basiCO

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GETTING STARTED

BasiCO is a simplified interface to using COPASI from python. It is a collection of utility python scripts, that hide the complexity of the underlying SWIG generated language bindings.

CHAPTER

ONE

GETTING STARTED

1.1 Installation

BasiCO is is finally available in pypi:

```
pip install copasi-basico
```

however you can pip install it using:

```
pip install git+https://github.com/copasi/basico.git
```

Currently there is one additional package available that provides support for PEtab and petab-select, that can be installed using

```
pip install copasi-basico[petab]
```

or

```
pip install git+https://github.com/copasi/basico.git#egg=basico[petab]
```

1.2 Use the package

To start using the package, you simply import it:

```
>>> from basico import *
```

1.3 Loading a Model

You can load either COPASI, or SBML files directly using the *load_model()* command:

```
>>> load_model('brusselator.cps')
```

You can also load a model by providing a URL:

```
>>> load_model('https://fairdomhub.org/models/287/download?version-1')
```

We also provide a number of example models, that you can directly load with the installation. See *get_examples()* and *load_example()*.

Models from the BioModels Database and JWS can also be directly loaded (*jws_online*, *biomodels*, *load_biomodel()*)

```
>>> load_biomodel(206)
```

1.4 Interrogating the Model

To find out what is in a model, you could use the corresponding functions:

- *get_species()*
- *get_reactions()*
- *get_parameters()*
- *get_compartments()*

Analogous you can also set all of these, by providing the name of the element to modify:

- *set_species()*
- *set_reaction()*
- *set_parameters()*
- *set_compartment()*

New elements are added with:

- *add_species()*
- *add_reaction()*
- *add_parameter()*
- *add_compartment()*

And removed with:

- *remove_species()*
- *remove_reaction()*
- *remove_parameter()*
- *remove_compartment()*

1.5 Analyzing the Model

Currently the following analysis tasks have been included:

- *task_timecourse*
- *task_steadystate*
- *task_parameterestimation*

1.6 Saving a Model

Saving a model, is done by calling *save_model()*:

```
>>> save_model('model_3.cps')
```

will save the file *model_3.cps* in the current folder. To export the model to SBML use:

```
>>> save_model('model_3.xml', type-'sbml')
```

CHAPTER

TWO

ACCESSING MODELS FROM THE DATABASE

This example describes how to access models from BioModels and JWS. Further databases could be easily added later on.

2.1 BioModels

[1]:
```
import sys
if '../..' not in sys.path:
    sys.path.append('../..')

import basico.biomodels as biomodels
```

the BioModels REST API allows searching for models, just as one would do in the web interface on http://biomodels.net. So one can search by pathway, species or reactions or submitter / author by just entering them.

[2]:
```
glycolysis_models = biomodels.search_for_model('glycolysis')
for model in glycolysis_models:
    print ('Id: %s' % model['id'])
    print ('Name: %s' % model['name'])
    print ('Format: %s' % model['format'])
    print ('')
```

```
Id: BIOMD0000000042
Name: Nielsen1998_Glycolysis
Format: SBML

Id: BIOMD0000000051
Name: Chassagnole2002_Carbon_Metabolism
Format: SBML

Id: BIOMD0000000054
Name: Ataullahkhanov1996_Adenylate
Format: SBML

Id: BIOMD0000000061
Name: Hynne2001_Glycolysis
Format: SBML

Id: BIOMD0000000064
Name: Teusink2000_Glycolysis
```

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```
Format: SBML

Id: BIOMD0000000071
Name: Bakker2001_Glycolysis
Format: SBML

Id: BIOMD0000000172
Name: Pritchard2002_glycolysis
Format: SBML

Id: BIOMD0000000176
Name: Conant2007_WGD_glycolysis_2A3AB
Format: SBML

Id: BIOMD0000000177
Name: Conant2007_glycolysis_2C
Format: SBML

Id: BIOMD0000000206
Name: Wolf2000_Glycolytic_Oscillations
Format: SBML
```

to get more information about a particular model, the `get_model_info` function provides basic information. As all the runctions in this module they take either an integer or string biomodels id as parameter

[3]:
```
info = biomodels.get_model_info(206)
```

[4]:
```
print (info['name'])
print (info['description'])
```

```
Wolf2000_Glycolytic_Oscillations
<notes xmlns="http://www.sbml.org/sbml/level2/version3">
      <body xmlns="http://www.w3.org/1999/xhtml">
        <p>Model reproduces the dynamics of ATP and NADH as depicted in Fig 4 of the␣
↪paper.  Model successfully tested on Jarnac and MathSBML.</p>
        <br />
        <p>To the extent possible under law, all copyright and related or neighbouring␣
↪rights to this encoded model have been dedicated to the public domain worldwide.␣
↪Please refer to      <a href="http://creativecommons.org/publicdomain/zero/1.0/" title=
↪"Creative Commons CC0">CC0 Public Domain Dedication</a>
          for more information.      </p>
      <p>In summary, you are entitled to use this encoded model in absolutely any manner␣
↪you deem suitable, verbatim, or with modification, alone or embedded it in a larger␣
↪context, redistribute it, commercially or not, in a restricted way or not.</p>
      <br />
      <p>To cite BioModels Database, please use:      <a href="http://www.ncbi.nlm.nih.
↪gov/pubmed/20587024" target="_blank">Li C, Donizelli M, Rodriguez N, Dharuri H, Endler␣
↪L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novère N, Laibe C␣
↪(2010) BioModels Database: An enhanced, curated and annotated resource for published␣
↪quantitative kinetic models. BMC Syst Biol., 4:92.</a>
  </p>
```

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```
</body>
</notes>
```

the model information object also contains the list of file names associated with the entry. To just get that list the convenience function `get_files_for_model` exists. The main document is contained in a sublist called `main`. So the main entry can be retrieved using

[5]:
```
first_entry = info['files']['main'][0]
```

[6]:
```
print ("Main FileName is: '{0}' and has size {1} kb".format(first_entry['name'], first_
↪entry['fileSize']))
```

```
Main FileName is: 'BIOMD0000000206_url.xml' and has size 27693 kb
```

to actually get hold of the model itself, you can use the `get_content_for_model` function, that takes a model id, as well as an optional filename. If the filename is not given, the first main content will be chosen automatically. So to download the model of biomodel #206, once could simply call:

[7]:
```
sbml = biomodels.get_content_for_model(206)
```

[8]:
```
print(sbml[:1000])  # just printing the first couple of lines
```

```
<?xml version='1.0' encoding='UTF-8' standalone='no'?>
<sbml xmlns="http://www.sbml.org/sbml/level2/version3" level="2" metaid="metaid_0000001"␣
↪version="3">
  <model id="Wolf2000_Glycolytic_Oscillations" metaid="metaid_0000002" name="Wolf2000_
↪Glycolytic_Oscillations">
    <notes>
      <body xmlns="http://www.w3.org/1999/xhtml">
        <p>Model reproduces the dynamics of ATP and NADH as depicted in Fig 4 of the␣
↪paper.  Model successfully tested on Jarnac and MathSBML.</p>
        <br/>
        <p>To the extent possible under law, all copyright and related or neighbouring␣
↪rights to this encoded model have been dedicated to the public domain worldwide.␣
↪Please refer to      <a href="http://creativecommons.org/publicdomain/zero/1.0/" title=
↪"Creative Commons CC0">CC0 Public Domain Dedication</a>
          for more information.      </p>
      <p>In summary, you are entitled to use this encoded model in absolutely any manner␣
↪you deem suitable, verbatim, or with modification, alone or embedd
```

of course you can simply call `load_biomodel(206)` to load a biomodel into basico.

[9]:
```
biomodels.search_for_model('kummer2000')
```

[9]:
```
[{'format': 'SBML',
  'id': 'BIOMD0000000329',
  'lastModified': '2014-12-11T00:00:00Z',
  'name': 'Kummer2000 - Oscillations in Calcium Signalling',
  'submissionDate': '2014-12-11T00:00:00Z',
  'submitter': 'Vijayalakshmi Chelliah',
  'url': 'https://www.ebi.ac.uk/biomodels/BIOMD0000000329'}]
```

2.2 JWS Online

we also provide access to models from JWS online.

[10]:
```
import basico.jws_online as jws
```

with `get_all_models` you would get a list of all the models in JWS online. To search for models, you have 2 options. One is to search for models by species. For example to search for all models involving 'atp'

[11]:
```
atp_models = jws.get_models_for_species('atp')
for model in atp_models:
    print(model['slug'])
```

```
achcar1
achcar10
achcar11
achcar12
achcar13
achcar14
achcar2
achcar3
achcar4
achcar5
achcar6
achcar7
achcar8
achcar9
albert1
arnold10
arnold10-2
arnold11
arnold6
arnold7
arnold8
arnold9
assmus
bali
bier2
bradshaw
bray2
bruggeman1
bulik1
bulik2
bulik3
chance1
chassagnole1
chassagnole3
conant1
conant2
curto1
dano1
dano2
dano3
```

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```
dupreez1
dupreez2
dupreez3
dupreez4
dupreez5
dupreez6
dupreez7
fribourg1
fribourg2
fridlyand1
galazzo1
gustavsson1
gustavsson2
gustavsson3
gustavsson4
gustavsson5
hald
heinrich
hoefnagel1
hoefnagel2
hoefnagel_mixedacid
holzhutter
hynne
jamshidi
jiang1
kerkhovena
kerkhovenc
kolmeisky1
kongas1
kouril2
kouril3
kouril4
kouril6
kouril7
kouril8
kouril9
lambeth
levering1
levering2
maher1
marinhernandez1
marinhernandez2
marinhernandez3
mayya1
mosca1
mulquiney
mulquiney1
mulquiney2
nazaret1
neves1
nielsen
nishio1
```

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```
olah
orth1
penkler1
penkler2
penkler2aa
poolman
pritchard1
proctor1
rohwer1
rovers1
saavedra
sengupta1
smallbone0
smallbone1
smallbone10
smallbone11
smallbone12
smallbone13
smallbone14
smallbone15
smallbone16
smallbone17
smallbone18
smallbone19
smallbone2
smallbone3
smallbone4
smallbone5
smallbone6
smallbone7
smallbone8
smallbone9
tang1
teusink2
uys
valero
vaneunen1
vanheerden1
vanheerden2
vanniekerk1
whillier4
wolf
wolf1
```

or you could get the models for a specific reaction for example, all models involving 'pfk' would be:

[12]:
```
pfk_models = jws.get_models_for_reaction('pfk')
for model in pfk_models:
    print(model['slug'])
```

```
achcar1
achcar10
achcar11
```

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```
achcar12
achcar13
achcar14
achcar2
achcar3
achcar4
achcar5
achcar6
achcar7
achcar8
achcar9
albert1
chassagnole2
conant1
conant2
dupreez1
dupreez2
dupreez3
dupreez4
dupreez5
dupreez6
dupreez7
gustavsson1
gustavsson2
gustavsson3
gustavsson4
gustavsson5
hald
kerkhovena
kerkhovenc
levering1
levering2
machado1
marinhernandez1
marinhernandez2
marinhernandez3
mosca1
mulquiney
mulquiney1
mulquiney2
orth1
penkler1
penkler2
penkler2aa
pritchard1
ralser1
smallbone0
smallbone1
smallbone10
smallbone11
smallbone12
smallbone13
```

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```
smallbone14
smallbone15
smallbone16
smallbone17
smallbone18
smallbone2
smallbone3
smallbone4
smallbone5
smallbone6
smallbone7
smallbone8
smallbone9
vanniekerk1
```

for each of these ids, you can get the manuscript, to find out what the model is all about, or the sbml model itself

[13]:
```
manuscript = jws.get_manuscript('wolf')
```

[14]:
```
print(manuscript['title'])
```

```
Transduction of intracellular and intercellular dynamics in yeast glycolytic␣
↪oscillations.
```

[15]:
```
print(manuscript['abstract'])
```

```
Under certain well-defined conditions, a population of yeast cells exhibits glycolytic␣
↪oscillations that synchronize through intercellular acetaldehyde. This implies that␣
↪the dynamic phenomenon of the oscillation propagates within and between cells. We here␣
↪develop a method to establish by which route dynamics propagate through a biological␣
↪reaction network. Application of the method to yeast demonstrates how the oscillations␣
↪and the synchronization signal can be transduced. That transduction is not so much␣
↪through the backbone of glycolysis, as via the Gibbs energy and redox coenzyme couples␣
↪(ATP/ADP, and NADH/NAD), and via both intra- and intercellular acetaldehyde.
```

[16]:
```
sbml = jws.get_sbml_model('wolf')
```

[17]:
```
print(sbml[:1000])
```

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core" level="3" version="1">
  <model id="wolf" name="wolf">
    <listOfCompartments>
      <compartment metaid="metaid_0" sboTerm="SBO:0000410" id="default_compartment"␣
↪spatialDimensions="3" size="1" constant="true"/>
    </listOfCompartments>
    <listOfSpecies>
      <species metaid="metaid_1" id="at" name="ATP" compartment="default_compartment"␣
↪initialConcentration="2" hasOnlySubstanceUnits="false" boundaryCondition="false"␣
↪constant="false">
        <annotation>
          <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#" xmlns:dc=
↪"http://purl.org/dc/elements/1.1/" xmlns:dcterms="http://purl.org/dc/terms/" xmlns:
```

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```
↪vCard="http://www.w3.org/2001/vcard-rdf/3.0#" xmlns:bqbiol="http://biomodels.net/
↪biology-qualifiers/" xmlns:bqmodel="http://biomodels.net/model-qualifiers/">
            <rdf:Description rdf:about="#metaid_1">
              <bqbiol:is>
                <rdf:Bag>
```

[ ]:

```

```

[ ]:

```

```

CHAPTER

THREE

CREATING AND SIMULATING A SIMPLE MODEL

Here we show how to create a basic model using basiCO, and simulating it. We start as usual by importing basiCO.

[1]:
```
import sys
if '../..' not in sys.path:
    sys.path.append('../..')
try:
  from basico import *
except ImportError:
  !pip install -q copasi-basico
  from basico import *
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

Now lets create a new model, passing along the `name` that we want to give it. Additional supported parameters for the model consist of:

- `quantity_unit`: which sets the unit to use for species concentrations (defaults to mol)
- `volume_unit`: the unit to use for three dimensional compartments (defaults to litre (l))
- `time_unit`: the unit to use for time (defaults to second (s))
- `area_unit`: the unit to use for two dimensional compartments
- `length_unit`: the unit to use for one dimensional compartments

[2]:
```
new_model(name='Simple Model');
```

now we add a basic reaction that converts a chemical species `A` irreversibly into `B`. We can do that by just calling `addReaction` with the chemical formula to use. In this case this would be: `A -> B`. The reaction will be automatically created using mass action kinetics.

[3]:
```
add_reaction('R1', 'A -> B');
```

Since we had a new model, this created the Species `A` and `B` as well as a compartment `compartment`, in which those chemicals reside. The species have an initial concentration of 1. To verify we can call `get_species`, which returns a dataframe with all information about the species (either all species, or the one filtered to):

[4]:
```
get_species().initial_concentration
```

[4]:
```
name
A    1.0
```

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```
B    1.0
Name: initial_concentration, dtype: float64
```

to change the initial concentration, we use `set_species`, and specify which property we want to change:

[5]:
```
set_species('B', initial_concentration=0)
set_species('A', initial_concentration=10)
get_species().initial_concentration
```

[5]:
```
name
A    10.0
B     0.0
Name: initial_concentration, dtype: float64
```

to see the kinetic paramters of our recation we can use `get_reaction_parameters`, and we see that the parameter has been created by default with a value of `0.1`

[6]:
```
get_reaction_parameters()
```

[6]:
```
         value reaction   type mapped_to
name
(R1).k1    0.1       R1  local
```

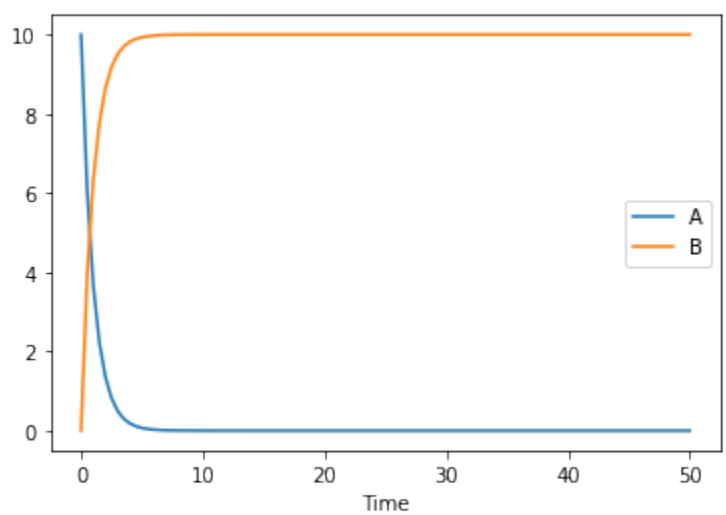
to change that parameter, we use `set_reaction_parameters`, specifying the value to be changed:

[7]:
```
set_reaction_parameters('(R1).k1', value=1)
get_reaction_parameters('k1')
```

[7]:
```
         value reaction   type mapped_to
name
(R1).k1    1.0       R1  local
```

now lets simulate our model for 10 seconds:

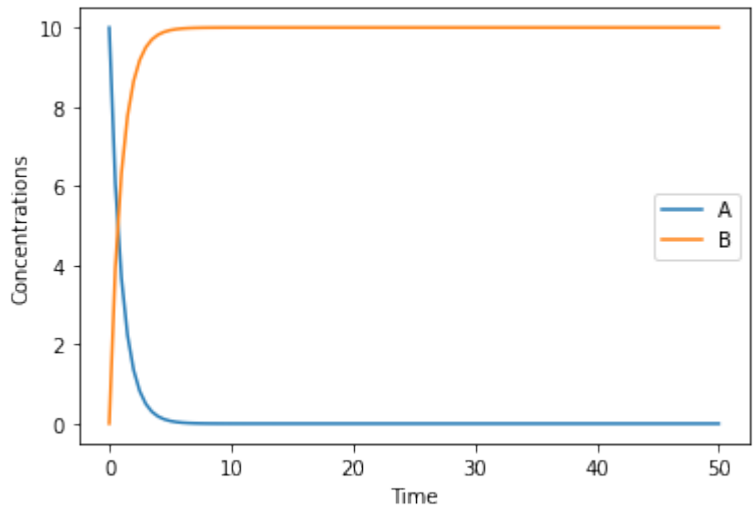
[8]:
```
result = run_time_course(duration=50)
result.plot();
```



this basic plot is done by pandas, and returns a `matplotlib.axes.AxesSubplot` object, that can be used to modify

it further (full documantation is in the pandas documentation), if you wanted to change the Y label for example you could run:

[9]:
```
ax = result.plot();
ax.set_ylabel('Concentrations');
```



to simulate the model stochastically, you can specify the simulation method. COPASI supports many different simulations methods:

- `deterministic`: using the COPASI LSODA implementation
- `stochastic`: using the Gibson Bruck algorithm
- `directMethod`: using the Gillespie direct method

others are:

- `tauleap`, `adaptivesa`, `radau5`, `hybridlsoda`, `hybridode45`

So lets try and simulate the model stochastically:

[10]:
```
result = run_time_course(duration=50, method='stochastic')
```

```
Error while initializing the simulation: >ERROR 2023-08-10T13:20:07<
  At least one particle number in the initial state is too big.
```

simulation failed in this time because the particle numbers, that the stochastic simulation is based upon is too high! Lets check:

[11]:
```
get_species().initial_particle_number
```

[11]:
```
name
A    6.022141e+24
B    0.000000e+00
Name: initial_particle_number, dtype: float64
```

so we just set the initial particle number of a to be smaller, and run the simulation again, this time returning particle numbers rather than concentrations for the resulting dataframe

[12]:
```
set_species('A', initial_particle_number=100)
```

Alternatively we could have modified the models quantity unit, which currently was set to:

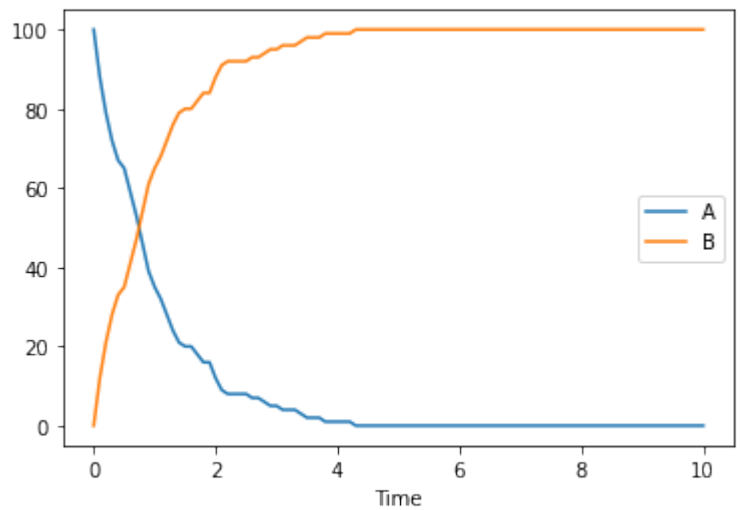
[13]:
```
get_model_units()
```

[13]:
```
{'time_unit': 's',
 'quantity_unit': 'mol',
 'length_unit': 'm',
 'area_unit': 'm²',
 'volume_unit': 'l'}
```

So initially we had a concentration of 10 mol/l, which does not lend itself for stochastic simulation. Using the `set_model_unit` command with a more apropriate `quantity_unit` and `volume_unit` would be the propper solution.

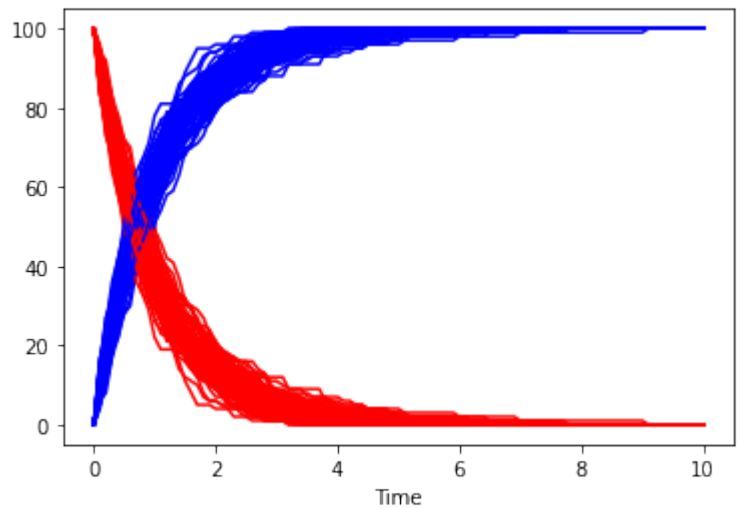
When running stochastic simulations, you might want to specify the `seed` to be used, so that traces become reproducible. In COPASI you have two parameters for that `seed`, the actual seed, and `use_seed` a boolean indicating whether that seed is to be used for the next simulation. For a single trace we use both:

[14]:
```
result = run_time_course(duration=10, method='stochastic', use_numbers=True, seed=1234,␣
↪use_seed=True)
result.plot();
```



of course one stochastic trace will not be enough, so lets run many of them. This time the species will be plotted separately, so that it is easy to reuse the same color. This time we also don't use the seed specified before.

[15]:
```
fig, ax = plt.subplots()
for i in range(100):
    result = run_time_course(duration=10, method='stochastic', use_numbers=True, use_
↪seed=False)
    result.plot(y='A', color='r', ax=ax, legend=None);
    result.plot(y='B', color='b', ax=ax, legend=None);
```



so far, we were only using mass action kinetics, but of course we could use any other kinetic as well. COPASI comes with a large number of functions already inbuilt. You can see those, running the `get_functions` command. It is filterable by name, and whether or not the formula is reversible, or general (general reactions can be used for either reversibility). Since we modelled our reaction as irreversible, lets look at the irreversible functions we have:

[16]:
```
get_functions(reversible=False)
```

[16]:
```
                                    reversible  \
name
Allosteric inhibition (MWC)                False
Catalytic activation (irrev)               False
Competitive inhibition (irr)               False
Constant flux (irreversible)               False
Henri-Michaelis-Menten (irreversible)      False
Hill Cooperativity                         False
Hyperbolic modifier (irrev)                False
Mass action (irreversible)                 False
Mixed activation (irrev)                   False
Mixed inhibition (irr)                     False
Noncompetitive inhibition (irr)            False
Specific activation (irrev)                False
Substrate activation (irr)                 False
Substrate inhibition (irr)                 False
Uncompetitive inhibition (irr)             False
Bi (irreversible)                          False
Arrhenius Bimolecular (irr)                False
Arrhenius Unimolecular (irr)               False

                                                                    formula␣
↪ \
name
Allosteric inhibition (MWC)            V*(substrate/Ks)*(1+(substrate/Ks))^(n-1)/(L*(...
Catalytic activation (irrev)           V*substrate*Activator/((Kms+substrate)*(Ka+Act...
Competitive inhibition (irr)                  V*substrate/(Km+substrate+Km*Inhibitor/Ki)
Constant flux (irreversible)                                                          v
Henri-Michaelis-Menten (irreversible)                          V*substrate/(Km+substrate)
```

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```
Hill Cooperativity                      V*(substrate/Shalve)^h/(1+(substrate/Shalve)^h)
Hyperbolic modifier (irrev)           V*substrate*(1+b*Modifier/(a*Kd))/(Km*(1+Modif...
Mass action (irreversible)                                   k1*PRODUCT<substrate_i>
Mixed activation (irrev)              V*substrate*Activator/(Kms*(Kas+Activator)+sub...
Mixed inhibition (irr)                V*substrate/(Km*(1+Inhibitor/Kis)+substrate*(1...
Noncompetitive inhibition (irr)           V*substrate/((Km+substrate)*(1+Inhibitor/Ki))
Specific activation (irrev)           V*substrate*Activator/(Kms*Ka+(Kms+substrate)*...
Substrate activation (irr)            V*(substrate/Ksa)^2/(1+substrate/Ksc+substrate...
Substrate inhibition (irr)               V*substrate/(Km+substrate+Km*(substrate/Ki)^2)
Uncompetitive inhibition (irr)              V*substrate/(Km+substrate*(1+Inhibitor/Ki))
Bi (irreversible)                              vmax*A*B/(Kma*Kmb + A*Kmb + B*Kma + A*B)
Arrhenius Bimolecular (irr)                                   A*exp(-Ea/(R*T))*S1*S2
Arrhenius Unimolecular (irr)                                      A*exp(-Ea/(R*T))*S

                                      general  \
name
Allosteric inhibition (MWC)             False
Catalytic activation (irrev)            False
Competitive inhibition (irr)            False
Constant flux (irreversible)            False
Henri-Michaelis-Menten (irreversible)   False
Hill Cooperativity                      False
Hyperbolic modifier (irrev)             False
Mass action (irreversible)              False
Mixed activation (irrev)                False
Mixed inhibition (irr)                  False
Noncompetitive inhibition (irr)         False
Specific activation (irrev)             False
Substrate activation (irr)              False
Substrate inhibition (irr)              False
Uncompetitive inhibition (irr)          False
Bi (irreversible)                       False
Arrhenius Bimolecular (irr)             False
Arrhenius Unimolecular (irr)            False

                                                                                mapping
name
Allosteric inhibition (MWC)           {'substrate': 'substrate', 'Inhibitor': 'modif...
Catalytic activation (irrev)          {'substrate': 'substrate', 'Activator': 'modif...
Competitive inhibition (irr)          {'substrate': 'substrate', 'Inhibitor': 'modif...
Constant flux (irreversible)                                      {'v': 'parameter'}
Henri-Michaelis-Menten (irreversible) {'substrate': 'substrate', 'Km': 'parameter', ...
Hill Cooperativity                    {'substrate': 'substrate', 'Shalve': 'paramete...
Hyperbolic modifier (irrev)           {'substrate': 'substrate', 'Modifier': 'modifi...
Mass action (irreversible)                {'k1': 'parameter', 'substrate': 'substrate'}
Mixed activation (irrev)              {'substrate': 'substrate', 'Activator': 'modif...
Mixed inhibition (irr)                {'substrate': 'substrate', 'Inhibitor': 'modif...
Noncompetitive inhibition (irr)       {'substrate': 'substrate', 'Inhibitor': 'modif...
Specific activation (irrev)           {'substrate': 'substrate', 'Activator': 'modif...
Substrate activation (irr)            {'substrate': 'substrate', 'V': 'parameter', '...
Substrate inhibition (irr)            {'substrate': 'substrate', 'Km': 'parameter', ...
Uncompetitive inhibition (irr)        {'substrate': 'substrate', 'Inhibitor': 'modif...
```

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(continued from previous page)

```
Bi (irreversible)                        {'vmax': 'parameter', 'A': 'substrate', 'B': '...
Arrhenius Bimolecular (irr)              {'A': 'parameter', 'Ea': 'parameter', 'R': 'pa...
Arrhenius Unimolecular (irr)             {'A': 'parameter', 'Ea': 'parameter', 'R': 'pa...
```

So lets change the kinetic function that our reaction should use. Here we simply specify the function name that we got from the call before. This will introduce new local parameters, for `Km` and `Vmax` to the model. (We of course could have used the function parameter already add the `add_reaction` command above.

[17]:
```
set_reaction('R1', function='Henri-Michaelis-Menten (irreversible)')
```

[18]:
```
get_reactions()
```

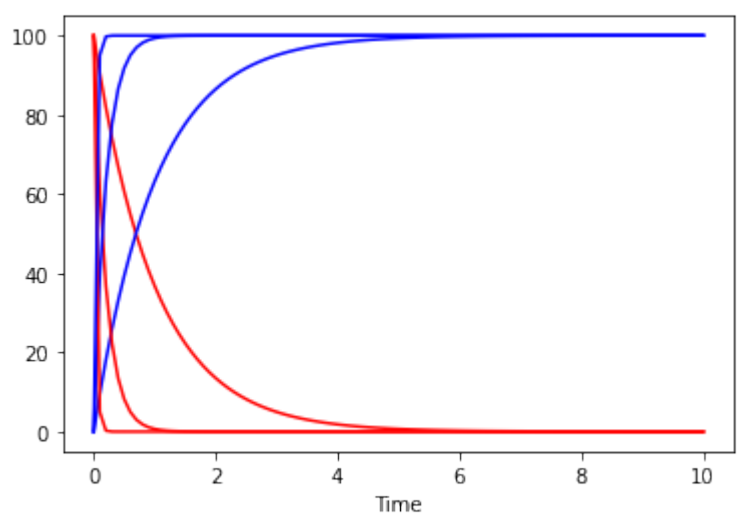
[18]:
```
      scheme  flux  particle_flux                                function  \
name
R1    A -> B   0.0            0.0  Henri-Michaelis-Menten (irreversible)

             key sbml_id                                     mapping
name
R1    Reaction_0          {'substrate': 'A', 'Km': 0.1, 'V': 0.1}
```

[19]:
```
get_reaction_parameters()
```

[19]:
```
         value reaction   type mapped_to
name
(R1).Km    0.1       R1  local
(R1).V     0.1       R1  local
```

and now we can look at how the plot would look at repeating the simulation for several vmax values:

[20]:
```
fig, ax = plt.subplots()
for vm in [0.1, 0.5, 3]:
    set_reaction_parameters('(R1).V', value=vm)
    result = run_time_course(duration=10, method='deterministic', use_numbers=True)
    result.plot(y='A', color='r', ax=ax, legend=None);
    result.plot(y='B', color='b', ax=ax, legend=None);
```



CHAPTER

FOUR

GETTING AND SETTING REACTION PARAMETERS AND REACTIONS

[1]:
```
import sys
sys.path.append('../..')
%matplotlib inline
```

[2]:
```
from basico import *
```

4.1 Load model

[3]:
```
biomod = load_example("LM-test1")
```

4.2 Getting/setting global quantities

```
It is possible to set:
    'initial_value'
    'initial_expression'
    'expression'
    'status'
    'type'
```

[4]:
```
get_parameters()
```

[4]:
```
               type unit  initial_value initial_expression  \
name
epsilon       fixed                0.78
offset        fixed                0.10
signal   assignment                0.10

                                   expression  value  rate           key
name
epsilon                                               NaN   0.0  ModelValue_0
offset                                                NaN   0.0  ModelValue_1
signal   [P] * Values[epsilon] + Values[offset]       NaN   NaN  ModelValue_2
```

[5]:
```
set_parameters(name= 'offset', initial_value = 50)
```

[6]:
```
set_parameters('signal', expression='[P] * Values[epsilon] + Values[offset]')
```

[7]:
```
get_parameters()
```

[7]:
```
               type unit  initial_value initial_expression  \
name
epsilon       fixed                0.78
offset        fixed               50.00
signal   assignment               50.00

                                   expression  value  rate           key
name
epsilon                                           NaN   0.0  ModelValue_0
offset                                            NaN   0.0  ModelValue_1
signal   [P] * Values[epsilon] + Values[offset]    NaN   NaN  ModelValue_2
```

4.3 Getting/setting species (metabolites)

[8]:
```
get_species()
```

[8]:
```
      compartment       type     unit  initial_concentration  \
name
E     compartment  reactions  mmol/ml               0.010000
S     compartment  reactions  mmol/ml              10.000001
ES    compartment  reactions  mmol/ml               0.000000
P     compartment  reactions  mmol/ml               0.000000

      initial_particle_number initial_expression expression  concentration  \
name
E                6.022142e+18                                          NaN
S                6.022142e+21                                          NaN
ES               0.000000e+00                                          NaN
P                0.000000e+00                                          NaN

      particle_number  rate  particle_number_rate           key
name
E                 NaN   NaN                   NaN  Metabolite_1
S                 NaN   NaN                   NaN  Metabolite_0
ES                NaN   NaN                   NaN  Metabolite_2
P                 NaN   NaN                   NaN  Metabolite_3
```

[9]:
```
get_species(name = 'E')['initial_concentration']
```

[9]:
```
name
E     0.01
ES    0.00
Name: initial_concentration, dtype: float64
```

4.3.1 Setting

```
if 'name' in kwargs:
    metab.setObjectName(kwargs['name'])

if 'unit' in kwargs:
    metab.setUnitExpression(kwargs['unit'])

if 'initial_concentration' in kwargs:
    metab.setInitialConcentration(kwargs['initial_concentration']),

if 'initial_particle_number' in kwargs:
    metab.setInitialValue(kwargs['initial_particle_number']),

if 'initial_expression' in kwargs:
    metab.setInitialExpression(kwargs['initial_expression'])

if 'expression' in kwargs:
    metab.setExpression(kwargs['expression'])
```

[10]:
```
set_species(name = 'E', new_name = 'Lilija')
```

[11]:
```
set_species(name = 'Lilija', initial_concentration = 123456)
```

[12]:
```
get_species(name = 'Lilija')
```

[12]:
```
        compartment       type     unit  initial_concentration  \
name
Lilija  compartment  reactions  mmol/ml               123456.0

        initial_particle_number initial_expression expression  concentration  \
name
Lilija             7.434694e+25                                          NaN

        particle_number  rate  particle_number_rate           key
name
Lilija              NaN   NaN                   NaN  Metabolite_1
```

[13]:
```
# change it back
set_species(new_name = 'E', name = 'Lilija')
```

4.4 Getting/setting reaction parameters

[14]:
```
get_reaction_parameters()
```

[14]:
```
         value reaction   type mapped_to
name
(R1).k1  130.0       R1  local
(R1).k2    1.0       R1  local
(R2).k1    1.0       R2  local
```

```
Setting only the following is possible:
'new_name'
'value'
```

[15]:
```
set_reaction_parameters(name = '(R1).k1', value=123)
```

[16]:
```
get_reaction_parameters()
```

[16]:
```
         value reaction   type mapped_to
name
(R1).k1  123.0       R1  local
(R1).k2    1.0       R1  local
(R2).k1    1.0       R2  local
```

4.5 Getting/setting reactions

[17]:
```
get_reactions()
```

[17]:
```
           scheme  flux  particle_flux                    function
name
R1     S + E = ES   NaN            NaN    Mass action (reversible)
R2    ES -> E + P   NaN            NaN  Mass action (irreversible)
```

4.6 Setting scheme

[18]:
```
set_reaction(name = 'R1', scheme = 'S + E + F = ES')
```

[19]:
```
get_reactions()
```

[19]:
```
              scheme  flux  particle_flux                    function
name
R1    S + E + F = ES   NaN            NaN    Mass action (reversible)
R2       ES -> E + P   NaN            NaN  Mass action (irreversible)
```

4.7 Setting reaction name

[20]:
```
set_reaction(name = 'R1', new_name = 'Reaction 1')
```

[21]:
```
get_reactions()
```

[21]:
```
                    scheme  flux  particle_flux                    function
name
Reaction 1  S + E + F = ES   NaN            NaN    Mass action (reversible)
R2             ES -> E + P   NaN            NaN  Mass action (irreversible)
```

```
[ ]:
```

CHAPTER

FIVE

EDITING REACTION KINETICS

Previous examples showed how to create models using basico, and using kinetic functions from the reaction database. Here, I want to expand on that showing how to map kinetic functions to reactions involving modifiers as well. Lets start as usual by importing basico:

[1]:
```
from basico import *
```

now lets create a new model:

[2]:
```
new_model(name='Reactions');
```

we know we can create a reaction, by using the `add_reaction` command. It requires at the very least two arguments:

- `name`: the name of the reaction
- `scheme`: the reaction scheme

If nothing else is specified, this will create the reaction with the given `name` and reaction `scheme`, assigning it mass action kinetics with local parameters defaulting to a value of `0.1`. All species will be created if they do not exist yet in the model. For example:

[3]:
```
add_reaction('R1', 'A -> B');
```

creates the reaction `R1`, species `A` and `B` and a local parameter `(R1).k1`. With `get_reactions` we can have a look at what was created:

[4]:
```
get_reactions()[['scheme', 'function', 'mapping']]
```

[4]:
```
      scheme                    function                        mapping
name
R1    A -> B  Mass action (irreversible)  {'k1': 0.1, 'substrate': 'A'}
```

here I want to point out, the `mapping` column. It shows that the parameter `k1` is a local one, as it is mapped to a value. And that the substrate of the function is mapped to `A`. We can specify the mapping directly in the `add_reaction` call, or we can specify it using `set_reaction`. So for example, if we wanted to modify the reaction, to map the reactions `k1` parameter to a global quantity `global_k`, we could to that as follows:

[5]:
```
add_parameter(name='global_k', initial_value=0.2)
set_reaction('R1', mapping={'k1': 'global_k'})
```

[6]:
```
get_reactions()[['scheme', 'function', 'mapping']]
```

[6]:
```
      scheme                    function                                mapping
name
R1    A -> B  Mass action (irreversible)  {'k1': 'global_k', 'substrate': 'A'}
```

next let us assume, i wanted to use a kinetic from the function database, that includes inhibition for the reaction. Using `get_functions` we can filter the functiondatabase, for suitable functions for our reaction, and then filter for ones that contain inhibition:

[7]:
```
suitable_functions = get_functions(suitable_for='R1')[['formula', 'mapping']]
suitable_inhibitions = suitable_functions[suitable_functions.index.str.contains(
↪'inhibition')]
suitable_inhibitions
```

[7]:
```
                                                                  formula  \
name
Allosteric inhibition (MWC)      V*(substrate/Ks)*(1+(substrate/Ks))^(n-1)/(L*(...
Competitive inhibition (irr)            V*substrate/(Km+substrate+Km*Inhibitor/Ki)
Mixed inhibition (irr)           V*substrate/(Km*(1+Inhibitor/Kis)+substrate*(1...
Noncompetitive inhibition (irr)      V*substrate/((Km+substrate)*(1+Inhibitor/Ki))
Substrate inhibition (irr)          V*substrate/(Km+substrate+Km*(substrate/Ki)^2)
Uncompetitive inhibition (irr)         V*substrate/(Km+substrate*(1+Inhibitor/Ki))

                                                                  mapping
name
Allosteric inhibition (MWC)      {'substrate': 'substrate', 'Inhibitor': 'modif...
Competitive inhibition (irr)     {'substrate': 'substrate', 'Inhibitor': 'modif...
Mixed inhibition (irr)           {'substrate': 'substrate', 'Inhibitor': 'modif...
Noncompetitive inhibition (irr)  {'substrate': 'substrate', 'Inhibitor': 'modif...
Substrate inhibition (irr)       {'substrate': 'substrate', 'Km': 'parameter', ...
Uncompetitive inhibition (irr)   {'substrate': 'substrate', 'Inhibitor': 'modif...
```

let us use `Allosteric inhibition (MWC)` here, lets have a look at the formula and the mapping table:

[8]:
```
as_dict(suitable_inhibitions)[0]
```

[8]:
```
{'name': 'Allosteric inhibition (MWC)',
 'formula': 'V*(substrate/Ks)*(1+(substrate/Ks))^(n-1)/(L*(1+Inhibitor/Ki)^
↪n+(1+(substrate/Ks))^n)',
 'mapping': {'substrate': 'substrate',
  'Inhibitor': 'modifier',
  'V': 'parameter',
  'Ks': 'parameter',
  'n': 'parameter',
  'L': 'parameter',
  'Ki': 'parameter'}}
```

since this function requires a modifier, we also change the reaction scheme to include a modifier. This is done by adding a semicolon at the end of the reaction scheme, and listing the modifiers space separated there. Then we an assign that function directly.

[9]:
```
set_reaction('R1', scheme='A -> B; C', function='Allosteric inhibition (MWC)')
get_reactions()[['scheme', 'function', 'mapping']]
```

[9]:
```
          scheme                     function  \
name
R1    A -> B;  C  Allosteric inhibition (MWC)

                                                mapping
name
R1    {'substrate': 'A', 'Inhibitor': 'C', 'V': 0.1,...
```

Note: that here, the mapping is not necessary, as the function has only one modifier, had we multiple modifiers defined, then we'd want to specify the mapping dictionary and map the `Inhibitor` to the respective modifier in our reaction scheme:

[10]:
```
set_reaction('R1', scheme='A -> B; C D', function='Allosteric inhibition (MWC)', mapping=
↪{'Inhibitor': 'D'})
get_reactions()[['scheme', 'function', 'mapping']]
```

[10]:
```
          scheme                     function  \
name
R1    A -> B;  D  Allosteric inhibition (MWC)

                                                mapping
name
R1    {'substrate': 'A', 'Inhibitor': 'D', 'V': 0.1,...
```

Note: Assigning a function that uses modifiers, *requires* that modifiers are present in the reaction scheme, or that *all modifiers* are specified in the mapping parameter. So assigning the function above would fail with error, if no modifier is declared:

[11]:
```
add_reaction('error', scheme='A -> B', function='Allosteric inhibition (MWC)');
get_reactions()[['scheme', 'function', 'mapping']]
```

```
ERROR:root:the mapping for reaction "error" with function "Allosteric inhibition (MWC)"␣
↪is not valid and cannot be applied.
```

[11]:
```
           scheme                     function  \
name
R1     A -> B;  D  Allosteric inhibition (MWC)
error      A -> B   Mass action (irreversible)

                                                 mapping
name
R1     {'substrate': 'A', 'Inhibitor': 'D', 'V': 0.1,...
error                       {'k1': 0.1, 'substrate': 'A'}
```

However, it will succeeed, if the modifier is specified. in the mapping parameter:

[12]:
```
set_reaction('error', new_name='now_it_works', function='Allosteric inhibition (MWC)',␣
↪mapping={'Inhibitor': 'D'})
get_reactions()[['scheme', 'function', 'mapping']]
```

[12]:
```
                  scheme                     function  \
name
R1            A -> B;  D  Allosteric inhibition (MWC)
now_it_works  A -> B;  D  Allosteric inhibition (MWC)

                                                       mapping
name
R1            {'substrate': 'A', 'Inhibitor': 'D', 'V': 0.1,...
now_it_works  {'substrate': 'A', 'Inhibitor': 'D', 'V': 0.1,...
```

CHAPTER

SIX

PARAMETER ESTIMATION

This document describes how to use BasiCO for paramter estimation tasks. This document assumes, that the parameter estimation task was already set up using COPASI. Look for another example, to set up a parameter estimation task directly from basiCO.

We start as normal:

[1]:
```
import sys
if '../..' not in sys.path:
    sys.path.append('../..')

from basico import *
%matplotlib inline
```

Now we load an example model, that already has paramter estimation set up:

[2]:
```
dm = load_example('LM')
```

with `get_fit_parameters` we can look at the paramters, that will be estimated, along with their bounds, and a list of experiments they apply to. If that list is empty, the parameter applies to all experiment, otherwise only the one mentioned.

[3]:
```
get_fit_parameters()
```

[3]:
```
               lower upper  start        affected  \
name
(R1).k2         1e-6   1e6    1.0              []
(R2).k1         1e-6   1e6    1.0              []
Values[offset]  -0.2   0.4    0.1  [Experiment_1]
Values[offset]  -0.2   0.4    0.1  [Experiment_3]
Values[offset]  -0.2   0.4    0.1    [Experiment]
Values[offset]  -0.2   0.4    0.1  [Experiment_4]
Values[offset]  -0.2   0.4    0.1  [Experiment_2]

                                                          cn
name
(R1).k2         CN=Root,Model=Kinetics of a  Michaelian enzyme...
(R2).k1         CN=Root,Model=Kinetics of a  Michaelian enzyme...
Values[offset]  CN=Root,Model=Kinetics of a  Michaelian enzyme...
Values[offset]  CN=Root,Model=Kinetics of a  Michaelian enzyme...
Values[offset]  CN=Root,Model=Kinetics of a  Michaelian enzyme...
Values[offset]  CN=Root,Model=Kinetics of a  Michaelian enzyme...
Values[offset]  CN=Root,Model=Kinetics of a  Michaelian enzyme...
```

Now lets see how well the current fit is:

[4]:
```
run_parameter_estimation(method='Statistics')
```

[4]:
```
                lower upper        sol        affected
name
(R1).k2          1e-6   1e6   0.000002              []
(R2).k1          1e-6   1e6  44.661715              []
Values[offset]  -0.2   0.4   0.043018  [Experiment_1]
Values[offset]  -0.2   0.4   0.054167  [Experiment_3]
Values[offset]  -0.2   0.4  -0.050941    [Experiment]
Values[offset]  -0.2   0.4   0.045922  [Experiment_4]
Values[offset]  -0.2   0.4   0.048025  [Experiment_2]
```

if ever you wanted to get the solution of the last run, you can execute `get_parameters_solution`

[5]:
```
get_parameters_solution()
```

[5]:
```
                lower upper        sol        affected
name
(R1).k2          1e-6   1e6   0.000002              []
(R2).k1          1e-6   1e6  44.661715              []
Values[offset]  -0.2   0.4   0.043018  [Experiment_1]
Values[offset]  -0.2   0.4   0.054167  [Experiment_3]
Values[offset]  -0.2   0.4  -0.050941    [Experiment]
Values[offset]  -0.2   0.4   0.045922  [Experiment_4]
Values[offset]  -0.2   0.4   0.048025  [Experiment_2]
```

the experimental data can be obtained like so:

[6]:
```
data = get_experiment_data_from_model()
```

[7]:
```
data[1]
```

[7]:
```
      [S]_0  Time  Values[signal]
0   0.31623   0.3         0.08568
1   0.31623   0.6         0.12849
2   0.31623   0.9         0.16599
3   0.31623   1.2         0.19788
4   0.31623   1.5         0.22046
..      ...   ...             ...
95  0.31623  28.8         0.27933
96  0.31623  29.1         0.28938
97  0.31623  29.4         0.28208
98  0.31623  29.7         0.25544
99  0.31623  30.0         0.29552

[100 rows x 3 columns]
```

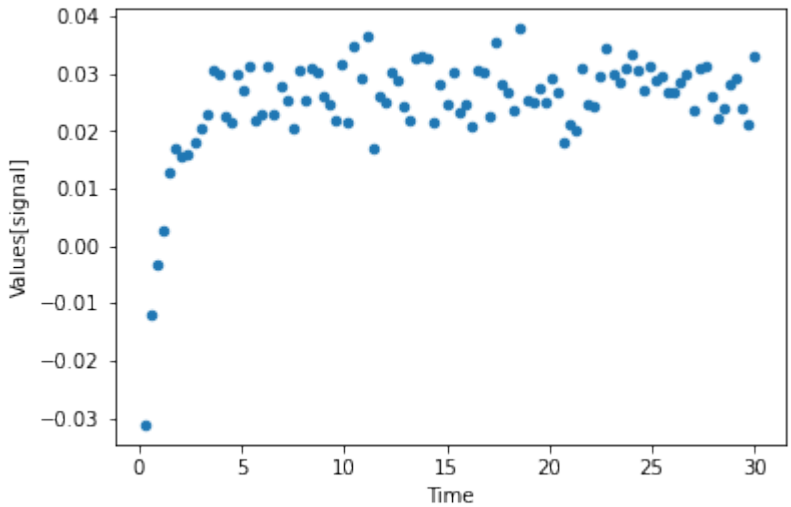
[8]:
```
len(data)
```

[8]:
```
5
```

or to get a specific data set you can get it directly from the name:

[9]:
```
df = get_data_from_experiment('Experiment')
```

[10]:
```
df.plot(kind='scatter', x='Time', y="Values[signal]");
```



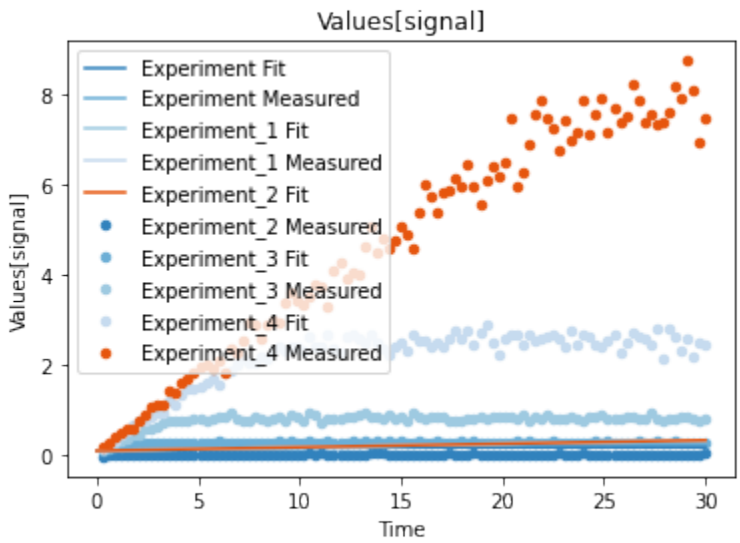
you can also look directly at the mapping, of the data. in this `independent` will mean that it is an initial value that is different in this experiment. `dependent` is the mapping to a model variable such as the transient concentration or a transient value of a model parameter.

[11]:
```
get_experiment_mapping('Experiment')
```

[11]:
```
               type         mapping  \
column
0       independent           [S]_0
1              time
2         dependent  Values[signal]


                                                      cn
column
0       CN=Root,Model=Kinetics of a  Michaelian enzyme...
1
2       CN=Root,Model=Kinetics of a  Michaelian enzyme...
```

you can also plot the current fit, by running:

[12]:
```
plot_per_dependent_variable();
```



now lets combine it, by actyally running the parameter estimation (here using the Levenberg Marquardt algorithm)

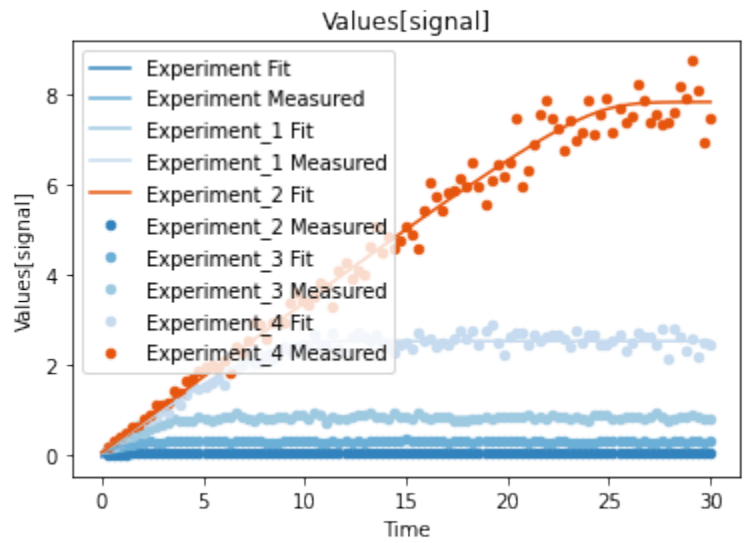
[13]:
```
run_parameter_estimation(method='Levenberg - Marquardt', update_model=True)
```

[13]:

name	lower	upper	sol	affected
(R1).k2	1e-6	1e6	0.000002	[]
(R2).k1	1e-6	1e6	44.729444	[]
Values[offset]	-0.2	0.4	0.043013	[Experiment_1]
Values[offset]	-0.2	0.4	0.054212	[Experiment_3]
Values[offset]	-0.2	0.4	-0.050942	[Experiment]
Values[offset]	-0.2	0.4	0.040968	[Experiment_4]
Values[offset]	-0.2	0.4	0.047976	[Experiment_2]

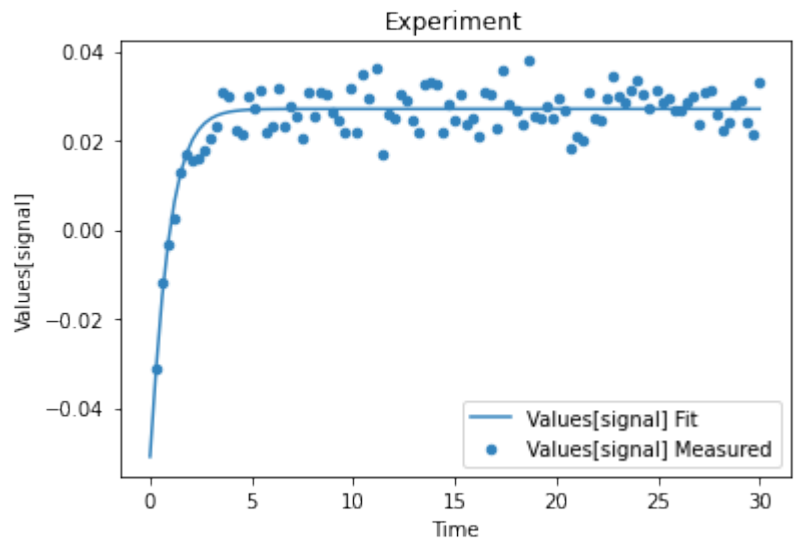
A first predefined plot function creates one plot for each defined dependent variable, containing all experiments in which it appears.

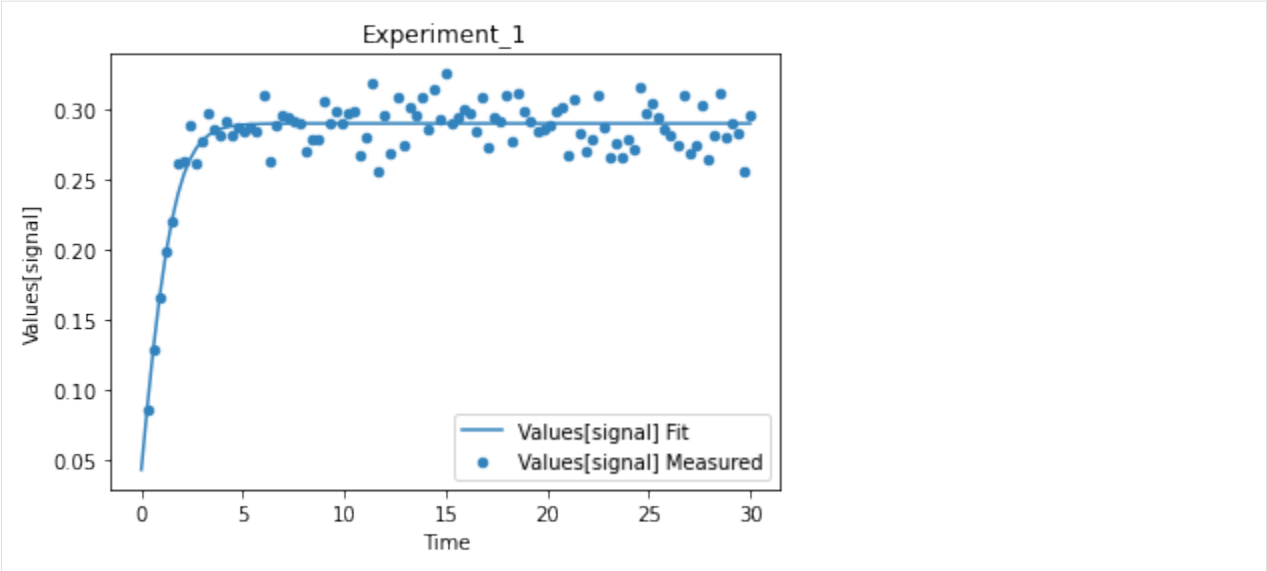
[14]:
```
plot_per_dependent_variable();
```

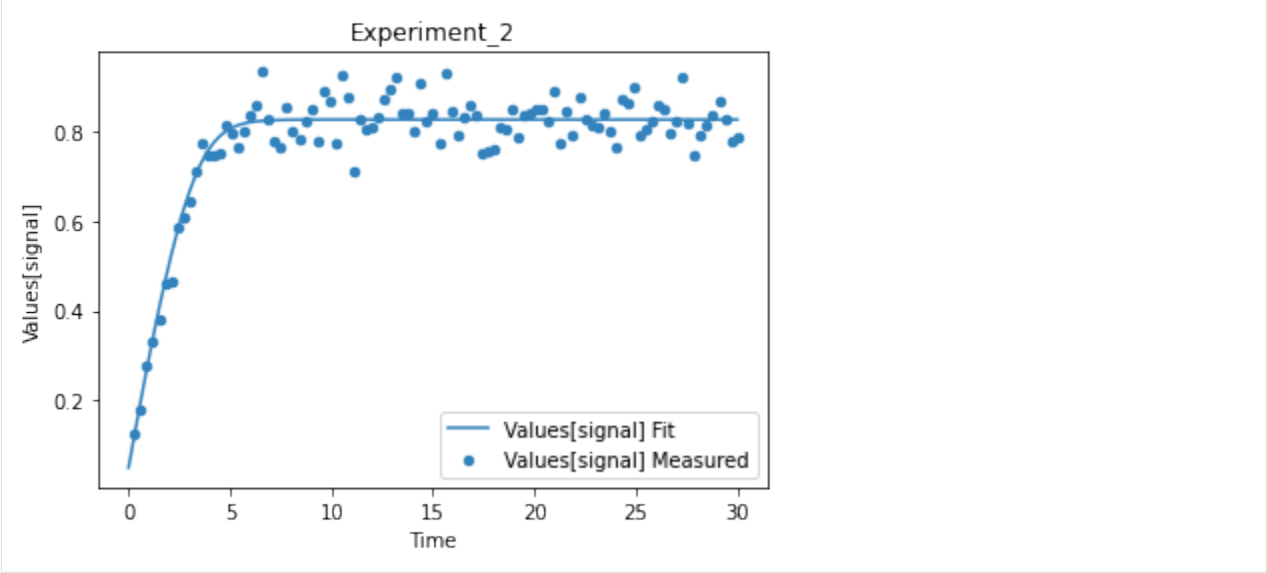


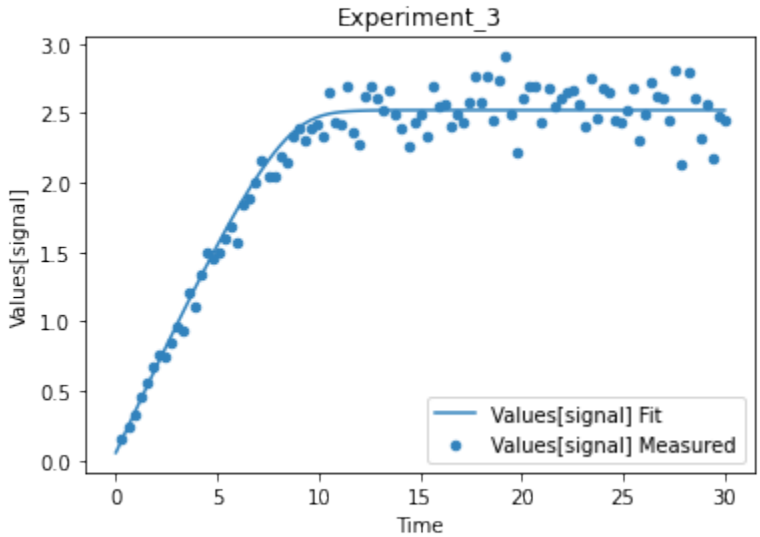
a second predefined plot function created one plot for each experiment, including all contained dependent values:

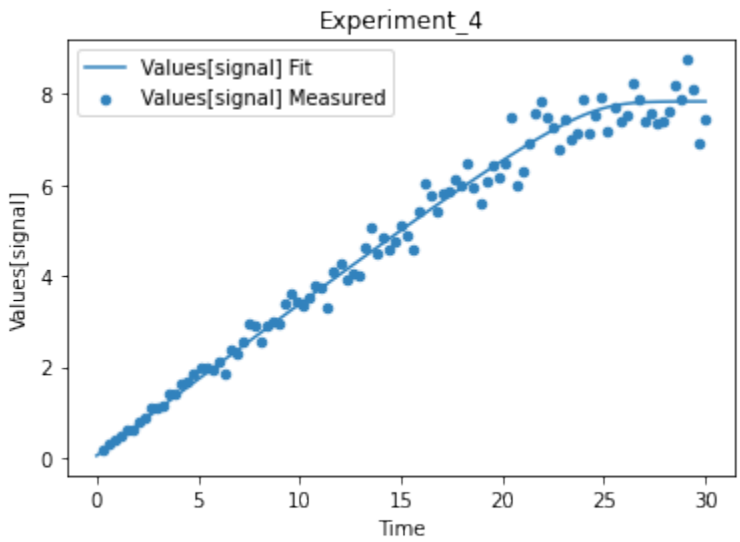
[15]:
```
plot_per_experiment();
```




Experiment_1
Values[signal]
Time
Values[signal] Fit
Values[signal] Measured

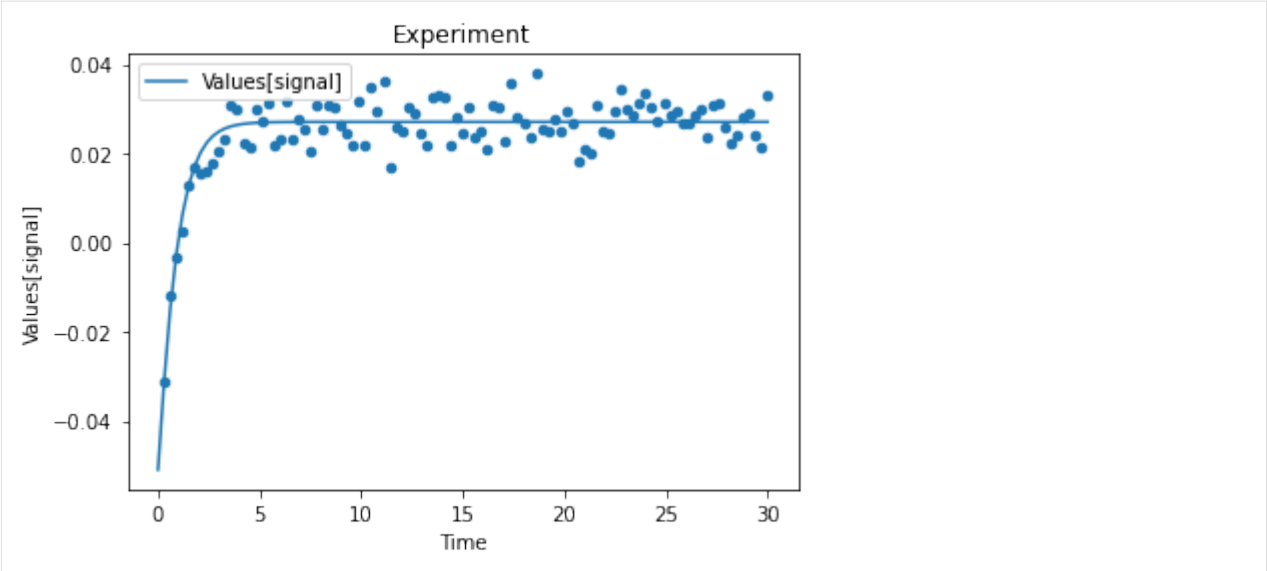

Experiment_2
Values[signal]
Time
Values[signal] Fit
Values[signal] Measured

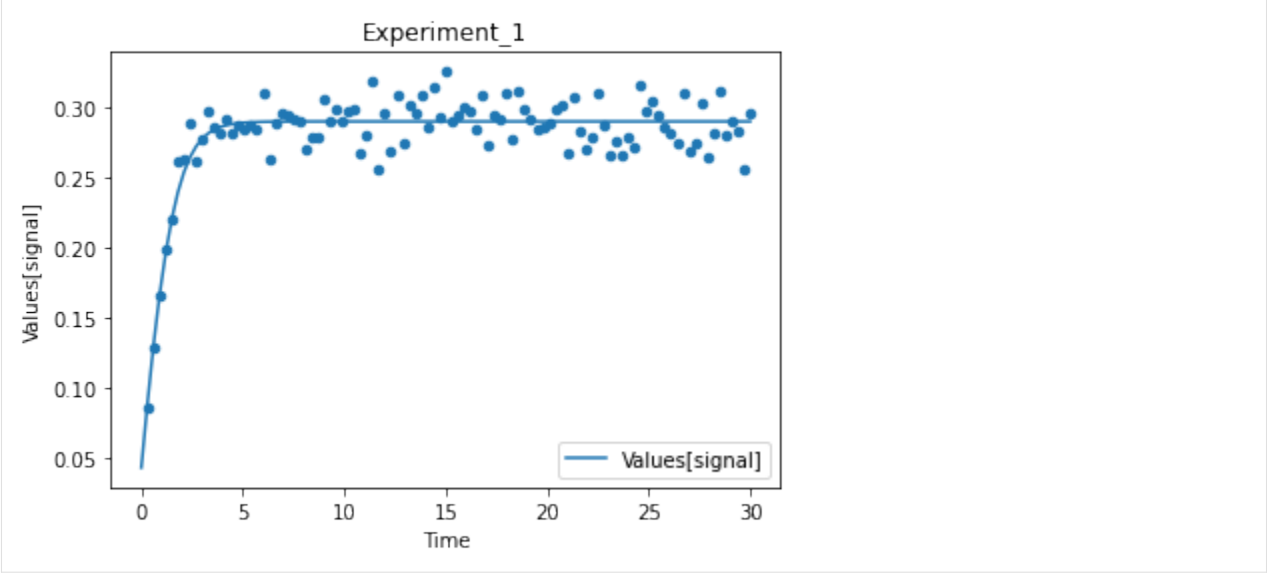


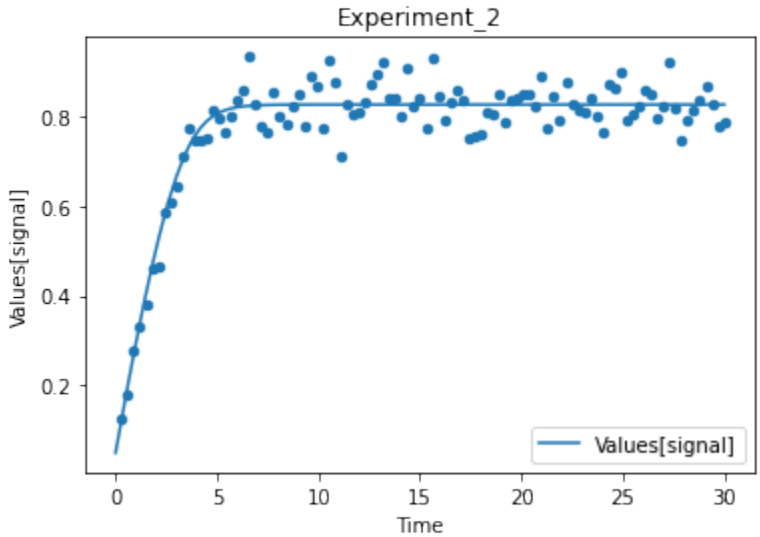


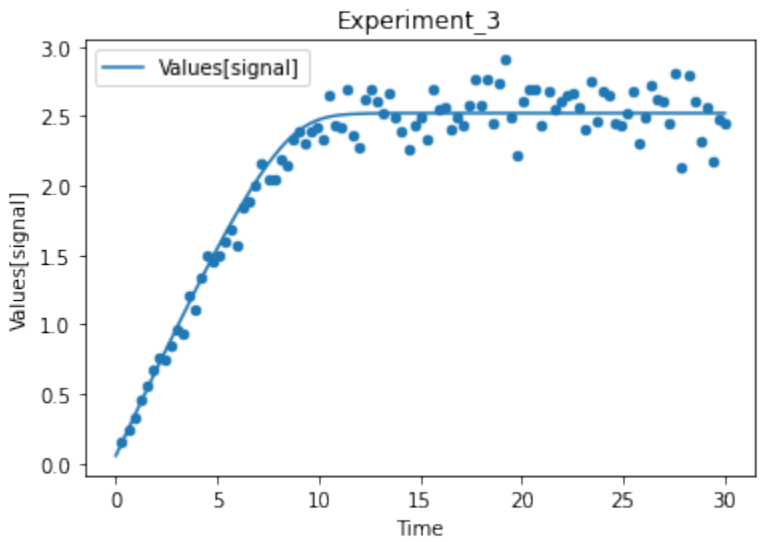
you also get all the data sets returned, so you can plot them yourself howerver you like

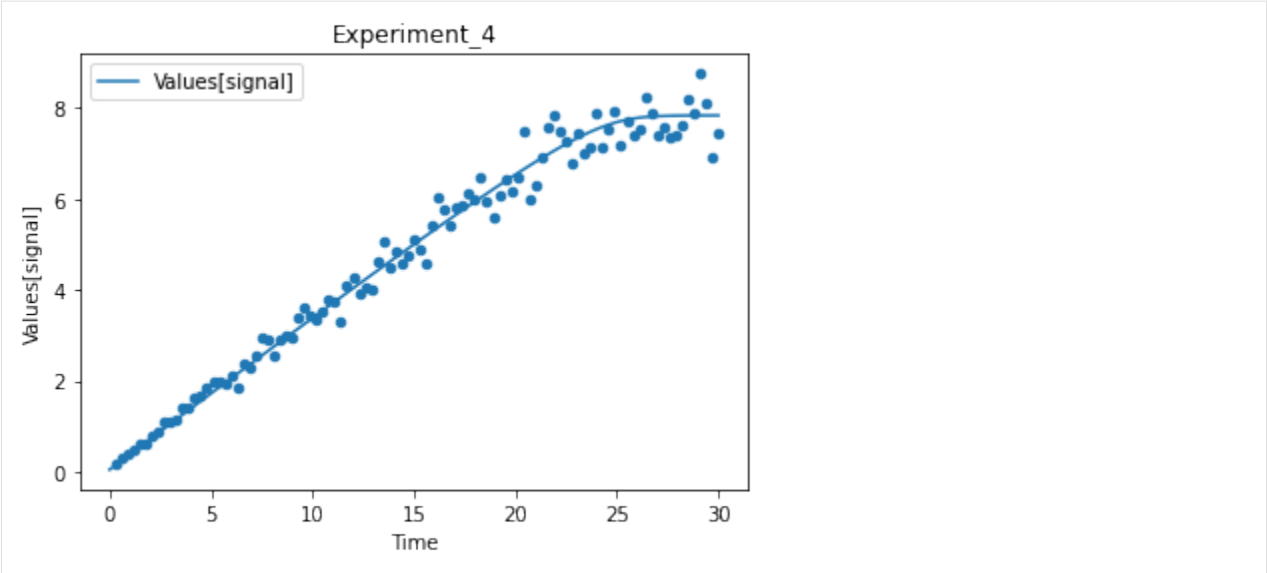
[16]:
```
exp, sim = get_simulation_results()
experiment_names = get_experiment_names()
for i in range(len(exp)):
    ax = exp[i].plot.scatter(x='Time', y='Values[signal]')
    sim[i].reset_index().plot(x='Time', y='Values[signal]', ax=ax)
    ax.set_title(experiment_names[i])
```


Experiment
Values[signal]
0.04
0.02
0.00
−0.02
−0.04
Values[signal]
0
5
10
15
20
25
30
Time


Experiment_1
0.30
0.25
0.20
0.15
0.10
0.05
Values[signal]
Values[signal]
0
5
10
15
20
25
30
Time


Experiment_2
Values[signal]
Time
Values[signal]
0.2
0.4
0.6
0.8
0
5
10
15
20
25
30


Experiment_3
Values[signal]
Time
Values[signal]
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
5
10
15
20
25
30


Experiment_4
Values[signal]
Values[signal]
Time
0
2
4
6
8
0
5
10
15
20
25
30

CHAPTER

SEVEN

PARAMETER ESTIMATION SETUP

This example goes through the steps of setting up the parameter estimation task directly from basiCO. Experimental data is provided through pandas dataframes, and mapping of the columns will be done by convention using specially crafted column names.

We start as usual:

[1]:
```
import sys
if '../..' not in sys.path:
    sys.path.append('../..')
from basico import *
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
%matplotlib inline
```

7.1 preparing the data

In this example we generate the data set by modifying the brusselator model, to produce some noisy data, and we will take that data set as a starting point for the parameter estimation later on. So lets start loading the brusselator model, and adding two observable variables that follow the model species with some noise added:

[2]:
```
load_example('brusselator')
add_parameter('obs_x', type='assignment', expression='[X] + UNIFORM(0,1) - 0.5')
add_parameter('obs_y', type='assignment', expression='[Y] + UNIFORM(0,1) - 0.5');
```

now we simulate the model, ensuring to return all result columns (not just the concentration ones)

[3]:
```
result = run_time_course(start_time=0, use_number=True)
```

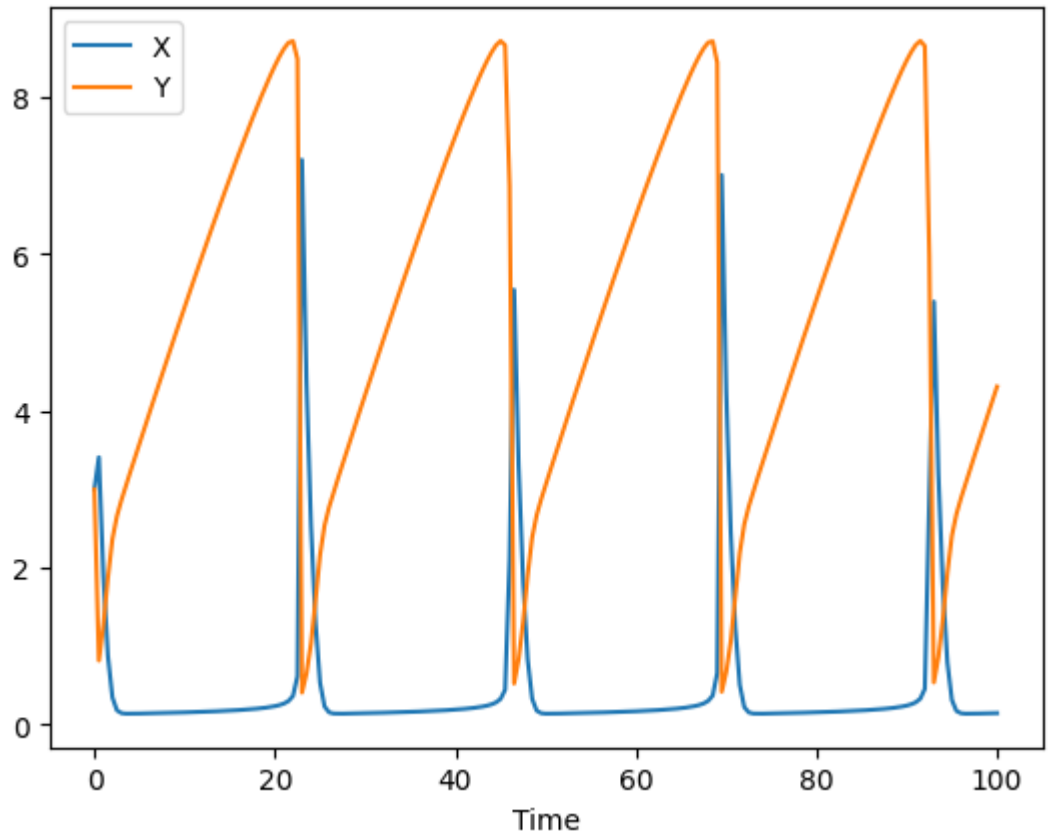
[4]:
```
result.head()
```

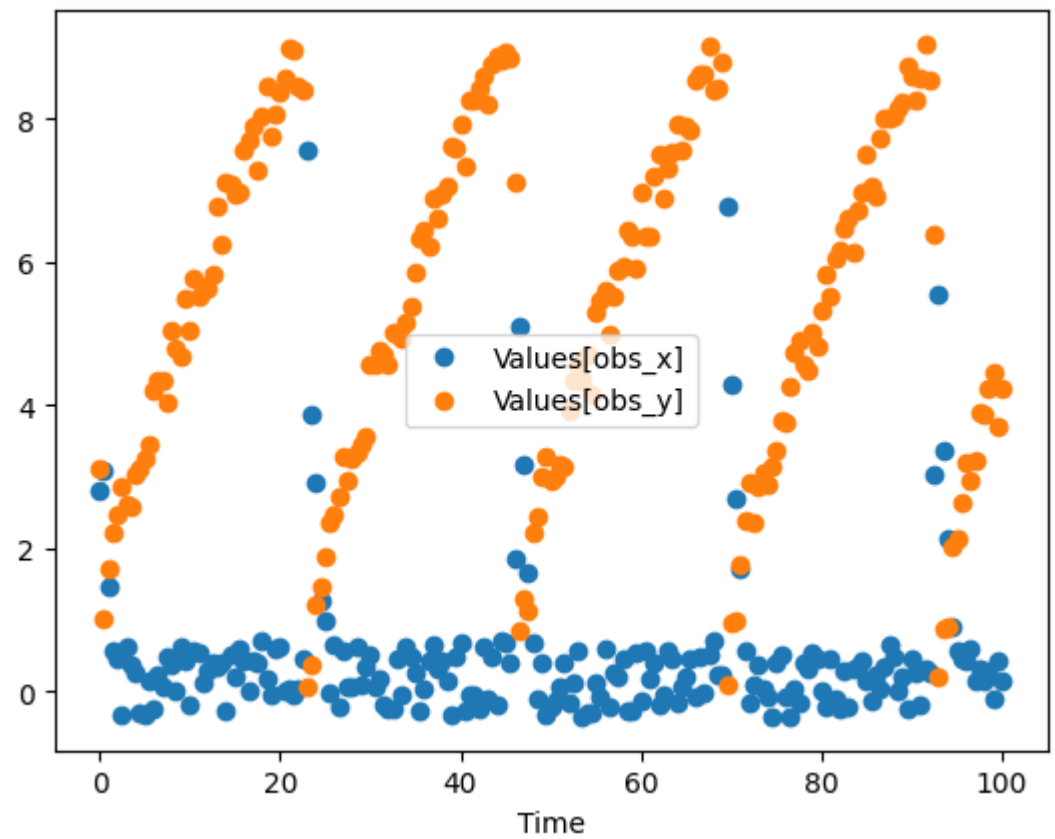
[4]:

	X	Y	Values[obs_x]	Values[obs_y]
Time				
0.0	2.999996	2.999996	2.795629	3.114868
0.5	3.408155	0.817484	3.086833	1.012499
1.0	1.896454	1.276790	1.456064	1.714168
1.5	0.876253	1.872929	0.579525	2.232427
2.0	0.345934	2.368188	0.448776	2.465324

lets plot the simulation data (first plot) and the noisy data (second plot)

[5]:
```
ax = result.plot(y='X')
result.plot(y='Y', ax=ax)

ax = result.plot(y='Values[obs_x]', style='o')
result.plot(y='Values[obs_y]', style='o' , ax=ax);
```





so our experimental data is the data frame with just the 2 last columns. I also rename the columns, so it makes it clear that i want to map it later to the transient concentrations. I'll also reset the index, so Time is a separate column:

[6]:
```
data = result.drop(columns=['X', 'Y'])
data.rename(columns = {'Values[obs_x]':'[X]', 'Values[obs_y]':'[Y]'}, inplace=True)
data = data.reset_index()
```

[7]:
```
data.head()
```

[7]:
```
   Time       [X]       [Y]
0   0.0  2.795629  3.114868
1   0.5  3.086833  1.012499
2   1.0  1.456064  1.714168
3   1.5  0.579525  2.232427
4   2.0  0.448776  2.465324
```

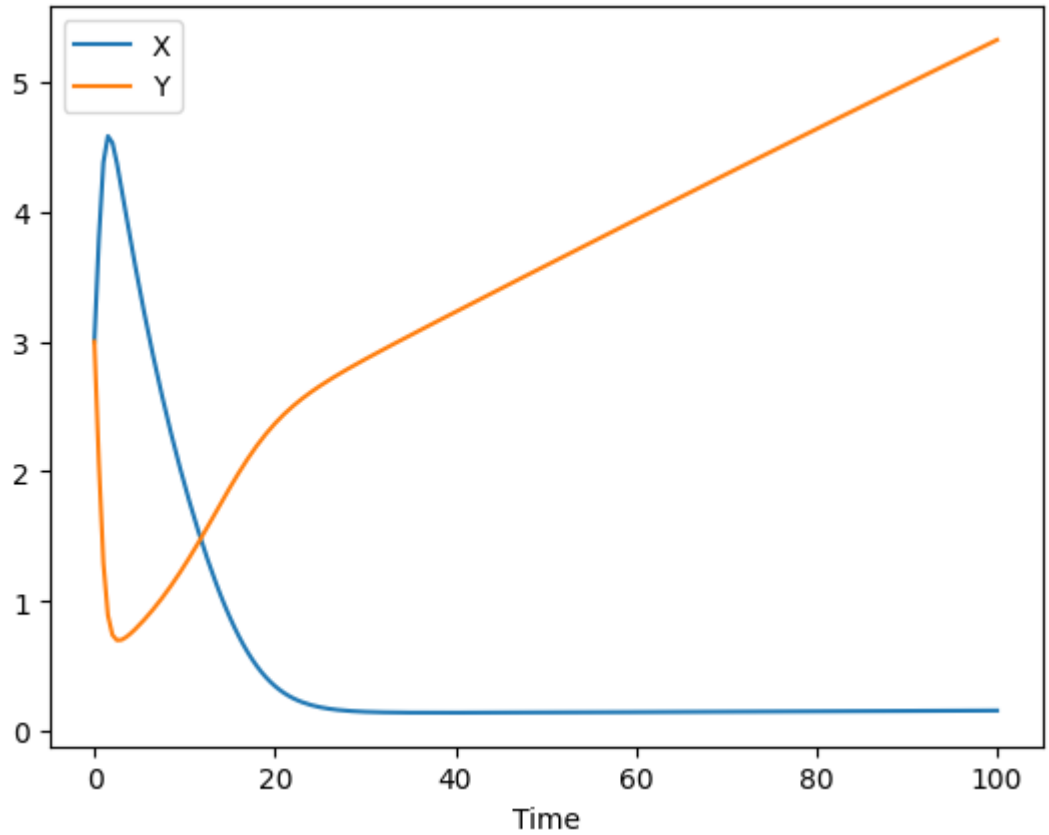
the parameters that gave rise to the solution were:

[8]:
```
get_reaction_parameters()
```

[8]:
```
         value reaction   type mapped_to
name
(R1).k1    1.0       R1  local
(R2).k1    1.0       R2  local
(R3).k1    1.0       R3  local
(R4).k1    1.0       R4  local
```

lets set them to something, else, so that the parameter estimation task will have something to do to find them again (we also remove the observable variables as we won't need them anymore):

[9]:
```
set_reaction_parameters(['(R1).k1', '(R2).k1', '(R3).k1', '(R4).k1'], value=0.1)
remove_parameter('obs_x')
remove_parameter('obs_y')
run_time_course(start_time=0).plot();
```



[10]:
```
get_reaction_parameters()
```

[10]:
```
         value reaction   type mapped_to
name
(R1).k1    0.1       R1  local
(R2).k1    0.1       R2  local
(R3).k1    0.1       R3  local
(R4).k1    0.1       R4  local
```

7.2 setting up the parameter estimation

the next step is to setup the paramter estimation task, first we add the experiment, and it will tell us where the experiment file has been created in case you want to delete it later.

[11]:
```
add_experiment('exp1', data)
```

[11]:
```
'/Users/frank/Development/basico/docs/notebooks/exp1.txt'
```

now lets verify that the experiment is there:

[12]:
```
get_experiment('exp1')
```

[12]:
```
<CExperiment "exp1">
```

and we have the mapping we were expecting:

[13]:
```
get_experiment_mapping('exp1')
```

[13]:
```
             type mapping                                                cn  \
column
0            time
1       dependent     [X]  CN=Root,Model=The Brusselator,Vector=Compartme...
2       dependent     [Y]  CN=Root,Model=The Brusselator,Vector=Compartme...

       column_name
column
0             Time
1              [X]
2              [Y]
```

now we are ready to add the parameters we want to fit, in our case this will be the reaction parameters:

[14]:
```
fit_items = [
            {'name': '(R1).k1', 'lower': 0.001, 'upper': 2},
            {'name': '(R2).k1', 'lower': 0.001, 'upper': 2},
            {'name': '(R3).k1', 'lower': 0.001, 'upper': 2},
            {'name': '(R4).k1', 'lower': 0.001, 'upper': 2},
        ]
```

[15]:
```
set_fit_parameters(fit_items)
```

[16]:
```
get_fit_parameters()
```

[16]:
```
         lower upper  start affected  \
name
(R1).k1  0.001     2    0.1       []
(R2).k1  0.001     2    0.1       []
(R3).k1  0.001     2    0.1       []
(R4).k1  0.001     2    0.1       []

                                                      cn
name
(R1).k1  CN=Root,Model=The Brusselator,Vector=Reactions...
(R2).k1  CN=Root,Model=The Brusselator,Vector=Reactions...
```

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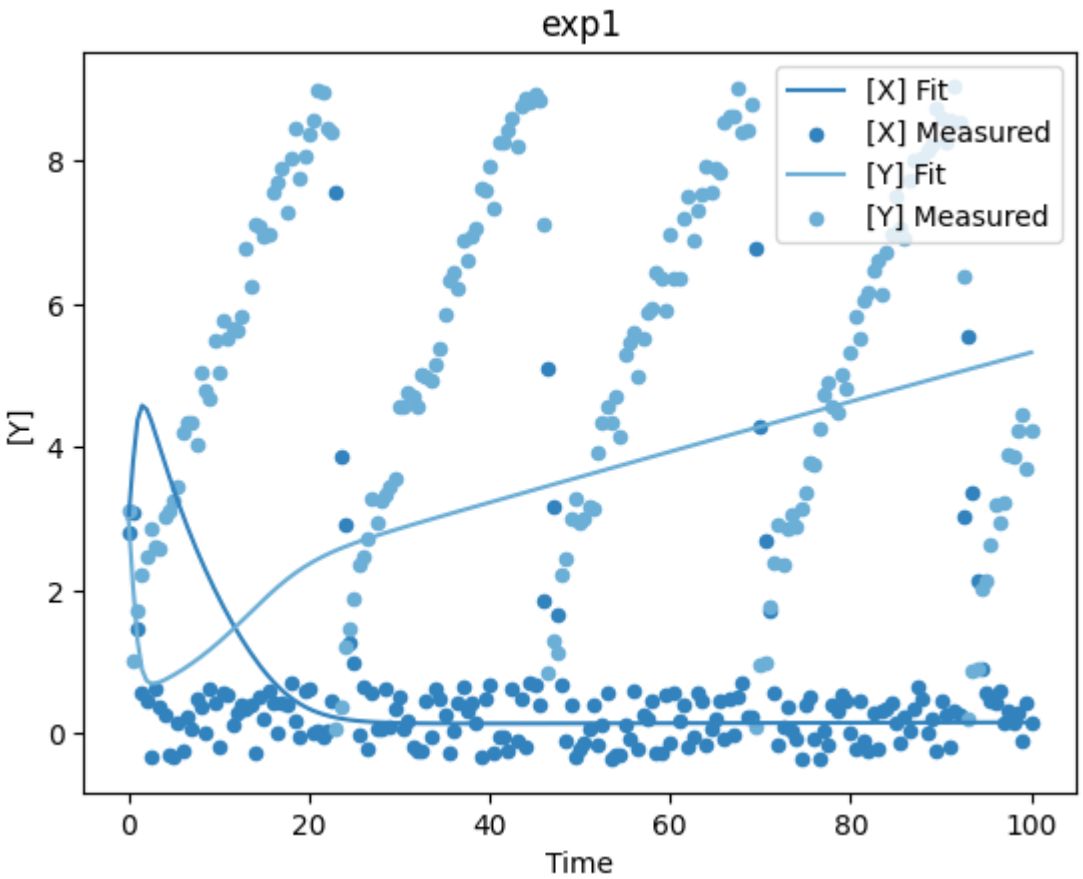
```
(R3).k1  CN=Root,Model=The Brusselator,Vector=Reactions...
(R4).k1  CN=Root,Model=The Brusselator,Vector=Reactions...
```

and with that we are ready to run the parameter estimation. Lets see how the fit looks now, it should be bad, since we set the parameters way off:

[17]:
```
plot_per_experiment();
```



Now lets run the parameter estimation, all the task names from the COPASI GUI are valid, algorithms here:

Current Solution:

- `Current Solution Statistics`,

Global Methods:

- `Random Search`,
- `Simulated Annealing`,
- `Differential Evolution`,
- `Scatter Search`,
- `Genetic Algorithm`,
- `Evolutionary Programming`,
- `Genetic Algorithm SR`,

- Evolution Strategy (SRES),
- Particle Swarm,

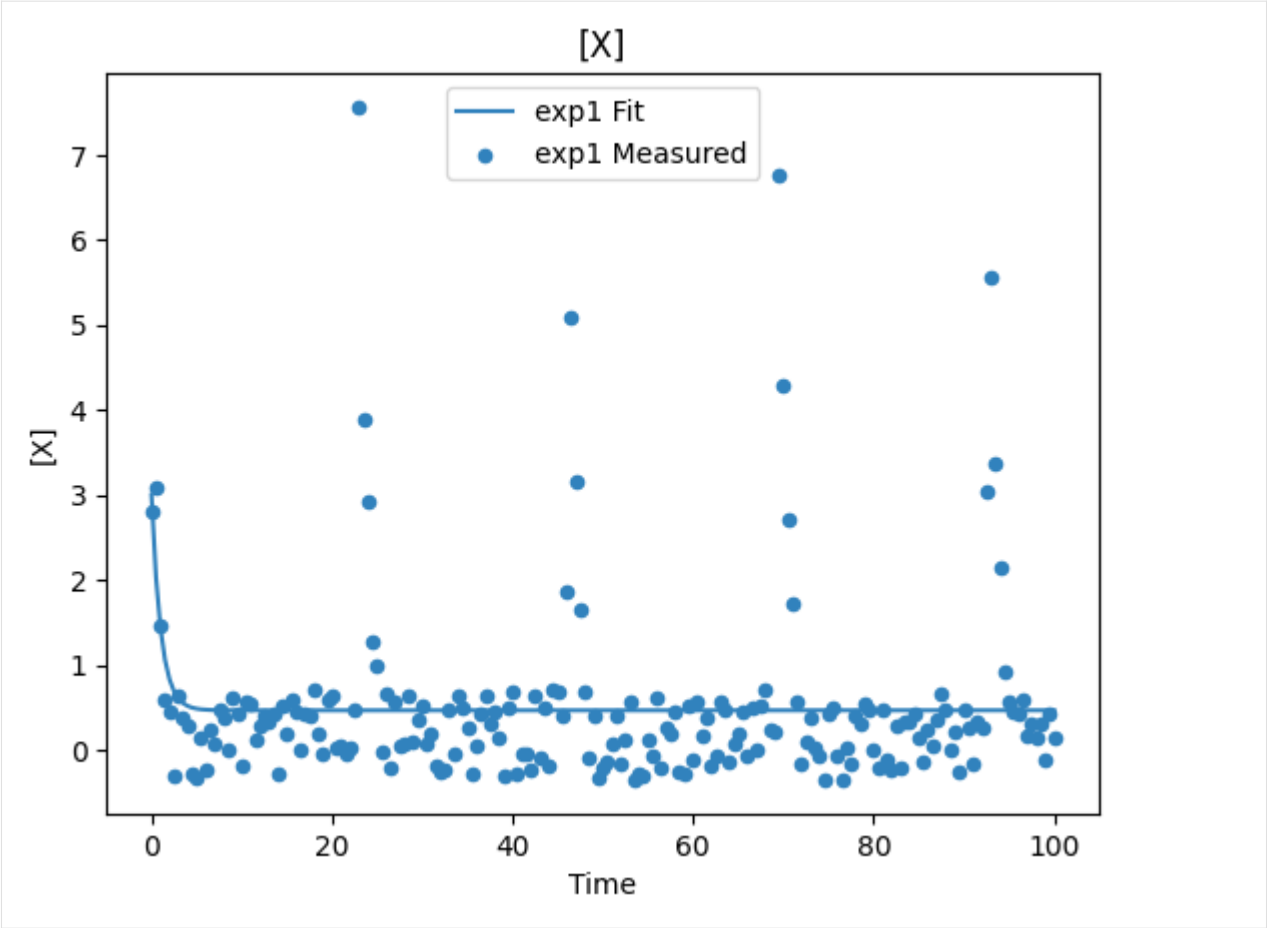
Local Methods:

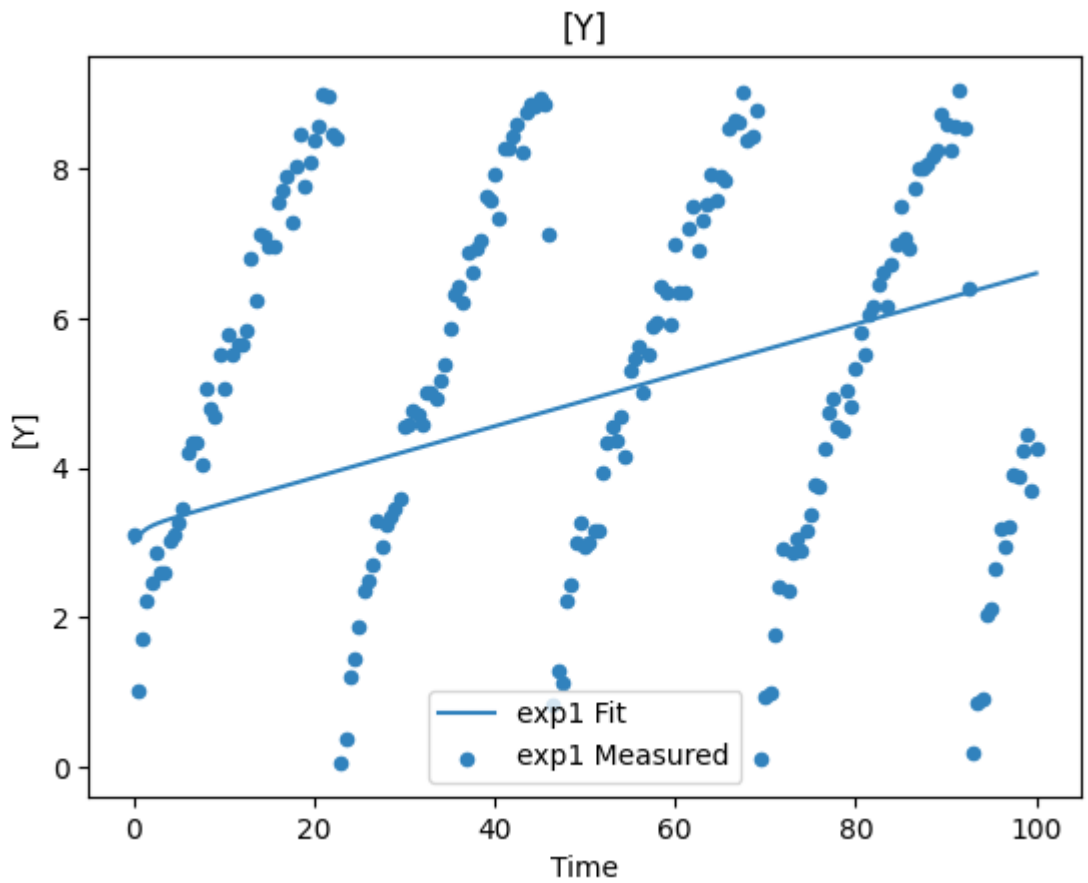
- Levenberg - Marquardt,
- Hooke & Jeeves,
- Nelder - Mead,
- Steepest Descent,
- NL2SOL,
- Praxis,
- Truncated Newton,

[18]:
```
run_parameter_estimation(method='Evolution Strategy (SRES)', update_model=True)
```

[18]:
```
         lower upper       sol affected
name
(R1).k1  0.001     2  0.908366       []
(R2).k1  0.001     2  0.001000       []
(R3).k1  0.001     2  0.025244       []
(R4).k1  0.001     2  0.902824       []
```

[19]:
```
plot_per_dependent_variable();
```


[X]
exp1 Fit
exp1 Measured
[X]
Time
0
1
2
3
4
5
6
7
0
20
40
60
80
100



7.3 Constraints

Additionally, you can add constraints to the parameter estimation problem. These constraint will be evaluated after each simulation, and allow to ensure, for example that solutions with concentrations outside a certain range are rejected.

Constraints are defined, just as the fit parameters specified above, when using `set_fit_constraints`. To see the constraints defined, you would use `get_fit_constraints`.

To demonstrate, lets create a constraint for this example, that rejects solutions, where the concentration of `[Y]` is outside the range of 2…10.

[20]:
```
set_fit_constraints([
    {'name': 'Y', 'lower': 2, 'upper': 10}
])
```

`get_fit_constraints` returns a pandas dataframe of the constraints, and as usual we can trasnform them to a dictionary if needed using `as_dict`.

[21]:
```
get_fit_constraints()
```

[21]:
```
     lower upper     start affected  \
name
Y        2    10  6.597017       []
```

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```
                                                    cn
name
Y     CN=Root,Model=The Brusselator,Vector=Compartme...
```

[22]:
```
as_dict(get_fit_constraints())
```

[22]:
```
{'name': 'Y',
 'lower': '2',
 'upper': '10',
 'start': 6.597017117106328,
 'affected': [],
 'cn': CN=Root,Model=The Brusselator,Vector=Compartments[compartment],
↪Vector=Metabolites[Y],Reference=Concentration}
```

now lets try to run the parameter estimation again, using this constraint:

[23]:
```
run_parameter_estimation(method=PE.LEVENBERG_MARQUARDT)
get_fit_statistic()
```

[23]:
```
{'obj': 295.53087769380215,
 'rms': 0.8574097253059701,
 'sd': 0.8617075453441385,
 'f_evals': 147,
 'failed_evals_exception': 0,
 'failed_evals_nan': 0,
 'constraint_evals': 2,
 'failed_constraint_evals': 0,
 'cpu_time': 0.028593999999999998,
 'data_points': 402,
 'valid_data_points': 402,
 'evals_per_sec': 0.00019451700680272107}
```

If we look at the fit statistic, we see that the evalations failed. This happened, because the allowed interval in the constraint was too small. Setting the lower bound of the constraint, fixes that issue:

[24]:
```
set_fit_constraints([
    {'name': 'Y', 'lower': 0, 'upper': 10}
])
run_parameter_estimation(method=PE.LEVENBERG_MARQUARDT)
get_fit_statistic()
```

[24]:
```
{'obj': 295.53087769380215,
 'rms': 0.8574097253059701,
 'sd': 0.8617075453441385,
 'f_evals': 147,
 'failed_evals_exception': 0,
 'failed_evals_nan': 0,
 'constraint_evals': 2,
 'failed_constraint_evals': 0,
 'cpu_time': 0.026792,
 'data_points': 402,
 'valid_data_points': 402,
 'evals_per_sec': 0.00018225850340136056}
```

We've seen how to add constraints to the parameter estimation problem, and how it would look if the constraint causes the parameter estimation procedure to fail.

CHAPTER

EIGHT

PARAMETER ESTIMATION (IMPORT / EXPORT)

This example describes how to export the parameter estimation setup to a YaML file (or string), so that it can be easily modified later, and then loaded back (or applied to a different model).

8.1 The Format

When saving the file, it will be exported as a sequence, of experiments of the following form:

```
name: Experiment
  filename: data.txt
  type: Time-Course
  separator: "\t"
  first_row: 1
  last_row: 102
  header_row: 1
  weight_method: Mean Square
  normalize_per_experiment: true
  mapping:
  - column: '# Time'
    type: time
  - column: Values[F16BP_obs]
    type: dependent
    cn: CN=Root, ...
    object: '[Fru1,6-P2]'
```

the individual fields are:

- `name`: the name of the experiment
- `type`: `Time-Course` for time course data (requires a mapping of type `time` to be specified), or `Steady-State` for steady state data.
- `separator`: the separator being used
- `first_row`: the beginning of the experiment in the file (1 based)
- `last_row`: the last row of the experiment
- `header_row`: (optional) row with header information that can be later used in the `column` field of the mappings.
- `weight_method`: one of: `Mean`, `Mean Square`, `Standard Deviation` or `Value Scaling`.
- `normalize_per_experiment`: boolean indicating whether experiments should be scaled individual (`True`) or over all defined experimentes (`False`).

- `mapping`: sequence of column mappings described as follows.

The mapping descriptions contain the fields:

- `column`: either an integer index (zero based), describing which column the mapping applies to. If the experiment has header information, the column may be a string with the (case sensitive) header the mapping applies to.
- `type`: the type of the mapping for this column. One of `ignored`, `time`, `dependent` or `independent`.
- `object`: display name of the element to map to
- `cn`: (optional) the CN to the reference to map to.

  For columns of type `dependent` or `independent` at least on of `object` or `cn` needs to be defined. (The `cn` value takes preference).
- `weight`: may be used for columns of type `dependent` to customize the scale to be applied to the column. If not specified it will be automatically calculated based on the selected `weight_method`.

8.2 Example

We start by importing basico as usual (should that fail for you just `!pip install copasi-basico`:

[1]:
```
from basico import *
```

here we load an existing parameter estimation example, included with the distribution as example:

[2]:
```
dm = load_example('PK')
```

now we can directly export the setup of the experimental data files as yaml string (or if you supply a filename to the function, it will be saved as file):

[3]:
```
yaml_str = save_experiments_to_yaml()
print("\n".join(yaml_str.split('\n')[:24])) # just restricting the amount of yaml to be
↪printed here to the first experiment
```

```
- name: Experiment
  filename: e:/development/basico/basico/data\data_2.txt
  type: Time-Course
  separator: "\t"
  first_row: 1
  last_row: 102
  weight_method: Mean Square
  normalize_per_experiment: true
  header_row: 1
  mapping:
  - column: '# Time'
    type: time
  - column: Values[F16BP_obs]
    type: dependent
    cn: CN=Root,Model=Pritchard2002_glycolysis,Vector=Compartments[cytosol],
↪Vector=Metabolites[Fru1\,6-P2],Reference=Concentration
    object: '[Fru1,6-P2]'
  - column: Values[Glu_obs]
    type: dependent
    cn: CN=Root,Model=Pritchard2002_glycolysis,Vector=Compartments[cytosol],
```

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```
↪Vector=Metabolites[Glc(int)],Reference=Concentration
    object: '[Glc(int)]'
  - column: Values[Pyr_obs]
    type: dependent
    cn: CN=Root,Model=Pritchard2002_glycolysis,Vector=Compartments[cytosol],
↪Vector=Metabolites[pyruvate],Reference=Concentration
    object: '[pyruvate]'
```

at this point you'd make modifications to you'd want to it. Remember, that the `cn` is optional. The key points to keep in mind:

- ensure that the row number for the experiment are consistent with the changes you make
- if it is a time course experiment, ensure you have a column of type `time`.
- the column specifier is either the index of the column, or the name if the experiment has headers.

once the changes are made, you can load the setup back into the model, using the `load_experiments_from_yaml` function. This will remove all existing experiments from the file first.

[4]:
```
load_experiments_from_yaml(yaml_str)
```

CHAPTER

NINE

OPTIMIZATION

This notebook walks through the steps of setting up / running optimizations using basico. We start as usual:

[1]:
```
from basico import *
```

9.1 Model

The first step is to load a model (this can be done as usual using `load_model`, `load_biomodel` or by `load_example`) or create a new one. Here I'll create one with a typical optimization problem, the himmelblau function:

$$f(x, y) = (x^2 + y - 11)^2 + (x + y^2 - 7)^2$$

In basico this is easily done using global parameters for x and y, and then an assignment for the function

[2]:
```
new_model(name="Himmelblau",
          notes="""A model implementing the himmelau function

          Maxima is known to be at (-0.270845, -0.923039) with
          max value 181.617

          4 Minima: (3,2), (-2.805118, 3.131313),
                    (-3.779310, -3.2383186),
                    (3.584428, -1.848126) with value 0

          """);
```

[3]:
```
add_parameter('x', initial_value=0)
add_parameter('y', initial_value=0)
add_parameter('f', type='assignment',
              expression='({Values[x].InitialValue}^2+{Values[y].InitialValue}-11)^2+(
↪{Values[x].InitialValue}+{Values[y].InitialValue}^2-7)^2');
```

9.2 The Setup

Now we setup the parameters to be varied during the optimization. For each item we need to specify, what to vary, as well as the lower and upper bounds. The utility function `get_opt_item_template` allows to retrieve all the global / local parameters and sets default bounds:

[4]:
```
get_opt_item_template(include_global=True, default_lb=-1)
```

[4]:
```
[{'name': 'Values[x].InitialValue', 'lower': -1, 'upper': 1000, 'start': 0.0},
 {'name': 'Values[y].InitialValue', 'lower': -1, 'upper': 1000, 'start': 0.0}]
```

lets use them:

[5]:
```
set_opt_parameters(get_opt_item_template(include_global=True, default_lb=-1))
```

the next thing is to set up the objective function. Any expression with the names of model elements will work, here we want to minimize the value of the global parameter `f`:

[6]:
```
set_objective_function(expression='Values[f].InitialValue', minimize=True)
```

additional settings can be modified using `set_opt_settings`, such as specifying the method to be used and their parameters:

[7]:
```
set_opt_settings(settings={
    'subtask': T.TIME_COURSE,
    'method': {
        'name': PE.LEVENBERG_MARQUARDT
}})
```

to verify the setup you can use `get_opt_parameters` to retrieve all the parameters and bounds and `get_opt_settings` to retrieve all settings:

[8]:
```
get_opt_settings()
```

[8]:
```
{'scheduled': False,
 'update_model': False,
 'problem': {'Maximize': False,
  'Randomize Start Values': False,
  'Calculate Statistics': True},
 'method': {'Iteration Limit': 2000,
  'Tolerance': 1e-06,
  'name': 'Levenberg - Marquardt'},
 'report': {'filename': '',
  'report_definition': 'Optimization',
  'append': True,
  'confirm_overwrite': True},
 'expression': 'Values[f].InitialValue',
 'subtask': 'Time-Course'}
```

9.3 Running the optimization

Now that everything is set up, we can simply run the optimization:

[9]:
```
run_optimization()
```

[9]:
```
          lower upper       sol
name
Values[x]    -1  1000  2.999999
Values[y]    -1  1000  2.000000
```

we got close to one of the minima, to see more information about the run, you can use:

[10]:
```
get_opt_statistic()
```

[10]:
```
{'obj': 8.352969862744543e-11,
 'f_evals': 321,
 'failed_evals_exception': 0,
 'failed_evals_nan': 0,
 'constraint_evals': 0,
 'failed_constraint_evals': 0,
 'cpu_time': 0.001112,
 'evals_per_sec': 3.46417445482866e-06}
```

9.4 Customn Output

normally when you run an optimization `run_optimization` will return a data frame of the best parameters found, just as when you run `get_opt_solution`. So, since we get to the results in any case, there is an optional parameter that you can pass to `run_optimization`, to collect any element you would like during the run.

This is an advanced feature, as for many things we only have Common Names, that are a bit wieldy to use, still lets do that here.

NOTE: this will only work for real valued CN's right now

In the next run, i collect the number of function evaluation and the objective function value:

[11]:
```
run_optimization(output=[
    'Values[x].InitialValue',
    'Values[y].InitialValue',
    'CN=Root,Vector=TaskList[Optimization],Problem=Optimization,Reference=Best Value'
])
```

[11]:
```
    Values[x].InitialValue  Values[y].InitialValue  \
0                 0.000000                0.000000
1                 0.875001                1.375001
2                 2.108645                2.656495
3                 2.185752                2.641869
4                 2.303988                2.611787
5                 2.461318                2.552965
6                 2.637356                2.451114
7                 2.797570                2.308062
8                 2.911844                2.158941
9                 2.972712                2.053942
```

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```
10                2.994778                2.010172
11                2.999459                2.000957
12                2.999970                2.000046
13                2.999998                2.000001
14                2.999999                2.000000
15                2.999999                2.000000
16                2.999999                2.000000
17                2.999999                2.000000

    TaskList[Optimization].(Problem)Optimization.Best Value
0                                        1.700000e+02
1                                        9.641837e+01
2                                        1.987741e+01
3                                        1.750903e+01
4                                        1.400292e+01
5                                        9.623309e+00
6                                        5.245471e+00
7                                        2.014153e+00
8                                        4.593865e-01
9                                        4.851944e-02
10                                       1.711901e-03
11                                       1.604411e-05
12                                       4.073483e-08
13                                       1.515858e-10
14                                       8.410451e-11
15                                       8.353344e-11
16                                       8.352971e-11
17                                       8.352970e-11
```

9.5 Constraints

You can further constrain the optimization problem, by defining constraints that will be evaluated when the model is simulated. This is useful for example, when you want to ensure concentrations are in a specific range.

You can modify constraints using the `set_opt_contraints` function and retrieve them using `get_opt_constraints`. As example here, we constrain the solution to be greater than `170` when maximizing:

[29]:
```
set_opt_constraints([
    {'name': 'Values[f]', 'lower': 170, 'upper': 200}
])
```

[30]:
```
get_opt_constraints()
```

[30]:
```
          lower upper       start  \
name
Values[f]   170   200  181.616522


                                                        cn
name
Values[f]  CN=Root,Model=Himmelblau,Vector=Values[f],Refe...
```

[31]:
```
settings = get_opt_settings()
settings['problem']['Maximize'] = True
run_optimization(settings=settings)
get_opt_statistic()
```

[31]:
```
{'obj': 181.6165215225808,
 'f_evals': 282,
 'failed_evals_exception': 0,
 'failed_evals_nan': 0,
 'constraint_evals': 33,
 'failed_constraint_evals': 0,
 'cpu_time': 0.001709,
 'evals_per_sec': 6.060283687943263e-06}
```

Note: Keep in mind, that setting constraints will make finding the solution harder for the algorithms. So when in doubt, it might be a good idea to take them out.

[ ]:
```

```

CHAPTER

TEN

SIMPLE SIMULATIONS AND PLOTTING

In this file, we load a model from the BioModels database, and simulate it for varying durations. We start as usual:

[2]:
```
from basico import *
```

10.1 Load a model

to load the model, we use the `load_biomodel` function, it takes in either an integer, which will be transformed into a valid biomodels id, or you can pass in a valid biomodels id to begin with:

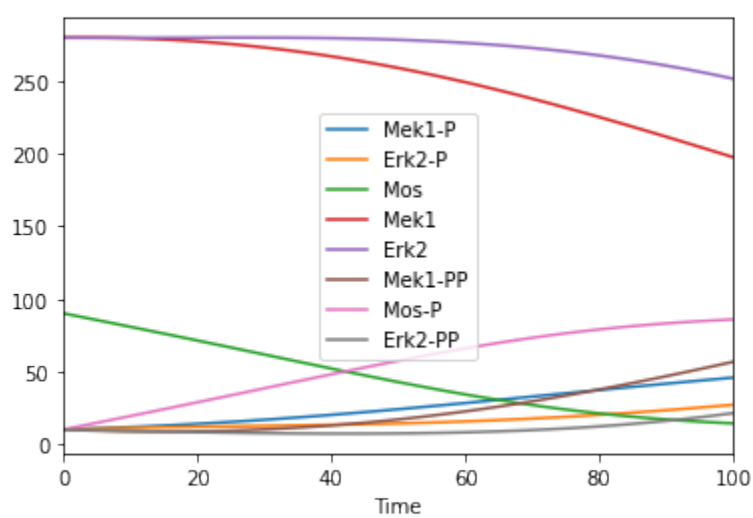
[3]:
```
biomod = load_biomodel(10)
```

10.2 Run time course

After the model is loaded, it is ready to be simulated, here we try it for varying durations:

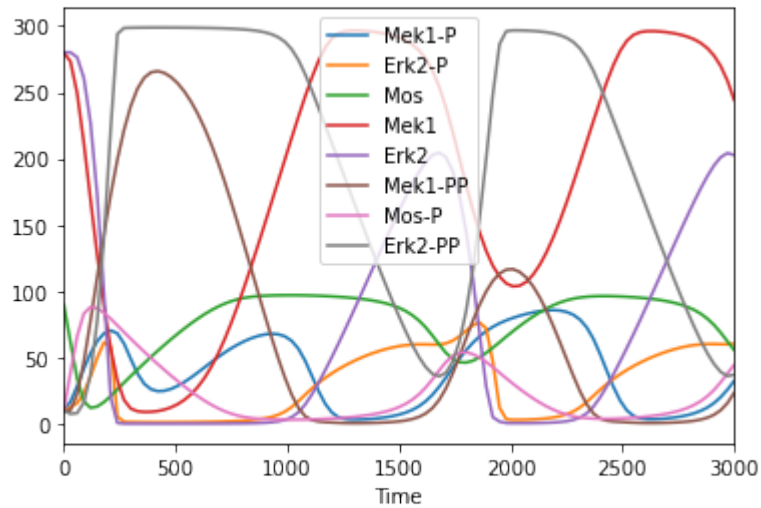
10.2.1 Time course duration 100

[4]:
```
tc = run_time_course(duration = 100)
tc.plot();
```



10.2.2 Time course duration 3000

[5]:
```
tc = run_time_course(duration = 3000)
tc.plot();
```



10.3 Get compartments

To get an overview of what elements the model entails, we can query the individual elements, yielding each time a pandas dataframe with the information:

[6]:
```
get_compartments()
```

[6]:
```
       type unit  initial_size initial_expression  dimensionality expression  \
name
uVol  fixed    l           1.0                                   3

      size  rate            key
name
uVol   1.0   0.0  Compartment_0
```

10.4 Get parameters ("global quantities")

[7]:
```
get_parameters() # no global quantities
```

10.5 Run steady state

we can also run the model to steady state, in order to see the steady state concentrations:

[9]:
```
run_steadystate()
# now call get_species, to get the steady state concentration and particle numbers
get_species()[['concentration', 'particle_number']]
```

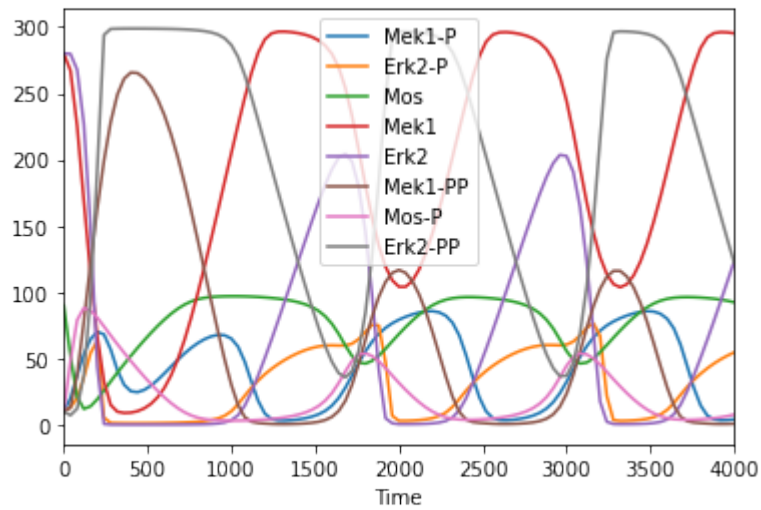
[9]:
```
        compartment       type    unit  initial_concentration  \
name
Mek1-P         uVol  reactions  nmol/l                   10.0
Erk2-P         uVol  reactions  nmol/l                   10.0
Mos            uVol  reactions  nmol/l                   90.0
Mek1           uVol  reactions  nmol/l                  280.0
Erk2           uVol  reactions  nmol/l                  280.0
Mek1-PP        uVol  reactions  nmol/l                   10.0
Mos-P          uVol  reactions  nmol/l                   10.0
Erk2-PP        uVol  reactions  nmol/l                   10.0

         initial_particle_number initial_expression expression  concentration  \
name
Mek1-P              6.022141e+15                                     41.142140
Erk2-P              6.022141e+15                                     99.971352
Mos                 5.419927e+16                                     76.635083
Mek1                1.686199e+17                                    238.913726
Erk2                1.686199e+17                                    102.158541
Mek1-PP             6.022141e+15                                     19.944135
Mos-P               6.022141e+15                                     23.364917
Erk2-PP             6.022141e+15                                     97.870107

         particle_number          rate  particle_number_rate           key
name
Mek1-P      2.477638e+16  3.113511e-16              0.187500  Metabolite_3
Erk2-P      6.020416e+16  0.000000e+00              0.000000  Metabolite_6
Mos         4.615073e+16 -7.783777e-17             -0.046875  Metabolite_0
Mek1        1.438772e+17  0.000000e+00              0.000000  Metabolite_2
Erk2        6.152131e+16 -6.745940e-16             -0.406250  Metabolite_5
Mek1-PP     1.201064e+16 -3.113511e-16             -0.187500  Metabolite_4
Mos-P       1.407068e+16  7.783777e-17              0.046875  Metabolite_1
Erk2-PP     5.893876e+16  6.745940e-16              0.406250  Metabolite_7
```

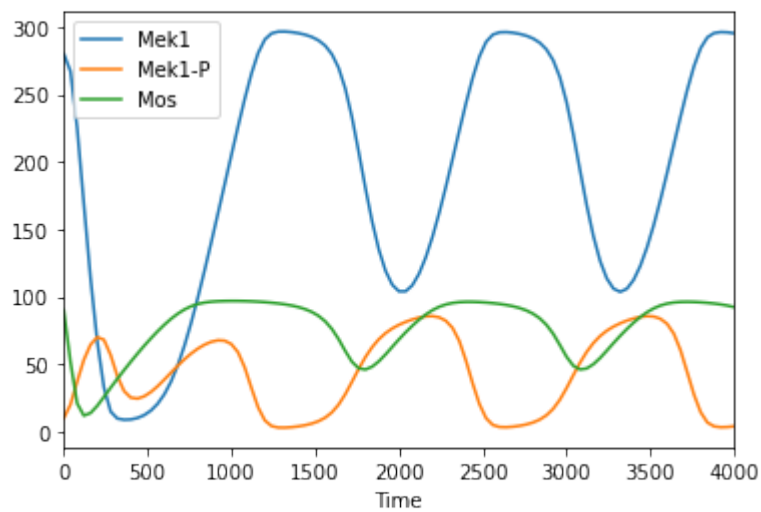
10.6 Use pandas syntax for indexing and plotting

[10]:
```
tc = run_time_course(model = biomod, duration = 4000)
tc.plot();
```



[11]:
```
tc.loc[:, ['Mek1', 'Mek1-P', 'Mos']].plot()
```

[11]:
```
<AxesSubplot:xlabel='Time'>
```



CHAPTER

ELEVEN

SIMULATING A MODEL WITH BASICO

First some jupyter magic for plotting and convenience

[1]:
```
%pylab
%matplotlib inline
import sys
if not '../..' in sys.path:
    sys.path.append('../..')
```

```
Using matplotlib backend: Qt5Agg
Populating the interactive namespace from numpy and matplotlib
```

Now import basico

[2]:
```
from basico import *
```

now we are ready to load a model, just adjust the file_name variable, to match yours. The file can be a COPASI or SBML file. For this example, we use the brusselator model, that is distributed with the package.

[3]:
```
file_name = get_examples('brusselator')[0]
```

[4]:
```
model = load_model(file_name)
```

now we are ready to simulate. Calling `run_time_course` will run the simulation as specified in the COPASI file and return a pandas dataframe for it.

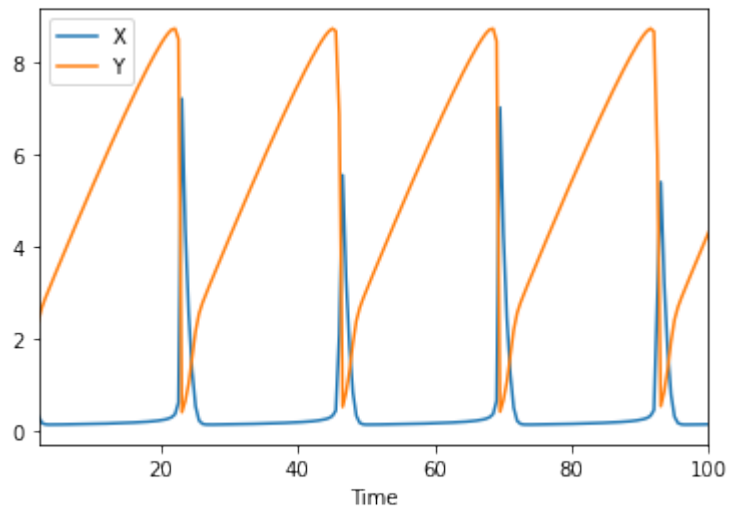
[5]:
```
run_time_course().head()
```

[5]:
```
             X         Y
Time
2.0   0.345934  2.368188
2.5   0.182762  2.658596
3.0   0.147433  2.863681
3.5   0.141129  3.048319
4.0   0.140734  3.228345
```

for plotting you would then just plot that as one does

[6]:
```
df = run_time_course()
df.plot()
```

[6]:
```
<AxesSubplot:xlabel='Time'>
```



11.1 The run_time_course command

you can change different options for the time course by adding named parameters into the `run_time_course_command`. Supported are:

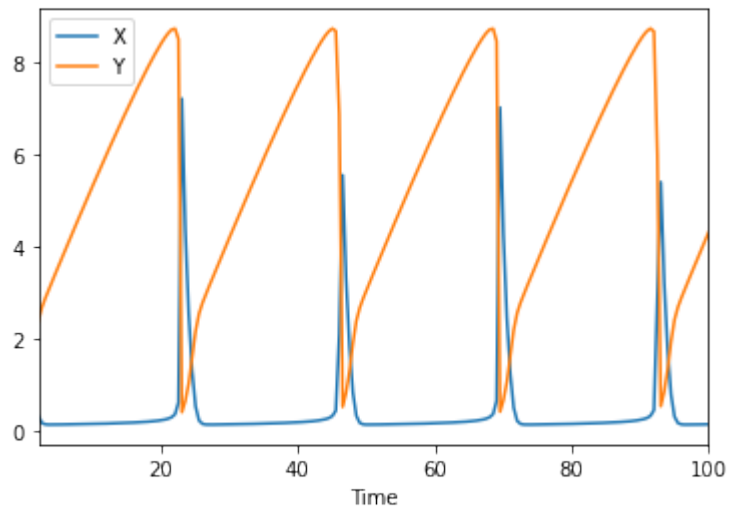
- `model`: incase you want to use another model than the one last loaded
- `scheduled`: to mark the model as scheduled
- `update_model`: to update the initial state after the simulation is run
- `duration`: to specify how long the simulation is run
- `automatic`: in case you would like automatic step size being used
- `output_event`: in case you would like to have the event values before and after the event hit listed
- `start_time`: to change the start time
- `step_number` or `intervals`: to overwrite the number of steps being used
- `method`: a method name to use for the simulation.

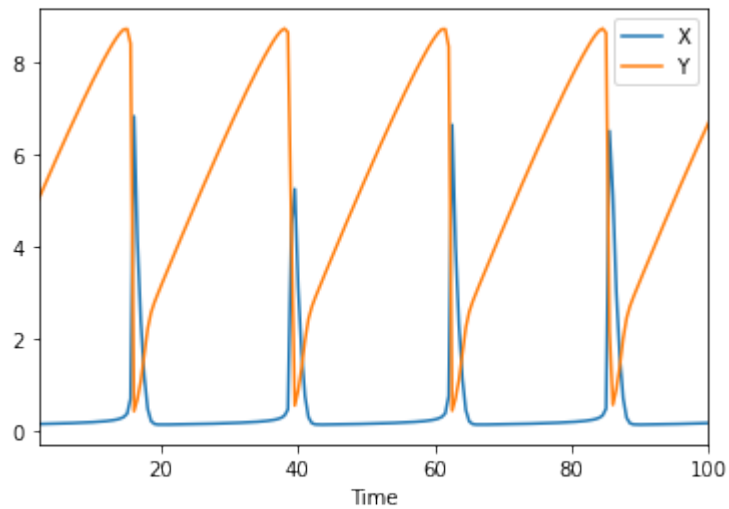
so lets run two simulations that will be different slightly, as we will use the `update_model` flag:

[7]:
```
df1 = run_time_course(update_model=True)
df2 = run_time_course(update_model=True)
```

[8]:
```
df1.plot(), df2.plot()
```

[8]:
```
(<AxesSubplot:xlabel='Time'>, <AxesSubplot:xlabel='Time'>)
```

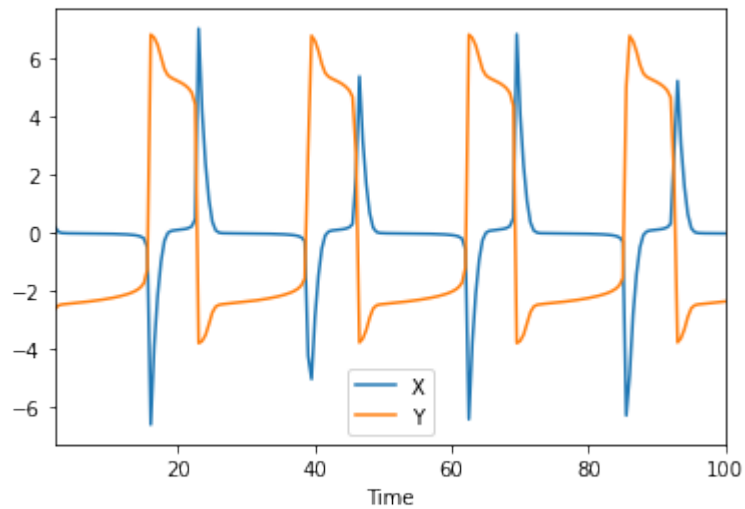




And now you could plot the difference between them too:

[9]:
```
(df1-df2).plot()
```

[9]:
```
<AxesSubplot:xlabel='Time'>
```



[10]:
```
(df1-df2).describe()
```

[10]:

	X	Y
count	197.000000	197.000000
mean	-0.014562	-0.123916
std	1.592729	3.615933
min	-6.630084	-3.816620
25%	-0.056936	-2.428037
50%	-0.024780	-2.245888
75%	0.077394	4.837513
max	7.051794	6.844179

[ ]:

CHAPTER

TWELVE

SIMULATING WITH CUSTOM RESULTS

In this example, we'll load a model, and simulate it, fine tuning the simulation results returned. We start as usual:

[1]:
```
from basico import *
```

lets load a model, i'll choose a model from the BioModels Database:

[2]:
```
load_biomodel(206);
```

[3]:
```
get_species()
```

[3]:
```
                           compartment       type    unit  \
name
ATP                        compartment  reactions  mmol/l
Triose_Gly3Phos_DHAP       compartment  reactions  mmol/l
Acetaldehyde               compartment  reactions  mmol/l
NAD                        compartment  reactions  mmol/l
Pyruvate                   compartment  reactions  mmol/l
Glucose                    compartment  reactions  mmol/l
extracellular acetaldehyde compartment  reactions  mmol/l
3PG                        compartment  reactions  mmol/l
F16P                       compartment  reactions  mmol/l

                           initial_concentration  initial_particle_number  \
name
ATP                                         2.00             1.204428e+21
Triose_Gly3Phos_DHAP                        0.60             3.613284e+20
Acetaldehyde                                0.08             4.817713e+19
NAD                                         0.60             3.613284e+20
Pyruvate                                    8.00             4.817713e+21
Glucose                                     1.00             6.022141e+20
extracellular acetaldehyde                  0.02             1.204428e+19
3PG                                         0.70             4.215499e+20
F16P                                        5.00             3.011070e+21

                          initial_expression expression  concentration  \
name
ATP                                                                NaN
Triose_Gly3Phos_DHAP                                               NaN
Acetaldehyde                                                       NaN
NAD                                                                NaN
Pyruvate                                                           NaN
```

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```
Glucose                                                          NaN
extracellular acetaldehyde                                       NaN
3PG                                                              NaN
F16P                                                             NaN

                            particle_number  rate  particle_number_rate  \
name
ATP                                     NaN   0.0                   0.0
Triose_Gly3Phos_DHAP                    NaN   0.0                   0.0
Acetaldehyde                            NaN   0.0                   0.0
NAD                                     NaN   0.0                   0.0
Pyruvate                                NaN   0.0                   0.0
Glucose                                 NaN   0.0                   0.0
extracellular acetaldehyde              NaN   0.0                   0.0
3PG                                     NaN   0.0                   0.0
F16P                                    NaN   0.0                   0.0

                                   key sbml_id
name
ATP                         Metabolite_1      at
Triose_Gly3Phos_DHAP        Metabolite_3      s3
Acetaldehyde                Metabolite_7      s6
NAD                         Metabolite_4      na
Pyruvate                    Metabolite_6      s5
Glucose                     Metabolite_0      s1
extracellular acetaldehyde  Metabolite_8     s6o
3PG                         Metabolite_5      s4
F16P                        Metabolite_2      s2
```

[4]:
```
get_reactions()
```

[4]:
```
                                                scheme  flux  particle_flux  \
name
v1                              Glucose + 2 * ATP = F16P   0.0            0.0
v2                        F16P = 2 * Triose_Gly3Phos_DHAP   0.0            0.0
v3                 Triose_Gly3Phos_DHAP + NAD = 3PG + ATP   0.0            0.0
v4                                  3PG = Pyruvate + ATP   0.0            0.0
v5                               Pyruvate = Acetaldehyde   0.0            0.0
v7                                                ATP =    0.0            0.0
v8                            Triose_Gly3Phos_DHAP = NAD   0.0            0.0
v9                        "extracellular acetaldehyde" =   0.0            0.0
v10   Acetaldehyde = 0.1 * "extracellular acetaldehyde"   0.0            0.0
v6                                   Acetaldehyde = NAD   0.0            0.0
v0                                            = Glucose   0.0            0.0

                        function          key sbml_id
name
v1                Function for v1   Reaction_0      v1
v2                Function for v2   Reaction_1      v2
v3                Function for v3   Reaction_2      v3
v4                Function for v4   Reaction_3      v4
v5                Function for v5   Reaction_4      v5
```

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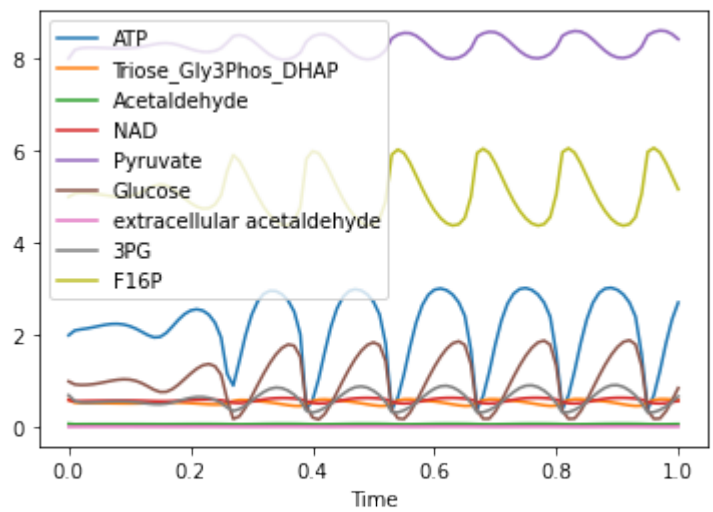
```
v7                Function for v7   Reaction_5      v7
v8                Function for v8   Reaction_6      v8
v9                Function for v9   Reaction_7      v9
v10              Function for v10   Reaction_8     v10
v6                Function for v6   Reaction_9      v6
v0     Constant flux (reversible)  Reaction_10      v0
```

12.1 Simulations:

[5]:
```
run_time_course(duration=1).plot()
```

[5]:
```
<AxesSubplot:xlabel='Time'>
```



12.2 Custom Selection list

Sometimes you just want to select certain elements, for which you want to select the output. This can be done using `run_time_course_with_output`, where the first element is an array of display names, for which you'd like to collect the output

[6]:
```
run_time_course_with_output(['Time', '[ATP]', 'ATP.Rate', '(v1).Flux'], duration=1)
```

[6]:
```
     Time     [ATP]   ATP.Rate  (v1).Flux
0    0.00  2.000000  23.471501  64.705882
1    0.01  2.103916  23.471501  52.477019
2    0.02  2.127439  23.471501  50.238184
3    0.03  2.147108  23.471501  49.133261
4    0.04  2.172374  23.471501  48.222173
..    ...       ...        ...        ...
96   0.96  0.700117  23.471501  58.593102
97   0.97  1.226780  23.471501  40.493568
98   0.98  1.833802  23.471501  29.080133
99   0.99  2.349971  23.471501  24.298749
```

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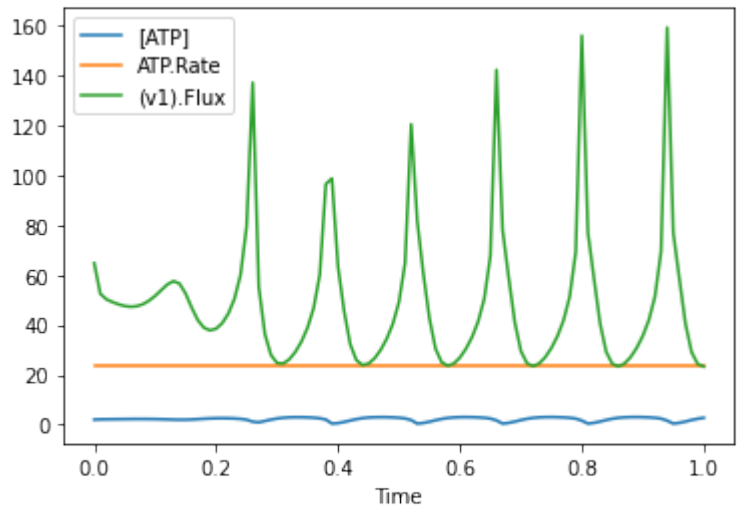
```
100  1.00  2.708829  23.471501  23.269926

[101 rows x 4 columns]
```

as you see just, as with `run_time_course` a pandas dataframe is returned, the only difference is, that the index column is not automatically set to the time column (as you might not want to collect time!).

[7]:
```
run_time_course_with_output(['Time', '[ATP]', 'ATP.Rate', '(v1).Flux'], duration=1).set_
↪index('Time').plot()
```

[7]:
```
<AxesSubplot:xlabel='Time'>
```



The other difference, hen using this method is, that the selection is not automatically saved to COPASI, so when you prepare a model and run it later in the COPASI UI, the output selection is not persisted. You would have to create plot elements or reports for that.

12.3 Custom Time Points

Some times you might only want to return values at certain times, this is possible as well (with either `run_time_course` and `run_time_course_with_output`, adding the 'values' argument:

[8]:
```
run_time_course(values=[0, 1, 2, 4])
```

[8]:
```
           ATP  Triose_Gly3Phos_DHAP  Acetaldehyde       NAD  Pyruvate  \
Time
0.0   2.000000              0.600000      0.080000  0.600000  8.000000
1.0   2.708848              0.593576      0.074087  0.579888  8.415963
2.0   3.001586              0.574146      0.078183  0.620547  8.217482
4.0   2.923411              0.508574      0.080717  0.645962  8.019722

       Glucose  extracellular acetaldehyde       3PG      F16P
Time
0.0   1.000000                    0.020000  0.700000  5.000000
1.0   0.856600                    0.023069  0.672236  5.160410
```

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```
2.0   1.290106                    0.024351  0.848794  4.759722
4.0   1.851914                    0.025662  0.903727  4.376452
```

[9]:
```
run_time_course_with_output(['Time', '[ATP]', 'ATP.Rate'], values=[0, 1, 2, 4])
```

[9]:
```
   Time     [ATP]   ATP.Rate
0   0.0  2.000000  23.471501
1   1.0  2.708848  23.471501
2   2.0  3.001586  23.471501
3   4.0  2.923411  23.471501
```

12.4 For expert users

For some elements, we do not have an easy mapping between object and display names, to help around that issue `run_time_course_with_output` allows the use of CN's as well. Though of course they are quite error prone and not as nice to read!

[10]:
```
run_time_course_with_output([
    'CN=Root,Model=Wolf2000_Glycolytic_Oscillations,Reference=Time',
    'CN=Root,Model=Wolf2000_Glycolytic_Oscillations,Vector=Compartments[compartment],
↪Vector=Metabolites[Glucose],Reference=ParticleNumber',
    'CN=Root,Model=Wolf2000_Glycolytic_Oscillations,Vector=Compartments[compartment],
↪Reference=Volume'],
    values=[0, 1, 2, 4])
```

[10]:
```
   Time  Glucose.ParticleNumber  Compartments[compartment].Volume
0   0.0            6.022141e+20                               1.0
1   1.0            5.158565e+20                               1.0
2   2.0            7.769203e+20                               1.0
3   4.0            1.115249e+21                               1.0
```

[ ]:
```

```

CHAPTER

THIRTEEN

PARAMETER SCANS

This notebook demonstrates how to edit / change parameter scan tasks. While most scans can be done using basico, by using simple loops, here we create the scans for the COPASI `Parameter Scan` task. That means, that these scans can be carried out later, using the COPASI graphical user interface, or the command line interface.

[1]:
```
from basico import *
```

lets start by using the brusselator example, where a scan task is already set up. Using `get_scan_settings`, we can see all the individual settings:

[2]:
```
load_example('brusselator')
get_scan_settings()
```

[2]:
```
{'update_model': False,
 'scheduled': False,
 'subtask': 'Steady-State',
 'output_during_subtask': False,
 'continue_from_current_state': False,
 'continue_on_error': False,
 'scan_items': [{'type': 'scan',
   'num_steps': 10,
   'log': False,
   'min': 0.5,
   'max': 2.0,
   'values': '',
   'use_values': False,
   'item': '(R1).k1',
   'cn': 'CN=Root,Model=The Brusselator,Vector=Reactions[R1],ParameterGroup=Parameters,
↪Parameter=k1,Reference=Value'}]}
```

the dictionary that is returned, contains all the information stored in the COPASI file. Altenatively you could also just retrieve the scan items using `get_scan_items`.

[3]:
```
get_scan_items()
```

[3]:
```
[{'type': 'scan',
  'num_steps': 10,
  'log': False,
  'min': 0.5,
  'max': 2.0,
  'values': '',
  'use_values': False,
  'item': '(R1).k1',
```

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```
  'cn': 'CN=Root,Model=The Brusselator,Vector=Reactions[R1],ParameterGroup=Parameters,
↪Parameter=k1,Reference=Value'}]
```

13.1 Modifying Scan Settings

Analogue to retrieving the settings, they can be set as well, using the same keys, as displayed above. Again, you can change all settings using `set_scan_settings`. Or just change the scan_items using `set_scan_items`. If the scan settings dictionary contain a `scan_items` element, or if `set_scan_items` is called, then all scan items are replaced with the ones given. Alternatively `add_scan_item` can be used to add one or more scan items directly.

Lets change the scan item from above, so that the `(R1).k1` parameter is changed to the specific values of 0.5, 1.0 and 2.0:

[4]:
```
set_scan_items([{'item': '(R1).k1', 'values': [0.5, 1.0, 2]}])
```

[5]:
```
get_scan_items()
```

[5]:
```
[{'type': 'scan',
  'num_steps': 0,
  'log': False,
  'min': 0.0,
  'max': 1.0,
  'values': [0.5, 1.0, 2.0],
  'use_values': True,
  'item': '(R1).k1',
  'cn': 'CN=Root,Model=The Brusselator,Vector=Reactions[R1],ParameterGroup=Parameters,
↪Parameter=k1'}]
```

scan items can be specified, either through their display name by specifying the `item` key, or by specifying the `cn` directly.

The scan item can be of one of three types:

- `scan`: this is the default (so will be used if not specifie), here a model element is varied either through values, or between a specified `min` and `max` value
- `repeat`: here the subtask is repeated `num_steps` times
- `random`: here the value for the specified model element is sampled from the specified `distribution` (which can be `uniform`, `normal`, `poisson` or `gamma`)

For example to specify a repeat you'd use:

[6]:
```
add_scan_item(type='repeat', num_steps=10)
```

[7]:
```
get_scan_items()
```

[7]:
```
[{'type': 'scan',
  'num_steps': 0,
  'log': False,
  'min': 0.0,
  'max': 1.0,
  'values': [0.5, 1.0, 2.0],
```

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```
  'use_values': True,
  'item': '(R1).k1',
  'cn': 'CN=Root,Model=The Brusselator,Vector=Reactions[R1],ParameterGroup=Parameters,
↪Parameter=k1'},
 {'type': 'repeat', 'num_steps': 10, 'log': None, 'min': None, 'max': None}]
```

as you can see, by using `add_scan_items`, the repeat item is added at the end of the scan list. In COPASI, when multiple scan items are defined, the semantics of those is that for each value of scan item 1, all values of scan item 2 are processed.

For scan items of type `distribution`, the min/max element take up different meaning:

- `uniform`: here the value is between the min and max value
- `normal`: min=`mean` and max=`standard deviation`
- `poisson`: min=`mean` and max has no meaning
- `gamma`: min=`shape` and max=`scale`

As a last example, lets change it to sample the initial concentration of species `A` from a normal distribution between around 2, and we want to do that 5 times:

[8]:
```
set_scan_items([
    {
        'type': 'repeat',
        'num_steps': 5
    },
    {
        'item': '[A]_0',
        'type':'random',
        'distribution': 'normal',
        'min': 2,
        'max': 0.1
    }])
```

[9]:
```
get_scan_items()
```

[9]:
```
[{'type': 'repeat', 'num_steps': 5, 'log': None, 'min': None, 'max': None},
 {'type': 'random',
  'num_steps': 0,
  'log': False,
  'min': 2.0,
  'max': 0.1,
  'distribution': 'normal',
  'item': '[A]_0',
  'cn': 'CN=Root,Model=The Brusselator,Vector=Compartments[compartment],
↪Vector=Metabolites[A],Reference=InitialConcentration'}]
```

13.2 Runnin a scan:

You can run these scans in basico using the `run_scan` method. Where you can optionally pass along a `settings` parameter to reconfigure the scan, or an `output` selection, to grab some data directly.

So lets run the configured scan task, changing it to run a the steady state task, collecting the final concentrations of `X` and `Y`:

[10]:
```
run_scan(settings={'subtask': T.STEADY_STATE}, output=['[A]_0', '[X]', '[Y]'])
```

[10]:

	[A]_0	[X]	[Y]
0	2.041315	2.041315	1.469639
1	1.925778	1.925778	1.557810
2	2.116724	2.116724	1.417283
3	2.088708	2.088708	1.436292
4	1.950328	1.950328	1.538201

CHAPTER

FOURTEEN

SENSITIVITY ANALYSIS

This notebook demonstrates how to use sensitivity analysis using basico.

We start as always by importing basico, and loading a model. Here I load the brusselator model from the examples.

[1]:
```
from basico import *
```

[2]:
```
load_example('brusselator');
get_reactions()[['scheme']]
```

[2]:
```
                  scheme
name
R1                A -> X
R2    2 * X + Y -> 3 * X
R3        X + B -> Y + D
R4                X -> E
```

14.1 Settings

The settings for the sensitivities task are controlled using the functions `get_sensitivity_settings()` and `set_sensitivity_settings()`. The core attributes to change here would be:

- the subtask to use (can be one of 'Evaluation', 'Steady State', 'Time Series', 'Parameter Estimation', 'Optimization', 'Cross Section'). They are available in the `SENS_ST` constant class.
- `effect`: this specifies the element (or elements that we want to observe)
- `cause` and `secondary_cause`: these are the elements to be varied, that we expect to have an effect on the observed element.

If we look at the current settings, we see that the steady state subtask is run to observe what happens to non-constant concentratiosn of species when parameter values are varied.

[3]:
```
get_sensitivity_settings()
```

[3]:
```
{'scheduled': False,
 'update_model': False,
 'method': {'Delta factor': 0.001,
  'Delta minimum': 1e-12,
  'name': 'Sensitivities Method'},
 'report': {'filename': '',
  'report_definition': 'Sensitivities',
  'append': True,
```

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```
 'confirm_overwrite': False},
'sub_task': 'Steady State',
'effect': 'Non-Constant Concentrations of Species',
'cause': 'All Parameter Values',
'secondary_cause': 'Not Set'}
```

Valid values for `cause` and `effect` are either a specific element, specified by using either the display name or the CN of an element. Or an element from the `SENS` constant class.

14.2 Running the Analysis

`run_sensitivities()` will run the sensitivity task, after which the result is available by calling:

- get_scaled_sensitivities()
- get_unscaled_sensitivities()
- get_summarized_sensitivities()

[4]:
```
run_sensitivities()
```

[5]:
```
get_scaled_sensitivities()
```

[5]:
```
      (R1).k1   (R2).k1       (R3).k1   (R4).k1
[X]  1.000000  0.000000  4.440893e-13 -0.999001
[Y] -0.999001 -0.999001  1.000000e+00  1.000000
```

[6]:
```
get_unscaled_sensitivities()
```

[6]:
```
      (R1).k1   (R2).k1       (R3).k1   (R4).k1
[X]  0.500000  0.000000  2.220446e-13 -0.499500
[Y] -5.993999 -5.993999  5.999993e+00  5.999993
```

[7]:
```
get_summarized_sensitivities()
```

[7]:
```
                0
(R1).k1  1.413507
(R2).k1  0.999001
(R3).k1  1.000000
(R4).k1  1.413507
```

Convenience overloads exist, so that the settings can directly be passed on to the run method. If `run_first=True` is given to the functions retrieving the result, the sensitivities will be computed before obtaining the result.

So for example, if we just wanted to see how the initial concentration of `A` would affect the transient concentration of `X`, we could directly call:

[8]:
```
get_scaled_sensitivities(run_first=True, settings={'effect': '[X]', 'cause': '[A]_0'})
```

[8]:
```
1.0000000000004075
```

To see what effect it would have on all metabolite concentrations:

[9]:
```
get_scaled_sensitivities(run_first=True,
                         settings={'effect': SENS.NON_CONST_METAB_CONCENTRATIONS,
                                   'cause': '[A]_0'})
```

[9]:
```
            0
[X]  1.000000
[Y] -0.999001
```

The changed settings of the last run will persist, so that it can be reproduced in the COPASI user interface as well:

[10]:
```
get_sensitivity_settings()
```

[10]:
```
{'scheduled': False,
 'update_model': False,
 'method': {'Delta factor': 0.001,
  'Delta minimum': 1e-12,
  'name': 'Sensitivities Method'},
 'report': {'filename': '',
  'report_definition': 'Sensitivities',
  'append': True,
  'confirm_overwrite': False},
 'sub_task': 'Steady State',
 'effect': 'Non-Constant Concentrations of Species',
 'cause': '[A]_0',
 'secondary_cause': 'Not Set'}
```

CHAPTER

FIFTEEN

WORKING WITH ARRAYS OF COMPARTMENTS

COPASI allows working with arrays of compartments, that is taking a model that is set up, and multiplying it either in a linear chain, or in an rectangular array. This example shows how to do that using basico. We start with the usual imports:

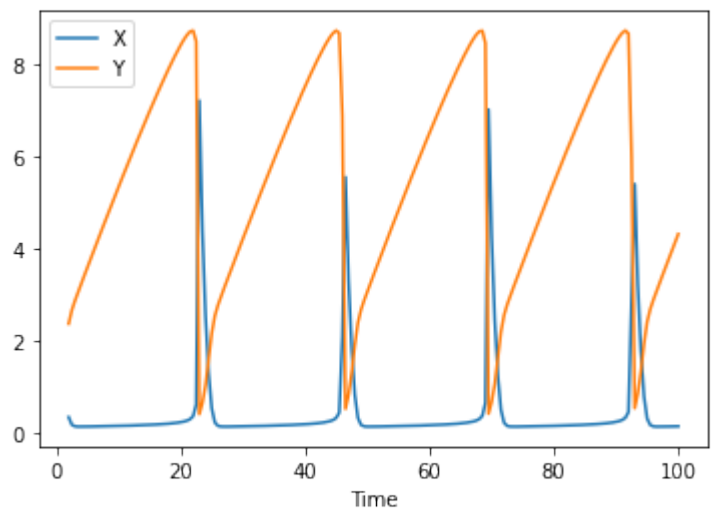
[1]:
```
from basico import *
```

now we import the brusselator example model

[2]:
```
dm = load_example('brusselator')
```

and obviouslky, we can run time courses just as usual:

[3]:
```
data = run_time_course()
data.plot();
```



For initialization it is useful, to add events to the model. The parameters are:

- name
- trigger expression
- array of arrays for assignments, with the inner array containing a target, and an expression what to assign.

for example the following would add an event `e2` that triggers at time 10, and assigns 10 to `X`

[4]:
```
add_event('e0', 'Time > 30', [['X', '10']]);
```

to display what events we have use `get_events()`

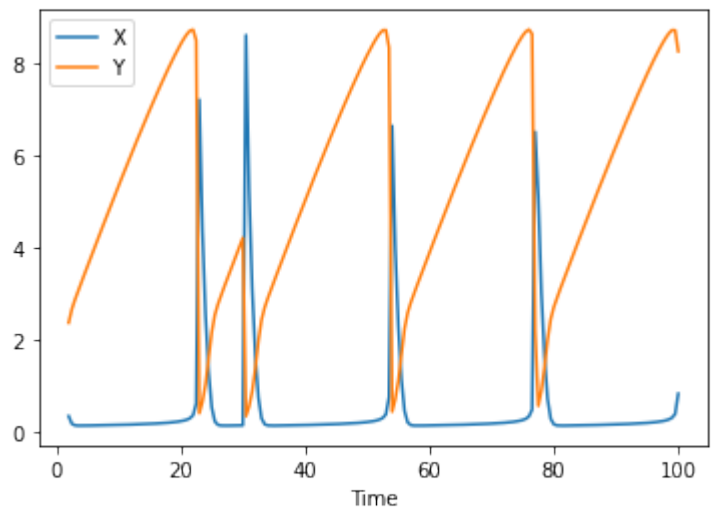
[5]:
```
get_events()
```

[5]:
```
        trigger delay                                assignments      key  \
name
e0    Time > 30        [{'target': '[X]', 'expression': '10'}]  Event_0

     sbml_id
name
e0
```

so running the time course again, we do see that at time 30, the event is triggered:

[6]:
```
run_time_course().plot();
```



15.1 Linear arrays of compartments

now lets run this model in a linear chain of 15 cells, allowing the species X and Y to diffuse linearly between them, with diffusion coefficients 0.16 and 0.08 respectively. We also remove the existing compartment afterwards, as it will not be part of the linear chain:

[7]:
```
create_linear_array(15, ['X', 'Y'], [0.16, 0.8], delete_template=True)
```

now we have many more species, compartments, and reactions, all parameterized exactly as the template model was

[8]:
```
print(overview())
get_species().head()
```

```
Name:            The Brusselator
# Compartments: 15
# Species:      90# Parameters:   2# Reactions:    88# Events:       1
```

[8]:
```
         compartment       type     unit  initial_concentration  \
name
X     compartment[0]  reactions  mmol/ml               2.999996
```

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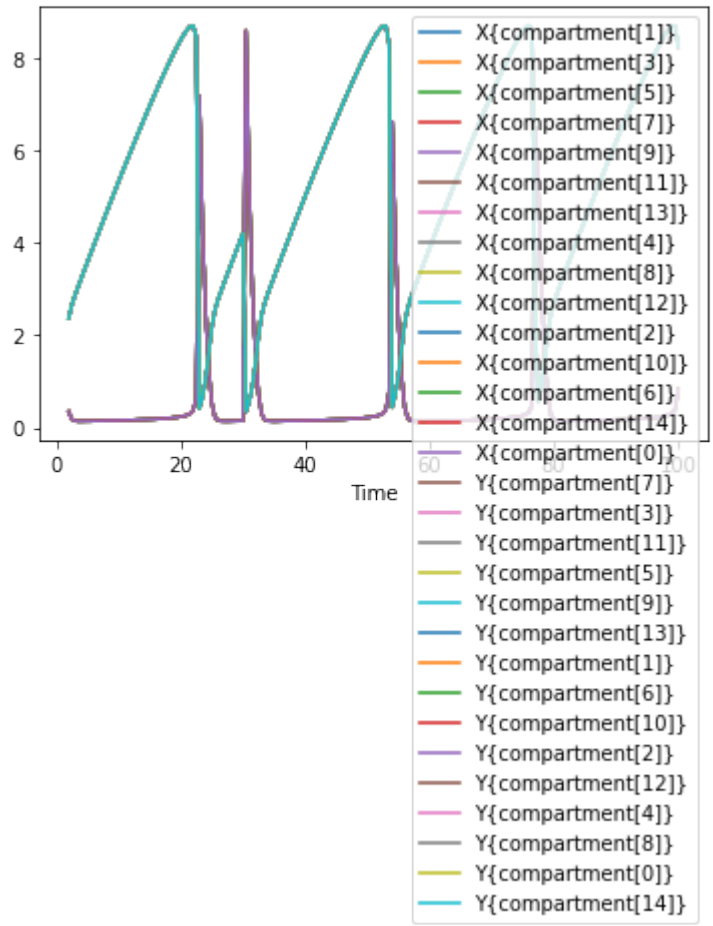
```
E     compartment[0]      fixed  mmol/ml               0.000000
B     compartment[0]      fixed  mmol/ml               2.999996
D     compartment[0]      fixed  mmol/ml               0.000000
Y     compartment[0]  reactions  mmol/ml               2.999996

      initial_particle_number initial_expression expression  concentration  \
name
X                1.806640e+21                                          NaN
E                0.000000e+00                                          NaN
B                1.806640e+21                                          NaN
D                0.000000e+00                                          NaN
Y                1.806640e+21                                          NaN

      particle_number  rate  particle_number_rate            key sbml_id
name
X                 NaN   0.0                   0.0   Metabolite_6
E                 NaN   0.0                   0.0   Metabolite_7
B                 NaN   0.0                   0.0   Metabolite_8
D                 NaN   0.0                   0.0   Metabolite_9
Y                 NaN   0.0                   0.0  Metabolite_10
```

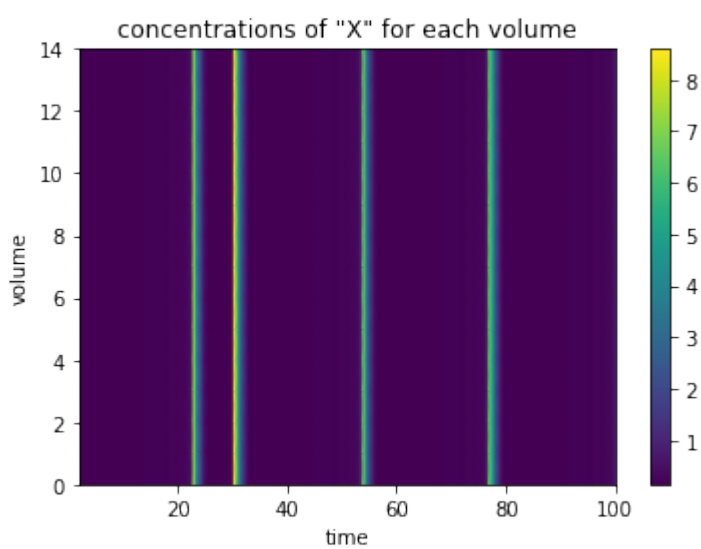
lets simulate again:

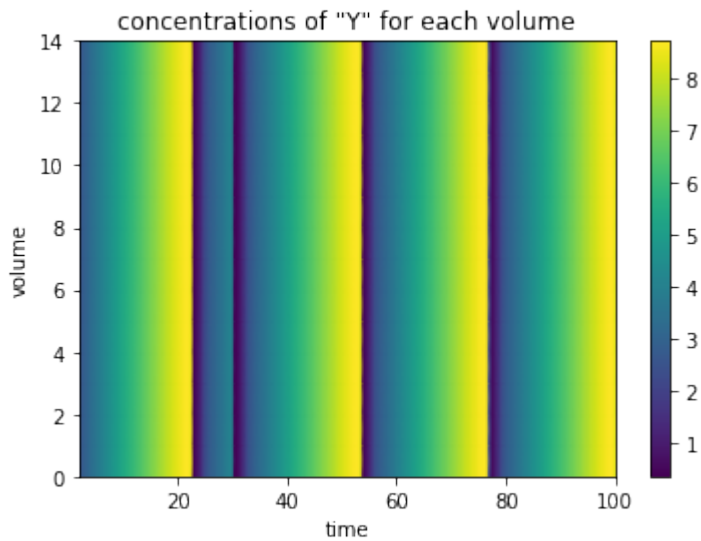
[9]:
```
data = run_time_course()
data.plot();
```



Seeing all these lines plotted over each other might not be too helpful, so we can also plot this as a clor mesh, with the time on the x axis, and the individal created compartments along the y axis.

[10]:
```
plot_linear_time_course(data, 'compartment');
```





15.2 Creating 2D array of compartments

the same can be done by createing a rectangular array of compartments. Note that this results in quickly getting large amounts of model variables, so it might prove prohibitive to be used in numbers. So i'll start over, loading the model again (as i don't want the linear chain anymore)

```
[ ]: dm = load_example('brusselator')
     create_rectangular_array(15, 15, ['X', 'Y'], [0.16, 0.8], delete_template=True)
     print(overview())
```

Lots of variables indeed. So simulation will take a bit longer. But before we come to that, i would like to change the concentration of X at time 10 of the simulation, just so that we don't just use uniform values (that would be boring to look at. So i add the events as before:

```
[ ]: add_event('change_x', 'Time > 10', [['X{compartment[2,2]}', '10'],
                                          ['X{compartment[2,3]}', '10'],
                                          ['X{compartment[3,2]}', '10'],
                                          ['X{compartment[3,3]}', '10']
                                         ])
```

```
[ ]: data = run_time_course(duration=100, start_time=0)
```

plotting all times of the time course might not be too interesting, so instead i select plots only at specific times. I also override the min / max scaling of the plots, to the range between 0 and 10, if those are not given the data will be scaled to each min / max value.

```
[ ]: plot_rectangular_time_course(data, times=[10.5, 30 , 60, 90], min_range=0, max_range=10);
```

To display it as animation we'll need an extra import, and you'll need to have ffmpeg installed

```
[ ]: from IPython.display import HTML
     HTML(animate_rectangular_time_course(data, metab='Y', min_range=0, max_range=10).to_
     ↪html5_video())
```

CHAPTER

SIXTEEN

USING CALLBACKS

When using basico, usually there is no feedback given when running tasks. That is fine when tasks dont take a long time, but for optimizations or parameter estimation runs, it would be nice to know how long things could go. Setting a callback also allows for interrupting a running task through interrupting by pressing `Ctrl+C`. Lets see how this works. We start as always by import basico. Additionally we also import the callbacks module (since i consider it an experimental module at the time of writing this, it is not done automatically):

[1]:
```
from basico import *
from basico.callbacks import create_default_handler
```

For now i have wrapped the tqdm library, others could easily be added later on let me know if you have a preference! The `create_default_handler` function sets up a tdqm handler, that will be used for all longer running operations. It takes the following arguments:

- `delay`: delay in seconds before showing the first message (defaults to 1)
- `leave`: boolean flag, that indicates whether messages should remain on screen after being completed (defaults to `False`)
- `unit`: a string to display as unit for the iterations (by default tqdm will use it/s)

additional key value pairs will be passed on to tqdm. So let us just create a handler, and run some tasks:

[2]:
```
create_default_handler()
```

we start with a simple example model that has parameter estimation set up on it already

[3]:
```
load_example('LM');
```

it uses a local method and runs for 500 iterations, or until the tolerance of 1e-16 is reached:

[4]:
```
get_task_settings(T.PARAMETER_ESTIMATION)['method']
```

[4]:
```
{'Iteration Limit': 500,
 'Tolerance': 1e-16,
 'Stop after # Stalled Iterations': 0,
 '#LogVerbosity': 0,
 'name': 'Levenberg - Marquardt'}
```

[5]:
```
run_parameter_estimation()
```

[5]:
```
               lower upper        sol        affected
name
(R1).k2         1e-6   1e6   0.000002              []
(R2).k1         1e-6   1e6  44.661715              []
```

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```
Values[offset]  -0.2   0.4   0.043018  [Experiment_1]
Values[offset]  -0.2   0.4   0.054167  [Experiment_3]
Values[offset]  -0.2   0.4  -0.050941    [Experiment]
Values[offset]  -0.2   0.4   0.045922  [Experiment_4]
Values[offset]  -0.2   0.4   0.048025  [Experiment_2]
```

lets choose just random search, which will take much longer, this will make the callbacks show up, and we will see the #function evaluations, as well as the best value reached. At any point we can interrup the execution of the cell (by presing the stop button on the notebook), this will cause the parameter estimation to stop after the next iteration, with partial results being returned:

[6]:
```
run_parameter_estimation(method=PE.RANDOM_SEARCH)
```

```
Function Evaluations: 1311 [00:01, 1309.69/s]
```

```
Best Value: 22.32126236098639 [00:01, 2516.34/s]
```

[6]:
```
               lower upper        sol        affected
name
(R1).k2         1e-6   1e6   0.000123              []
(R2).k1         1e-6   1e6  40.864396              []
Values[offset]  -0.2   0.4   0.108320  [Experiment_1]
Values[offset]  -0.2   0.4   0.216139  [Experiment_3]
Values[offset]  -0.2   0.4   0.010154    [Experiment]
Values[offset]  -0.2   0.4   0.368608  [Experiment_4]
Values[offset]  -0.2   0.4  -0.057231  [Experiment_2]
```

to remove the default handler again, the `reset_default_handler` function can be used. As it turns out, the output of the handler could not be seen on the html version of the notebook. So here a screenshot of the operation in action.

16.1 Timeouts

callbacks can also be used, to ensure that tasks are automatically interrupted after a certain number of seconds. So if we repeat the example from above, and stop the parameter estimation automatically after 10seconds, we could use:

[7]:
```
create_default_handler(max_time=10)
```

[8]:
```
run_parameter_estimation(method=PE.RANDOM_SEARCH)
```

```
Function Evaluations: 1330 [00:01, 1328.85/s]
```

```
Best Value: 18.52026239524136 [00:01, 2366.75/s]
```

[8]:
```
               lower upper        sol        affected
name
(R1).k2         1e-6   1e6   0.000002              []
(R2).k1         1e-6   1e6  43.882694              []
Values[offset]  -0.2   0.4  -0.061506  [Experiment_1]
Values[offset]  -0.2   0.4   0.062814  [Experiment_3]
Values[offset]  -0.2   0.4  -0.016544    [Experiment]
Values[offset]  -0.2   0.4   0.001578  [Experiment_4]
Values[offset]  -0.2   0.4   0.096818  [Experiment_2]
```

CHAPTER

SEVENTEEN

WORKING WITH PLOTS

This example describes how to read / edit plot specifications, so that they can appear in the COPASI User Interface.

[1]:
```
import sys
if '../..' not in sys.path:
    sys.path.append('../..')
from basico import *
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

lets start with the Brusselator example, that we have in the examples

[2]:
```
load_example('brusselator');
```

now let us have a look at the plots defined in the file:

[3]:
```
get_plots()
```

[3]:
```
                                                 active  log_x  log_y  \
name
Concentrations, Volumes, and Global Quantity Va...    True  False  False
Phase Plot                                            True  False  False

                                                 tasks  \
name
Concentrations, Volumes, and Global Quantity Va...
Phase Plot


                                                                                 ␣
↪      curves
name
Concentrations, Volumes, and Global Quantity Va...  [{'name': '[X]', 'type': 'curve2d',
↪'channels'...
Phase Plot                                          [{'name': '[Y]|[X]', 'type': 'curve2d
↪', 'chann...
```

To filter the plot specification, by name you can specify a substring to be used:

[4]:
```
get_plots('Phase Plot')
```

[4]:
```
            active  log_x  log_y tasks  \
name
```

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```
Phase Plot    True  False  False

                                                        curves
name
Phase Plot  [{'name': '[Y]|[X]', 'type': 'curve2d', 'chann...
```

the plot specification can also be retrieved directly as dictionary:

[5]:
```
get_plot_dict('Phase Plot')
```

[5]:
```
{'name': 'Phase Plot',
 'active': True,
 'log_x': False,
 'log_y': False,
 'tasks': '',
 'curves': [{'name': '[Y]|[X]',
   'type': 'curve2d',
   'channels': ['[X]', '[Y]'],
   'color': 'auto',
   'line_type': 'lines',
   'line_subtype': 'solid',
   'line_width': 2.0,
   'symbol': 'small_cross',
   'activity': 'during'}]}
```

Now let us add a new plot. Ensure to compare with :func:`.set_plot_dict` and :func:`.set_plot_curves` for all parameters. Note that the only parameters necessary for the curve are a name for the curve (which will be displayed in the legend), and the data channels of what information to collect. These channels again use the display names of the elements that you want to plot (so `[X]` for the concentration of species `X`).

[6]:
```
add_plot('test plot', curves=[{'name': 'x vs time', 'color': '#ff8800','channels':['Time
↪', '[X]']}]);
```

and verify, that it is there and has gotten all the default values expected:

[7]:
```
get_plot_dict('test plot')
```

[7]:
```
{'name': 'test plot',
 'active': True,
 'log_x': False,
 'log_y': False,
 'tasks': '',
 'curves': [{'name': 'x vs time',
   'type': 'curve2d',
   'channels': ['Time', '[X]'],
   'color': '#ff8800',
   'line_type': 'lines',
   'line_subtype': 'solid',
   'line_width': 2.0,
   'symbol': 'small_cross',
   'activity': 'during'}]}
```

changing is possible as well, by using `set_plot_dict` directly.

finally the plot can also be deleted using `remove_plot`.

[8]:
```
remove_plot('test plot')
```

CHAPTER

EIGHTEEN

WORKING WITH REPORTS

For the use case, where you are using basico to prepare files to run later (say on a cluster environment or such). It is often useful to manipulate the report definitions we store in COPASI files. This notebook demonstrate to work with them. Lets just start by importing basico.

[1]:
```
from basico import *
```

here we simply load the brusselator example:

[2]:
```
load_example('brusselator');
```

18.1 Retrieving Report Definitions

The first function to look into is `get_reports` which will retrieve all report definition encoded in the file and returns its content as a data frame. You can filter by name, task or whether or not the reports is an automatically generated one. So while the following line reports there are 11 reports in the model, we can ignore them if we so choose (hence not getting a result printed at the end)

[3]:
```
print('there are {0} reports in the model'.format(len(get_reports())))
get_reports(ignore_automatic=True)
```

```
there are 11 reports in the model
```

lets look at the reports that apply to steady state tasks:

[4]:
```
get_reports(task=T.STEADY_STATE)
```

[4]:
```
             separator  precision          task  \
name
Steady-State        \t          6  Steady-State

                                                     comment  is_table  \
name
Steady-State  <body xmlns="http://www.w3.org/1999/xhtml">\n ...     False

             header body                                   footer
name
Steady-State     []   []  [CN=Root,Vector=TaskList[Steady-State]]
```

analoge as to when working with plots, the reports can be retrieved as dictionaries, by specifying the name of the report to retrieve. The dictionary will either include a key `body` with lists of elements to collect (in that case `is_table` will

be `True`), or as seen below, a `header`, `body` and `footer` entries. Each entry in those lists can be either a display name, or common name (as not all elements can be retrieved via names).

The key thing to keep in mind, is that `header` entries will be collected before runing the task, `body` and `table` entries during running of the task. And `footer` entries, once the task is complete.

[5]:
```
get_report_dict('Steady-State')
```

[5]:
```
{'name': 'Steady-State',
 'separator': '\t',
 'precision': 6,
 'task': 'Steady-State',
 'comment': '<body xmlns="http://www.w3.org/1999/xhtml">\n          Automatically␣
↪generated report.\n        </body>',
 'is_table': False,
 'header': [],
 'body': [],
 'footer': ['CN=Root,Vector=TaskList[Steady-State]']}
```

18.2 Adding Reports

lets add a new report for a custom time course in which we collect the models time, the concentration of the species `X` and their rate of change:

[6]:
```
add_report('X Time-Course', task=T.TIME_COURSE, table=['Time', '[X]', 'X.Rate']);
```

[7]:
```
get_report_dict('X Time-Course')
```

[7]:
```
{'name': 'X Time-Course',
 'separator': '\t',
 'precision': 6,
 'task': 'Time-Course',
 'comment': '',
 'is_table': True,
 'print_headers': True,
 'table': ['Time', '[X]', 'X.Rate']}
```

the value in `print_headers` indicates, whether the name of the elements will be printed in the header column.

using the `table` element directly, does only work for tasks that generate output *during* the execution of the task, as in the time course example above. Other tasks, such as steady state computation only provide results *after* the task has completed. In the following we add a report for the steady state concentration (and rate of X). We use the function `wrap_copasi_string`, to indicate that we want to have the literal string `[X]` in the header, rather than the initial concentration.

One other important thing to note, is that when specifying headers manually, the separators also need to be included manually. That can be done using the separator char manually, or the special String `Separator=\t` to indicate that it is the separator of the report. Alternatively, you can specify the boolean flagg `add_sepratator=True`, so that between header, footer and body entries the separator is automatically added.

[9]:
```
add_report('X Steady-State', task=T.STEADY_STATE,
           header=[wrap_copasi_string('[X]'), wrap_copasi_string('X.Rate')],
           footer=['[X]','X.Rate'], add_separator=True);
```

[10]:
```
get_report_dict('X Steady-State')
```

[10]:
```
{'name': 'X Steady-State',
 'separator': '\t',
 'precision': 6,
 'task': 'Steady-State',
 'comment': '',
 'is_table': False,
 'header': ['String=\\[X\\]', 'Separator=\t', 'String=X.Rate'],
 'body': [],
 'footer': ['[X]', 'Separator=\t', 'X.Rate']}
```

18.3 Changing values

of course all the values can be changed using the `set_report_dict` function, say we wanted to collect CSV information for the plot above, we would specify to use `,` as separator:

[11]:
```
set_report_dict('X Time-Course', separator=',')
```

[12]:
```
get_report_dict('X Time-Course')
```

[12]:
```
{'name': 'X Time-Course',
 'separator': ',',
 'precision': 6,
 'task': 'Time-Course',
 'comment': '',
 'is_table': True,
 'print_headers': True,
 'table': ['Time', '[X]', 'X.Rate']}
```

if you at any point set the `header`, `body` or `footer`, the `table` entries will be removed.

18.4 Assigning to task

In order to use a report definition, it has to be assigned to a task. COPASI will only create the report if a filename is assigned to it.

[13]:
```
assign_report('X Time-Course', task=T.TIME_COURSE, filename='out.txt', append=True)
```

Alternatively, it is also possible to assign a report directly using the `set_task_settings` method, so for example:

[14]:
```
set_task_settings(T.TIME_COURSE,
   settings = {'report':
               {'report_definition': 'X Time-Course'}})
```

that with `get_task_settings` you can query which report is assigned to a given task:

[15]:
```
get_task_settings(T.TIME_COURSE)['report']['report_definition']
```

[15]:
```
'X Time-Course'
```

CHAPTER

NINETEEN

WORKING WITH SBML IDS

Usually basico uses the COPASI display names, to work with model elements. That way a consistent naming scheme between the COPASI graphical user interface, and the scripts can be easily maintained. However, for someone inspecting an SBML model, it might be convenient to also look at the SBML ids and identify elements that way. For this reason the data frames returned for compartments, events, parameters, species and reactions now also contain a column `sbml_id`.

Lets start as usual with the common imports:

[1]:
```
import sys
if '../..' not in sys.path:
    sys.path.append('../..')
from basico import *
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

Next lets load a model from the BioModels Database, and look at the elments:

[2]:
```
load_biomodel(64);
```

Now we have not just the element name availabe, but also their respective `sbml_id`:

[3]:
```
get_species()[['sbml_id', 'initial_concentration']]
```

[3]:
```
                          sbml_id  initial_concentration
name
High energy phosphates          P               6.310000
Glucose 6 Phosphate           G6P               2.450000
Triose-phosphate             TRIO               0.960000
NAD                           NAD               1.200000
Acetaldehyde                  ACE               0.170000
2-phosphoglycerate            P2G               0.120000
1,3-bisphosphoglycerate       BPG               0.000000
Glucose in Cytosol           GLCi               0.087000
Fructose 6 Phosphate          F6P               0.620000
Phosphoenolpyruvate           PEP               0.070000
Pyruvate                      PYR               1.850000
Fructose-1,6 bisphosphate    F16P               5.510000
3-phosphoglycerate            P3G               0.900000
NADH                         NADH               0.390000
ATP concentration             ATP               2.509190
ADP concentration             ADP               1.291619
```

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```
AMP concentration            AMP              0.299190
Extracellular Glucose       GLCo             50.000000
Glycogen                    Glyc              0.000000
Trehalose                    Trh              0.000000
CO2                          CO2              1.000000
Succinate                   SUCC              0.000000
Ethanol                     ETOH             50.000000
Glycerol                     GLY              0.150000
sum of AXP conc            SUM_P              4.100000
F2,6P                      F26BP              0.020000
```

similarly we can get the elements by SBML id as well:

[4]:
```
get_species(sbml_id='ATP')
```

[4]:
```
                  compartment        type    unit  initial_concentration  \
name
ATP concentration     cytosol  assignment  mmol/l                2.50919

                   initial_particle_number initial_expression  \
name
ATP concentration             1.511070e+21

                                                     expression  \
name
ATP concentration  ( [High energy phosphates] - [ADP concentratio...

                   concentration  particle_number  rate  particle_number_rate  \
name
ATP concentration            NaN              NaN   NaN                   NaN

                             key sbml_id
name
ATP concentration  Metabolite_21     ATP
```

Whereas in COPASI each element has a concentration and a particle number, in SBML usually elements deal only with concentrations and amounts. To make it easy to access them, it is convenient to add the expressions for the amount to the model, so that they can be accessed at any point in time. For that a utility function exists. If `use_sbml_ids` is specified, the sbml id of the species will be used in the name (i.e: `amount(sbml_id)`), otherwise it will be named `amount(display name)`. In case `ignore_fixed` is specified, no expressions for fixed species will be created, and similarly assignment expressions can be ignored:

[5]:
```
add_amount_expressions(use_sbml_ids=True, ignore_fixed=True)
```

lets look at the expressions created, we see it is just the concentration multiplied with the compartment size the species is in:

[6]:
```
get_parameters(name='amount(')[['initial_value', 'expression']]
```

[6]:
```
              initial_value                                          expression
name
amount(GLCi)       0.087000  [Glucose in Cytosol] * Compartments[cytosol].V...
amount(G6P)        2.450000  [Glucose 6 Phosphate] * Compartments[cytosol]...
amount(F6P)        0.620000  [Fructose 6 Phosphate] * Compartments[cytosol]...
```

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```
amount(F16P)       5.510000  [Fructose-1,6 bisphosphate] * Compartments[cyt...
amount(TRIO)       0.960000  [Triose-phosphate] * Compartments[cytosol].Volume
amount(BPG)        0.000000  [1,3-bisphosphoglycerate] * Compartments[cytos...
amount(P3G)        0.900000  [3-phosphoglycerate] * Compartments[cytosol].V...
amount(P2G)        0.120000  [2-phosphoglycerate] * Compartments[cytosol].V...
amount(PEP)        0.070000  [Phosphoenolpyruvate] * Compartments[cytosol]...
amount(PYR)        1.850000          [Pyruvate] * Compartments[cytosol].Volume
amount(ACE)        0.170000      [Acetaldehyde] * Compartments[cytosol].Volume
amount(P)          6.310000  [High energy phosphates] * Compartments[cytoso...
amount(NAD)        1.200000               [NAD] * Compartments[cytosol].Volume
amount(NADH)       0.390000              [NADH] * Compartments[cytosol].Volume
amount(ATP)        2.509190  [ATP concentration] * Compartments[cytosol].Vo...
amount(ADP)        1.291619  [ADP concentration] * Compartments[cytosol].Vo...
amount(AMP)        0.299190  [AMP concentration] * Compartments[cytosol].Vo...
```

the `run_time_course` function now also takes a parameter to use sbml id's if they are present (it will still use the display names in case an element has no sbml id.

[7]:
```
run_time_course(use_sbml_id=True)
```

[7]:
```
             P       G6P      TRIO       NAD       ACE       P2G       BPG  \
Time
0.00  6.310000  2.450000  0.960000  1.200000  0.170000  0.120000  0.000000
0.01  6.530115  2.491309  2.325367  1.055557  0.011908  0.051758  0.000412
0.02  6.481760  2.428287  2.355642  1.010053  0.012240  0.039849  0.000327
0.03  6.419771  2.357805  2.326751  1.033128  0.013500  0.040591  0.000326
0.04  6.465266  2.295451  2.288924  1.076765  0.015151  0.043923  0.000361
...        ...       ...       ...       ...       ...       ...       ...
0.96  6.470716  1.124734  0.799562  1.550632  0.195576  0.049470  0.000391
0.97  6.463801  1.120309  0.798489  1.550554  0.195101  0.049284  0.000388
0.98  6.457177  1.116112  0.797470  1.550473  0.194615  0.049106  0.000385
0.99  6.450834  1.112132  0.796503  1.550390  0.194118  0.048936  0.000383
1.00  6.444763  1.108357  0.795584  1.550304  0.193613  0.048772  0.000380

          GLCi       F6P       PEP  ...  Values[amount(P2G)]  \
Time                                ...
0.00  0.087000  0.620000  0.070000  ...             0.120000
0.01  0.097408  0.351027  0.075957  ...             0.051758
0.02  0.097234  0.341946  0.062268  ...             0.039849
0.03  0.099157  0.328112  0.062661  ...             0.040591
0.04  0.098315  0.323283  0.068018  ...             0.043923
...        ...       ...       ...  ...                  ...
0.96  0.094281  0.127878  0.084961  ...             0.049470
0.97  0.094464  0.127152  0.084495  ...             0.049284
0.98  0.094640  0.126464  0.084049  ...             0.049106
0.99  0.094809  0.125811  0.083622  ...             0.048936
1.00  0.094971  0.125191  0.083214  ...             0.048772

      Values[amount(PEP)]  Values[amount(PYR)]  Values[amount(ACE)]  \
Time
0.00             0.070000             1.850000             0.170000
0.01             0.075957             3.176736             0.011908
0.02             0.062268             3.864468             0.012240
```

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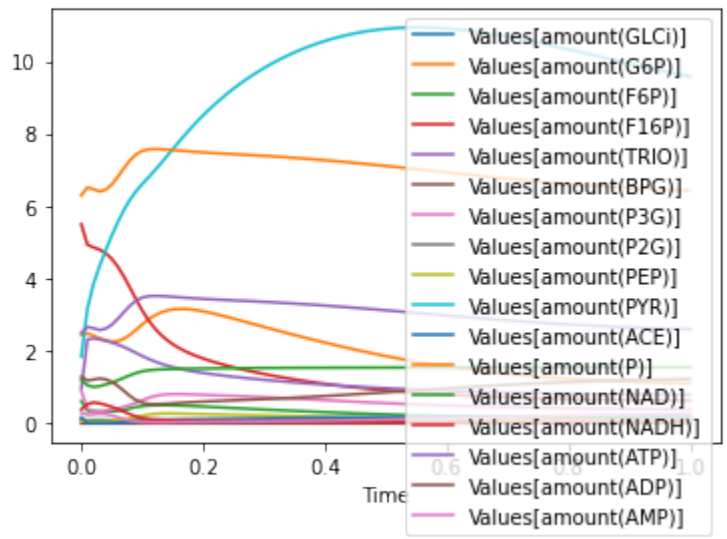
```
0.03             0.062661             4.355273             0.013500
0.04             0.068018             4.792030             0.015151
...                   ...                  ...                  ...
0.96             0.084961             9.734328             0.195576
0.97             0.084495             9.698833             0.195101
0.98             0.084049             9.663914             0.194615
0.99             0.083622             9.629595             0.194118
1.00             0.083214             9.595898             0.193613

      Values[amount(P)]  Values[amount(NAD)]  Values[amount(NADH)]  \
Time
0.00           6.310000             1.200000              0.390000
0.01           6.530115             1.055557              0.534443
0.02           6.481760             1.010053              0.579947
0.03           6.419771             1.033128              0.556872
0.04           6.465266             1.076765              0.513235
...                 ...                  ...                   ...
0.96           6.470716             1.550632              0.039368
0.97           6.463801             1.550554              0.039446
0.98           6.457177             1.550473              0.039527
0.99           6.450834             1.550390              0.039610
1.00           6.444763             1.550304              0.039696

      Values[amount(ATP)]  Values[amount(ADP)]  Values[amount(AMP)]
Time
0.00             2.509190             1.291619             0.299190
0.01             2.669381             1.191352             0.239267
0.02             2.633713             1.214334             0.251953
0.03             2.588384             1.243002             0.268613
0.04             2.621609             1.222048             0.256343
...                   ...                  ...                  ...
0.96             2.625605             1.219506             0.254889
0.97             2.620535             1.222730             0.256734
0.98             2.615684             1.225809             0.258507
0.99             2.611044             1.228747             0.260209
1.00             2.606606             1.231551             0.261843

[101 rows x 34 columns]
```

[8]:
```
df = run_time_course()
```

so lets plot just the amounts we got:

[9]:
```
amount_columns = list(df.columns)
amount_columns = [name for name in amount_columns if 'amount(' in name]
```

[10]:
```
df[amount_columns].plot();
```

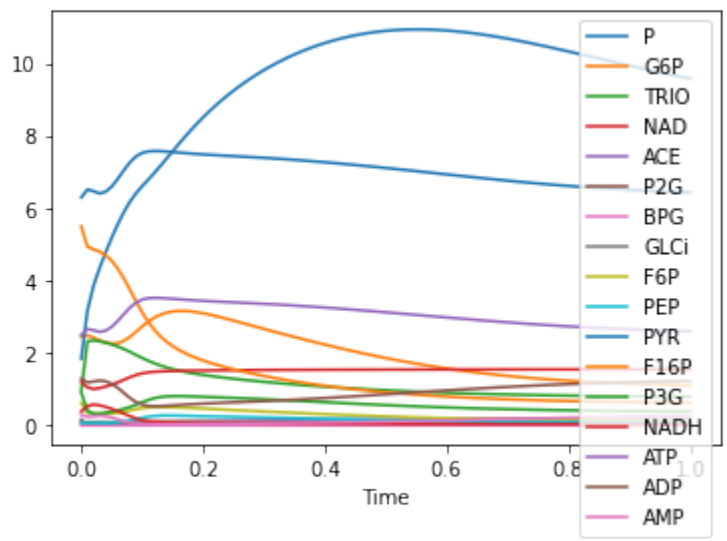


of course the added global parameters can be easily removed:

[11]:
```
remove_amount_expressions()
```

and now we can plot the concentrations:

[14]:
```
run_time_course(use_sbml_id=True).plot();
```



[ ]:

CHAPTER

TWENTY

WORKING WITH ANNOTATIONS

COPASI and SBML files can be annotated with MIRIAM annotations. These annotations describe what the model and its constituents actually represent. In basico you can ask for these annotations using the `get_miriam_annotation` function, simmilarly, you can set them using the `set_miriam_annotation` commands.

So lets start as usual, loading basico:

[1]:
```
import sys
if '../..' not in sys.path:
    sys.path.append('../..')


from basico import *
from ipywidgets import HTML
%matplotlib inline
```

20.1 Resource Lists / Updating

For the resolving of MIRIAM entries to work, occasionally COPASI needs to update the list of MIRIAM resources. This will be necessary on systems, where the graphical user interface to COAPSI has not been installed. To see whether it is necessary, you can call:

[2]:
```
have_miriam_resources()
```

[2]:
```
True
```

Should that call return false, simply update the resources using:

[3]:
```
update_miriam_resources()
```

To see the list of terms currently known by COPASI you can use the function:

[4]:
```
get_miriam_resources().head()
```

[4]:
```
                       is_citation                            uri
resource
BIND                         False     http://identifiers.org/bind
ChEBI                        False    http://identifiers.org/CHEBI
Ensembl                      False  http://identifiers.org/ensembl
Enzyme Nomenclature          False  http://identifiers.org/ec-code
UniProt Knowledgebase        False  http://identifiers.org/uniprot
```

and of course you can filter elements as usual, for example here to see the resources suitable for citations:

[5]:
```
resources = get_miriam_resources()
resources[resources.is_citation == True]
```

[5]:
```
          is_citation                          uri
resource
PubMed           True  http://identifiers.org/pubmed
DOI              True     http://identifiers.org/doi
arXiv            True   http://identifiers.org/arxiv
ISBN             True    http://identifiers.org/isbn
```

20.2 Displaying Annotations:

Now we load a fully annotated model, to display its annotations:

[6]:
```
load_biomodel(64);
```

Then we can display the Notes of the model:

[7]:
```
display(HTML(get_notes()))
```

```
HTML(value='\n  <body xmlns="http://www.w3.org/1999/xhtml">\n    <p>\n      <b>Can yeast␣
↪glycolysis be underst...
```

Similarly, we could get to all annotations. As with the `get_notes` call, if no element is specified, the annotations of the model element will be displayed:

[8]:
```
get_miriam_annotation()
```

[8]:
```
{'creators': [{'first_name': 'Lukas',
   'last_name': 'Endler',
   'email': 'lukas@ebi.ac.uk',
   'organization': 'EMBL-EBI'},
  {'first_name': 'Harish',
   'last_name': 'Dharuri',
   'email': 'hdharuri@cds.caltech.edu',
   'organization': 'California Institute of Technology'},
  {'first_name': 'Jacky L',
   'last_name': 'Snoep',
   'email': 'jls@sun.ac.za',
   'organization': 'Stellenbosh University'}],
 'references': [{'id': '10951190',
   'uri': 'http://identifiers.org/pubmed/10951190',
   'resource': 'PubMed',
   'description': ''}],
 'descriptions': [{'id': 'MODEL6623915522',
   'qualifier': 'is',
   'uri': 'http://identifiers.org/biomodels.db/MODEL6623915522',
   'resource': 'BioModels Database'},
  {'id': 'GO:0006096',
   'qualifier': 'is',
   'uri': 'http://identifiers.org/GO:0006096',
```

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```
   'resource': 'Gene Ontology'},
  {'id': 'sce00010',
   'qualifier': 'is',
   'uri': 'http://identifiers.org/kegg.pathway/sce00010',
   'resource': 'KEGG Pathway'},
  {'id': 'BIOMD0000000064',
   'qualifier': 'is',
   'uri': 'http://identifiers.org/biomodels.db/BIOMD0000000064',
   'resource': 'BioModels Database'},
  {'id': 'REACT_723',
   'qualifier': 'is homolog to',
   'uri': 'http://identifiers.org/reactome/REACT_723',
   'resource': 'Reactome'},
  {'id': '4932',
   'qualifier': 'has taxon',
   'uri': 'http://identifiers.org/taxonomy/4932',
   'resource': 'Taxonomy'}],
 'modifications': [datetime.datetime(2012, 7, 19, 18, 26, 7, tzinfo=tzutc())],
 'created': datetime.datetime(2008, 9, 16, 14, 0, 6, tzinfo=tzutc())}
```

To display the annotations of a specific species, or reaction just enter its name as the element to get the information for. Here we do this for `NADH` to return the dictionary of descriptions as given:

[9]:
```
get_miriam_annotation(name='NADH')
```

[9]:
```
{'descriptions': [{'id': 'C00004',
   'qualifier': 'is',
   'uri': 'http://identifiers.org/kegg.compound/C00004',
   'resource': 'KEGG Compound'},
  {'id': 'CHEBI:16908',
   'qualifier': 'is',
   'uri': 'http://identifiers.org/CHEBI:16908',
   'resource': 'ChEBI'}]}
```

20.3 Setting annotations

Lets start over with a new model, and annotate it as we go along:

[10]:
```
new_model(name='simple model', notes='A simple decay model');
```

The `set_miriam_annotation` accepts the following arguments:

- `creators`: a list of creator dictionary entries with: `first_name`, `last_name`, `email` and `organization`
- `references`: a list of reference dictionary entries with: `id`, `uri`, `resource` and `description`
- `descriptions`: a list of description dictionary entries with: `qualifier`, `resource` and `id`
- `modifications`: a list of DateTime objects representing the modification dates
- `created`: a DateTime object representing the creation date
- `replace`: a boolean indicating, whether the current annotation entries should be replaced ('True' default), or if new entries should be added to the existing ones ('False')

[11]:
```
set_miriam_annotation(creators=[
    {
        'first_name': 'Frank',
        'last_name': 'Bergmann',
        'email':'fbergman@caltech.edu',
        'organization':'Heidelberg University'
    }], replace=True)
```

[12]:
```
get_miriam_annotation()
```

[12]:
```
{'creators': [{'first_name': 'Frank',
   'last_name': 'Bergmann',
   'email': 'fbergman@caltech.edu',
   'organization': 'Heidelberg University'}],
 'created': datetime.datetime(2023, 7, 6, 9, 20, 43, tzinfo=tzutc())}
```

[13]:
```
set_miriam_annotation(descriptions=[
    {
        'qualifier': 'is',
        'resource': 'BioModels Database',
        'id': 'MODEL6623915522',
    }
])
```

[14]:
```
get_miriam_annotation()
```

[14]:
```
{'creators': [{'first_name': 'Frank',
   'last_name': 'Bergmann',
   'email': 'fbergman@caltech.edu',
   'organization': 'Heidelberg University'}],
 'descriptions': [{'id': 'MODEL6623915522',
   'qualifier': 'is',
   'uri': 'http://identifiers.org/biomodels.db/MODEL6623915522',
   'resource': 'BioModels Database'}],
 'created': datetime.datetime(2023, 7, 6, 9, 20, 43, tzinfo=tzutc())}
```

[15]:
```
set_miriam_annotation(references=[
    {
      'id': '10951190',
      'resource': 'PubMed',
    }
])
```

[16]:
```
get_miriam_annotation()
```

[16]:
```
{'creators': [{'first_name': 'Frank',
   'last_name': 'Bergmann',
   'email': 'fbergman@caltech.edu',
   'organization': 'Heidelberg University'}],
 'references': [{'id': '10951190',
   'uri': 'http://identifiers.org/pubmed/10951190',
   'resource': 'PubMed',
   'description': ''}],
```

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```
 'descriptions': [{'id': 'MODEL6623915522',
   'qualifier': 'is',
   'uri': 'http://identifiers.org/biomodels.db/MODEL6623915522',
   'resource': 'BioModels Database'}],
 'created': datetime.datetime(2023, 7, 6, 9, 20, 43, tzinfo=tzutc())}
```

[17]:
```
set_miriam_annotation(modifications=[datetime.datetime.now(datetime.timezone.utc)],␣
↪replace=True)
```

[18]:
```
get_miriam_annotation()
```

[18]:
```
{'creators': [{'first_name': 'Frank',
   'last_name': 'Bergmann',
   'email': 'fbergman@caltech.edu',
   'organization': 'Heidelberg University'}],
 'references': [{'id': '10951190',
   'uri': 'http://identifiers.org/pubmed/10951190',
   'resource': 'PubMed',
   'description': ''}],
 'descriptions': [{'id': 'MODEL6623915522',
   'qualifier': 'is',
   'uri': 'http://identifiers.org/biomodels.db/MODEL6623915522',
   'resource': 'BioModels Database'}],
 'modifications': [datetime.datetime(2023, 7, 6, 9, 20, 43, 723553, tzinfo=tzutc())],
 'created': datetime.datetime(2023, 7, 6, 9, 20, 43, tzinfo=tzutc())}
```

CHAPTER

TWENTYONE

WORKING WITH IPYPARALLEL

In this example we want to use basico from ipython, in a `ipyparallel`, as the normal approach with using `multiprocessing` does not seem to work across operating systems within the jupyter notebooks (read: i could not make it work on Windows).

This means, that to run this example, you will need the `ipyparallel` package installed, which can be achieved by uncommenting the folling line:

[1]:
```
#!pip install -q ipyparallel
```

once that is installed, you will to switch to the home screen of the jupyter notebook, and start the cluster manually:

otherwise this notebook will fail with an error like:

```
---------------------------------------------------------------------------
FileNotFoundError                         Traceback (most recent call last)
Cell In[3], line 1
----> 1 cluster = ipp.Cluster.from_file()
      2 rc = cluster.connect_client_sync()
      3 # wait to get the engines and print their id

File ~/env/lib/python3.11/site-packages/ipyparallel/cluster/cluster.py:556, in Cluster.
↪from_file(cls, cluster_file, profile, profile_dir, cluster_id, **kwargs)
    554 # ensure from_file preserves cluster_file, even if it moved
    555 kwargs.setdefault("cluster_file", cluster_file)
--> 556 with open(cluster_file) as f:
    557     return cls.from_dict(json.load(f), **kwargs)

FileNotFoundError: [Errno 2] No such file or directory:
'~/.ipython/profile_default/security/cluster-.json'
```

Once the ipyparallel is installed and the cluster is running continue as follows:

[2]:
```
from basico import *
import ipyparallel as ipp
```

we could create a cluster manually, in my case i just created one in the cluster menu in the jupyter setup, so to access it we just need to run:

[3]:
```
cluster = ipp.Cluster.from_file()
rc = cluster.connect_client_sync()
```

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```
# wait to get the engines and print their id
rc.wait_for_engines(6); rc.ids
```

[3]:
```
[0, 1, 2, 3, 4, 5, 6, 7]
```

Now we create a direct view with all of the workers:

[4]:
```
dview = rc[:]
```

The model we use is the BioModel 68, since we will need the model many times, i download it once and save it to a local file:

[5]:
```
m = load_biomodel(68)
save_model('bm68.cps', model=m)
remove_datamodel(m)
```

And define the worker method, the worker just loads a biomodel (in case it was not loaded into the worker before, otherwise it accesses the current model). It then chooses a random initial concentration for 2 species, and computes the steady state of the model. Finally the initial concentrations used and the fluxes computed are return. In case a `seed` is specified, it will be used to initialize the rng:

[6]:
```
def worker_method(seed=None):
    import basico
    import random
    if seed is not None:
        random.seed(seed)
    if basico.get_num_loaded_models() == 0:
        m = basico.load_model('bm68.cps')
    else:
        m = basico.get_current_model()

    # we sample the model as described in Mendes (2009)
    cysteine = 0.3 * 10 ** random.uniform(0, 3)
    adomed = random.uniform(0, 100)

    # set the sampled initial concentration.
    basico.set_species('Cysteine', initial_concentration=cysteine, model=m)
    basico.set_species('S-adenosylmethionine', initial_concentration=adomed, model=m)

    # compute the steady state
    _ = basico.run_steadystate(model=m)

    # retrieve the current flux values
    fluxes = basico.get_reactions(model=m).flux

    # and return as tuple
    return (cysteine, adomed, fluxes[1], fluxes[2])
```

We can invoke this method synchronusly in the notebook to obtain the result:

[7]:
```
worker_method()
```

[7]:
```
(1.5236813977490542,
 29.805870872058716,
```

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```
0.04158430196391732,
0.9584156980360827)
```

now we want to do that many times over (passing along the index to set the seed every time to get about the same result on my machine):

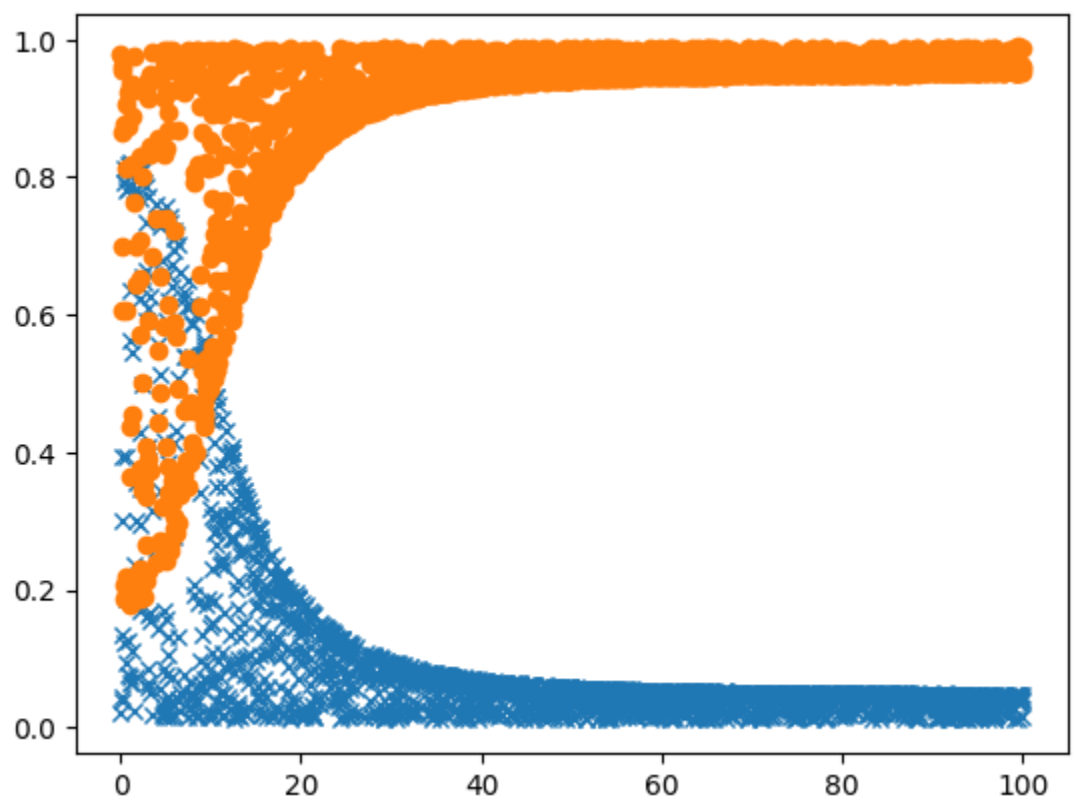
[8]:
```
%%time
sync_results = []
for i in range(2000):
    sync_results.append(worker_method(i))
```

```
CPU times: user 2.06 s, sys: 55 ms, total: 2.12 s
Wall time: 2.08 s
```

here a utility method plotting the result:

[9]:
```
def plot_result(results):
    cys = [x[0] for x in results]
    ado = [x[1] for x in results]
    y1 = [x[2] for x in results]
    y2 = [x[3] for x in results]
    plt.plot(ado, y1, 'x')
    plt.plot(ado, y2, 'o')
    plt.show()
```

[10]:
```
plot_result(sync_results)
```



So that for me took some 10 seconds (even though the model was loaded already), so the next thing to do is to run it in parallel. Here i start 10000 runs, passing along the seed for each one, to make it reproducible:

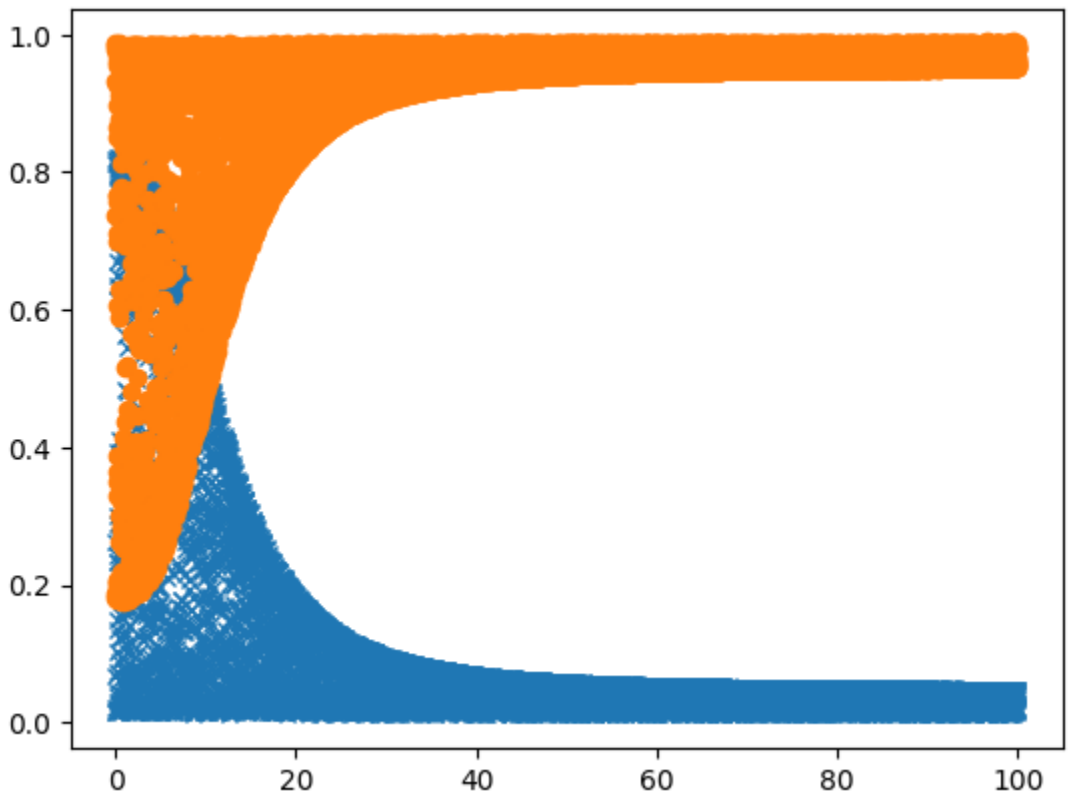
[11]:
```
%%time
ar_map = dview.map_async(worker_method, [i for i in range(10000)])
ar_map.wait_for_output()
```

```
CPU times: user 412 ms, sys: 259 ms, total: 671 ms
Wall time: 3.72 s
```

[11]:
```
True
```

And now we can plot that as well:

[12]:
```
plot_result(ar_map.get())
```



CHAPTER

TWENTYTWO

WORKING WITH PETAB

PEtab is a standard file format, describing parameter estimation problems. While COPASI does not support the full feature set of PEtab, with basico we can import PEtab problems, and analyze them. THis is an optional dependency, that is only installed, when basico is installed using:

```
pip install copasi-basico[petab]
```

assuming this is done, and that a petab problem is in the local directory, you can load it and analyze it like so:

[1]:
```
from basico import *
import basico.petab
```

```
using COPASI: 4.39.272 (Source)
```

within the `basico.petab` module we define a PetabSimulator, that automatically imports a PEtab file, and transforms the experimental data files as needed by COPASI. It implementes the `petab.simulate.Simulator` interface that can be used for other libraries using libpetab.

So lets start by loading a PEtab problem

[2]:
```
from petab import Problem
pp = Problem.from_yaml('./Elowitz_Nature2000/Elowitz_Nature2000.yaml')
```

now lets instantiate the simulator with:

- `pp`: the petab problem
- `working_dir`: the directory where temp files can be stored

we are not specifying any additional optimization settings, so the parameter estimation task will be set to 'Current Solution Statistics', meaning that no actual optimization will be performed:

[3]:
```
sim = basico.petab.PetabSimulator(pp, working_dir='./temp_dir/')
```

now lets simulate it:

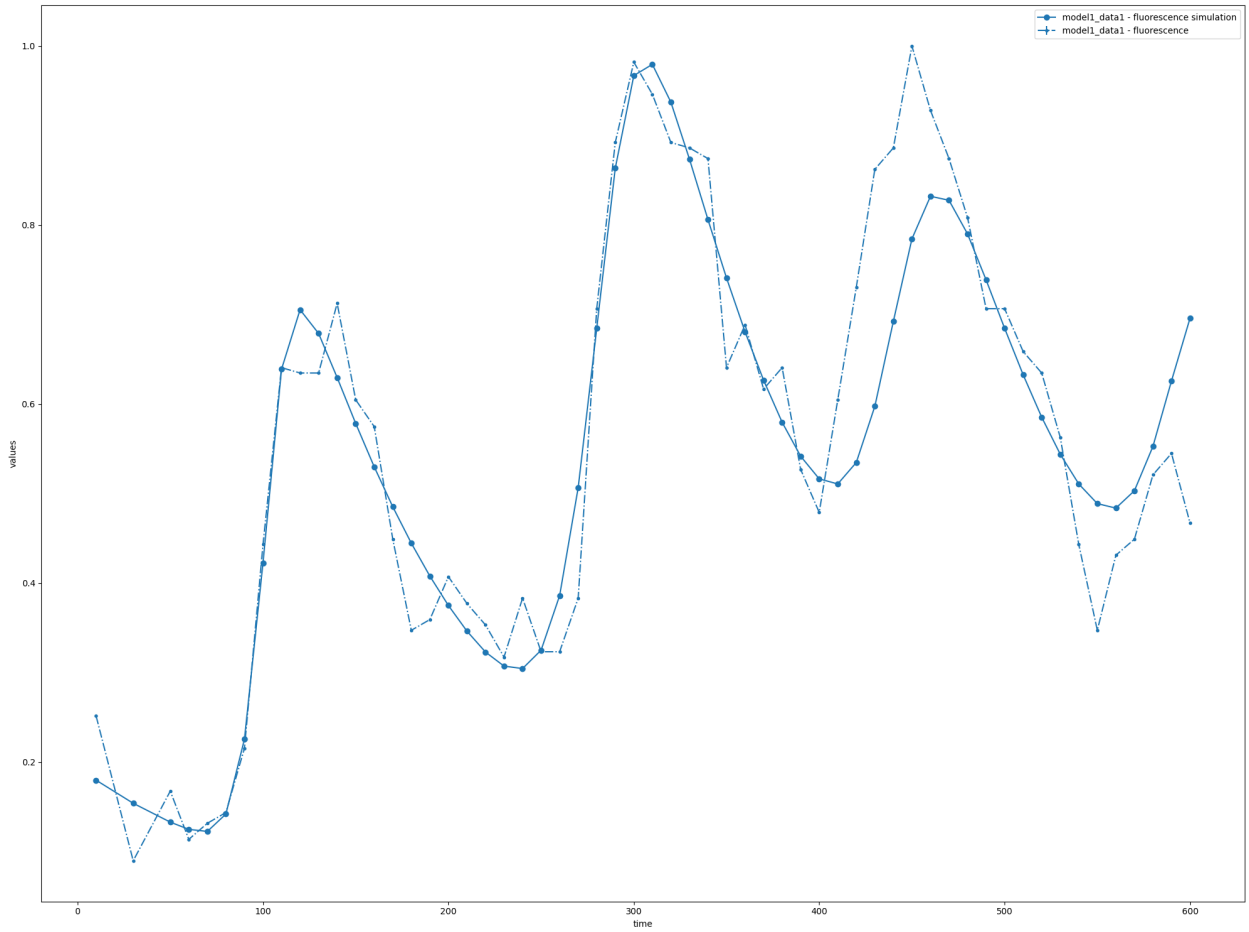
[4]:
```
df = sim.simulate()
```

At this point the file can be opened directly in COPASI using `open_copasi()`, or here I use the visualization library from libpetab, to plot the problem and simulation obtained:

[5]:
```
import petab.visualize
```

[6]:
```
petab.visualize.plot_problem(pp, simulations_df=df)
```

[6]:
```
{'plot1': <Axes: xlabel='time', ylabel='values'>}
```



CHAPTER

TWENTYTHREE

MODEL SELECTION

Using the `petab_select` library, model selection is also wrapped within basico. It will instantiate the petab problem, and explore all models according to the specified method:

[7]:
```
import petab_select
```

[8]:
```
problem = petab_select.Problem.from_yaml('./model_selection/petab_select_problem.yaml')
```

evaluating the problem will perform the calibrations. While COPASI uses different errorscaling than other PEtab scales, we would expect the same models being chosen:

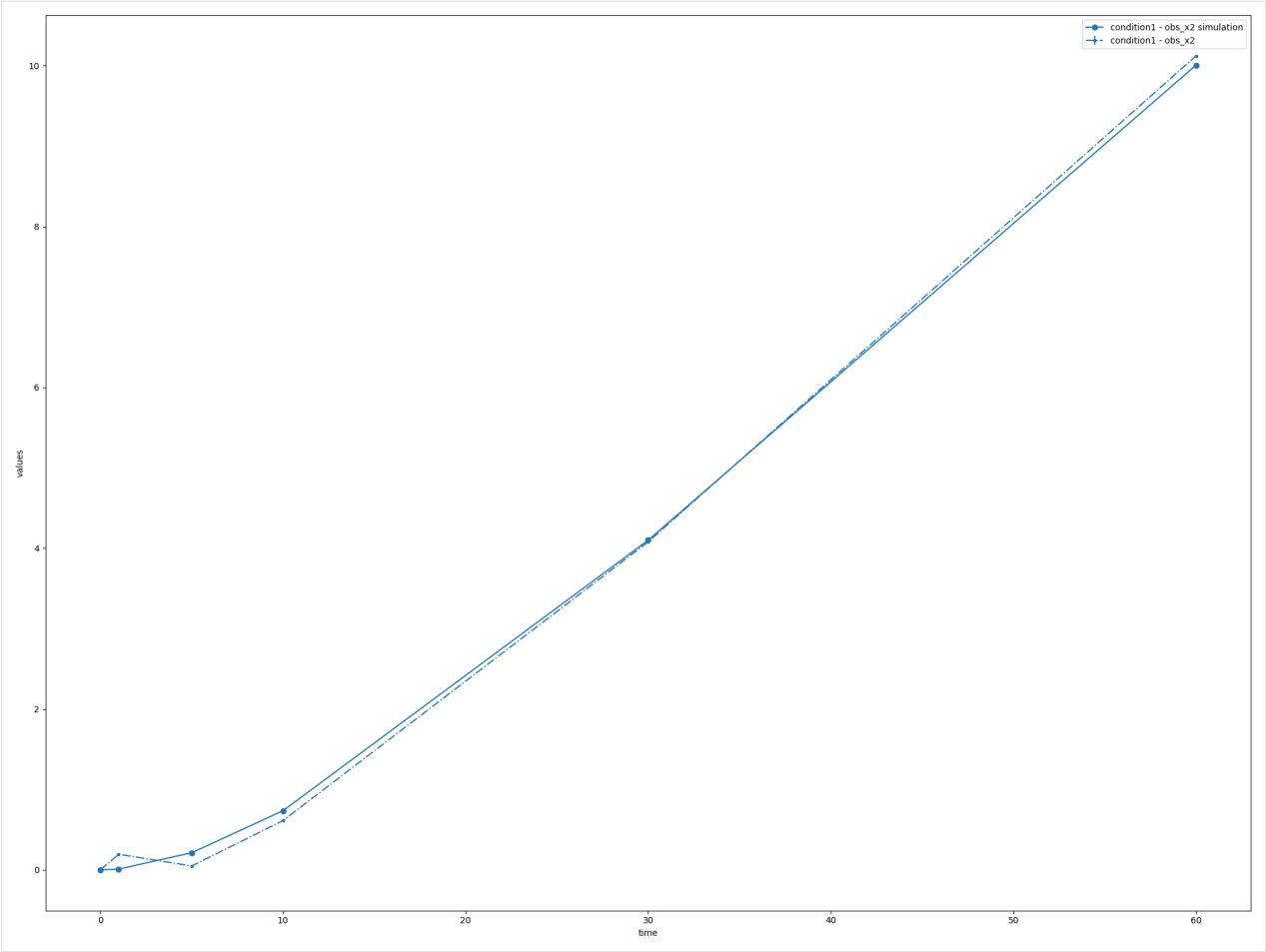
[9]:
```
best = basico.petab.evaluate_problem(problem, temp_dir='./temp_dir/', delete_temp_
↪files=False)
print(best.model_subspace_id)
```

```
M1_3
```

at this point the best model returned could be turned into its own PEtab problem, and simulated as above:

[10]:
```
pp = best.to_petab()['petab_problem']
sim = basico.petab.PetabSimulator(pp, working_dir='./temp_dir/')
petab.visualize.plot_problem(pp, simulations_df=sim.simulate())
```

[10]:
```
{'plot1': <Axes: xlabel='time', ylabel='values'>}
```



finally lets clean up after ourselfes and delete all the temp files generated:

[11]:
```
import shutil
shutil.rmtree('./temp_dir')
```

CHAPTER

TWENTYFOUR

WORKING WITH PARAMETER SETS

COPASI supports storing multiple parameter sets for a model. This tutorial describes how to work with them. We start by loading the brusselator example model:

[1]:
```
from basico import *
```

[2]:
```
brusselator = load_example('brus')
```

Currently we dont have any parameter sets in this file:

[3]:
```
get_parameter_sets()
```

[3]:
```
[]
```

so lets create a new parameter set from the current state:

[4]:
```
add_parameter_set('InitialState')
```

24.1 Looking at parameter sets

now let us look at it using the `get_parameter_sets` method. If no name is specified, `get_parameter_sets` returns all parameter sets in the file as a list of dictionaries, in each one you will find the following keys:

- `name`: the name of the parameter set
- `description`: notes if any
- `Initial Time`: a dictionary with the initial time of the model
- `Initial Compartment Sizes`: a dictionary with the compartment sizes of all compartments
- `Initial Species Values`: a dictionary with the initial concentration of all species
- `Initial Global Quantities`: a dictionary with the initial values of all global parameters
- `Kinetic Parameters`: a dictionary of all local reaction parameters

`get_parameter_sets` takes 3 arguments:

- `name`: the name of the parameter set to return (can be a substring, to return multiple)
- `exact`: whether the name has to be precisely matched
- `values_only`: if true, only the initial values will be returned, otherwise also the type of model parameter

so you will see either:

[5]:
```
get_parameter_sets(values_only=True)
```

[5]:
```
[{'name': 'InitialState',
  'description': '',
  'Initial Time': {'The Brusselator': 0.0},
  'Initial Compartment Sizes': {'compartment': 1.0},
  'Initial Species Values': {'X': 2.9999959316797846,
   'Y': 2.9999959316797846,
   'A': 0.49999987545958524,
   'B': 2.9999959316797846,
   'D': 0.0,
   'E': 0.0},
  'Initial Global Quantities': {},
  'Kinetic Parameters': {'R1': {'k1': 1.0},
   'R2': {'k1': 1.0},
   'R3': {'k1': 1.0},
   'R4': {'k1': 1.0}}}]
```

or the much more verbose variant (I'll restrict it here to just one of the species to avoid clutter):

[6]:
```
get_parameter_sets()[0]['Initial Species Values']['X']
```

[6]:
```
{'concentration': 2.9999959316797846,
 'particle_number': 1.80664e+21,
 'parameter_type': 'species',
 'simulation_type': 'reactions'}
```

24.2 Creating / Modifying Parameter sets

As we saw above, we can add a new parameter set using `add_parameter_set` with only a name parameter, you can also specify the parameter set, by providing the dictionary as it was returned above. It does not have to be complete, you can can also create a partial one, containing only those values you want to specify.

NOTE: when specifying concentrations, you will also have to specify the initial compartment volume for those species.

[7]:
```
add_parameter_set('Partial', {
         'Initial Compartment Sizes': {'compartment': 1},
         'Initial Species Values': {'X': 3, 'Y': 1}})
```

[8]:
```
get_parameter_sets('Partial', values_only=True)[0]
```

[8]:
```
{'name': 'Partial',
 'description': '',
 'Initial Time': {},
 'Initial Compartment Sizes': {'compartment': 1.0},
 'Initial Species Values': {'X': 3.0, 'Y': 1.0},
 'Initial Global Quantities': {},
 'Kinetic Parameters': {}}
```

to change certain values in a parameter set, you can use the `set_parameter_set`, this will set all the values specified, and by default leave all entries not specified at their old values. You'd use the argument `remove_others=True`, to remove all entries not specified. For example, let me set the initial concentration of `Y` in the Partial parameter set to 3:

[9]:
```
set_parameter_set('Partial', param_set_dict={'Initial Species Values': {'Y': 3}}, remove_
↪others=False)
get_parameter_sets('Partial', values_only=True)[0]['Initial Species Values']
```

[9]:
```
{'X': 3.0, 'Y': 3.0}
```

To change the current model state, to use the values specified in a certain parameter set, you'd use the function `apply_parameter_set`:

[10]:
```
apply_parameter_set('Partial')
get_species()[['initial_concentration']]
```

[10]:
```
      initial_concentration
name
X                  3.000000
Y                  3.000000
A                  0.500000
B                  2.999996
D                  0.000000
E                  0.000000
```

If you wanted to update a parameter set, with all the values from the current model state, you can use `update_parameter_set`. Lets use that here, to update the `InitialState` parameter set from above, to contain the updated concentrations:

[11]:
```
update_parameter_set('InitialState')
get_parameter_sets('InitialState', values_only=True)[0]['Initial Species Values']
```

[11]:
```
{'X': 3.0,
 'Y': 3.0,
 'A': 0.49999987545958524,
 'B': 2.9999959316797846,
 'D': 0.0,
 'E': 0.0}
```

24.3 Removing parameter sets

The `remove_parameter_sets` function can be used to remove parameter sets if no argument is specified, all paraemter sets will be removed, otherwise the once matching the given name. Here i just want to remove the partial one defined above:

[12]:
```
remove_parameter_sets('Partial')
```

[13]:
```
for p_set in get_parameter_sets():
    print(p_set['name'])
```

```
InitialState
```

[14]:
```
remove_datamodel(brusselator)
```

24.4 Parameter sets and Parameter Estimation

Parameter sets are mainly in use in parameter estimations, with multiple experiments. Since each experiment can have different initial conditions or even dependent values can differ between experiments, the parameter sets can capture those differences, when a parameter estimation is run with `create_parametersets=True`, lets try this here for a small test model that has parameter estimation set up:

[15]:
```
lm = load_example('LM')
```

we don't have any parameter sets yet, but when we run the the parameter estimation we can have some created:

[16]:
```
get_parameter_sets()
```

[16]:
```
[]
```

[17]:
```
run_parameter_estimation(create_parametersets=True)
```

[17]:
```
               lower upper        sol        affected
name
(R1).k2         1e-6   1e6   0.000002              []
(R2).k1         1e-6   1e6  44.661715              []
Values[offset]  -0.2   0.4   0.043018  [Experiment_1]
Values[offset]  -0.2   0.4   0.054167  [Experiment_3]
Values[offset]  -0.2   0.4  -0.050941    [Experiment]
Values[offset]  -0.2   0.4   0.045922  [Experiment_4]
Values[offset]  -0.2   0.4   0.048025  [Experiment_2]
```

we can look at the fit statistic, to see which objective value was reached:

[18]:
```
get_fit_statistic()['obj']
```

[18]:
```
inf
```

and we also see all the generated parameter sets, one for the original model state, and one for each individual experiment:

[19]:
```
for p_set in get_parameter_sets():
    print(p_set['name'])
```

```
PE: 2023-12-06T09:14:46Z Exp: Original
PE: 2023-12-06T09:14:46Z Exp: Experiment
PE: 2023-12-06T09:14:46Z Exp: Experiment_1
PE: 2023-12-06T09:14:46Z Exp: Experiment_2
PE: 2023-12-06T09:14:46Z Exp: Experiment_3
PE: 2023-12-06T09:14:46Z Exp: Experiment_4
```

we can run the parameter estimation again, maybe using a different algorithm, and this new run would give as further parameter sets:

[20]:
```
run_parameter_estimation(method=PE.HOOKE_JEEVES, create_parametersets=True)
print(f"Objective value reached: {get_fit_statistic()['obj']}")
```

```
Objective value reached: inf
```

[21]:
```
for p_set in get_parameter_sets():
    print(p_set['name'])
```

```
PE: 2023-12-06T09:14:46Z Exp: Original
PE: 2023-12-06T09:14:46Z Exp: Experiment
PE: 2023-12-06T09:14:46Z Exp: Experiment_1
PE: 2023-12-06T09:14:46Z Exp: Experiment_2
PE: 2023-12-06T09:14:46Z Exp: Experiment_3
PE: 2023-12-06T09:14:46Z Exp: Experiment_4
PE: 2023-12-06T09:14:52Z Exp: Original
PE: 2023-12-06T09:14:52Z Exp: Experiment
PE: 2023-12-06T09:14:52Z Exp: Experiment_1
PE: 2023-12-06T09:14:52Z Exp: Experiment_2
PE: 2023-12-06T09:14:52Z Exp: Experiment_3
PE: 2023-12-06T09:14:52Z Exp: Experiment_4
```

since the objective value is better for the second run, let us assume we want to remove the parameter sets from the first run. We can do this like so:

[22]:
```
psets =  get_parameter_sets()
first_time_stamp = psets[0]['name'][:psets[0]['name'].rfind('Exp:')]
remove_parameter_sets(first_time_stamp, exact=False)
```

[23]:
```
for p_set in get_parameter_sets():
    print(p_set['name'])
```

```
PE: 2023-12-06T09:14:52Z Exp: Original
PE: 2023-12-06T09:14:52Z Exp: Experiment
PE: 2023-12-06T09:14:52Z Exp: Experiment_1
PE: 2023-12-06T09:14:52Z Exp: Experiment_2
PE: 2023-12-06T09:14:52Z Exp: Experiment_3
PE: 2023-12-06T09:14:52Z Exp: Experiment_4
```

[24]:
```
remove_datamodel(lm)
```

Once a model has several parameter sets, we can also use them in a parameter scan. To give an example, here we load the brusselator example again, create a parameter set for the initial state, and then one for the steady state. Then running a scan over the two parameter sets we can see them both being applied:

[25]:
```
brusselator = load_example('brus')
add_parameter_set('InitialState')
run_steadystate(update_model=True)
add_parameter_set('steady_state')
```

lets look at the parametersets we have, and the concentrations of `X` and `Y` in them

[26]:
```
for param_set in get_parameter_sets():
    print(param_set['name'])
    concentrations = param_set['Initial Species Values']
    for species in ['X', 'Y']:
        print(f"{species}: {concentrations[species]['concentration']}")
```

```
InitialState
X: 2.9999959316797846
Y: 2.9999959316797846
steady_state
```

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```
X: 0.49999987545958524
Y: 5.999993357842892
```

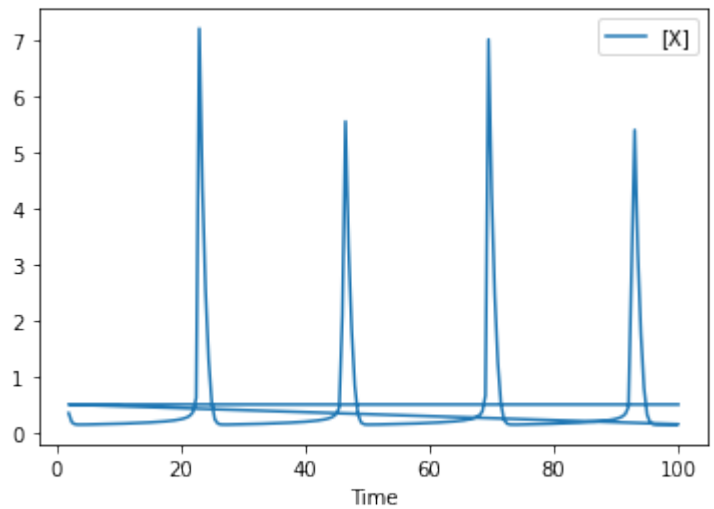
Now we can setup a scan over both parameter sets as example, for that we switch the subtask to time course, capture output while the task is running and set the scan item to be the parameter sets:

[27]:
```
set_scan_settings( subtask=T.TIME_COURSE, output_during_subtask=True, scan_items=[
    {'parameter_sets':['InitialState', 'steady_state'],}
])
```

when we now run this task, and capture the output for time and the concentration for `X` we want to see the time course to be performed twice, once for the initial state, and once for steadystate:

[28]:
```
run_scan(output=['Time', '[X]']).plot(x='Time', y='[X]')
```

[28]:
```
<Axes: xlabel='Time'>
```



CHAPTER

TWENTYFIVE

PROFILE LIKELIHOOD

To perform a basic profile likelihood analysis of a fit obtained, basico implements the Schaber method that in turn fixes each optimization parameter, while reoptimizing the remaining parameters. This scan is performed in both directions. Ideally, what we would want to see for identified parameters, is that the result gets worse, as we go away from the found solution. If we find a flat line, that means the parameter is not identifiable, if we find a curve that is flat on one side, we can only identify the corresponding bound.

Since this could potentially take quite some time basico breaks this task into three steps:

- generating different copasi models for each of the scans. (these files could then be moved to a cluster environment for parallel computation)
- running the the scans (here basico uses the python mulitiprocessing library), which places reports into a specified directory
- plotting the result, by specifying the directory where the reports have been stashed.

Let's try this on an example model.

[1]:
```
from basico import *
from basico.task_profile_likelihood import prepare_files, process_dir, plot_data
```

25.1 Preparing files

The first step is to prepare the files, here we load an example model, run the parameter estimation

[2]:
```
example_model = load_example('LM')
run_parameter_estimation(method=PE.HOOKE_JEEVES, update_model=True)
```

[2]:
```
                lower upper        sol        affected
name
(R1).k2          1e-6   1e6  26.353601              []
(R2).k1          1e-6   1e6  46.699200              []
Values[offset]  -0.2   0.4   0.046461  [Experiment_1]
Values[offset]  -0.2   0.4   0.077161  [Experiment_3]
Values[offset]  -0.2   0.4  -0.049828    [Experiment]
Values[offset]  -0.2   0.4   0.030610  [Experiment_4]
Values[offset]  -0.2   0.4   0.058074  [Experiment_2]
```

at this point we also want to make sure, that we have reached a good fit, so we look at the fit statistic:

[3]:
```
get_fit_statistic()
```

[3]:
```
{'obj': 12.501488024131111,
 'rms': 0.15812329381929224,
 'sd': 0.15924191621103437,
 'f_evals': 3008,
 'failed_evals_exception': 0,
 'failed_evals_nan': 0,
 'cpu_time': 5.0625,
 'data_points': 500,
 'valid_data_points': 500,
 'evals_per_sec': 0.0016830119680851063}
```

now we create a temporary directory, and save the file and experimental data into it. After that i unload the model.

[4]:
```
from tempfile import mkdtemp
data_dir = mkdtemp()
original_model = os.path.join(data_dir, 'original.cps')
save_model(original_model)
remove_datamodel(example_model)
```

the code has just been ported from an earlier version, so lets debug it for now

[5]:
```
#import logging
#logging.basicConfig()
#logging.getLogger().setLevel(logging.DEBUG)
```

the data will be stored in those files:

[6]:
```
#print(data_dir)
#print(original_model)
```

now we go ahead and prepare all the files, this is done by the `prepare_files` function that accepts the following arguments:

- `filename`: the template file with the fit we want to analyze
- `data_dir`: the directory in which to store the files in

the remaining parameters are optional:

- `iterations=50`: if not specified hooks & Jeeves / Levenberg Marquardt will perform `50` iterations
- `scan_interval=40`: if not specified 40 scan intervals will be taken (40 in each direction!)
- `lower_adjustment='-50%'`: the multiplier for the lower bound of the scan. By default the interval will be -50% of the found parmeter value.
- `upper_adjustment='+50%'`: the multiplier for the upper bound of the scan, defaults to '+50%' found
- `modulation=0.01`: modulation parameter for Levenberg Marquardt
- `tolerance=1e-06`: tolerance for the optimization method
- `disable_plots=True`: if true, other plots in the file will be removed
- `disable_tasks=True`: if true, other tasks in the file will be deleted
- `use_hooke=False`: if true, use hooks & jeaves otherwise Levenberg Marquadt
- `prefix="out_"`: the prefix for each file generated.

For this example we just do a scan of 8 values in each direction for 20 iterations:

[7]:
```
prepare_files(original_model, scan_interval=8, iterations=20, data_dir=data_dir)
```

[7]:
```
{'num_params': 7,
 'num_data': 500,
 'obj': 12.501488024131111,
 'param_sds': {'(R1).k2': 5.433042366390387,
  '(R2).k1': 0.5087112193172452,
  'Values[offset].InitialValue': 0.01143802470807778}}
```

25.2 Processing the files:

Here we use the python multiprocessing pool, to launch `CopasiSE` to process all the files we have generated in the data directory we process 4 files at the same time, but you can supply a `pool_size` parameter to change that. This step can be skipped, if you copy the files to a cluster environment and run them there.

To specify a specific CopasiSE version to use you can pass it along the module's `COPASI_SE` field. For example like so:

`basico.task_profile_likelihood.COPASI_SE = '/opt/COPASI/COPASI-4.38.268-Linux-64bit/bin/CopasiSE'`

alternatively, `process_dir` also accepts the following named arguments:

- `copasi_se`: if you dont want to change the global default for CopasiSE, but just pass it along here
- `max_time`: normally, we'd let the model run to completion, but if you specify a max time in seconds, then the computation will be stopped after that time.

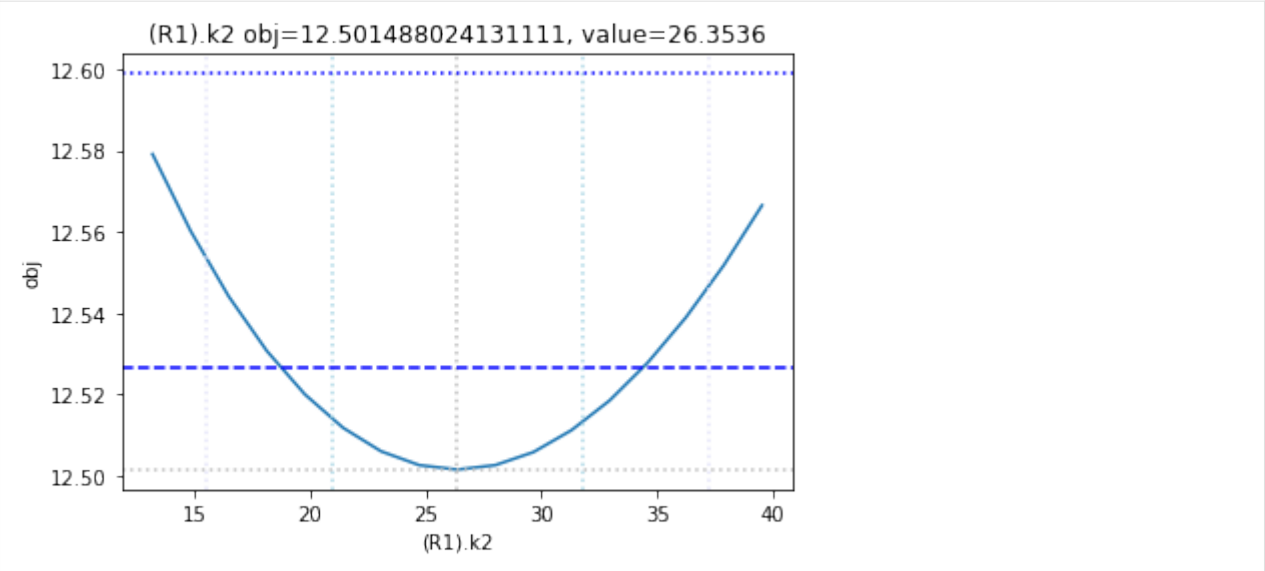
so lets runt the files we have generated above, and restrict each run to 10 seconds:

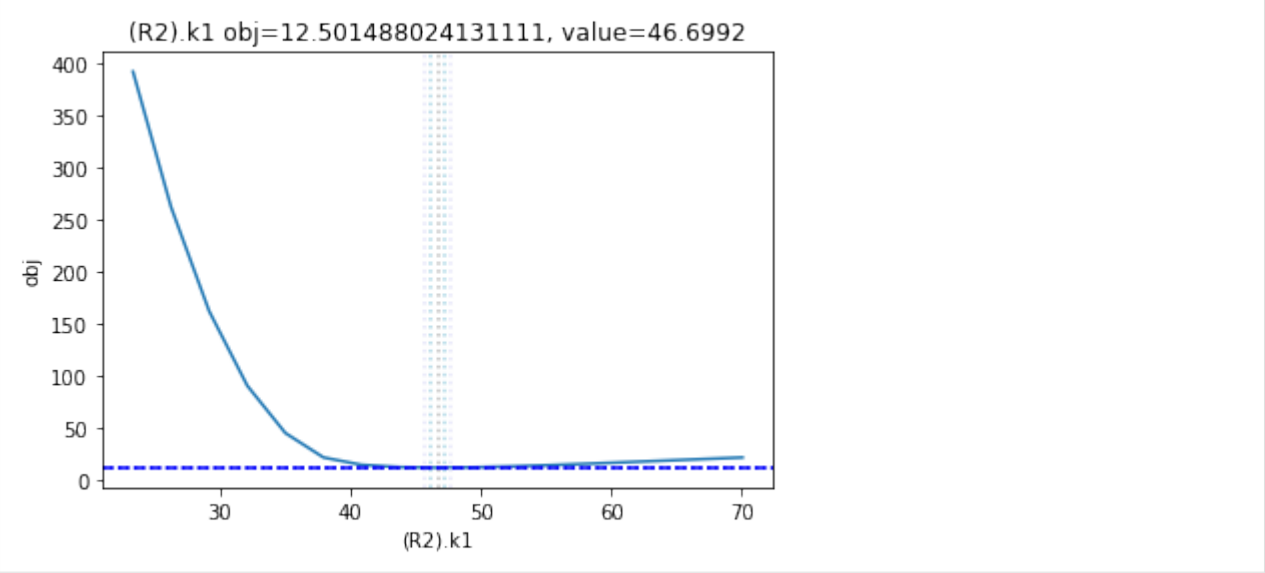
[8]:
```
process_dir(data_dir, max_time=10)
```

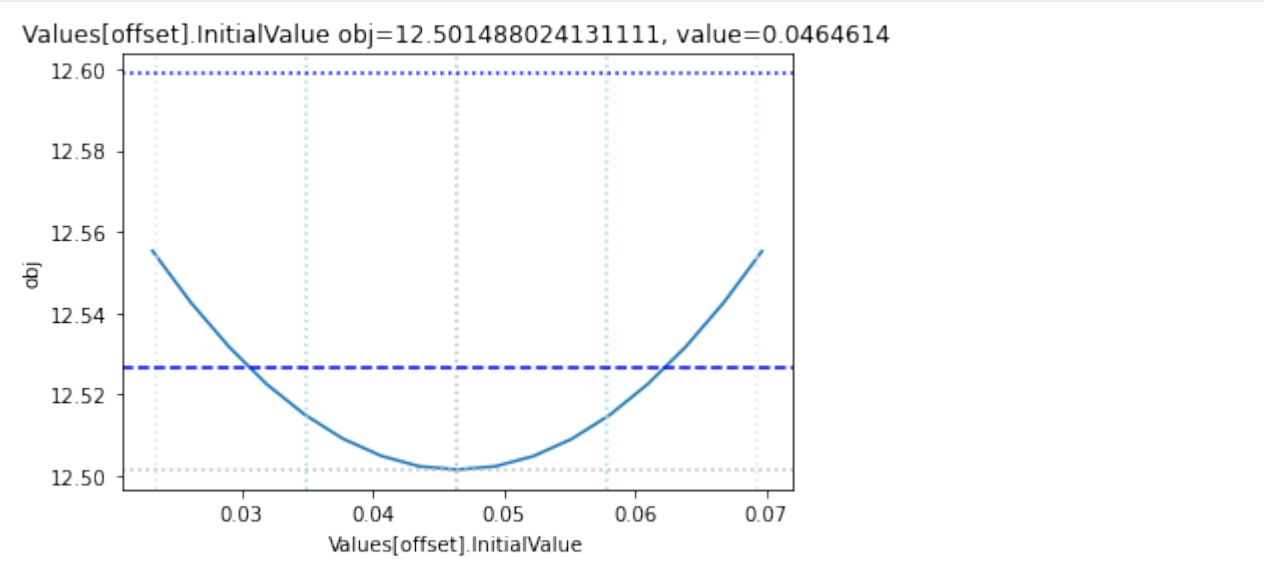
25.3 Looking at the results

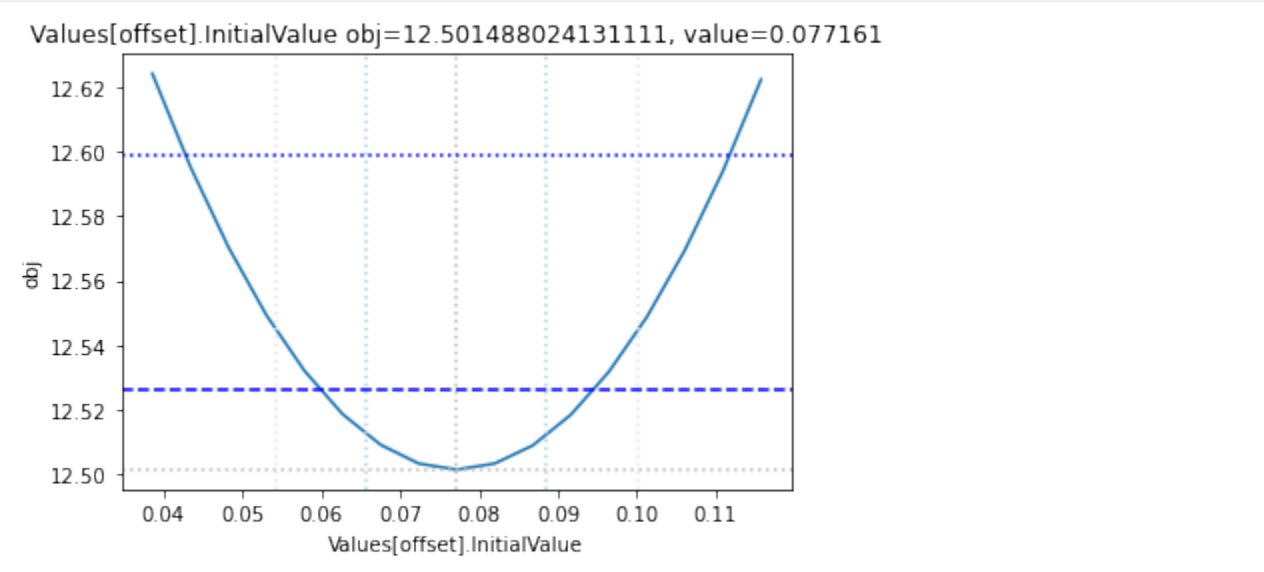
The `plot_data` function reads all the report files from the `data_dir`, and combines the scans from both directions to one plot.

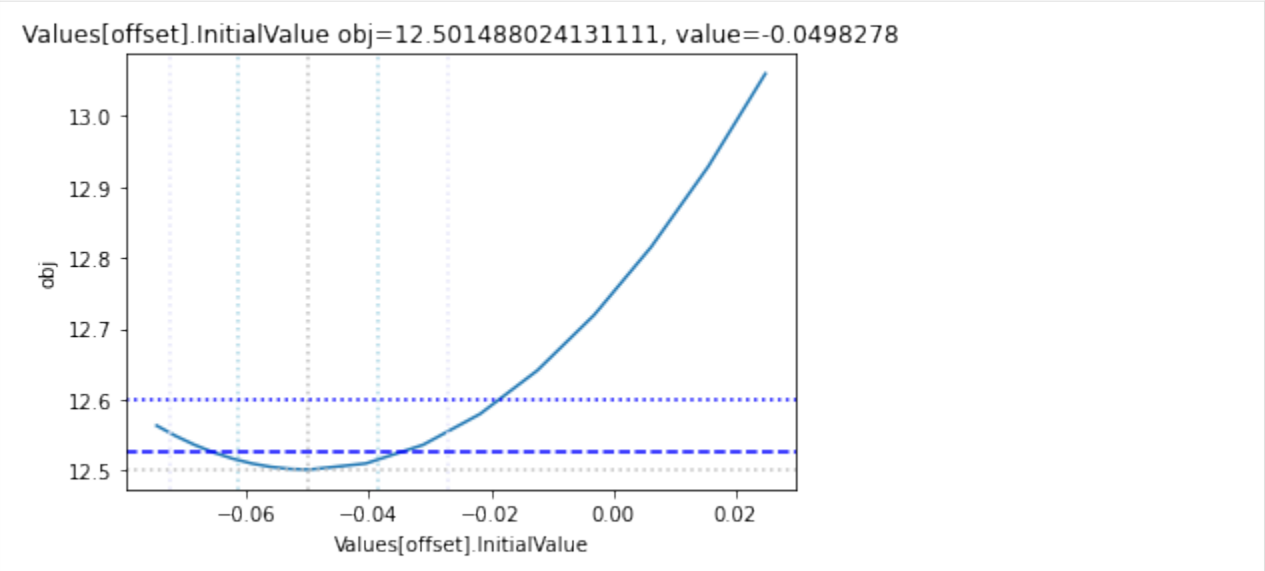
[9]:
```
plots = plot_data(data_dir)
```

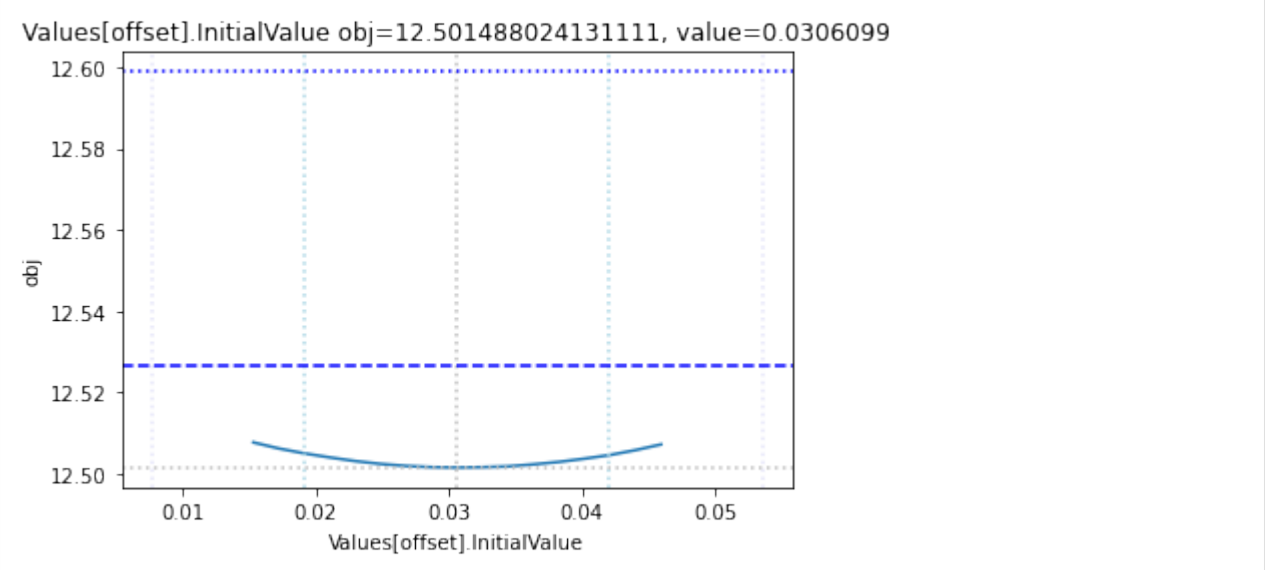

(R1).k2 obj=12.501488024131111, value=26.3536
12.60
12.58
12.56
12.54
12.52
12.50
obj
15
20
25
30
35
40
(R1).k2

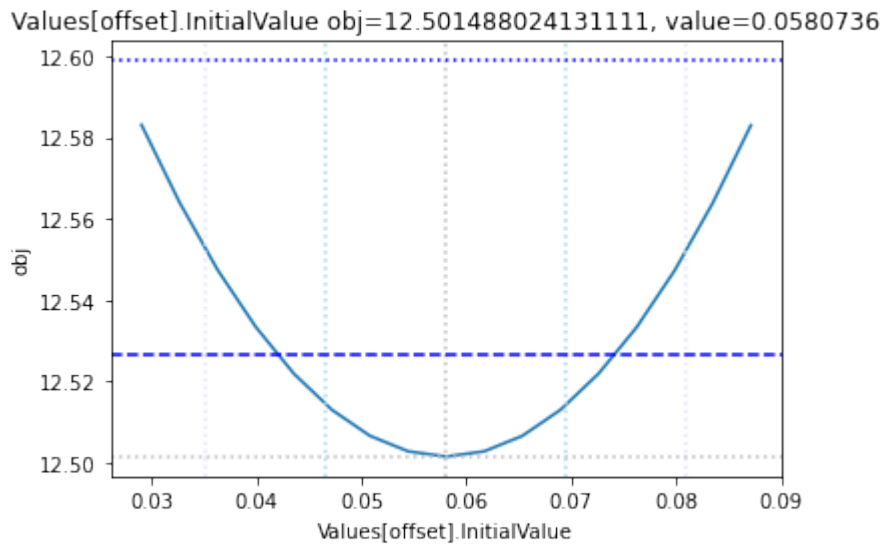

(R2).k1 obj=12.501488024131111, value=46.6992
400
350
300
250
200
150
100
50
0
obj
30
40
50
60
70
(R2).k1


Values[offset].InitialValue obj=12.501488024131111, value=0.0464614
12.60
12.58
12.56
12.54
12.52
12.50
obj
0.03
0.04
0.05
0.06
0.07
Values[offset].InitialValue


Values[offset].InitialValue obj=12.501488024131111, value=0.077161
12.62
12.60
12.58
12.56
12.54
12.52
12.50
obj
0.04
0.05
0.06
0.07
0.08
0.09
0.10
0.11
Values[offset].InitialValue


Values[offset].InitialValue obj=12.501488024131111, value=-0.0498278
13.0
12.9
12.8
12.7
12.6
12.5
obj
−0.06
−0.04
−0.02
0.00
0.02
Values[offset].InitialValue


Values[offset].InitialValue obj=12.501488024131111, value=0.0306099
12.60
12.58
12.56
12.54
12.52
12.50
obj
0.01
0.02
0.03
0.04
0.05
Values[offset].InitialValue



and finally, let us remove the temporary files:

[10]:
```
#import shutil
#shutil.rmtree(data_dir, ignore_errors=True)
```

25.4 Everything together

Lets use a second example, this time we recreate the model from Schabers publication from scratch, and then run the parameter estimation using a convenience method:

[11]:
```
from basico import *
from basico.task_profile_likelihood import get_profiles_for_model
```

[12]:
```
new_model(name='Schaber Example', notes="""
The example from the supplement, originally described in

Schaber, J. and Klipp, E. (2011) Model-based inference of biochemical parameters and
dynamic properties of microbial signal transduction networks, Curr Opin Biotechnol, 22,␣
↪109-
116 (https://doi.org/10.1016/j.copbio.2010.09.014)

""");
```

[13]:
```
add_function('mod. MA',
             'k * S * T',
             'irreversible',
             mapping={'S': 'modifier', 'T': 'substrate'}
);
```

[14]:
```
add_reaction('v1', 'T -> Tp; S', function='mod. MA')
add_reaction('v2', 'Tp -> T')
```

(continues on next page)

(continued from previous page)

```
add_reaction('decay', 'S ->', mapping={'k1': 0.5})
get_reactions()[['scheme', 'function', 'mapping']]
```

[14]:
```
            scheme                    function                          mapping
name
v1     T -> Tp;  S                     mod. MA  {'k': 0.1, 'S': 'S', 'T': 'T'}
v2         Tp -> T  Mass action (irreversible)  {'k1': 0.1, 'substrate': 'Tp'}
decay        S ->   Mass action (irreversible)   {'k1': 0.5, 'substrate': 'S'}
```

[15]:
```
set_species('Tp', initial_concentration=0)
# observable
add_species('TpFit', status='assignment', expression='{[Tp]}/0.5')
get_species()[['initial_concentration']]
```

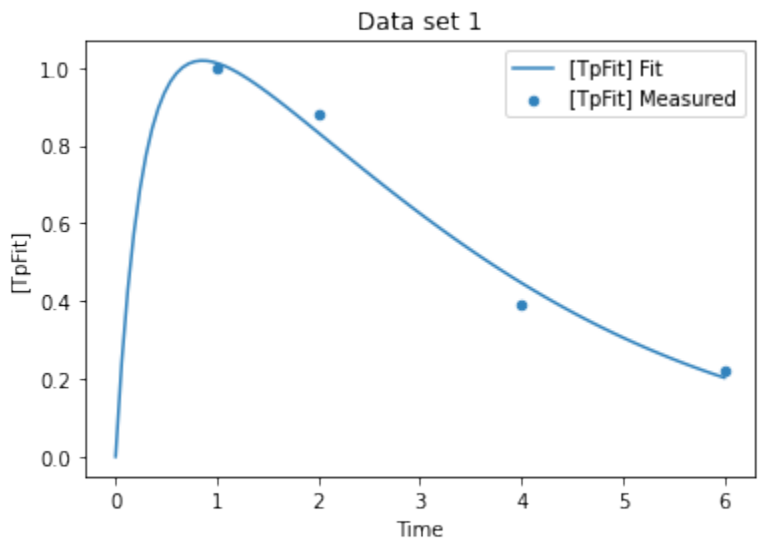
[15]:
```
       initial_concentration
name
S                        1.0
T                        1.0
Tp                       0.0
TpFit                    0.0
```

[16]:
```
add_experiment('Data set 1', pd.DataFrame(data = {
    'Time': [1, 2, 4, 6],
    '[TpFit]': [1, 0.88, 0.39, 0.22],
    #'sd': [0.09, 0.09, 0.09, 0.09]
}
));
```

[17]:
```
set_fit_parameters([
    {'name': '(v1).k', 'lower': 0, 'upper': 100},
    {'name': '(v2).k1', 'lower': 0, 'upper': 100},
])

sol = run_parameter_estimation(method=PE.HOOKE_JEEVES, update_model=True)
sol[['sol']]
```

[17]:
```
              sol
name
(v1).k   2.267945
(v2).k1  1.425208
```

[18]:
```
plot_per_experiment(solution=sol);
```

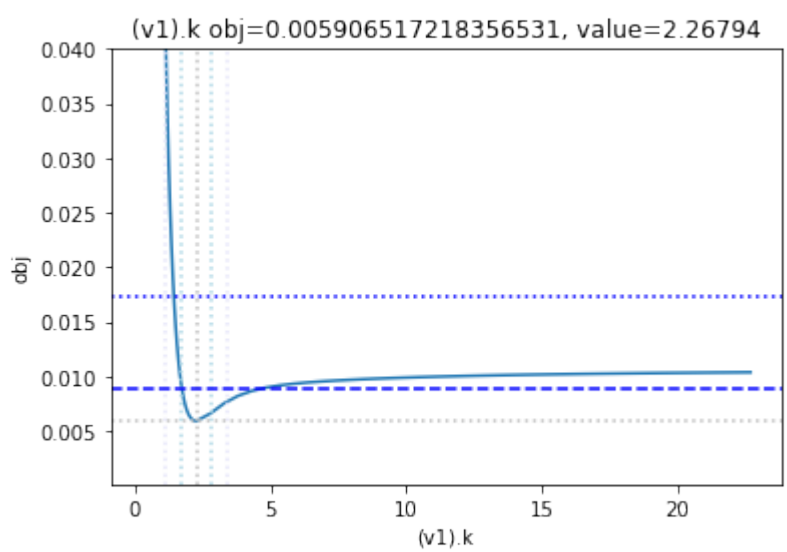


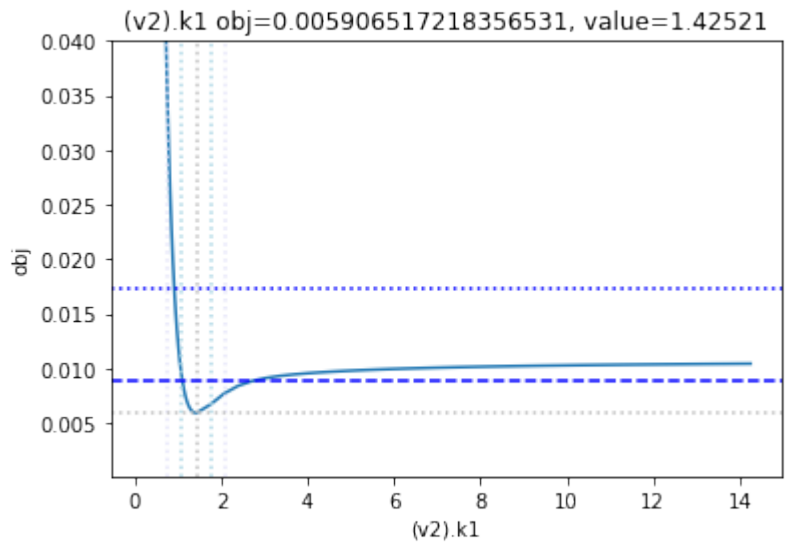
while the fit looks ok, lets have a look at the likelyhood profile

the utility method `get_profiles_for_model` combines all of the above and runs the profile likelihood for the currently loaded model and fit. You can supply all the arguments of `prepare_files` and `process_dir`. By defaut `get_profiles_for_model` will use a temporary directory, and remove the files afterwards. If you would like the files to stay on your disc, you can supply a `data_dir`, in which all files will be generated, and reports placed.

We additionally use the `scale_mode` parameter, that allows to limit the y_axis to desired limits.

[19]:
```
get_profiles_for_model(lower_adjustment=0.1, upper_adjustment=10, scale_mode={'top': 0.
↪04, 'bottom': 0.0001});
```



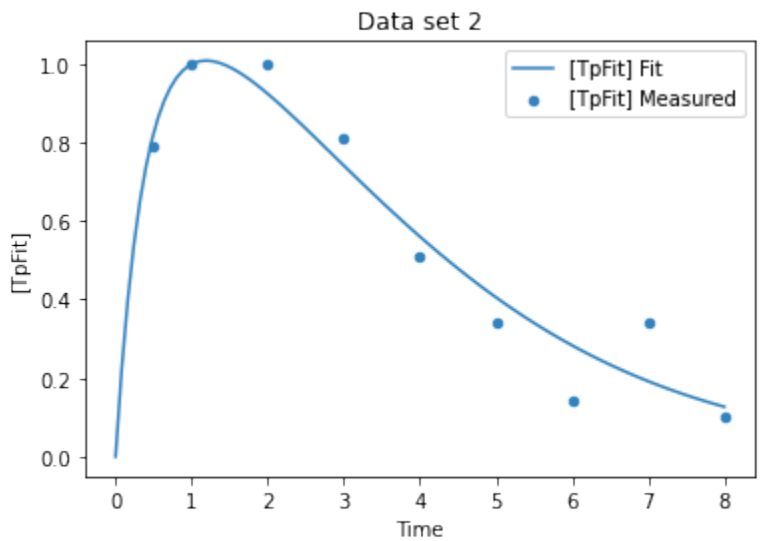


as the result from the publication suggests, the parameter is not identifiable. No lets the run the second dataset as well:

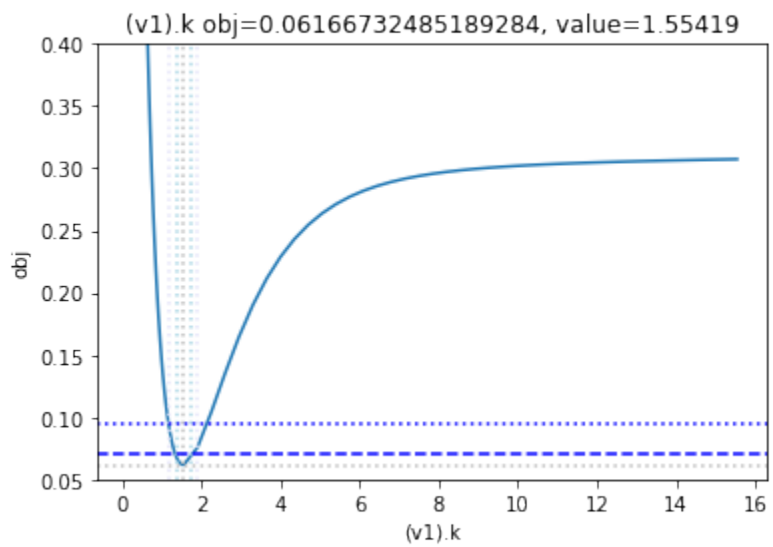
[20]:
```
remove_experiments()
add_experiment('Data set 2',pd.DataFrame(data = {
    'Time': [0.5, 1, 2, 3, 4, 5, 6, 7, 8],
    '[TpFit]': [0.79, 1, 1, 0.81, 0.51, 0.34, 0.14, 0.34, 0.1],
    #'sd': [0.1,0.1,0.1,0.1,0.1,0.1,0.1,0.1,0.1]
}))

sol = run_parameter_estimation(method=PE.HOOKE_JEEVES, update_model=True)
sol[['sol']]
```

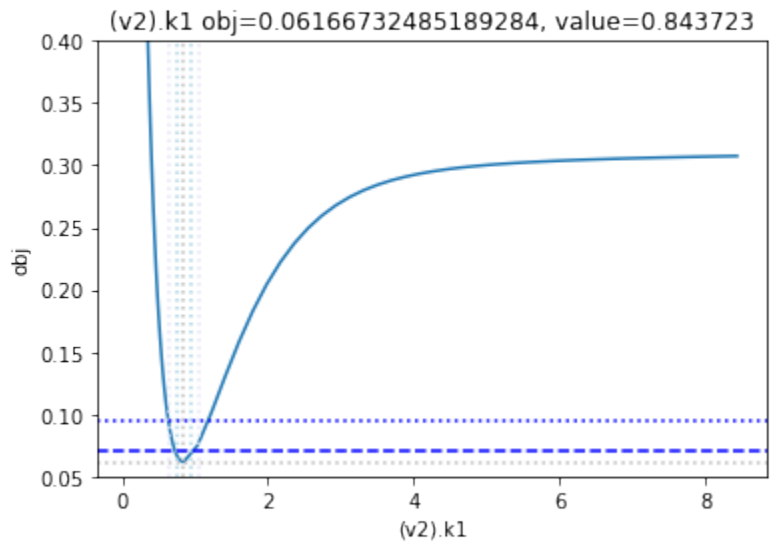
[20]:
```
              sol
name
(v1).k   1.554192
(v2).k1  0.843723
```

[21]:
```
plot_per_experiment(solution=sol);
```



[22]:
```
get_profiles_for_model(lower_adjustment=0.1, upper_adjustment=10, scale_mode={'top': 0.4,
↪ 'bottom': 0.05});
```

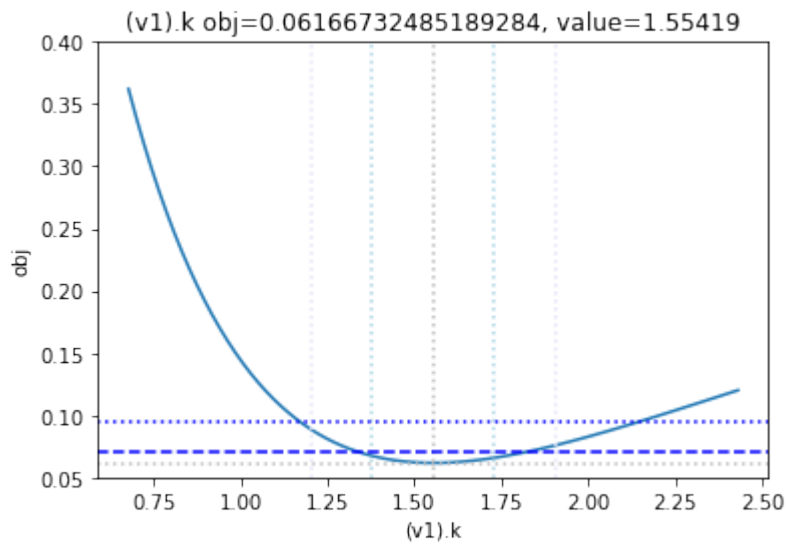


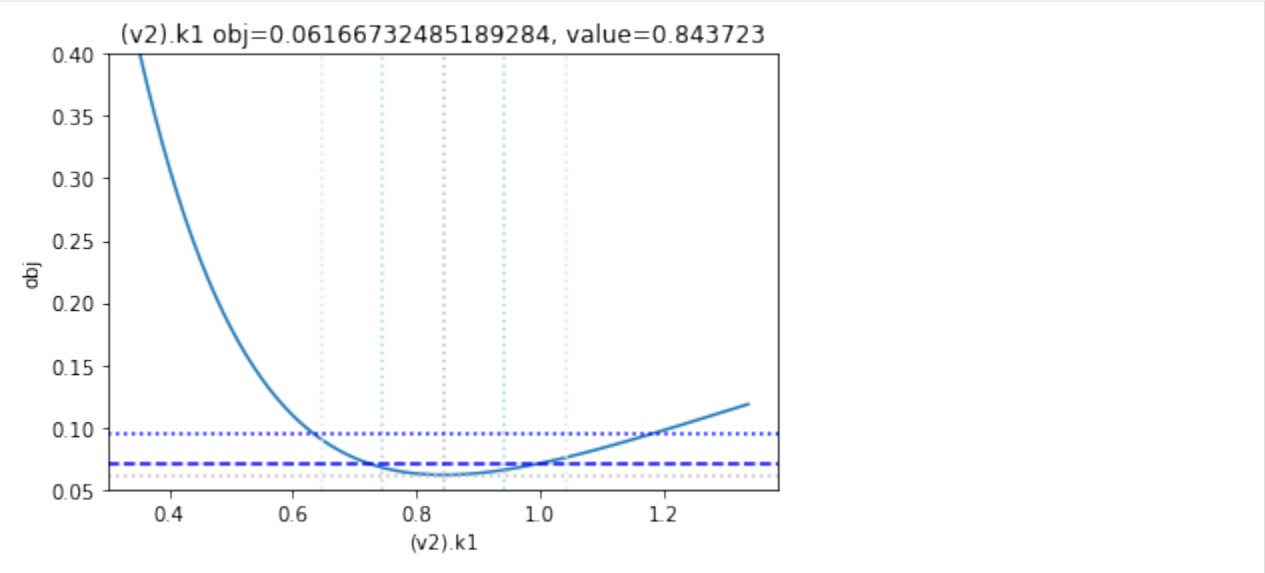


looking at the profile we find what we want to see.

A new option added, is to generate the profiles for a certain number of standard deviations as calculated by the COPASI fit. Lets try this here, by going to the ranges of -5 / +5 standard deviations from the value found:

[23]:
```
get_profiles_for_model(lower_adjustment="-5SD", upper_adjustment="+5SD", scale_mode={'top
↪': 0.4, 'bottom': 0.05});
```




(v2).k1 obj=0.06166732485189284, value=0.843723
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
obj
0.4
0.6
0.8
1.0
1.2
(v2).k1

CHAPTER

TWENTYSIX

METABOLIC CONTROL ANALYSIS

This notebook demonstrates how to use Metabolic Control Analysis using basico. We start as always, by importing basico:

[1]:
```
from basico import *
```

next we load the Brusselator example model

[2]:
```
brusselator = load_example('brusselator')
```

running the MCA can be done explicitly by calling `run_mca`, or implicitly by passing allong `run_first=True` to the functions that retrieve the elasticities or control coefficients. The task needs to be run only once so that all matrices are available. These functions additionally include a `scaled` flag, that indicates, whether the scaled or unscaled values should be returned. By default `run_first=False` and `scaled=True`.

So here we pass `run_first=True` for the first call, and then just retrieve the remaining functions. First the elasticities.

Running the MCA can be done explicitly by calling `run_mca`, or implicitly by passing along `run_first=True` to the functions that retrieve the elasticities or control coefficients. The task needs to be run only once so that all matrices are available. These functions additionally include a `scaled` flag, that indicates whether the scaled or unscaled values should be returned. By default, `run_first=False` and `scaled=True`.

So here we pass `run_first=True` for the first call, and then just retrieve the remaining functions.

Elasticities define how much impact do changes of the metabolite concentration *Si* have on the reaction rate *vk*.

[3]:
```
get_elasticities(run_first=True)
```

[3]:

	X	Y
(R1)	0.0	0.0
(R2)	2.0	1.0
(R3)	1.0	0.0
(R4)	1.0	0.0

Concentration control coefficients tell us about how much impact changes of a single reaction rate have on the steady state concentrations of the metabolites. The sum of entries in each row should be `0`, the `Summation Error` column shows the deviation from that, that can be the result of numeric operations.

Concentration coefficients are only available if a steady state was found when running the task.

[4]:
```
get_concentration_control_coefficients(scaled=True)
```

[4]:

	(R1)	(R2)	(R3)	(R4)	'Summation Error'
X	1.0	0.0	0.0	-1.0	0.0
Y	-1.0	-1.0	1.0	1.0	0.0

Finally, the flux control coefficients tell us about how much changes of a single reaction rate impact the steady state flux of (another) reaction. The sum of each row should be 1, deviations will again be shown in the `Summation Error` column when the scaled results are retrieved.

Flux control coefficients are only available if a steady state was found when running the task.

[5]:
```
get_flux_control_coefficients()
```

[5]:
```
      (R1)          (R2)  (R3)  (R4)  'Summation Error'
(R1)   1.0  0.000000e+00   0.0   0.0       0.000000e+00
(R2)   1.0 -2.220446e-16   1.0  -1.0       0.000000e+00
(R3)   1.0  0.000000e+00   1.0  -1.0       2.220446e-16
(R4)   1.0  0.000000e+00   0.0   0.0       0.000000e+00
```

CHAPTER

TWENTYSEVEN

WORKING WITH WIDGETS

Here we create an interactive example, using ipywidgets and matplotlib for plotting, lets first import those. If the script does not run for you try:

```
!pip install -q --upgrade ipympl ipywidgets matplotlib
!jupyter labextension install jupyter-matplotlib
```

and reload the kernel.

[1]:
```
%matplotlib widget
import ipywidgets as widgets
import matplotlib.pyplot as plt
import numpy as np

from basico import *
```

We start by creating the lorenz model, right from the ODEs:

[2]:
```
new_model(name='Lorenz Model')

add_species('X', initial_concentration=0)
add_species('Y', initial_concentration=1)
add_species('Z', initial_concentration=1.05)

add_parameter('beta', initial_value=8./3.)
add_parameter('rho', initial_value=28.)
add_parameter('sigma', initial_value=10.0)

add_equation('d[X]/dt=sigma*([Y]-[X])')
add_equation('d[Y]/dt=rho*[X]-[Y]-[X]*[Z]')
add_equation('d[Z]/dt=[X]*[Y]-beta*[Z]')
```

Now we use the ipywidgets interact decroator, to allow to modify the values for sigma, rho and beta.

[3]:
```
fig = plt.figure()
ax = fig.add_subplot(projection='3d')
ax.set_xlabel("X Axis")
ax.set_ylabel("Y Axis")
ax.set_zlabel("Z Axis")
ax.set_title("Lorenz Attractor")

@widgets.interact(sigma=(1, 50, 0.01), rho=(0.1, 50, .01), beta=(-0.1, 10, 0.01),␣
```

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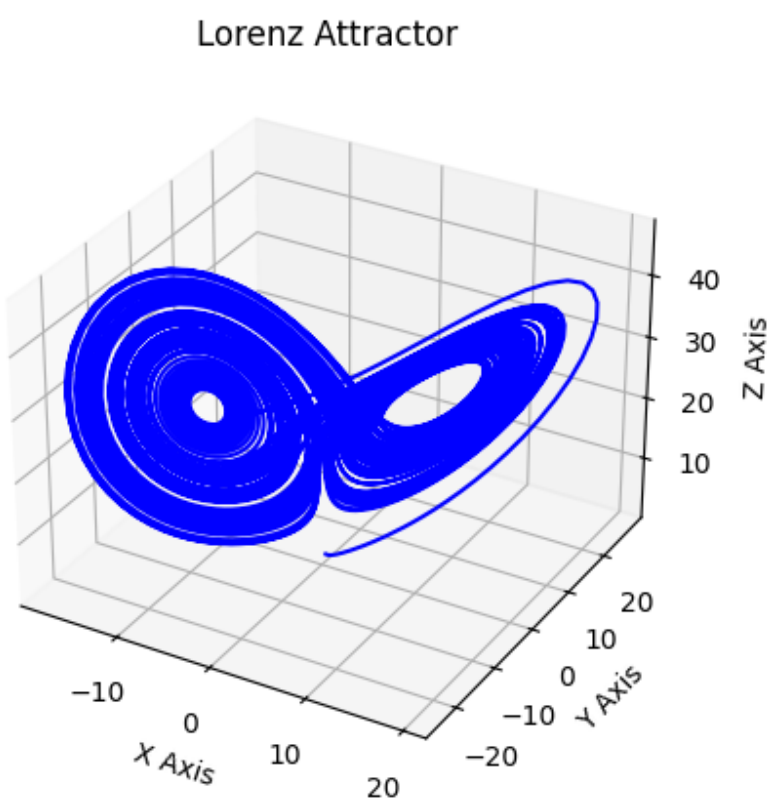
```
↪duration=(10, 1000), start_time=(0, 10))
def update(sigma = 10, rho=28, beta=8.0/3.0, duration=100, start_time=0.01):
    # remove existing lines
    [l.remove() for l in ax.lines]

    # set new parameter values
    set_parameters('sigma', initial_value=sigma)
    set_parameters('rho', initial_value=rho)
    set_parameters('beta', initial_value=beta)

    # run time course
    df = run_time_course_with_output(['[X]', '[Y]', '[Z]'], duration=duration,␣
↪intervals=10000, start_time=start_time)

    # create 3d plot for x,y and z (remember to set color otherwise it'll be overwritten)
    ax.plot(df['[X]'].values, df['[Y]'].values, df['[Z]'].values, color='blue');
```

```
interactive(children=(FloatSlider(value=10.0, description='sigma', max=50.0, min=1.0,␣
↪step=0.01), FloatSlider(...
```



I've noticed, that the result is not visible when rendering the result as html, so here a gif showing the result:

CHAPTER

TWENTYEIGHT

BASICO

28.1 basico package

BasiCO is a simplified interface to COPASI.

This module provides convenience functions to quickly get a model loaded and simulated:

Example

```
>>> from basico import *
>>> load_biomodel(10)
>>> run_time_course().plot()
```

28.1.1 Submodules

28.1.2 basico.biomodels module

A submodule for accessing the BioModels API.

This submodule accesses the BioModels REST api as described on:

<https://www.ebi.ac.uk/biomodels/docs/>

Examples

```
>>> # get info for a specific model
>>> info = get_model_info(12)
>>> print(info['name'], info['files']['main'][0]['name'])
```

```
>>> # get all files for one model
>>> files = get_files_for_model(12)
>>> print(files['main'][0]['name'])
```

```
>>> # get content of specific model
>>> sbml = get_content_for_model(12)
>>> print(sbml)
```

```
>>> # search for model
>>> models = search_for_model('repressilator')
>>> for model in models:
>>>     print(model['id'], model['name'], model['format'])
```

basico.biomodels.**download_from**(*url*)

Convenience method reading content from a URL.

This convenience method uses urlopen on either python 2.7 or 3.x

Parameters
url (*str*) – the url to read from

Returns
the contents of the URL as str

Return type
str

basico.biomodels.**download_json**(*url*)

Convenience method reading the content of the url as JSON.

Parameters
url (*str*) – the url to read from

Returns
a python object representing the json content loaded

Return type
dict

basico.biomodels.**get_content_for_model**(*model_id*, *file_name=None*)

Downloads the specified file from biomodels

Parameters

- **model_id** – the model id as int, or string
- **file_name** – the filename to download (or None, to download the main file)

Returns
the content of the specified file

basico.biomodels.**get_files_for_model**(*model_id*)

Retrieves the json structure for all files for the given biomodel.

The structure is of form:

```
>>> get_files_for_model(10)
{
    'additional': [
        {'description': 'Auto-generated Scilab file',
         'fileSize': '3873',
         'name': 'BIOMD0000000010.sci'},
         ...
    ],
    'main': [
        {'fileSize': '31568',
         'name': 'BIOMD0000000010_url.xml'
```

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```
        }
    ]
}
```

Parameters
model_id – the model id (as int or string)

Returns
json structure

basico.biomodels.**get_model_info**(*model_id*)

Return the model info for the provided *model_id*.

Parameters
model_id – either an integer, or a valid model id

Returns
a python object describing the model

basico.biomodels.**search_for_model**(*query*, *offset=0*, *num_results=10*, *sort='id-asc'*)

Queries the biomodel database

Queries the database, for information about the query system see: <https://www.ebi.ac.uk/biomodels-static/jummp-biomodels-help/model_search.html>

Example

```
>>> search_for_model('glycolysis')
[...,
    {
    'format': 'SBML',
    'id': 'BIOMD0000000206',
    'lastModified': '2012-07-04T23:00:00Z',
    'name': 'Wolf2000_Glycolytic_Oscillations',
    'submissionDate': '2008-11-27T00:00:00Z',
    'submitter': 'Harish Dharuri',
    'url': 'https://www.ebi.ac.uk/biomodels/BIOMD0000000206'
    }
]
```

Note by default, it will include only manually curated models, to obtain Non-curated models you would use:

```
>>> search_for_model('Hodgkin AND curationstatus:"Non-curated"')
[...,
    {
    'format': 'SBML',
    'id': 'MODEL1006230012',
    'lastModified': '2012-02-02T00:00:00Z'',
    'name': 'Stewart2009_ActionPotential_PurkinjeFibreCells',
    'submissionDate': '2010-06-22T23:00:00Z',
    'submitter': 'Camille Laibe',
    'url': 'https://www.ebi.ac.uk/biomodels/MODEL1006230012'
```

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```
    }
]
```

Parameters

- **query** – the query to use (it will be encoded with quote_plus before send out, so it is safe to use spaces)
- **offset** – offset (defaults to 0)
- **num_results** – number of results to obtain (defaults to 10)
- **sort** – sort criteria to be used (defaults to id-asc)

Returns

the search result as [{}]

28.1.3 basico.compartment_array_tools module

This module provides convenience functions for array of compartments.

COPASI can duplicate the current model in either a rectangular or linear manner, with diffusion reactions added in between the created model. This allows for a simplified spatial simulation.

This submodule adds functions, to create such an array, to delete the template model. Additionally some basic plotting functionality is available as well.

Example

```
>>> dm = load_example('brusselator')
>>> create_rectangular_array(10, 10, ['X', 'Y'], [0.16, 0.8], delete_template=True)
>>> set_species(['X{compartment[1,1]}',
...             'X{compartment[1,2]}',
...             'X{compartment[2,1]}',
...             'X{compartment[2,2]}'], initial_concentration=10)
```

```
>>> add_event('E0', 'Time > 10', [['X{compartment[1,1]}', '10'],
...                               ['X{compartment[1,2]}', '10'],
...                               ['X{compartment[2,1]}', '10'],
...                               ['X{compartment[2,2]}', '10']])
```

```
>>> data = run_time_course(start_time=0, duration=500)
>>> animate_rectangular_time_course_as_image(data, metabs=["X", "Y"], min_range=0, max_
↪range=10)
```

basico.compartment_array_tools.**animate_rectangular_time_course**(*data*, *metab=None*, *prefix=None*, *shading='gouraud'*, *min_range=nan*, *max_range=nan*, *filename=None*, ***kwargs*)

Plots the simulation data on the loaded model assuming that this is in the format of an array of compartments as generated by COPASI. This will create a figure for each species at each of the specified time points.

Parameters

- **data** – timecourse simulation result
- **metab** – optional parameter specifying the species to animate. If not given, one the first metab will be chosen
- **prefix** – string of compartment prefix to indicate which compartment should be visualized. This is expected to not include the indices, so it would be 'compartment' rather than 'compartment[0]'
- **shading** – optional shading for the color mesh, defaults to 'gouraud' can also be 'flat'
- **min_range** – optional min range, defaults to NaN, meaning that it is to be the minimum value of the data
- **max_range** – optional max range, defaults to NaN, meaning that it is to be the maximum value of the data
- **filename** – optional filename to a file to which to save the animation to
- **kwargs** –
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

the FuncAnimation constructed

`basico.compartment_array_tools.`**`animate_rectangular_time_course_as_image`**(*data*, *metabs=None*, *prefix=None*, *min_range=nan*, *max_range=nan*, *filename=None*, ***kwargs*)

Plots the data as image.

Parameters

- **data** – data frame with results to plot
- **metabs**
- **prefix** – string of compartment prefix to indicate which compartment should be visualized. This is expected to not include the indices, so it would be 'compartment' rather than 'compartment[0]'
- **min_range** – optional min range, defaults to NaN, meaning that it is to be the minimum value of the data
- **max_range** – optional max range, defaults to NaN, meaning that it is to be the maximum value of the data
- **filename** – optional filename to safe the image as
- **kwargs** –
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

FuncAnimation result

basico.compartment_array_tools.**create_linear_array**(*num_steps*, *species=None*, *diffusion_coefficients=None*, *compartment_names=None*, *delete_template=False*, ***kwargs*)

Utility function to create a linear duplicating the specified species, their reactions in the given compartments and created diffusion reactions between the newly created array

Parameters

- **num_steps** – the number of steps to create
- **species** – array of species names, that should be diffusing between compartments
- **compartment_names** – optional compartment names (will default to the compartment the species is in)
- **diffusion_coefficients** – optional array of diffusion coefficients in the same order as the species (otherwise they will be set to 1)
- **delete_template** – if True, the original template model in the specified compartment will be deleted.
- **kwargs** –
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

basico.compartment_array_tools.**create_rectangular_array**(*num_steps_x*, *num_steps_y*, *species=None*, *diffusion_coefficients=None*, *compartment_names=None*, *delete_template=False*, ***kwargs*)

Utility function to create a rectangular array duplicating the specified species, their reactions in the given compartments and created diffusion reactions between the newly created array

Parameters

- **num_steps_x** – the number of compartments to create along the x direction
- **num_steps_y** – the number of compartments to create along the y direction
- **species** – array of species names, that should be diffusing between compartments
- **compartment_names** – optional compartment names (will default to the compartment the species is in)
- **diffusion_coefficients** – optional array of diffusion coefficients in the same order as the species (otherwise they will be set to 1)
- **delete_template** – if True, the original template model in the specified compartment will be deleted.
- **kwargs** –
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

basico.compartment_array_tools.**delete_compartments**(*selection*, ***kwargs*)

utility function for deleting a selection of compartments from the datamodel. This will also delete the species and reactions included.

Parameters

- **selection** – an array of tuples of indices at which the compartments should be deleted
- **kwargs** –
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

basico.compartment_array_tools.**plot_linear_time_course**(*data*, *prefix=None*, *metab_names=None*, *shading='gouraud'*, *min_range=nan*, *max_range=nan*, ***kwargs*)

Plots the simulation data on the loaded model assuming that this is in the format of an array of compartments as generated by COPASI. This will create a figure for each species

Parameters

- **data** – timecourse simulation result
- **prefix** – string of compartment prefix to indicate which compartment should be visualized. This is expected to not include the indices, so it would be 'compartment' rather than 'compartment[0]'
- **metab_names** – optional array of metabolite names that should be plotted (defaults to all)
- **shading** – optional shading for the color mesh, defaults to 'gouraud' can also be 'flat'
- **min_range** – optional min range, defaults to NaN, meaning that it is to be the minimum value of the data
- **max_range** – optional max range, defaults to NaN, meaning that it is to be the maximum value of the data
- **kwargs** –
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
array with tuple of figures and their axis

basico.compartment_array_tools.**plot_rectangular_time_course**(*data*, *times=None*, *prefix=None*, *shading='gouraud'*, *min_range=nan*, *max_range=nan*, ***kwargs*)

Plots the simulation data on the loaded model assuming that this is in the format of an array of compartments as generated by COPASI. This will create a figure for each species at each of the specified time points.

Parameters

- **data** – timecourse simulation result
- **times** – optional parameter specifying the times for which to plot the results. If not given, one figure will be created for each output time point in the data

- **prefix** – string of compartment prefix to indicate which compartment should be visualized. This is expected to not include the indices, so it would be 'compartment' rather than 'compartment[0]'
- **shading** – optional shading for the color mesh, defaults to 'gouraud' can also be 'flat'
- **min_range** – optional min range, defaults to NaN, meaning that it is to be the minimum value of the data
- **max_range** – optional max range, defaults to NaN, meaning that it is to be the maximum value of the data
- **kwargs** –
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
array with tuple of figures and their axis

28.1.4 basico.jws_online module

Convenience module to access JWS models

This module provides convenience functions for accessing models from JWS Online <https://jjj.mib.ac.uk> using the netherlands endpoint.

Example

```
>>> # get all models with ATP
>>> atp_models = get_models_for_species('atp')
```

```
>>> # get all models with PFK
>>> pfk_models = get_models_for_reaction('pfk')
```

```
>>> # get all_models (this will take a while)
>>> all = get_all_models()
```

```
>>> # get manuscript information
>>> manuscript = get_manuscript('teusink')
>>> print(manuscript['title'], manuscript['abstract'], manuscript['url'])
```

```
>>> # get info for a specific model
>>> info = get_model_info('teusink')
>>> print(info['name'], info['status'])
```

```
>>> # get content of specific model
>>> sbml = get_sbml_model('teusink')
>>> print(sbml)
```

basico.jws_online.**download_from**(*url*)

Convenience method reading content from a URL.

This convenience method uses urlopen on either python 2.7 or 3.x

Parameters
url (*str*) – the url to read from

Returns
the contents of the URL as str

Return type
str

basico.jws_online.**download_json**(*url*)

Convenience method reading the content of the url as JSON.

Parameters
url (*str*) – the url to read from

Returns
a python object representing the json content loaded

Return type
dict

basico.jws_online.**get_all_models**()

Returns the list of all models

```
>>> get_all_models()
[...,
    {
    'slug': 'zi1',
    'name': 'zi1',
    'cbm': False,
    'status': 'CURATED',
    'details': 'https://jjj.bio.vu.nl/rest/models/zi1/',
    'manuscript': 'https://jjj.bio.vu.nl/rest/models/zi1/manuscript/',
    'experiments': 'https://jjj.bio.vu.nl/rest/models/zi1/experiments/'
    }
]
```

Returns
list of model ids

basico.jws_online.**get_manuscript**(*model_id*)

Returns information about the model manuscript

```
>>> get_manuscript('wolf')
```

Parameters
model_id – valid model slug

Returns
manuscript structure (list of dictionary)

basico.jws_online.**get_mathematica_model**(*model_id*)

Return the mathematica model for the slug

Parameters
model_id – valid model slug

Returns
the model as mathematica notebook

basico.jws_online.**get_model_info**(*model_id*)

Returns information about the JWS model

```
>>> get_model_info('wolf')
{
    'slug': 'wolf',
    'id': 'wolf',
    'name': 'wolf',
    'cbm': False,
    'status': 'CURATED',
    'species_set': ['at (ATP)', ... ],
    'reaction_set': ['v_1 (glucose transporter)', ...],
    'event_set': [],
    'parameter_set': ['atot',...]
}
```

Parameters
model_id – a valid jws slug

Returns
structure with information about the model [{}]

basico.jws_online.**get_models_for_reaction**(*reaction*)

Searches for models containing a specific reaction

```
>>> get_models_for_reaction('pfk')
```

Parameters
reaction – name of the reaction to search for

Returns
(list of dictionary) of all models containing the reaction

basico.jws_online.**get_models_for_species**(*species*)

Searches for models containing a specific chemical species

```
>>> get_models_for_species('atp')
```

Parameters
species – the species name to search for

Returns
(list of dictionary) of all models containing this species

basico.jws_online.**get_sbml_model**(*model_id*)

Returns the SBML for the model.

Parameters
model_id – valid model slug

Returns
the model as sbml string

28.1.5 basico.model_info module

The model_info module contains basic functionality for interrogating the model.

Here all functionality for interrogating and manipulating the model is hosted. For each of the elements:

- compartments
- species
- parameters
- events
- reactions

you will find functions to add, get, set, and remove them.

class basico.model_info.**T**

Bases: object

Constants for Task names

Convert between task names to enums

```
>>> T.from_enum(0)
Steady-State
```

```
>>> T.to_enum('Steady-State')
0
```

CROSS_SECTION = 'Cross Section'

EFM = 'Elementary Flux Modes'

LNA = 'Linear Noise Approximation'

LYAPUNOV_EXPONENTS = 'Lyapunov Exponents'

MCA = 'Metabolic Control Analysis'

MOIETIES = 'Moieties'

OPTIMIZATION = 'Optimization'

PARAMETER_ESTIMATION = 'Parameter Estimation'

SCAN = 'Scan'

SENSITIVITIES = 'Sensitivities'

STEADY_STATE = 'Steady-State'

TIME_COURSE = 'Time-Course'

TIME_COURSE_SENSITIVITIES = 'Time-Course Sensitivities'

TIME_SCALE_SEPARATION = 'Time Scale Separation Analysis'

classmethod all_task_names()

classmethod from_enum(*int_value*)

classmethod to_enum(*value*)

basico.model_info.**add_amount_expressions**(***kwargs*)

Utility function that adds model values for all metabolites to the model to compute the amount

The global parameters created will be named amount(metab_name), and so can be accessed at any time. Should the amount already exist, it will not be modified.

Parameters

kwargs – optional parameters

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

None

basico.model_info.**add_compartment**(*name*, *initial_size=1.0*, ***kwargs*)

Adds a new compartment to the model.

Parameters

- **name** (*str*) – the name for the new compartment
- **initial_size** (*float*) – the initial size for the compartment
- **kwargs** – optional parameters, recognized are:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
  - all other parameters from `set_compartment()`.

Returns

the compartment added

basico.model_info.**add_default_plot**(*name*, ***kwargs*)

Adds a default plot to the list of plots

Parameters

- **name** (*str*) – name of the default plot
- **kwargs** – optional arguments
  - *new_name*: to rename the plot specification
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

none or the name of the plot created

Return type

str or None

basico.model_info.**add_equation**(*eqn*, *time_symbol='t'*, ***kwargs*)

This function allows to add arbitrary equations to the current model.

This function allows adding arbitrary ODE's / assignments to the model. Nonexisting model entities will be created.

Parameters

- **eqn** (*str*) – the equation for example of form: d[X]/dt = k1 * exp({Time})

- **time_symbol** (*str*) – optional symbol that will be used for time (defaults to t)
- **kwargs**

Returns

basico.model_info.**add_event**(*name*, *trigger*, *assignments*, ***kwargs*)

Adds a new event to the model.

Parameters

- **name** (*str*) – the name for the new event
- **trigger** (*str*) – the trigger expression to be used. The expression can consist of all display names. for example *Time > 10* would make the event trigger at time 10.
- **assignments** (*[(str,str)]*) – All the assignments that should be made, when the event fires. This should be a list of tuples where the first element is the name of the element to change, and the second element the assignment expression.
- **kwargs** – optional parameters, recognized are:
  - *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)
  - 'new_name': the new name for the event
  - 'delay': the delay expression
  - 'priority': the priority expression
  - 'persistent': boolean indicating if the event is persistent
  - **'delay_calculation': boolean indicating whether just the assignment is delayed, or the** calculation as well
  - 'fire_at_initial_time': boolean indicating if the event should fire at the initial time

Returns

the newly created event

basico.model_info.**add_event_assignment**(*name*, *assignment*, *exact=False*, ***kwargs*)

Adds an event assignment to the named event

Parameters

- **name** (*str*) – the name (or substring of name) of an event
- **assignment** (*[(str,str)] or (str, str)*) – tuple or list of tuples of event assignments of form (target, expression)
- **exact** (*bool*) – boolean indicating whether the named expression has to be exact

Returns

None

basico.model_info.**add_function**(*name*, *infix*, *type='general'*, *mapping=None*, ***kwargs*)

Adds a new function definition if none with that name already exists

Parameters

- **name** (*str*) – the name for the new function
- **infix** (*str*) – the formula for the new function (e.g: $V * S / (K + S)$)

- **type** (*str*) – optional flag specifying whether the function is 'reversible', 'irreversible' or 'general'
- **mapping** (*dict*) – optional dictionary mapping the elements of the infix to their usage. If not specified, the usage will default to *parameter*, other values possible would be *substrate*, *product*, *modifier*, *volume or `time*. One example for the infix for the infix above we would specify that *S* is *substrate*:

  { 'S': 'substrate' }
- **kwargs** – optional parameters, recognized are:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

basico.model_info.**add_parameter**(*name*, *initial_value=1.0*, ***kwargs*)

Adds a new global parameter to the model.

Parameters

- **name** (*str*) – the name for the new global parameter
- **initial_value** (*float*) – optional the initial value of the parameter (defaults to 1)
- **kwargs** – optional parameters, recognized are:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
  - all other parameters from `set_parameters()`.

Returns

the newly created parameter

basico.model_info.**add_parameter_set**(*name*, *param_set_dict=None*, ***kwargs*)

Adds a new parameter set to the model with the values from the dictionary

Parameters

- **name** (*str*) – name of the parameter set to add
- **param_set_dict** (*dict or None*) – dictionary with the parameter set values if empty, the current state of the model will be used
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

basico.model_info.**add_plot**(*name*, ***kwargs*)

Adds a new plot specification to the model.

Parameters

- **name** (*str*) – the name for the new plot specification
- **kwargs** – optional parameters, recognized are:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
  - all other parameters from `set_plot_dict()`.

Returns
the plot

`basico.model_info.add_reaction(name, scheme, **kwargs)`

Adds a new reaction to the model

Parameters

- **name** (*str*) – the name for the new reaction
- **scheme** (*str*) – the reaction scheme for the new reaction, if it includes Species that do not exist yet in the model they will be created. So for example a scheme of *A* -> *B* would create species *A* and *B* if they would not exist in the model, before creating the irreversible reaction.
- **kwargs** – optional parameters, recognized are:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
  - all other parameters from `set_reaction()`.

Returns
the newly created reaction

`basico.model_info.add_report(name, **kwargs)`

Adds a new report specification to the model.

Examples

The following would adds a report definition 'Time Course' to include Time and the concentration of S, in a report that is separated by tabs.

```
>>> add_report('Time Course', body=['Time', '[S]']
```

The following defines a report for the Steady State concentration of S. To disambiguate, that the string '[S]' in the header should be used literally, we call the function wrap_copasi_string.

```
>>> add_report('Steady State', task=T.STEADY_STATE, header=[wrap_copasi_string('[S]
↪')], footer=['[S]'])
```

Parameters

- **name** (*str*) – the name for the new plot specification
- **kwargs** – optional parameters, recognized are:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
  - all other parameters from `set_report_dict()`.

Returns
the report definition

`basico.model_info.add_species(name, compartment_name='', initial_concentration=1.0, **kwargs)`

Adds a new species to the model.

Parameters

- **name** (*str*) – the name for the new species
- **compartment_name** (*str*) – optional the name of the compartment in which the species should be created, it will default to the first compartment. If no compartment is present, a unit compartment named *compartment* will be created.
- **initial_concentration** (*float*) – optional the initial concentration of the species
- **kwargs** – optional parameters, recognized are:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
  - all other parameters from `set_species()`.

Returns
the newly created species

basico.model_info.**apply_parameter_set**(*name*, *exact=False*, ***kwargs*)

Applies the parameter set with the given name to the model

Parameters

- **name** – the name of the parameter set or a substring of the name
- **exact** – boolean indicating whether the name has to match exactly
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

basico.model_info.**as_dict**(*df*, *fold_list=True*)

Convenience function returning the data frame as dictionary

Parameters

- **df** (*pd.DataFrame*) – the data frame
- **fold_list** (*bool*) – optional boolean indicating whether to fold lists into a single dictionary, if there is only one entry (defaults to true)

Returns
the contents of the dataframe as [{}] if there are multiple ones, otherwise the dictionary if just one, or None

Return type
List[Dict] or Dict or None

basico.model_info.**assign_report**(*name*, *task*, *filename=''*, *append=True*, *confirm_overwrite=True*, ***kwargs*)

Assigns the named report to the specified task

Parameters

- **name** (*str*) – the name of the report definition to assign
- **task** (*Union[int, str, COPASI.CCopasiTask]*) – the task to assign the report to
- **filename** (*str*) – the filename to write the result to or ''', if it is the empty, it resets the target of the task, and COPASI will not create that report
- **append** (*bool*) – boolean indicating whether output should be appended (defaults to True)

- **confirm_overwrite** (*bool*) – boolean indicating whether the copasi should ask before overwriting a file
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

`basico.model_info.get_cn(name_or_reference, initial=False, **kwargs)`

Gets the cn of the named element or none

Parameters

- **name_or_reference** (*str or COPASI.CDataObject*) – display name of model element
- **initial** (*bool*) – if True, an initial reference cn will be returned, rather than a transient one
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
the cn if found or None

Return type
str or None

`basico.model_info.get_compartments(name=None, exact=False, **kwargs)`

Returns all information about the compartments as pandas dataframe.

Parameters

- **name** (*str*) – optional filter expression for the compartment, if it is not included in the name, the compartment will not be added to the data set.
- **exact** (*bool*) – boolean indicating, that the name has to be exact
- **kwargs** – optional arguments:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
a pandas dataframe with the information about the compartment

Return type
pandas.DataFrame

`basico.model_info.get_copasi_messages(num_messages_before, filters=None)`

Returns error messages that occurred while initializing or running the simulation

Parameters

- **num_messages_before** – number of messages before calling initialization or process
- **filters** (*list of str or str or None*) – optional list of filter expressions of what messages to ignore

Returns
error messages in form of a string

basico.model_info.**get_default_plot_names**(*filter=None*, ***kwargs*)

Returns a list of default plot names

Parameters

- **filter** – optional filter of substring to be in the name
- **kwargs**

Returns

basico.model_info.**get_events**(*name=None*, *exact=False*, ***kwargs*)

Returns all information about the events as pandas dataframe.

Parameters

- **name** (*str*) – optional filter expression for the event, if it is not included in the event name, the event will not be added to the data set.
- **exact** (*bool*) – boolean indicating whether the name has to be exact
- **kwargs** – optional arguments:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
a pandas dataframe with the information about the event

Return type
pandas.DataFrame

basico.model_info.**get_functions**(*name=None*, ***kwargs*)

Returns all available functions as pandas dataframe.

Parameters

- **name** (*str*) – optional filter expression for the functions, if it is not included in the name, the function will not be added to the data set.
- **kwargs** – optional arguments:
  - *reversible*: to further filter for functions that are only reversible
  - *suitable_for*: an optional reaction for which to filter the function list. Only functions suitable for the reaction will be returned
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
a pandas dataframe with the information about the functions

Return type
pandas.DataFrame

basico.model_info.**get_jacobian_matrix**(*apply_initial_values=False*, ***kwargs*)

Returns the jacobian matrix of the model at the current state

Parameters

- **apply_initial_values** (*bool*) – if set to the the initial values will be applied, otherwise the jacobian from the current state will be returned
- **kwargs** – optional parameters

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
the stoichiometry matrix of the current model

Return type
pd.DataFrame

`basico.model_info.get_miriam_annotation(**kwargs)`

Returns the elements miriam annotations as dictionary of the form:

{

'created': datetime, 'creators': [{

'first_name': '…', 'last_name': '…', 'email': '…', 'organization': '…'

},…],

'references': [{
'id': '…', 'uri': 'identifiers.org uri', 'resource': 'human readable name of resource', 'description', '…'

},…],

'descriptions': [{
'id': '…', 'qualifier': 'human readable qualifier string', 'uri': 'identifiers.org uri', 'resource': 'name of the resource referenced'

},…], 'modifications': [datetime,…]

}

Parameters
kwargs – optional parameters, recognized are:

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
- *name*: the display name of the element to set the notes on. otherwise the main model will be taken.
- *element*: any model element

Returns
the elements annotation as dictionary as described

Return type
{}

`basico.model_info.get_miriam_resources(compact=True)`

Retrieves the current MIRIAM resources from the configuration

Parameters
compact (*bool*) – whether to return a compact version of the resources (default: True)

Returns
dataframe with the list of current miriam resources

Return type
pandas.DataFrame

basico.model_info.**get_model_name**(***kwargs*)

Returns the name of the current model.

Parameters

kwargs – optional parameters

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

the name of the model

basico.model_info.**get_model_units**(***kwargs*)

Returns all model units as dictionary.

Parameters

kwargs – optional parameters

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

a dictionary containing the model units in the form: | { | 'time_unit': '', | 'quantity_unit': '', | 'length_unit': '', | 'area_unit': '', | 'volume_unit': '', | }

basico.model_info.**get_notes**(***kwargs*)

Returns all notes on the element or model.

Parameters

kwargs – optional parameters, recognized are:

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
- *name*: the display name of the element to set the notes on. otherwise the main model will be taken.
- *element*: any model element

Returns

the notes string (plain text, or xhtml)

Return type

str

basico.model_info.**get_parameter_sets**(*name=None*, *exact=False*, *values_only=False*, ***kwargs*)

Returns the list of parameter sets

Parameters

- **name** (*str*) – name of the parameter set to return (or a substring of the name)
- **exact** (*bool*) – boolean indicating whether the name has to be exact or not (default: False)
- **values_only** (*bool*) – boolean indicating whether to return only the values of the entries of the parameter set or a dictionary describing it (default: False)
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

basico.model_info.**get_parameters**(*name=None*, *exact=False*, ***kwargs*)

Returns all information about the global parameters as pandas dataframe.

Parameters

- **name** (*str*) – optional filter expression for the parameters, if it is not included in the name, the parameter will not be added to the data set.
- **exact** (*bool*) – boolean indicating that the name has to be exact
- **kwargs** – optional arguments:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

a pandas dataframe with the information about the parameter

Return type

pandas.DataFrame

basico.model_info.**get_plot_dict**(*plot_spec*, ***kwargs*)

Returns the information for the specified plot

Parameters

- **plot_spec** (*Union[str,int,COPASI.CPlotSpecification]*) – the name, index or plot specification object
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

dictionary of the form: | { | 'name': 'Phase Plot', | 'active': True, | 'log_x': False, | 'log_y': False, | 'tasks': '', | 'curves': | [| { | 'name': '[Y]|[X]', # the name of the curve | 'type': 'curve2d',# type of the curve (one of *curve2d*, *histoItem1d*, *bandedGraph* | or *spectogram*) | 'channels': ['[X]', '[Y]'], # display names of all the items to be plotted | 'color': 'auto', # color as hex rgb value (i.e '#ff0000' for red) or 'auto' | 'line_type': 'lines',# the line type (one of *lines*, *points*, *symbols* or | *lines_and_symbols*) | 'line_subtype': 'solid', # line subtype (one of *solid*, *dotted*, *dashed*, *dot_dash* or | *dot_dot_dash*) | 'line_width': 2.0, # line width | 'symbol': 'small_cross', # the symbol to be used (one of *small_cross*, *large_cross* | or *circle*) | 'activity': 'during' # when the data should be collected (one of 'before', 'during', 'after') | from task | } |] | }

basico.model_info.**get_plots**(*name=None*, ***kwargs*)

Returns all information about the plot definitions as pandas dataframe.

Parameters

- **name** (*str*) – optional filter expression for the plots, if it is not included in the plot name, the plot will not be added to the data set.
- **kwargs** – optional arguments:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

a pandas dataframe with the information about the plot see also `get_plot_dict()`

Return type

pandas.DataFrame

basico.model_info.**get_reaction_mapping**(*reaction*, ***kwargs*)

Returns the reaction mapping of the given reaction

Parameters

- **reaction** (*str or COPASI.CReaction*) – name of a reaction, or the reaction object
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
the dictionary with the reaction mapping

Return type
{}

basico.model_info.**get_reaction_parameters**(*name=None*, ***kwargs*)

Returns all local parameters as pandas dataframe.

This also includes global parameters that are mapped to local ones.

Parameters

- **name** (*str*) – optional filter expression, if it is not included in the name, the function will not be added to the data set.
- **kwargs** – optional arguments:
  - *reaction_name*: to further filter for local parameters of only certain reactions (that contain the substring)
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
a pandas dataframe with the information about local parameters

Return type
pandas.DataFrame

basico.model_info.**get_reactions**(*name=None*, *exact=False*, ***kwargs*)

Returns all reactions as pandas dataframe.

Parameters

- **name** (*str*) – optional filter expression, if it is not included in the name, the reaction will not be added to the data set.
- **exact** (*bool*) – boolean indicating, that the name has to be exact
- **kwargs** – optional arguments:
  - *reaction_name*: to further filter for local parameters of only certain reactions (that contain the substring)
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
a pandas dataframe with the information about local parameters

Return type
pandas.DataFrame

basico.model_info.**get_reduced_jacobian_matrix**(*apply_initial_values=False*, ***kwargs*)

Returns the jacobian matrix of the reduced model at the current state

Parameters

- **apply_initial_values** (*bool*) – if set to the the initial values will be applied, otherwise the jacobian from the current state will be returned
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
the stoichiometry matrix of the reduced current model

Return type
pd.DataFrame

basico.model_info.**get_reduced_stoichiometry_matrix**(***kwargs*)

Returns the reduced stoichiometry matrix of the model

Returns
the stoichiometry matrix of the current model

Return type
pd.DataFrame

basico.model_info.**get_report_dict**(*report*, ***kwargs*)

Returns all information about the plot as dictionary

Parameters

- **report** (*COPASI.CReportDefinition or int or str*) – report definition, index or name
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
a dictionary with all information about the plot

Return type
dict

basico.model_info.**get_reports**(*name=None*, *ignore_automatic=False*, *task=None*, ***kwargs*)

Returns the reports as dataframe

Parameters

- **name** – optional filter by name
- **ignore_automatic** – if true, only manually created reports are returned
- **task** – optional task name, to the get the report for
- **kwargs** – optional arguments:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
a data frame with all the report information

Return type
pd.DataFrame

`basico.model_info.get_scheduled_tasks(**kwargs)`

Returns the list of scheduled tasks

Parameters
kwargs – optional parameters

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
list of tasks that are scheduled

Return type
[str]

`basico.model_info.get_species(name=None, exact=False, **kwargs)`

Returns all information about the species as pandas dataframe.

Example:

Assume you have the brusselator example loaded *load_example('brusselator')*

```
>>> get_species()
```

returns you a dataframe of all species with the species name as index.

```
>>> get_species('X')
```

returns you only those species, that include *X* in the name.

Parameters

- **name** (*str*) – optional filter expression for the species, if it is not included in the species name, the species will not be added to the data set.
- **exact** (*bool*) – if true, the name has to match precisely the name of the species
- **kwargs** – optional arguments to further filter down the species. recognized are:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
  - *compartment*: to filter down only species in specific compartments
  - *type*: to filter for species of specific simulation type

Returns
a pandas dataframe with the information about the species

Return type
pandas.DataFrame

`basico.model_info.get_stoichiometry_matrix(**kwargs)`

Returns the stoichiometry matrix of the model

Returns
the stoichiometry matrix of the current model

Return type
pd.DataFrame

basico.model_info.**get_task_settings**(*task*, *basic_only=True*, ***kwargs*)

Returns the settings of the given task

Parameters

- **task** (*COPASI.CCopasiTask or str*) – the task to read the settings of
- **basic_only** (*bool*) – boolean flag, indicating that only the basic parameters should be returned
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)

Returns
dict of task settings

Return type
{}

basico.model_info.**get_time_unit**(***kwargs*)

Returns the time unit of the model

basico.model_info.**get_value**(*name_or_reference*, *initial=False*, ***kwargs*)

Gets the value of the named element or nones

Parameters

- **name_or_reference** (*str or COPASI.CDataObject*) – display name of model element
- **initial** (*bool or None*) – if True, an initial value will be returned, rather than a transient one. If set to *None*, the default reference will be returned and not coerced.
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)

Returns
the value if found or None

Return type
float or None

basico.model_info.**have_miriam_resources**()

Utility function returning whether MIRIAM resources are avaialble

Returns
boolean indicating whether there are MIRIAM resources available or not

Return type
bool

basico.model_info.**remove_amount_expressions**(***kwargs*)

Utility function that removes model values created using *add_amount_expressions*.

The global parameters created will be named amount(metab_name), and so can be accessed at any time.

Parameters
kwargs – optional parameters

- *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)

Returns
None

`basico.model_info.remove_compartment(name, **kwargs)`

Deletes the named compartment (and everything included)

Parameters

- **name** (*str*) – the name of a compartment in the model
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

`basico.model_info.remove_event(name, **kwargs)`

Deletes the named event

Parameters

- **name** (*str*) – the name of an event in the model
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

`basico.model_info.remove_function(name, **kwargs)`

Removes the function with the given name

Parameters

- **name** (*str*) – the name of the function to be removed
- **kwargs** – optional parameters, recognized are:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

`basico.model_info.remove_parameter(name, **kwargs)`

Deletes the named global parameter

This will also delete any model element that uses this parameter, so if it appears in any model expression, the elements using these expressions will also be deleted. To prevent that, use the recursive parameter.

Parameters

- **name** (*str | List[str]*) – the name of a parameter in the model
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

basico.model_info.**remove_parameter_sets**(*name=None*, *exact=False*, ***kwargs*)

remove the named parameter set(s)

Parameters

- **name** (*str*) – name of the parameter set to remove (or a substring of the name)
- **exact** (*bool*) – boolean indicating whether the name has to be exact
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

basico.model_info.**remove_plot**(*name*, ***kwargs*)

Deletes the named plot

Parameters

- **name** (*str*) – the name of an plot in the model
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

None

basico.model_info.**remove_reaction**(*name*, ***kwargs*)

Deletes the named reaction

Parameters

- **name** (*str*) – the name of a reaction in the model
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

None

basico.model_info.**remove_report**(*name*, ***kwargs*)

Deletes the named report

Parameters

- **name** (*str*) – the name of a report in the model
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

None

basico.model_info.**remove_report_from_task**(*task*, ***kwargs*)

Clears the report filename from the specified task

Parameters

- **task** (*Union[int, str, COPASI.CCopasiTask]*) – the task to assign the report to
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)

Returns
None

basico.model_info.**remove_species**(*name*, ***kwargs*)

Deletes the named species

Parameters

- **name** (*str*) – the name of a species in the model
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)

Returns
None

basico.model_info.**remove_user_defined_functions**()

Removes all user defined functions along with all elements that still use them

basico.model_info.**run_scheduled_tasks**(*include_plots=True*, *include_general_plots=False*, *plots=None*, *reports=None*, ***kwargs*)

Runs all scheduled tasks, optionally producing plots and reports

Parameters

- **include_plots** – boolean indicating whether to produce the plots associated with the task
- **include_general_plots** – boolean indicating whether to produce the general plots
- **plots** – optional list of plot dataframes computed by the task
- **reports** – optional list of report dataframes computed by the task

Returns
Figure produced if *include_plots* is true, otherwise None

basico.model_info.**run_task**(*task_name*, *include_plots=True*, *include_general_plots=False*, *plots=None*, *reports=None*, ***kwargs*)

Utility function that runs the named task and returns the result

Parameters

- **task_name** (*str*) – the name of the task e.g. 'Time-Course' to run the timecourse task. See the basico.T for all the task names.
- **include_plots** (*bool*) – boolean indicating whether to produce the plots associated with the task
- **include_general_plots** (*bool*) – boolean indicating whether to produce the general plots (those not specified to a particular task)
- **plots** (*list[pandas.DataFrame] or None*) – optional list of plot dataframes computed by the task
- **reports** (*list[pandas.DataFrame] or None*) – optional list of report dataframes computed by the task

Returns
Figures produced if *include_plots* is true, otherwise None

`basico.model_info.set_compartment(name=None, exact=False, **kwargs)`

Sets properties of the named compartment

Parameters

- **name** (*str*) – the name of the compartment (or a substring of the name)
- **exact** (*bool*) – boolean indicating whether the name has to be exact
- **kwargs** – optional arguments
  - *new_name*: the new name for the compartment
  - *initial_value* or *initial_size*: to set the initial size of the compartment
  - *value* or *size*: to set the transient size of the compartment
  - *initial_expression*: the initial expression for the compartment
  - *status* or *type*: the type of the compartment one of *fixed*, *assignment* or *ode*
  - *expression*: the expression for the compartment (only valid when type is *ode* or *assignment*)
  - *dimensionality*: sets the dimensionality of the compartment (int value 1..3)
  - *notes*: sets notes for the compartment (either plain text, or valid xhtml)
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

`basico.model_info.set_element_name(element, new_name, **kwargs)`

Sets the name of the element

Parameters

- **element** (*COPASI.CDataObject or str*) – the element whose name to change
- **new_name** (*str*) – the new name for the element
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

`basico.model_info.set_event(name, exact=False, trigger=None, assignments=None, **kwargs)`

Sets properties of the named event

Parameters

- **name** (*str*) – the name of the event (or a substring of the name)
- **exact** (*bool*) – boolean indicating, that the name has to be exact
- **trigger** (*str or None*) – the trigger expression to be used. The expression can consist of all display names. for example *Time > 10* would make the event trigger at time 10.
- **assignments** (*[(str,str)] or None*) – All the assignments that should be made, when the event fires. This should be a list of tuples where the first element is the name of the element to change, and the second element the assignment expression.

- **kwargs** – optional parameters, recognized are:
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
  - 'new_name': the new name for the event
  - 'delay': the delay expression
  - 'priority': the priority expression
  - 'persistent': boolean indicating if the event is persistent
  - 'delay_calculation': boolean indicating whether just the assignment is delayed, or the calculation as well
  - 'fire_at_initial_time': boolean indicating if the event should fire at the initial time

Returns

`basico.model_info.set_miriam_annotation(created=None, creators=None, references=None, descriptions=None, modifications=None, replace=True, **kwargs)`

Sets the MIRIAM annotations for the provided element or model

Parameters

- **created** (*datetime.datetime or None*) – the date/time to set as the objects creation time or None, if not to be set
- **creators** (*list or None*) –

  None, if not to be modified, otherwise list of creators of the form:

  {
  'first_name': '...',
  'last_name': '...',
  'email': '...',
  'organization': '...'
  }

- **references** (*list or None*) –

  None if not to be modified, otherwise list of references of the form:

  {
  'resource': 'human readable name of resource',
  'id': '...',
  'uri': 'identifiers.org uri',
  'description', '...'
  }

  only the uri needs to be provided, or alternatively id + resource.

- **descriptions** (*list or None*) –

  None if not to be modified, otherwise list of descriptions of the form:

  {
  'resource': 'human readable name of resource',

```
        'id': '...',
        'qualifier': '...',
        'uri': 'identifiers.org uri',
    }
```

only the uri needs to be provided, or alternatively id + resource.

- **modifications** (*list or None*) –

  None if not to be modified, otherwise list of datetime objects representing modification dates

- **replace** – Boolean indicating whether existing entries should be removed.

Returns
None

basico.model_info.**set_model_name**(*new_name*, ***kwargs*)

Renames the model to the provided new name

Parameters

- **new_name** (*str*) – the new name of the model
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)

Returns
None

basico.model_info.**set_model_unit**(***kwargs*)

Sets the model units.

Parameters
kwargs – optional parameters

- *time_unit*: time unit expression
- *substance_unit* or *quantity_unit*: substance unit expression
- *length_unit*: length unit expression
- *area_unit*: area unit expression
- *volume_unit*: volume unit expression
- *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)

basico.model_info.**set_notes**(*notes*, ***kwargs*)

Sets notes on the provided element

Parameters

- **notes** (*str*) – the notes to be set, can be either plain text, or valid xhtml
- **kwargs** – optional parameters, recognized are:
  - *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)
  - *name*: the display name of the element to set the notes on.

otherwise the main model will be taken.

- *element*: any model element

Returns
None

`basico.model_info.set_parameter_set(name, exact=False, param_set_dict=None, remove_others=False, **kwargs)`

sets the named parameter sets to the given dictionary values

Parameters

- **name** (*str*) – name of the parameter set to change (or a substring of the name)
- **exact** (*bool*) – boolean indicating whether the name has to be exact
- **param_set_dict** (*dict or None*) – dictionary with the parameter set values
- **remove_others** (*bool*) – boolean indicating whether to remove entries, that are not specified in the dictionary (default: False)
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

`basico.model_info.set_parameters(name=None, exact=False, **kwargs)`

Sets properties of the named parameter(s).

Parameters

- **name** (*str*) – the name of the parameter (or a substring of the name)
- **exact** (*bool*) – boolean indicating whether the name has to be exact or not
- **kwargs** – optional arguments
  - *new_name*: the new name for the parameter
  - *unit*: the unit expression to be set
  - *initial_value*: to set the initial value for the parameter
  - *value*: set the transient value for the parameter
  - *initial_expression*: the initial expression
  - *status* or *type*: the type of the parameter one of *fixed*, *assignment* or *ode*
  - *expression*: the expression for the parameter (only valid when type is *ode* or *assignment*)
  - *notes*: sets notes for the parameter (either plain text, or valid xhtml)
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

`basico.model_info.set_plot_curves(plot_spec, curves, **kwargs)`

Sets all curves of the named plot specification (all curves will be replaced)

Parameters

- **plot_spec** (*Union[str,int,COPASI.CPlotSpecification]*) – the name, index or plot specification object
- **curves** (*[{}]*) –

  list of dictionaries of curve items to be added. For example

  [
  {
  'name': '[Y]|[X]', # the name of the curve
  'type': 'curve2d', # type of the curve (one of *curve2d*, *histoItem1d*, *bandedGraph*
  or *spectogram*)
  'channels': ['[X]', '[Y]'], # display names of all the items to be plotted
  'color': 'auto', # color as hex rgb value (i.e '#ff0000' for red) or 'auto'
  'line_type': 'lines', # the line type (one of *lines*, *points*, *symbols* or
  lines_and_symbols)
  'line_subtype': 'solid', # line subtype (one of *solid*, *dotted*, *dashed*, *dot_dash* or
  dot_dot_dash)
  'line_width': 2.0, # line width
  'symbol': 'small_cross', # the symbol to be used (one of *small_cross*, *large_cross* or *circle*)
  'activity': 'during' # when the data should be collected (one of 'before', 'during', 'after')
  }
  ]

  Additionally, histograms may have the bin size in a *increment* element. Spectograms can have
  log_z, *color_map* (one of 'Default', 'Yellow-Red', 'Grayscale' or 'Blue-White-Red'),
  'bilinear' (should the plot interpolate between values), 'contours' (at which values to draw contours)
  'max_z' (max z value).
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

`basico.model_info.`**`set_plot_dict`**(*plot_spec*, *active=True*, *log_x=False*, *log_y=False*, *tasks=''*, ***kwargs*)

Sets properties of the named plot specification.

Parameters

- **plot_spec** (*Union[str,int,COPASI.CPlotSpecification]*) – the name, index or plot specification object
- **active** (*bool*) – boolean indicating whether plot should be active (defaults to true)
- **log_x** (*bool*) – boolean indicating that the x axis should be logarithmic
- **log_y** (*bool*) – boolean indicating that the y axis should be logarithmic

- **tasks** (*str*) –

  task type (or colon separated list of task types) for which the plot should be brought up

- **kwargs** – optional arguments
  - *new_name*: to rename the plot specification
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
  - *curves*: dictionary in the format as described in `set_plot_curves()`.

Returns
None

basico.model_info.**set_reaction**(*name=None*, *exact=False*, ***kwargs*)

Sets attributes of the named reaction.

Parameters

- **name** (*str*) – the name of the reaction (or a substring of the name)
- **exact** (*bool*) – boolean indicating whether the name has to be exact
- **kwargs** – optional arguments
  - *new_name*: new name of the reaction
  - *scheme*: the reaction scheme, new species will be created automatically
  - *function*: the function from the function database to set
  - *mapping*: an optional dictionary that maps model elements to the function parameters. (can be any volume, species, modelvalue or in case of local parameters a value)
  - *notes*: sets notes for the reaction (either plain text, or valid xhtml)
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

basico.model_info.**set_reaction_mapping**(*reaction*, *mapping*, ***kwargs*)

Sets the reaction mapping of the parameters as specified in the mapping dictionary

Parameters

- **reaction** (*str or COPASI.CReaction*) – the name of the reaction (or reaction object)
- **mapping** (*{}*) –

  dictionary that maps model elements to the function
  parameters. (can be any volume, species, modelvalue or in case of

  local parameters a value)

- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
boolean indicating whether the reaction was changed

Return type
bool

`basico.model_info.set_reaction_parameters(name=None, **kwargs)`

Sets local parameter values.

Parameters

- **name** (*str*) – the name of the parameter (or a substring of the name)
- **kwargs** – optional arguments
  - *reaction_name*: if specified only parameters of the named reaction will be changed
  - *value*: the new value of the parameter to set. (only one of *value* / *mapped_to* should be defined)
  - *mapped_to*: the name of a global parameter to map the local parameter to
  - *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)

Returns
None

`basico.model_info.set_report_dict(spec, precision=None, separator=None, table=None, print_headers=True, header=None, body=None, footer=None, task=None, comment=None, add_separator=None, **kwargs)`

Sets properties of the named report definition.

Examples:

The following would set a report definition 'Time Course' to include Time and the concentration of S, in a report that is separated by tabs.

```
>>> set_report_dict('Time Course', body=['Time', '[S]']
```

The following defines a report for the Steady State concentration of S. To disambiguate, that the string '[S]' in the header should be used literally, we call the function wrap_copasi_string.

```
>>> set_report_dict('Steady State', task=T.STEADY_STATE, header=[wrap_copasi_string(
↪'[S]')], footer=['[S]'])
```

Parameters

- **spec** (*Union[str,int,COPASI.CReportDefinition]*) – the name, index or report definition object
- **precision** (*Optional[int]*) – number of digits to print (defaults to 6)
- **separator** (*Optional[str]*) – the separator to use between elements (defaults to)
- **table** (*[str]*) – a list of CNs or display names of elements to collect in a table. If *table* is specified the header, body, footer argument will be ignored. Note that setting table elements is only useful for tasks that generate output *during* the task. If that is not the case, you will have to specify the footer and header element directly.
- **print_headers** (*bool*) – optional arguments, indicating whether table headers will be printed (only applies when the *table* argument is given

- **header** (*[str]*) – a list of CNs or display names of elements to collect in the header column
- **body** (*[str]*) – a list of CNs or display names of elements to collect in the body rows
- **footer** (*[str]*) – a list of CNs or display names of elements to collect in the footer column
- **task** (*Optional[str]*) –

  task name for which the report should be used
- **comment** (*Optional[str]*) – a documentation string for the report (can bei either string, or xhtml string)
- **add_separator** (*Optional[bool]*) – an optional boolean flag, to automatically add seprators between header, body and footer entries since this is not necessary for table entries.
- **kwargs** – optional arguments
  - *new_name*: to rename the report
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

basico.model_info.**set_scheduled_tasks**(*task_name*, ***kwargs*)

Sets the scheduled tasks

Only the tasks with the listed names will be set to be scheduled.

Parameters

- **task_name** (*str or [str]*) – name or list of names of tasks set to be scheduled
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

basico.model_info.**set_species**(*name=None*, *exact=False*, ***kwargs*)

Sets properties of the named species

Parameters

- **name** (*str*) – the name of the species (or a substring of the name)
- **exact** (*bool*) – boolean indicating, that the name has to be exact
- **kwargs** – optional arguments
  - *new_name*: the new name for the species
  - *initial_concentration*: to set the initial concentration for the species
  - *initial_particle_number*: to set the initial particle number for the species
  - *initial_expression*: the initial expression for the species
  - *concentration*: the new transient concentration for the species
  - *particle_number*: the new transient particle number for the species

- *status* or *type*: the type of the species one of *fixed*, *assignment* or *ode*
- *expression*: the expression for the species (only valid when type is *ode* or *assignment*)
- *notes*: sets notes for the species (either plain text, or valid xhtml)
- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

`basico.model_info.set_task_settings(task, settings, **kwargs)`

Applies the task settings present in the settings object

Parameters

- **task** (*COPASI.CCopasiTask or str*) – the task to set
- **settings** (*dict*) – dictionary in the same format as the ones obtained from `get_task_settings()`
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

`basico.model_info.set_time_unit(unit, **kwargs)`

Sets the time unit of the model.

Parameters

- **unit** (*str*) – the time unit expression
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

`basico.model_info.set_value(name_or_reference, new_value, initial=False, **kwargs)`

Gets the value of the named element or nones

Parameters

- **name_or_reference** (*str or COPASI.CDataObject*) – display name of model element
- **new_value** (*float*) – the new value to set
- **initial** (*bool or None*) – if True, an initial value will be set, rather than a transient one. If set to *None*, the default reference will be returned and not coerced.
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
the value if found or None

Return type
float or None

basico.model_info.**simplify_names**(***kwargs*)

Simplifies the names of the model elements by removing all special characters and replacing them with underscores

Parameters

kwargs

- model: the model to simplify
- drop: a list of substrings to drop from the names

Returns

None

basico.model_info.**update_miriam_resources**()

This method downloads the latest miriam resources from the COPASI website and stores the configuration

basico.model_info.**update_parameter_set**(*name*, *exact=False*, ***kwargs*)

Updates the specified parameter set with values from the model

Parameters

- **name** – the name of the parameter set or a substring of the name
- **exact** – boolean indicating whether the name has to match exactly
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

basico.model_info.**wrap_copasi_string**(*text*)

Utility function wrapping the given text into a COPASI string

Parameters

text – the text to wrap

Returns

an escaped COPASI string, that can be used in reports

28.1.6 basico.model_io module

This module hosts all method for loading/saving new models.

All methods for loading / saving a new model are within this module. As well as the functionality to get/set the currently loaded model. Whenever a function needs the currently loaded model, and no model was provided in the *kwargs*, the `get_current_model()` function retrieves the model loaded last. There are also convenience methods to load models directly from BioModels or from url.

basico.model_io.**create_datamodel**()

creates a new data model

Returns

new data model

Return type

COPASI.CDataModel

basico.model_io.**get_current_model**()

Returns the current model.

This function returns the current model. That is the model loaded / created last. If no model exists a new one will be created first.

Returns
the current model

Return type
COPASI.CDataModel

basico.model_io.**get_examples**(*selector=''*)

Returns the filenames of examples bundled with this version.

A number of example models are included with the distribution. This method returns the filenames to those examples. Filtered by the argument.

Parameters
selector (*str*) – a filter expression to be used, only files matching **{selector}.[cps|xml]* will be returned

Returns
the list of examples matching

Return type
[str]

basico.model_io.**get_model_from_dict_or_default**(*d*, *key='model'*)

Convenience function returning the data model from the dictionary

Parameters

- **d** – the dictionary optionally containing the data model
- **key** – the key that the model is under (defaults to 'model')

Returns
the data model if found, or the one from *get_current_model()*

Return type
COPASI.CDataModel

basico.model_io.**get_num_loaded_models**()

Returns
the number of loaded models

basico.model_io.**load_biomodel**(*model_id*, *remove_user_defined_functions=False*)

Loads a model from the BioModels Database.

Parameters

- **model_id** (*Union[int,str]*) – either an integer of the biomodels id, or a valid biomodels id
- **remove_user_defined_functions** (*bool*) – optional flag, indicating that user defined functions should be removed before loading the model. Since function definitions are global, this can be helpful to ensure that function names remain the same as in the loaded file. (default: False)

Returns

Return type
COPASI.CDataModel

basico.model_io.**load_example**(*selector*)

Loads the example matching the selector.

Parameters
selector (*str*) – the filter expression to use for the examples see *get_examples()*

Returns
the loaded model, or None, if none matched

Return type
COPASI.CDataModel or None

`basico.model_io.load_model(location, remove_user_defined_functions=False)`

Loads the model and sets it as current

Parameters

- **location** (*str*) – either a filename, url or raw string of a COPASI / SBML model
- **remove_user_defined_functions** (*bool*) – optional flag, indicating that user defined functions should be removed before loading the model. Since function definitions are global, this can be helpful to ensure that function names remain the same as in the loaded file. (default: False)

Returns
the loaded model

Return type
COPASI.CDataModel

`basico.model_io.load_model_from_string(content)`

Loads either COPASI model / SBML model from the raw string given.

Parameters
content (*str or bytes*) – the copasi / sbml model serialized as string

Returns
the loaded model

Return type
COPASI.CDataModel

`basico.model_io.load_model_from_url(url)`

Loads either COPASI model / SBML model from the url.

Parameters
url (*str*) – url to a copasi / sbml model

Returns
the loaded model

Return type
COPASI.CDataModel

`basico.model_io.new_model(**kwargs)`

Creates a new model and sets it as current.

Parameters
kwargs – optional arguments

- *name* (str): the name for the new model
- *quantity_unit* (str): the unit to use for species
- *time_unit* (str): the time unit to use
- *volume_unit* (str): the unit to use for 3D compartments
- *area_unit* (str): the unit to use for 2D compartments
- *length_unit* (str): the unit to use for 1D compartments
- *remove_user_defined_functions* (bool): whether to remove user defined functions when creating the model
- *notes*: sets notes for the model (either plain text, or valid xhtml)

Returns
the new model

Return type
COPASI.CDataModel

`basico.model_io.open_copasi(filename='', **kwargs)`

Saves the model as COPASI file and opens it in COPASI.

The file will be written to a temporary file, and then it will be executed, so that the application registered to open it will start.

Parameters

- **filename** (*str*) – the file name to write to, if not given a temp file will be created that will be deleted at the end of the python session.
- **kwargs** – optional arguments:

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

`basico.model_io.overview(model=None)`

Returns a basic representation of the model.

Parameters
model (*COPASI.CDataModel or None*) – the model to get the overview for

Returns
a string, consisting of name, # compartments, # species, # parameters, # reaction

Return type
str

`basico.model_io.print_model(model=None)`

Prints the model overview.

See also `overview()`

Parameters
model (*COPASI.CDataModel*) – the model

Returns
None

`basico.model_io.remove_datamodel(model)`

Removes the model from the internal list of loaded models.

The model is removed from the list of models, and current model, before it is freed

Parameters
model – the model to be removed
:type model:COPASI.CDataModel :return: None

`basico.model_io.remove_loaded_models()`

Removes all loaded models

Returns
None

`basico.model_io.save_model(filename, **kwargs)`

Saves the model to the given filename.

Parameters

- **filename** (*str*) – the file to be written

- **kwargs** – optional arguments:

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
- *type* (str): *copasi* to write COPASI files, *sbml* to write SBML files (defaults to *copasi*), *sedml* to write SED-ML files, *omex* to write a COMBINE archive
- *overwrite* (bool): whether the file should be overwritten if present (defaults to True)
- *sbml_level* (int): SBML level to export
- *sbml_version* (int): SBML version to export
- *sedml_level* (int): SEDML level to export
- *sedml_version* (int): SEDML version to export
- *export_copasi_miriam* (bool): whether to export copasi miriam annotations
- *export_incomplete* (bool): whether to export incomplete SBML model
- *include_copasi* (bool): whether to include the COPASI file in the COMBINE archive (defaults to True)
- *include_data* (bool): whether to include the data file in the COMBINE archive (defaults to True)
- *include_sbml* (bool): whether to include the SBML file in the COMBINE archive (defaults to True)
- *include_sedml* (bool): whether to include the SED-ML file in the COMBINE archive (defaults to False)

Returns
None

`basico.model_io.save_model_and_data(filename, **kwargs)`

Saves the model to the give filename, along with all experimental data files.

Parameters

- **filename** – the filename of the COPASI file to write
- **filename** – str
- **kwargs** – optional arguments:

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
- *delete_data_on_exit* (bool): a flag indicating whether the files should be deleted at the end of the python session (defaults to False)

Returns
None

`basico.model_io.save_model_to_string(**kwargs)`

Saves the current model to string

Parameters
kwargs – optional arguments:

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
- *type* (str): *copasi* to write COPASI files, *sbml* to write SBML files (defaults to *copasi*), *sedml* to write SED-ML files
- *sbml_level* (int): SBML level to export
- *sbml_version* (int): SBML version to export
- *sedml_level* (int): SEDML level to export
- *sedml_version* (int): SEDML version to export

Returns
the copasi model as string

Return type
str

basico.model_io.**set_current_model**(*model*)

Sets the current model.

The current model, is the one that all functions will use if not is provided explicitly.

Parameters

model (*COPASI.CDataModel*) – the model to be set as current

Returns

the model

Return type

COPASI.CDataModel

28.1.7 basico.task_parameterestimation module

Submodule with utility methods for carrying out and plotting of parameter estimations.

The main function provided by this submodule is *run_parameter_estimation()*. Without any parameters, the previously set up parameter estimation as stored in the file will be carried out. And the parameters found will be returned.

It is also possible to set up parameter estimation problems from scratch. To make it as simple as possible, pandas data frames are used, the mapping from the columns to the model element will be done implicitly by naming the columns like the corresponding model elements.

Example

```
>>> from basico import *
>>> m = model_io.load_example("LM-test1")
>>> print(get_fit_parameters())
>>> print(get_parameters_solution())
>>> run_parameter_estimation(method='Levenberg - Marquardt')
>>> print(get_parameters_solution())
```

class basico.task_parameterestimation.**PE**

Bases: `object`

Constants for Parameter estimation method names

Convert between method names to enums

```
>>> PE.from_enum(0)
'Current Solution Statistics'
```

```
>>> PE.to_enum('Current Solution Statistics')
17
```

CURRENT_SOLUTION = 'Current Solution Statistics'

DIFFERENTIAL_EVOLUTION = 'Differential Evolution'

EVOLUTIONARY_PROGRAMMING = 'Evolutionary Programming'

EVOLUTIONARY_STRATEGY_SRES = 'Evolution Strategy (SRES)'

GENETIC_ALGORITHM = 'Genetic Algorithm'

GENETIC_ALGORITHM_SR = 'Genetic Algorithm SR'

HOOKE_JEEVES = 'Hooke & Jeeves'

LEVENBERG_MARQUARDT = 'Levenberg - Marquardt'

NELDER_MEAD = 'Nelder - Mead'

NL2SOL = 'NL2SOL'

PARTICLE_SWARM = 'Particle Swarm'

PRAXIS = 'Praxis'

RANDOM_SEARCH = 'Random Search'

SCATTER_SEARCH = 'Scatter Search'

SIMULATED_ANNEALING = 'Simulated Annealing'

STEEPEST_DESCENT = 'Steepest Descent'

TRUNCATED_NEWTON = 'Truncated Newton'

classmethod all_method_names()

classmethod from_enum(*int_value*)

classmethod to_enum(*value*)

basico.task_parameterestimation.**add_experiment**(*name*, *data*, ***kwargs*)

Adds a new experiment to the model.

This method adds a new experiment file to the parameter estimation task. The provided data frame will be written into the current directory as *experiment_name.txt* unless a filename has been provided.

The mapping between the columns and the model elements should be done by having the columns of the data frame be model element names in question. So for example *[A]* to note that the transient concentrations of a species *A* is to be mapped as dependent variable. or *[A]_0* to note that the initial concentration of a species *A* is to be mapped as independent variable.

Parameters

- **name** (*str*) – the name of the experiment
- **data** (*pandas.DataFrame*) – the data frame with the experimental data
- **kwargs**

- *model*: to specify the data model to be used (if not specified
  the one from *get_current_model()* will be taken)
- *file_name* (str): the file name to save the experimental data to (otherwise it will be name.txt)
- *data_dir* (str): the directory to save the experimental data to (otherwise it will be the current directory)

Returns

the filename of the generated data file

Return type

str

basico.task_parameterestimation.**add_experiment_from_dict**(*exp_dict*, ***kwargs*)

Adds an experiment from dictionary

Parameters

exp_dict

Returns

basico.task_parameterestimation.**get_data_from_experiment**(*experiment*, ***kwargs*)

Returns the data of the given experiment as dataframe

Parameters

- **experiment** – the experiment
- **kwargs**

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
- *rename_headers* (bool): if true (default) the columns of the headers will be renamed with the names of the element it is mapped to. Also all ignored columns will be removed from the dataset

Returns

dataframe with experimental data

Return type

pandas.DataFrame

basico.task_parameterestimation.**get_experiment**(*experiment*, ***kwargs*)

Returns the specified experiment.

Parameters

- **experiment** (*int or str or COPASI.CExperiment*) – experiment name or index
- **kwargs**

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

the experiment or an error if none existent

basico.task_parameterestimation.**get_experiment_data_from_model**(*model=None*)

Returns all experimental data from the model

Parameters

model (*COPASI.CDataModel or None*) – the model to get the data from

Returns

list of dataframes with experimental data (with columns renamed and unmapped columns dropped)

Return type

[pandas.DataFrame]

basico.task_parameterestimation.**get_experiment_dict**(*experiment*, ***kwargs*)

Returns all information about the experiment as dictionary

Parameters

- **experiment** – copasi experiment, experiment name or index
- **kwargs** – optional arguments

- *model*: to specify the data model to be used (if not specified

the one from `get_current_model()` will be taken)

- *raise_error*: boolean indicating that an error should be raised if the experimentfile is not present (default: False)
- *return_relative*: to indicate that relative experiment filenames should be returned (default: True)

Returns
all information about the experiment as dictionary

`basico.task_parameterestimation.`**`get_experiment_filenames`**(*model=None*)

Returns filenames of all experiments

Parameters
model (*COPASI.CDataModel or None*) – the model to get the data from

Returns
list of filenames of experimental data

Return type
[str]

`basico.task_parameterestimation.`**`get_experiment_mapping`**(*experiment*, ***kwargs*)

Retrieves a data frame of the experiment mapping.

The resulting data frame will have the columns: * *column* (int): index of the column in the file * *type* (str): 'time', 'dependent', 'indepenent' or 'ignored' * 'mapping' (str): the name of the element it is mapped to * 'cn' (str): internal identifier

Parameters

- **experiment** – the experiment to get the mapping from
- **kwargs**

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
data frame with the mapping as described

Return type
pandas.DataFrame

`basico.task_parameterestimation.`**`get_experiment_names`**(***kwargs*)

Returns the list of experiment names

Parameters
kwargs

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
list of experiment names defined

Return type
[str]

`basico.task_parameterestimation.`**`get_fit_constraints`**(*model=None*)

Returns a data frame with all fit constraints

The resulting dataframe will have the following columns:

- *name*: the name of the fit parameter
- *lower*: the lower bound of the parameter

- *upper*: the upper bound of the parameter
- *start*: the start value
- *affected*: a list of all experiments (names) the fit parameter should apply to. If empty the parameter should

  be varied for all experiments.
- *cn*: internal identifier

Parameters
model (*COPASI.CDataModel or None*) – the model to get the fit parameters from

Returns
data frame with the fit parameters

Return type
pandas.DataFrame

basico.task_parameterestimation.**get_fit_item_template**(*include_local=False*, *include_global=False*, *default_lb=0.001*, *default_ub=1000*, *model=None*)

Returns a template list of items to be used for the parameter estimation

Parameters

- **include_local** (*bool*) – boolean, indicating whether to include local parameters
- **include_global** (*bool*) – boolean indicating whether to include global parameters
- **default_lb** (*float*) – default lower bound to be used
- **default_ub** (*float*) – default upper bound to be used
- **model** (*COPASI.CDataModel or None*) – the model or None

Returns
List of dictionaries, with the local / global parameters in the format needed by: *set_fit_parameters()*.

Return type
[{}]

basico.task_parameterestimation.**get_fit_parameters**(*model=None*)

Returns a data frame with all fit parameters

The resulting dataframe will have the following columns:

- *name*: the name of the fit parameter
- *lower*: the lower bound of the parameter
- *upper*: the upper bound of the parameter
- *start*: the start value
- *affected*: a list of all experiments (names) the fit parameter should apply to. If empty the parameter should

  be varied for all experiments.
- *cn*: internal identifier

Parameters
model (*COPASI.CDataModel or None*) – the model to get the fit parameters from

Returns
data frame with the fit parameters

Return type
pandas.DataFrame

basico.task_parameterestimation.**get_fit_statistic**(*include_parameters=False*, *include_experiments=False*, *include_fitted=False*, ***kwargs*)

Return information about the last fit.

Parameters

- **include_parameters** (*bool*) – whether to include information about the parameters in a result entry with key *parameters*
- **include_experiments** (*bool*) – whether to include information about the experiments in a result entry with key *experiments*
- **include_fitted** (*bool*) – whether to include information about the fitted values in a result entry with key *fitted*
- **kwargs**

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

dictionary with the fit statistic

Return type

{}

basico.task_parameterestimation.**get_parameters_solution**(*model=None*)

Returns the solution found for the fit parameters as data frame

The resulting data frame will have the columns:

- *name*: the name of the parameter
- *lower*: the parameters lower bound
- *upper*: the parameters upper bound
- *sol*: the solution found in the last run (or NaN, if not run yet, or no solution found)
- *affected*: the experiments this parameter applies to (or an empty list if it applies to all)

Parameters

model (*COPASI.CDataModel or None*) – the model to use, or None

Returns

data frame as described

Return type

pandas.DataFrame

basico.task_parameterestimation.**get_simulation_results**(*values_only=False*, *update_parameters=True*, ***kwargs*)

Runs the current solution statistics and returns result of simulation and experimental data

Parameters

- **values_only** (*bool*) – if true, only time points at the measurements will be returned
- **update_parameters** (*bool*) – if set true, the model will be updated with the parameters found from the solution. (defaults to True)
- **kwargs**

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
- *solution*: a solution data frame to use, if not specified a current solution statistic will be computed

Returns
tuple of lists of experiment data, and a list of simulation data

Return type
([pandas.DataFrame],[pandas.DataFrame])

`basico.task_parameterestimation.`**`load_experiments_from_dict`**(*experiments*, ***kwargs*)

Loads all experiments from the specified experiment description

All existing experiments will be replaced with the ones from the specified file.

Parameters

- **`experiments`** – list of experiment dictionaries
- **`kwargs`** – optional arguments

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

`basico.task_parameterestimation.`**`load_experiments_from_yaml`**(*experiment_description*, ***kwargs*)

Loads all experiments from the specified experiment description

All existing experiments will be replaced with the ones from the specified file.

Parameters

- **`experiment_description`** – filename or yamlstring
- **`kwargs`** – optional arguments

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

`basico.task_parameterestimation.`**`num_experiment_files`**(***kwargs*)

Return the number of experiment files defined.

Parameters
`kwargs`

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
number of experiment files

Return type
int

`basico.task_parameterestimation.`**`num_validations_files`**(***kwargs*)

Returns the number of cross validation experiment files

Parameters
`kwargs`

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
number of cross validation experiment files

Return type
int

basico.task_parameterestimation.**plot_per_dependent_variable**(**kwargs)

This function creates a figure for each dependent variable, with traces for all experiments.

Parameters

kwargs

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

array of tuples (fig, ax) for each figure created

basico.task_parameterestimation.**plot_per_experiment**(**kwargs)

This function creates one figure per experiment defined, with plots of all dependent variables and their fit in it.

Parameters

kwargs

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

array of tuples (fig, ax) for the figures created

basico.task_parameterestimation.**prune_simulation_results**(*simulation_results*)

Removes all columns & time points from the simulation set, that are not available in the measurement set

Parameters

simulation_results – the simulation result as obtained by get_simulation_results

Returns

basico.task_parameterestimation.**remove_experiments**(**kwargs)

Removes all experiments from the model

Parameters

kwargs

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

None

basico.task_parameterestimation.**remove_fit_parameters**(**kwargs)

Removes all fit items

Parameters

kwargs

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

None

basico.task_parameterestimation.**run_parameter_estimation**(**kwargs)

Runs the parameter estimation task as specified:

The following are valid methods to be used for the parameter estimation task.

Current Solution:

- *Current Solution Statistics*,

Global Methods:

- *Random Search*,
- *Simulated Annealing*,
- *Differential Evolution*,
- *Scatter Search*,
- *Genetic Algorithm*,
- *Evolutionary Programming*,
- *Genetic Algorithm SR*,
- *Evolution Strategy (SRES)*,
- *Particle Swarm*,

Local Methods:

- *Levenberg - Marquardt*,
- *Hooke & Jeeves*,
- *Nelder - Mead*,
- *Steepest Descent*,
- *NL2SOL*,
- *Praxis*,
- *Truncated Newton*,

Parameters
kwargs

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
- *method* (str): one of the strings from above
- *randomize_start_values* (bool): if true, parameters will be randomized before starting otherwise the parameters starting value will be taken.
- *calculate_statistics* (bool): if true, the statistics will be calculated at the end of the task
- *create_parametersets* (bool): if true, parameter sets will be created for all experiments
- *use_initial_values* (bool): whether to use initial values
- *scheduled* (bool): sets whether the task is scheduled or not
- *update_model* (bool): sets whether the model should be updated, or reset to initial conditions.
- ***settings* (dict): a dictionary with settings to use, in the same format as the ones obtained from** `get_task_settings()`
- *write_report* (bool): overrides the writing of a report file of filename is specified. (defaults to True)

Returns
the solution for the fit parameters see `get_parameters_solution()`.

Return type
pandas.DataFrame

`basico.task_parameterestimation.`**`save_experiments_to_dict`**`(`***kwargs*`)`

Returns a list of dictionaries with the parameter estimation experiments

Parameters
kwargs – optional arguments

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

- *raise_error*: boolean indicating that an error should be raised if the experimentfile is not present (default: False)
- *return_relative*: to indicate that relative experiment filenames should be returned (default: True)

Returns
the parameter estimation experimetns as list of dictionary

Return type
[{}]

basico.task_parameterestimation.**save_experiments_to_yaml**(*filename=None*, ***kwargs*)

Saves the experiment to yaml

Parameters

- **filename** – optional filename to write to
- **kwargs** – optional arguments

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
the yaml string

basico.task_parameterestimation.**set_fit_constraints**(*fit_constraints*, *model=None*)

Replaces all existing fit constraints with the ones provided

Parameters

- **fit_constraints** (*pandas.DataFrame or [{}]*) – the fit parameters as pandas data frame of list of dictionaries with keys:
  - 'name' str: the display name of the model element to map the column to.
  - 'lower': the lower bound of the parameter
  - 'upper': the upper bound of the parameter
  - 'start' (float, optional): the start value
  - 'affected' (list[str], optional): a list of affected experiment names.
  - 'cn' (str, optional): internal identifier
- **model** (*COPASI.CDataModel or None*) – the model or None

Returns
None

basico.task_parameterestimation.**set_fit_parameters**(*fit_parameters*, *model=None*)

Replaces all existing fit items with the ones provided

Parameters

- **fit_parameters** (*pandas.DataFrame or [{}]*) – the fit parameters as pandas data frame of list of dictionaries with keys:
  - 'name' str: the display name of the model element to map the column to.
  - 'lower': the lower bound of the parameter
  - 'upper': the upper bound of the parameter
  - 'start' (float, optional): the start value
  - 'affected' (list[str], optional): a list of affected experiment names.

- 'cn' (str, optional): internal identifier

- **model** (*COPASI.CDataModel or None*) – the model or None

Returns
None

28.1.8 basico.task_steadystate module

This module is concerned with brining the model to steady state.

The *run_steadystate()* method brings the currently loaded model to steady state supporting a number of parameters you could set. Once done, additional calls to functions like *get_species()* or *get_reactions()* will contain the steady state values.

Example

```
>>> run_steadystate()
>>> get_species()
```

basico.task_steadystate.**run_steadystate**(***kwargs*)

Brings the model to steady state.

The function will use the *get_current_model()* unless one is provided.

Parameters

kwargs – optional arguments:

- *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)
- *use_initial_values* (bool): whether to use initial values
- *scheduled* (bool): sets whether the task is scheduled or not
- *update_model* (bool): sets whether the model should be updated, or reset to initial conditions.
- *criterion* (str): specifies the acceptance criterion to be used for a steady state can be one of:

  * *Distance and Rate*: both the Distance and the Rate criterion have to be fulfilled to accept
  * *Distance*: the distance criterion
  * *Rate*: the rate of change has to be sufficiently small

- ***settings* (dict): a dictionary with settings to use, in the same format as the ones obtained from** *get_task_settings()*

Returns

integer status information whether the steady state was reached:

- *0*: not found
- *1*: steady state found
- *2*: equillibrium steady state found

- *3*: steady state with negative concentrations found

Return type
int

28.1.9 basico.task_timecourse module

This module encapsulates methods for running time course simulations.

main method provided is the `run_time_course()` method, that will simulate the given model (or the current `get_current_model()`).

Examples

To run a time course for the duration of 10 time units use

```
>>> run_time_course(10)
```

To run a time course for the duration of 10 time units, in 50 simulation steps use

```
>>> run_time_course(10, 50)
```

To run a time course from 0, for the duration of 10 time units, in 50 simulation steps use:

```
>>> run_time_course(0, 10, 50)
```

all parameters can also be given as key value pairs.

`basico.task_timecourse.`**`create_data_handler`**(*output_selection*, *during=None*, *after=None*, *before=None*, *model=None*)

Creates an output handler for the given selection

Parameters

- **`output_selection`** (*[str]*) – list of display names or cns, of elements to capture
- **`during`** (*[str]*) – optional list of elements from the output selection, that should be collected during the run of the task
- **`after`** (*[str]*) – optional list of elements from the output selection, that should be collected after the run of the task
- **`before`** (*[str]*) – optional list of elements from the output selection, that should be collected before the run of the task
- **`model`** – the model in which to resolve the display names

Returns
tuple of the data handler from which to retrieve output later, and their columns

Return type
(COPASI.CDataHandler, [])

`basico.task_timecourse.`**`get_data_from_data_handler`**(*dh*, *columns*)

`basico.task_timecourse.`**`run_time_course`**(**args*, ***kwargs*)

Simulates the current or given model, returning a data frame with the results

Parameters

- **`args`** – positional arguments

  - 1 argument: the duration to simulate the model
  - 2 arguments: the duration and number of steps to take
  - 3 arguments: start time, duration, number of steps
- **kwargs** – additional arguments
  - *model*: to specify the data model to be used (if not specified
    the one from `get_current_model()` will be taken)
  - *use_initial_values* (bool): whether to use initial values
  - *scheduled* (bool): sets whether the task is scheduled or not
  - *update_model* (bool): sets whether the model should be updated, or reset to initial conditions.
  - *method* (str): sets the simulation method to use (otherwise the previously set method will be used)
    support methods:

    * *deterministic* / *lsoda*: the LSODA implementation
    * *stochastic*: the Gibson & Bruck Gillespie implementation
    * *directMethod*: Gillespie Direct Method
    * others: *hybrid*, *hybridode45*, *hybridlsoda*, *adaptivesa*, *tauleap*, *radau5*, *sde*
  - *duration* (float): the duration in time units for how long to simulate
  - *automatic* (bool): whether to use automatic determined steps (True), or the specified interval / number of steps
  - *output_event* (bool): if true, output will be collected at the time a discrete event occurs.
  - *values* ([float]): if given, output will only returned at the output points specified
    for example use *values=[0, 1, 4]* to return output only for those three times
  - *start_time* (float): the output start time. If the model is not at that start time, a simulation
    will be performed in one step, to reach it before starting to collect output.
  - *step_number* or *intervals* (int): the number of output steps. (will only be used if *automatic*
    or *stepsize* is not used.
  - *stepsize* (float): the output step size (will only be used if *automatic* is False).
  - *seed* (int): set the seed that will be used if *use_seed* is true, using this stochastic trajectories can
    be repeated
  - 'use_seed' (bool): if true, the specified seed will be used.
  - *a_tol* (float): the absolute tolerance to be used
  - *r_tol* (float): the relative tolerance to be used
  - *max_steps* (int): the maximum number of internal steps the integrator is allowed to use.
  - *use_concentrations* (bool): whether to return just the concentrations (default)

- *use_numbers* (bool): return all elements collected

Returns
data frame with simulation results

Return type
pandas.DataFrame

`basico.task_timecourse.run_time_course_with_output(output_selection, *args, **kwargs)`

Simulates the current model, returning only the data specified in the output_selection array

Parameters

- **output_selection** – selection of elements to return, for example ['Time', '[ATP]', 'ATP.Rate'] to return the time column, ATP concentration and the rate of change of ATP. The strings can be either the Display names as can be found in COPASI, or the CN's of the elements.
- **args** – positional arguments
  - 1 argument: the duration to simulate the model
  - 2 arguments: the duration and number of steps to take
  - 3 arguments: start time, duration, number of steps
- **kwargs** – additional arguments
  - *model*: to specify the data model to be used (if not specified
    the one from `get_current_model()` will be taken)
  - *use_initial_values* (bool): whether to use initial values
  - *scheduled* (bool): sets whether the task is scheduled or not
  - *update_model* (bool): sets whether the model should be updated, or reset to initial conditions.
  - *method* (str): sets the simulation method to use (otherwise the previously set method will be used)
    support methods:

    * *deterministic* / *lsoda*: the LSODA implementation
    * *stochastic*: the Gibson & Bruck Gillespie implementation
    * *directMethod*: Gillespie Direct Method
    * others: *hybrid*, *hybridode45*, *hybridlsoda*, *adaptivesa*, *tauleap*, *radau5*, *sde*
  - *duration* (float): the duration in time units for how long to simulate
  - *automatic* (bool): whether to use automatic determined steps (True), or the specified interval / number of steps
  - *output_event* (bool): if true, output will be collected at the time a discrete event occurs.
  - *values* ([float]): if given, output will only returned at the output points specified
    for example use *values=[0, 1, 4]* to return output only for those three times
  - *start_time* (float): the output start time. If the model is not at that start time, a simulation
    will be performed in one step, to reach it before starting to collect output.

- *step_number* or *intervals* (int): the number of output steps. (will only be used if *automatic*
  or *stepsize* is not used.
- *stepsize* (float): the output step size (will only be used if *automatic* is False).
- *seed* (int): set the seed that will be used if *use_seed* is true, using this stochastic trajectories can
  be repeated
- 'use_seed' (bool): if true, the specified seed will be used.
- *a_tol* (float): the absolute tolerance to be used
- *r_tol* (float): the relative tolerance to be used
- *max_steps* (int): the maximum number of internal steps the integrator is allowed to use.

28.1.10 basico.task_scan module

Utility functions for dealing with scan tasks

While usually it is easier to encode scan functionality directly in python code, the utility methods here make it easy to set up scan tasks as supported by COPASI directly. That way they can be carried out from the command line version of COPASI, or from the graphical user interface.

`basico.task_scan.`**`add_scan_item`**`(`***kwargs*`)`

Adds the scan item to the model

Parameters

kwargs – optional parameters

- *model*: to specify the data model to be used (if not specified
  the one from `get_current_model()` will be taken)
- *type (str)*: the type for the scan item can be one of *scan*,
  repeat, *random* or *parameter_set*. If not specified *scan* will be used.
- *cn (str)*: the cn of the element to use in the scan item (use when
  no suitable display names for the item you are interested in exist)
  if you specify cn, don't use the *item* optional paramter
- *item (str)*: the display name of the item you want to use, for example
  [Signal]_0 for the initial concentration of species *Signal*, or
  (r1).k for the local parameter *k* of reaction *r1*.
- *values(str or [float])*: if you want to scan over specific values,
  rather than a range, specify them here e.g.: *[0.1, 0.5, 1, 2]*. Using
  this parameter also sets *use_values* to *True*
- *parameter_sets([str])*: if you want to scan over parameter sets, add the
  list of parameter set names here.
- *use_values (bool)*: indicates that the values specified should be used
  rather than the min / max range
- *num_steps (int)*: the number of steps in the range of [min, max] or the
  number of repeats.

- *min (float)*: minimum value for the range or first distribution parameter
- *max (float)*: maximum value for the range, or the 2nd distributon parameter
- *log (bool)*: boolean indicating that the range should be used logarithmically.
- *distribution (str)*: one of *uniform*, *normal*, *poisson* or *gamma*

Returns

`basico.task_scan.get_scan_items(**kwargs)`

Retrieves the scan items specified on the scan task:

```
>>> get_scan_items()
[
   {
     'type': 'scan',
     'num_steps': 10,
     'log': False,
     'min': 0.5,
     'max': 2.0,
     'item': '(R1).k1',
   }
]
```

Parameters

kwargs – optional parameters

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

array of dictionary with the scan items specified

Return type

[{}]

`basico.task_scan.get_scan_items_frame(**kwargs)`

Returns all the scan items as pandas DataFrame

Parameters

kwargs – optional parameters

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns

data frame of scan items

`basico.task_scan.get_scan_settings(**kwargs)`

Returns the scan settings as dictionary

```
>>> get_scan_settings()
{
    'update_model': False,
    'scheduled': False,
    'subtask': 'Steady-State',
    'output_during_subtask': False,
    'continue_from_current_state': False,
    'continue_on_error': False,
```

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```
    'scan_items': [ ... ]
}
```

Parameters
kwargs – optional parameters

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
dictionary of scan settings

Return type
{}

`basico.task_scan.run_scan(**kwargs)`

Runs the scan task

Parameters
kwargs – optional parameters

- settings: optional dictionary with the scan settings
- scan_items: a list of scan items see `set_scan_items()`
- output ([(str)]): optional list of cns or display names, of elements to collect in the scan.
- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None if output is not specified, otherwise the collected output as dataframe.

Return type
None or pd.DataFrame

`basico.task_scan.set_scan_items(scan_items, **kwargs)`

Replaces the scan items in the task, with the scan items passed in

If you just wanted to change a specific entry, you could would retrieve the current set of scan items, make the change and then set them again:

```
>>> scan_items = get_scan_items()
```

the list of scan items is returned as array of dictionary items, and can be freely modified (say change the number of steps of the first item to a new value), or add new entries, remove some

```
>>> scan_items[0]['num_steps'] = 20
```

Finally a call to scan items, will replace the ones in the model with the ones from the array.

```
>>> set_scan_items(scan_items)
```

Parameters

- **scan_items** (*[{}]*) – list of dictionaries as returned by `get_scan_items()`.
- **kwargs** – optional parameters
  - *model*: to specify the data model to be used (if not specified

the one from *get_current_model()* will be taken)

Returns

None

basico.task_scan.**set_scan_settings**(***kwargs*)

Changes the scan settings

Parameters

kwargs – optional parameters

- settings: dictionary with the scan settings
- subtask: sub task name
- output_during_subtask: boolean, indicating whether ouput should be collected during the subtask execution
- **continue_from_current_state: boolean indicating, whether the subtask should be reset to initial values (False)**
  or not (True)
- continue_on_error: boolean indicating, whether executions should continue, in case one subtask execution failed (True) or not.
- scan_items: a list of scan items see *set_scan_items()*
- *model*: to specify the data model to be used (if not specified
  the one from *get_current_model()* will be taken)

Returns

28.1.11 basico.task_optimization module

Submodule with utility methods for setting up and carrying out optimization tasks.

The main function provided by this submodule is *run_optimization()*. Without any parameters, the previously set up parameter estimation as stored in the file will be carried out. And the parameters found will be returned.

Example

Create an optimization problem

```
>>> from bascio import *
>>> new_model(name='Square')
>>> add_parameter('x', initial_value=0)
>>> add_parameter('y', initial_value=0)
>>> add_parameter('f', type='assignment',
...                    expression='(1+{Values[x].InitialValue})^2+(1 + {Values[y].
↪InitialValue})^2')
```

Setup the optimization

```
>>> set_opt_settings({
...       'expression': 'Values[f].InitialValue',
...       'subtask': T.TIME_COURSE,
...       'method': {'name': PE.LEVENBERG_MARQUARDT}
... })
```

Specifiy which paramters to vary:

```
>>> set_opt_parameters(get_opt_item_template(include_global=True))
```

Run the optimization

```
>>> run_optimization()
```

Get statistic, to see how good the fit was:

```
>>> get_opt_statistic()
```

basico.task_optimization.**get_opt_constraints**(*model=None*)

Returns a data frame with all constraints to be adhered to during optimization

The resulting dataframe will have the following columns:

- *name*: the name of the fit parameter
- *lower*: the lower bound of the parameter
- *upper*: the upper bound of the parameter
- *start*: the start value
- *cn*: internal identifier

Parameters

model (*COPASI.CDataModel or None*) – the model to get the optitems from

Returns

data frame with the constraints

Return type

pandas.DataFrame

basico.task_optimization.**get_opt_item_template**(*include_local=False*, *include_global=False*, *default_lb=0.001*, *default_ub=1000*, *model=None*)

Returns a template dictionary with optimization items

Parameters

- **include_local** (*bool*) – boolean, indicating whether to include local parameters
- **include_global** (*bool*) – boolean indicating whether to include global parameters
- **default_lb** (*float*) – default lower bound to be used
- **default_ub** (*float*) – default upper bound to be used
- **model** (*COPASI.CDataModel or None*) – the model or None

Returns

List of dictionaries, with the local / global parameters in the format needed by: *set_opt_parameters()*.

Return type

[{}]

basico.task_optimization.**get_opt_parameters**(*model=None*)

Returns a data frame with all parameters to be varied during optimization

The resulting dataframe will have the following columns:

- *name*: the name of the fit parameter
- *lower*: the lower bound of the parameter
- *upper*: the upper bound of the parameter
- *start*: the start value

- *cn*: internal identifier

Parameters
model (*COPASI.CDataModel or None*) – the model to get the optitems from

Returns
data frame with the fit parameters

Return type
pandas.DataFrame

`basico.task_optimization.get_opt_settings(model=None, basic_only=True)`

Returns a dictionary with the optimization setup
The result int dictionary includes the objective function, and the subtask.

Parameters

- **model** – the model or None for the current one
- **basic_only** (*bool*) – boolean flag indicating whether only basic settings should be returned

Returns
dictionary with settings

`basico.task_optimization.get_opt_solution(model=None)`

Returns the solution found for the optimization parameters as data frame

The resulting data frame will have the columns:
- *name*: the name of the parameter
- *lower*: the parameters lower bound
- *upper*: the parameters upper bound
- *sol*: the solution found in the last run (or NaN, if not run yet, or no solution found)

Parameters
model (*COPASI.CDataModel or None*) – the model to use, or None

Returns
data frame as described

Return type
pandas.DataFrame

`basico.task_optimization.get_opt_statistic(**kwargs)`

Return information about the last optimization run.
Parameters
kwargs

- *model*: to specify the data model to be used (if not specified
the one from *get_current_model()* will be taken)

Returns
dictionary with the statistic

Return type
{}

`basico.task_optimization.run_optimization(expression=None, output=None, settings=None, **kwargs)`

Runs the optimization
Parameters

- **expression** – optional objective function to be used

- **settings** – optional settings dictionary
- **output** – optional list of output to collect
- **kwargs** – optional arguments

Returns
pandas data frame of the specified output, or the resulting solution for the parameters

basico.task_optimization.**set_objective_function**(*expression*, *maximize=None*, *minimize=None*, *model=None*)

Sets the objective function to be used

Parameters

- **expression** – the expression to be used as objective function, it can contain any display names of model elements. So for example to minimize an initial value of a global parameter *x* the expression would look like *Values[x].InitialValue*.
- **maximize** – optional boolean indicating whether the expression should be maximized
- **minimize** – optional boolean indicating whether the expression should be minimized
- **model** – the model to be used or None

Returns
None

basico.task_optimization.**set_opt_constraints**(*opt_constraints*, *model=None*)

Replaces all existing opt constraints with the ones provided

Parameters

- **opt_constraints** (*pandas.DataFrame or [{}]*) – the optimization parameters as pandas data frame of list of dictionaries with keys:
  - 'name' str: the display name of the model element to map the column to.
  - 'lower': the lower bound of the parameter
  - 'upper': the upper bound of the parameter
  - 'start' (float, optional): the start value
  - 'cn' (str, optional): internal identifier
- **model** (*COPASI.CDataModel or None*) – the model or None

Returns
None

basico.task_optimization.**set_opt_parameters**(*opt_parameters*, *model=None*)

Replaces all existing opt items with the ones provided

Parameters

- **opt_parameters** (*pandas.DataFrame or [{}]*) – the optimization parameters as pandas data frame of list of dictionaries with keys:
  - 'name' str: the display name of the model element to map the column to.
  - 'lower': the lower bound of the parameter
  - 'upper': the upper bound of the parameter
  - 'start' (float, optional): the start value
  - 'cn' (str, optional): internal identifier

- **model** (*COPASI.CDataModel or None*) – the model or None

Returns
None

basico.task_optimization.**set_opt_settings**(*settings*, *model=None*)

Changes the optimization setup

Parameters

- **settings** – a dictionary as returned by *get_opt_parameters()*
- **model** – the model to be used, nor None

Returns

28.1.12 basico.task_sensitivities module

Utility methods for working with the sensitivity task

class basico.task_sensitivities.**EnumHelper**

Bases: object

Utility class for dealing with mapping from names to enums easier

classmethod from_enum(*int_value*)

classmethod get_all_names()

classmethod to_enum(*value*)

class basico.task_sensitivities.**SENS**

Bases: *EnumHelper*

Class for Sensitivity object lists

ALL_INITIAL_VALUES = 'All initial Values'

ALL_LOCAL_PARAMETER_VALUES = 'Local Parameter Values'

ALL_ODE_VARIABLES = 'All independent Variables of the model'

ALL_PARAMETER_AND_INITIAL_VALUES = 'All Parameter and Initial Values'

ALL_PARAMETER_VALUES = 'All Parameter Values'

ALL_VARIABLES = 'All Variables of the model'

ASS_COMPARTMENT_VOLUMES = 'Values of Compartment Volumes with Assignment'

ASS_GLOBAL_PARAMETER_VALUES = 'Values of Global Quantities with Assignment'

ASS_METAB_CONCENTRATIONS = 'Concentrations of Species with Assignment'

ASS_METAB_NUMBERS = 'Numbers of Species with Assignment'

COMPARTMENTS = 'Compartments'

COMPARTMENT_INITIAL_VOLUMES = 'Compartment Initial Volumes'

COMPARTMENT_RATES = 'Compartment Volume Rates'

```
COMPARTMENT_VOLUMES = 'Compartment Volumes'

CONST_COMPARTMENT_VOLUMES = 'Constant Compartment Volumes'

CONST_GLOBAL_PARAMETER_INITIAL_VALUES = 'Constant Global Quantity Values'

CONST_METAB_CONCENTRATIONS = 'Constant Concentrations of Species'

CONST_METAB_NUMBERS = 'Constant Numbers of Species'

EMPTY_LIST = 'Not Set'

GLOBAL_PARAMETERS = 'Global Quantity'

GLOBAL_PARAMETER_INITIAL_VALUES = 'Global Quantity Initial Values'

GLOBAL_PARAMETER_RATES = 'Global Quantity Rates'

GLOBAL_PARAMETER_VALUES = 'Global Quantity Values'

METABS = 'Species'

METAB_CONCENTRATIONS = 'Concentrations of Species'

METAB_CONC_RATES = 'Concentration Rates'

METAB_INITIAL_CONCENTRATIONS = 'Initial Concentrations'

METAB_INITIAL_NUMBERS = 'Initial Numbers'

METAB_NUMBERS = 'Numbers of Species'

METAB_PART_RATES = 'Particle Rates'

METAB_TRANSITION_TIME = 'Transition Time'

NON_CONST_COMPARTMENT_VOLUMES = 'Non-Constant Compartment Volumes'

NON_CONST_GLOBAL_PARAMETER_VALUES = 'Non-Constant Global Quantity Values'

NON_CONST_METAB_CONCENTRATIONS = 'Non-Constant Concentrations of Species'

NON_CONST_METAB_NUMBERS = 'Non-Constant Numbers of Species'

ODE_COMPARTMENT_VOLUMES = 'Values of Compartment Volumes with ODE'

ODE_GLOBAL_PARAMETER_VALUES = 'Values of Global Quantities with ODE'

ODE_METAB_CONCENTRATIONS = 'Concentrations of Species with ODE'

ODE_METAB_NUMBERS = 'Numbers of Species with ODE'

REACTIONS = 'Reactions'

REACTION_CONC_FLUXES = 'Concentration Fluxes of Reactions'

REACTION_METAB_CONCENTRATIONS = 'Concentrations of Species determined by Reactions'

REACTION_METAB_NUMBERS = 'Numbers of Species determined by Reactions'

REACTION_PART_FLUXES = 'Particle Fluxes of Reactions'
```

REDUCED_JACOBIAN_EV_IM = 'Imaginary part of eigenvalues of the reduced jacobian'

REDUCED_JACOBIAN_EV_RE = 'Real part of eigenvalues of the reduced jacobian'

SINGLE_OBJECT = 'Single Object'

class basico.task_sensitivities.**SENS_ST**

Bases: *EnumHelper*

Enumeration of Sensitivity Subtasks

CrossSection = 'Cross Section'

Evaluation = 'Evaluation'

Optimization = 'Optimization'

ParameterEstimation = 'Parameter Estimation'

SteadyState = 'Steady State'

TimeSeries = 'Time Series'

basico.task_sensitivities.**get_scaled_sensitivities**(***kwargs*)

Returns the scaled sensitivity matrix as pandas data frame

Parameters

kwargs – optional arguments

- *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)
- *run_first*: boolean flag indicating that the task should be run first (defaults to false)
- *settings*: a dictionary with the settings to apply first
- *use_initial_values*: boolean flag indicating whether initial values should be used (true by default)

Returns

the scaled sensitivity matrix

Return type

pd.DataFrame

basico.task_sensitivities.**get_sensitivity_settings**(*basic_only=True*, ***kwargs*)

Returns the settings of the sensitivity task

Parameters

- **basic_only** (*bool*) – if true, only basic parameters will be returned
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from *get_current_model()* will be taken)

Returns

the settings as dictionary

Return type

dict

`basico.task_sensitivities.get_summarized_sensitivities(**kwargs)`

Returns the summarized sensitivity matrix as pandas data frame

The summarized result is computed as the 2 norm of the scaled result, thus collapsing the dimension

Parameters

kwargs – optional arguments

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
- *run_first*: boolean flag indicating that the task should be run first (defaults to false)
- *settings*: a dictionary with the settings to apply first
- *use_initial_values*: boolean flag indicating whether initial values should be used (true by default)

Returns

the summarized sensitivity matrix

Return type

pd.DataFrame or None

`basico.task_sensitivities.get_unscaled_sensitivities(**kwargs)`

Returns the unscaled sensitivity matrix as pandas data frame

Parameters

kwargs – optional arguments

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
- *run_first*: boolean flag indicating that the task should be run first (defaults to false)
- *settings*: a dictionary with the settings to apply first
- *use_initial_values*: boolean flag indicating whether initial values should be used (true by default)

Returns

the unscaled sensitivity matrix

Return type

pd.DataFrame

`basico.task_sensitivities.run_sensitivities(**kwargs)`

Runs the sensitivity task, the result is obtained

by calling:

- *get_scaled_sensitivies*
- *get_unscaled_sensitivies* or
- *get_summarized_sensitivites*

Parameters

kwargs – optional arguments

- *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)
- *settings*: a dictionary with the settings to apply first
- *use_initial_values*: boolean flag indicating whether initial values should be used (true by default)

Returns
None

`basico.task_sensitivities.set_sensitivity_settings(settings, **kwargs)`

Applies the settings to the sensitivity task

Parameters

- **settings** (*dict*) – the setting dictionary with keys, as obtained by get_sensitivity_settings
- **kwargs** – optional arguments
  - *model*: to specify the data model to be used (if not specified the one from `get_current_model()` will be taken)

Returns
None

PYTHON MODULE INDEX

b

INDEX

A

B

C

D

E

F

G

H

L

M

N

O

P

R

S

T

U

W