

Create an overview table with model properties

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INTRODUCTION

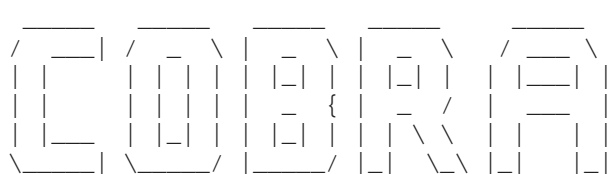
In this tutorial, we evaluate the basic properties of the metabolic model, such as the number of reactions, unique metabolites, blocked reactions, dead-end metabolites, and store the information in a table ('Table_Prop').

EQUIPMENT SETUP

Initialize the COBRA Toolbox.

If necessary, initialize The Cobra Toolbox using the `initCobraToolbox` function.

```
initCobraToolbox(false) % false, as we don't want to update
```



CONstraint-Based Reconstruction and Analysis
The COBRA Toolbox - 2017

Documentation:
<http://opencobra.github.io/cobratoolbox>

```
> Checking if git is installed ... Done.
> Checking if the repository is tracked using git ... Done.
> Checking if curl is installed ... Done.
> Checking if remote can be reached ... Done.
> Initializing and updating submodules ... Done.
> Adding all the files of The COBRA Toolbox ... Done.
> Define CB map output... set to svg.
> Retrieving models ... Done.
> TranslateSBML is installed and working properly.
> Configuring solver environment variables ...
- [---*] ILOG_CPLEX_PATH: C:\Program Files\IBM\ILOG\CPLEX_Studio1271\cplex\matlab\x64_win64
- [----] GUROBI_PATH : --> set this path manually after installing the solver ( see instructions )
- [---*] TOMLAB_PATH: C:\Program Files\tomlab\
- [----] MOSEK_PATH : --> set this path manually after installing the solver ( see instructions )
Done.
> Checking available solvers and solver interfaces ... Done.
> Setting default solvers ... Done.
> Saving the MATLAB path ... Done.
- The MATLAB path was saved in the default location.

> Summary of available solvers and solver interfaces
```

	Support	LP	MILP	QP	MIQP	NLP
cplex_direct	full	0	0	0	0	-
dqqMinos	full	0	-	-	-	-
glpk	full	1	1	-	-	-
gurobi	full	1	1	1	1	-
ibm_cplex	full	1	1	1	-	-

matlab	full	1	-	-	-	1
mosek	full	0	0	0	-	-
pdco	full	1	-	1	-	-
quadMinos	full	0	-	-	-	0
tomlab_cplex	full	1	1	1	1	-
qpng	experimental	-	-	1	-	-
tomlab_snopt	experimental	-	-	-	-	1
gurobi_mex	legacy	0	0	0	0	-
lindo_old	legacy	0	-	-	-	-
lindo_legacy	legacy	0	-	-	-	-
lp_solve	legacy	1	-	-	-	-
opti	legacy	0	0	0	0	0

Total	-	7	4	5	2	2

+ Legend: - = not applicable, 0 = solver not compatible or not installed, 1 = solver installed.

```
> You can solve LP problems using: 'glpk' - 'gurobi' - 'ibm_cplex' - 'matlab' - 'pdco' - 'tomlab_cplex' -
> You can solve MILP problems using: 'glpk' - 'gurobi' - 'ibm_cplex' - 'tomlab_cplex'
> You can solve QP problems using: 'gurobi' - 'ibm_cplex' - 'pdco' - 'tomlab_cplex' - 'qpng'
> You can solve MIQP problems using: 'gurobi' - 'tomlab_cplex'
> You can solve NLP problems using: 'matlab' - 'tomlab_snopt'

> Checking for available updates ...
--> You cannot update your fork using updateCobraToolbox(). [3d2698 @ Tutorial-modelProperties].
    Please use the MATLAB.devTools (https://github.com/opencobra/MATLAB.devTools).
```

Setting the optimization solver.

This tutorial will be run with a 'glpk' package, which is a linear programming ('LP') solver. The 'glpk' package does not require additional instalation and configuration.

```
solverName='glpk';
solverType='LP';
changeCobraSolver(solverName,solverType);
```

However, for the analysis of large models, such as Recon 2.04, it is not recommended to use the 'glpk' package but rather an industrial strength solver, such as the 'gurobi' package.

A solver package may offer different types of optimization programmes to solve a problem. The above example used a LP optimization, other types of optimization programmes include; mixed-integer linear programming ('MILP'), quadratic programming ('QP'), and mixed-integer quadratic programming ('MIQP').

```
warning off MATLAB:subscripting:noSubscriptsSpecified
```

COBRA model.

In this tutorial, the model used is the generic reconstruction of human metabolism, the Recon 2.04 [1], which is provided in the COBRA Toolbox. The Recon 2.04 model can also be downloaded from the [Virtual Metabolic Human](#) webpage. Before proceeding with the simulations, the path to the model needs to be set up and the model loaded:

```
modelFileName = 'Recon2.v04.mat';
```

```

modelDirectory = getDistributedModelFolder(modelFileName); %Look up the
folder for the distributed Models.
modelFileName= [modelDirectory filesep modelFileName]; % Get the full path.
Necessary to be sure, that the right model is loaded
model = readCbModel(modelFileName);

```

PROCEDURE

We first initialize the table

```

clear TableProp
r = 1;
TableProp(r, :) = {'Model'}; r = r+1;

```

Determine the number of reactions in the model.

```

TableProp(r, 1) = {'Reactions'};
TableProp{r, 2} = num2str(length(model.rxns));
r = r + 1;

```

Determine the number of metabolites in the model.

```

TableProp(r, 1) = {'Metabolites'};
TableProp{r, 2} = num2str(length(model.mets));
r = r + 1;

```

Determine the number of unique metabolites in the model.

```

TableProp(r, 1) = {'Metabolites (unique)'};
[g, remR3M] = strtok(model.mets, '[');
TableProp{r, 2} = num2str(length(unique(g)));
r = r + 1;

```

Determine the number of compartments in model.

```

TableProp(r, 1) = {'Compartments (unique)'};
TableProp{r, 2} = num2str(length(unique(remR3M)));
r = r + 1;

```

Determine the number of unique genes.

```

TableProp(r, 1) = {'Genes (unique)'};
[g,rem]=strtok(model.genes, '.');
TableProp{r, 2} = num2str(length(unique(g)));
r = r + 1;

```

Determine the number of subsystems.

```

TableProp(r, 1) = {'Subsystems'};
TableProp{r, 2} = num2str(length(unique(model.subSystems)));
r = r + 1;

```

Determine the number of deadends.

```
TableProp(r, 1) = {'Deadends'};  
D3M = detectDeadEnds(model);  
TableProp{r, 2} = num2str(length(D3M));  
r = r + 1;
```

Determine the size of the S matrix.

```
TableProp(r, 1) = {'Size of S'};  
TableProp{r, 2} = strcat(num2str(size(model.S,1)), ';' ,  
num2str(size(model.S,2)));  
r = r + 1;
```

Determine the rank of S.

```
TableProp(r, 1) = {'Rank of S'};  
TableProp{r, 2} = strcat(num2str(rank(full(model.S))));  
r = r + 1;
```

Determine the percentage of non-zero entries in the S matrix (nnz)

```
TableProp(r, 1) = {'Percentage nz'};  
TableProp{r, 2} = strcat(num2str((nnz(model.S)/  
(size(model.S,1)*size(model.S,2))));  
r = r + 1;
```

View table.

TableProp

```
TableProp =  
    'Model'                                []  
    'Reactions'                            '7440'  
    'Metabolites'                          '5063'  
    'Metabolites (unique)'                  '2626'  
    'Compartments (unique)'                  '8'  
    'Genes (unique)'                        '1733'  
    'Subsystems'                           '100'  
    'Deadends'                             '1332'  
    'Size of S'                            '5063;7440'  
    'Rank of S'                            '4666'  
    'Percentage nz'                        '0.0008373'
```

Determine blocked reactions properties (optional).

To evaluate the following model properties of blocked reactions, the solver package of IBM ILOG CPLEX is required. To install CPLEX refer to [solver installation guide](#), and change the solver to 'ibm_cplex' using the changeCobraSolver as shown above in equipment set-up.

- Determine the number of blocked reactions using fastFVA with 4 parallel workers (optional).

```
nworkers = 2;
solver = 'ibm_cplex';
setWorkerCount(nworkers);
```

Starting parallel pool (parpool) using the 'local' profile ...
connected to 2 workers.
Parallel computation initialized

```
tol = 1e-6;
```

```
TableProp(r, 1) = {'Blocked Reactions'};
[minFluxR3M, maxFluxR3M] = fastFVA(model, 0, 'max', solver);
```

```
> The CPLEX version has been determined as 1271.

-- Warning:: You may only output 4, 7 or 9 variables.

>> Solving Model.S. (uncoupled)
>> The number of arguments is: input: 4, output 2.
>> Size of stoichiometric matrix: (5063,7440)
>> All reactions are solved (7440 reactions - 100%).
>> 0 reactions out of 7440 are minimized (0.00%).
>> 0 reactions out of 7440 are maximized (0.00%).
>> 7440 reactions out of 7440 are minimized and maximized (100.00%).

-- Starting to loop through the 2 workers. --

-- The splitting strategy is 0. --

-----
-- Task Launched // TaskID: 2 / 2 (LoopID = 2) <> [3721, 7440] / [5063, 7440].
>> Number of reactions given to the worker: 3720
>> The number of reactions retrieved is 3720
>> Log files will be stored at P:\Gitlab\fork-cobratoolbox\src\analysis\FVA\fastFVA\logFiles
-- Start time:      Tue Jul 11 16:59:08 2017
>> #Task.ID = 2; logfile: cplexint_logfile_2.log
    -- Minimization (iRound = 0). Number of reactions: 3720.
    -- Maximization (iRound = 1). Number of reactions: 3720.
-- End time:      Tue Jul 11 17:05:21 2017
>> Time spent in FVAc: 373.9 seconds.
-----
==> 50.0% done. Please wait ...

-----
-- Task Launched // TaskID: 1 / 2 (LoopID = 1) <> [1, 3720] / [5063, 7440].
>> Number of reactions given to the worker: 3720
>> The number of reactions retrieved is 3720
>> Log files will be stored at P:\Gitlab\fork-cobratoolbox\src\analysis\FVA\fastFVA\logFiles
-- Start time:      Tue Jul 11 16:59:08 2017
>> #Task.ID = 1; logfile: cplexint_logfile_1.log
    -- Minimization (iRound = 0). Number of reactions: 3720.
    -- Maximization (iRound = 1). Number of reactions: 3720.
-- End time:      Tue Jul 11 17:07:21 2017
>> Time spent in FVAc: 499.0 seconds.
-----
==> 100% done. Analysis completed.
```

```
TableProp{r, 2} = num2str(length(intersect(find(abs(minFluxR3M) < tol),
find(abs(maxFluxR3M) < tol))));
r = r + 1;
```

- Determine the percentage of blocked reactions.

```
TableProp(r, 1) = {'Blocked Reactions (Percentage)'};
TableProp{r, 2} = num2str(length(intersect(find(abs(minFluxR3M) < tol),
find(abs(maxFluxR3M) < tol)))/length(model.rxns));
r = r + 1;
```

View table

TableProp

```
TableProp =
    'Model'                                []
    'Reactions'                            '7440'
    'Metabolites'                          '5063'
    'Metabolites (unique)'                 '2626'
    'Compartments (unique)'                 '8'
    'Genes (unique)'                       '1733'
    'Subsystems'                           '100'
    'Deadends'                             '1332'
    'Size of S'                            '5063;7440'
    'Rank of S'                            '4666'
    'Percentage nz'                        '0.0008373'
    'Blocked Reactions'                    '2123'
    'Blocked Reactions (Percentage)'        '0.28535'
```

TIMING

This tutorial takes a few minutes depending on solver, computer, and model size. The most time consuming step is the flux variability analysis.

References

[1] [Thiele et al., A community-driven global reconstruction of human metabolism, Nat Biotech, 2013.](#)