Simulation

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Simulation as an Analysis Method

"Execution of the model", which results in a "sample of the possible behaviour".

Any model type can be simulated.

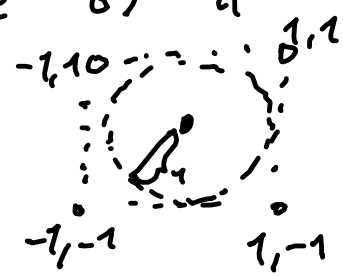
- ✗ Deterministic and Discrete; ⇝ Entire reachable space
- ✓ Deterministic and Continuous; ⇝ Numerical simulations
- ✗ Non-Deterministic; ⇝ Rather sampling
- ✓ Stochastic;

Monte Carlo Method

Repeated sampling of a random variable.

Kinetic Monte Carlo method for stochastic processes (evolution in time).

→ estimate the value of π

draw points in the 

square

n ... number of trials (points)

m ... number of points in the unit cycle

$$\pi \approx \frac{4m}{n}$$

Gillespie Algorithm

Stochastic simulation algorithm

First described by Joseph Doob (1945).

Reinvented and popularised by Daniel Gillespie (1975).

Statistically correct solutions of a stochastic system with known transition rates.

Key assumptions:

- The transition rates are statistically independent.
- The stochastic system is Markovian.

1. Initialise $t = t_0$ and $x = x_0$
2. If (t, x) satisfies whatever stopping criterion: exit
3. evaluate $\lambda_i(x)$ and the $\sum_{i=1}^{m} \lambda_i(x) = \lambda$
   ($\lambda_i(x)$: $q_{x\,i(x)}$; λ: $-q_{xx}$)
4. compute τ and j - index of the transition
   "Direct" sample two variables $r, r' \in [0, 1]$ uniformly

$$\tau = \frac{1}{\lambda} \ln\left(\frac{1}{r}\right) \qquad j = \min_{j \in \{1,\dots,m\}} \left(\sum_{\lambda_i(x)}^{j} \lambda_i(x) > r' \lambda \right)$$

5. Set $t \leftarrow t + \tau$ and $x \leftarrow x + \nu_j$ → effect of transition j
6. Return to step (2.)

Optimisations

First-reaction method.

$r_1, \dots, r_m \in [0,1]$ uniformly

$\forall k \in \{1,\dots,m\} \quad \tau_k = \frac{1}{\lambda_k(x)} \cdot \ln\left(\frac{1}{r_k}\right) \qquad \tau = \min_{k \in \{1,\dots,m\}} (\tau_k)$

j = index of τ

First-family method.

transitions are partitioned into classes $F_1, \dots, F_l$

$r_1, \dots, r_{l+1} \in [0,1]$ uniformly

$\forall k \in \{1,\dots,l\} \quad \tau_k = \frac{1}{\sum_{i_k=1}^{m_k} \lambda_{i_k}(x)} \cdot \ln\left(\frac{1}{r_k}\right) \qquad \tau = \min_{k \in \{1,\dots,l\}} (\tau_k)$

l is index of τ

$j = \min_{j \in \{1,\dots,m_l\}} \left(\sum_{i_l=1}^{m_l} \lambda_{i_l}(x) > r_{l+1} \lambda_l \right)$

τ-leaping

Let τ be the such that $\forall i \in 1, \ldots, m, \lambda_1(\mathbf{x})$ remain essentially constant over the interval $[t, t + \tau]$.

→ The number of times a transition i fires in the interval $[t, t+\tau]$ is given by a random variable distributed with Poisson dist. and both mean and variance are $\lambda_i(x).\tau$

$$X(t+\tau) \simeq x + \sum_{i=1}^{m} P(\lambda_i(x)\tau)\, v_i$$

$P(\lambda_i(x)\tau)$: sample from the Poisson dist.

v_i: net change caused by transition i

Mass Action Kinetics

Chemical Reaction Networks.

Assuming:

- The mixture of chemical species is well mixed.
- The system is spatially confined.
- External factors are in an equilibrium.

$\frac{d\lambda_i(x)}{dt} \triangleq$ probability of r_i occurring in $x = X_t$ within the next infinitesmal interval $[t, t+dt]$

each reaction r_i has a "base propensity" c_i

$\frac{dc_i}{dt} \Rightarrow$ The probability that reaction occurs in the infinitesmal interval given that all reactants "met".

unimolecular reactions: $\lambda_i(x) = c_i \cdot x_j$ j is the sole reactant

bimolecular reactions: $j \neq k$ are the reactants,

$\lambda_i(x) = c_i \cdot x_j \cdot x_k$

j reacts with itself

$\lambda_i(x) = c_i \frac{x_j(x_j - 1)}{2}$