cobra Documentation

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Contents

For installation instructions, please see INSTALL.rst.

Many of the examples below are viewable as IPython notebooks, which can be viewed at nbviewer.

CHAPTER 1

Getting Started

Loading a model and inspecting it

To begin with, cobrapy comes with bundled models for *Salmonella* and *E. coli*, as well as a "textbook" model of *E. coli* core metabolism. To load a test model, type

```
In [1]: from __future__ import print_function

        import cobra
        import cobra.test

        # "ecoli" and "salmonella" are also valid arguments
        model = cobra.test.create_test_model("textbook")
```

The reactions, metabolites, and genes attributes of the cobrapy model are a special type of list called a `cobra.DictList`, and each one is made up of `cobra.Reaction`, `cobra.Metabolite` and `cobra.Gene` objects respectively.

```
In [2]: print(len(model.reactions))
        print(len(model.metabolites))
        print(len(model.genes))
```

```
95
72
137
```

When using Jupyter notebook this type of information is rendered as a table.

```
In [3]: model
```

```
Out[3]: <Model e_coli_core at 0x1116ea9e8>
```

Just like a regular list, objects in the `DictList` can be retrieved by index. For example, to get the 30th reaction in the model (at index 29 because of 0-indexing):

```
In [4]: model.reactions[29]
```

```
Out[4]: <Reaction EX_glu__L_e at 0x11b8643c8>
```

Additionally, items can be retrieved by their `id` using the `DictList.get_by_id()` function. For example, to get the cytosolic atp metabolite object (the id is "atp_c"), we can do the following:

```
In [5]: model.metabolites.get_by_id("atp_c")
```

```
Out[5]: <Metabolite atp_c at 0x11b7f82b0>
```

As an added bonus, users with an interactive shell such as IPython will be able to tab-complete to list elements inside a list. While this is not recommended behavior for most code because of the possibility for characters like "-" inside ids, this is very useful while in an interactive prompt:

```
In [6]: model.reactions.EX_glc__D_e.bounds
```

```
Out[6]: (-10.0, 1000.0)
```

Reactions

We will consider the reaction glucose 6-phosphate isomerase, which interconverts glucose 6-phosphate and fructose 6-phosphate. The reaction id for this reaction in our test model is PGI.

```
In [7]: pgi = model.reactions.get_by_id("PGI")
        pgi
```

```
Out[7]: <Reaction PGI at 0x11b886a90>
```

We can view the full name and reaction catalyzed as strings

```
In [8]: print(pgi.name)
        print(pgi.reaction)
```

```
glucose-6-phosphate isomerase
g6p_c <=> f6p_c
```

We can also view reaction upper and lower bounds. Because the `pgi.lower_bound` < 0, and `pgi.upper_bound` > 0, `pgi` is reversible.

```
In [9]: print(pgi.lower_bound, "< pgi <", pgi.upper_bound)
        print(pgi.reversibility)
```

```
-1000.0 < pgi < 1000.0
True
```

We can also ensure the reaction is mass balanced. This function will return elements which violate mass balance. If it comes back empty, then the reaction is mass balanced.

```
In [10]: pgi.check_mass_balance()
```

```
Out[10]: {}
```

In order to add a metabolite, we pass in a `dict` with the metabolite object and its coefficient

```
In [11]: pgi.add_metabolites({model.metabolites.get_by_id("h_c"): -1})
         pgi.reaction
```

```
Out[11]: 'g6p_c + h_c <=> f6p_c'
```

The reaction is no longer mass balanced

```
In [11]: pgi.check_mass_balance()
```

```
Out[11]: {'H': -1.0, 'charge': -1.0}
```

We can remove the metabolite, and the reaction will be balanced once again.

```
In [12]: pgi.subtract_metabolites({model.metabolites.get_by_id("h_c"): -1})
         print(pgi.reaction)
         print(pgi.check_mass_balance())
```

```
g6p_c <=> f6p_c
```

It is also possible to build the reaction from a string. However, care must be taken when doing this to ensure reaction id's match those in the model. The direction of the arrow is also used to update the upper and lower bounds.

```
In [13]: pgi.reaction = "g6p_c --> f6p_c + h_c + green_eggs + ham"
```

```
unknown metabolite 'green_eggs' created
unknown metabolite 'ham' created
```

```
In [14]: pgi.reaction
```

```
Out[14]: 'g6p_c --> f6p_c + green_eggs + h_c + ham'
```

```
In [15]: pgi.reaction = "g6p_c <=> f6p_c"
         pgi.reaction
```

```
Out[15]: 'g6p_c <=> f6p_c'
```

Metabolites

We will consider cytosolic atp as our metabolite, which has the id `"atp_c"` in our test model.

```
In [16]: atp = model.metabolites.get_by_id("atp_c")
         atp
```

```
Out[16]: <Metabolite atp_c at 0x11b7f82b0>
```

We can print out the metabolite name and compartment (cytosol in this case) directly as string.

```
In [17]: print(atp.name)
         print(atp.compartment)
```

```
ATP
c
```

We can see that ATP is a charged molecule in our model.

```
In [18]: atp.charge
```

```
Out[18]: -4
```

We can see the chemical formula for the metabolite as well.

```
In [19]: print(atp.formula)
```

```
C10H12N5O13P3
```

The reactions attribute gives a `frozenset` of all reactions using the given metabolite. We can use this to count the number of reactions which use atp.

```
In [20]: len(atp.reactions)
```

```
Out[20]: 13
```

A metabolite like glucose 6-phosphate will participate in fewer reactions.

```
In [21]: model.metabolites.get_by_id("g6p_c").reactions
```

```
Out[21]: frozenset({<Reaction G6PDH2r at 0x11b870c88>,
                    <Reaction GLCpts at 0x11b870f98>,
                    <Reaction PGI at 0x11b886a90>,
                    <Reaction Biomass_Ecoli_core at 0x11b85a5f8>})
```

Genes

The `gene_reaction_rule` is a boolean representation of the gene requirements for this reaction to be active as described in Schellenberger et al 2011 Nature Protocols 6(9):1290-307.

The GPR is stored as the gene_reaction_rule for a Reaction object as a string.

```
In [22]: gpr = pgi.gene_reaction_rule
         gpr

Out[22]: 'b4025'
```

Corresponding gene objects also exist. These objects are tracked by the reactions itself, as well as by the model

```
In [23]: pgi.genes

Out[23]: frozenset({<Gene b4025 at 0x11b844cc0>})

In [24]: pgi_gene = model.genes.get_by_id("b4025")
         pgi_gene

Out[24]: <Gene b4025 at 0x11b844cc0>
```

Each gene keeps track of the reactions it catalyzes

```
In [25]: pgi_gene.reactions

Out[25]: frozenset({<Reaction PGI at 0x11b886a90>})
```

Altering the gene_reaction_rule will create new gene objects if necessary and update all relationships.

```
In [26]: pgi.gene_reaction_rule = "(spam or eggs)"
         pgi.genes

Out[26]: frozenset({<Gene spam at 0x11b850908>, <Gene eggs at 0x11b850eb8>})

In [27]: pgi_gene.reactions

Out[27]: frozenset()
```

Newly created genes are also added to the model

```
In [28]: model.genes.get_by_id("spam")

Out[28]: <Gene spam at 0x11b850908>
```

The `delete_model_genes` function will evaluate the GPR and set the upper and lower bounds to 0 if the reaction is knocked out. This function can preserve existing deletions or reset them using the `cumulative_deletions` flag.

```
In [29]: cobra.manipulation.delete_model_genes(
             model, ["spam"], cumulative_deletions=True)
         print("after 1 KO: %4d < flux_PGI < %4d" % (pgi.lower_bound, pgi.upper_bound))

         cobra.manipulation.delete_model_genes(
             model, ["eggs"], cumulative_deletions=True)
         print("after 2 KO:  %4d < flux_PGI < %4d" % (pgi.lower_bound, pgi.upper_bound))

after 1 KO: -1000 < flux_PGI < 1000
after 2 KO:     0 < flux_PGI <    0
```

The undelete_model_genes can be used to reset a gene deletion

```
In [30]: cobra.manipulation.undelete_model_genes(model)
         print(pgi.lower_bound, "< pgi <", pgi.upper_bound)
```

```
-1000 < pgi < 1000
```

Making changes reversibly using models as contexts

Quite often, one wants to make small changes to a model and evaluate the impacts of these. For example, we may want to knock-out all reactions sequentially, and see what the impact of this is on the objective function. One way of doing this would be to create a new copy of the model before each knock-out with `model.copy()`. However, even with small models, this is a very slow approach as models are quite complex objects. Better then would be to do the knock-out, optimizing and then manually resetting the reaction bounds before proceeding with the next reaction. Since this is such a common scenario however, cobrapy allows us to use the model as a context, to have changes reverted automatically.

```
In [31]: model = cobra.test.create_test_model('textbook')
         for reaction in model.reactions[:5]:
             with model as model:
                 reaction.knock_out()
                 model.optimize()
                 print('%s blocked (bounds: %s), new growth rate %f' %
                       (reaction.id, str(reaction.bounds), model.objective.value))
```

```
ACALD blocked (bounds: (0, 0)), new growth rate 0.873922
ACALDt blocked (bounds: (0, 0)), new growth rate 0.873922
ACKr blocked (bounds: (0, 0)), new growth rate 0.873922
ACONTa blocked (bounds: (0, 0)), new growth rate -0.000000
ACONTb blocked (bounds: (0, 0)), new growth rate -0.000000
```

If we look at those knocked reactions, see that their bounds have all been reverted.

```
In [32]: [reaction.bounds for reaction in model.reactions[:5]]
```

```
Out[32]: [(-1000.0, 1000.0),
          (-1000.0, 1000.0),
          (-1000.0, 1000.0),
          (-1000.0, 1000.0),
          (-1000.0, 1000.0)]
```

Nested contexts are also supported

```
In [33]: print('original objective: ', model.objective.expression)
         with model:
             model.objective = 'ATPM'
             print('print objective in first context:', model.objective.expression)
             with model:
                 model.objective = 'ACALD'
                 print('print objective in second context:', model.objective.expression)
             print('objective after exiting second context:',
                   model.objective.expression)
         print('back to original objective:', model.objective.expression)
```

```
original objective:  -1.0*Biomass_Ecoli_core_reverse_2cdba + 1.0*Biomass_Ecoli_core
print objective in first context: -1.0*ATPM_reverse_5b752 + 1.0*ATPM
print objective in second context: 1.0*ACALD - 1.0*ACALD_reverse_fda2b
objective after exiting second context: -1.0*ATPM_reverse_5b752 + 1.0*ATPM
back to original objective: -1.0*Biomass_Ecoli_core_reverse_2cdba + 1.0*Biomass_Ecoli_core
```

Most methods that modify the model are supported like this including adding and removing reactions and metabolites and setting the objective. Supported methods and functions mention this in the corresponding documentation.

While it does not have any actual effect, for syntactic convenience it is also possible to refer to the model by a different name than outside the context. Such as

```
In [34]: with model as inner:
             inner.reactions.PFK.knock_out
```

CHAPTER 2

Building a Model

This simple example demonstrates how to create a model, create a reaction, and then add the reaction to the model.

We'll use the '3OAS140' reaction from the STM_1.0 model:

1.0 malACP[c] + 1.0 h[c] + 1.0 ddcaACP[c] → 1.0 co2[c] + 1.0 ACP[c] + 1.0 3omrsACP[c]

First, create the model and reaction.

```
In [1]: from __future__ import print_function
```

```
In [2]: from cobra import Model, Reaction, Metabolite
        # Best practise: SBML compliant IDs
        model = Model('example_model')

        reaction = Reaction('3OAS140')
        reaction.name = '3 oxoacyl acyl carrier protein synthase n C140 '
        reaction.subsystem = 'Cell Envelope Biosynthesis'
        reaction.lower_bound = 0.  # This is the default
        reaction.upper_bound = 1000.  # This is the default
```

We need to create metabolites as well. If we were using an existing model, we could use `Model.get_by_id` to get the appropriate Metabolite objects instead.

```
In [3]: ACP_c = Metabolite(
            'ACP_c',
            formula='C11H21N2O7PRS',
            name='acyl-carrier-protein',
            compartment='c')
        omrsACP_c = Metabolite(
            '3omrsACP_c',
            formula='C25H45N2O9PRS',
            name='3-Oxotetradecanoyl-acyl-carrier-protein',
            compartment='c')
        co2_c = Metabolite('co2_c', formula='CO2', name='CO2', compartment='c')
        malACP_c = Metabolite(
            'malACP_c',
            formula='C14H22N2O10PRS',
            name='Malonyl-acyl-carrier-protein',
```

```
        compartment='c')
    h_c = Metabolite('h_c', formula='H', name='H', compartment='c')
    ddcaACP_c = Metabolite(
        'ddcaACP_c',
        formula='C23H43N2O8PRS',
        name='Dodecanoyl-ACP-n-C120ACP',
        compartment='c')
```

Adding metabolites to a reaction requires using a dictionary of the metabolites and their stoichiometric coefficients. A group of metabolites can be added all at once, or they can be added one at a time.

```
In [4]: reaction.add_metabolites({
            malACP_c: -1.0,
            h_c: -1.0,
            ddcaACP_c: -1.0,
            co2_c: 1.0,
            ACP_c: 1.0,
            omrsACP_c: 1.0
        })

        reaction.reaction  # This gives a string representation of the reaction
```

```
Out[4]: 'ddcaACP_c + h_c + malACP_c --> 3omrsACP_c + ACP_c + co2_c'
```

The gene_reaction_rule is a boolean representation of the gene requirements for this reaction to be active as described in Schellenberger et al 2011 Nature Protocols 6(9):1290-307. We will assign the gene reaction rule string, which will automatically create the corresponding gene objects.

```
In [5]: reaction.gene_reaction_rule = '( STM2378 or STM1197 )'
        reaction.genes
```

```
Out[5]: frozenset({<Gene STM1197 at 0x7f2d85786898>, <Gene STM2378 at 0x7f2dc45437f0>})
```

At this point in time, the model is still empty

```
In [6]: print('%i reactions initially' % len(model.reactions))
        print('%i metabolites initially' % len(model.metabolites))
        print('%i genes initially' % len(model.genes))
```

```
0 reactions initially
0 metabolites initially
0 genes initially
```

We will add the reaction to the model, which will also add all associated metabolites and genes

```
In [7]: model.add_reactions([reaction])

        # Now there are things in the model
        print('%i reaction' % len(model.reactions))
        print('%i metabolites' % len(model.metabolites))
        print('%i genes' % len(model.genes))
```

```
1 reaction
6 metabolites
2 genes
```

We can iterate through the model objects to observe the contents

```
In [8]: # Iterate through the the objects in the model
        print("Reactions")
        print("---------")
        for x in model.reactions:
            print("%s : %s" % (x.id, x.reaction))
```

```
        print("")
        print("Metabolites")
        print("-----------")
        for x in model.metabolites:
            print('%9s : %s' % (x.id, x.formula))

        print("")
        print("Genes")
        print("-----")
        for x in model.genes:
            associated_ids = (i.id for i in x.reactions)
            print("%s is associated with reactions: %s" %
                  (x.id, "{" + ", ".join(associated_ids) + "}"))
```

```
Reactions
---------
3OAS140 : ddcaACP_c + h_c + malACP_c --> 3omrsACP_c + ACP_c + co2_c

Metabolites
-----------
    co2_c : CO2
 malACP_c : C14H22N2O10PRS
      h_c : H
3omrsACP_c : C25H45N2O9PRS
ddcaACP_c : C23H43N2O8PRS
    ACP_c : C11H21N2O7PRS

Genes
-----
STM1197 is associated with reactions: 3OAS140
STM2378 is associated with reactions: 3OAS140
```

Last we need to set the objective of the model. Here, we just want this to be the maximization of the flux in the single reaction we added and we do this by assigning the reaction's identifier to the `objective` property of the model.

```
In [9]: model.objective = '3OAS140'
```

The created objective is a symbolic algebraic expression and we can examine it by printing it

```
In [10]: print(model.objective.expression)
         print(model.objective.direction)
```

```
-1.0*3OAS140_reverse_65ddc + 1.0*3OAS140
max
```

which here shows that the solver will maximize the flux in the forward direction.

CHAPTER 3

Reading and Writing Models

Cobrapy supports reading and writing models in SBML (with and without FBC), JSON, YAML, MAT, and pickle formats. Generally, SBML with FBC version 2 is the preferred format for general use. The JSON format may be more useful for cobrapy-specific functionality.

The package also ships with test models in various formats for testing purposes.

```
In [1]: import cobra.test
        import os
        from os.path import join

        data_dir = cobra.test.data_dir

        print("mini test files: ")
        print(", ".join(i for i in os.listdir(data_dir) if i.startswith("mini")))

        textbook_model = cobra.test.create_test_model("textbook")
        ecoli_model = cobra.test.create_test_model("ecoli")
        salmonella_model = cobra.test.create_test_model("salmonella")
```

```
mini test files:
mini.json, mini.mat, mini.pickle, mini.yml, mini_cobra.xml, mini_fbc1.xml, mini_fbc2.xml, mini_fbc2.x
```

SBML

The Systems Biology Markup Language is an XML-based standard format for distributing models which has support for COBRA models through the FBC extension version 2.

Cobrapy has native support for reading and writing SBML with FBCv2. Please note that all id's in the model must conform to the SBML SID requirements in order to generate a valid SBML file.

```
In [2]: cobra.io.read_sbml_model(join(data_dir, "mini_fbc2.xml"))
```

```
Out[2]: <Model mini_textbook at 0x1074fd080>
```

```
In [3]: cobra.io.write_sbml_model(textbook_model, "test_fbc2.xml")
```

There are other dialects of SBML prior to FBC 2 which have previously been use to encode COBRA models. The primary ones is the "COBRA" dialect which used the "notes" fields in SBML files.

Cobrapy can use libsbml, which must be installed separately (see installation instructions) to read and write these files. When reading in a model, it will automatically detect whether FBC was used or not. When writing a model, the use_fbc_package flag can be used can be used to write files in this legacy "cobra" format.

Consider having the lxml package installed as it can speed up parsing considerably.

```
In [4]: cobra.io.read_sbml_model(join(data_dir, "mini_cobra.xml"))

Out[4]: <Model mini_textbook at 0x112fa6b38>

In [5]: cobra.io.write_sbml_model(
            textbook_model, "test_cobra.xml", use_fbc_package=False)
```

JSON

Cobrapy models have a JSON (JavaScript Object Notation) representation. This format was created for interoperability with escher.

```
In [6]: cobra.io.load_json_model(join(data_dir, "mini.json"))

Out[6]: <Model mini_textbook at 0x113061080>

In [7]: cobra.io.save_json_model(textbook_model, "test.json")
```

YAML

Cobrapy models have a YAML (YAML Ain't Markup Language) representation. This format was created for more human readable model representations and automatic diffs between models.

```
In [8]: cobra.io.load_yaml_model(join(data_dir, "mini.yml"))

Out[8]: <Model mini_textbook at 0x113013390>

In [9]: cobra.io.save_yaml_model(textbook_model, "test.yml")
```

MATLAB

Often, models may be imported and exported solely for the purposes of working with the same models in cobrapy and the MATLAB cobra toolbox. MATLAB has its own ".mat" format for storing variables. Reading and writing to these mat files from python requires scipy.

A mat file can contain multiple MATLAB variables. Therefore, the variable name of the model in the MATLAB file can be passed into the reading function:

```
In [10]: cobra.io.load_matlab_model(
             join(data_dir, "mini.mat"), variable_name="mini_textbook")

Out[10]: <Model mini_textbook at 0x113000b70>
```

If the mat file contains only a single model, cobra can figure out which variable to read from, and the variable_name parameter is unnecessary.

```
In [11]: cobra.io.load_matlab_model(join(data_dir, "mini.mat"))

Out[11]: <Model mini_textbook at 0x113758438>
```

Saving models to mat files is also relatively straightforward

```
In [12]: cobra.io.save_matlab_model(textbook_model, "test.mat")
```

Pickle

Cobra models can be serialized using the python serialization format, pickle.

Please note that use of the pickle format is generally not recommended for most use cases. JSON, SBML, and MAT are generally the preferred formats.

CHAPTER 4

Simulating with FBA

Simulations using flux balance analysis can be solved using `Model.optimize()`. This will maximize or minimize (maximizing is the default) flux through the objective reactions.

```
In [1]: import cobra.test
        model = cobra.test.create_test_model("textbook")
```

Running FBA

```
In [2]: solution = model.optimize()
        print(solution)
```

```
<Solution 0.874 at 0x112eb3d30>
```

The Model.optimize() function will return a Solution object. A solution object has several attributes:

- `objective_value`: the objective value
- `status`: the status from the linear programming solver
- `fluxes`: a pandas series with flux indexed by reaction identifier. The flux for a reaction variable is the difference of the primal values for the forward and reverse reaction variables.
- `shadow_prices`: a pandas series with shadow price indexed by the metabolite identifier.

For example, after the last call to `model.optimize()`, if the optimization succeeds it's status will be optimal. In case the model is infeasible an error is raised.

```
In [3]: solution.objective_value
```

```
Out[3]: 0.8739215069684307
```

The solvers that can be used with cobrapy are so fast that for many small to mid-size models computing the solution can be even faster than it takes to collect the values from the solver and convert to them python objects. With `model.optimize`, we gather values for all reactions and metabolites and that can take a significant amount of time if done repeatedly. If we are only interested in the flux value of a single reaction or the objective, it is faster to instead use `model.slim_optimize` which only does the optimization and returns the objective value leaving it up to you to fetch other values that you may need.

```
In [4]: %%time
        model.optimize().objective_value

CPU times: user 3.84 ms, sys: 672 µs, total: 4.51 ms
Wall time: 6.16 ms

Out[4]: 0.8739215069684307

In [5]: %%time
        model.slim_optimize()

CPU times: user 229 µs, sys: 19 µs, total: 248 µs
Wall time: 257 µs

Out[5]: 0.8739215069684307
```

Analyzing FBA solutions

Models solved using FBA can be further analyzed by using summary methods, which output printed text to give a quick representation of model behavior. Calling the summary method on the entire model displays information on the input and output behavior of the model, along with the optimized objective.

```
In [6]: model.summary()

IN FLUXES        OUT FLUXES    OBJECTIVES
---------------  ------------  ----------------------
o2_e      21.8   h2o_e  29.2   Biomass_Ecol...  0.874
glc__D_e  10     co2_e  22.8
nh4_e      4.77  h_e    17.5
pi_e       3.21
```

In addition, the input-output behavior of individual metabolites can also be inspected using summary methods. For instance, the following commands can be used to examine the overall redox balance of the model

```
In [7]: model.metabolites.nadh_c.summary()

PRODUCING REACTIONS -- Nicotinamide adenine dinucleotide - reduced (nadh_c)
---------------------------------------------------------------------------
%       FLUX  RXN ID      REACTION
----  ------  ----------  ------------------------------------------------
42%    16     GAPD        g3p_c + nad_c + pi_c <=> 13dpg_c + h_c + nadh_c
24%     9.28  PDH         coa_c + nad_c + pyr_c --> accoa_c + co2_c + nadh_c
13%     5.06  AKGDH       akg_c + coa_c + nad_c --> co2_c + nadh_c + succ...
13%     5.06  MDH         mal__L_c + nad_c <=> h_c + nadh_c + oaa_c
8%      3.1   Biomass...  1.496 3pg_c + 3.7478 accoa_c + 59.81 atp_c + 0....

CONSUMING REACTIONS -- Nicotinamide adenine dinucleotide - reduced (nadh_c)
---------------------------------------------------------------------------
%       FLUX  RXN ID      REACTION
----  ------  ----------  ------------------------------------------------
100%   38.5   NADH16      4.0 h_c + nadh_c + q8_c --> 3.0 h_e + nad_c + q...
```

Or to get a sense of the main energy production and consumption reactions

```
In [8]: model.metabolites.atp_c.summary()

PRODUCING REACTIONS -- ATP (atp_c)
----------------------------------
%      FLUX  RXN ID      REACTION
---  ------  ----------  ------------------------------------------------
67%  45.5    ATPS4r      adp_c + 4.0 h_e + pi_c <=> atp_c + h2o_c + 3.0 h_c
23%  16      PGK         3pg_c + atp_c <=> 13dpg_c + adp_c
7%    5.06   SUCOAS      atp_c + coa_c + succ_c <=> adp_c + pi_c + succoa_c
```

```
3%    1.76   PYK         adp_c + h_c + pep_c --> atp_c + pyr_c

CONSUMING REACTIONS -- ATP (atp_c)
----------------------------------
%      FLUX  RXN ID      REACTION
---  ------  ----------  --------------------------------------------------
76%  52.3    Biomass...  1.496 3pg_c + 3.7478 accoa_c + 59.81 atp_c + 0....
12%   8.39   ATPM        atp_c + h2o_c --> adp_c + h_c + pi_c
11%   7.48   PFK         atp_c + f6p_c --> adp_c + fdp_c + h_c
0%    0.223  GLNS        atp_c + glu__L_c + nh4_c --> adp_c + gln__L_c +...
```

Changing the Objectives

The objective function is determined from the objective_coefficient attribute of the objective reaction(s). Generally, a "biomass" function which describes the composition of metabolites which make up a cell is used.

```
In [9]: biomass_rxn = model.reactions.get_by_id("Biomass_Ecoli_core")
```

Currently in the model, there is only one reaction in the objective (the biomass reaction), with an linear coefficient of 1.

```
In [10]: from cobra.util.solver import linear_reaction_coefficients
         linear_reaction_coefficients(model)
```

```
Out[10]: {<Reaction Biomass_Ecoli_core at 0x112eab4a8>: 1.0}
```

The objective function can be changed by assigning Model.objective, which can be a reaction object (or just it's name), or a `dict` of `{Reaction: objective_coefficient}`.

```
In [11]: # change the objective to ATPM
         model.objective = "ATPM"

         # The upper bound should be 1000, so that we get
         # the actual optimal value
         model.reactions.get_by_id("ATPM").upper_bound = 1000.
         linear_reaction_coefficients(model)
```

```
Out[11]: {<Reaction ATPM at 0x112eab470>: 1.0}
```

```
In [12]: model.optimize().objective_value
```

```
Out[12]: 174.99999999999966
```

We can also have more complicated objectives including quadratic terms.

Running FVA

FBA will not give always give unique solution, because multiple flux states can achieve the same optimum. FVA (or flux variability analysis) finds the ranges of each metabolic flux at the optimum.

```
In [13]: from cobra.flux_analysis import flux_variability_analysis
```

```
In [14]: flux_variability_analysis(model, model.reactions[:10])
```

```
Out[14]: maximum       minimum
         ACALD  -2.208811e-30 -5.247085e-14
         ACALDt  0.000000e+00 -5.247085e-14
         ACKr    0.000000e+00 -8.024953e-14
         ACONTa  2.000000e+01  2.000000e+01
         ACONTb  2.000000e+01  2.000000e+01
```

```
ACt2r   0.000000e+00 -8.024953e-14
ADK1    3.410605e-13  0.000000e+00
AKGDH   2.000000e+01  2.000000e+01
AKGt2r  0.000000e+00 -2.902643e-14
ALCD2x  0.000000e+00 -4.547474e-14
```

Setting parameter `fraction_of_optimium=0.90` would give the flux ranges for reactions at 90% optimality.

```
In [15]: cobra.flux_analysis.flux_variability_analysis(
             model, model.reactions[:10], fraction_of_optimum=0.9)
```

```
Out[15]: maximum   minimum
         ACALD   0.000000e+00 -2.692308
         ACALDt  0.000000e+00 -2.692308
         ACKr    6.635712e-30 -4.117647
         ACONTa  2.000000e+01  8.461538
         ACONTb  2.000000e+01  8.461538
         ACt2r   0.000000e+00 -4.117647
         ADK1    1.750000e+01  0.000000
         AKGDH   2.000000e+01  2.500000
         AKGt2r  2.651196e-16 -1.489362
         ALCD2x  0.000000e+00 -2.333333
```

The standard FVA may contain loops, i.e. high absolute flux values that only can be high if they are allowed to participate in loops (a mathematical artifact that cannot happen in vivo). Use the `loopless` argument to avoid such loops. Below, we can see that FRD7 and SUCDi reactions can participate in loops but that this is avoided when using the looplesss FVA.

```
In [16]: loop_reactions = [model.reactions.FRD7, model.reactions.SUCDi]
         flux_variability_analysis(model, reaction_list=loop_reactions, loopless=False)
```

```
Out[16]: maximum  minimum
         FRD7     980.0      0.0
         SUCDi   1000.0     20.0
```

```
In [17]: flux_variability_analysis(model, reaction_list=loop_reactions, loopless=True)
```

```
Out[17]: maximum  minimum
         FRD7       0.0      0.0
         SUCDi     20.0     20.0
```

Running FVA in summary methods

Flux variability analysis can also be embedded in calls to summary methods. For instance, the expected variability in substrate consumption and product formation can be quickly found by

```
In [18]: model.optimize()
         model.summary(fva=0.95)
```

```
IN FLUXES                    OUT FLUXES                   OBJECTIVES
---------------------------  ---------------------------  ------------
id          Flux  Range      id          Flux  Range      ATPM  175
--------  ------  ----------  --------  ------  ----------
o2_e          60  [55.9, 60]  co2_e         60  [54.2, 60]
glc__D_e      10  [9.5, 10]   h2o_e         60  [54.2, 60]
nh4_e          0  [0, 0.673]  for_e          0  [0, 5.83]
pi_e           0  [0, 0.171]  h_e            0  [0, 5.83]
                               ac_e           0  [0, 2.06]
                               acald_e        0  [0, 1.35]
                               pyr_e          0  [0, 1.35]
                               etoh_e         0  [0, 1.17]
```

```
lac__D_e        0   [0, 1.13]
succ_e          0   [0, 0.875]
akg_e           0   [0, 0.745]
glu__L_e        0   [0, 0.673]
```

Similarly, variability in metabolite mass balances can also be checked with flux variability analysis.

```
In [19]: model.metabolites.pyr_c.summary(fva=0.95)
```

```
PRODUCING REACTIONS -- Pyruvate (pyr_c)
---------------------------------------
%       FLUX  RANGE          RXN ID      REACTION
----  ------  ------------  ----------  ----------------------------------------
50%       10  [1.25, 18.8]  PYK         adp_c + h_c + pep_c --> atp_c + pyr_c
50%       10  [9.5, 10]     GLCpts      glc__D_e + pep_c --> g6p_c + pyr_c
0%         0  [0, 8.75]     ME1         mal__L_c + nad_c --> co2_c + nadh_c +...
0%         0  [0, 8.75]     ME2         mal__L_c + nadp_c --> co2_c + nadph_c...

CONSUMING REACTIONS -- Pyruvate (pyr_c)
---------------------------------------
%       FLUX  RANGE          RXN ID      REACTION
----  ------  ------------  ----------  ----------------------------------------
100%      20  [13, 28.8]    PDH         coa_c + nad_c + pyr_c --> accoa_c + c...
0%         0  [0, 8.75]     PPS         atp_c + h2o_c + pyr_c --> amp_c + 2.0...
0%         0  [0, 5.83]     PFL         coa_c + pyr_c --> accoa_c + for_c
0%         0  [0, 1.35]     PYRt2       h_e + pyr_e <=> h_c + pyr_c
0%         0  [0, 1.13]     LDH_D       lac__D_c + nad_c <=> h_c + nadh_c + p...
0%         0  [0, 0.132]    Biomass...  1.496 3pg_c + 3.7478 accoa_c + 59.81 ...
```

In these summary methods, the values are reported as a the center point +/- the range of the FVA solution, calculated from the maximum and minimum values.

Running pFBA

Parsimonious FBA (often written pFBA) finds a flux distribution which gives the optimal growth rate, but minimizes the total sum of flux. This involves solving two sequential linear programs, but is handled transparently by cobrapy. For more details on pFBA, please see Lewis et al. (2010).

```
In [20]: model.objective = 'Biomass_Ecoli_core'
         fba_solution = model.optimize()
         pfba_solution = cobra.flux_analysis.pfba(model)
```

These functions should give approximately the same objective value.

```
In [21]: abs(fba_solution.fluxes["Biomass_Ecoli_core"] - pfba_solution.fluxes[
             "Biomass_Ecoli_core"])
```

```
Out[21]: 7.7715611723760958e-16
```

CHAPTER 5

Simulating Deletions

```
In [1]: import pandas
        from time import time

        import cobra.test
        from cobra.flux_analysis import (
            single_gene_deletion, single_reaction_deletion, double_gene_deletion,
            double_reaction_deletion)

        cobra_model = cobra.test.create_test_model("textbook")
        ecoli_model = cobra.test.create_test_model("ecoli")
```

Knocking out single genes and reactions

A commonly asked question when analyzing metabolic models is what will happen if a certain reaction was not allowed to have any flux at all. This can tested using cobrapy by

```
In [2]: print('complete model: ', cobra_model.optimize())
        with cobra_model:
            cobra_model.reactions.PFK.knock_out()
            print('pfk knocked out: ', cobra_model.optimize())
```

```
complete model:  <Solution 0.874 at 0x1118cc898>
pfk knocked out:  <Solution 0.704 at 0x1118cc5c0>
```

For evaluating genetic manipulation strategies, it is more interesting to examine what happens if given genes are knocked out as doing so can affect no reactions in case of redundancy, or more reactions if gene when is participating in more than one reaction.

```
In [3]: print('complete model: ', cobra_model.optimize())
        with cobra_model:
            cobra_model.genes.b1723.knock_out()
            print('pfkA knocked out: ', cobra_model.optimize())
            cobra_model.genes.b3916.knock_out()
            print('pfkB knocked out: ', cobra_model.optimize())
```

```
complete model:  <Solution 0.874 at 0x1108b81d0>
pfkA knocked out:  <Solution 0.874 at 0x1108b80b8>
pfkB knocked out:  <Solution 0.704 at 0x1108b8128>
```

Single Deletions

Perform all single gene deletions on a model

```
In [4]: deletion_results = single_gene_deletion(cobra_model)
```

These can also be done for only a subset of genes

```
In [5]: single_gene_deletion(cobra_model, cobra_model.genes[:20])
```

```
Out[5]: flux   status
        b0116  0.782351  optimal
        b0118  0.873922  optimal
        b0351  0.873922  optimal
        b0356  0.873922  optimal
        b0474  0.873922  optimal
        b0726  0.858307  optimal
        b0727  0.858307  optimal
        b1241  0.873922  optimal
        b1276  0.873922  optimal
        b1478  0.873922  optimal
        b1849  0.873922  optimal
        b2296  0.873922  optimal
        b2587  0.873922  optimal
        b3115  0.873922  optimal
        b3732  0.374230  optimal
        b3733  0.374230  optimal
        b3734  0.374230  optimal
        b3735  0.374230  optimal
        b3736  0.374230  optimal
        s0001  0.211141  optimal
```

This can also be done for reactions

```
In [6]: single_reaction_deletion(cobra_model, cobra_model.reactions[:20])
```

```
Out[6]: flux   status
        ACALD                8.739215e-01  optimal
        ACALDt               8.739215e-01  optimal
        ACKr                 8.739215e-01  optimal
        ACONTa              -5.039994e-13  optimal
        ACONTb              -1.477823e-12  optimal
        ACt2r                8.739215e-01  optimal
        ADK1                 8.739215e-01  optimal
        AKGDH                8.583074e-01  optimal
        AKGt2r               8.739215e-01  optimal
        ALCD2x               8.739215e-01  optimal
        ATPM                 9.166475e-01  optimal
        ATPS4r               3.742299e-01  optimal
        Biomass_Ecoli_core   0.000000e+00  optimal
        CO2t                 4.616696e-01  optimal
        CS                   1.129472e-12  optimal
        CYTBD                2.116629e-01  optimal
        D_LACt2              8.739215e-01  optimal
        ENO                  1.161773e-14  optimal
```

```
ETOHt2r              8.739215e-01  optimal
EX_ac_e              8.739215e-01  optimal
```

Double Deletions

Double deletions run in a similar way. Passing in `return_frame=True` will cause them to format the results as a `pandas.DataFrame`.

```
In [7]: double_gene_deletion(
            cobra_model, cobra_model.genes[-5:], return_frame=True).round(4)
```

```
Out[7]: b2464   b0008   b2935   b2465  b3919
        b2464  0.8739  0.8648  0.8739  0.8739  0.704
        b0008  0.8648  0.8739  0.8739  0.8739  0.704
        b2935  0.8739  0.8739  0.8739  0.0000  0.704
        b2465  0.8739  0.8739  0.0000  0.8739  0.704
        b3919  0.7040  0.7040  0.7040  0.7040  0.704
```

By default, the double deletion function will automatically use multiprocessing, splitting the task over up to 4 cores if they are available. The number of cores can be manually specified as well. Setting use of a single core will disable use of the multiprocessing library, which often aids debugging.

```
In [8]: start = time()  # start timer()
        double_gene_deletion(
            ecoli_model, ecoli_model.genes[:300], number_of_processes=2)
        t1 = time() - start
        print("Double gene deletions for 200 genes completed in "
              "%.2f sec with 2 cores" % t1)

        start = time()  # start timer()
        double_gene_deletion(
            ecoli_model, ecoli_model.genes[:300], number_of_processes=1)
        t2 = time() - start
        print("Double gene deletions for 200 genes completed in "
              "%.2f sec with 1 core" % t2)

        print("Speedup of %.2fx" % (t2 / t1))
```

```
Double gene deletions for 200 genes completed in 33.26 sec with 2 cores
Double gene deletions for 200 genes completed in 45.38 sec with 1 core
Speedup of 1.36x
```

Double deletions can also be run for reactions.

```
In [9]: double_reaction_deletion(
            cobra_model, cobra_model.reactions[2:7], return_frame=True).round(4)
```

```
Out[9]: ACKr   ACONTa  ACONTb   ACt2r    ADK1
        ACKr    0.8739     0.0     0.0  0.8739  0.8739
        ACONTa  0.0000     0.0     0.0  0.0000  0.0000
        ACONTb  0.0000     0.0     0.0  0.0000 -0.0000
        ACt2r   0.8739     0.0     0.0  0.8739  0.8739
        ADK1    0.8739     0.0    -0.0  0.8739  0.8739
```

CHAPTER 6

Production envelopes

Production envelopes (aka phenotype phase planes) will show distinct phases of optimal growth with different use of two different substrates. For more information, see Edwards et al.

Cobrapy supports calculating these production envelopes and they can easily be plotted using your favorite plotting package. Here, we will make one for the "textbook" *E. coli* core model and demonstrate plotting using matplotlib.

```
In [1]: import cobra.test
        from cobra.flux_analysis import production_envelope

        model = cobra.test.create_test_model("textbook")
```

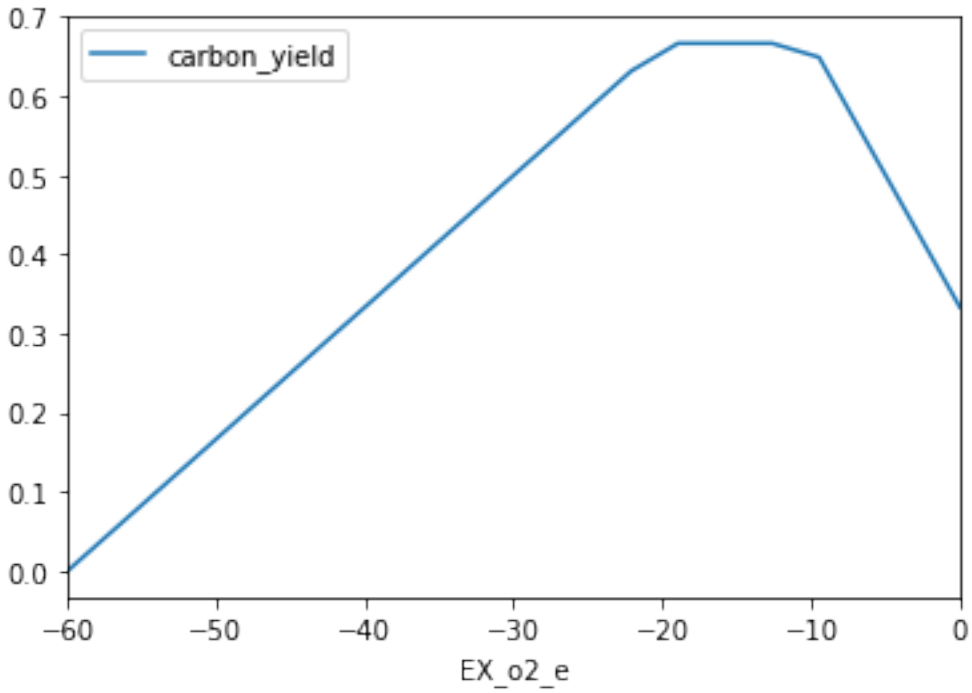
We want to make a phenotype phase plane to evaluate uptakes of Glucose and Oxygen.

```
In [2]: prod_env = production_envelope(model, ["EX_glc__D_e", "EX_o2_e"])

In [3]: prod_env.head()

Out[3]: EX_glc__D_e    EX_o2_e direction  flux
        0        -10.0 -60.000000   minimum   0.0
        1        -10.0 -56.842105   minimum   0.0
        2        -10.0 -53.684211   minimum   0.0
        3        -10.0 -50.526316   minimum   0.0
        4        -10.0 -47.368421   minimum   0.0
```

If we specify the carbon source, we can also get the carbon and mass yield. For example, temporarily setting the objective to produce acetate instead we could get production envelope as follows and pandas to quickly plot the results.

```
In [4]: prod_env = production_envelope(
            model, ["EX_o2_e"], objective="EX_ac_e", c_source="EX_glc__D_e")

In [5]: prod_env.head()

Out[5]: EX_o2_e carbon_source  carbon_yield direction  flux  mass_yield
        0 -60.000000   EX_glc__D_e           0.0   minimum   0.0         0.0
        1 -56.842105   EX_glc__D_e           0.0   minimum   0.0         0.0
        2 -53.684211   EX_glc__D_e           0.0   minimum   0.0         0.0
        3 -50.526316   EX_glc__D_e           0.0   minimum   0.0         0.0
        4 -47.368421   EX_glc__D_e           0.0   minimum   0.0         0.0
```

```
In [6]: %matplotlib inline

In [7]: prod_env[prod_env.direction == 'maximum'].plot(
            kind='line', x='EX_o2_e', y='carbon_yield')

Out[7]: <matplotlib.axes._subplots.AxesSubplot at 0x10fc37630>
```



Previous versions of cobrapy included more tailored plots for phase planes which have now been dropped in order to improve maintainability and enhance the focus of cobrapy. Plotting for cobra models is intended for another package.

CHAPTER 7

Flux sampling

Basic usage

The easiest way to get started with flux sampling is using the `sample` function in the `flux_analysis` submodule. `sample` takes at least two arguments: a cobra model and the number of samples you want to generate.

```
In [1]: from cobra.test import create_test_model
        from cobra.flux_analysis import sample

        model = create_test_model("textbook")
        s = sample(model, 100)
        s.head()
```

```
Out[1]: ACALD    ACALDt      ACKr     ACONTa     ACONTb     ACt2r       ADK1  \
        0 -3.706944 -0.163964 -0.295823   8.975852   8.975852 -0.295823   4.847986
        1 -1.340710 -0.175665 -0.429169  11.047827  11.047827 -0.429169   2.901598
        2 -1.964087 -0.160334 -0.618029   9.811474   9.811474 -0.618029  17.513791
        3 -0.838442 -0.123865 -0.376067  11.869552  11.869552 -0.376067   7.769872
        4 -0.232088 -0.034346 -1.067684   7.972039   7.972039 -1.067684   5.114975

              AKGDH    AKGt2r    ALCD2x    ...          RPI   SUCCt2_2     SUCCt3  \
        0  6.406533 -0.081797 -3.542980    ...    -1.649393  20.917568  20.977290
        1  7.992916 -0.230564 -1.165045    ...    -0.066975  24.735567  24.850041
        2  8.635576 -0.284992 -1.803753    ...    -4.075515  23.425719  23.470968
        3  9.765178 -0.325219 -0.714577    ...    -0.838094  23.446704  23.913036
        4  5.438125 -0.787864 -0.197742    ...    -3.109205   8.902309   9.888083

                SUCDi    SUCOAS      TALA       THD2      TKT1      TKT2       TPI
        0  744.206008 -6.406533  1.639515   1.670533  1.639515  1.635542  6.256787
        1  710.481004 -7.992916  0.056442   9.680476  0.056442  0.052207  7.184752
        2  696.114154 -8.635576  4.063291  52.316496  4.063291  4.058376  5.122237
        3  595.787313 -9.765178  0.822987  36.019720  0.822987  0.816912  8.364314
        4  584.552692 -5.438125  3.088152  12.621811  3.088152  3.079686  6.185089

        [5 rows x 95 columns]
```

By default sample uses the `optgp` method based on the method presented here as it is suited for larger models and can run in parallel. By default the sampler uses a single process. This can be changed by using the `processes` argument.

```
In [2]: print("One process:")
        %time s = sample(model, 1000)
        print("Two processes:")
        %time s = sample(model, 1000, processes=2)
```

```
One process:
CPU times: user 5.31 s, sys: 433 ms, total: 5.74 s
Wall time: 5.27 s
Two processes:
CPU times: user 217 ms, sys: 488 ms, total: 705 ms
Wall time: 2.8 s
```

Alternatively you can also user Artificial Centering Hit-and-Run for sampling by setting the method to `achr`. `achr` does not support parallel execution but has good convergence and is almost Markovian.

```
In [3]: s = sample(model, 100, method="achr")
```

In general setting up the sampler is expensive since initial search directions are generated by solving many linear programming problems. Thus, we recommend to generate as many samples as possible in one go. However, this might require finer control over the sampling procedure as described in the following section.

Advanced usage

Sampler objects

The sampling process can be controlled on a lower level by using the sampler classes directly.

```
In [4]: from cobra.flux_analysis.sampling import OptGPSampler, ACHRSampler
```

Both sampler classes have standardized interfaces and take some additional argument. For instance the `thinning` factor. "Thinning" means only recording samples every n iterations. A higher thinning factors mean less correlated samples but also larger computation times. By default the samplers use a thinning factor of 100 which creates roughly uncorrelated samples. If you want less samples but better mixing feel free to increase this parameter. If you want to study convergence for your own model you might want to set it to 1 to obtain all iterates.

```
In [5]: achr = ACHRSampler(model, thinning=10)
```

`OptGPSampler` has an additional `processes` argument specifying how many processes are used to create parallel sampling chains. This should be in the order of your CPU cores for maximum efficiency. As noted before class initialization can take up to a few minutes due to generation of initial search directions. Sampling on the other hand is quick.

```
In [6]: optgp = OptGPSampler(model, processes=4)
```

Sampling and validation

Both samplers have a sample function that generates samples from the initialized object and act like the `sample` function described above, only that this time it will only accept a single argument, the number of samples. For `OptGPSampler` the number of samples should be a multiple of the number of processes, otherwise it will be increased to the nearest multiple automatically.

```
In [7]: s1 = achr.sample(100)

        s2 = optgp.sample(100)
```

You can call `sample` repeatedly and both samplers are optimized to generate large amount of samples without falling into "numerical traps". All sampler objects have a `validate` function in order to check if a set of points are feasible and give detailed information about feasibility violations in a form of a short code denoting feasibility. Here the short code is a combination of any of the following letters:

- "v" - valid point
- "l" - lower bound violation
- "u" - upper bound violation
- "e" - equality violation (meaning the point is not a steady state)

For instance for a random flux distribution (should not be feasible):

```
In [8]: import numpy as np

        bad = np.random.uniform(-1000, 1000, size=len(model.reactions))
        achr.validate(np.atleast_2d(bad))
```

```
Out[8]: array(['le'],
              dtype='<U3')
```

And for our generated samples:

```
In [9]: achr.validate(s1)
```

```
Out[9]: array(['v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v',
               'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v',
               'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v',
               'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v',
               'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v',
               'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v',
               'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v',
               'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v', 'v'],
              dtype='<U3')
```

Batch sampling

Sampler objects are made for generating billions of samples, however using the `sample` function might quickly fill up your RAM when working with genome-scale models. Here, the `batch` method of the sampler objects might come in handy. `batch` takes two arguments, the number of samples in each batch and the number of batches. This will make sense with a small example.

Let's assume we want to quantify what proportion of our samples will grow. For that we might want to generate 10 batches of 50 samples each and measure what percentage of the individual 100 samples show a growth rate larger than 0.1. Finally, we want to calculate the mean and standard deviation of those individual percentages.

```
In [10]: counts = [np.mean(s.Biomass_Ecoli_core > 0.1) for s in optgp.batch(100, 10)]
         print("Usually {:.2f}% +- {:.2f}% grow...".format(
             np.mean(counts) * 100.0, np.std(counts) * 100.0))
```

```
Usually 8.70% +- 2.72% grow...
```

Adding constraints

Flux sampling will respect additional contraints defined in the model. For instance we can add a constraint enforcing growth in asimilar manner as the section before.

```
In [11]: co = model.problem.Constraint(model.reactions.Biomass_Ecoli_core.flux_expression, lb=0.1)
         model.add_cons_vars([co])
```

Note that this is only for demonstration purposes. usually you could set the lower bound of the reaction directly instead of creating a new constraint.

```
In [12]: s = sample(model, 10)
         print(s.Biomass_Ecoli_core)
```

```
0    0.175547
1    0.111499
2    0.123073
3    0.151874
4    0.122541
5    0.121878
6    0.147333
7    0.106499
8    0.174448
9    0.143273
Name: Biomass_Ecoli_core, dtype: float64
```

As we can see our new constraint was respected.

CHAPTER 8

Loopless FBA

The goal of this procedure is identification of a thermodynamically consistent flux state without loops, as implied by the name. You can find a more detailed description in the *method* section at the end of the notebook.

```
In [1]: %matplotlib inline
        import plot_helper

        import cobra.test
        from cobra import Reaction, Metabolite, Model
        from cobra.flux_analysis.loopless import add_loopless, loopless_solution
        from cobra.flux_analysis import pfba
```

Loopless solution

Classical loopless approaches as described below are computationally expensive to solve due to the added mixed-integer constraints. A much faster, and pragmatic approach is instead to post-process flux distributions to simply set fluxes to zero wherever they can be zero without changing the fluxes of any exchange reactions in the model. CycleFreeFlux is an algorithm that can be used to achieve this and in cobrapy it is implemented in the `cobra.flux_analysis.loopless_solution` function. `loopless_solution` will identify the closest flux distribution (using only loopless elementary flux modes) to the original one. Note that this will not remove loops which you explicitly requested, for instance by forcing a loop reaction to carry non-zero flux.

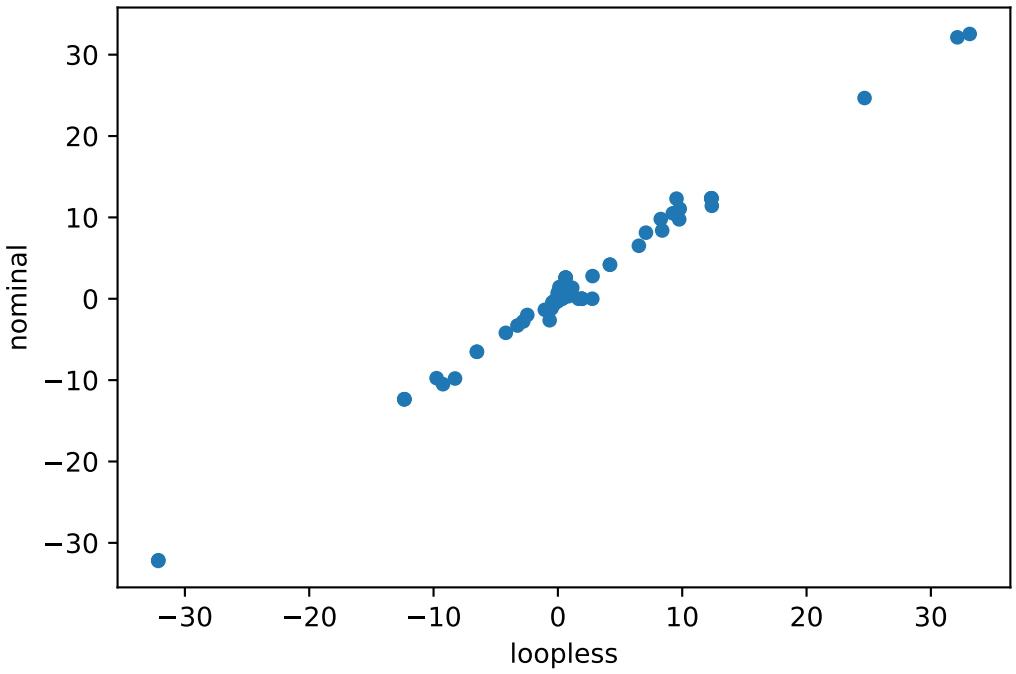
Using a larger model than the simple example above, this can be demonstrated as follows

```
In [2]: salmonella = cobra.test.create_test_model('salmonella')
        nominal = salmonella.optimize()
        loopless = loopless_solution(salmonella)
```

```
In [3]: import pandas
        df = pandas.DataFrame(dict(loopless=loopless.fluxes, nominal=nominal.fluxes))
```

```
In [4]: df.plot.scatter(x='loopless', y='nominal')
```

```
Out[4]: <matplotlib.axes._subplots.AxesSubplot at 0x10f7cb3c8>
```



This functionality can also be used in FVA by using the `loopless=True` argument to avoid getting high flux ranges for reactions that essentially only can reach high fluxes if they are allowed to participate in loops (see the simulation notebook) leading to much narrower flux ranges.

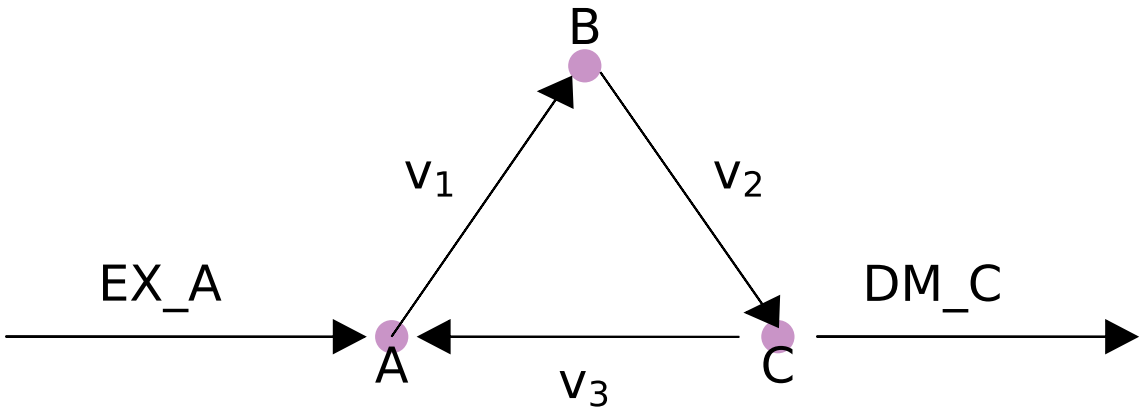
Loopless model

Cobrapy also includes the "classical" loopless formulation by Schellenberger et. al. implemented in `cobra.flux_analysis.add_loopless` modify the model with additional mixed-integer constraints that make thermodynamically infeasible loops impossible. This is much slower than the strategy provided above and should only be used if one of the two following cases applies:

1. You want to combine a non-linear (e.g. quadratic) objective with the loopless condition
2. You want to force the model to be infeasible in the presence of loops independent of the set reaction bounds.

We will demonstrate this with a toy model which has a simple loop cycling A $\rightarrow$ B $\rightarrow$ C $\rightarrow$ A, with A allowed to enter the system and C allowed to leave. A graphical view of the system is drawn below:

```
In [5]: plot_helper.plot_loop()
```




```
In [6]: model = Model()
        model.add_metabolites([Metabolite(i) for i in "ABC"])
        model.add_reactions([Reaction(i) for i in ["EX_A", "DM_C", "v1", "v2", "v3"]])

        model.reactions.EX_A.add_metabolites({"A": 1})
        model.reactions.DM_C.add_metabolites({"C": -1})

        model.reactions.v1.add_metabolites({"A": -1, "B": 1})
        model.reactions.v2.add_metabolites({"B": -1, "C": 1})
        model.reactions.v3.add_metabolites({"C": -1, "A": 1})

        model.objective = 'DM_C'
```

While this model contains a loop, a flux state exists which has no flux through reaction v_3, and is identified by loopless FBA.

```
In [7]: with model:
            add_loopless(model)
            solution = model.optimize()
        print("loopless solution: status = " + solution.status)
        print("loopless solution flux: v3 = %.1f" % solution.fluxes["v3"])
```

```
loopless solution: status = optimal
loopless solution flux: v3 = 0.0
```

If there is no forced flux through a loopless reaction, parsimonious FBA will also have no flux through the loop.

```
In [8]: solution = pfba(model)
        print("parsimonious solution: status = " + solution.status)
        print("loopless solution flux: v3 = %.1f" % solution.fluxes["v3"])
```

```
parsimonious solution: status = optimal
loopless solution flux: v3 = 0.0
```

However, if flux is forced through v_3, then there is no longer a feasible loopless solution, but the parsimonious solution will still exist.

```
In [9]: model.reactions.v3.lower_bound = 1
        with model:
            add_loopless(model)
            try:
                solution = model.optimize()
```

```
            except:
                print('model is infeasible')
```

```
model is infeasible
```

```
cobra/util/solver.py:398 UserWarning: solver status is 'infeasible'
```

```
In [10]: solution = pfba(model)
         print("parsimonious solution: status = " + solution.status)
         print("loopless solution flux: v3 = %.1f" % solution.fluxes["v3"])
```

```
parsimonious solution: status = optimal
loopless solution flux: v3 = 1.0
```

Method

`loopless_solution` is based on a given reference flux distribution. It will look for a new flux distribution with the following requirements:

1. The objective value is the same as in the reference fluxes.
2. All exchange fluxes have the same value as in the reference distribution.
3. All non-exchange fluxes have the same sign (flow in the same direction) as the reference fluxes.
4. The sum of absolute non-exchange fluxes is minimized.

As proven in the original publication this will identify the "least-loopy" solution closest to the reference fluxes.

If you are using `add_loopless` this will use the method described here. In summary, it will add $G \approx \Delta G$ proxy variables and make loops thermodynamically infeasible. This is achieved by the following formulation.

to

$$
\begin{aligned}
&\text{maximize } v_{obj} \\
s.t. \quad & Sv = 0 \\
& lb_j \leq v_j \leq ub_j \\
& -M \cdot (1 - a_i) \leq v_i \leq M \cdot a_i \\
& -1000 a_i + (1 - a_i) \leq G_i \leq -a_i + 1000(1 - a_i) \\
& N_{int} G = 0 \\
& a_i \in \{0, 1\} (8.1)
\end{aligned}
$$

$$
\begin{aligned}
& Sv = 0 \\
& -M \cdot (1 - a_i) \leq v_i \leq M \cdot a_i \\
& N_{int} G = 0
\end{aligned}
$$

Here the index j runs over all reactions and the index i only over internal ones. a_i are indicator variables which equal one if the reaction flux flows in hte forward direction and 0 otherwise. They are used to force the G proxies to always carry the opposite sign of the flux (as it is the case for the "real" ΔG values). N_{int} is the nullspace matrix for internal reactions and is used to find thermodinamically "correct" values for G.

CHAPTER 9

Gapfillling

Model gap filling is the task of figuring out which reactions have to be added to a model to make it feasible. Several such algorithms have been reported e.g. Kumar et al. 2009 and Reed et al. 2006. Cobrapy has a gap filling implementation that is very similar to that of Reed et al. where we use a mixed-integer linear program to figure out the smallest number of reactions that need to be added for a user-defined collection of reactions, i.e. a universal model. Briefly, the problem that we try to solve is

Minimize:

$$\sum_i c_i * z_i$$

subject to

$$Sv = 0$$

$$v^\star \geq t$$

$$l_i \leq v_i \leq u_i$$

$$v_i = 0 \text{ if } z_i = 0$$

Where *l*, *u* are lower and upper bounds for reaction *i* and *z* is an indicator variable that is zero if the reaction is not used and otherwise 1, *c* is a user-defined cost associated with using the *i*th reaction, $v^\star$ is the flux of the objective and *t* a lower bound for that objective. To demonstrate, let's take a model and remove some essential reactions from it.

```
In [1]: import cobra.test
        from cobra.flux_analysis import gapfill
        model = cobra.test.create_test_model("salmonella")
```

In this model D-Fructose-6-phosphate is an essential metabolite. We will remove all the reactions using it, and at them to a separate model.

```
In [2]: universal = cobra.Model("universal_reactions")
        for i in [i.id for i in model.metabolites.f6p_c.reactions]:
            reaction = model.reactions.get_by_id(i)
            universal.add_reaction(reaction.copy())
            model.remove_reactions([reaction])
```

Now, because of these gaps, the model won't grow.

```
In [3]: model.optimize().objective_value
```

```
Out[3]: 0.0
```

We will use can use the model's original objective, growth, to figure out which of the removed reactions are required for the model be feasible again. This is very similar to making the 'no-growth but growth (NGG)' predictions of Kumar et al. 2009.

```
In [4]: solution = gapfill(model, universal, demand_reactions=False)
        for reaction in solution[0]:
            print(reaction.id)
```

```
GF6PTA
F6PP
TKT2
FBP
MAN6PI
```

We can obtain multiple possible reaction sets by having the algorithm go through multiple iterations.

```
In [5]: result = gapfill(model, universal, demand_reactions=False, iterations=4)
        for i, entries in enumerate(result):
            print("---- Run %d ----" % (i + 1))
            for e in entries:
                print(e.id)
```

```
---- Run 1 ----
GF6PTA
F6PP
TKT2
FBP
MAN6PI
---- Run 2 ----
GF6PTA
TALA
PGI
F6PA
MAN6PI
---- Run 3 ----
GF6PTA
F6PP
TKT2
FBP
MAN6PI
---- Run 4 ----
GF6PTA
TALA
PGI
F6PA
MAN6PI
```

We can also instead of using the original objective, specify a given metabolite that we want the model to be able to produce.

```
In [6]: with model:
            model.objective = model.add_boundary(model.metabolites.f6p_c, type='demand')
            solution = gapfill(model, universal)
            for reaction in solution[0]:
                print(reaction.id)
```

```
FBP
```

Finally, note that using mixed-integer linear programming is computationally quite expensive and for larger models you may want to consider alternative gap filling methods and reconstruction methods.

CHAPTER 10

Solvers

A constraints-based reconstruction and analysis model for biological systems is actually just an application of a class of discrete optimization problems typically solved with linear, mixed integer or quadratic programming techniques. Cobrapy does not implement any algorithms to find solutions to such problems but rather creates an biologically motivated abstraction to these techniques to make it easier to think of how metabolic systems work without paying much attention to how that formulates to an optimization problem.

The actual solving is instead done by tools such as the free software glpk or commercial tools gurobi and cplex which are all made available as a common programmers interface via the optlang package.

When you have defined your model, you can switch solver backend by simply assigning to the `model.solver` property.

```
In [1]: import cobra.test
        model = cobra.test.create_test_model('textbook')
```

```
In [2]: model.solver = 'glpk'
        # or if you have cplex installed
        model.solver = 'cplex'
```

For information on how to configure and tune the solver, please see the documentation for optlang project and note that `model.solver` is simply an object optlang of class `Model`.

```
In [3]: type(model.solver)
```

```
Out[3]: optlang.cplex_interface.Model
```

Internal solver interfaces

Cobrapy also contains its own solver interfaces but these are now deprecated and will be removed completely in the near future. For documentation of how to use these, please refer to older documentation.

CHAPTER 11

Tailored constraints, variables and objectives

Thanks to the use of symbolic expressions via the optlang mathematical modeling package, it is relatively straightforward to add new variables, constraints and advanced objectives that can not easily be formulated as a combination of different reaction and their corresponding upper and lower bounds. Here we demonstrate this optlang functionality which is exposed via the `model.solver.interface`.

Constraints

Suppose we want to ensure that two reactions have the same flux in our model. We can add this criteria as constraint to our model using the optlang solver interface by simply defining the relevant expression as follows.

```
In [1]: import cobra.test
        model = cobra.test.create_test_model('textbook')
```

```
In [2]: same_flux = model.problem.Constraint(
            model.reactions.FBA.flux_expression - model.reactions.NH4t.flux_expression,
            lb=0,
            ub=0)
        model.add_cons_vars(same_flux)
```

The flux for our reaction of interest is obtained by the `model.reactions.FBA.flux_expression` which is simply the sum of the forward and reverse flux, i.e.,

```
In [3]: model.reactions.FBA.flux_expression
```

```
Out[3]: 1.0*FBA - 1.0*FBA_reverse_84806
```

Now I can maximize growth rate whilst the fluxes of reactions 'FBA' and 'NH4t' are constrained to be (near) identical.

```
In [4]: solution = model.optimize()
        print(solution.fluxes['FBA'], solution.fluxes['NH4t'],
              solution.objective_value)
```

```
4.66274904774 4.66274904774 0.855110960926157
```

Objectives

Simple objective such as the maximization of the flux through one or more reactions can conveniently be done by simply assigning to the `model.objective` property as we have seen in previous chapters, e.g.,

```
In [5]: model = cobra.test.create_test_model('textbook')
        with model:
            model.objective = {model.reactions.Biomass_Ecoli_core: 1}
            model.optimize()
            print(model.reactions.Biomass_Ecoli_core.flux)
```

```
0.8739215069684307
```

The objectives mathematical expression is seen by

```
In [6]: model.objective.expression
```

```
Out[6]: -1.0*Biomass_Ecoli_core_reverse_2cdba + 1.0*Biomass_Ecoli_core
```

But suppose we need a more complicated objective, such as minimizing the Euclidean distance of the solution to the origin minus another variable, while subject to additional linear constraints. This is an objective function with both linear and quadratic components.

Consider the example problem:

$$\textbf{min } \tfrac{1}{2}\left(x^2 + y^2\right) - y$$

subject to

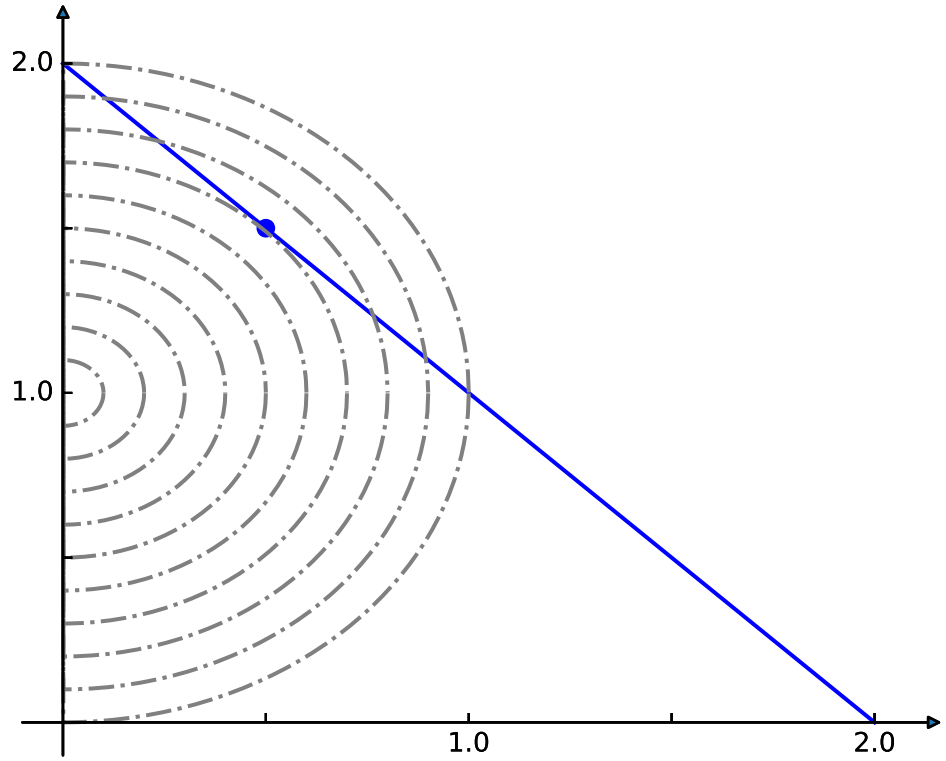
$$x + y = 2$$

$$x \geq 0$$

$$y \geq 0$$

This (admittedly very artificial) problem can be visualized graphically where the optimum is indicated by the blue dot on the line of feasible solutions.

```
In [7]: %matplotlib inline
        import plot_helper

        plot_helper.plot_qp2()
```



We return to the textbook model and set the solver to one that can handle quadratic objectives such as cplex. We then add the linear constraint that the sum of our x and y reactions, that we set to FBA and NH4t, must equal 2.

```
In [8]: model.solver = 'cplex'
        sum_two = model.problem.Constraint(
            model.reactions.FBA.flux_expression + model.reactions.NH4t.flux_expression,
            lb=2,
            ub=2)
        model.add_cons_vars(sum_two)
```

Next we add the quadratic objective

```
In [9]: quadratic_objective = model.problem.Objective(
            0.5 * model.reactions.NH4t.flux_expression**2 + 0.5 *
            model.reactions.FBA.flux_expression**2 -
            model.reactions.FBA.flux_expression,
            direction='min')
        model.objective = quadratic_objective
        solution = model.optimize(objective_sense=None)

In [10]: print(solution.fluxes['NH4t'], solution.fluxes['FBA'])

0.5 1.5
```

Variables

We can also create additional variables to facilitate studying the effects of new constraints and variables. Suppose we want to study the difference in flux between nitrogen and carbon uptake whilst we block other reactions. For this it will may help to add another variable representing this difference.

```
In [11]: model = cobra.test.create_test_model('textbook')
         difference = model.problem.Variable('difference')
```

We use constraints to define what values this variable shall take

```
In [12]: constraint = model.problem.Constraint(
             model.reactions.EX_glc__D_e.flux_expression -
             model.reactions.EX_nh4_e.flux_expression - difference,
             lb=0,
             ub=0)
         model.add_cons_vars([difference, constraint])
```

Now we can access that difference directly during our knock-out exploration by looking at its primal value.

```
In [13]: for reaction in model.reactions[:5]:
             with model:
                 reaction.knock_out()
                 model.optimize()
                 print(model.solver.variables.difference.primal)
```

```
-5.234680806802543
-5.2346808068025386
-5.234680806802525
-1.8644444444444337
-1.8644444444444466
```

CHAPTER 12

Using the COBRA toolbox with cobrapy

This example demonstrates using COBRA toolbox commands in MATLAB from python through pymatbridge.

```
In [1]: %load_ext pymatbridge
```

```
Starting MATLAB on ZMQ socket ipc:///tmp/pymatbridge-57ff5429-02d9-4e1a-8ed0-44e391fb0df7
Send 'exit' command to kill the server
....MATLAB started and connected!
```

```
In [2]: import cobra.test
        m = cobra.test.create_test_model("textbook")
```

The model_to_pymatbridge function will send the model to the workspace with the given variable name.

```
In [3]: from cobra.io.mat import model_to_pymatbridge
        model_to_pymatbridge(m, variable_name="model")
```

Now in the MATLAB workspace, the variable name 'model' holds a COBRA toolbox struct encoding the model.

```
In [4]: %%matlab
        model
```

```
model =

            rev: [95x1 double]
       metNames: {72x1 cell}
              b: [72x1 double]
      metCharge: [72x1 double]
              c: [95x1 double]
         csense: [72x1 char]
          genes: {137x1 cell}
    metFormulas: {72x1 cell}
           rxns: {95x1 cell}
        grRules: {95x1 cell}
       rxnNames: {95x1 cell}
    description: [11x1 char]
              S: [72x95 double]
             ub: [95x1 double]
```

```
            lb: [95x1 double]
          mets: {72x1 cell}
    subSystems: {95x1 cell}
```

First, we have to initialize the COBRA toolbox in MATLAB.

```
In [5]: %%matlab --silent
        warning('off'); % this works around a pymatbridge bug
        addpath(genpath('~/cobratoolbox/'));
        initCobraToolbox();
```

Commands from the COBRA toolbox can now be run on the model

```
In [6]: %%matlab
        optimizeCbModel(model)
```

```
ans =

           x: [95x1 double]
           f: 0.8739
           y: [71x1 double]
           w: [95x1 double]
        stat: 1
    origStat: 5
      solver: 'glpk'
        time: 3.2911
```

FBA in the COBRA toolbox should give the same result as cobrapy (but maybe just a little bit slower :))

```
In [7]: %time
        m.optimize().f
```

```
CPU times: user 0 ns, sys: 0 ns, total: 0 ns
Wall time: 5.48 µs
```

```
Out[7]: 0.8739215069684909
```

CHAPTER 13

FAQ

This document will address frequently asked questions not addressed in other pages of the documentation.

How do I install cobrapy?

Please see the INSTALL.rst file.

How do I cite cobrapy?

Please cite the 2013 publication: 10.1186/1752-0509-7-74

How do I rename reactions or metabolites?

TL;DR Use `Model.repair` afterwards

When renaming metabolites or reactions, there are issues because cobra indexes based off of ID's, which can cause errors. For example:

```
In [1]: from __future__ import print_function
        import cobra.test
        model = cobra.test.create_test_model()

        for metabolite in model.metabolites:
            metabolite.id = "test_" + metabolite.id

        try:
            model.metabolites.get_by_id(model.metabolites[0].id)
        except KeyError as e:
            print(repr(e))
```

The Model.repair function will rebuild the necessary indexes

```
In [2]: model.repair()
        model.metabolites.get_by_id(model.metabolites[0].id)
```

```
Out[2]: <Metabolite test_dcaACP_c at 0x110f09630>
```

How do I delete a gene?

That depends on what precisely you mean by delete a gene.

If you want to simulate the model with a gene knockout, use the `cobra.manipulation.delete_model_genes` function. The effects of this function are reversed by `cobra.manipulation.undelete_model_genes`.

```
In [3]: model = cobra.test.create_test_model()
        PGI = model.reactions.get_by_id("PGI")
        print("bounds before knockout:", (PGI.lower_bound, PGI.upper_bound))
        cobra.manipulation.delete_model_genes(model, ["STM4221"])
        print("bounds after knockouts", (PGI.lower_bound, PGI.upper_bound))
```

```
bounds before knockout: (-1000.0, 1000.0)
bounds after knockouts (0.0, 0.0)
```

If you want to actually remove all traces of a gene from a model, this is more difficult because this will require changing all the `gene_reaction_rule` strings for reactions involving the gene.

How do I change the reversibility of a Reaction?

`Reaction.reversibility` is a property in cobra which is computed when it is requested from the lower and upper bounds.

```
In [4]: model = cobra.test.create_test_model()
        model.reactions.get_by_id("PGI").reversibility
```

```
Out[4]: True
```

Trying to set it directly will result in an error or warning:

```
In [5]: try:
            model.reactions.get_by_id("PGI").reversibility = False
        except Exception as e:
            print(repr(e))
```

```
cobra/core/reaction.py:501 UserWarning: Setting reaction reversibility is ignored
```

The way to change the reversibility is to change the bounds to make the reaction irreversible.

```
In [6]: model.reactions.get_by_id("PGI").lower_bound = 10
        model.reactions.get_by_id("PGI").reversibility
```

```
Out[6]: False
```

How do I generate an LP file from a COBRA model?

For optlang based solvers

With optlang solvers, the LP formulation of a model is obtained by it's string representation. All solvers behave the same way.

```
In [7]: with open('test.lp', 'w') as out:
            out.write(str(model.solver))
```

For cobrapy's internal solvers

With the internal solvers, we first create the problem and use functions bundled with the solver.

Please note that unlike the LP file format, the MPS file format does not specify objective direction and is always a minimization. Some (but not all) solvers will rewrite the maximization as a minimization.

```
In [8]: model = cobra.test.create_test_model()
        # glpk through cglpk
        glpk = cobra.solvers.cglpk.create_problem(model)
        glpk.write("test.lp")
        glpk.write("test.mps")  # will not rewrite objective
        # cplex
        cplex = cobra.solvers.cplex_solver.create_problem(model)
        cplex.write("test.lp")
        cplex.write("test.mps")  # rewrites objective
```

How do I visualize my flux solutions?

cobrapy works well with the escher package, which is well suited to this purpose. Consult the escher documentation for examples.

CHAPTER 14

cobra package

Subpackages

cobra.core package

Submodules

cobra.core.arraybasedmodel module

class cobra.core.arraybasedmodel.**ArrayBasedModel**(*description=None*, *deep-copy_model=False*, *ma-trix_type='scipy.lil_matrix'*)

Bases: *cobra.core.model.Model*

ArrayBasedModel is a class that adds arrays and vectors to a cobra.Model to make it easier to perform linear algebra operations.

S

Stoichiometric matrix of the model

This will be formatted as either `lil_matrix` or `dok_matrix`

add_metabolites(*metabolite_list*, *expand_stoichiometric_matrix=True*)

Will add a list of metabolites to the the object, if they do not exist and then expand the stochiometric matrix

metabolite_list: A list of `Metabolite` objects

expand_stoichimetric_matrix: Boolean. If True and self.S is not None then it will add rows to self.S. self.S must be created after adding reactions and metabolites to self before it can be expanded. Trying to expand self.S when self only contains metabolites is ludacris.

add_reactions(*reaction_list*, *update_matrices=True*)

Will add a cobra.Reaction object to the model, if reaction.id is not in self.reactions.

reaction_list: A `Reaction` object or a list of them

update_matrices: Boolean. If true populate / update matrices S, lower_bounds, upper_bounds, ... Note this is slow to run for very large models and using this option with repeated calls will degrade performance. Better to call self.update() after adding all reactions.

If the stoichiometric matrix is initially empty then initialize a 1x1 sparse matrix and add more rows as needed in the self.add_metabolites function

b
bounds for metabolites as `numpy.ndarray`

constraint_sense

copy()
Provides a partial 'deepcopy' of the Model. All of the Metabolite, Gene, and Reaction objects are created anew but in a faster fashion than deepcopy

lower_bounds

objective_coefficients

remove_reactions(*reactions*, *update_matrices=True*, ***kwargs*)
remove reactions from the model

See `cobra.core.Model.Model.remove_reactions()`

update_matrices: Boolean If true populate / update matrices S, lower_bounds, upper_bounds. Note that this is slow to run for very large models, and using this option with repeated calls will degrade performance.

update()
Regenerates the stoichiometric matrix and vectors

upper_bounds

cobra.core.dictlist module

class `cobra.core.dictlist.`**DictList**(**args*)
Bases: `list`

A combined dict and list

This object behaves like a list, but has the O(1) speed benefits of a dict when looking up elements by their id.

Parameters ***args** (*iterable*) – iterable as single argument to create new DictList from

add(*x*)
Opposite of *remove*. Mirrors set.add

append(*object*)
append object to end

extend(*iterable*)
extend list by appending elements from the iterable

get_by_any(*iterable*)
Get a list of members using several different ways of indexing

Parameters **iterable** (*list (if not, turned into single element list)*) – list where each element is either int (referring to an index in in this DictList), string (a id of a member in this DictList) or member of this DictList for pass-through

Returns a list of members

Return type list

get_by_id(*id*)
return the element with a matching id

has_id(*id*)

index(*id*, **args*)
Determine the position in the list

id: A string or a `Object`

insert(*index*, *object*)
insert object before index

list_attr(*attribute*)
return a list of the given attribute for every object

pop(**args*)
remove and return item at index (default last).

query(*search_function*, *attribute=None*)
Query the list

Parameters

- **search_function** (*a string, regular expression or function*) – used to find the matching elements in the list.

  – a regular expression (possibly compiled), in which case the

  given attribute of the object should match the regular expression.

  – a function which takes one argument and returns True for

  desired values

- **attribute** (*string or None*) – the name attribute of the object to passed as argument to the *search_function*. If this is None, the object itself is used.

Returns a new list of objects which match the query

Return type *DictList*

Examples

```
>>> import cobra.test
>>> model = cobra.test.create_test_model('textbook')
>>> model.reactions.query(lambda x: x.boundary)
>>> import re
>>> regex = re.compile('^g', flags=re.IGNORECASE)
>>> model.metabolites.query(regex, attribute='name')
```

remove(*x*)

> **Warning:** Internal use only

reverse()
reverse *IN PLACE*

sort (*cmp=None*, *key=None*, *reverse=False*)
stable sort *IN PLACE*

cmp(x, y) -> -1, 0, 1

union (*iterable*)
adds elements with id's not already in the model

cobra.core.formula module

class cobra.core.formula.**Formula** (*formula=None*)
Bases: *cobra.core.object.Object*

Describes a Chemical Formula

Parameters **formula** (*string*) – A legal formula string contains only letters and numbers.

parse_composition ()
Breaks the chemical formula down by element.

weight
Calculate the mol mass of the compound

Returns the mol mass

Return type float

cobra.core.gene module

class cobra.core.gene.**GPRCleaner**
Bases: ast.NodeTransformer

Parses compiled ast of a gene_reaction_rule and identifies genes

Parts of the tree are rewritten to allow periods in gene ID's and bitwise boolean operations

visit_BinOp (*node*)

visit_Name (*node*)

class cobra.core.gene.**Gene** (*id=None*, *name=''*, *functional=True*)
Bases: *cobra.core.species.Species*

A Gene in a cobra model

Parameters

- **id** (*string*) – The identifier to associate the gene with
- **name** (*string*) – A longer human readable name for the gene
- **functional** (*bool*) – Indicates whether the gene is functional. If it is not functional then it cannot be used in an enzyme complex nor can its products be used.

functional
A flag indicating if the gene is functional.

Changing the flag is reverted upon exit if executed within the model as context.

knock_out ()
Knockout gene by marking it as non-functional and setting all associated reactions bounds to zero.

The change is reverted upon exit if executed within the model as context.

remove_from_model(*model=None*, *make_dependent_reactions_nonfunctional=True*)
Removes the association

Parameters

- **model** (*cobra model*) – The model to remove the gene from
- **make_dependent_reactions_nonfunctional** (*bool*) – If True then replace the gene with 'False' in the gene association, else replace the gene with 'True'

Deprecated since version 0.4: Use cobra.manipulation.delete_model_genes to simulate knockouts and cobra.manipulation.remove_genes to remove genes from the model.

cobra.core.gene.**ast2str**(*expr*, *level=0*, *names=None*)
convert compiled ast to gene_reaction_rule str

Parameters

- **expr** (*str*) – string for a gene reaction rule, e.g "a and b"
- **level** (*int*) – internal use only
- **names** (*dict*) – Dict where each element id a gene identifier and the value is the gene name. Use this to get a rule str which uses names instead. This should be done for display purposes only. All gene_reaction_rule strings which are computed with should use the id.

Returns The gene reaction rule

Return type string

cobra.core.gene.**eval_gpr**(*expr*, *knockouts*)
evaluate compiled ast of gene_reaction_rule with knockouts

Parameters

- **expr** (*Expression*) – The ast of the gene reaction rule
- **knockouts** (*DictList, set*) – Set of genes that are knocked out

Returns True if the gene reaction rule is true with the given knockouts otherwise false

Return type bool

cobra.core.gene.**parse_gpr**(*str_expr*)
parse gpr into AST

Parameters **str_expr** (*string*) – string with the gene reaction rule to parse

Returns elements ast_tree and gene_ids as a set

Return type tuple

cobra.core.metabolite module

class cobra.core.metabolite.**Metabolite**(*id=None*, *formula=None*, *name=''*, *charge=None*, *compartment=None*)
Bases: *cobra.core.species.Species*

Metabolite is a class for holding information regarding a metabolite in a cobra.Reaction object.

Parameters

- **id** (*str*) – the identifier to associate with the metabolite
- **formula** (*str*) – Chemical formula (e.g. H2O)

- **name** (*str*) – A human readable name.
- **charge** (*float*) – The charge number of the metabolite
- **compartment** (*str or None*) – Compartment of the metabolite.

constraint
Get the constraints associated with this metabolite from the solve

Returns the optlang constraint for this metabolite

Return type optlang.<interface>.Constraint

elements
Dictionary of elements as keys and their count in the metabolite as integer. When set, the *formula* property is update accordingly

formula_weight
Calculate the formula weight

remove_from_model (*destructive=False*)
Removes the association from self.model

The change is reverted upon exit when using the model as a context.

Parameters **destructive** (*bool*) – If False then the metabolite is removed from all associated reactions. If True then all associated reactions are removed from the Model.

shadow_price
The shadow price in the most recent solution.

Shadow price is the dual value of the corresponding constraint in the model.

Warning:

•Accessing shadow prices through a *Solution* object is the safer, preferred, and only guaranteed to be correct way. You can see how to do so easily in the examples.

•Shadow price is retrieved from the currently defined *self._model.solver*. The solver status is checked but there are no guarantees that the current solver state is the one you are looking for.

•If you modify the underlying model after an optimization, you will retrieve the old optimization values.

Raises

- RuntimeError – If the underlying model was never optimized beforehand or the metabolite is not part of a model.
- OptimizationError – If the solver status is anything other than 'optimal'.

Examples

```
>>> import cobra
>>> import cobra.test
>>> model = cobra.test.create_test_model("textbook")
>>> solution = model.optimize()
>>> model.metabolites.glc__D_e.shadow_price
-0.09166474637510488
```

```
>>> solution.shadow_prices.glc__D_e
-0.091664746375104883
```

summary (*threshold=0.01*, *fva=False*, *floatfmt='.3g'*, ***kwargs*)
Print a summary of the reactions which produce and consume this metabolite.

This method requires the model for which this metabolite is a part to be solved.

Parameters

- **threshold** (*float*) – a value below which to ignore reaction fluxes
- **fva** (*float (0->1), or None*) – Whether or not to include flux variability analysis in the output. If given, fva should be a float between 0 and 1, representing the fraction of the optimum objective to be searched.
- **floatfmt** (*string*) – format method for floats, passed to tabulate. Default is '.3g'.

y
The shadow price for the metabolite in the most recent solution

Shadow prices are computed from the dual values of the bounds in the solution.

cobra.core.model module

class cobra.core.model.**Model** (*id_or_model=None*, *name=None*)
Bases: *cobra.core.object.Object*

Class representation for a cobra model

Parameters

- **id_or_model** (*Model, string*) – Either an existing Model object in which case a new model object is instantiated with the same properties as the original model, or a the identifier to associate with the model as a string.
- **name** (*string*) – Human readable name for the model

reactions
DictList – A DictList where the key is the reaction identifier and the value a Reaction

metabolites
DictList – A DictList where the key is the metabolite identifier and the value a Metabolite

genes
DictList – A DictList where the key is the gene identifier and the value a Gene

solution
Solution – The last obtained solution from optimizing the model.

add_boundary (*metabolite*, *type='exchange'*, *reaction_id=None*, *lb=None*, *ub=1000.0*)
Add a boundary reaction for a given metabolite.

There are three different types of pre-defined boundary reactions: exchange, demand, and sink reactions. An exchange reaction is a reversible, imbalanced reaction that adds to or removes an extracellular metabolite from the extracellular compartment. A demand reaction is an irreversible reaction that consumes an intracellular metabolite. A sink is similar to an exchange but specifically for intracellular metabolites.

If you set the reaction *type* to something else, you must specify the desired identifier of the created reaction along with its upper and

lower bound. The name will be given by the metabolite name and the given *type*.

Parameters

- **metabolite** (*cobra.Metabolite*) – Any given metabolite. The compartment is not checked but you are encouraged to stick to the definition of exchanges and sinks.
- **type** (*str, {"exchange", "demand", "sink"}*) – Using one of the predefined reaction types is easiest. If you want to create your own kind of boundary reaction choose any other string, e.g., 'my-boundary'.
- **reaction_id** (*str, optional*) – The ID of the resulting reaction. Only used for custom reactions.
- **lb** (*float, optional*) – The lower bound of the resulting reaction. Only used for custom reactions.
- **ub** (*float, optional*) – The upper bound of the resulting reaction. For the predefined reactions this default value determines all bounds.

Returns The created boundary reaction.

Return type cobra.Reaction

Examples

```
>>> import cobra.test
>>> model = cobra.test.create_test_model("textbook")
>>> demand = model.add_boundary(model.metabolites.atp_c, type="demand")
>>> demand.id
'DM_atp_c'
>>> demand.name
'ATP demand'
>>> demand.bounds
(0, 1000.0)
>>> demand.build_reaction_string()
'atp_c --> '
```

add_cons_vars (*what*, ***kwargs*)

Add constraints and variables to the model's mathematical problem.

Useful for variables and constraints that can not be expressed with reactions and simple lower and upper bounds.

Additions are reversed upon exit if the model itself is used as context.

Parameters

- **what** (*list or tuple of optlang variables or constraints.*) – The variables or constraints to add to the model. Must be of class *optlang.interface.Variable* or *optlang.interface.Constraint*.
- ****kwargs** (*keyword arguments*) – Passed to solver.add()

add_metabolites (*metabolite_list*)

Will add a list of metabolites to the model object and add new constraints accordingly.

The change is reverted upon exit when using the model as a context.

Parameters **metabolite_list** (A list of *cobra.core.Metabolite* objects) –

add_reaction (*reaction*)

Will add a cobra.Reaction object to the model, if reaction.id is not in self.reactions.

Parameters

- **reaction** (*cobra.Reaction*) – The reaction to add
- **(0.6)Use ~cobra.Model.add_reactions instead** (*Deprecated*) –

add_reactions (*reaction_list*)
Add reactions to the model.

Reactions with identifiers identical to a reaction already in the model are ignored.

The change is reverted upon exit when using the model as a context.

Parameters **reaction_list** (*list*) – A list of *cobra.Reaction* objects

constraints
The constraints in the cobra model.

In a cobra model, most constraints are metabolites and their stoichiometries. However, for specific use cases, it may also be useful to have other types of constraints. This property defines all constraints currently associated with the model's problem.

Returns A container with all associated constraints.

Return type optlang.container.Container

copy ()
Provides a partial 'deepcopy' of the Model. All of the Metabolite, Gene, and Reaction objects are created anew but in a faster fashion than deepcopy

description

exchanges
Exchange reactions in model.

Reactions that either don't have products or substrates.

get_metabolite_compartments ()
Return all metabolites' compartments.

medium

merge (*right*, *prefix_existing=None*, *inplace=True*, *objective='left'*)
Merge two models to create a model with the reactions from both models.

Custom constraints and variables from right models are also copied to left model, however note that, constraints and variables are assumed to be the same if they have the same name.

right [cobra.Model] The model to add reactions from

prefix_existing [string] Prefix the reaction identifier in the right that already exist in the left model with this string.

inplace [bool] Add reactions from right directly to left model object. Otherwise, create a new model leaving the left model untouched. When done within the model as context, changes to the models are reverted upon exit.

objective [string] One of 'left', 'right' or 'sum' for setting the objective of the resulting model to that of the corresponding model or the sum of both.

objective
Get or set the solver objective

Before introduction of the optlang based problems, this function returned the objective reactions as a list. With optlang, the objective is not limited a simple linear summation of individual reaction fluxes,

making that return value ambiguous. Henceforth, use *cobra.util.solver.linear_reaction_coefficients* to get a dictionary of reactions with their linear coefficients (empty if there are none)

The set value can be dictionary (reactions as keys, linear coefficients as values), string (reaction identifier), int (reaction index), Reaction or problem.Objective or sympy expression directly interpreted as objectives.

When using a *HistoryManager* context, this attribute can be set temporarily, reversed when the exiting the context.

optimize(*objective_sense=None*, *raise_error=False*, ***kwargs*)

Optimize the model using flux balance analysis.

Parameters

- **objective_sense** (*{None, 'maximize' 'minimize'}, optional*) – Whether fluxes should be maximized or minimized. In case of None, the previous direction is used.
- **raise_error** (*bool*) –

  If true, raise an OptimizationError if solver status is not optimal.
- **solver** (*{None, 'glpk', 'cglpk', 'gurobi', 'cplex'}, optional*) – If unspecified will use the currently defined *self.solver* otherwise it will use the given solver and update the attribute.
- **quadratic_component** (*{None, scipy.sparse.dok_matrix}, optional*) – The dimensions should be (n, n) where n is the number of reactions. This sets the quadratic component (Q) of the objective coefficient, adding $\frac{1}{2} v^T \cdot Q \cdot v$ to the objective. Ignored for optlang based solvers.
- **tolerance_feasibility** (*float*) – Solver tolerance for feasibility. Ignored for optlang based solvers
- **tolerance_markowitz** (*float*) – Solver threshold during pivot. Ignored for optlang based solvers
- **time_limit** (*float*) – Maximum solver time (in seconds). Ignored for optlang based solvers

Notes

Only the most commonly used parameters are presented here. Additional parameters for cobra.solvers may be available and specified with the appropriate keyword argument.

problem

The interface to the model's underlying mathematical problem.

Solutions to cobra models are obtained by formulating a mathematical problem and solving it. Cobrapy uses the optlang package to accomplish that and with this property you can get access to the problem interface directly.

Returns The problem interface that defines methods for interacting with the problem and associated solver directly.

Return type optlang.interface

remove_cons_vars(*what*)

Remove variables and constraints from the model's mathematical problem.

Remove variables and constraints that were added directly to the model's underlying mathematical problem. Removals are reversed upon exit if the model itself is used as context.

Parameters **what** (*list or tuple of optlang variables or constraints.*) – The variables or constraints to add to the model. Must be of class *optlang.interface.Variable* or *optlang.interface.Constraint*.

remove_metabolites(*metabolite_list*, *destructive=False*)
Remove a list of metabolites from the the object.

The change is reverted upon exit when using the model as a context.

Parameters

- **metabolite_list** (*list*) – A list with *cobra.Metabolite* objects as elements.
- **destructive** (*bool*) – If False then the metabolite is removed from all associated reactions. If True then all associated reactions are removed from the Model.

remove_reactions(*reactions*, *remove_orphans=False*)
Remove reactions from the model.

The change is reverted upon exit when using the model as a context.

Parameters

- **reactions** (*list*) – A list with reactions (*cobra.Reaction*), or their id's, to remove
- **remove_orphans** (*bool*) – Remove orphaned genes and metabolites from the model as well

repair(*rebuild_index=True*, *rebuild_relationships=True*)
Update all indexes and pointers in a model

Parameters

- **rebuild_index** (*bool*) – rebuild the indices kept in reactions, metabolites and genes
- **rebuild_relationships** (*bool*) – reset all associations between genes, metabolites, model and then re-add them.

slim_optimize(*error_value=nan*, *message=None*)
Optimize model without creating a solution object.

Creating a full solution object implies fetching shadow prices and flux values for all reactions and metabolites from the solver object. This necessarily takes some time and in cases where only one or two values are of interest, it is recommended to instead use this function which does not create a solution object returning only the value of the objective. Note however that the *optimize()* function uses efficient means to fetch values so if you need fluxes/shadow prices for more than say 4 reactions/metabolites, then the total speed increase of *slim_optimize* versus *optimize* is expected to be small or even negative depending on how you fetch the values after optimization.

Parameters

- **error_value** (*float, None*) – The value to return if optimization failed due to e.g. infeasibility. If None, raise *OptimizationError* if the optimization fails.
- **message** (*string*) – Error message to use if the model optimization did not succeed.

Returns The objective value.

Return type float

solver
Get or set the attached solver instance.

The associated the solver object, which manages the interaction with the associated solver, e.g. glpk.

This property is useful for accessing the optimization problem directly and to define additional non-metabolic constraints.

Examples

```
>>> import cobra.test
>>> model = cobra.test.create_test_model("textbook")
>>> new = model.problem.Constraint(model.objective.expression,
>>> lb=0.99)
>>> model.solver.add(new)
```

summary (*threshold=1e-08*, *fva=None*, *floatfmt='.3g'*, ***kwargs*)
Print a summary of the input and output fluxes of the model. This method requires the model to have been previously solved.

Parameters

- **threshold** (*float*) – tolerance for determining if a flux is zero (not printed)
- **fva** (*int or None*) – Whether or not to calculate and report flux variability in the output summary
- **floatfmt** (*string*) – format method for floats, passed to tabulate. Default is '.3g'.

to_array_based_model (*deepcopy_model=False*, ***kwargs*)
Makes a *cobra.core.ArrayBasedModel* from a cobra.Model which may be used to perform linear algebra operations with the stoichiometric matrix.

Deprecated (0.6). Use *cobra.util.array.create_stoichiometric_matrix* instead.

Parameters **deepcopy_model** (*bool*) – If False then the ArrayBasedModel points to the Model

variables
The mathematical variables in the cobra model.

In a cobra model, most variables are reactions. However, for specific use cases, it may also be useful to have other types of variables. This property defines all variables currently associated with the model's problem.

Returns A container with all associated variables.

Return type optlang.container.Container

cobra.core.object module

class cobra.core.object.**Object** (*id=None*, *name=''*)
Bases: object

Defines common behavior of object in cobra.core

id

cobra.core.reaction module

class cobra.core.reaction.**Reaction** (*id=None*, *name=''*, *subsystem=''*, *lower_bound=0.0*, *upper_bound=1000.0*, *objective_coefficient=0.0*)
Bases: *cobra.core.object.Object*

Reaction is a class for holding information regarding a biochemical reaction in a cobra.Model object.

Parameters

- **id** (*string*) – The identifier to associate with this reaction
- **name** (*string*) – A human readable name for the reaction
- **subsystem** (*string*) – Subsystem where the reaction is meant to occur
- **lower_bound** (*float*) – The lower flux bound
- **upper_bound** (*float*) – The upper flux bound

add_metabolites(*metabolites_to_add*, *combine=True*, *reversibly=True*)

Add metabolites and stoichiometric coefficients to the reaction. If the final coefficient for a metabolite is 0 then it is removed from the reaction.

The change is reverted upon exit when using the model as a context.

Parameters

- **metabolites_to_add** (*dict*) – Dictionary with metabolite objects or metabolite identifiers as keys and coefficients as values. If keys are strings (name of a metabolite) the reaction must already be part of a model and a metabolite with the given name must exist in the model.
- **combine** (*bool*) – Describes behavior a metabolite already exists in the reaction. True causes the coefficients to be added. False causes the coefficient to be replaced.
- **reversibly** (*bool*) – Whether to add the change to the context to make the change reversibly or not (primarily intended for internal use).

boundary

Whether or not this reaction is an exchange reaction.

Returns *True* if the reaction has either no products or reactants.

bounds

Get or set the bounds directly from a tuple

Convenience method for setting upper and lower bounds in one line using a tuple of lower and upper bound. Invalid bounds will raise an AssertionError.

When using a *HistoryManager* context, this attribute can be set temporarily, reversed when the exiting the context.

build_reaction_from_string(*reaction_str*, *verbose=True*, *fwd_arrow=None*, *rev_arrow=None*, *reversible_arrow=None*, *term_split='+'*)

Builds reaction from reaction equation reaction_str using parser

Takes a string and using the specifications supplied in the optional arguments infers a set of metabolites, metabolite compartments and stoichiometries for the reaction. It also infers the reversibility of the reaction from the reaction arrow.

Changes to the associated model are reverted upon exit when using the model as a context.

Parameters

- **reaction_str** (*string*) – a string containing a reaction formula (equation)
- **verbose** (*bool*) – setting verbosity of function
- **fwd_arrow** (*re.compile*) – for forward irreversible reaction arrows
- **rev_arrow** (*re.compile*) – for backward irreversible reaction arrows

- **reversible_arrow** (*re.compile*) – for reversible reaction arrows
- **term_split** (*string*) – dividing individual metabolite entries

build_reaction_string(*use_metabolite_names=False*)
Generate a human readable reaction string

check_mass_balance()
Compute mass and charge balance for the reaction

returns a dict of {element: amount} for unbalanced elements. "charge" is treated as an element in this dict This should be empty for balanced reactions.

compartments
lists compartments the metabolites are in

copy()
Copy a reaction

The referenced metabolites and genes are also copied.

delete(*remove_orphans=False*)
Removes the reaction from a model.

This removes all associations between a reaction the associated model, metabolites and genes.

The change is reverted upon exit when using the model as a context.

Deprecated, use *reaction.remove_from_model* instead.

Parameters **remove_orphans** (*bool*) – Remove orphaned genes and metabolites from the model as well

flux
The flux value in the most recent solution.

Flux is the primal value of the corresponding variable in the model.

Warning:

•Accessing reaction fluxes through a *Solution* object is the safer, preferred, and only guaranteed to be correct way. You can see how to do so easily in the examples.

•Reaction flux is retrieved from the currently defined *self._model.solver*. The solver status is checked but there are no guarantees that the current solver state is the one you are looking for.

•If you modify the underlying model after an optimization, you will retrieve the old optimization values.

Raises

- RuntimeError – If the underlying model was never optimized beforehand or the reaction is not part of a model.
- OptimizationError – If the solver status is anything other than 'optimal'.
- AssertionError – If the flux value is not within the bounds.

Examples

```
>>> import cobra.test
>>> model = cobra.test.create_test_model("textbook")
>>> solution = model.optimize()
>>> model.reactions.PFK.flux
7.477381962160283
>>> solution.fluxes.PFK
7.4773819621602833
```

flux_expression
Forward flux expression

Returns The expression repreeenting the the forward flux (if associated with model), otherwise None. Representing the net flux if model.reversible_encoding == 'unsplit' or None if reaction is not associated with a model

Return type sympy expression

forward_variable
An optlang variable representing the forward flux

Returns An optlang variable for the forward flux or None if reaction is not associated with a model.

Return type optlang.interface.Variable

functional
All required enzymes for reaction are functional.

Returns True if the gene-protein-reaction (GPR) rule is fulfilled for this reaction, or if reaction is not associated to a model, otherwise False.

Return type bool

gene_name_reaction_rule
Display gene_reaction_rule with names intead.

Do NOT use this string for computation. It is intended to give a representation of the rule using more familiar gene names instead of the often cryptic ids.

gene_reaction_rule

genes

get_coefficient(*metabolite_id*)
Return the stoichiometric coefficient of a metabolite.

Parameters **metabolite_id** (*str or cobra.Metabolite*) –

get_coefficients(*metabolite_ids*)
Return the stoichiometric coefficients for a list of metabolites in the reaction.

Parameters **metabolite_ids** (*iterable*) – Containing str or ‘‘cobra.Metabolite‘‘s.

get_compartments()
lists compartments the metabolites are in

knock_out()
Knockout reaction by setting its bounds to zero.

lower_bound
Get or set the lower bound

Setting the lower bound (float) will also adjust the associated optlang variables associated with the reaction. Infeasible combinations, such as a lower bound higher than the current upper bound will update the other bound.

When using a *HistoryManager* context, this attribute can be set temporarily, reversed when the exiting the context.

metabolites

model
returns the model the reaction is a part of

objective_coefficient
Get the coefficient for this reaction in a linear objective (float)

Assuming that the objective of the associated model is summation of fluxes from a set of reactions, the coefficient for each reaction can be obtained individually using this property. A more general way is to use the *model.objective* property directly.

products
Return a list of products for the reaction

reactants
Return a list of reactants for the reaction.

reaction
Human readable reaction string

reduced_cost
The reduced cost in the most recent solution.

Reduced cost is the dual value of the corresponding variable in the model.

Warning:

- Accessing reduced costs through a *Solution* object is the safer, preferred, and only guaranteed to be correct way. You can see how to do so easily in the examples.
- Reduced cost is retrieved from the currently defined *self._model.solver*. The solver status is checked but there are no guarantees that the current solver state is the one you are looking for.
- If you modify the underlying model after an optimization, you will retrieve the old optimization values.

Raises

- `RuntimeError` – If the underlying model was never optimized beforehand or the reaction is not part of a model.
- `OptimizationError` – If the solver status is anything other than 'optimal'.

Examples

```
>>> import cobra.test
>>> model = cobra.test.create_test_model("textbook")
>>> solution = model.optimize()
>>> model.reactions.PFK.reduced_cost
-8.673617379884035e-18
```

```
>>> solution.reduced_costs.PFK
-8.6736173798840355e-18
```

remove_from_model (*remove_orphans=False*)
Removes the reaction from a model.

This removes all associations between a reaction the associated model, metabolites and genes.

The change is reverted upon exit when using the model as a context.

Parameters **remove_orphans** (*bool*) – Remove orphaned genes and metabolites from the model as well

reverse_id
Generate the id of reverse_variable from the reaction's id.

reverse_variable
An optlang variable representing the reverse flux

Returns An optlang variable for the reverse flux or None if reaction is not associated with a model.

Return type optlang.interface.Variable

reversibility
Whether the reaction can proceed in both directions (reversible)

This is computed from the current upper and lower bounds.

subtract_metabolites (*metabolites*, *combine=True*, *reversibly=True*)
This function will 'subtract' metabolites from a reaction, which means add the metabolites with -1*coefficient. If the final coefficient for a metabolite is 0 then the metabolite is removed from the reaction.

The change is reverted upon exit when using the model as a context.

Parameters

- **metabolites** (*dict*) – Dictionary where the keys are of class Metabolite and the values are the coefficients. These metabolites will be added to the reaction.
- **combine** (*bool*) – Describes behavior a metabolite already exists in the reaction. True causes the coefficients to be added. False causes the coefficient to be replaced.
- **reversibly** (*bool*) – Whether to add the change to the context to make the change reversibly or not (primarily intended for internal use).

:param .. note:: A final coefficient < 0 implies a reactant.:

upper_bound
Get or set the upper bound

Setting the upper bound (float) will also adjust the associated optlang variables associated with the reaction. Infeasible combinations, such as a upper bound lower than the current lower bound will update the other bound.

When using a *HistoryManager* context, this attribute can be set temporarily, reversed when the exiting the context.

x
The flux through the reaction in the most recent solution.

Flux values are computed from the primal values of the variables in the solution.

y
The reduced cost of the reaction in the most recent solution.

Reduced costs are computed from the dual values of the variables in the solution.

cobra.core.reaction.**separate_forward_and_reverse_bounds**(*lower_bound*, *upper_bound*)
Split a given (lower_bound, upper_bound) interval into a negative component and a positive component. Negative components are negated (returns positive ranges) and flipped for usage with forward and reverse reactions bounds

Parameters

- **lower_bound** (*float*) – The lower flux bound
- **upper_bound** (*float*) – The upper flux bound

cobra.core.reaction.**update_forward_and_reverse_bounds**(*reaction*, *direction='both'*)
For the given reaction, update the bounds in the forward and reverse variable bounds.

Parameters

- **reaction** (*cobra.Reaction*) – The reaction to operate on
- **direction** (*string*) – Either 'both', 'upper' or 'lower' for updating the corresponding flux bounds.

cobra.core.solution module

Provide unified interfaces to optimization solutions.

class cobra.core.solution.**Solution**(*objective_value*, *status*, *reactions*, *fluxes*, *reduced_costs=None*, *metabolites=None*, *shadow_prices=None*, ***kwargs*)
Bases: object

A unified interface to a *cobra.Model* optimization solution.

Notes

Solution is meant to be constructed by *get_solution* please look at that function to fully understand the *Solution* class.

objective_value
float – The (optimal) value for the objective function.

status
str – The solver status related to the solution.

reactions
list – A list of *cobra.Reaction* objects for which the solution is retrieved.

fluxes
pandas.Series – Contains the reaction fluxes (primal values of variables).

reduced_costs
pandas.Series – Contains reaction reduced costs (dual values of variables).

metabolites
list – A list of *cobra.Metabolite* objects for which the solution is retrieved.

shadow_prices
pandas.Series – Contains metabolite shadow prices (dual values of constraints).

Deprecated Attributes

----

f
float – Use *objective_value* instead.

x
list – Use *fluxes.values* instead.

x_dict
pandas.Series – Use *fluxes* instead.

y
list – Use *reduced_costs.values* instead.

y_dict
pandas.Series – Use *reduced_costs* instead.

f
Deprecated property for getting the objective value.

get_primal_by_id(*reaction_id*)
Return the flux of a reaction.

Parameters **reaction** (*str*) – A model reaction ID.

to_frame()
Return the fluxes and reduced costs as a data frame

x
Deprecated property for getting flux values.

x_dict
Deprecated property for getting fluxes.

y
Deprecated property for getting reduced cost values.

y_dict
Deprecated property for getting reduced costs.

class cobra.core.solution.**LegacySolution**(*f*, *x=None*, *x_dict=None*, *y=None*, *y_dict=None*, *solver=None*, *the_time=0*, *status='NA'*, ***kwargs*)
Bases: object

Legacy support for an interface to a *cobra.Model* optimization solution.

f
float – The objective value

solver
str – A string indicating which solver package was used.

x
iterable – List or Array of the fluxes (primal values).

x_dict
dict – A dictionary of reaction IDs that maps to the respective primal values.

y
iterable – List or Array of the dual values.

y_dict
dict – A dictionary of reaction IDs that maps to the respective dual values.

> **Warning:** The LegacySolution class and its interface is deprecated.

dress_results(*model*)
Method could be intended as a decorator.

> **Warning:** deprecated

cobra.core.solution.**get_solution**(*model*, *reactions=None*, *metabolites=None*, *raise_error=False*)
Generate a solution representation of the current solver state.

Parameters

- **model** (*cobra.Model*) – The model whose reactions to retrieve values for.
- **reactions** (*list, optional*) – An iterable of *cobra.Reaction* objects. Uses *model.reactions* by default.
- **metabolites** (*list, optional*) – An iterable of *cobra.Metabolite* objects. Uses *model.metabolites* by default.
- **raise_error** (*bool*) – If true, raise an OptimizationError if solver status is not optimal.

Returns

Return type cobra.Solution

Note: This is only intended for the *optlang* solver interfaces and not the legacy solvers.

cobra.core.species module

class cobra.core.species.**Species**(*id=None*, *name=None*)
Bases: *cobra.core.object.Object*

Species is a class for holding information regarding a chemical Species

Parameters

- **id** (*string*) – An identifier for the chemical species
- **name** (*string*) – A human readable name.

copy()
When copying a reaction, it is necessary to deepcopy the components so the list references aren't carried over.

Additionally, a copy of a reaction is no longer in a cobra.Model.

This should be fixed with self.__deepcopy__ if possible

model

reactions

Module contents

cobra.design package

Submodules

cobra.design.design_algorithms module

cobra.design.design_algorithms.**set_up_optknock**(**args*, ***kwargs*)

cobra.design.design_algorithms.**dual_problem**(**args*, ***kwargs*)

Module contents

cobra.flux_analysis package

Submodules

cobra.flux_analysis.deletion_worker module

class cobra.flux_analysis.deletion_worker.**CobraDeletionMockPool**(*cobra_model*, *n_processes=1*, *solver=None*, ***kwargs*)

Bases: object

Mock pool solves LP's in the same process

receive_all()

receive_one()

start()

submit(*indexes*, *label=None*)

terminate()

class cobra.flux_analysis.deletion_worker.**CobraDeletionPool**(*cobra_model*, *n_processes=None*, *solver=None*, ***kwargs*)

Bases: object

A pool of workers for solving deletions

submit jobs to the pool using submit and recieve results using receive_all

pids

receive_all()

receive_one()
This function blocks

start()

submit(*indexes*, *label=None*)

terminate()

cobra.flux_analysis.deletion_worker.**compute_fba_deletion**(*lp*, *solver_object*, *model*, *indexes*, ***kwargs*)

cobra.flux_analysis.deletion_worker.**compute_fba_deletion_worker**(*cobra_model*, *solver*, *job_queue*, *output_queue*, ***kwargs*)

cobra.flux_analysis.double_deletion module

cobra.flux_analysis.double_deletion.**double_deletion**(*cobra_model*, *element_list_1=None*, *element_list_2=None*, *element_type='gene'*, ***kwargs*)

Wrapper for double_gene_deletion and double_reaction_deletion

Deprecated since version 0.4: Use double_reaction_deletion and double_gene_deletion

cobra.flux_analysis.double_deletion.**double_gene_deletion**(*cobra_model*, *gene_list1=None*, *gene_list2=None*, *method='fba'*, *return_frame=False*, *solver=None*, *zero_cutoff=1e-12*, ***kwargs*)

sequentially knocks out pairs of genes in a model

cobra_model [`Model`] cobra model in which to perform deletions

gene_list1 [[`Gene`:] (or their id's)] Genes to be deleted. These will be the rows in the result. If not provided, all reactions will be used.

gene_list1 [[`Gene`:] (or their id's)] Genes to be deleted. These will be the rows in the result. If not provided, reaction_list1 will be used.

method: "fba" or "moma" Procedure used to predict the growth rate

solver: str for solver name This must be a QP-capable solver for MOMA. If left unspecified, a suitable solver will be automatically chosen.

zero_cutoff: float When checking to see if a value is 0, this threshold is used.

number_of_processes: int for number of processes to use. If unspecified, the number of parallel processes to use will be automatically determined. Setting this to 1 explicitly disables used of the multiprocessing library.

Note: multiprocessing is not supported with method=moma

---

return_frame: bool If true, formats the results as a pandas.Dataframe. Otherwise returns a dict of the form: {"x": row_labels, "y": column_labels", "data": 2D matrix}

cobra.flux_analysis.double_deletion.**double_reaction_deletion**(*cobra_model*, *reaction_list1=None*, *reaction_list2=None*, *method='fba'*, *return_frame=False*, *solver=None*, *zero_cutoff=1e-12*, ***kwargs*)

sequentially knocks out pairs of reactions in a model

cobra_model [Model] cobra model in which to perform deletions

reaction_list1 [[Reaction:] (or their id's)] Reactions to be deleted. These will be the rows in the result. If not provided, all reactions will be used.

reaction_list2 [[Reaction:] (or their id's)] Reactions to be deleted. These will be the rows in the result. If not provided, reaction_list1 will be used.

method: "fba" or "moma" Procedure used to predict the growth rate

solver: str for solver name This must be a QP-capable solver for MOMA. If left unspecified, a suitable solver will be automatically chosen.

zero_cutoff: float When checking to see if a value is 0, this threshold is used.

return_frame: bool If true, formats the results as a pandas.Dataframe. Otherwise returns a dict of the form: {"x": row_labels, "y": column_labels", "data": 2D matrix}

cobra.flux_analysis.double_deletion.**format_results_frame**(*row_ids*, *column_ids*, *matrix*, *return_frame=False*)

format results as a pandas.DataFrame if desired/possible

Otherwise returns a dict of {"x": row_ids, "y": column_ids", "data": result_matrx}

cobra.flux_analysis.double_deletion.**generate_matrix_indexes**(*ids1*, *ids2*)

map an identifier to an entry in the square result matrix

cobra.flux_analysis.double_deletion.**yield_upper_tria_indexes**(*ids1*, *ids2*, *id_to_index*)

gives the necessary indexes in the upper triangle

ids1 and ids2 are lists of the identifiers i.e. gene id's or reaction indexes to be knocked out. id_to_index maps each identifier to its index in the result matrix.

Note that this does not return indexes for the diagonal. Those have to be computed separately.

cobra.flux_analysis.gapfilling module

class cobra.flux_analysis.gapfilling.**GapFiller**(*model*, *universal=None*, *lower_bound=0.05*, *penalties=None*, *exchange_reactions=False*, *demand_reactions=True*, *integer_threshold=1e-06*)

Bases: object

Class for performing gap filling.

This class implements gap filling based on a mixed-integer approach, very similar to that described in [1]_ and the 'no-growth but growth' part of [2]_ but with minor adjustments. In short, we add indicator variables for using the reactions in the universal model, z_i and then solve problem

minimize sum_i c_i * z_i s.t. Sv = 0

v_o >= t lb_i <= v_i <= ub_i v_i = 0 if z_i = 0

where lb, ub are the upper, lower flux bounds for reaction i, c_i is a cost parameter and the objective v_o is greater than the lower bound t. The default costs are 1 for reactions from the universal model, 100 for exchange (uptake) reactions added and 1 for added demand reactions.

Note that this is a mixed-integer linear program and as such will expensive to solve for large models. Consider using alternatives [3]_ such as CORDA instead [4,5]_.

Parameters

- **model** (*cobra.Model*) – The model to perform gap filling on.
- **universal** (*cobra.Model*) – A universal model with reactions that can be used to complete the model.
- **lower_bound** (*float*) – The minimally accepted flux for the objective in the filled model.
- **penalties** (*dict, None*) – A dictionary with keys being 'universal' (all reactions included in the universal model), 'exchange' and 'demand' (all additionally added exchange and demand reactions) for the three reaction types. Can also have reaction identifiers for reaction specific costs. Defaults are 1, 100 and 1 respectively.
- **integer_threshold** (*float*) – The threshold at which a value is considered non-zero (aka integrality threshold). If gapfilled models fail to validate, you may want to lower this value.
- **exchange_reactions** (*bool*) – Consider adding exchange (uptake) reactions for all metabolites in the model.
- **demand_reactions** (*bool*) – Consider adding demand reactions for all metabolites.

References

add_switches_and_objective()
Update gapfilling model with switches and the indicator objective.

extend_model(*exchange_reactions=False*, *demand_reactions=True*)
Extend gapfilling model.

Add reactions from universal model and optionally exchange and demand reactions for all metabolites in the model to perform gapfilling on.

Parameters

- **exchange_reactions** (*bool*) – Consider adding exchange (uptake) reactions for all metabolites in the model.
- **demand_reactions** (*bool*) – Consider adding demand reactions for all metabolites.

fill(*iterations=1*)
Perform the gapfilling by iteratively solving the model, updating the costs and recording the used reactions.

Parameters **iterations** (*int*) – The number of rounds of gapfilling to perform. For every iteration, the penalty for every used reaction increases linearly. This way, the algorithm is encouraged to search for alternative solutions which may include previously used reactions. I.e., with enough iterations pathways including 10 steps will eventually be reported even if the shortest pathway is a single reaction.

Returns A list of lists where each element is a list reactions that were used to gapfill the model.

Return type iterable

Raises `RuntimeError` – If the model fails to be validated (i.e. the original model with the proposed reactions added, still cannot get the required flux through the objective).

update_costs()
Update the coefficients for the indicator variables in the objective.

Done incrementally so that second time the function is called, active indicators in the current solutions gets higher cost than the unused indicators.

validate(*reactions*)

cobra.flux_analysis.gapfilling.**SMILEY**(*model*, *metabolite_id*, *Universal*, *dm_rxns=False*, *ex_rxns=False*, *penalties=None*, ***solver_parameters*)
runs the SMILEY algorithm. Legacy function, to be removed in future version of cobrapy in favor of gapfill.

cobra.flux_analysis.gapfilling.**gapfill**(*model*, *universal=None*, *lower_bound=0.05*, *penalties=None*, *demand_reactions=True*, *exchange_reactions=False*, *iterations=1*)
Perform gapfilling on a model.

See documentation for the class GapFiller.

Parameters

- **model** (*cobra.Model*) – The model to perform gap filling on.
- **universal** (*cobra.Model, None*) – A universal model with reactions that can be used to complete the model. Only gapfill considering demand and exchange reactions if left missing.
- **lower_bound** (*float*) – The minimally accepted flux for the objective in the filled model.
- **penalties** (*dict, None*) – A dictionary with keys being 'universal' (all reactions included in the universal model), 'exchange' and 'demand' (all additionally added exchange and demand reactions) for the three reaction types. Can also have reaction identifiers for reaction specific costs. Defaults are 1, 100 and 1 respectively.
- **iterations** (*int*) – The number of rounds of gapfilling to perform. For every iteration, the penalty for every used reaction increases linearly. This way, the algorithm is encouraged to search for alternative solutions which may include previously used reactions. I.e., with enough iterations pathways including 10 steps will eventually be reported even if the shortest pathway is a single reaction.
- **exchange_reactions** (*bool*) – Consider adding exchange (uptake) reactions for all metabolites in the model.
- **demand_reactions** (*bool*) – Consider adding demand reactions for all metabolites.

Returns list of lists with on set of reactions that completes the model per requested iteration.

Return type iterable

Examples

```
>>> import cobra.test as ct
>>> from cobra import Model
>>> from cobra.flux_analysis import gapfill
>>> model = ct.create_test_model("salmonella")
>>> universal = Model('universal')
>>> universal.add_reactions(model.reactions.GF6PTA.copy())
>>> model.remove_reactions([model.reactions.GF6PTA])
>>> gapfill(model, universal)
```

cobra.flux_analysis.gapfilling.**growMatch**(*model*, *Universal*, *dm_rxns=False*, *ex_rxns=False*, *penalties=None*, *iterations=1*, ***solver_parameters*)

runs (partial implementation of) growMatch. Legacy function, to be removed in future version of cobrapy in favor of gapfill.

cobra.flux_analysis.loopless module

Provides functions to remove thermodynamically infeasible loops.

cobra.flux_analysis.loopless.**add_loopless**(*model*, *zero_cutoff=1e-12*)

Modify a model so all feasible flux distributions are loopless.

In most cases you probably want to use the much faster *loopless_solution*. May be used in cases where you want to add complex constraints and objecives (for instance quadratic objectives) to the model afterwards or use an approximation of Gibbs free energy directions in you model. Adds variables and constraints to a model which will disallow flux distributions with loops. The used formulation is described in [1]_. This function *will* modify your model.

Parameters

- **model** (*cobra.Model*) – The model to which to add the constraints.
- **zero_cutoff** (*positive float, optional*) – Cutoff used for null space. Coefficients with an absolute value smaller than *zero_cutoff* are considered to be zero.

Returns

Return type Nothing

References

cobra.flux_analysis.loopless.**construct_loopless_model**(*cobra_model*)

Construct a loopless model.

This adds MILP constraints to prevent flux from proceeding in a loop, as done in http://dx.doi.org/10.1016/j.bpj.2010.12.3707 Please see the documentation for an explanation of the algorithm.

This must be solved with an MILP capable solver.

cobra.flux_analysis.loopless.**loopless_fva_iter**(*model*, *reaction*, *solution=False*, *zero_cutoff=1e-06*)

Plugin to get a loopless FVA solution from single FVA iteration.

Assumes the following about *model* and *reaction*: 1. the model objective is set to be *reaction* 2. the model has been optimized and contains the minimum/maximum flux for

reaction

3.the model contains an auxiliary variable called “fva_old_objective” denoting the previous objective

Parameters

- **model** (*cobra.Model*) – The model to be used.
- **reaction** (*cobra.Reaction*) – The reaction currently minimized/maximized.
- **solution** (*boolean, optional*) – Whether to return the entire solution or only the minimum/maximum for *reaction*.
- **zero_cutoff** (*positive float, optional*) – Cutoff used for loop removal. Fluxes with an absolute value smaller than *zero_cutoff* are considered to be zero.

Returns Returns the minimized/maximized flux through *reaction* if all_fluxes == False (default). Otherwise returns a loopless flux solution containing the minimum/maximum flux for *reaction*.

Return type single float or dict

cobra.flux_analysis.loopless.**loopless_solution**(*model*, *fluxes=None*)

Convert an existing solution to a loopless one.

Removes as many loops as possible (see Notes). Uses the method from CycleFreeFlux [1]_ and is much faster than *add_loopless* and should therefore be the preferred option to get loopless flux distributions.

Parameters

- **model** (*cobra.Model*) – The model to which to add the constraints.
- **fluxes** (*dict*) – A dictionary {rxn_id: flux} that assigns a flux to each reaction. If not None will use the provided flux values to obtain a close loopless solution. Note that this requires a linear objective function involving only the model reactions. This is the case if *linear_reaction_coefficients(model)* is a correct representation of the objective.

Returns A solution object containing the fluxes with the least amount of loops possible or None if the optimization failed (usually happening if the flux distribution in *fluxes* is infeasible).

Return type cobra.Solution

Notes

The returned flux solution has the following properties:

•it contains the minimal number of loops possible and no loops at all if all flux bounds include zero

•it has the same exact objective value as the previous solution

•it has the same exact exchange fluxes as the previous solution

•all fluxes have the same sign (flow in the same direction) as the previous solution

References

cobra.flux_analysis.moma module

Contains functions to run minimization of metabolic adjustment (MOMA).

cobra.flux_analysis.moma.**add_moma**(*model*, *solution=None*, *linear=False*)

Add constraints and objective representing for MOMA.

This adds variables and constraints for the minimization of metabolic adjustment (MOMA) to the model.

Parameters

- **model** (*cobra.Model*) – The model to add MOMA constraints and objective to.
- **solution** (*cobra.Solution*) – A previous solution to use as a reference.
- **linear** (*bool*) – Whether to use the linear MOMA formulation or not.

Returns

Return type Nothing.

Notes

In the original MOMA specification one looks for the flux distribution of the deletion (v^d) closest to the fluxes without the deletion (v). In math this means:

minimize sum_i (v^d_i - v_i)^2 s.t. Sv^d = 0

lb_i <= v^d_i <= ub_i

Here, we use a variable transformation v^t := v^d_i - v_i. Substituting and using the fact that Sv = 0 gives:

minimize sum_i (v^t_i)^2 s.t. Sv^d = 0

v^t = v^d_i - v_i lb_i <= v^d_i <= ub_i

So basically we just re-center the flux space at the old solution and than find the flux distribution closest to the new zero (center). This is the same strategy as used in cameo.

In the case of linear MOMA, we instead minimize sum_i abs(v^t_i). The linear MOMA is typically significantly faster. Also quadratic MOMA tends to give flux distributions in which all fluxes deviate from the reference fluxes a little bit whereas linear MOMA tends to give flux distributions where the majority of fluxes are the same reference which few fluxes deviating a lot (typical effect of L2 norm vs L1 norm).

The former objective function is saved in the optlang solver interface as "moma_old_objective" and this can be used to immediately extract the value of the former objective after MOMA optimization.

cobra.flux_analysis.moma.**create_euclidian_distance_lp**(*moma_model*, *solver*)
Create the distance linear program (legacy method).

cobra.flux_analysis.moma.**create_euclidian_distance_objective**(*n_moma_reactions*)
Return a matrix which will minimize the euclidian distance (legacy).

This matrix has the structure [I -I] [-I I] where I is the identity matrix the same size as the number of reactions in the original model.

Parameters **n_moma_reactions** (*int*) – This is the number of reactions in the MOMA model, which should be twice the number of reactions in the original model

Returns A matrix describing the distance objective.

Return type scipy.sparse.dok_matrix

cobra.flux_analysis.moma.**create_euclidian_moma_model**(*cobra_model*, *wt_model=None*, ***solver_args*)
Create a new moma model (legacy function).

cobra.flux_analysis.moma.**moma**(*wt_model*, *mutant_model*, *solver=None*, ***solver_args*)
Run MOMA on models (legacy method).

cobra.flux_analysis.moma.**moma_knockout**(*moma_model*, *moma_objective*, *reaction_indexes*, ***moma_args*)
Compute result of reaction_knockouts using moma.

cobra.flux_analysis.moma.**solve_moma_model**(*moma_model*, *objective_id*, *solver=None*, ***solver_args*)

Solve the MOMA LP (legacy method).

cobra.flux_analysis.parsimonious module

cobra.flux_analysis.parsimonious.**add_pfba**(*model*, *objective=None*, *fraction_of_optimum=1.0*)

Add pFBA objective

Add objective to minimize the summed flux of all reactions to the current objective.

See also:

pfba()

Parameters

- **model** (*cobra.Model*) – The model to add the objective to
- **objective** – An objective to set in combination with the pFBA objective.
- **fraction_of_optimum** (*float*) – Fraction of optimum which must be maintained. The original objective reaction is constrained to be greater than maximal_value * fraction_of_optimum.

cobra.flux_analysis.parsimonious.**optimize_minimal_flux**(**args*, ***kwargs*)

cobra.flux_analysis.parsimonious.**pfba**(*model*, *already_irreversible=False*, *fraction_of_optimum=1.0*, *solver=None*, *desired_objective_value=None*, *objective=None*, *reactions=None*, ***optimize_kwargs*)

Perform basic pFBA (parsimonious Enzyme Usage Flux Balance Analysis) to minimize total flux.

pFBA [1] adds the minimization of all fluxes the the objective of the model. This approach is motivated by the idea that high fluxes have a higher enzyme turn-over and that since producing enzymes is costly, the cell will try to minimize overall flux while still maximizing the original objective function, e.g. the growth rate.

Parameters

- **model** (*cobra.Model*) – The model
- **already_irreversible** (*bool, optional*) – By default, the model is converted to an irreversible one. However, if the model is already irreversible, this step can be skipped. Ignored for optlang solvers as not relevant.
- **fraction_of_optimum** (*float, optional*) – Fraction of optimum which must be maintained. The original objective reaction is constrained to be greater than maximal_value * fraction_of_optimum.
- **solver** (*str, optional*) – Name of the solver to be used. If None it will respect the solver set in the model (model.solver).
- **desired_objective_value** (*float, optional*) – A desired objective value for the minimal solution that bypasses the initial optimization result. Ignored for optlang solvers, instead, define your objective separately and pass using the *objective* argument.
- **objective** (*dict or model.problem.Objective*) – A desired objective to use during optimization in addition to the pFBA objective. Dictionaries (reaction as key, coefficient as value) can be used for linear objectives. Not used for non-optlang solvers.

- **reactions** (*iterable*) – List of reactions or reaction identifiers. Implies *return_frame* to be true. Only return fluxes for the given reactions. Faster than fetching all fluxes if only a few are needed. Only supported for optlang solvers.
- ****optimize_kwargs** (*additional arguments for legacy solver, optional*) – Additional arguments passed to the legacy solver. Ignored for optlang solver (those can be configured using

  model.solver.configuration).

Returns The solution object to the optimized model with pFBA constraints added.

Return type cobra.Solution

References

cobra.flux_analysis.phenotype_phase_plane module

cobra.flux_analysis.phenotype_phase_plane.**calculate_phenotype_phase_plane**(*model*, *reaction1_name*, *reaction2_name*, *reaction1_range_max=20*, *reaction2_range_max=20*, *reaction1_npoints=50*, *reaction2_npoints=50*, *solver=None*, *n_processes=1*, *tolerance=1e-06*)

calculates the growth rates while varying the uptake rates for two reactions.

Returns a *phenotypePhasePlaneData* object containing the growth rates

for the uptake rates. To plot the result, call the plot function of the returned object.

Example

```
>>> import cobra.test
>>> model = cobra.test.create_test_model("textbook")
>>> ppp = calculate_phenotype_phase_plane(model, "EX_glc__D_e", "EX_o2_e")
>>> ppp.plot()
```

cobra.flux_analysis.phenotype_phase_plane.**carbon_yield**(*c_input_output*)

mol product per mol carbon input

Returns the mol carbon atoms in the product (as defined by the model objective) divided by the mol carbon in the input reactions (as defined by the model medium) or zero in case of division by zero arises

Return type float

cobra.flux_analysis.phenotype_phase_plane.**envelope_for_points**(*model*, *reactions*, *grid*, *carbon_io*)

cobra.flux_analysis.phenotype_phase_plane.**get_c_input**(*model*)
carbon source reactions

Returns The medium reaction with highest input carbon flux

Return type *Reaction*

cobra.flux_analysis.phenotype_phase_plane.**mass_yield**(*c_input_output*)
Gram product divided by gram of carbon input source

Parameters **c_input_output** (*tuple*) – Two reactions, the one that feeds carbon to the system and the one that produces carbon containing compound.

Returns gram product per 1 g of feeding source

Return type float

class cobra.flux_analysis.phenotype_phase_plane.**phenotypePhasePlaneData**(*reaction1_name*, *reaction2_name*, *reaction1_range_max*, *reaction2_range_max*, *reaction1_npoints*, *reaction2_npoints*)

Bases: object

class to hold results of a phenotype phase plane analysis

plot()
plot the phenotype phase plane in 3D using any available backend

plot_matplotlib(*theme='Paired'*, *scale_grid=False*)
Use matplotlib to plot a phenotype phase plane in 3D.

theme: color theme to use (requires palettable)

returns: maptlotlib 3d subplot object

plot_mayavi()
Use mayavi to plot a phenotype phase plane in 3D. The resulting figure will be quick to interact with in real time, but might be difficult to save as a vector figure. returns: mlab figure object

segment(*threshold=0.01*)
attempt to segment the data and identify the various phases

cobra.flux_analysis.phenotype_phase_plane.**production_envelope**(*model*, *reactions*, *objective=None*, *c_source=None*, *points=20*, *solver=None*)
Calculate the objective value conditioned on all combinations of fluxes for a set of chosen reactions

The production envelope can be used to analyze a models ability to produce a given compound conditional on the fluxes for another set of reaction, such as the uptake rates. The model is alternately optimize with respect to minimizing and maximizing the objective and record the obtained fluxes. Ranges to compute production is set to the effective bounds, i.e. the minimum / maximum fluxes that can be obtained given current reaction bounds.

Parameters

- **model** (*cobra.Model*) – The model to compute the production envelope for.
- **reactions** (*list or string*) – A list of reactions, reaction identifiers or single reaction
- **objective** (*string, dict, model.solver.interface.Objective*) – The objective (reaction) to use for the production envelope. Use the model's current objective is left missing.
- **c_source** (*cobra.Reaction or string*) – A reaction or reaction identifier that is the source of carbon for computing carbon (mol carbon in output over mol carbon in input) and mass yield (gram product over gram output). Only objectives with a carbon containing input and output metabolite is supported.
- **points** (*int*) – The number of points to calculate production for.
- **solver** (*string*) – The solver to use - only here for consistency with older implementations (this argument will be removed in the future). The solver should be set using *model.solver* directly. Only optlang based solvers are supported.

Returns

A data frame with one row per evaluated point and

- reaction id : one column per input reaction indicating the flux at each given point,
- flux: the objective flux
- carbon_yield: if carbon source is defined and the product is a single metabolite (mol carbon product per mol carbon feeding source)
- mass_yield: if carbon source is defined and the product is a single metabolite (gram product per 1 g of feeding source)
- direction: the direction of the optimization.

Only points that give a valid solution are returned.

Return type pandas.DataFrame

Examples

```
>>> import cobra.test
>>> from cobra.flux_analysis import production_envelope
>>> model = cobra.test.create_test_model("textbook")
>>> production_envelope(model, ["EX_glc__D_e", "EX_o2_e"])
```

cobra.flux_analysis.phenotype_phase_plane.**single_flux**(*reaction*, *consumption=True*)

flux into single product for a reaction

only defined for reactions with single products

Parameters

- **reaction** (Reaction) – the reaction to product flux for

- **consumption** (*bool*) – flux for consumed metabolite, else produced

Returns metabolite, flux for the metabolite

Return type tuple

cobra.flux_analysis.phenotype_phase_plane.**total_carbon_flux**(*reaction*, *consumption=True*)

summed product carbon flux for a reaction

Parameters

- **reaction** (Reaction) – the reaction to carbon return flux for
- **consumption** (*bool*) – flux for consumed metabolite, else produced

Returns reaction flux multiplied by number of carbon for the products of the reaction

Return type float

cobra.flux_analysis.reaction module

functions for analyzing / creating objective functions

cobra.flux_analysis.reaction.**assess**(*model*, *reaction*, *flux_coefficient_cutoff=0.001*, *solver=None*)

Assesses production capacity.

Assesses the capacity of the model to produce the precursors for the reaction and absorb the production of the reaction while the reaction is operating at, or above, the specified cutoff.

Parameters

- **model** (*cobra.Model*) – The cobra model to assess production capacity for
- **reaction** (*reaction identifier or cobra.Reaction*) – The reaction to assess
- **flux_coefficient_cutoff** (*float*) – The minimum flux that reaction must carry to be considered active.
- **solver** (*basestring*) – Solver name. If None, the default solver will be used.

Returns True if the model can produce the precursors and absorb the products for the reaction operating at, or above, flux_coefficient_cutoff. Otherwise, a dictionary of {'precursor': Status, 'product': Status}. Where Status is the results from assess_precursors and assess_products, respectively.

Return type bool or dict

cobra.flux_analysis.reaction.**assess_component**(*model*, *reaction*, *side*, *flux_coefficient_cutoff=0.001*, *solver=None*)

Assesses the ability of the model to provide sufficient precursors, or absorb products, for a reaction operating at, or beyond, the specified cutoff.

Parameters

- **model** (*cobra.Model*) – The cobra model to assess production capacity for
- **reaction** (*reaction identifier or cobra.Reaction*) – The reaction to assess
- **side** (*basestring*) – Side of the reaction, 'products' or 'reactants'

- **flux_coefficient_cutoff** (*float*) – The minimum flux that reaction must carry to be considered active.
- **solver** (*basestring*) – Solver name. If None, the default solver will be used.

Returns True if the precursors can be simultaneously produced at the specified cutoff. False, if the model has the capacity to produce each individual precursor at the specified threshold but not all precursors at the required level simultaneously. Otherwise a dictionary of the required and the produced fluxes for each reactant that is not produced in sufficient quantities.

Return type bool or dict

cobra.flux_analysis.reaction.**assess_precursors**(*model*, *reaction*, *flux_coefficient_cutoff=0.001*, *solver=None*)

Assesses the ability of the model to provide sufficient precursors for a reaction operating at, or beyond, the specified cutoff.

Deprecated: use assess_component instead

Parameters

- **model** (*cobra.Model*) – The cobra model to assess production capacity for
- **reaction** (*reaction identifier or cobra.Reaction*) – The reaction to assess
- **flux_coefficient_cutoff** (*float*) – The minimum flux that reaction must carry to be considered active.
- **solver** (*basestring*) – Solver name. If None, the default solver will be used.

Returns True if the precursors can be simultaneously produced at the specified cutoff. False, if the model has the capacity to produce each individual precursor at the specified threshold but not all precursors at the required level simultaneously. Otherwise a dictionary of the required and the produced fluxes for each reactant that is not produced in sufficient quantities.

Return type bool or dict

cobra.flux_analysis.reaction.**assess_products**(*model*, *reaction*, *flux_coefficient_cutoff=0.001*, *solver=None*)

Assesses whether the model has the capacity to absorb the products of a reaction at a given flux rate.

Useful for identifying which components might be blocking a reaction from achieving a specific flux rate.

Deprecated: use assess_component instead

Parameters

- **model** (*cobra.Model*) – The cobra model to assess production capacity for
- **reaction** (*reaction identifier or cobra.Reaction*) – The reaction to assess
- **flux_coefficient_cutoff** (*float*) – The minimum flux that reaction must carry to be considered active.
- **solver** (*basestring*) – Solver name. If None, the default solver will be used.

Returns True if the model has the capacity to absorb all the reaction products being simultaneously given the specified cutoff. False, if the model has the capacity to absorb each individual product but not all products at the required level simultaneously. Otherwise a dictionary of the required and the capacity fluxes for each product that is not absorbed in sufficient quantities.

Return type bool or dict

cobra.flux_analysis.sampling module

Module implementing flux sampling for cobra models.

New samplers should derive from the abstract *HRSampler* class where possible to provide a uniform interface.

class cobra.flux_analysis.sampling.**ACHRSampler**(*model*, *thinning=100*, *seed=None*)
Bases: *cobra.flux_analysis.sampling.HRSampler*

Artificial Centering Hit-and-Run sampler.

A sampler with low memory foot print and good convergence.

Parameters

- **model** (*a cobra model*) – The cobra model from which to generate samples.
- **thinning** (*int, optional*) – The thinning factor of the generated sampling chain. A thinning of 10 means samples are returned every 10 steps.
- **seed** (*positive integer, optional*) – Sets the random number seed. Initialized to the current time stamp if None.

model
cobra.Model – The cobra model from which the samples get generated.

thinning
int – The currently used thinning factor.

n_samples
int – The total number of samples that have been generated by this sampler instance.

problem
collections.namedtuple – A python object whose attributes define the entire sampling problem in matrix form. See docstring of *Problem*.

warmup
a numpy matrix – A matrix of with as many columns as reactions in the model and more than 3 rows containing a warmup sample in each row. None if no warmup points have been generated yet.

seed
positive integer, optional – Sets the random number seed. Initialized to the current time stamp if None.

fwd_idx
np.array – Has one entry for each reaction in the model containing the index of the respective forward variable.

rev_idx
np.array – Has one entry for each reaction in the model containing the index of the respective reverse variable.

prev
numpy array – The current/last flux sample generated.

center
numpy array – The center of the sampling space as estimated by the mean of all previously generated samples.

Notes

ACHR generates samples by choosing new directions from the sampling space's center and the warmup points. The implementation used here is the same as in the Matlab Cobra Toolbox [2]_ and uses only the initial warmup points to generate new directions and not any other previous iterates. This usually gives better mixing since the startup points are chosen to span the space in a wide manner. This also makes the generated sampling chain quasi-markovian since the center converges rapidly.

Memory usage is roughly in the order of (2 * number reactions)^2 due to the required projection matrices and warmup points. So large models easily take up a few GB of RAM.

References

sample (*n*, *fluxes=True*)
Generate a set of samples.

This is the basic sampling function for all hit-and-run samplers.

Parameters

- **n** (*int*) – The number of samples that are generated at once.
- **fluxes** (*boolean*) – Whether to return fluxes or the internal solver variables. If set to False will return a variable for each forward and backward flux as well as all additional variables you might have defined in the model.

Returns Returns a matrix with *n* rows, each containing a flux sample.

Return type numpy.matrix

Notes

Performance of this function linearly depends on the number of reactions in your model and the thinning factor.

class cobra.flux_analysis.sampling.**HRSampler** (*model*, *thinning*, *seed=None*)
Bases: object

The abstract base class for hit-and-run samplers.

Parameters

- **model** (*cobra.Model*) – The cobra model from which to generate samples.
- **thinning** (*int*) – The thinning factor of the generated sampling chain. A thinning of 10 means samples are returned every 10 steps.

model
cobra.Model – The cobra model from which the samples get generated.

thinning
int – The currently used thinning factor.

n_samples
int – The total number of samples that have been generated by this sampler instance.

problem
collections.namedtuple – A python object whose attributes define the entire sampling problem in matrix form. See docstring of *Problem*.

warmup
a numpy matrix – A matrix of with as many columns as reactions in the model and more than 3 rows containing a warmup sample in each row. None if no warmup points have been generated yet.

seed
positive integer, optional – Sets the random number seed. Initialized to the current time stamp if None.

fwd_idx
np.array – Has one entry for each reaction in the model containing the index of the respective forward variable.

rev_idx
np.array – Has one entry for each reaction in the model containing the index of the respective reverse variable.

batch(*batch_size*, *batch_num*, *fluxes=True*)
Create a batch generator.

This is useful to generate n batches of m samples each.

Parameters

- **batch_size** (*int*) – The number of samples contained in each batch (m).
- **batch_num** (*int*) – The number of batches in the generator (n).
- **fluxes** (*boolean*) – Whether to return fluxes or the internal solver variables. If set to False will return a variable for each forward and backward flux as well as all additional variables you might have defined in the model.

Yields *pandas.DataFrame* – A DataFrame with dimensions (batch_size x n_r) containing a valid flux sample for a total of n_r reactions (or variables if fluxes=False) in each row.

generate_fva_warmup()
Generate the warmup points for the sampler.

Generates warmup points by setting each flux as the sole objective and minimizing/maximizing it. Also caches the projection of the warmup points into the nullspace for non-homogeneous problems (only if necessary).

sample(*n*, *fluxes=True*)
Abstract sampling function.

Should be overwritten by child classes.

validate(*samples*)
Validate a set of samples for equality and inequality feasibility.

Can be used to check whether the generated samples and warmup points are feasible.

Parameters **samples** (*numpy.matrix*) – Must be of dimension (n_samples x n_reactions). Contains the samples to be validated. Samples must be from fluxes.

Returns

A one-dimensional numpy array of length containing a code of 1 to 3 letters denoting the validation result:

- 'v' means feasible in bounds and equality constraints
- 'l' means a lower bound violation
- 'u' means a lower bound validation
- 'e' means and equality constraint violation

Return type numpy.array

class cobra.flux_analysis.sampling.**OptGPSampler**(*model*, *processes*, *thinning=100*, *seed=None*)

Bases: *cobra.flux_analysis.sampling.HRSampler*

A parallel optimized sampler.

A parallel sampler with fast convergence and parallel execution. See [1]_ for details.

Parameters

- **model** (*cobra.Model*) – The cobra model from which to generate samples.
- **processes** (*int*) – The number of processes used during sampling.
- **thinning** (*int, optional*) – The thinning factor of the generated sampling chain. A thinning of 10 means samples are returned every 10 steps.
- **seed** (*positive integer, optional*) – Sets the random number seed. Initialized to the current time stamp if None.

model
cobra.Model – The cobra model from which the samples get generated.

thinning
int – The currently used thinning factor.

n_samples
int – The total number of samples that have been generated by this sampler instance.

problem
collections.namedtuple – A python object whose attributes define the entire sampling problem in matrix form. See docstring of *Problem*.

warmup
a numpy matrix – A matrix of with as many columns as reactions in the model and more than 3 rows containing a warmup sample in each row. None if no warmup points have been generated yet.

seed
positive integer, optional – Sets the random number seed. Initialized to the current time stamp if None.

fwd_idx
np.array – Has one entry for each reaction in the model containing the index of the respective forward variable.

rev_idx
np.array – Has one entry for each reaction in the model containing the index of the respective reverse variable.

prev
numpy.array – The current/last flux sample generated.

center
numpy.array – The center of the sampling space as estimated by the mean of all previously generated samples.

Notes

The sampler is very similar to artificial centering where each process samples its own chain. Initial points are chosen randomly from the warmup points followed by a linear transformation that pulls the points towards the a little bit towards the center of the sampling space.

If the number of processes used is larger than one the requested number of samples is adjusted to the smallest multiple of the number of processes larger than the requested sample number. For instance, if you have 3 processes and request 8 samples you will receive 9.

Memory usage is roughly in the order of (2 * number reactions)^2 due to the required projection matrices and warmup points. So large models easily take up a few GB of RAM. However, most of the large matrices are kept in shared memory. So the RAM usage is independent of the number of processes.

References

sample(*n*, *fluxes=True*)

Generate a set of samples.

This is the basic sampling function for all hit-and-run samplers.

n [int] The minimum number of samples that are generated at once (see Notes).

fluxes [boolean] Whether to return fluxes or the internal solver variables. If set to False will return a variable for each forward and backward flux as well as all additional variables you might have defined in the model.

Returns Returns a matrix with *n* rows, each containing a flux sample.

Return type numpy.matrix

Notes

Performance of this function linearly depends on the number of reactions in your model and the thinning factor.

If the number of processes is larger than one, computation is split across as the CPUs of your machine. This may shorten computation time. However, there is also overhead in setting up parallel computation so we recommend to calculate large numbers of samples at once ($n > 1000$).

class cobra.flux_analysis.sampling.**Problem**(*equalities*, *b*, *inequalities*, *bounds*, *variable_fixed*, *variable_bounds*, *projection*, *homogeneous*)

Bases: tuple

Defines the matrix representation of a sampling problem.

equalities
numpy.array – All equality constraints in the model.

b
numpy.array – The right side of the equality constraints.

inequalities
numpy.array – All inequality constraints in the model.

bounds
numpy.array – The lower and upper bounds for the inequality constraints.

variable_bounds
numpy.array – The lower and upper bounds for the variables.

homogeneous
boolean – Indicates whether the sampling problem is homogenous, e.g. whether there exist no non-zero fixed variables or constraints.

projection
numpy.matrix – A projection matrix that projects an arbitrary point into the nullspace of the problem.

b
Alias for field number 1

bounds
Alias for field number 3

equalities
Alias for field number 0

homogeneous
Alias for field number 7

inequalities
Alias for field number 2

projection
Alias for field number 6

variable_bounds
Alias for field number 5

variable_fixed
Alias for field number 4

cobra.flux_analysis.sampling.**bounds_tol**
The tolerance used for checking bounds feasibility.

cobra.flux_analysis.sampling.**feasibility_tol**
The tolerance used for checking equalities feasibility.

cobra.flux_analysis.sampling.**mp_init**(*obj*)
Initialize the multiprocessing pool.

cobra.flux_analysis.sampling.**nproj = 1000000**
Reproject the solution into the feasibility space every nproj iterations.

cobra.flux_analysis.sampling.**sample**(*model*, *n*, *method='optgp'*, *thinning=100*, *processes=1*, *seed=None*)
Sample valid flux distributions from a cobra model.

The function samples valid flux distributions from a cobra model. Currently we support two methods:

1. **'optgp' (default) which uses the OptGPSampler that supports parallel** sampling [1]_. Requires large numbers of samples to be performant (n < 1000). For smaller samples 'achr' might be better suited.

or

2. 'achr' which uses artificial centering hit-and-run. This is a single process method with good convergence [2]_.

Parameters

- **model** (*cobra.Model*) – The model from which to sample flux distributions.
- **n** (*int*) – The number of samples to obtain. When using 'optgp' this must be a multiple of *processes*, otherwise a larger number of samples will be returned.
- **method** (*str, optional*) – The sampling algorithm to use.
- **thinning** (*int, optional*) – The thinning factor of the generated sampling chain. A thinning of 10 means samples are returned every 10 steps. Defaults to 100 which in benchmarks gives approximately uncorrelated samples. If set to one will return all iterates.

- **processes** (*int, optional*) – Only used for 'optgp'. The number of processes used to generate samples.
- **seed** (*positive integer, optional*) – The random number seed to be used. Initialized to current time stamp if None.

Returns The generated flux samples. Each row corresponds to a sample of the fluxes and the columns are the reactions.

Return type pandas.DataFrame

Notes

The samplers have a correction method to ensure equality feasibility for long-running chains, however this will only work for homogeneous models, meaning models with no non-zero fixed variables or constraints (right-hand side of the equalities are zero).

References

cobra.flux_analysis.sampling.**shared_np_array**(*shape*, *data=None*)

Create a new numpy array that resides in shared memory.

shape [tuple of ints] The shape of the new array.

data [numpy.array] Data to copy to the new array. Has to have the same shape.

cobra.flux_analysis.single_deletion module

Bundles functions for successively deleting a set of genes or reactions.

cobra.flux_analysis.single_deletion.**single_gene_deletion**(*cobra_model*, *gene_list=None*, *solver=None*, *method='fba'*, ***solver_args*)

Sequentially knocks out each gene from a given gene list.

Parameters

- **cobra_model** (*a cobra model*) – The model from which to delete the genes. The model will not be modified.
- **gene_list** (*iterable*) – List of gene IDs or cobra.Gene. If None (default) will use all genes in the model.
- **method** (*str, optional*) – The method used to obtain fluxes. Must be one of "fba", "moma" or "linear moma".
- **solver** (*str, optional*) – Name of the solver to be used.
- **solver_args** (*optional*) – Additional arguments for the solver. Ignored for optlang solver, please use *model.solver.configuration* instead.

Returns

Data frame with two column and reaction id as index: - flux: the value of the objective after the knockout - status: the solution's status, (for instance "optimal" for each

knockout)

Return type pandas.DataFrame

cobra.flux_analysis.single_deletion.**single_gene_deletion_fba**(*cobra_model*, *gene_list*, *solver=None*, ***solver_args*)

Sequentially knocks out each gene in a model using FBA.

Not supposed to be called directly use *single_reactions_deletion(..., method="fba")* instead.

Parameters

- **gene_list** (*iterable*) – List of gene IDs or cobra.Reaction.
- **solver** (*str, optional*) – The name of the solver to be used.

Returns A tuple ({reaction_id: growth_rate}, {reaction_id: status})

Return type tuple of dicts

cobra.flux_analysis.single_deletion.**single_gene_deletion_moma**(*cobra_model*, *gene_list*, *linear=False*, *solver=None*, ***solver_args*)

Sequentially knocks out each gene in a model using MOMA.

Not supposed to be called directly use *single_reactions_deletion(..., method="moma")* instead.

Parameters

- **gene_list** (*iterable*) – List of gene IDs or cobra.Reaction.
- **linear** (*bool*) – Whether to use linear MOMA.
- **solver** (*str, optional*) – The name of the solver to be used.

Returns A tuple ({reaction_id: growth_rate}, {reaction_id: status})

Return type tuple of dicts

cobra.flux_analysis.single_deletion.**single_reaction_deletion**(*cobra_model*, *reaction_list=None*, *solver=None*, *method='fba'*, ***solver_args*)

Sequentially knocks out each reaction from a given reaction list.

Parameters

- **cobra_model** (*cobra.Model*) – The model from which to delete the reactions. The model will not be modified.
- **reaction_list** (*iterable*) – List of reaction IDs or cobra.Reaction. If None (default) will use all reactions in the model.
- **method** (*str, optional*) – The method used to obtain fluxes. Must be one of "fba", "moma" or "linear moma".
- **solver** (*str, optional*) – Name of the solver to be used.
- **solver_args** (*optional*) – Additional arguments for the solver. Ignored for optlang solver, please use *model.solver.configuration* instead.

Returns

Data frame with two column and reaction id as index: - flux: the value of the objective after the knockout - status: the solution's status, (for instance "optimal" for each

knockout)

Return type pandas.DataFrame

cobra.flux_analysis.single_deletion.**single_reaction_deletion_fba**(*cobra_model*, *reaction_list*, *solver=None*, ***solver_args*)

Sequentially knocks out each reaction in a model using FBA.

Not supposed to be called directly use *single_reactions_deletion(..., method="fba")* instead.

Parameters

- **cobra_model** (*cobra.Model*) – The model from which to delete the reactions. The model will not be modified.
- **reaction_list** (*iterable*) – List of reaction Ids or cobra.Reaction.
- **solver** (*str, optional*) – The name of the solver to be used.

Returns A tuple ({reaction_id: growth_rate}, {reaction_id: status})

Return type tuple of dicts

cobra.flux_analysis.single_deletion.**single_reaction_deletion_moma**(*cobra_model*, *reaction_list*, *linear=False*, *solver=None*, ***solver_args*)

Sequentially knocks out each reaction in a model using MOMA.

Not supposed to be called directly use *single_reactions_deletion(..., method="moma")* instead.

Parameters

- **cobra_model** (*cobra.Model*) – The model from which to delete the reactions. The model will not be modified.
- **reaction_list** (*iterable*) – List of reaction IDs or cobra.Reaction.
- **linear** (*bool*) – Whether to use linear MOMA.
- **solver** (*str, optional*) – The name of the solver to be used.

Returns A tuple ({reaction_id: growth_rate}, {reaction_id: status})

Return type tuple of dicts

cobra.flux_analysis.summary module

cobra.flux_analysis.summary.**format_long_string**(*string*, *max_length*)

cobra.flux_analysis.summary.**metabolite_summary**(*met*, *threshold=0.01*, *fva=False*, *floatfmt='.3g'*, ***solver_args*)

Print a summary of the reactions which produce and consume this metabolite

threshold: float a value below which to ignore reaction fluxes

fva: float (0->1), or None Whether or not to include flux variability analysis in the output. If given, fva should be a float between 0 and 1, representing the fraction of the optimum objective to be searched.

floatfmt: string format method for floats, passed to tabulate. Default is '.3g'.

cobra.flux_analysis.summary.**model_summary**(*model*, *threshold=1e-08*, *fva=None*, *floatfmt='.3g'*, ***solver_args*)

Print a summary of the input and output fluxes of the model.

threshold: float tolerance for determining if a flux is zero (not printed)

fva: int or None Whether or not to calculate and report flux variability in the output summary

floatfmt: string format method for floats, passed to tabulate. Default is '.3g'.

cobra.flux_analysis.variability module

cobra.flux_analysis.variability.**calculate_lp_variability**(*lp*, *solver*, *cobra_model*, *reaction_list*, ***solver_args*)

calculate max and min of selected variables in an LP

cobra.flux_analysis.variability.**find_blocked_reactions**(*model*, *reaction_list=None*, *solver=None*, *zero_cutoff=1e-09*, *open_exchanges=False*, ***solver_args*)

Finds reactions that cannot carry a flux with the current exchange reaction settings for a cobra model, using flux variability analysis.

Parameters

- **model** (*cobra.Model*) – The model to analyze
- **reaction_list** (*list*) – List of reactions to consider, use all if left missing
- **solver** (*string*) – The name of the solver to use
- **zero_cutoff** (*float*) – Flux value which is considered to effectively be zero.
- **open_exchanges** (*bool*) – If true, set bounds on exchange reactions to very high values to avoid that being the bottle-neck.
- ****solver_args** – Additional arguments to the solver. Ignored for optlang based solvers.

Returns List with the blocked reactions

Return type list

cobra.flux_analysis.variability.**find_essential_genes**(*model*, *threshold=0.01*)

Return a set of essential genes.

A gene is considered essential if restricting the flux of all reactions that depends on it to zero causes the objective (e.g. the growth rate) to also be zero.

Parameters

- **model** (*cobra.Model*) – The model to find the essential genes for.
- **threshold** (*float (default 0.01)*) – Minimal objective flux to be considered viable.

Returns Set of essential genes

Return type set

cobra.flux_analysis.variability.**find_essential_reactions**(*model*, *threshold=0.01*)

Return a set of essential reactions.

A reaction is considered essential if restricting its flux to zero causes the objective (e.g. the growth rate) to also be zero.

Parameters

- **model** (*cobra.Model*) – The model to find the essential reactions for.
- **threshold** (*float (default 0.01)*) – Minimal objective flux to be considered viable.

Returns Set of essential reactions

Return type set

cobra.flux_analysis.variability.**flux_variability_analysis**(*model*, *reaction_list=None*, *loopless=False*, *fraction_of_optimum=1.0*, *pfba_factor=None*, *solver=None*, ***solver_args*)

Runs flux variability analysis to find the min/max flux values for each each reaction in *reaction_list*.

Parameters

- **model** (*a cobra model*) – The model for which to run the analysis. It will *not* be modified.
- **reaction_list** (*list of cobra.Reaction or str, optional*) – The reactions for which to obtain min/max fluxes. If None will use all reactions in the model.
- **loopless** (*boolean, optional*) – Whether to return only loopless solutions. Ignored for legacy solvers, also see *Notes*.
- **fraction_of_optimum** (*float, optional*) – Must be <= 1.0. Requires that the objective value is at least fraction * max_objective_value. A value of 0.85 for instance means that the objective has to be at least at 85% percent of its maximum.
- **pfba_factor** (*float, optional*) – Add additional constraint to the model that the total sum of absolute fluxes must not be larger than this value times the smallest possible sum of absolute fluxes, i.e., by setting the value to 1.1 then the total sum of absolute fluxes must not be more than 10% larger than the pfba solution. Since the pfba solution is the one that optimally minimizes the total flux sum, the pfba_factor should, if set, be larger than one. Setting this value may lead to more realistic predictions of the effective flux bounds.
- **solver** (*str, optional*) – Name of the solver to be used. If None it will respect the solver set in the model (model.solver).
- ****solver_args** (*additional arguments for legacy solver, optional*) – Additional arguments passed to the legacy solver. Ignored for optlang solver (those can be configured using model.solver.configuration).

Returns

DataFrame with reaction identifier as the index columns

- maximum: indicating the highest possible flux
- minimum: indicating the lowest possible flux

Return type pandas.DataFrame

Notes

This implements the fast version as described in [1]_. Please note that the flux distribution containing all minimal/maximal fluxes does not have to be a feasible solution for the model. Fluxes are minimized/maximized individually and a single minimal flux might require all others to be suboptimal.

Using the loopless option will lead to a significant increase in computation time (about a factor of 100 for large models). However, the algorithm used here (see [2]_) is still more than 1000x faster than the "naive" version using *add_loopless(model)*. Also note that if you have included constraints that force a loop (for instance by setting all fluxes in a loop to be non-zero) this loop will be included in the solution.

References

Module contents

cobra.io package

Submodules

cobra.io.json module

cobra.io.json.**from_json**(*document*)
Load a cobra model from a JSON document.

Parameters **document** (*str*) – The JSON document representation of a cobra model.

Returns The cobra model as represented in the JSON document.

Return type cobra.Model

See also:

load_json_model() Load directly from a file.

cobra.io.json.**load_json_model**(*filename*)
Load a cobra model from a file in JSON format.

Parameters **filename** (*str or file-like*) – File path or descriptor that contains the JSON document describing the cobra model.

Returns The cobra model as represented in the JSON document.

Return type cobra.Model

See also:

from_json() Load from a string.

cobra.io.json.**save_json_model**(*model*, *filename*, *pretty=False*, ***kwargs*)
Write the cobra model to a file in JSON format.

`kwargs` are passed on to `json.dump`.

Parameters

- **model** (*cobra.Model*) – The cobra model to represent.
- **filename** (*str or file-like*) – File path or descriptor that the JSON representation should be written to.

- **pretty** (*bool, optional*) – Whether to format the JSON more compactly (default) or in a more verbose but easier to read fashion. Can be partially overwritten by the `kwargs`.

See also:

to_json() Return a string representation.

json.dump() Base function.

cobra.io.json.**to_json**(*model*, ***kwargs*)
Return the model as a JSON document.

`kwargs` are passed on to `json.dumps`.

Parameters **model** (*cobra.Model*) – The cobra model to represent.

Returns String representation of the cobra model as a JSON document.

Return type str

See also:

save_json_model() Write directly to a file.

json.dumps() Base function.

cobra.io.mat module

cobra.io.mat.**create_mat_dict**(*model*)
create a dict mapping model attributes to arrays

cobra.io.mat.**create_mat_metabolite_id**(*model*)

cobra.io.mat.**from_mat_struct**(*mat_struct*, *model_id=None*, *inf=<Mock object>*)
create a model from the COBRA toolbox struct

The struct will be a dict read in by scipy.io.loadmat

cobra.io.mat.**load_matlab_model**(*infile_path*, *variable_name=None*, *inf=<Mock object>*)
Load a cobra model stored as a .mat file

Parameters

- **infile_path** (*str*) – path to the file to to read
- **variable_name** (*str, optional*) – The variable name of the model in the .mat file. If this is not specified, then the first MATLAB variable which looks like a COBRA model will be used
- **inf** (*value*) – The value to use for infinite bounds. Some solvers do not handle infinite values so for using those, set this to a high numeric value.

Returns The resulting cobra model

Return type cobra.core.Model.Model

cobra.io.mat.**model_to_pymatbridge**(*model*, *variable_name='model'*, *matlab=None*)
send the model to a MATLAB workspace through pymatbridge

This model can then be manipulated through the COBRA toolbox

Parameters

- **variable_name** (*str*) – The variable name to which the model will be assigned in the MATLAB workspace
- **matlab** (*None or pymatbridge.Matlab instance*) – The MATLAB workspace to which the variable will be sent. If this is None, then this will be sent to the same environment used in IPython magics.

cobra.io.mat.**save_matlab_model**(*model*, *file_name*, *varname=None*)

Save the cobra model as a .mat file.

This .mat file can be used directly in the MATLAB version of COBRA.

Parameters

- **model** (*cobra.core.Model.Model object*) – The model to save
- **file_name** (*str or file-like object*) – The file to save to
- **varname** (*string*) – The name of the variable within the workspace

cobra.io.sbml module

cobra.io.sbml.**add_sbml_species**(*sbml_model*, *cobra_metabolite*, *note_start_tag*, *note_end_tag*, *boundary_metabolite=False*)

A helper function for adding cobra metabolites to an sbml model.

Parameters

- **sbml_model** (*sbml_model object*) –
- **cobra_metabolite** (*a cobra.Metabolite object*) –
- **note_start_tag** (*string*) – the start tag for parsing cobra notes. this will eventually be supplanted when COBRA is worked into sbml.
- **note_end_tag** (*string*) – the end tag for parsing cobra notes. this will eventually be supplanted when COBRA is worked into sbml.
- **boundary_metabolite** (*bool*) – if metabolite boundary condition should be set or not

Returns string

Return type the created metabolite identifier

cobra.io.sbml.**create_cobra_model_from_sbml_file**(*sbml_filename*, *old_sbml=False*, *legacy_metabolite=False*, *print_time=False*, *use_hyphens=False*)

convert an SBML XML file into a cobra.Model object.

Supports SBML Level 2 Versions 1 and 4. The function will detect if the SBML fbc package is used in the file and run the converter if the fbc package is used.

Parameters

- **sbml_filename** (*string*) –
- **old_sbml** (*bool*) – Set to True if the XML file has metabolite formula appended to metabolite names. This was a poorly designed artifact that persists in some models.
- **legacy_metabolite** (*bool*) –

  If True then assume that the metabolite id has the compartment id appended after an underscore (e.g. _c for cytosol). This has not been implemented but will be soon.

- **print_time** (*bool*) – deprecated
- **use_hyphens** (*bool*) – If True, double underscores (__) in an SBML ID will be converted to hyphens

Returns Model

Return type The parsed cobra model

cobra.io.sbml.**fix_legacy_id**(*id*, *use_hyphens=False*, *fix_compartments=False*)

cobra.io.sbml.**get_libsbml_document**(*cobra_model*, *sbml_level=2*, *sbml_version=1*, *print_time=False*, *use_fbc_package=True*)

Return a libsbml document object for writing to a file. This function is used by write_cobra_model_to_sbml_file().

cobra.io.sbml.**parse_legacy_id**(*the_id*, *the_compartment=None*, *the_type='metabolite'*, *use_hyphens=False*)

Deals with a bunch of problems due to bigg.ucsd.edu not following SBML standards

Parameters

- **the_id** (*String.*) –
- **the_compartment** (*String*) –
- **the_type** (*String*) – Currently only 'metabolite' is supported
- **use_hyphens** (*Boolean*) – If True, double underscores (__) in an SBML ID will be converted to hyphens

Returns string

Return type the identifier

cobra.io.sbml.**parse_legacy_sbml_notes**(*note_string*, *note_delimiter=':'*)

Deal with legacy SBML format issues arising from the COBRA Toolbox for MATLAB and BiGG.ucsd.edu developers.

cobra.io.sbml.**read_legacy_sbml**(*filename*, *use_hyphens=False*)

read in an sbml file and fix the sbml id's

cobra.io.sbml.**write_cobra_model_to_sbml_file**(*cobra_model*, *sbml_filename*, *sbml_level=2*, *sbml_version=1*, *print_time=False*, *use_fbc_package=True*)

Write a cobra.Model object to an SBML XML file.

Parameters

- **cobra_model** (*cobra.core.Model.Model*) – The model object to write
- **sbml_filename** (*string*) – The file to write the SBML XML to.
- **sbml_level** (*int*) – 2 is the only supported level.
- **sbml_version** (*int*) – 1 is the only supported version.
- **print_time** (*bool*) – deprecated
- **use_fbc_package** (*bool*) – Convert the model to the FBC package format to improve portability. http://sbml.org/Documents/Specifications/SBML_Level_3/Packages/Flux_Balance_Constraints_(flux)

Notes

TODO: Update the NOTES to match the SBML standard and provide support for Level 2 Version 4

cobra.io.sbml3 module

exception cobra.io.sbml3.**CobraSBMLError**
Bases: Exception

cobra.io.sbml3.**annotate_cobra_from_sbml**(*cobra_element*, *sbml_element*)

cobra.io.sbml3.**annotate_sbml_from_cobra**(*sbml_element*, *cobra_element*)

cobra.io.sbml3.**clip**(*string*, *prefix*)
clips a prefix from the beginning of a string if it exists

```
>>> clip("R_pgi", "R_")
"pgi"
```

cobra.io.sbml3.**construct_gpr_xml**(*parent*, *expression*)
create gpr xml under parent node

cobra.io.sbml3.**get_attrib**(*tag*, *attribute*, *type=<function <lambda>>*, *require=False*)

cobra.io.sbml3.**indent_xml**(*elem*, *level=0*)
indent xml for pretty printing

cobra.io.sbml3.**model_to_xml**(*cobra_model*, *units=True*)

cobra.io.sbml3.**ns**(*query*)
replace prefixes with namespace

cobra.io.sbml3.**parse_stream**(*filename*)
parses filename or compressed stream to xml

cobra.io.sbml3.**parse_xml_into_model**(*xml*, *number=<class 'float'>*)

cobra.io.sbml3.**read_sbml_model**(*filename*, *number=<class 'float'>*, ***kwargs*)

cobra.io.sbml3.**set_attrib**(*xml*, *attribute_name*, *value*)

cobra.io.sbml3.**strnum**(*number*)
Utility function to convert a number to a string

cobra.io.sbml3.**validate_sbml_model**(*filename*, *check_model=True*)
Returns the model along with a list of errors.

Parameters

- **filename** (*str*) – The filename of the SBML model to be validated.
- **check_model** (*bool, optional*) – Whether to also check some basic model properties such as reaction boundaries and compartment formulas.

Returns

- **model** (Model object) – The cobra model if the file could be read succesfully or None otherwise.
- **errors** (*dict*) – Warnings and errors grouped by their respective types.

Raises *CobraSBMLError* – If the file is not a valid SBML Level 3 file with FBC.

cobra.io.sbml3.**write_sbml_model**(*cobra_model*, *filename*, *use_fbc_package=True*, ***kwargs*)

Module contents

cobra.manipulation package

Submodules

cobra.manipulation.annotate module

cobra.manipulation.annotate.**add_SBO**(*model*)
adds SBO terms for demands and exchanges

This works for models which follow the standard convention for constructing and naming these reactions.

The reaction should only contain the single metabolite being exchanged, and the id should be EX_metid or DM_metid

cobra.manipulation.delete module

cobra.manipulation.delete.**delete_model_genes**(*cobra_model*, *gene_list*, *cumulative_deletions=True*, *disable_orphans=False*)
delete_model_genes will set the upper and lower bounds for reactions catalysed by the genes in gene_list if deleting the genes means that the reaction cannot proceed according to cobra_model.reactions[:].gene_reaction_rule

cumulative_deletions: False or True. If True then any previous deletions will be maintained in the model.

cobra.manipulation.delete.**find_gene_knockout_reactions**(*cobra_model*, *gene_list*, *compiled_gene_reaction_rules=None*)
identify reactions which will be disabled when the genes are knocked out

cobra_model: `Model`

gene_list: iterable of `Gene`

compiled_gene_reaction_rules: dict of {reaction_id: compiled_string} If provided, this gives pre-compiled gene_reaction_rule strings. The compiled rule strings can be evaluated much faster. If a rule is not provided, the regular expression evaluation will be used. Because not all gene_reaction_rule strings can be evaluated, this dict must exclude any rules which can not be used with eval.

cobra.manipulation.delete.**get_compiled_gene_reaction_rules**(*cobra_model*)
Generates a dict of compiled gene_reaction_rules

Any gene_reaction_rule expressions which cannot be compiled or do not evaluate after compiling will be excluded. The result can be used in the find_gene_knockout_reactions function to speed up evaluation of these rules.

cobra.manipulation.delete.**prune_unused_metabolites**(*cobra_model*)
Remove metabolites that are not involved in any reactions

Parameters **cobra_model** (*cobra.Model*) – the model to remove unused metabolites from

Returns list of metabolites that were removed

Return type list

cobra.manipulation.delete.**prune_unused_reactions**(*cobra_model*)
Remove reactions that have no assigned metabolites

Parameters **cobra_model** (*cobra.Model*) – the model to remove unused reactions from

Returns list of reactions that were removed

Return type list

cobra.manipulation.delete.**remove_genes**(*cobra_model*, *gene_list*, *remove_reactions=True*)
remove genes entirely from the model

This will also simplify all gene_reaction_rules with this gene inactivated.

cobra.manipulation.delete.**undelete_model_genes**(*cobra_model*)
Undoes the effects of a call to delete_model_genes in place.

cobra_model: A cobra.Model which will be modified in place

cobra.manipulation.modify module

cobra.manipulation.modify.**canonical_form**(*model*, *objective_sense='maximize'*, *already_irreversible=False*, *copy=True*)
Return a model (problem in canonical_form).

Converts a minimization problem to a maximization, makes all variables positive by making reactions irreversible, and converts all constraints to <= constraints.

model: class:~*cobra.core.Model*. The model/problem to convert.

objective_sense: str. The objective sense of the starting problem, either 'maximize' or 'minimize'. A minimization problems will be converted to a maximization.

already_irreversible: bool. If the model is already irreversible, then pass True.

copy: bool. Copy the model before making any modifications.

cobra.manipulation.modify.**convert_to_irreversible**(*cobra_model*)
Split reversible reactions into two irreversible reactions

These two reactions will proceed in opposite directions. This guarentees that all reactions in the model will only allow positive flux values, which is useful for some modeling problems.

cobra_model: A Model object which will be modified in place.

cobra.manipulation.modify.**escape_ID**(*cobra_model*)
makes all ids SBML compliant

cobra.manipulation.modify.**rename_genes**(*cobra_model*, *rename_dict*)
renames genes in a model from the rename_dict

cobra.manipulation.modify.**revert_to_reversible**(*cobra_model*, *update_solution=True*)
This function will convert an irreversible model made by convert_to_irreversible into a reversible model.

cobra_model [cobra.Model] A model which will be modified in place.

update_solution: bool This option is ignored since *model.solution* was removed.

cobra.manipulation.validate module

cobra.manipulation.validate.**check_mass_balance**(*model*)

cobra.manipulation.validate.**check_metabolite_compartment_formula**(*model*)

cobra.manipulation.validate.**check_reaction_bounds**(*model*)

Module contents

cobra.topology package

Submodules

cobra.topology.reporter_metabolites module

cobra.topology.reporter_metabolites.**identify_reporter_metabolites**(**args*, ***kwargs*)

Module contents

cobra.util package

Submodules

cobra.util.array module

cobra.util.array.**constraint_matrices**(*model*, *array_type='dense'*, *include_vars=False*, *zero_tol=1e-06*)

Create a matrix representation of the problem.

This is used for alternative solution approaches that do not use optlang. The function will construct the equality matrix, inequality matrix and bounds for the complete problem.

Notes

To accomodate non-zero equalities the problem will add the variable "const_one" which is a variable that equals one.

Parameters

- **model** (*cobra.Model*) – The model from which to obtain the LP problem.
- **array_type** (*string*) – The type of array to construct. if 'dense', return a standard numpy.array, 'dok', or 'lil' will construct a sparse array using scipy of the corresponding type and 'DataFrame' will give a pandas *DataFrame* with metabolite indices and reaction columns.
- **zero_tol** (*float*) – The zero tolerance used to judge whether two bounds are the same.

Returns

A named tuple consisting of 6 matrices and 2 vectors: - "equalities" is a matrix S such that S*vars = b. It includes a row

for each constraint and one column for each variable.

- "b" the right side of the equality equation such that S*vars = b.
- "inequalities" is a matrix M such that lb <= M*vars <= ub. It contains a row for each inequality and as many columns as variables.
- "bounds" is a compound matrix [lb ub] containing the lower and upper bounds for the inequality constraints in M.

- "variable_fixed" is a boolean vector indicating whether the variable at that index is fixed (lower bound == upper_bound) and is thus bounded by an equality constraint.
- "variable_bounds" is a compound matrix [lb ub] containing the lower and upper bounds for all variables.

Return type collections.namedtuple

cobra.util.array.**create_stoichiometric_matrix**(*model*, *array_type='dense'*, *dtype=None*)

Return a stoichiometric array representation of the given model.

The the columns represent the reactions and rows represent metabolites. S[i,j] therefore contains the quantity of metabolite *i* produced (negative for consumed) by reaction *j*.

Parameters

- **model** (*cobra.Model*) – The cobra model to construct the matrix for.
- **array_type** (*string*) – The type of array to construct. if 'dense', return a standard numpy.array, 'dok', or 'lil' will construct a sparse array using scipy of the corresponding type and 'DataFrame' will give a pandas *DataFrame* with metabolite indices and reaction columns
- **dtype** (*data-type*) – The desired data-type for the array. If not given, defaults to float.

Returns The stoichiometric matrix for the given model.

Return type matrix of class *dtype*

cobra.util.array.**nullspace**(*A*, *atol=1e-13*, *rtol=0*)

Compute an approximate basis for the nullspace of A. The algorithm used by this function is based on the singular value decomposition of *A*.

Parameters

- **A** (*numpy.ndarray*) – A should be at most 2-D. A 1-D array with length k will be treated as a 2-D with shape (1, k)
- **atol** (*float*) – The absolute tolerance for a zero singular value. Singular values smaller than *atol* are considered to be zero.
- **rtol** (*float*) – The relative tolerance. Singular values less than rtol*smax are considered to be zero, where smax is the largest singular value.
- **both atol and rtol are positive, the combined tolerance is the** (*If*) –

:param maximum of the two; that is::: :param tol = max(atol, rtol * smax): :param Singular values smaller than *tol* are considered to be zero.:

Returns If *A* is an array with shape (m, k), then *ns* will be an array with shape (k, n), where n is the estimated dimension of the nullspace of *A*. The columns of *ns* are a basis for the nullspace; each element in numpy.dot(A, ns) will be approximately zero.

Return type numpy.ndarray

Notes

Taken from the numpy cookbook.

cobra.util.context module

class cobra.util.context.**HistoryManager**
Bases: object

Record a list of actions to be taken at a later time. Used to implement context managers that allow temporary changes to a Model.

reset()
Trigger executions for all items in the stack in reverse order

cobra.util.context.**get_context**(*obj*)
Search for a context manager

cobra.util.context.**resettable**(*f*)
A decorator to simplify the context management of simple object attributes. Gets the value of the attribute prior to setting it, and stores a function to set the value to the old value in the HistoryManager.

cobra.util.solver module

Additional helper functions for the optlang solvers.

All functions integrate well with the context manager, meaning that all operations defined here are automatically reverted when used in a *with model:* block.

The functions defined here together with the existing model functions should allow you to implement custom flux analysis methods with ease.

exception cobra.util.solver.**SolverNotFound**
Bases: Exception

A simple Exception when a solver can not be found.

cobra.util.solver.**add_absolute_expression**(*model*, *expression*, *name='abs_var'*, *ub=None*, *difference=0*, *add=True*)
Add the absolute value of an expression to the model.

Also defines a variable for the absolute value that can be used in other objectives or constraints.

Parameters

- **model** (*a cobra model*) – The model to which to add the absolute expression.
- **expression** (*A sympy expression*) – Must be a valid expression within the Model's solver object. The absolute value is applied automatically on the expression.
- **name** (*string*) – The name of the newly created variable.
- **ub** (*positive float*) – The upper bound for the variable.
- **difference** (*positive float*) – The difference between the expression and the variable.
- **add** (*bool*) – Whether to add the variable to the model at once.

Returns A named tuple with variable and two constraints (upper_constraint, lower_constraint) describing the new variable and the constraints that assign the absolute value of the expression to it.

Return type namedtuple

cobra.util.solver.**add_cons_vars_to_problem**(*model*, *what*, ***kwargs*)
Add variables and constraints to a Model's solver object.

Useful for variables and constraints that can not be expressed with reactions and lower/upper bounds. Will integrate with the Model's context manager in order to revert changes upon leaving the context.

Parameters

- **model** (*a cobra model*) – The model to which to add the variables and constraints.
- **what** (*list or tuple of optlang variables or constraints.*) – The variables or constraints to add to the model. Must be of class *model.problem.Variable* or *model.problem.Constraint*.
- ****kwargs** (*keyword arguments*) – passed to solver.add()

cobra.util.solver.**assert_optimal**(*model*, *message='optimization failed'*)
Assert model solver status is optimal.

Do nothing if model solver status is optimal, otherwise throw appropriate exception depending on the status.

Parameters

- **model** (*cobra.Model*) – The model to check the solver status for.
- **message** (*str (optional)*) – Message to for the exception if solver status was not optimal.

cobra.util.solver.**check_solver_status**(*status*, *raise_error=False*)
Perform standard checks on a solver's status.

cobra.util.solver.**choose_solver**(*model*, *solver=None*, *qp=False*)
Choose a solver given a solver name and model.

This will choose a solver compatible with the model and required capabilities. Also respects model.solver where it can.

Parameters

- **model** (*a cobra model*) – The model for which to choose the solver.
- **solver** (*str, optional*) – The name of the solver to be used. Optlang solvers should be prefixed by "optlang-", for instance "optlang-glpk".
- **qp** (*boolean, optional*) – Whether the solver needs Quadratic Programming capabilities.

Returns

- **legacy** (*boolean*) – Whether the returned solver is a legacy (old cobra solvers) version or an optlang solver (legacy = False).
- **solver** (*a cobra or optlang solver interface*) – Returns a valid solver for the problem. May be a cobra solver or an optlang interface.

Raises *SolverNotFound* – If no suitable solver could be found.

cobra.util.solver.**fix_objective_as_constraint**(*model*, *fraction=1*, *bound=None*, *name='fixed_objective_{}'*)
Fix current objective as an additional constraint.

When adding constraints to a model, such as done in pFBA which minimizes total flux, these constraints can become too powerful, resulting in solutions that satisfy optimality but sacrifices too much for the original objective function. To avoid that, we can fix the current objective value as a constraint to ignore solutions that give a lower (or higher depending on the optimization direction) objective value than the original model.

When done with the model as a context, the modification to the objective will be reverted when exiting that context.

Parameters

- **model** (*cobra.Model*) – The model to operate on
- **fraction** (*float*) – The fraction of the optimum the objective is allowed to reach.
- **bound** (*float, None*) – The bound to use instead of fraction of maximum optimal value. If not None, fraction is ignored.
- **name** (*str*) – Name of the objective. May contain one *{}* placeholder which is filled with the name of the old objective.

cobra.util.solver.**get_solver_name**(*mip=False*, *qp=False*)
Select a solver for a given optimization problem.

Parameters

- **mip** (*bool*) – Does the solver require mixed integer linear programming capabilities?
- **qp** (*bool*) – Does the solver require quadratic programming capabilities?

Returns The name of feasible solver.

Return type string

Raises *SolverNotFound* – If no suitable solver could be found.

cobra.util.solver.**interface_to_str**(*interface*)
Give a string representation for an optlang interface.

Parameters **interface** (*string, ModuleType*) – Full name of the interface in optlang or cobra representation. For instance 'optlang.glpk_interface' or 'optlang-glpk'.

Returns The name of the interface as a string

Return type string

cobra.util.solver.**linear_reaction_coefficients**(*model*, *reactions=None*)
Coefficient for the reactions in a linear objective.

Parameters

- **model** (*cobra model*) – the model object that defined the objective
- **reactions** (*list*) – an optional list for the reactions to get the coefficients for. All reactions if left missing.

Returns A dictionary where the key is the reaction object and the value is the corresponding coefficient. Empty dictionary if there are no linear terms in the objective.

Return type dict

cobra.util.solver.**remove_cons_vars_from_problem**(*model*, *what*)
Remove variables and constraints from a Model's solver object.

Useful to temporarily remove variables and constraints from a Models's solver object.

Parameters

- **model** (*a cobra model*) – The model from which to remove the variables and constraints.

- **what** (*list or tuple of optlang variables or constraints.*) – The variables or constraints to remove from the model. Must be of class *model.problem.Variable* or *model.problem.Constraint*.

cobra.util.solver.**set_objective**(*model*, *value*, *additive=False*)
Set the model objective.

Parameters

- **model** (*cobra model*) – The model to set the objective for
- **value** (*model.problem.Objective,*) – e.g. optlang.glpk_interface.Objective, sympy.Basic or dict

  If the model objective is linear, the value can be a new Objective object or a dictionary with linear coefficients where each key is a reaction and the element the new coefficient (float).

  If the objective is not linear and *additive* is true, only values of class Objective.
- **additive** (*bool*) – If true, add the terms to the current objective, otherwise start with an empty objective.

cobra.util.util module

class cobra.util.util.**AutoVivification**
Bases: dict

Implementation of perl's autovivification feature. Checkout http://stackoverflow.com/a/652284/280182

Module contents

Submodules

cobra.config module

cobra.exceptions module

exception cobra.exceptions.**DefunctError**(*what*, *alternative=None*, *url=None*)
Bases: Exception

Exception for retired functionality

Parameters

- **what** (*string*) – The name of the retired object
- **alternative** (*string*) – Suggestion for an alternative
- **url** (*string*) – A url to alternative resource

exception cobra.exceptions.**FeasibleButNotOptimal**(*message*)
Bases: *cobra.exceptions.OptimizationError*

exception cobra.exceptions.**Infeasible**(*message*)
Bases: *cobra.exceptions.OptimizationError*

exception cobra.exceptions.**OptimizationError**(*message*)
Bases: Exception

exception cobra.exceptions.**Unbounded**(*message*)
Bases: *cobra.exceptions.OptimizationError*

exception cobra.exceptions.**UndefinedSolution**(*message*)
Bases: *cobra.exceptions.OptimizationError*

Module contents

CHAPTER 15

Indices and tables

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