Outline

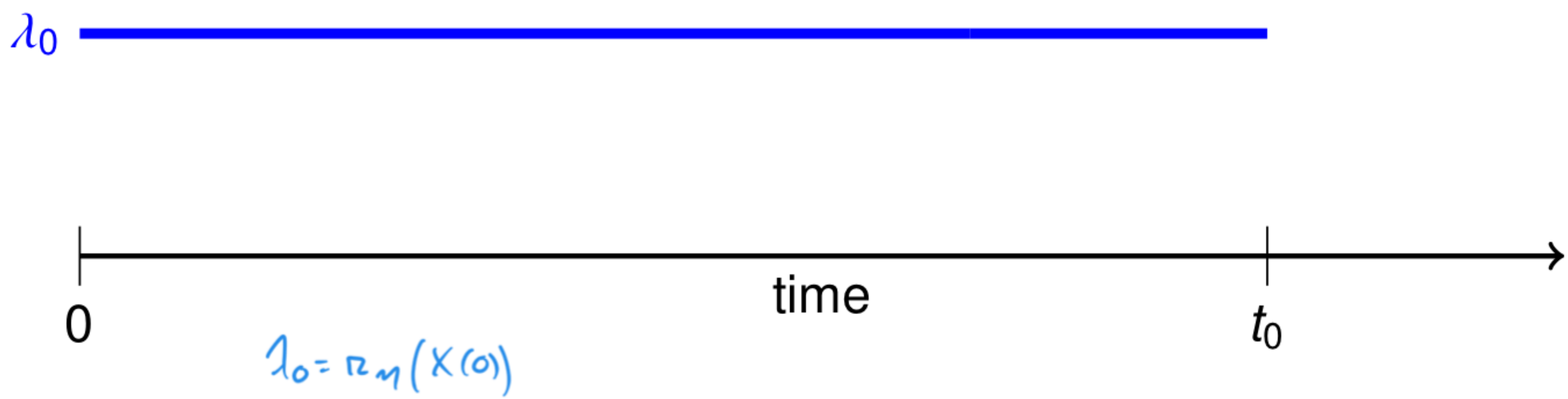
1. Continuous Time Markov Chains
   - Main concepts
   - Poisson Process
   - Time-inhomogeneous rates
2. Population Continuous Time Markov Chains
3. Simulation
   - SSA
   - Next Reaction Method
   - τ-leaping

NEXT REACTION METHOD/GIBSON-BRUCK (SKETCH)

- Consider a single η transition in a time interval $[0, t]$ in which it never fires.
- As other transitions may fire, its rate $r_\eta(\mathbf{X}(s))$ is a time-dependent function.
- Therefore, we can sample the firing time of η using the inversion method for time-inhomogeneous exponential distribution, solving for t

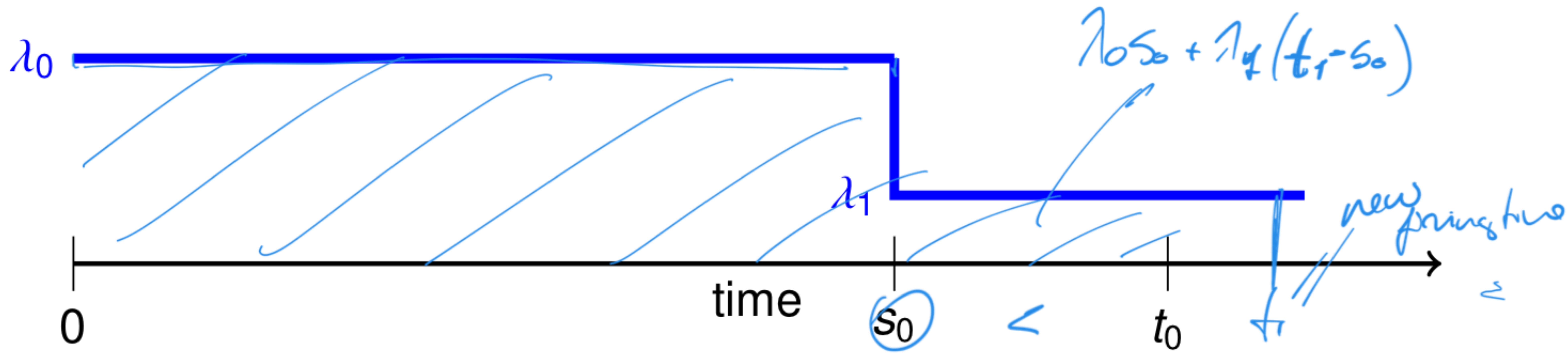
$$\Lambda_\eta(t) = \int_0^t r_\eta(\mathbf{X}(s))ds = \xi \sim Exp(1).$$

NEXT REACTION METHOD/GIBSON-BRUCK (SKETCH)



- Start at time 0, and suppose the rate of η is λ_0. Assuming it does not change in time, the firing time would be $t_0 = \frac{1}{\lambda_0}\xi \sim Exp(\lambda_0)$.

NEXT REACTION METHOD/GIBSON-BRUCK (SKETCH)

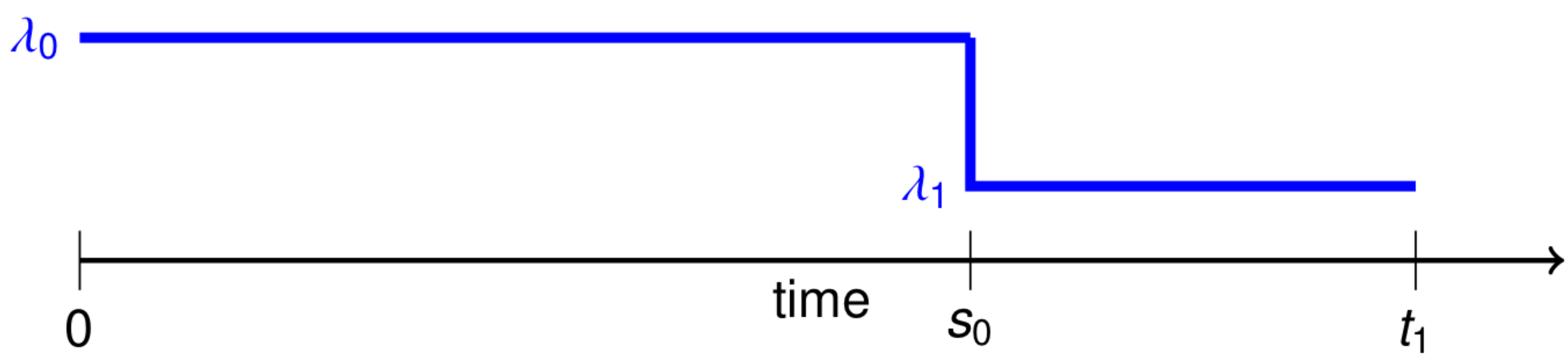


- Start at time 0, and suppose the rate of η is λ_0. Assuming it does not change in time, the firing time would be $t_0 = \frac{1}{\lambda_0}\xi \sim Exp(\lambda_0)$.
- Now, suppose at time s_0 another event η' fires, and this changes the rate of η to λ_1.

$\lambda_0 s_0 + \lambda_1 (t_1 - s_0) = \xi$

$\lambda_1 t_1 + \lambda_0 s_0 - \lambda_1 s_0 = \xi$

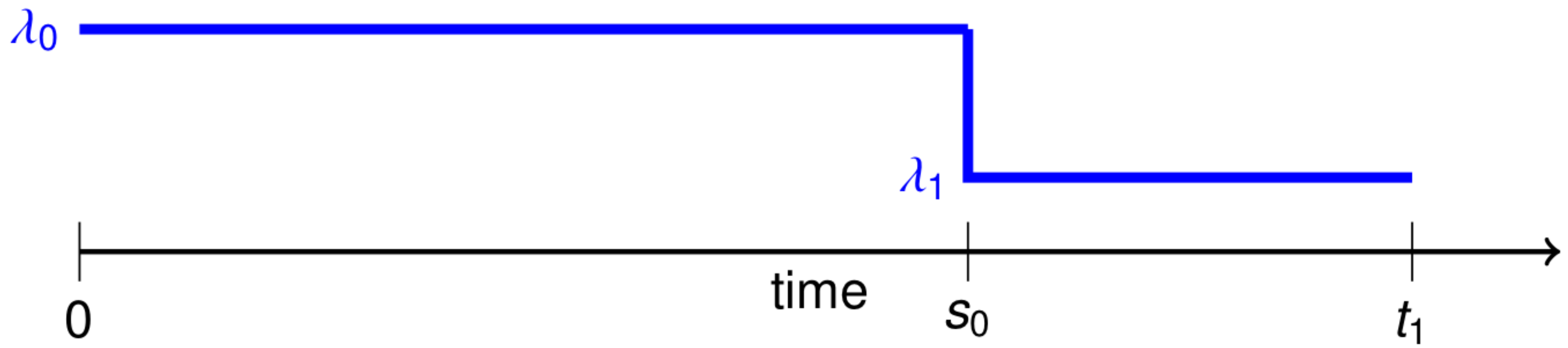
NEXT REACTION METHOD/GIBSON-BRUCK (SKETCH)



- Start at time 0, and suppose the rate of η is λ_0. Assuming it does not change in time, the firing time would be $t_0 = \frac{1}{\lambda_0}\xi \sim Exp(\lambda_0)$.
- Now, suppose at time s_0 another event η' fires, and this changes the rate of η to λ_1.
- Then the firing time of η would be found by solving $\lambda_0 s_0 + \lambda_1(t_1 - s_0) = \xi$, from which

$$t_1 = s_0 + \frac{\lambda_0}{\lambda_1}\left(\frac{1}{\lambda_0}\xi - s_0\right) = s_0 + \frac{\lambda_0}{\lambda_1}(t_0 - s_0).$$

NEXT REACTION METHOD/GIBSON-BRUCK (SKETCH)



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- Now, suppose at time s_0 another event η' fires, and this changes the rate of η to λ_1.
- Then the firing time of η would be found by solving $\lambda_0 s_0 + \lambda_1(t_1 - s_0) = \xi$, from which

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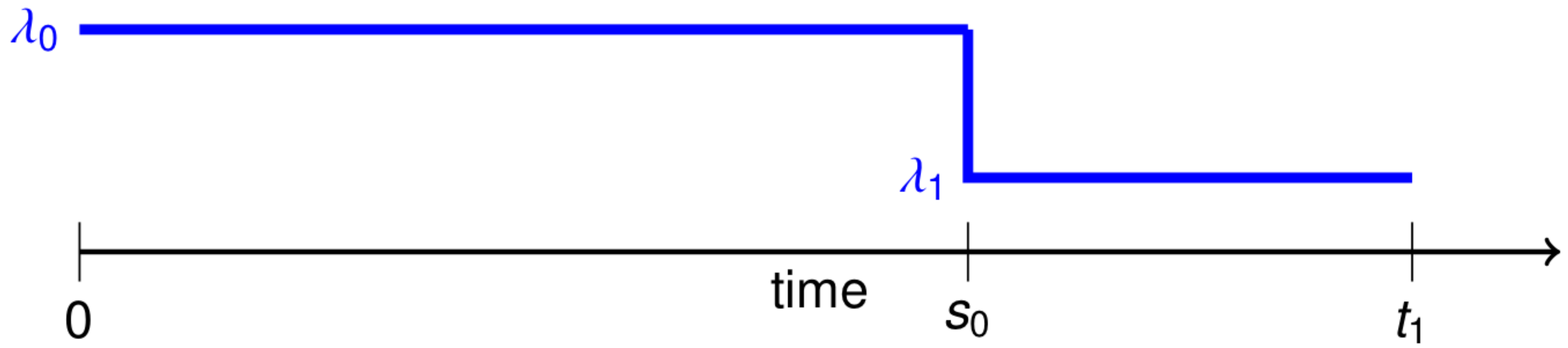
- This is the update formula of Gibson-Bruck algorithm (can be easily generalized to n intermediate events by induction).

NEXT REACTION METHOD/GIBSON-BRUCK (SKETCH)



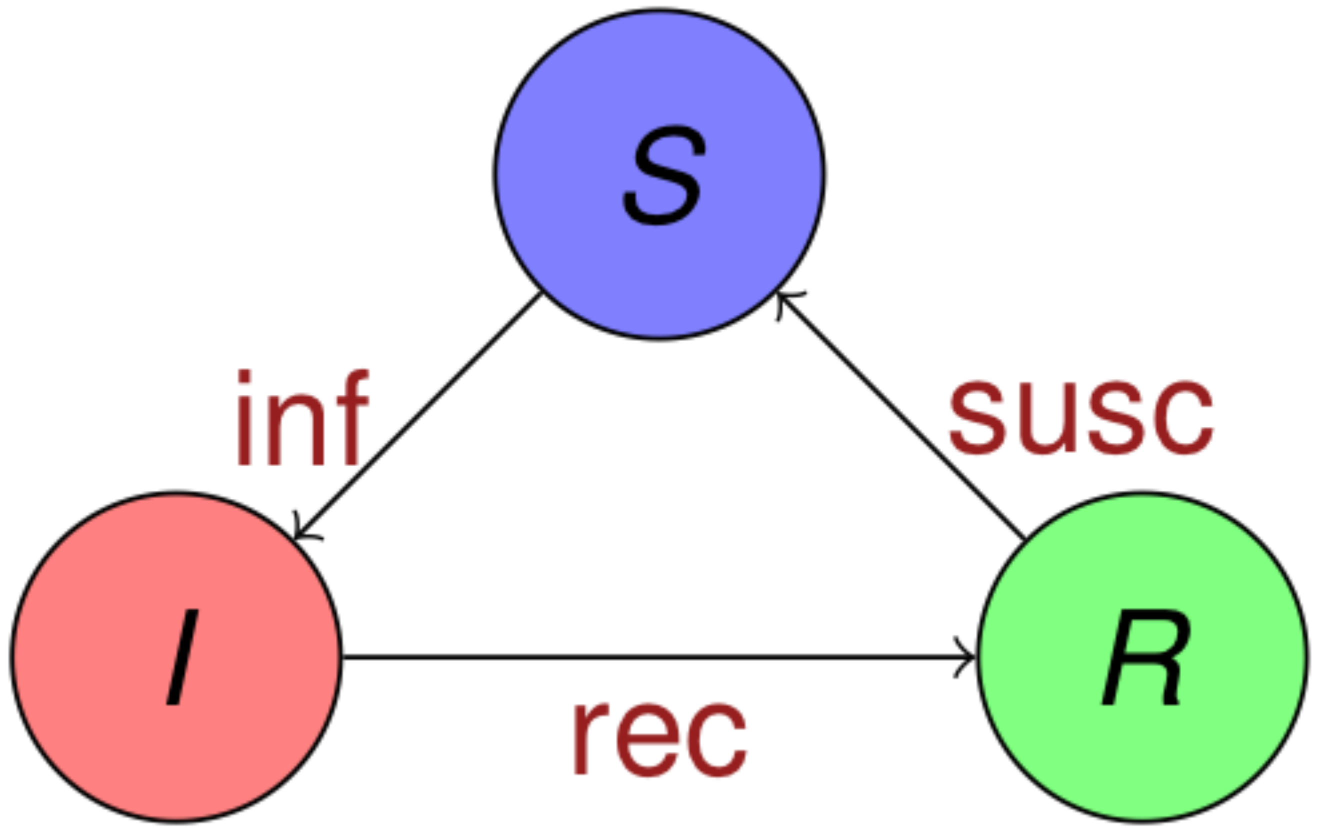
NEXT REACTION METHOD

At each step, with current state **x** and current time t

1. execute transition η with smallest time;
2. update rates and firing times of other transitions;
3. sample a new firing time for η.

the algorithm uses a priority queue and a dependency graph to speed up operations.

EXAMPLE: SIR EPIDEMICS



$N = 10$, $k_I = 1$, $k_R = 0.05$, $k_S = 0.01$
$X_S(0) = 8$, $X_I(0) = 2$, $X_R(0) = 0$.

STEP 1: RATES OF TRANSITIONS

INFECTION: $\frac{1}{10} \cdot 8 \cdot 2 = 1.6$

RECOVERY: $0.05 \cdot 2 = 0.1$

IMMUNITY LOSS: 0

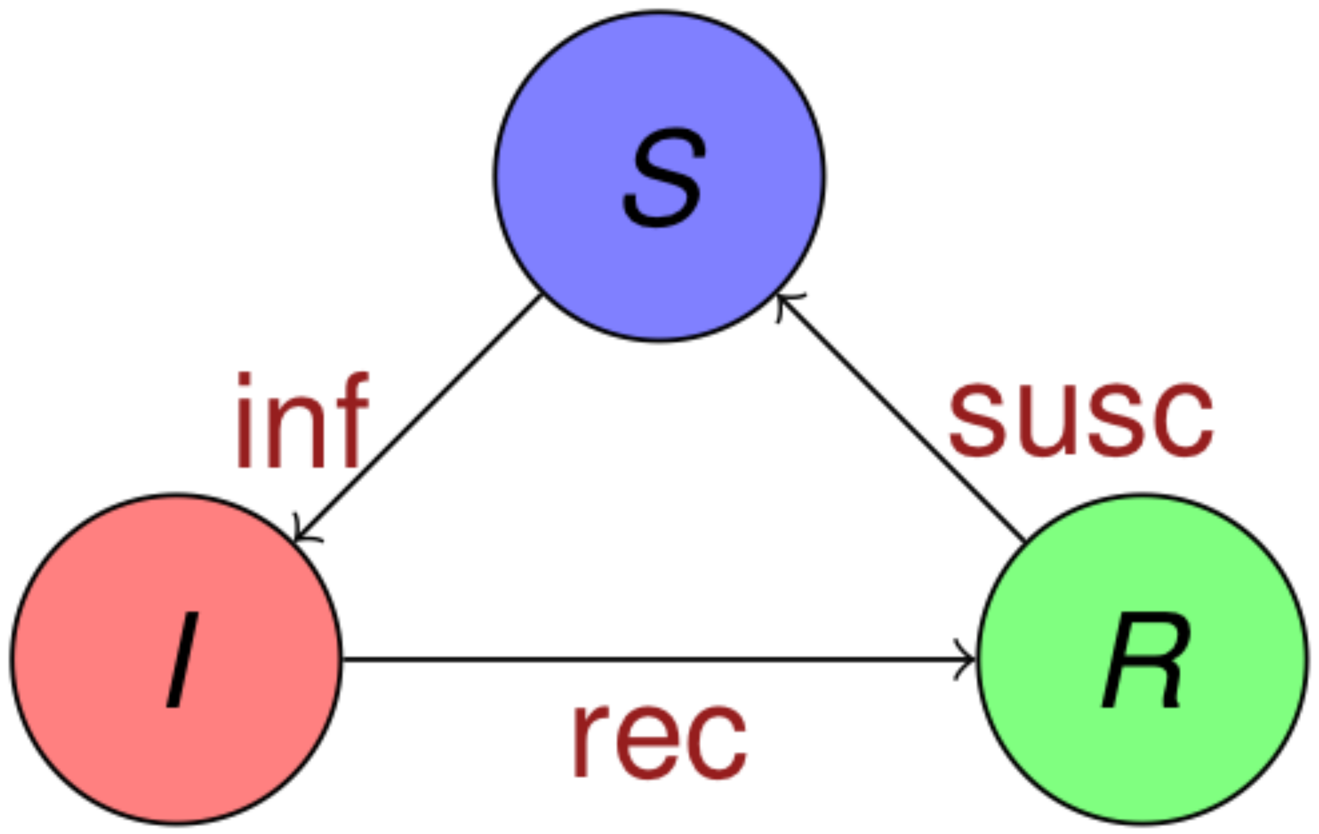
STEP 2: COMPUTE FIRING TIMES

INFECTION: $\frac{1}{1.6} \cdot 0.2228 = 0.1392$

RECOVERY: $\frac{1}{0.1} \cdot 1.9527 = 19.5273$

IMMUNITY LOSS: $\frac{1}{0} \cdot 0 = \infty$

EXAMPLE: SIR EPIDEMICS



$N = 10$, $k_I = 1$, $k_R = 0.05$, $k_S = 0.01$
$X_S(0.1392) = 7$, $X_I(0.1392) = 3$,
$X_R(0.1392) = 0$.

STEP 1: RATES OF TRANSITIONS

INFECTION: $\frac{1}{10} \cdot 7 \cdot 3 = 2.1$

RECOVERY: $0.05 \cdot 3 = 0.15$

IMMUNITY LOSS: 0

STEP 2: REEVALUATE FIRING TIMES

INFECTION: $\frac{1}{2.1} \cdot 3.3323 = 1.5868$

RECOVERY: $0.1392 + \frac{0.1}{0.15} \cdot (19.5273 - 0.1392)$
$= 13.0646$

IMMUNITY LOSS: ∞

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τ-LEAPING (SKETCH)

Consider the Poisson representation of a population CTMC at time τ

$$X(\tau) = X(0) + \sum_{\eta \in \mathcal{T}} \mathbf{v}_\eta \mathcal{Y}_\eta \left(\int_0^\tau r_\eta(X(s)) ds \right).$$

If τ is sufficiently small, we may assume that the rates $r_\eta(X(s))$ are approximately constant in $[0, \tau]$ and equal to a_η.
Then $\int_0^t r_\eta(X(s)) ds \approx a_\eta \tau$, hence

$$X(\tau) \approx X(0) + \sum_{\eta \in \mathcal{T}} \mathbf{v}_\eta \mathcal{Y}_\eta \left(a_\eta \tau \right).$$

τ-LEAPING (SKETCH)

τ-LEAPING

At each step, with current state $\mathbf{x}$ and current time t

1. choose τ;
2. for each η, sample n_η from the Poisson r.v. $\mathcal{Y}_\eta\left(a_\eta\tau\right)$;
3. update $\mathbf{x}$ to $\mathbf{x} + \sum_\eta \mathbf{v}_\eta n_\eta$ and time to $t + \tau$.

CHOICE OF τ: LEAPING CONDITION

The choice of τ is an art:

- it has to be small for rates to be approximately constant in $[t, t + \tau]$;
- it has to be as large as possible to make $\mathcal{Y}_\eta(a_\eta\tau)$ large to gain in computational efficiency;
- one has to avoid the generation of negative populations.

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