$1\quad \hbox{Double branch simulations with alpha}=0, \ beta=0$

Double branch model with artificial data (noise-free kinetic data, noise-free state data) - alpha = 0, beta = 0

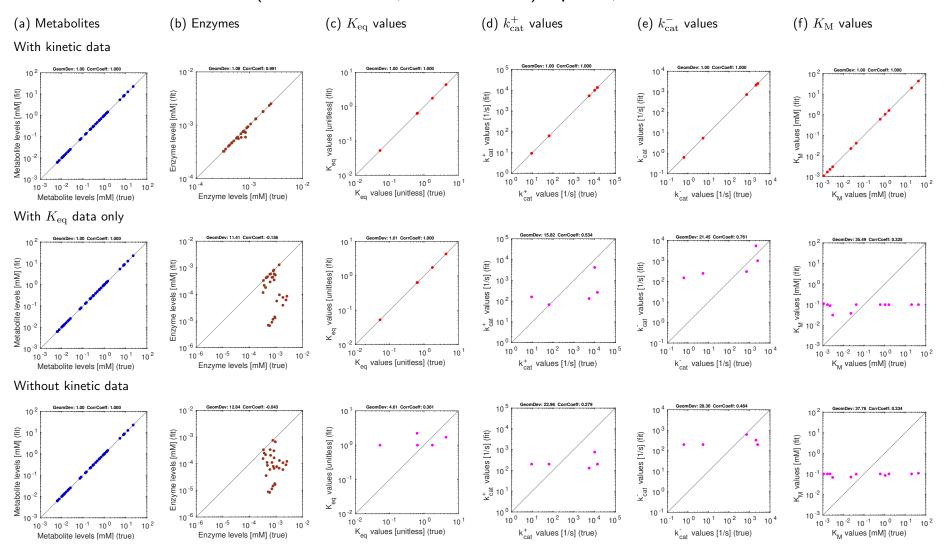


Figure 3: Model balancing results for Double branch model with artificial data. The model structure is shown in Figure ??. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation coefficients ("CorrCoeff"). (a) Metabolite levels. (b) Enzyme levels. (c)-(f) Different types of kinetic constants. Rows show different estimation scenarios (see Figure) Upper row: simple scenario S1 (noise-free artificial data, data for kinetic constants). Centre row: scenario S1K (noise-free artificial data, kinetic data given only for equilibrium constants). Lower row: scenario S2 (noise-free artificial data, no data for kinetic constants). Depending on the scenario, kinetic constants are either fitted (red dots) or predicted (magenta dots).

Double branch model with artificial data (noisy kinetic data, noise-free state data) - alpha = 0, beta = 0(d) $k_{\rm cat}^+$ values (e) $k_{\rm cat}^-$ values (a) Metabolites (b) Enzymes (c) $K_{\rm eq}$ values (f) $K_{ m M}$ values With kinetic data GeomDev: 1.40 CorrCoeff: 0.998 10 ⁴ 10 10-2 10 values [1/s] (fit) values [unitless] (fit) 10¹ Metabolite levels [mM] (fit) 103 Enzyme levels [mM] (fit) values [1/s] (fit) values [mM] (fit) 10 ⁰ 10⁰ 10³ 10² 10 -10² 10 ¹ 10 10 -2 + tg 10 , tg 10 ℃ 10² 10³ 10⁴ 10 ⁻² 10¹ 10⁻¹ 10⁰ 10¹ 10² 10³ 10⁰ 10 ¹ 10⁻⁴ 10⁻³ 10⁻² 10⁻¹ 10⁰ 10¹ 10² 10⁻⁵ 10 ⁻⁴ 10⁻³ 10-3 10-2 10-1 100 101 K_{eq} values [unitless] (true) k+ values [1/s] (true) k at values [1/s] (true) K_M values [mM] (true) Enzyme levels [mM] (true) Metabolite levels [mM] (true) With $K_{\rm eq}$ data only GeomDev: 15.11 CorrCoeff: 0.563 GeomDev: 21.27 CorrCoeff: 0.676 10 10-10 4 10 values [1/s] (fit) levels [mM] (fit) values [unitless] (fit) 10³ values [1/s] (fit) values [mM] (fit) 10⁰ 10³ 10² 10⁰ 10² 10¹ 10⁻¹ + tg 10 ' ag 10 g 10² 10³ 10⁴ 10¹ 10⁰ 10¹ 10² 10³ 10 ¹ 10-3 10-2 10-1 100 101 102 10 -3 10 -2 10 -1 10 0 10 1 10⁻⁶ 10⁻⁵ 10⁻⁴ 10⁻³ k at values [1/s] (true) k_{cat}^+ values [1/s] (true) K_M values [mM] (true) Ken values [unitless] (true) Metabolite levels [mM] (true) Enzyme levels [mM] (true) Without kinetic data GeomDev: 28.36 CorrCoeff: 0.484 GeomDev: 12.84 CorrCoeff: -0.043 10 10 GeomDev: 37.78 CorrCoeff: 0.334 10² 10-2 10 values [1/s] (fit) levels [mM] (fit) Metabolite levels [mM] (fit) values [unitless] (fit) 10³ values [mM] (fit) values [1/s] (fit)

Figure 4: Same as Figure 13, with noisy kinetic data

10 ¹

10 ⁰

K_{eq} values [unitless] (true)

10³

10²

10 ¹

10² 10³ 10⁴ 10⁵

k_{cat} values [1/s] (true)

10 gt +

10²

10 ¹

10⁰ 10¹ 10² 10³

k-at values [1/s] (true)

`å 10 g

10⁰

10⁻³ 10⁻² 10⁻¹ 10⁰ 10¹ 10²

K_M values [mM] (true)

10⁰

10

10⁻⁶ 10 ⁻⁵

10 -3 10 -2 10 -1 10 0 10 1

Metabolite levels [mM] (true)

10 ⁻⁴ 10 ⁻³

Enzyme levels [mM] (true)

Double branch model with artificial data (noise-free kinetic data, noisy state data) - alpha = 0, beta = 0

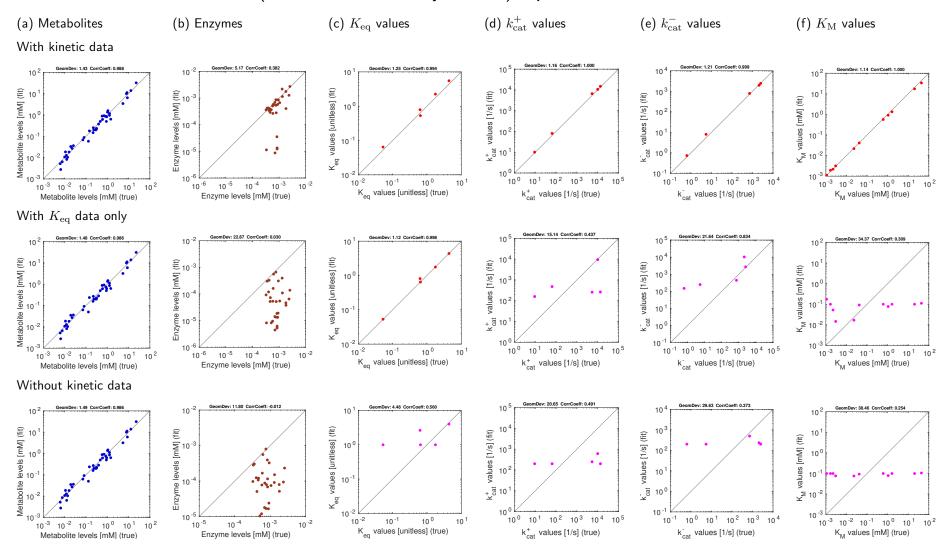


Figure 5: Results for Double branch with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial data, no data for kinetic constants).

Double branch model with artificial data (noisy kinetic data, noisy state data) - alpha = 0, beta = 0(d) $k_{\rm cat}^+$ values (a) Metabolites (b) Enzymes (c) $K_{\rm eq}$ values (e) $k_{\rm cat}^-$ values (f) $K_{ m M}$ values With kinetic data GeomDev: 1.62 CorrCoeff: 0.994 10 ⁴ 10 10-2 values [1/s] (fit) levels [mM] (fit) values [unitless] (fit) Metabolite levels [mM] (fit) 103 values [1/s] (fit) values [mM] (fit) 10 ⁰ 10³ 10² 10⁰ 10² 10 ¹ 10 + tg 10 , tg 10 ℃ . ≥ 10 10² 10³ 10⁴ 10 ⁻² 10¹ 10⁻¹ 10⁰ 10¹ 10² 10³ 10⁰ 10 ¹ 10 -3 10 -2 10 -1 10 0 10 1 10⁻⁶ 10 ⁻⁵ 10 ⁻⁴ 10⁻³ 10-3 10-2 10-1 100 101 K_{eq} values [unitless] (true) k at values [1/s] (true) k+ values [1/s] (true) K_M values [mM] (true) Enzyme levels [mM] (true) Metabolite levels [mM] (true) With $K_{\rm eq}$ data only GeomDev: 15.10 CorrCoeff: 0.502 GeomDev: 23.35 CorrCoeff: 0.765 GeomDev: 1.55 CorrCoeff: 0.957 10 10-10 4 10 values [1/s] (fit) levels [mM] (fit) values [unitless] (fit) 10³ values [1/s] (fit) values [mM] (fit) 10⁰ 10³ 10² 10⁰ 10² 10¹ 10⁻¹ + tg 10 ' ag 10 g 10² 10³ 10⁴ 10¹ 10⁰ 10¹ 10² 10³ 10 ¹ 10-3 10-2 10-1 100 101 102 10 -3 10 -2 10 -1 10 0 10 1 10⁻⁶ 10⁻⁵ 10⁻⁴ 10⁻³ k at values [1/s] (true) K_{eq} values [unitless] (true) k_{cat}^+ values [1/s] (true) K_M values [mM] (true) Metabolite levels [mM] (true) Enzyme levels [mM] (true) Without kinetic data GeomDev: 29.63 CorrCoeff: 0.373 GeomDev: 11.80 CorrCoeff: -0.012 10 10 10² 10 -2 10 Metabolite levels [mM] (fit) Enzyme levels [mM] (fit) values [1/s] (fit) values [unitless] (fit) 10³ values [mM] (fit) values [1/s] (fit) 10³ 10² 10⁰ 10² 10 ¹ 10 10 gt `å 10 g 10 ¹ 10² 10³ 10⁴ 10⁵ 10⁰ 10¹ 10² 10³

Figure 6: Same as Figure 15, with noisy kinetic data

k_{cat} values [1/s] (true)

10⁻³ 10⁻² 10⁻¹ 10⁰ 10¹ 10²

K_M values [mM] (true)

k at values [1/s] (true)

10 ¹

10 ⁰

K_{eq} values [unitless] (true)

10 ⁻⁴

Enzyme levels [mM] (true)

10⁻⁵

10 -3 10 -2 10 -1 10 0 10 1

Metabolite levels [mM] (true)

10⁻³

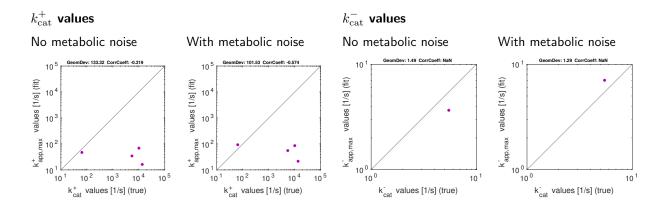


Figure 7: Catalytic constants in Double branch (artificial data), estimated by kinetic profiling. Note that $k_{\rm cat}$ values can only be estimated in the direction of fluxes (e.g. $k_{\rm cat}^+$ for reactions with forward fluxe).

- 2 Double branch model Simulations with alpha = 0.1
- 3 Double branch simulations with alpha = 0.1, beta = 0

Double branch model with artificial data (noise-free kinetic data, noise-free state data) - alpha = 0.1, beta = 0

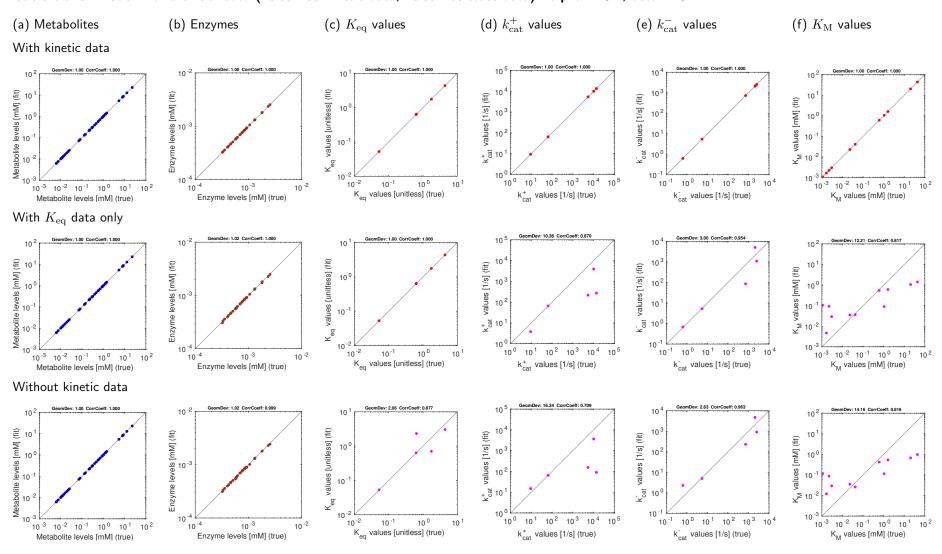


Figure 8: Model balancing results for Double branch model with artificial data. The model structure is shown in Figure ??. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation coefficients ("CorrCoeff"). (a) Metabolite levels. (b) Enzyme levels. (c)-(f) Different types of kinetic constants. Rows show different estimation scenarios (see Figure) Upper row: simple scenario S1 (noise-free artificial data, data for kinetic constants). Centre row: scenario S1K (noise-free artificial data, kinetic data given only for equilibrium constants). Lower row: scenario S2 (noise-free artificial data, no data for kinetic constants). Depending on the scenario, kinetic constants are either fitted (red dots) or predicted (magenta dots).

10 -3 10 -2 10 -1 10 0 10 1

Metabolite levels [mM] (true)

Double branch model with artificial data (noisy kinetic data, noise-free state data) - alpha = 0.1, beta = 0(d) $k_{\rm cat}^+$ values (e) $k_{\rm cat}^-$ values (a) Metabolites (b) Enzymes (c) $K_{\rm eq}$ values (f) $K_{ m M}$ values With kinetic data GeomDev: 1.35 CorrCoeff: 0.999 10 ⁴ 10 10-2 10 values [1/s] (fit) values [unitless] (fit) 10¹ Metabolite levels [mM] (fit) 103 Enzyme levels [mM] (fit) values [1/s] (fit) values [mM] (fit) 10 ⁰ 10⁰ 10³ 10² 10² 10 ¹ 10 + tg 10 , tg 10 °C 10² 10³ 10⁴ 10 ⁻² 10 ¹ 10⁻¹ 10⁰ 10¹ 10² 10³ 10⁰ 10 ¹ 10⁻⁴ 10⁻³ 10⁻² 10⁻¹ 10⁰ 10¹ 10² 10-3 10-2 10-1 100 101 K_{eq} values [unitless] (true) k at values [1/s] (true) k+ values [1/s] (true) K_M values [mM] (true) Metabolite levels [mM] (true) Enzyme levels [mM] (true) With $K_{\rm eq}$ data only GeomDev: 10.89 CorrCoeff: 0.790 GeomDev: 13.92 CorrCoeff: 0.760 GeomDev: 1.37 CorrCoeff: 0.982 10 10 4 10-10 Metabolite levels [mM] (fit) values [1/s] (fit) values [unitless] (fit) 10³ Enzyme levels [mM] (fit) values [1/s] (fit) values [mM] (fit) 10⁰ 10³ 10² 10⁰ 10² 10¹ 10 + tg 10 ' ag 10 g 10² 10³ 10⁴ 10⁵ 10¹ 10⁰ 10¹ 10² 10³ 10 ¹ 10-3 10-2 10-1 100 101 102 10 -3 10 -2 10 -1 10 0 10 1 10⁻⁴ 10 ⁻³ 10 ⁻² k at values [1/s] (true) K_{eq} values [unitless] (true) k_{cat}^+ values [1/s] (true) K_M values [mM] (true) Metabolite levels [mM] (true) Enzyme levels [mM] (true) Without kinetic data GeomDev: 2.63 CorrCoeff: 0.963 10 10 GeomDev: 14.16 CorrCoeff: 0.816 10² 10-2 10 Metabolite levels [mM] (fit) values [1/s] (fit) Enzyme levels [mM] (fit) values [unitless] (fit) 10³ values [mM] (fit) values [1/s] (fit) 10⁰ 10³ 10² 10⁰ 10² 10 ¹ 10 10 gt + `å 10 g

Figure 9: Same as Figure 13, with noisy kinetic data

10 ¹

10 ⁰

K_{eq} values [unitless] (true)

10 ⁻³

Enzyme levels [mM] (true)

10⁻⁴

10 ⁻²

10 ¹

10² 10³ 10⁴ 10⁵

k_{cat} values [1/s] (true)

10⁰ 10¹ 10² 10³

k-at values [1/s] (true)

10⁻³ 10⁻² 10⁻¹ 10⁰ 10¹ 10²

K_M values [mM] (true)

Double branch model with artificial data (noise-free kinetic data, noisy state data) - alpha = 0.1, beta = 0

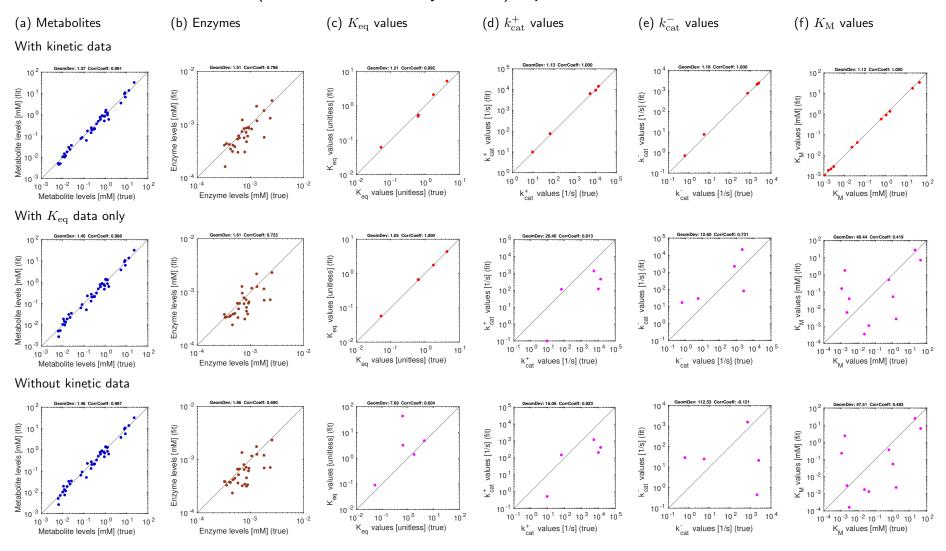


Figure 10: Results for Double branch with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial data, no data for kinetic constants).

10 -3 10 -2 10 -1 10 0 10 1

Metabolite levels [mM] (true)

Enzyme levels [mM] (true)

Double branch model with artificial data (noisy kinetic data, noisy state data) - alpha = 0.1, beta = 0(d) $k_{\rm cat}^+$ values (e) $k_{\rm cat}^-$ values (a) Metabolites (b) Enzymes (c) $K_{\rm eq}$ values (f) $K_{ m M}$ values With kinetic data GeomDev: 1.56 CorrCoeff: 0.994 10 ⁴ 10 10-2 10 values [1/s] (fit) values [unitless] (fit) Metabolite levels [mM] (fit) 103 Enzyme levels [mM] (fit) values [1/s] (fit) values [mM] (fit) 10 ⁰ 10³ 10² 10⁰ 10² 10 ¹ 10 + tg 10 , tg 10 ℃ . ≥ 10 10² 10³ 10⁴ 10¹ 10⁻¹ 10⁰ 10¹ 10² 10³ 10⁻² 10⁰ 10 ¹ 10 -3 10 -2 10 -1 10 0 10 1 10 ⁻⁴ 10⁻³ 10-3 10-2 10-1 100 101 K_{eq} values [unitless] (true) k at values [1/s] (true) k+ values [1/s] (true) K_M values [mM] (true) Enzyme levels [mM] (true) Metabolite levels [mM] (true) With $K_{\rm eq}$ data only GeomDev: 33.01 CorrCoeff: 0.135 GeomDev: 1.65 CorrCoeff: 0.708 GeomDev: 1.56 CorrCoeff: 0.956 GeomDev: 28.09 CorrCoeff: 0.801 10 10 4 10 10 values [unitless] (fit) 10³ Enzyme levels [mM] (fit) values [1/s] (fit) values [1/s] (fit) values [mM] (fit) 10³ 10⁰ 10² 10² 10 ⁻¹ 10 ¹ 10 ¹ 10⁻¹ 10 ⁻² Metabolite I , tg 10 ° , cat 10 0 10 1 10 2 10 3 10 4 10 5 10⁻¹ 10⁰ 10¹ 10² 10³ 10⁴ 10⁰ 10⁻¹ 10 ¹ 10⁻⁴ 10⁻³ 10⁻² 10⁻¹ 10⁰ 10¹ 10² 10 -3 10 -2 10 -1 10 0 10 1 10⁻⁴ 10⁻³ K_{eq} values [unitless] (true) k at values [1/s] (true) k_{cat} values [1/s] (true) K_M values [mM] (true) Metabolite levels [mM] (true) Enzyme levels [mM] (true) Without kinetic data GeomDev: 16.06 CorrCoeff: 0.823 GeomDev: 47.51 CorrCoeff: 0.483 104 10⁻² 10 10 10 10 Metabolite levels [mM] (fit) values [unitless] (fit) 103 Enzyme levels [mM] (fit) values [1/s] (fit) 10 values [1/s] (fit) values [mM] (fit) 10³ 10⁰ 10² 10⁰ 10² 10¹ 10 ¹ 10 ⁻² 10 و 10 g +⁷g 10 c

Figure 11: Same as Figure 15, with noisy kinetic data

10⁰ 10¹ 10² 10³ 10⁴ 10⁵

k+ values [1/s] (true)

10 ¹

10⁰

K_{eq} values [unitless] (true)

10³

10 -4 10 -3 10 -2 10 -1 10 0 10 1 10 2

K_M values [mM] (true)

10¹ 10²

k_{cat} values [1/s] (true)

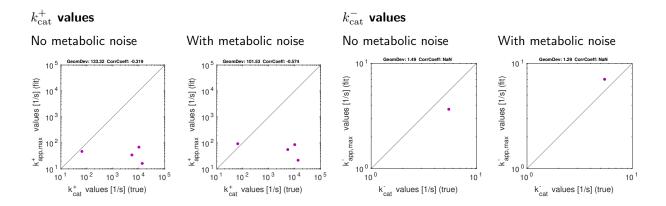


Figure 12: Catalytic constants in Double branch (artificial data), estimated by kinetic profiling. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k_{cat}^+ for reactions with forward fluxe).

- 4 Double branch model Simulations with alpha = 1
- 5 Double branch simulations with alpha = 1, beta = 0

Double branch model with artificial data (noise-free kinetic data, noise-free state data) - alpha = 1, beta = 0

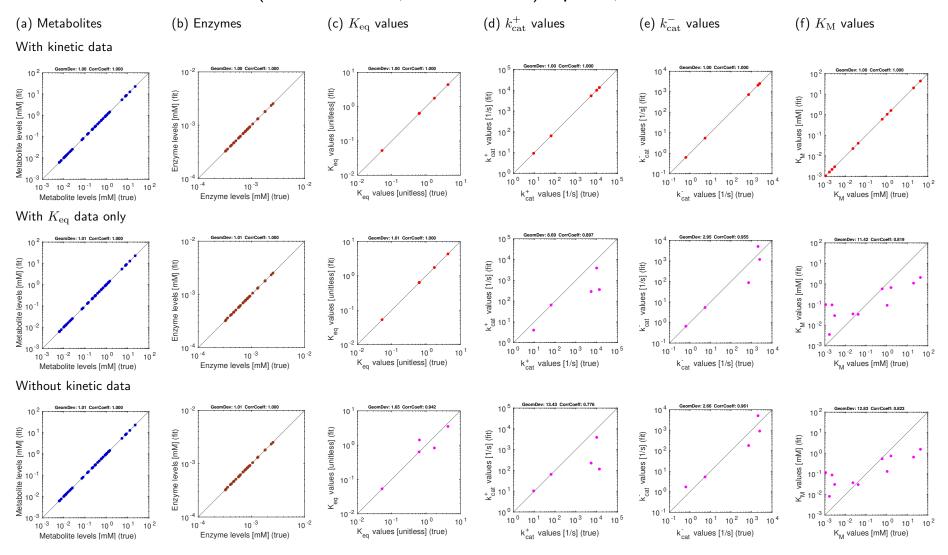


Figure 13: Model balancing results for Double branch model with artificial data. The model structure is shown in Figure ??. Each subfigure shows "true" values (x-axis) versus reconstructed values (y-axis). Similarities are quntified by geometric standard deviations ("GeomDev") and Pearson correlation coefficients ("CorrCoeff"). (a) Metabolite levels. (b) Enzyme levels. (c)-(f) Different types of kinetic constants. Rows show different estimation scenarios (see Figure) Upper row: simple scenario S1 (noise-free artificial data, data for kinetic constants). Centre row: scenario S1K (noise-free artificial data, kinetic data given only for equilibrium constants). Lower row: scenario S2 (noise-free artificial data, no data for kinetic constants). Depending on the scenario, kinetic constants are either fitted (red dots) or predicted (magenta dots).

10 -3 10 -2 10 -1 10 0 10 1

Metabolite levels [mM] (true)

Double branch model with artificial data (noisy kinetic data, noise-free state data) - alpha = 1, beta = 0(d) k_{cat}^+ values (e) $k_{\rm cat}^-$ values (a) Metabolites (b) Enzymes (c) $K_{\rm eq}$ values (f) $K_{ m M}$ values With kinetic data GeomDev: 1.33 CorrCoeff: 0.999 10 ⁴ 10 10-2 10 values [1/s] (fit) values [unitless] (fit) 10¹ Metabolite levels [mM] (fit) 103 Enzyme levels [mM] (fit) values [1/s] (fit) values [mM] (fit) 10 ⁰ 10⁰ 10³ 10² 10² 10 ¹ 10 + tg 10 , tg 10 ℃ 10² 10³ 10⁴ 10 ¹ 10⁻¹ 10⁰ 10¹ 10² 10³ 10⁻² 10⁰ 10 ¹ 10⁻⁴ 10⁻³ 10⁻² 10⁻¹ 10⁰ 10¹ 10² 10 ⁻³ 10-3 10-2 10-1 100 101 K_{eq} values [unitless] (true) k+ values [1/s] (true) k at values [1/s] (true) K_M values [mM] (true) Metabolite levels [mM] (true) Enzyme levels [mM] (true) With $K_{\rm eq}$ data only GeomDev: 9.47 CorrCoeff: 0.827 GeomDev: 14.11 CorrCoeff: 0.759 GeomDev: 1.37 CorrCoeff: 0.983 10 10 4 10-10 values [1/s] (fit) values [unitless] (fit) 10³ Enzyme levels [mM] (fit) values [1/s] (fit) values [mM] (fit) 10⁰ 10³ 10² 10⁰ 10² 10¹ 10 + tg 10 ' ag 10 g 10² 10³ 10⁴ 10⁵ 10¹ 10⁰ 10¹ 10² 10³ 10⁰ 10 ¹ 10-3 10-2 10-1 100 101 102 10 -3 10 -2 10 -1 10 0 10 1 10⁻⁴ 10 ⁻³ 10 ⁻² k at values [1/s] (true) K_{eq} values [unitless] (true) k_{cat}^+ values [1/s] (true) K_M values [mM] (true) Metabolite levels [mM] (true) Enzyme levels [mM] (true) Without kinetic data GeomDev: 13.43 CorrCoeff: 0.776 GeomDev: 2.66 CorrCoeff: 0.961 GeomDev: 1.65 CorrCoeff: 0.942 10 10 GeomDev: 12.83 CorrCoeff: 0.823 10² 10-2 10 Metabolite levels [mM] (fit) values [1/s] (fit) Enzyme levels [mM] (fit) values [unitless] (fit) 10³ values [mM] (fit) values [1/s] (fit) 10 ⁰ 10³ 10² 10⁰ 10² 10 ¹ 10 10 gt + `å 10 g

Figure 14: Same as Figure 13, with noisy kinetic data

10 ¹

10 ⁰

K_{eq} values [unitless] (true)

10 ⁻³

Enzyme levels [mM] (true)

10⁻⁴

10 ⁻²

10 ¹

10² 10³ 10⁴ 10⁵

k_{cat} values [1/s] (true)

10⁰ 10¹ 10² 10³

k-at values [1/s] (true)

10⁻³ 10⁻² 10⁻¹ 10⁰ 10¹ 10²

K_M values [mM] (true)

Double branch model with artificial data (noise-free kinetic data, noisy state data) - alpha = 1, beta = 0

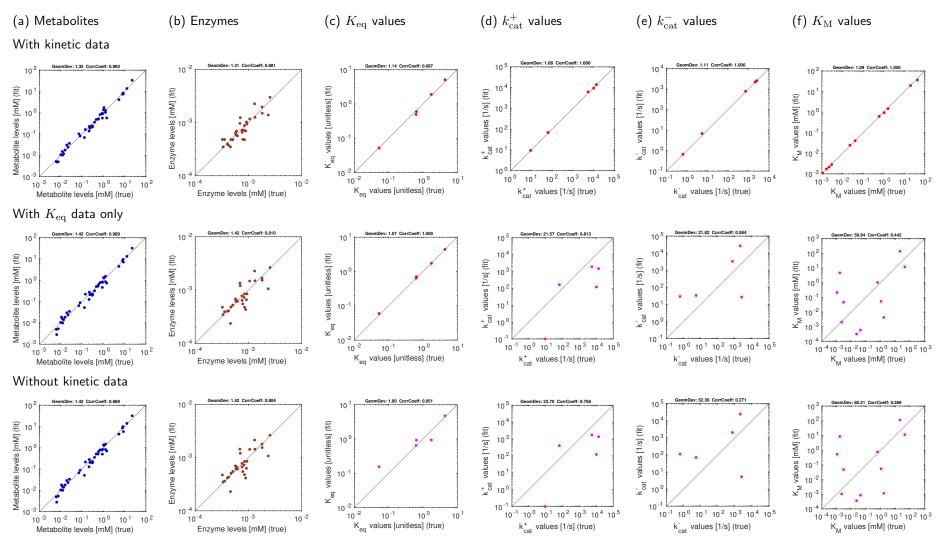


Figure 15: Results for Double branch with noisy artificial data. Top row: estimation scenario S3 (noisy artificial data, data used for kinetic constants). Centre row: estimation scenario S3K (noisy artificial data, data for equilibrium constants only). Bottom row: estimation scenario S4 (noisy artificial data, no data for kinetic constants).

Metabolite levels [mM] (true)

Enzyme levels [mM] (true)

Double branch model with artificial data (noisy kinetic data, noisy state data) - alpha = 1, beta = 0(d) $k_{\rm cat}^+$ values (a) Metabolites (b) Enzymes (c) $K_{\rm eq}$ values (e) $k_{\rm cat}^-$ values (f) $K_{ m M}$ values With kinetic data GeomDev: 1.48 CorrCoeff: 0.995 10 ⁴ 10 10 values [1/s] (fit) values [unitless] (fit) Metabolite levels [mM] (fit) 103 Enzyme levels [mM] (fit) values [1/s] (fit) values [mM] (fit) 10 ⁰ 10³ 10² 10⁰ 10² 10 ¹ 10 + tg 10 , tg 10 ℃ . ≥ 10 10² 10³ 10⁴ 10¹ 10⁻¹ 10⁰ 10¹ 10² 10³ 10⁻² 10⁰ 10 ¹ 10 -3 10 -2 10 -1 10 0 10 1 10-3 10-2 10-1 100 101 K_{eq} values [unitless] (true) k at values [1/s] (true) k+ values [1/s] (true) K_M values [mM] (true) Metabolite levels [mM] (true) Enzyme levels [mM] (true) With $K_{\rm eq}$ data only GeomDev: 50.36 CorrCoeff: -0.108 GeomDev: 1.41 CorrCoeff: 0.814 GeomDev: 1.50 CorrCoeff: 0.964 GeomDev: 18.09 CorrCoeff: 0.832 10 10 4 10² 10 values [unitless] (fit) 10³ Enzyme levels [mM] (fit) values [mM] (fit) 10 1 10 1 10 -2 values [1/s] (fit) values [1/s] (fit) 10³ 10² 10² 10 ¹ 10 ¹ 10⁻¹ Metabolite I , tg 10 ° , cat 10 0 10 1 10 2 10 3 10 4 10 5 10⁰ 10¹ 10² 10³ 10⁴ 10⁰ 10⁻¹ 10 ¹ 10 -4 10 -3 10 -2 10 -1 10 0 10 1 10 2 10 3 10 -3 10 -2 10 -1 10 0 10 1 10⁻⁴ 10⁻³ K_{eq} values [unitless] (true) k at values [1/s] (true) k_{cat} values [1/s] (true) K_M values [mM] (true) Metabolite levels [mM] (true) Enzyme levels [mM] (true) Without kinetic data GeomDev: 23.70 CorrCoeff: 0.758 10⁵ GeomDev: 85.21 CorrCoeff: 0.369 10⁻² 10 10 10 10² Metabolite levels [mM] (fit) values [unitless] (fit) Enzyme levels [mM] (fit) values [1/s] (fit) values [mM] (fit) 10 1 10 -1 10 -2 values [1/s] (fit) 10⁰ 10³ 10³ 10² 10² 10 ¹ 10 ¹ 10⁻¹ 10 و علم مح cat 10⁰ 10¹ 10² 10³ 10⁴ 10⁵ 10¹ 10² 10³ 10⁴ 10⁵ 10⁻¹ 10⁰ 10 ¹ 10 $^{-4}$ 10 $^{-3}$ 10 $^{-2}$ 10 $^{-1}$ 10 0 10 1 10 2 10 3 10 -3 10 -2 10 -1 10 0 10 1 K_{eq} values [unitless] (true) k_{cat} values [1/s] (true)

Figure 16: Same as Figure 15, with noisy kinetic data

k+ values [1/s] (true)

K_M values [mM] (true)

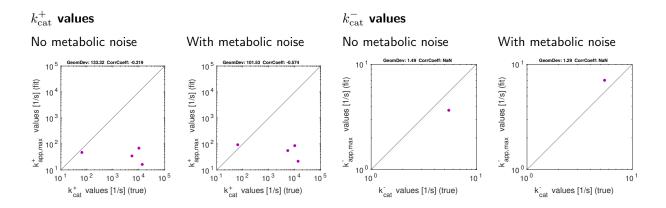


Figure 17: Catalytic constants in Double branch (artificial data), estimated by kinetic profiling. Note that k_{cat} values can only be estimated in the direction of fluxes (e.g. k_{cat}^+ for reactions with forward fluxe).