Let’s consider different terms that may appear in the Lagrangian:

**L0 - the basis equation**:

Then, using the matrix calculus:

Optimum is at:

But, the direct matrix inversion is not to be used.

**L1 – unnormalized flux constraint:**

Or:

A variation is with diagonal elements:

Then:

**L2 – constraint on the sum over the column or the row:**

**L3 – just minimize the fluxes (transformed with sigma-function):**

and

is a differentiable representation of the Heavyside step function.

Using

So:

So:

Also:

**L3b – just minimize the fluxes (transformed with sigma-function), also including the diagonal elements:**

In particular, we are interested in:

this is the total probability outflux from the state j.

**L4 – enforce the normalization of the probabilities for in-flux to be close to 1:**

Flux-based approach: , , are the rate constants, so

**L2 squared fluxes:**

a and b are constant matrices

is a differentiable representation of the Heavyside step function.

Flux-based approach: , , are the rate constants, so

That is: ;