

Metabolic modelling, Spring 07, Exercise 4, Thursday, 19.4.2007

1 Untrivial enzyme subsets:

- $\{ M_1 \rightarrow M_2, M_2 \rightarrow M_5 + M_8, M_5 + M_8 \rightarrow M_6 \}$;
- $\{ M_1 \rightarrow M_3 + M_4, M_3 \rightarrow M_8, M_4 \rightarrow, M_8 \rightarrow \}$;
- $\{ \rightarrow M_7, M_7 \rightarrow M_6 \}$

2 The rank of augmented system equals 9. There are 11 reactions, thus the augmented system is not of full rank.

4 Untrivial fragment equivalence sets:

- $\{ M_1, M_2 \}$;
- $\{ M_1 | C_1, M_2 | C_1, M_3, M_5 \}$;
- $\{ M_1 | C_2, M_2 | C_2, M_4 \}$

- 5
- $P(^0M_5) = P(^0M_2 | C_1) = P(^0M_1 | C_1) = P(^{00}M_1) + P(^{01}M_1) = 0.8$;
 - $P(^1M_5) = 1 - P(^0M_5)$;
 - $P(^xM_3) = P(^xM_5)$ (M_3 and M_5 in the same equivalence set.)
 - $P(^{xy}M_2) = P(^{xy}M_1)$ (M_1 and M_2 in the same equivalence set.)
 $\rightarrow P(^0M_2 | C_2) = P(^{00}M_1) + P(^{10}M_1) = 0.75$

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- A generalized balance equation for M_8 :

$$P(^0M_2 | C_2)v_{(M_2 \rightarrow M_5 + M_8)} + P(^0M_3)v_{(M_3 \rightarrow M_8)} = P(^0M_8) \left(v_{(M_5 + M_8 \rightarrow M_6)} + v_{(M_8 \rightarrow)} \right) =$$

$$0.75v_{(M_2 \rightarrow M_5 + M_8)} + 0.8v_{(M_3 \rightarrow M_8)} = 0.7833 \left(v_{(M_5 + M_8 \rightarrow M_6)} + v_{(M_8 \rightarrow)} \right)$$
 - A generalized balance equation for $M_6 | C_1$:

$$P(^0M_5)v_{(M_5 + M_8 \rightarrow M_6)} + P(^0M_7 | C_1)v_{(M_7 \rightarrow M_6)} = P(^0M_6 | C_1)v_{(M_6 \rightarrow)} =$$

$$0.8v_{(M_5 + M_8 \rightarrow M_6)} + 0.6v_{(M_7 \rightarrow M_6)} = 0.7v_{(M_6 \rightarrow)}$$
 - The flux distribution (the order of fluxes is the same as in Assingment 1): [3, 1, 2, 1, 2, 2, 1, 1, 2, 1, 2].