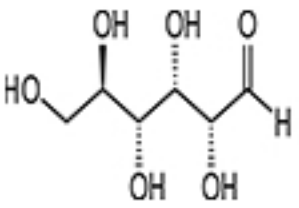
```
rxns: {2382x1 cell}
mets: {1668x1 cell}
   S: [1668x2382 double]
 rev: [2382x1 double]
  lb: [2382x1 double]
  ub: [2382x1 double]
   c: [2382x1 double]
```

E . *coli* Model

Growth Conditions

Carbon	*Nitrogen*
1. D-glucose	1. Ammonia
2. Pyruvate	2. Adenine
3. ...	3. ...



maximize {Biomass Composition}

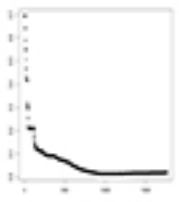
such that Sv=0, where
S=stoichiometric matrix,
v=reaction flux vector

Reaction flux bounds:
a(i) < v(i) < b(i) for each i.

Flux Balance Analysis

MATLAB with COBRA and SBML toolboxes

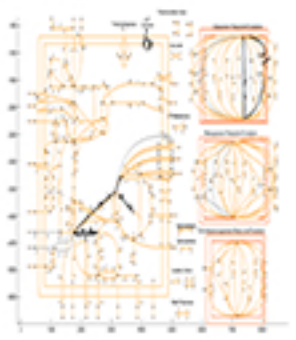
1. Simulated metabolic flux data for e. coli is generated with different combinations of growth nutrients.
2. For this, iAF1260 model containing ~2400 reactions and ~1700 metabolites is used.



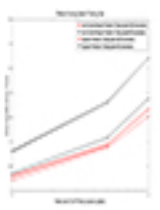
Multinomial Classification

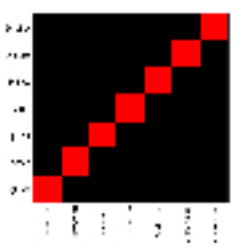
R with GLMNET package

Training, validation and testing of models using flux data.



E . *coli* Map





Results:

1. Pathways showing key reactions that discriminate a particular growth condition from others.
2. Heatmaps, histograms, plots showing the effects of misclassification with noise levels, training data size.