Report 2, deadline see Canvas

Exercise 7: Fitting a decay rate in combination with an IRF (Optional)
(1-2 pages in total, with a typical figures at upper and lower bound)
Now increase and decrease this decay rate and simulate and fit the new data. Fix the Stdev. noise at 0.01. Interpret the resulting *Fit diagnostics* tab. What decay rates can reliably be estimated? Give both upper and lower bound. Explain why.

Exercise 11: Fitting with a kinetic model (2 pages in total, with 3 typical figures) **(Optional)**
Try also (with a low noise level) a simulation where two components have either identical concentration profiles (figure), or identical spectra (figure). How does this affect the rank of the data matrix ?

The desired result of this exercise is a specification of the signal to noise level needed to **just** resolve three components (below this level two components are sufficient). Of course this depends upon the differences between the parameters describing these components. Assume spectral parameters (20000,3000,0.1), (21000,3000,0.1), (22000,3000,0.1), all amplitudes equal to 1, and decay rates 0.05,0.03 and 0.01, respectively. What is the estimated rank of the data matrix at the critical noise level? Verify this with three realizations of the noise.

Exercise 12: Fitting with a sequential kinetic model (2 pages in total, with 2 typical figures)

See lecture notes.

Exercise 13: Fitting unknown simulated data (3 pages in total, with figures for the final model with each data set a, b or c)

See lecture notes.

Exercise 15: Fitting with a spectral model (3 pages in total, with figures for the final model with each data set a, b or c)

See lecture notes.

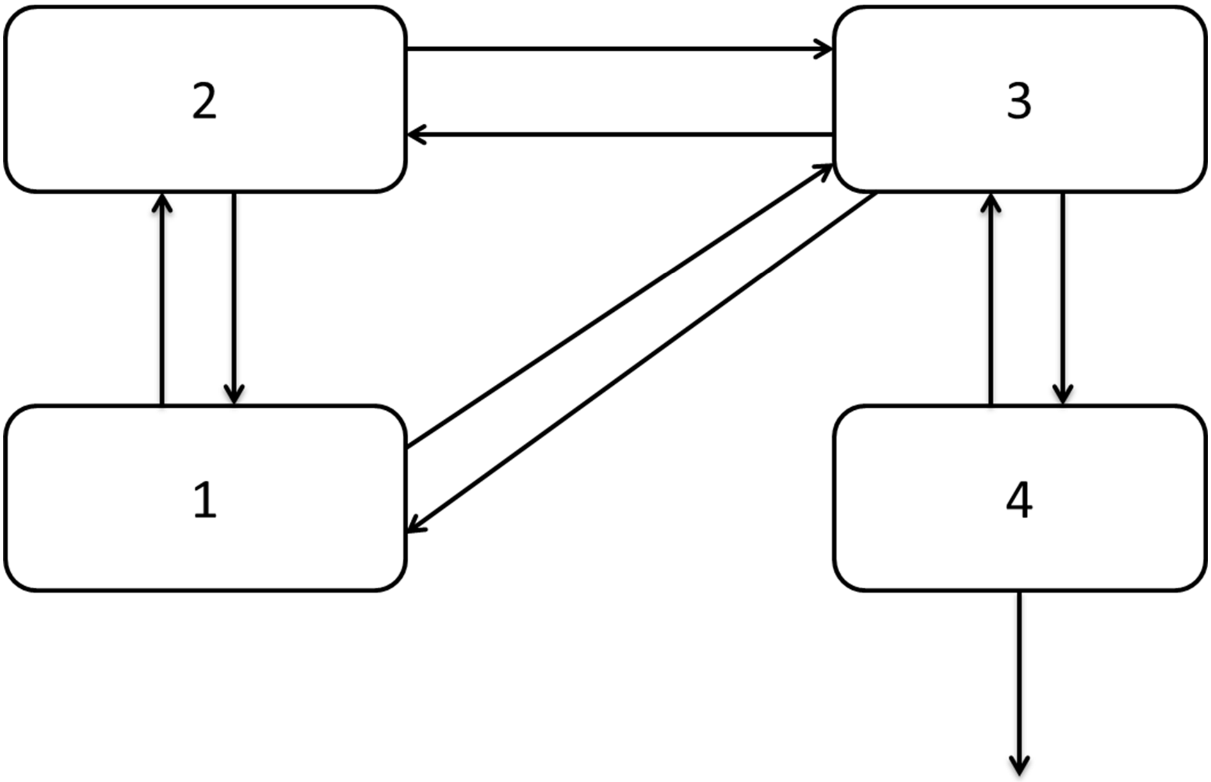
Exercise 16: Fitting with a spectrotemporal model (3 pages in total, with figures for the final model with each data set a, b or c)

See lecture notes.

Exercise 17: Fitting with a sequential kinetic model revisited (2 pages in total, with figures for the most appropriate data set a, b or c)

See lecture notes.

Question 3: compartmental model of a light harvesting antenna **(**30 points)



a. (6p) Add rate constant names k_{ij} describing the flow to and from all compartments.
Then write down the matrix/vector differential equation that describes the above compartment system, assuming that there is no external input, but only initial conditions $c_1(0) = c_2(0) = 1$, $c_3(0) = 0.75$ and $c_4(0) = 0$.

b. (4p) Write down the formal, analytical solution to the matrix equation from **a**, assuming that the initial condition is a vector **c(0)**.

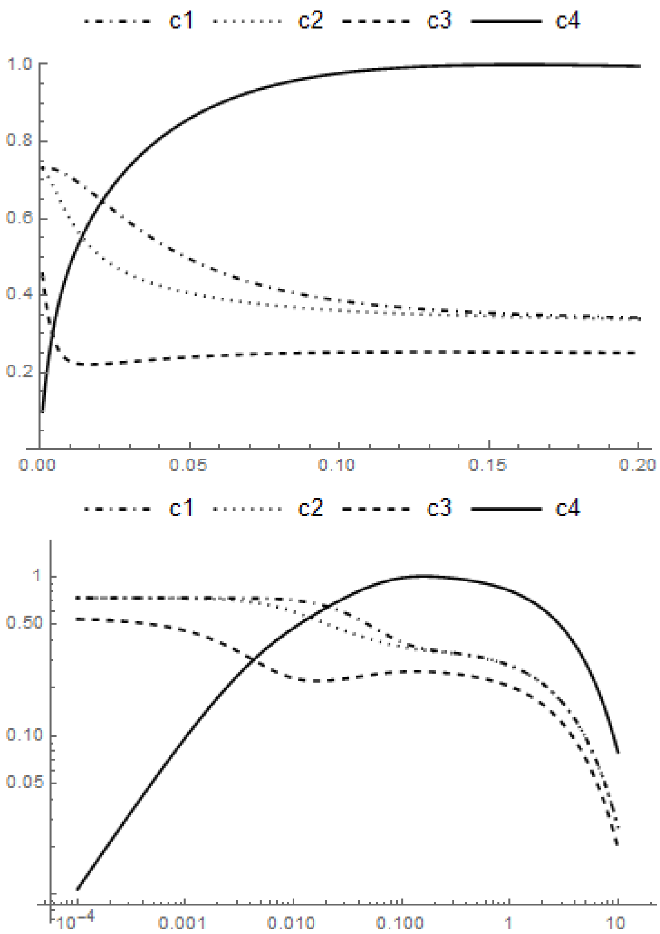
How do the observed decay rates (reciprocals of the observed lifetimes) relate to this solution?
(2 lines)

c. (4p) Formulate the detailed balance condition for this compartment system.
Assuming that the detailed balance condition holds, given the values $k_{31} = 1.2, k_{13} = 1.6, k_{12} = 40, k_{43} = 200, k_{34} = 50, k_{23} = 80, k_{32} = 60$, what is k_{21}?

d. (3p)What is the Gibbs free energy difference between compartments 1 and 3 (use $k_B T = 25$ meV) ?

e. (4p)Draw a Gibbs free energy level scheme for the four compartments, or describe this scheme in words.

f. (5p) Describe qualitatively what you observe in these two plots of this system. (3-5 lines)



g. (4p) Estimate the decay rate k_{04} from the plots in f.