MODEL FOR EFFICIENTLY SIMULATING DIFFUSION THROUGH A NETWORK

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1. First passage time distributions

A particle of diffusivity D is on a one-dimensional interval, with an absorbing state a distance $\tilde{x}$ in one direction, and a distance $\ell - \tilde{x}$ in the other direction. We want the first passage time $\tilde{T}_{\text{FPT}}$ to reach either of these absorbing state positions. Lengths and times are rescaled to nondimensionalized length units $x = \tilde{x}/\ell$ and nondimensionalized time units $t = \tilde{t}(\ell^2/D)$. ℓ is the distance between the two absorbing states, which is rescaled such that one absorbing state is a distance x to the left, and the other $1 - x$ to the right, so they are separated by a distance 1. The particle has a probability $1 - x$ of being absorbed by the left absorbing state a distance x from the initial particle position, and a probability x of being absorbed to the right at a distnace $1 - x$. The distribution of first passage times until the particle is absorbed depends on the distance of the absorbing state from the initial particle position. Below is the probability distribution for first passage time T_{FPT} for the case where the particle is absorbed by the absorbing state a distance $1 - x$ from the initial particle position. To find the probability distribution for the first passage time to be absorbed by the absorbing state a distance x from the initial particle position, simple replace x in the expressions below with $1 - x$. The first passage time probability distribution can be written in two ways.

Sine series:

$$P(T_{\text{FPT}} = T) = 1 + \sum_{n=1}^{\infty} (-1)^n \frac{2}{n\pi x} \sin(n\pi x) e^{-\pi^2 T n^2} \ . \tag{1}$$

Image method series:

$$P(T_{\text{FPT}} = T) = \frac{1}{x} \sum_{k=1}^{\infty} \left[\text{erf}\left(\frac{k+x}{2\sqrt{T}} \right) - \text{erf}\left(\frac{k-x}{2\sqrt{T}} \right) \right] \ . \tag{2}$$

These sums are obviously not computed to arbitrarily large order, but instead are truncated beyond $n = n_{\max}$ or $k = k_{\max}$. For accuracy ϵ,

$$n_{\max} = \sqrt{-\frac{\log \epsilon}{10\pi^2}} \ . \tag{3}$$

$$k_{\max} = \sqrt{-\log \epsilon} \ . \tag{4}$$

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2. Network propagation algorithm

This algorithm is for one dimensional diffusion in a spatial network defined by nodes with physical locations, and edges between those nodes of a length defined by the distance between nodes.

2.1. **Two neighboring nodes.** The particle can be either at a node or on an edge. The case that a particle is on an edge or at a node with two edges is the same for determining the first passage time to one of the neighboring nodes, because the particle is a distance x from a node in one direction, and a distance $1-x$ from a node in the other direction. First pick which node the particle will propagate to: probability to propagate to node at distance x with probability $1-x$, and to propagate to node at distance $1-x$ with probability x. Once the direction and distance the node will propagate is selected, use Eqs. 1 or 2 to determine the first passage time (these equations are equal, but one or the other converges more quickly depending on x). The cumulative probability of the first passage time,

$$\int_0^T P(T_{\mathrm{FPT}})dT_{\mathrm{FPT}} \ , \tag{5}$$

can be compared to a random number $\in [0,1]$ to choose a first passage time T. The particle is then moved to the chosen destination and the time increased by T.

2.2. **One neighboring node.** For a particle at a node with a single edge, simply pretend there is a second edge of the same length, and find the first passage time to either of the nodes ending these two edges. This works out because if there are two edges, and the particle returns to the initial node, it's equivalent to the particle returning to the node and going back out on the same edge.

2.3. **Four neighboring nodes.** For a particle at a node with four edges, put the edges in order from shortest to longest. The edges are divided into two groups: the two shortest edges, and the two longest edges. Together, the shortest edge and the third shortest edge (shorter of the two longest edges) then comprise a situation where there are only two edges for the node. Follow the steps for the two-edge node. If the short edge is chosen, the particle will go along one of the two shorter edges; and if the longer edge is chosen, the particle will go along one of the two longer edges. Thus the decision has been narrowed down to deciding within a pair of edges (choosing between the shortest and second shortest edges, or between the third-shortest and the longest edges). The particle chooses which edge of the selected pair to move down with equal probability — if the shorter edge of the pair is chosen, the particle goes to the node at the end of that edge; if the longer edge of the pair is chosen, the particle moves a distance equal to the shorter edge down the chosen edge.

2.4. **Three neighboring nodes.** For a particle at a node with three edges, assume there is an 'imaginary' fourth edge of length equal to the shortest of the three edges, then follow the steps for a node with four edges. If the imaginary edge is selected, the particle moves

a distance equal to the shortest edge length along one of the three real edges with equal probability.