

| | | | | | | | |
|-------------|----|----|---|----|----|----|----|
| Metabolites | 0 | 0 | 1 | 0 | 0 | -1 | 0 |
| | 0 | 0 | 0 | 0 | 0 | 1 | 0 |
| | 1 | 0 | 1 | -1 | 1 | 0 | 1 |
| | 0 | 1 | 0 | 0 | 0 | 0 | 0 |
| | -1 | 0 | 0 | 1 | -1 | 0 | 0 |
| | 0 | -1 | 0 | 0 | 0 | 0 | -1 |
| | 0 | 0 | 0 | 0 | 1 | 1 | 0 |
| Reactions | | | | | | | |

E. coli Model

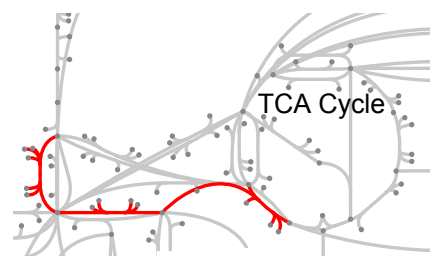
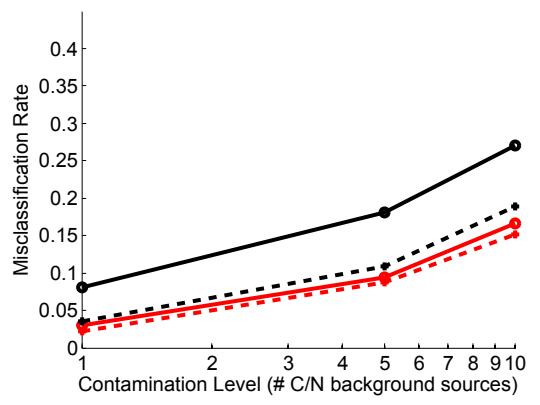
Growth Conditions

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

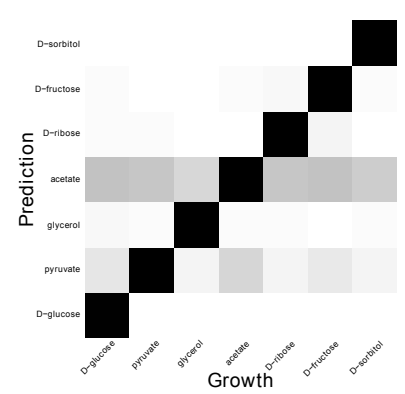
Flux Balance Analysis

$$\max. c^T v \quad s.t. \quad Sv = 0$$

Multinomial Classification



E. coli Map



Results

1. Misclassification rate
2. Key reactions that discriminate growth conditions