Simulationstechnik A
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Exercise 1 - Chemical Master Equation

For all our exercises, we will consider the following system consisting of substrate S_1, enzyme S_2, complex S_3 and product S_4:

$$S_1 + S_2 \xrightarrow{c_1} S_3$$
$$S_3 \xrightarrow{c_2} S_1 + S_2$$
$$S_3 \xrightarrow{c_3} S_4 + S_2$$

It is often referred to as Michaelis Menten Kinetics and will serve as a manageable system to train techniques and algorithms from the lecture.

1. **Defining state-transition vectors ν_j and the propensity function $a_j(X(t))$**
   Each chemical reaction j is defined by a state-transition vector ν_j and a propensity function $a_j(X(t))$ depending on the system state X at time t. While the first indicates the change induced by the specific reaction, the latter describes the frequency in which reaction j is likely to occur.
   a) Determine the state-change vectors ν_1, ν_2 and ν_3.
   b) Determine the propensity functions $a_1(X(t))$, $a_2(X(t))$ and $a_3(X(t))$ for a given system state $X(t)$.

2. **System reduction**
   The system state X seems to be four-dimensional.
   a) Show, that its actual dimension is lower than that by using conservation laws.
   b) How are ν_j and $a_j(X(t))$ $j = 1, 2, 3$ defined now?

3. **The Chemical Master Equation**
   Everything is set up to solve the system now. This actually means that we are interested in knowing the probability $P(X(t), t)$ of our System being in state $X(t)$ at time t for all possible states and times.
   a) Each probability density (and therefore also $P(X(t), t)$) must be normalized. State, how this normalization criterion is mathematically defined for $P(X(t), t)$.
   b) Derive the Chemical Master Equation (CME), the differential equation whose solution is $P(X(t), t)$

4. **Implementing the System**
   We will now implement, solve and visualize the system.

   a) Define the state-transition vectors and propensity functions in the provided code.
   b) How could you solve the CME derived in 3b) numerically? Implement your idea.
   c) Determine the algorithmic comlpexity of your solution.
   d) How could you visualize the solution $P(X(t), t)$? Implement your idea.