Workshop Day 2 - Introduction and motivations

Why do we need other methods?

Gillespie ♡

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1. Time-dependent rates (Lewis thinning)
2. Large population sizes (τ-leaping)
3. Applications
4. Exercises

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- The Gillespie algorithm is not suitable because the rates can change during the waiting time.
- But is it still possible to derive an exact method?

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- It is also possible to construct exact time-dependent methods by modifying the First-Reaction Method.

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Lewis thinning algorithm (1978)

SIMULATION OF NONHOMOGENEOUS POISSON PROCESSES BY THINNING

P. A. W. Lewis*

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Monterey, California

G. S. Shedler

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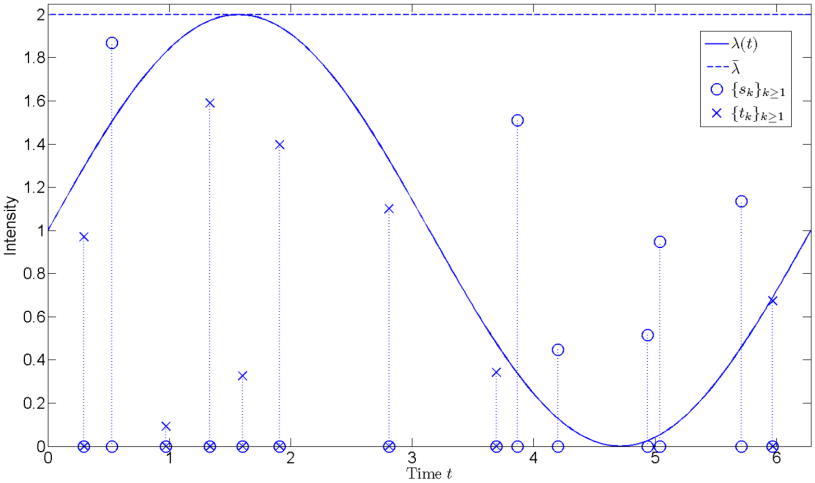
- It means that we are updating time more frequently than we should: **sometimes, no reaction should occur**
- One can prove that if we discard every update with probability $1 - \frac{a_0(t+\tau)}{\bar{a}_0}$, then this method actually sample from the joint distribution $p(\tau, i)$

An example with a single reaction

Here we assume that the propensity $\lambda(t) = 1 + \sin(t)$ does not depend on the system state $\boldsymbol{x}$



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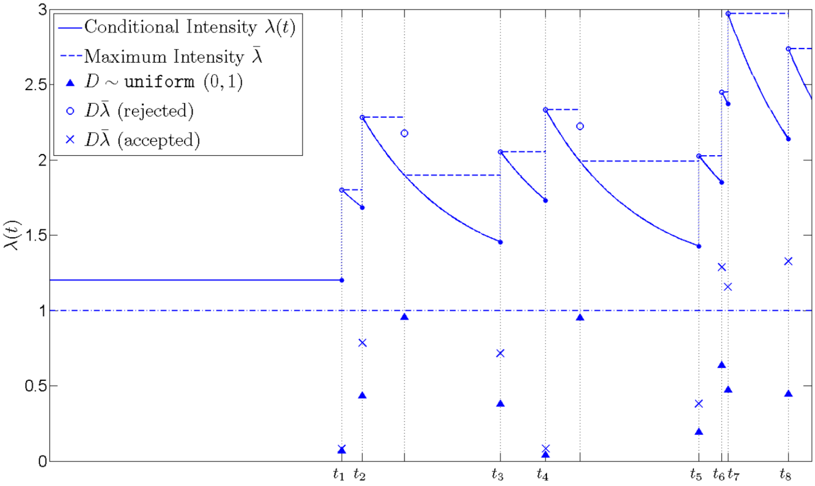
Now, the propensity $\lambda(t)$ depends on the system state $\boldsymbol{x}$



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- τ-leaping has other interesting properties, especially for large populations.

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- The probability of generating a given trajectory with an exact method is exactly the probability that would come out of the solution of the master / Kolmogorov forward equation.
- However, exact methods are usually slow for large dimensions and/or when the transitions occur very often (large population sizes for example). One transition at a time.

Logical structure of stochastic kinetics