

Continuous-Time Random Walks on Networks

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1 Introduction

Random walks are one of the fundamental concepts in probability theory and have been studied for well over 100 years [1]. Understanding the mathematical treatment of random walks provides a solid foundation for tackling a large range of mathematical problems. Not only are random walks and their many variants used in a wide range of scientific disciplines (biology, particle physics, network science, and economics, to name a few [2, 3, 4, 5]), but their treatment can be extended to Markov processes, the generalization of random walks.

A Markov process is a type of stochastic process, that is, a system that evolves in time and involves stochasticity. The fundamental assumption of Markov processes is that the future only depends on the current state. The mathematical treatment differs between discrete-time and continuous-time and discrete and continuous state space Markov processes [6, 7]. In this report, we study a specific continuous-time, discrete-space Markov process that can be understood as a random walk on a network and will serve as an example for understanding the more general case. How to go from random walks on networks to discrete-space Markov processes is discussed in detail in ref. [7].

In a random walk, a walker jumps between states according to some probability distribution. Unlike in discrete-time random walks, where jumps occur at fixed times, the time between jumps in continuous-time random walks follows a probability distribution called the waiting time distribution. In discrete-space random walks, the walker jumps between discrete states, which can be naturally represented by a network. A network consists of nodes and edges, where nodes represent the possible states and the weighted edges represent transition rates between states. In this generality, networks can describe any discrete-space Markov process [7], but we focus here on a specific subset where the network is undirected, meaning that the transition rates between nodes are the same in both directions. Additionally, for the specific random walk we discuss here, all transition rates are the same and equal to 1, and the random walk is thus described by the graph Laplacian [8]. This leaves us with an object of study that is simple enough to get concrete results without frequently having to address special cases but nonetheless covers most concepts for understanding general Markov processes. In order to underscore the importance of the graph Laplacian even without the applicability to more general cases, we refer to refs. [9, 10].

An interesting question is what changes when multiple random walkers move on the same network, either independently or interacting. Besides presenting the analysis of a single continuous-time random walk, the focus of this report is the analysis of the distribution of multiple independent random walkers on the network. Given m independent walkers we answer the question: How are the walkers distributed on the network at any point in time? To answer this question we look at three approaches that are useful for analysing many stochastic systems. The first approach deals with sums of independent variables and is the simplest, but still very powerful because mathematical tools such as the central limit theorem can be applied. The second approach is based on the Kronecker product, which allows the compact description of the state space of all possible combinations of walker positions. Besides the application presented here, the Kronecker product can be used in many other contexts [11, 12]. Lastly, an approach using a master equation on the node distribution directly is shortly described and a common scenario is encountered where the description of the resulting system is not closed.

In section 2, the mathematical analysis of a single continuous-time random walk on a network is described. We turn to the node distribution in section 3 and present the first approach in section 3.1. The Kronecker product is introduced in section 3.2 and a representation of the complete state space with a Kronecker sum is derived. In section 3.3, the Kronecker sum representation is used to derive an alternative derivation of the node distribution. section 3.4 covers a third approach for deriving the node distribution, leading to a description that is not closed. Some aspects of generalizing the approaches to interacting random walks are discussed in section 4. Finally, section 5 concludes the report with a discussion of the results.

2 Continuous-Time Random Walks on Networks

To set the stage, we introduce the continuous-time random walk (CTRW) and its mathematical analysis, as well as notation in this section.

Troughout the report, we consider random walks on a finite network, which we denote by $G = (V, E)$ and where $V = \{v_1, \dots, v_{|V|}\}$ is the set of nodes and $E = \{e_1, \dots, e_{|E|}\}$ is the set of edges. The number of nodes of G is denoted by $|V| = n$ and we write $\delta(j)$ for the degree of node v_j . We assume that the network only has a single component because the same analysis can be applied to each component separately if there is more than one. Additionally, only undirected networks are considered in the beginning, and directed networks are covered in the section on continuous-time Markov processes. The connections between nodes can be summarized by the adjacency matrix \mathbf{A} , whose entries a_{jk} are 1, if an edge exists between nodes v_j and v_k and 0 otherwise. Similarly, the vertex degrees can be compactly stored in the diagonal matrix \mathbf{D} , with entry $\delta(j)$ at \mathbf{D}_{jj} and 0 for all non-diagonal entries. The adjacency matrix and the degree matrix combine to form the Laplacian $\mathbf{L} = \mathbf{D} - \mathbf{A}$, which will be central for describing random walks on networks.

In the CTRW, a random walker starts at an initial node at time $t = 0$ and then moves along edges to connected nodes, choosing which edge to take according to some probability distribution. In the absence of a reason to prefer certain edges over others, it is natural to choose each edge with the same probability. Upon arriving at a new node at time t , a waiting time τ is drawn from a waiting-time distribution $\Psi(\tau)$ and the next move is made at time $t + \tau$. In this report, we will use an exponential distribution, $\Psi(\tau) = \beta e^{-\beta\tau}$, for the waiting time distribution, which we can interpret as the walker leaving the node at a constant rate, see [13] for a derivation of this result. We will consider edge-centric CTRWs, meaning that the rate of the random walker leaving a node depends on the degree of the node giving $\beta_j = \delta(j)$. The effect of this is that a walker leaves nodes of high degree more quickly than nodes of low degree.

Mathematically, these CTRWs can be described by a sequence of random variables $W(t)$ that each have the same state space, namely the nodes of the network, indexed by a continuous time $t \in \mathbb{R}_{\geq 0}$. We denote the probability of a random walker being at node v_j at time t as

$$y_j(t) := P(W(t) = v_j). \quad (1)$$

For this kind of random walk it is possible to determine $y_j(t)$ mathematically, giving a complete description of the random walk.

To do this, it is necessary to understand how $y_j(t)$ changes over time. The change of $y_j(t)$ is given by the master equation and can be derived using the Chapman-Kolmogorov equation

$$y_j(t + \tau) = \sum_{l=1}^n P(W(t + \tau) = j | W(t) = l) \cdot y_l(t) \quad (2)$$

where the conditional probability can be simplified by using the waiting time distribution and the adjacency matrix of the network. This leads to

$$\frac{dy_j(t)}{dt} = -\delta(j)y_j + \sum_{k=1}^n \mathbf{A}_{jk}y_k, \quad (3)$$

that is, the loss term is the probability of being at node v_j times the rate at which node v_j is left and the gain term is the sum over the neighbors of v_j where the rate of moving from node v_k to v_j is multiplied with the probability of being at v_k .

When the individual probabilities y_j are combined into a vector $\mathbf{y} = (y_1, \dots, y_n)^\top$, the master equation for \mathbf{x} can be compactly written as

$$\dot{\mathbf{y}} = -\mathbf{L}\mathbf{y}. \quad (4)$$

As we are focusing on undirected networks, \mathbf{L} is symmetric and can thus be written in terms of its eigenvalues and eigenvectors

$$\mathbf{L} = \sum_{k=1}^n \lambda_k \mathbf{v}_k \mathbf{v}_k^\top, \quad (5)$$

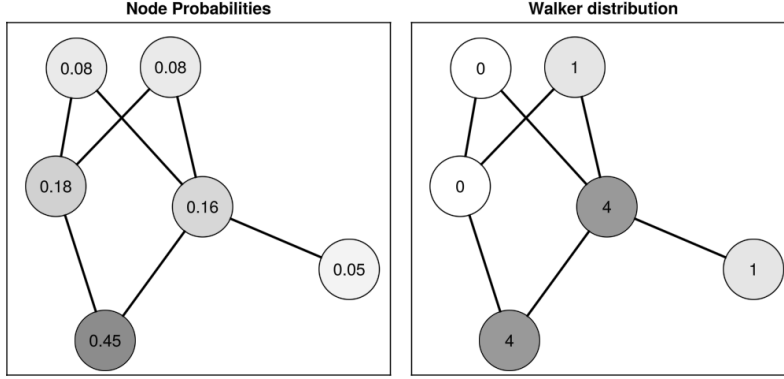


Figure 1: On the left, the probability of being at each node at time $t = 0.5$ is given for each individual walker, if the starting point is the bottom node. On the right, the number of walkers at each node at time $t = 0.5$ is shown for a simulation of 10 walkers that all started at the bottom node.

where for $k = 1, \dots, n$, λ_k are the eigenvalues, v_k are the eigenvectors [14]. Then the solution to Eq. 4 can be written as

$$\mathbf{y}(t) = \sum_{k=1}^n c_k e^{-\lambda_k t} \mathbf{v}_k. \quad (6)$$

The Laplacian of G is a positive semi-definite, symmetric matrix with all rows and columns summing to zero. The implication from linear algebra is that G has exactly one eigenvalue that is equal to $\lambda_1 = 0$ and a corresponding eigenvector $\mathbf{v}_1 = (1, \dots, 1)^\top$. Additionally, all other eigenvalues are bigger than zero, which means that the terms in Eq. 6 decay exponentially for $k \neq 1$. In the limit, the probabilities even out

$$\lim_{t \rightarrow \infty} \mathbf{y}(t) = c_1 \cdot (1, \dots, 1)^\top. \quad (7)$$

Since probabilities sum to 1, we find that $c_1 = 1/n$.

In a general continuous-time Markov process, the matrix describing the change of the distribution \mathbf{y} is a so-called intensity matrix \mathbf{Q} that is not necessarily symmetric. While the master equation still has the same structure $\dot{\mathbf{y}} = \mathbf{Q}\mathbf{y}$, there is less that can be said about the eigenvalues and eigenvectors of the matrix, although the general solution $\mathbf{y} = \exp(\mathbf{Q}t)$ is still correct. For a more detailed look on continuous-time Markov processes, see ref. [6].

3 Distributions of Multiple Random Walkers

In the previous section, we have seen that we can describe the time-evolution of a single CTRW on a network by finding the eigenvalues and eigenvectors of

the network Laplacian. Now, we consider multiple independent random walkers moving on the network. Specifically, we look at how the distribution of walkers on the nodes changes over time. In Figure 1, a visualization of these two different points of view is shown. If all walkers start at the same node, we would expect that, at least as the number of walkers goes to infinity, the proportion of walkers at any node v_j is just given by $y_j(t)$, because $y_j(t)$ describes the likelihood of each walker being at that node. The goal of this section is to show that the expected number of walkers at any node v_j is described by $y_j(t)$ for all m , not just in the limit. Additionally, methods for studying interacting random walks are developed.

There are three approaches that we will take to describe a system of multiple walkers. In the first approach, we use the independence of the walkers to study each of them individually and add up their contributions to study the distribution of the walkers on the nodes. For the second approach, we work with the multivariate distribution and derive the time evolution of the system using Kronecker products. This approach is more involved, but unlike the first one, it can be applied to study interacting walks as well. Lastly, we shortly discuss a third approach directly working on the node distribution.

We start by introducing the notation for describing a system of m walkers W_1, \dots, W_m . We write the probability of the system being in a given state at time t as

$$x_{j_1 \dots j_m}(t) := P(W_1(t) = v_{j_1}, \dots, W_m(t) = v_{j_m}). \quad (8)$$

Usually, we drop the argument t of the state variables for compactness. Because of independence, Eq. 8 can be decomposed into the probabilities for the individual walkers $y_{i,j_i}(t) = P(W_i(t) = v_{j_i})$, giving us

$$x_{j_1 \dots j_m} = \prod_{i=1}^m y_{i,j_i}. \quad (9)$$

We again combine the probabilities for each walker into a single vector $\mathbf{y}_i = (y_{i,1}, \dots, y_{i,n})^\top$.

To describe the distribution of the walkers on the nodes, we introduce the random variables $Z_j(t)$, which describe the proportion of walkers at node j at time t . Studying these random variables is the focus of the next sections.

3.1 Node Distributions: Individual Approach

The easiest way to find the distribution of the walkers on the nodes is by considering each walker for themselves. Because all walkers are independent, their time evolution is given individually by Eq. 4

$$\dot{\mathbf{y}}_i = -\mathbf{L}\mathbf{y}_i. \quad (10)$$

How \mathbf{y}_i evolves, also depends on the initial position of each walker, which can differ between walkers.

To describe Z_j , we construct it as a sum of random variables. Let Y_{ij} be a random variable that is 1, if walker i is at node j , and 0 otherwise. Then Z_j , the proportion of walkers at node j , is equal to

$$Z_j = \frac{1}{m} (Y_{1j} + Y_{2j} + \dots + Y_{mj}). \quad (11)$$

Because of the linearity of the expected value, we can easily calculate the expected value for Z_j

$$\langle Z_j \rangle = \frac{1}{m} \sum_{i=1}^m \langle Y_{ij} \rangle. \quad (12)$$

The terms in the sum are

$$\langle Y_{ij} \rangle = 0 \cdot P(W_i(t) \neq v_j) + 1 \cdot P(W_i(t) = v_j) = y_{i,j}. \quad (13)$$

Thus the expected value in Eq. 12 becomes

$$\langle Z_j \rangle = \frac{1}{m} \sum_{i=1}^m y_{i,j}. \quad (14)$$

This shows that the expected proportion of walkers at each node is given by adding up the probabilities of each walker being at that node.

To see how this is related to the dynamics of a single walker, we combine the expected values into a vector $\mathbf{Z} = (\langle Z_1 \rangle, \dots, \langle Z_m \rangle)^\top$. From this, we get

$$\mathbf{Z} = \frac{1}{m} \sum_{i=1}^m \mathbf{y}_i. \quad (15)$$

The last two equations are already enough to determine the expected distribution of walkers on the network at all times, because as we have seen in the first section, the exact solution for each walker is known. Let us write this out in more detail using Eq. 6

$$\mathbf{Z} = \frac{1}{m} \sum_{i=1}^m \sum_{k=1}^n c_{i,k} e^{-\lambda_k t} \mathbf{v}_k. \quad (16)$$

Only the constants $c_{i,k}$ depend on the walker and by introducing a new constant $\tilde{c}_k = \frac{1}{m} \sum_{i=1}^m c_{i,k}$, we can write Eq. 16 as

$$\mathbf{Z} = \sum_{k=1}^n \tilde{c}_k e^{-\lambda_k t} \mathbf{v}_k. \quad (17)$$

The expected value of the walker distribution is therefore governed by the same dynamics as the distribution of a single walker on the network, only that the constants \tilde{c}_k correspond to a different initial condition of the system. For example, if all walkers share the same initial distribution, then \tilde{c}_k is equal to $c_{i,k}$ for all i , and we thus have $\mathbf{Z}(t) = \mathbf{y}_i(t)$.

In the case that all walkers share the same initial distribution, the individual terms in Eq. 11 are independent and identically distributed, meaning that the central limit theorem applies and we can describe how fast the proportion of walkers approaches the mean as the number of walkers increases and how these proportions are distributed.

The only point where we used the independence of the walkers, was when we substituted the solution for the independent walkers into Eq. 15. Up until Eq. 15, the analysis also holds for interacting walks, although it is not always possible to describe how \mathbf{y}_i evolves which makes this approach insufficient in such cases.

3.2 Kronecker Product Representations

Because of the shortcomings of the previous approach, we turn to a more detailed description of the system. As in the single walker case, we derive how the system evolves in time, this time considering the states $x_{j_1 \dots j_m}$ as defined in Eq. 8. First, we show how the change of $x_{j_1 \dots j_m}$ in time can be written using Kronecker products and then solve the resulting ODE to find the time-evolution of the system. We then use the solution to find the distribution of walkers on the nodes.

When considering interacting random walks, the ODE describing the change of \mathbf{x} is, in most cases, linear and we can try similar approaches to the one described below to study them. It has to be said, however, that some of the results depend directly on the independence of the walkers.

To begin, we find the master equation for the states $x_{j_1 \dots j_m}$. By using the independence (Eq. 9), we get

$$\frac{dx_{j_1 \dots j_m}}{dt} = \sum_{i=1}^m \prod_{\substack{l=1 \\ l \neq i}}^m y_{l, j_l} \cdot \dot{y}_{i, j_i} \quad (18)$$

We substitute Eq. 4 for \dot{y}_{i, j_i} , and then write out the matrix-vector product explicitly, to get

$$\sum_{i=1}^m \prod_{\substack{l=1 \\ l \neq i}}^m y_{l, j_l} (-\mathbf{L}\mathbf{y}_i)_{j_i} = \sum_{i=1}^m \prod_{\substack{l=1 \\ l \neq i}}^m y_{l, j_l} \left(\sum_{k_i=1}^n A_{j_i k_i} (y_{i k_i} - y_{i j_i}) \right). \quad (19)$$

With some simple rearrangements, we can bring this in the form of a master equation

$$\frac{dx_{j_1 \dots j_m}}{dt} = \sum_{i=1}^m \left(\sum_{k_i=1}^n A_{j_i k_i} \cdot x_{j_1 \dots k_i \dots j_m} - \delta(j_i) \cdot x_{j_1 \dots j_m} \right). \quad (20)$$

Here, $x_{j_1 \dots k_i \dots j_m}$ corresponds to the state where the i -th walker is at node k_i and all other walkers are at the same state as in $x_{j_1 \dots j_m}$. The master equation shows that the states of the system change by adding up the changes in each

individual walker. We can summarize the master equation for all states using a matrix

$$\dot{\mathbf{x}} = \mathbf{L}_{\mathbf{m}} \mathbf{x}. \quad (21)$$

The structure of the master equation suggests that we can somehow write the matrix $\mathbf{L}_{\mathbf{m}}$ in terms of the Laplacian matrices of the individual walkers. For the following, we write $\mathbf{L}_1 := -\mathbf{L}$, that is, the subscript of the matrix indicates the number of walkers in the system that it describes. There is a mathematical concept that leads to $\mathbf{L}_{\mathbf{m}}$, called the Kronecker sum. The Kronecker sum allows us to describe $\mathbf{L}_{\mathbf{m}}$ in terms of \mathbf{L}_1 , as well as the eigenvalues and eigenvectors of $\mathbf{L}_{\mathbf{m}}$ and therefore leads to an exact solution of Eq. 21.

3.2.1 The Kronecker Product

First, we need to introduce the Kronecker product, which is used to define the Kronecker sum. The introduction follows the one in ref. [11]. Given two matrices $\mathbf{A} \in \mathbb{R}^{m_1 \times n_1}$ and $\mathbf{B} \in \mathbb{R}^{m_2 \times n_2}$ of arbitrary size (vectors are also understood as $n \times 1$ matrices), the *Kronecker product* $\mathbf{A} \otimes \mathbf{B}$ is an $m_1 \times n_1$ block matrix, where the block at index (i, j) is the matrix $a_{ij} \mathbf{B}$. For example,

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \otimes \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix} = \left(\begin{array}{ccc|ccc} a_{11}b_{11} & a_{11}b_{12} & a_{11}b_{13} & a_{12}b_{11} & a_{12}b_{12} & a_{12}b_{13} \\ a_{11}b_{21} & a_{11}b_{22} & a_{11}b_{23} & a_{12}b_{21} & a_{12}b_{22} & a_{12}b_{23} \\ a_{11}b_{31} & a_{11}b_{32} & a_{11}b_{33} & a_{12}b_{31} & a_{12}b_{32} & a_{12}b_{33} \\ \hline a_{21}b_{11} & a_{21}b_{12} & a_{21}b_{13} & a_{22}b_{11} & a_{22}b_{12} & a_{22}b_{13} \\ a_{21}b_{21} & a_{21}b_{22} & a_{21}b_{23} & a_{22}b_{21} & a_{22}b_{22} & a_{22}b_{23} \\ a_{21}b_{31} & a_{21}b_{32} & a_{21}b_{33} & a_{22}b_{31} & a_{22}b_{32} & a_{22}b_{33} \end{array} \right).$$

The Kronecker product has a number of nice properties, but for our purposes, we only need the following:

1. Distributivity: $(\mathbf{A} + \mathbf{B}) \otimes \mathbf{C} = (\mathbf{A} \otimes \mathbf{C}) + (\mathbf{B} \otimes \mathbf{C})$
2. Mixed Product: $(\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}) = (\mathbf{AC}) \otimes (\mathbf{BD})$
3. Scalar Multiplication: $c(\mathbf{A} \otimes \mathbf{B}) = (c\mathbf{A}) \otimes \mathbf{B} = \mathbf{A} \otimes (c\mathbf{B})$, for $c \in \mathbb{C}$.

A useful convention is to index the Kronecker product of multiple matrices $\mathbf{A} = \mathbf{A}^{(1)} \otimes \dots \otimes \mathbf{A}^{(m)}$ by using a mixed-base numbering index [6]. For instance, if all matrices are $n \times n$ matrices, the index written as $(j_1 \dots j_m, \tilde{j}_1 \dots \tilde{j}_m)$ refers to the row at position $\sum_{k=1}^m j_k n^k$ and column at position $\sum_{k=1}^m \tilde{j}_k n^k$. If we do this, then we have

$$\mathbf{A}_{(j_1 \dots j_m, \tilde{j}_1 \dots \tilde{j}_m)} = \prod_{k=1}^m \mathbf{A}_{j_k, \tilde{j}_k}^{(k)}. \quad (22)$$

Using the Kronecker product, we can define the Kronecker sum. Given $n \times n$ square matrices $\mathbf{A}^{(1)}, \dots, \mathbf{A}^{(m)}$, the *Kronecker sum* is defined as

$$\bigoplus_{i=1}^m \mathbf{A}^{(i)} = \sum_{i=1}^m \mathbf{I}_{n_1} \otimes \mathbf{I}_{n_2} \otimes \dots \otimes \mathbf{A}^{(i)} \otimes \mathbf{I}_{n_{i+1}} \otimes \dots \otimes \mathbf{I}_{n_m}. \quad (23)$$

One nice property of the Kronecker sum is that the eigenvalues and eigenvectors of the Kronecker sum can be expressed in terms of the eigenvalues and eigenvectors of the $\mathbf{A}^{(i)}$. This property is explored in more detail in the next section.

3.2.2 Kronecker Sum Structure of \mathbf{L}_m

In the following theorem, we see how to describe \mathbf{L}_m as a Kronecker sum.

Theorem 3.1. *The matrix \mathbf{L}_m , describing the dynamics of m walkers, can be written as*

$$\mathbf{L}_m = \bigoplus_{i=1}^m \mathbf{L}_1. \quad (24)$$

Proof. Consider a single index of the product

$$\left(\bigoplus_{i=1}^m \mathbf{L}_1 \cdot \mathbf{x} \right)_{j_1 \dots j_m} = \left(\sum_{i=1}^m (\mathbf{I}_{n_1} \otimes \dots \otimes \mathbf{I}_{n_{i-1}} \otimes \mathbf{L}_1 \otimes \dots \otimes \mathbf{I}_{n_m}) \cdot \mathbf{x} \right)_{j_1 \dots j_m}. \quad (25)$$

We show that this equation is equal to the RHS of Eq. 20. To make things less cluttered, we write $\mathbf{L}_m^{(i)} := \mathbf{I}_{n_1} \otimes \dots \otimes \mathbf{I}_{n_{i-1}} \otimes \mathbf{L}_1 \otimes \dots \otimes \mathbf{I}_{n_m}$. First, we only consider one of the summands and thus need to find the value of the matrix-vector product at a specific index

$$\left(\mathbf{L}_m^{(i)} \cdot \mathbf{x} \right)_{j_1 \dots j_m}. \quad (26)$$

By the definition of matrix multiplication, this is the same as multiplying the $j_1 \dots j_m$ -th row of the matrix componentwise with the vector \mathbf{x} . Let's look at a specific component $\tilde{j}_1 \dots \tilde{j}_m$ of \mathbf{x} and the result of multiplying it by the element of the matrix at index $(j_1 \dots j_m, \tilde{j}_1 \dots \tilde{j}_m)$. Then, by the indexing convention, this element of the matrix is

$$\mathbf{L}_m^{(i)}_{(j_1 \dots j_m, \tilde{j}_1 \dots \tilde{j}_m)} = \prod_{k \neq i}^m \mathbf{I}_{n_k}(j_k, \tilde{j}_k) \cdot \mathbf{L}_1(j_i, \tilde{j}_i). \quad (27)$$

We can now easily see that this product is 0, if $j_k \neq \tilde{j}_k$ for $k \neq i$, and 1 otherwise. Thus,

$$\mathbf{L}_m^{(i)}_{(j_1 \dots j_m, \tilde{j}_1 \dots \tilde{j}_m)} = \begin{cases} L_1(j_k, \tilde{j}_k) & \text{if } j_i = \tilde{j}_i \text{ for } i \neq k, \\ 0 & \text{else.} \end{cases} \quad (28)$$

We now see that the non-zero terms that get summed up in Eq. 25 are precisely the ones in the RHS of Eq. 20. Therefore, the dynamics of m walkers can be described by the matrix

$$\mathbf{L}_m = \bigoplus_{i=1}^m \mathbf{L}_1. \quad (29)$$

□

Now that we know how to represent \mathbf{L}_m as a Kronecker sum, we use the properties of the Kronecker sum and Kronecker product to find an exact solution to Eq. 21. Of course, since we have a linear ODE, a general solution is given by $\mathbf{x} = \exp(\mathbf{L}_m t)$, but we can say more about this solution using the eigenvalues and eigenvectors of \mathbf{L}_m .

The eigenvalues and eigenvectors of \mathbf{L}_m , can be found using the eigenvalues and eigenvectors of \mathbf{L}_1 . For $k = 1, \dots, n$, we denote the eigenvalues and eigenvectors of \mathbf{L}_1 by λ_k and \mathbf{v}_k , respectively. Now consider the vector $\mathbf{v}_{k_1 \dots k_n} := \mathbf{v}_{k_1} \otimes \dots \otimes \mathbf{v}_{k_n}$. If we multiply with \mathbf{L}_m , we get

$$\mathbf{L}_m \mathbf{v}_{k_1 \dots k_n} = \left(\sum_{i=1}^m \mathbf{I}_n \otimes \dots \otimes \mathbf{L} \otimes \dots \otimes \mathbf{I}_n \right) \cdot (\mathbf{v}_{k_1} \otimes \dots \otimes \mathbf{v}_{k_n}) \quad (30)$$

We can multiply the vector with every term in the sum and use the mixed product property to distribute the \mathbf{v}_{k_i} to get

$$\sum_{i=1}^m \mathbf{I}_n \mathbf{v}_{k_1} \otimes \dots \otimes \mathbf{L} \mathbf{v}_{k_i} \otimes \dots \otimes \mathbf{I}_n \mathbf{v}_{k_n} \quad (31)$$

Since \mathbf{I}_n is the identity matrix and \mathbf{v}_{k_i} is an eigenvector of \mathbf{L} , this is equal to

$$\sum_{i=1}^m \mathbf{v}_{k_1} \otimes \dots \otimes \lambda_{k_i} \mathbf{v}_{k_i} \otimes \dots \otimes \mathbf{v}_{k_n} \quad (32)$$

and now we can move the scalar outside the Kronecker product which leaves us with

$$(\lambda_{k_1} + \dots + \lambda_{k_m}) \cdot (\mathbf{v}_{k_1} \otimes \dots \otimes \mathbf{v}_{k_n}), \quad (33)$$

i.e. $\mathbf{v}_{k_1} \otimes \dots \otimes \mathbf{v}_{k_n}$ is an eigenvector, and $\lambda_{k_1} + \dots + \lambda_{k_m}$ is an eigenvalue of \mathbf{L}_m . This shows that every Kronecker product of m eigenvectors of \mathbf{L}_m is an eigenvector of \mathbf{L}_m . While this approach does not rule out that some of the eigenvectors found in this way are linearly dependent, a proof showing that indeed all eigenvalues of \mathbf{L}_m are obtained by this approach can be found in ref. [15].

For the sake of completeness, I state the solution to the ODE Eq. 21 in terms of eigenvalues and eigenvectors

$$\mathbf{x}(t) = \sum_{k_1 \dots k_m}^{n^m} c_{k_1 \dots k_m} e^{\lambda_{k_1 \dots k_m} t} \mathbf{v}_{k_1 \dots k_m}. \quad (34)$$

3.3 Node Distributions: Kronecker Sum Approach

We have seen how to use Kronecker products and Kronecker sums to fully describe the probability evolution of all possible states. Now we look at how to use this description to find how the distribution of m walkers on the nodes evolves.

Now, let \mathbf{S} be an $n \times n^m$ matrix whose entry at index $(j, j_1 \dots j_m)$ is the number of j_i that are equal to j or, in other words, the number of walkers in node j if walker 1 is at node v_{j_1} , walker 2 is at node v_{j_2} and so on. Then, the product

$$(\mathbf{S}\mathbf{x})_j = \sum_{j_1 \dots j_m} \mathbf{S}_{(j, j_1 \dots j_m)} x_{j_1 \dots j_m} \quad (35)$$

is equal to the expected number of walkers at node j , i.e. \mathbf{Z}_j .

So far, this does not look much simpler than before, but the matrix \mathbf{S} can be constructed using Kronecker products in a similar way to \mathbf{L}_m . If we define the matrices \mathbf{S}_i for $i = 1, 2, \dots, m$ as

$$\mathbf{S}_{i(j, j_1 \dots j_m)} = \begin{cases} 1 & , j_i = j \\ 0 & , j_i \neq j, \end{cases}$$

that is, \mathbf{S}_i is 1 for all states in which walker i is at node j , then $\mathbf{S} = \mathbf{S}_1 + \dots + \mathbf{S}_m$.

There is a nice way to write \mathbf{S}_i using Kronecker products, which is described in the following Lemma.

Lemma 3.2. *The $n \times n^m$ matrix \mathbf{S}_i can be written as*

$$\mathbf{S}_i = \mathbf{1} \otimes \dots \otimes \mathbf{I}_n \otimes \dots \otimes \mathbf{1},$$

where the tensor product has m terms, the i -th term is the $n \times n$ identity matrix and all other terms are $1 \times n$ vectors of all ones, denoted by $\mathbf{1} := (11 \dots 1)$.

Proof. By the definition of the Kronecker product

$$\begin{aligned} (\mathbf{1} \otimes \dots \otimes \mathbf{I}_n \otimes \dots \otimes \mathbf{1})_{(j, j_1 \dots j_m)} &= \mathbf{1}_{j_1} \cdot \mathbf{1}_{j_2} \cdot \dots \cdot \mathbf{I}_{n(j, j_i)} \cdot \dots \cdot \mathbf{1}_{j_m} \\ &= \mathbf{I}_{n(j, j_i)} \end{aligned}$$

Which is equal to 1, if $j_i = j$ and equal to 0, if $j_i \neq j$.

Thus, $\mathbf{S}_i = \mathbf{1} \otimes \dots \otimes \mathbf{I}_n \otimes \dots \otimes \mathbf{1}$. □

By using that $\mathbf{Z} = \mathbf{S}\mathbf{x}$, the time-evolution of \mathbf{Z} will be derived. As shown in the previous section, the state vector evolves over time as

$$\mathbf{x}(t) = \sum_{i_1 \dots i_n} c_{i_1 \dots i_n} e^{(\lambda_{i_1} + \dots + \lambda_{i_n})t} \cdot (\mathbf{v}_{i_1} \otimes \dots \otimes \mathbf{v}_{i_n}). \quad (36)$$

From above, it follows that the projection matrix \mathbf{S} has the form

$$\mathbf{S} = \mathbf{S}_1 + \dots + \mathbf{S}_m = \sum_{i=1}^m \mathbf{1}_1 \otimes \dots \otimes \mathbf{1}_{i-1} \otimes \mathbf{I}_n \otimes \dots \otimes \mathbf{1}_m$$

which is remarkably similar to the Kronecker sum. Let us now consider the product of \mathbf{S} with a single term in Eq. 36

$$\mathbf{S} \cdot c_{i_1 \dots i_n} e^{(\lambda_{i_1} + \dots + \lambda_{i_n})t} \cdot (\mathbf{v}_{i_1} \otimes \dots \otimes \mathbf{v}_{i_n}).$$

which is equal to

$$(\mathbf{S}_1 + \dots + \mathbf{S}_m) \cdot c_{i_1 \dots i_n} e^{(\lambda_{i_1} + \dots + \lambda_{i_n})t} \cdot (\mathbf{v}_{i_1} \otimes \dots \otimes \mathbf{v}_{i_n}). \quad (37)$$

Again, we look at one of the terms and use the properties of the Kronecker product to distribute the eigenvectors

$$\begin{aligned} &= (\mathbf{1} \otimes \dots \otimes \mathbf{I}_n \otimes \dots \otimes \mathbf{1}) \cdot c_{i_1 \dots i_n} e^{(\lambda_{i_1} + \dots + \lambda_{i_n})t} \cdot (\mathbf{v}_{i_1} \otimes \dots \otimes \mathbf{v}_{i_n}) \\ &= (\mathbf{1} \cdot \mathbf{v}_{i_1} \otimes \dots \otimes \mathbf{I}_n \cdot \mathbf{v}_{i_k} \otimes \dots \otimes \mathbf{1} \cdot \mathbf{v}_{i_1}) \cdot c_{i_1 \dots i_n} e^{(\lambda_{i_1} + \dots + \lambda_{i_n})t} \end{aligned} \quad (38)$$

The product $\mathbf{1} \cdot \mathbf{v}_{i_j} = \sum_{l=1}^n (\mathbf{v}_{i_j})_l$, is the sum over the components of the eigenvector \mathbf{v}_{i_j} but it can also be understood as the dot product of the left eigenvector $\mathbf{1}$ and the right eigenvector \mathbf{v}_{i_j} . If \mathbf{v}_{i_j} does not belong to the eigenvalue 0, the sum is 0. The term $\mathbf{1} \cdot \mathbf{v}_{i_j}$ is therefore 0, unless $\mathbf{v}_{i_j} = \mathbf{v}_1$. Thus, Eq. 38 is zero unless $\lambda_{i_j} = \lambda_1 = 0$ for $j \neq k$.

Now, consider the case where $\lambda_{i_j} = \lambda_1 = 0$ for $j \neq k$ and λ_{i_k} is any of the eigenvalues of \mathbf{L}_1 . Then, because $\mathbf{v}_1 = (1 \dots 1)^\top$, we have $\mathbf{1} \cdot \mathbf{v}_{i_j} = n$ for $j \neq k$ and $\mathbf{I}_n \cdot \mathbf{v}_{i_k} = \mathbf{v}_{i_k}$. In this case, Eq. 38 is thus equal to

$$n^{m-1} c_{1 \dots i_k \dots 1} e^{\lambda_{i_k} t} \cdot \mathbf{v}_{i_k}.$$

Also note that in Eq. 37, at most one of the terms of the sum is non-zero when multiplied with the eigenvector. Putting all non-zero terms together, we get

$$\mathbf{Z} = \sum_{k=1}^n \tilde{c}_k e^{\lambda_k t} \mathbf{v}_k,$$

where

$$\tilde{c}_k = n^{m-1} \cdot \sum_{k=1}^n c_{1 \dots i_k \dots 1}.$$

A comparison with Eq. 16 shows that we get the exact same solution, only that the constants are indexed differently. That these constants actually lead to a "physical" solution where probabilities are between 0 and 1 is shown in ref. [16]. Additionally, we can see that the matrix \mathbf{S}_i and the random variables Y_{ij} from section 3.1 do the same thing, that is, detecting whether a given walker is at a given node.

3.4 Node Distributions: Master Equations Approach

To end the discussion on the node distribution of independent random walks, we briefly discuss another angle that one might attempt to take, which doesn't work out in the end because it leads to a description that is not closed. It is again a master equation approach, but this time on the level of the walker distribution \mathbf{Z} . Because all approaches describe the same system, the non-closed description it should be possible to bring this description into the form found the previous sections.

Again, the random variables $Z_j(t)$ describe the proportion of walkers at node j at time t . Unlike before, we don't look at Z_j as a sum of random variables, but we work with the random variables directly. We denote by $z_{jk}(t)$ the propability that k walkers are at node j at time t , i.e. $z_{jk} = P(Z_j = k)$. Without going into the detailed derivation, we get the master equation

$$\frac{dz_{jk}}{dt} = \sum_{l=1}^n \mathbf{A}_{jl} \cdot \left[-kz_{jk} - \sum_{\tilde{k}=0}^m \tilde{k}P(\hat{Z}_j^m = k, \hat{Z}_l^m = \tilde{k}) \right. \quad (39)$$

$$\left. + (k+1)z_{jk+1} + \sum_{\tilde{k}=0}^m \tilde{k}P(\hat{Z}_j^m = k-1, \hat{Z}_l^m = \tilde{k}) \right] \quad (40)$$

As before, we are interested in the expected value $\langle Z_j \rangle = \sum_{k=0}^m \frac{k}{m} z_{jk}$ and we can use the master equation to get the derivative of $\langle Z_j \rangle$

$$\langle \dot{Z}_j \rangle = \sum_{k=0}^m \frac{k}{m} \dot{z}_{jk}. \quad (41)$$

If we substitute Eq. 39, we get

$$\sum_{k=0}^m \frac{k}{m} \sum_{l=1}^n \mathbf{A}_{jl} \cdot \left[-kz_{jk} - \sum_{\tilde{k}=0}^m \tilde{k}z_{jk,l\tilde{k}} + (k+1)z_{jk+1} + \sum_{\tilde{k}=0}^m \tilde{k}z_{jk-1,l\tilde{k}} \right], \quad (42)$$

where $z_{jk,l\tilde{k}} := P(\hat{Z}_j^m = k, \hat{Z}_l^m = \tilde{k})$. After some cancelations and rearrangements, we get

$$-\delta(v_j)\langle z_j \rangle + \sum_{l=1}^n \mathbf{A}_{jl} \sum_{k=0}^m z_{jk} \langle z_l | z_{jk} \rangle, \quad (43)$$

where $\langle z_l | z_{jk} \rangle$ is the expected value of walkers at node l , given that there are k walkers at node j . This has a very similar structure to the master equation of a single walker (Eq. 3), only the extra sum over conditional expected values. Because we already know from the last sections that both systems are described by the same dynamics, we get an equality of the form

$$\langle z_l \rangle = \sum_{k=0}^m z_{jk} \langle z_l | z_{jk} \rangle. \quad (44)$$

4 Interacting Random Walks

Now that we have seen how to study the node distribution of random walkers, we try to apply these insights to interacting random walks. This is done by considering the complete state space, for which the Kronecker product representation was described in the previous sections. While not going into much detail, we see how our previous approach fails and what still works. When considering chemical reactions, even on the level of the whole state space, the

master equation can not be described by a matrix most of the time [13]. In that case, our approach can not help us further. On the other hand, there are cases when describing the time derivative of the whole state space with a matrix is possible.

One example of such a case that we focus on is an avoiding/aggregating walk. This means that the rate at which a walker moves into a node that is already occupied by one or more other walkers is changed. In an avoiding walk this rate is reduced, while in an aggregating walk it is increased. Let us call the modified rate p .

We consider a small example of $m = 2$ walkers on $n = 3$ nodes, that nonetheless shows many interesting features that are likely present for any sizes. We denote the matrix describing the time-evolution of the avoiding/aggregating walk as \mathbf{A}_2 , so

$$\dot{\mathbf{x}} = \mathbf{A}_2 \mathbf{x}.$$

The rates where no interactions occur, for example between states x_{12} and x_{13} , are given by the corresponding entry of the matrix \mathbf{L}_2 . On the other hand, between states x_{11} and x_{12} , the rate of leaving state x_{11} to state x_{12} is unchanged, but the rate of moving from state x_{12} to state x_{11} is now different, because walker 2 moves to node v_1 which is already occupied by walker 1. The first consequence is that \mathbf{A}_2 is not symmetric. Additionally, we can see that there is still a close relation between \mathbf{A}_2 and \mathbf{L}_2 and this suggests writing

$$\mathbf{A}_2 = \mathbf{L}_2 + \mathbf{Q}. \quad (45)$$

The matrix \mathbf{Q} can be written using a sum of Kronecker products with a nice interpretation. We define the 3×3 detector matrices $\mathbf{D}_1, \mathbf{D}_2$ and \mathbf{D}_3 that in some sense detect whether a walker is in node v_1, v_2 , or v_3 . The entries of a detector matrix \mathbf{D}_j are all 0, except the j -th entry on the diagonal is equal to 1.

Suppose for example that walker 1 is in node v_1 . Then the transition rates of walker 2 into node v_1 need to be adjusted. We need to refer to the entries of the one-walker Laplacian \mathbf{L}_1 and do this by writing \mathbf{L}_{ij} . The modified transition rates can be expressed by the Kronecker product

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 & 0 \\ -(1-p)\mathbf{L}_{21} & (1-p)\mathbf{L}_{21} & 0 \\ -(1-p)\mathbf{L}_{31} & 0 & (1-p)\mathbf{L}_{31} \end{pmatrix}. \quad (46)$$

I recommend convincing yourself that adding this matrix to \mathbf{L}_2 indeed leads to the rate between state x_{12} and x_{11} being equal to p . Let us call the right matrix in the last equation \mathbf{M}_1 , describing the modified rate of moving into node v_1 if it is already occupied. By defining \mathbf{M}_2 and \mathbf{M}_3 in a similar way, we can find a description of \mathbf{Q} :

$$\mathbf{Q} = \mathbf{D}_1 \otimes \mathbf{M}_1 + \mathbf{M}_1 \otimes \mathbf{D}_1 + \mathbf{D}_2 \otimes \mathbf{M}_2 + \mathbf{M}_2 \otimes \mathbf{D}_2 + \mathbf{D}_3 \otimes \mathbf{M}_3 + \mathbf{M}_3 \otimes \mathbf{D}_3 \quad (47)$$

Since $\mathbf{L}_2 + \mathbf{Q}$ is just another matrix, the solution can be calculated. However, the eigenvalues and eigenvectors of \mathbf{L}_1 can not be used to find the eigenvalues

and eigenvectors of \mathbf{A}_2 , as we did with \mathbf{L}_2 . A perturbation analysis could likely give some insight into the behaviour when p is very close to 1. Additionally, \mathbf{Q} has a lot of structure that can likely be exploited to get a better understanding of the interacting system.

The approach can easily be extended to n nodes. When extending to more walkers, I am not quite sure whether some additional care is needed to handle different numbers of walkers that could be at a given node, but the general idea should still hold. One promising aspect of this result is that even though the number of states explodes with more nodes and walkers, growing like n^m , the number of terms in \mathbf{Q} is only nm .

5 Discussion

We have seen how CTRWs can be treated mathematically and showed that the average distribution of multiple walkers follows the same dynamics as the single walker system. To that end, multiple mathematical tools were presented that are useful in a wide range of applications. In section 4, for example, we saw how the Kronecker product could be helpful in understanding interacting random walkers.

While the treatment of interacting random walkers was only very briefly touched on and the benefit of the approach presented here remains unclear, a recent paper showed that a Kronecker product approach can lead to fast and storage-efficient algorithms for simulating epidemic models [12]. This highlights the potential of describing interacting systems with Kronecker products for studying high-dimensional systems.

The random walks that were discussed in this report are described by the graph Laplacian. While the graph Laplacian has many direct applications, replacing it by an arbitrary intensity matrix \mathbf{Q} , any discrete-space, continuous-time Markov process can be described by the ODE

$$\dot{\mathbf{y}} = \mathbf{Q}\mathbf{y}. \quad (48)$$

A description of intensity matrices and some of their properties are given in ref. [6]. Most of the derivations in this report can be applied directly to intensity matrices as well, although we need to be careful, when properties of the eigenvalues and eigenvectors of the graph Laplacian are used. For example, a general intensity matrix might have multiple 0 eigenvalues, which complicates the discussion slightly. The derivation of important properties in a more general setting is given in ref. [16].

To end this discussion, let us consider the use of random walks to create models of reality. Because of the immense complexity of the real world, it is impossible to account for the exact state of any given system. For example, as described in ref. [13], the dynamics of a chemically reacting system of N chemical species is, under the assumption of classical mechanics (so no quantum effects), a deterministic process in the full position-momentum phase space, but not deterministic when describing the system on the level of the number of

molecules of each chemical species. Another example is the spread of epidemics, where it may be possible to ascertain the (approximate) number of infected individuals but basically impossible to determine the infection state and the contacts of every single person. If only the number of infected individuals is known at some time, depending on who is infected and how well connected they are, different outcomes are possible. Thus, when a full description of a system is not available (which is effectively always the case), the possible trajectories contain fluctuations that can only be understood stochastically. In this light, random walks or more generally, stochastic processes are powerful tools for modeling systems with incomplete information.

Closely related is the additional observation that in the real world, there is often only one realisation of any given process. For instance, the number of infected people over time in an epidemic will be a single realisation of the epidemic spreading process. As noted above however, at any point in time there are multiple possible trajectories for a given number of infected individuals. Here, stochastic processes can help us understand the range of possible outcomes, while the observed trajectory only shows one outcome.

These considerations highlight the importance of incorporating stochasticity into our models of complex real world systems. Of course, the way we choose to incorporate randomness into our models will almost certainly result in other simplifications and imperfections. The large diversity of existing random walk variants then presumably stems from incorporating additional knowledge or assumptions to improve on the inevitable shortcomings of any given approach. As we have seen in this report, describing a process as a random walk allows us to determine the time evolution of the system exactly and make predictions of long term behaviour. Given a large number of random walkers moving independently on a network, we know that they will evenly distribute across the nodes. While more complicated stochastic processes can usually only be solved numerically, they still capture the whole range of possible trajectories. Thus, even though incomplete information makes it fundamentally impossible to calculate the future exactly, random walks and stochastic processes are important tools that allow us to describe and predict, at least some aspects of, the unpredictable.

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