Optimal non-Markovian search strategies

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Stochastic search processes are ubiquitous in nature and are expected to become more efficient when equipped with a memory, where the searcher has been before. A natural realization of a search process with long-lasting memory is a migrating cell that is repelled from the diffusive chemotactic signal that it secrets on its way, denoted as auto-chemotactic searcher. To analyze the efficiency of this class of non-Markovian search processes we present a general formalism that allows to compute the mean first passage time (MFPT) for a given set of conditional transition probabilities for non-Markovian random walks on a lattice. We show that the optimal choice of the $n$-step transition probabilities decreases the MFPT systematically and substantially with an increasing number of steps. It turns out that the optimal search strategies can be reduced to simple cycles defined by a small parameter set and that mirror-asymmetric walks are more efficient. For the auto-chemotactic searcher we show that an optimal coupling between the searcher and the chemical reduces the MFPT to $1/3$ of the one for a Markovian random walk.

The term search processes encompasses all phenomena in which an agent scans a domain, looking for a target to reach. Search for preys and/or wild food resources by animals, known as foraging \cite{1,2}, is one of the major examples of such processes. They can take various forms (blind or guided, individual or collective, random or deterministic, ...), but they all aim at being efficient, that is at minimizing the overall cost of the searching process. Several definitions for such a cost exist depending on the context, but it often simply reduces to the total duration of the search. In terms of statistical physics, the efficiency is usually quantified using first-passage time distributions: given all possible trajectories of the process considered, what is the probability that the agents will find the target in a certain amount of time? Optimizing the search efficiency therefore translates into minimizing of the first-passage time. The main statistical estimate is the mean first passage time (MFPT) although there are situations in which the whole FPT distribution is relevant \cite{4,5}.

Many biological organisms, from bacteria to mammals, have evolved in such a way that their searching strategies are optimized in a certain way \cite{6}. Modeling these phenomena in quantitative terms is a challenge that has motivated many of recent studies. Recently, various ways to transform simple blind random walks into efficient search processes have been suggested. Among other works, Bénichou and co-workers have e.g. shown that alternating periods of diffusive and ballistic motion can dramatically reduce first-passage times \cite{3,8}, and this strategy has actually been observed in various animal species. Other effects such as the impact of confinement \cite{1-3,10} or the topology of the scanned domain \cite{11}, have also been studied in different contexts.

Memory of a stochastic process is also expected to affect the MFPT \cite{12-16}. A natural realization of a search process with a long-lasting memory is a migrating cell that is repelled from the diffusive chemotactic signal that it secrets on its way, denoted as auto-chemotactic searcher. Chemotaxis, a process in which a migrating cell changes its motion direction due to a chemical gradient of a chemical cue in its immediate surrounding, has been extensively studied, by biologists as well as chemists and physicists \cite{17,28}, and is, for instance, used by immune cells to guide themselves towards areas of infection or to tumors \cite{29}. Experimental as well as theoretical studies of auto-chemotaxis are currently intensively studied in biophysics as it can help to understand the efficiency of a variety of biological processes \cite{30,50}. Mathematically, these search processes are non-Markovian since the searcher uses the chemical information it has released along its past path in order to move ahead.

A systematic study of the first passage properties of stochastic non-Markovian search processes with $n$-step memory has not been performed yet, which is what we will present here: we will analyze the efficiency of non-Markovian search processes in general and of the auto-chemotactic in particular, and present results for the optimal search strategies. We first introduce a general formalism that allows to compute the MFPT for a given set of conditional transition probabilities for non-Markovian random walks on a lattice, which is based on the backward equation for the MFPT and on the conditional probability for the walker to go in a certain direction given its $n$ past directions. Then we use this formalism to determine for a given $n$ the optimal conditional transition probabilities that minimize the MFPT. Finally we analyze the search efficiency of the auto-chemotactic walker and determine the optimal coupling of the searcher to the self-generated chemotactic concentration field.

In this letter we consider a minimal model for a non-Markovian searcher: a random walk on a discrete lattice of lateral size $L$ and with transition probabilities depending on the steps it made before. Formally this stochastic process is defined by the hierarchy of conditional tran-
We assumed periodic boundary conditions, which allows us to consider the backward equation of motion for the average first-passage time of a target that is placed at the center of the domain and that the jump directions of the last \( n \) steps. This allows us to write a backward equation of motion for the average first-passage time \( T_n(r, r_T; e_0, \ldots, e_{n-1}) \) to reach the target at position \( r_T \) for a walker starting at position \( r \) with \( n \) past directions \( \{e_0, \ldots, e_{n-1}\} \):

\[
T_n(r, r_T; e_0, \ldots, e_{n-1}) = 1 + \sum_k p_k(e_k | e_0, \ldots, e_{n-1}) T(r + e_k, r_T; e_1, \ldots, e_{n-1}, e_k)
\]

The sum runs over all \( z \) nearest neighbor sites the walker can jump to, with \( z \) the coordination number of the lattice. A sketch of equation (1) is shown in figure [1]. We assumed periodic boundary conditions, which is equivalent to an infinite lattice with periodically arranged targets. In addition, equation (1) also holds for reflecting boundary conditions if one assumes that the target is placed at the center of the domain and that the probabilities \( p_k(e_k | e_0, \ldots, e_{n-1}) \) are mirror-symmetric as we discuss in more detail below. Finally, eqn. (1) is obviously not correct if \( r = r_T \), for which the average passage-time is trivially 0. In this case, the right-hand side yields the average return time on the site \( r_T \), equal to \( V \) [37]. By applying a discrete Fourier transformation \( f(q) = \sum r \in \mathbb{Z} f(r) e^{-iqr} \) with \( q_i = 2\pi n_i / L \) and \( n_i \in [0, L-1] \), and properly accounting for the case \( r = r_T \), a closed set of linearly coupled equations for \( \tilde{T}_n(q, r_T; e_0, \ldots, e_{n-1}) \) for all possible paths \( \{e_0, \ldots, e_{n-1}\} \) is obtained, which can be cast into a matrix equation.

Let \( s_n \) be a vector of size \( z^n \) containing all possible paths \( \{e_0, \ldots, e_{n-1}\} \), and \( \tilde{t}_n \) a vector of equal size whose entries are defined as \( \tilde{t}_n(q, r_T) = T_n(q, r_T; s_{n\alpha}) \). The solution of the matrix equation then is

\[
\tilde{t}_n(q, r_T) = V \left[ \delta(q) - e^{-iqr_T} \right] (I - P_n E_n(q))^{-1} u_n
\]

Here \( u_n \) is a vector of size \( z^n \), all entries of which are equal to 1, \( E_n(q) \) is a square diagonal matrix whose elements are the complex exponentials \( e^{i\mathbf{q} \cdot \mathbf{e}_k} \), and \( P_n \) is a square matrix containing all conditional probabilities \( p(e_k | e_0, \ldots, e_{n-1}) \). Note that this matrix has only \( z^{n+1} \) non-zero elements, whose positions in the matrix depend on the ordering of the vector \( s_n \) [38].

Fourier inversion and averaging over all possible initial positions yields

\[
\langle t_n \rangle = \sum_{q \neq 0} (I - P_n E_n(q))^{-1} u_n
\]

The mean first-passage time is finally computed by summing all entries of this averaged vector \( \langle t \rangle \), weighted by the probability of the respective paths. These weights are found using the identity

\[ p(e_0, \ldots, e_{n-1}) = \sum_{i=1}^{z^n} p(e_0, \ldots, e_{n-1}) p(e_{i-1}, \ldots, e_{i-2}) \]

with the normalization constraint

\[ \sum_{i=1}^{z^n} p(e_0, \ldots, e_{n-1}) = 1. \]

These equations can again be cast into a matrix form \( M_n p_n = v_n \). Here, \( p_n \) is a vector containing all entries of \( p(e_0, \ldots, e_{n-1}) \). \( M_n \) is equal to \( I - P_n \) except for the last row, all elements of which are 1. Finally \( v_n \) is a vector containing only zeros except the last element being 1. The mean first-passage time is therefore obtained as the dot product \( \langle T_n \rangle = p_n \cdot \langle t_n \rangle \). This general formalism allows to infer the mean first-passage time of any non-Markovian random walk, provided the \( n \)-step conditional probability \( p(e_k | e_0, \ldots, e_{n-1}) \) is known [39].

One intuitively expects that the number of steps \( n \) kept in memory has a major impact on the search efficiency. As the case \( n = 0 \) consists in a blind random walk, the asymptotic case \( n \to \infty \) corresponds to a walk where the walker remembers all the sites it has visited and could thus elaborate a strategy to never visit twice the same site. To quantify this effect, one determines the optimal search strategy that maximizes the search efficiency for a certain value of \( n \) by finding the set of conditional probabilities \( p(e_k | e_0, \ldots, e_{n-1}) \) that minimizes the MFPT. For a lattice with coordination number \( z \), using the normalization constraint and assuming isotropic walks, this consists in finding the global minimum of a function of \( z^{n-1}(z-1) \) variables. Using a method of coordinate descent with constraint [42] for the MFPT optimization we obtain for a square lattice (\( z=4 \)):

- For \( n = 1 \), the optimal search strategy is found to be mirror-symmetric. More specifically, the probabilities \( p_l \) and \( p_r \) of turning left or right are found to be equal, while the probability of going forward is given by \( p_f = q_0^{(1)} = 1 - 2p_{l,r} \). The optimal 1-step
memory process is therefore found to prevent from going backward. Note that $q_0^{(1)}$ depends on the system size $L$ and approaches 1 as $L \to \infty$.

- For $n = 2$, the optimal strategy is mirror-asymmetric and follows the diagram shown in figure 2. Only one step in the cycle is chosen probabilistically, with probability $q_0^{(2)}$ that also depends on the system size. The resulting MFPT turns out to be much lower than the optimal 1-step memory process, as it is reduced by a factor $\sim 0.75$.

If mirror-symmetry is imposed, the optimal search process is governed by two parameters, $q_0^{(2)}$ and $q_0^{(1)}$. However this constraint makes the MFPT almost equal to the 1-step case.

- For $n = 3$, the optimal strategy is again mirror-asymmetric and governed by only one probabilistic parameter $p_0^{(3)}$. The corresponding diagram is shown in figure 2 and the MFPT is again reduced by a factor $\sim 0.86$ with respect to $n = 2$.

In all these cases, the MFPT scales proportionally to $L^2$ as $L \to \infty$. For $n > 3$, the minimization procedure becomes computationally expensive, but nothing indicates that mirror-symmetric search strategies would become more favorable. In the limit of infinite memory, the optimal strategy can be simply guessed. For $n \geq L^2$, the walker can in fact simply scan all sites by going row by row, which is a highly mirror-asymmetric process for which the MFPT would be equal to $(L^2 - 1) / 2$. These results prove that memory can be useful to enhance the search efficiency of random walks. Such effects, although they might not be perfectly optimized, actually exist in some real systems, such as e.g. chemotactic walks.

Next we consider the auto-chemotactic searcher, and focus on chemo-repulsive searcher-cue interactions since they avoid repeated visits of already scanned areas and thereby increasing the search efficiency. A simple lattice model for an autochemorepulsive walk can be constructed as an adaptation of the true self-avoiding walk with chemical diffusion 44, 45. A concentration field $c$ is defined on the lattice, and diffuses at each time step according to a discretized diffusion equation, with diffusion constant $D_c$. After the diffusive step, the searcher moves from site $i$ to site $j$ with probability

$$p_{i \to j} = \left[ 1 + \sum_{k \neq j} \exp \left( -\beta (c_i - c_j) \right) \right]^{-1}$$

where the sum runs over all neighbors of $i$, except $j$. Here, $\beta$ quantifies the coupling between the walker and the concentration field: for $\beta \to 0$, the process reduces to a unbiased blind random walk, while the limit $\beta \to \infty$ corresponds to the case where the walker always jumps to the neighboring site with the lowest concentration. Finally, once the walker has jumped to the site $j$, it adds an amount $\delta c$ to the concentration field at this site.

**FIG. 2:** Optimal search strategies on a 2-dimensional lattice for $n = 1, 2, 3$ (left panel). In the diagrams, the sum of all arrows coming out of one box is equal to 1, therefore only the necessary coefficients are shown and all others can be deduced from the normalization constraint. The corresponding MFPT normalized by the MFPT for a blind random walk 40, together with the optimal parameters in the inset, are shown as a function of the system size (right panel). For comparison, the optimal MFPT found by Tejedor et. al in 41 is plotted.
shows the mean first-passage time of the au-

tional probability

corporation to diffuse away, without source, to

However, as \( \beta \) gets larger, the MFPT abruptly increases. This effect can be understood as fol-

Because the profile of the concentration field at a cer-

tain time depends on the entire path of the walker, this

model is obviously a non-Markovian process. However, inferring a conditional probability \( p(\mathbf{e}_k|\mathbf{e}_{i_0},\cdots,\mathbf{e}_{i_{n-1}}) \) is not straightforward as this quantity would be exactly de-

finite only for \( n \to \infty \). \( \mathbf{e}_i \) is found by explic-

itly computing the concentration field generated by the

walk \( \{\mathbf{e}_{i_0},\cdots,\mathbf{e}_{i_{n-1}}\} \), starting from an initially empty

field. Constructing the entire matrix \( \mathbf{P}_n \) might become computationally expensive for large values of \( n \), but relatively low values of \( n \) can still predict the qualitative behavior of the MFPT.

Figure 3 shows the mean first-passage time of the au-

tochemorepulsive walk for a 2-dimensional lattice of size

\( L = 100 \), using the formalism presented in this paper,

together with simulation results (each point accounts for

\( 10^4 \) trajectories [41]). From both theory and simulations,

it appears clearly that for a certain value of \( D_c \), there

exists an optimal value for \( \beta \) that minimizes the search

time. At low values of \( \beta \) the MFPT slowly decreases as

the process goes from a blind random walk to a smarter

walk in which the chemical information from the envi-

ronment is used. However, as \( \beta \) gets larger, the MFPT

abruptly increases. This effect can be understood as fol-

Figure 3: MFPT as a function of \( \beta \) for an

autochemorepulsive walk, with \( D_c = 0.1 \), from

simulation (full line with error bars were computed via

Jackknife re-sampling [42]) and theory for various

values of \( n \) (dotted lines). Inset: sketch of the

auto-chemorepulsive searcher. Size of the arrows

correspond to \( p_{i\rightarrow j} \), color code to concentration values

of \( c_j \).

Figure 4 shows the mean first-passage time of the au-

tochemorepulsive walk for a 2-dimensional lattice of size

\( L = 100 \), using the formalism presented in this paper,

together with simulation results (each point accounts for

\( 10^4 \) trajectories [41]). From both theory and simulations,

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the process goes from a blind random walk to a smarter

walk in which the chemical information from the envi-

ronment is used. However, as \( \beta \) gets larger, the MFPT

abruptly increases. This effect can be understood as fol-

Figure 4: Persistence length for the autochemotactic walk

as a function of \( \beta \). The limit value \( l_p^{(0)} = 4/3 \) is

subtracted. Discrepancies between theory (dotted lines)

and simulations (full lines) as \( \beta \to \infty \) are mostly

finite-size effects.

nows : after the walker has jumped to a certain site, and

because it has released some cue behind it, the chemical

collection is expected to be lower on the forward site

than on the left and right sites, and even more than on the

backward site. For large values of \( \beta \), as the walker

jumps on the neighboring site with the lowest collection

with probability \( p \sim 1 \), it will thus tend to go for-

ward, and so over very long distances, turning its motion

into an almost ballistic behavior. Fully ballistic trajecto-

ries are obviously not efficient for a search process, which

we observe here with the very large values for the MFPT

for \( \beta \to \infty \). The persistence length \( l_p \), defined as the

mean number of consecutive steps in the same direction,

can in particular be calculated to quantify this effect. By

noting \( p_n \) the probability of continuing forward after \( n \)

steps in the same direction, it holds

\[
l_p = \sum_{n=1}^{\infty} n(1-p_n) \prod_{k=1}^{n-1} p_k
\]

Now, consider a walker that has changed its direction at

the previous step \( t_0 \). Although it will not be exact, the

probabilities \( p_n \) can be estimated by neglecting the con-

tribution of \( c(t_0) \) and only considering the contribution

of the newly deposited chemical. With such assumption,

\( p_n \) is of the form \( p_n^{-1} = 1 + \sum_{i=1}^{3} \exp \left( -\beta \sum_{j=0}^{n} \alpha_{ij} D_{ij} \right) \).

For relatively low values of \( D_c \), the sum in the exponen-

tial factor can be truncated to the second order. This

approximation yields in particular \( p_n = p_3 \) for \( n \geq 3 \),

and, after some algebra

\[
l_p = 1 + p_1 \left( 1 + \frac{p_2 p_3^{-1}}{p_3 - 1} \right)
\]

This approximate result only holds for low values of \( D_c \)

and assumes that the system resets its memory before

every turn. Nevertheless, it provides a good estimate of
the persistence length, consistent with simulation data, as shown in figure 3. This analysis confirms that the walker’s persistence length strongly increases for large values $\beta$. To optimize its search, an autochemotactic particle must find the right balance between a blind search that makes use of no chemical information and a strong coupling with the cue that makes it go in a straight line.

The results presented in this letter clearly indicate that non-Markovian features of search processes can be tuned in order to maximize search efficiency. Optimal search strategies are found to be mirror-asymmetric and more efficient with longer memory. However, search processes in nature are not necessarily as optimal, but the physical parameters that govern them can still be adjusted to improve efficiency. The formal and systematic tool introduced in this paper should be useful for other biologically relevant applications, many of which present non-negligible non-Markovian effects.

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See appendix C of the supplemental material.

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An animation of a simulated trajectory is available as a supplemental material.
Appendix A - Matrix structures

We show the structure of the matrix $\mathbf{P}_n$, that is at the core of our formalism. As explained in the main text, we first need to cast all possible paths $\{e_{i_0}, \ldots, e_{i_{n-1}}\}$ into a vector $s$ of size $z^n$. The most intuitive way to perform this operation is to vary hierarchically the directions in the path as one go from one entry of the vector to the next. Noting the unit vectors $\mathbf{e}_0, \ldots, \mathbf{e}_{z-1}$, a natural sorting would be as follows

\[
\begin{align*}
  s_0 &= \{ \mathbf{e}_0, \mathbf{e}_0, \cdots, \mathbf{e}_0, \mathbf{e}_0 \} \\
  s_1 &= \{ \mathbf{e}_0, \mathbf{e}_0, \cdots, \mathbf{e}_0, \mathbf{e}_1 \} \\
  &\vdots \\
  s_{z-1} &= \{ \mathbf{e}_0, \mathbf{e}_0, \cdots, \mathbf{e}_0, \mathbf{e}_{z-1} \} \\
  s_z &= \{ \mathbf{e}_0, \mathbf{e}_0, \cdots, \mathbf{e}_1, \mathbf{e}_0 \} \\
  s_{z+1} &= \{ \mathbf{e}_0, \mathbf{e}_0, \cdots, \mathbf{e}_1, \mathbf{e}_1 \} \\
  &\vdots \\
  s_{z^n-2} &= \{ \mathbf{e}_{z-1}, \mathbf{e}_{z-1}, \cdots, \mathbf{e}_{z-1}, \mathbf{e}_{z-2} \} \\
  s_{z^n-1} &= \{ \mathbf{e}_{z-1}, \mathbf{e}_{z-1}, \cdots, \mathbf{e}_{z-1}, \mathbf{e}_{z-1} \}
\end{align*}
\]

Using this ordering, the matrix $\mathbf{P}_n$ has the structure

\[
\mathbf{P}_n = \begin{pmatrix}
  \mathbf{P}_n^{(0)} \\
  \vdots \\
  \mathbf{P}_n^{(z^n-1)}
\end{pmatrix}
\]

where each submatrix $\mathbf{P}_n^{(i)}$ is of size $z \times z^n$ and is of the form

\[
\mathbf{P}_n^{(i)} = \begin{pmatrix}
  \mathbf{P}_n^{(i,0)} & 0 & \cdots & 0 \\
  0 & \mathbf{P}_n^{(i,1)} & \cdots & \vdots \\
  \vdots & \cdots & \ddots & 0 \\
  0 & \cdots & 0 & \mathbf{P}_n^{(i,z-1)}
\end{pmatrix}
\]

Here, each matrix $\mathbf{P}_n^{(i,j)}$ is a row matrix with $z$ columns, namely

\[
\mathbf{P}_n^{(i,j)} = (p(e_{i_0}|s_{\alpha(i,j)}) \cdots p(e_{z-1}|s_{\alpha(i,j)}))
\]

where $\alpha(i, j) = iz + j$. The non-zero elements of these matrices can be gathered into matrices $\mathbf{Q}_n^{(i)}$ of the form

\[
\mathbf{Q}_n^{(i)} = \begin{pmatrix}
  \mathbf{P}_n^{(i,0)} \\
  \vdots \\
  \mathbf{P}_n^{(i,z-1)}
\end{pmatrix}
\]

For isotropic walks, all matrix $\mathbf{Q}_n^{(i)}$ contain exactly the same elements in different orders such that the matrix $\mathbf{Q}_n^{(0)}$ is the building block of the formalism. More precisely, the matrix $\mathbf{Q}_n^{(i)}$ contains all probabilities $p(e_{i_0}|e_{i_0}, \cdots, e_{i_{n-1}})$ with $i_0 = i$. To draw a connection between different values of $i$, consider $\mathbf{R}$ a transformation that maps the lattice onto itself. It holds

\[
p(e_{i}|e_{i}, \cdots, e_{i_{n-1}}) = p(\mathbf{R}e_{i}|e_{i}, \cdots, e_{i_{n-1}})
\]

Now, let $\mathbf{R}_j$ be a transformation such that $e_j = \mathbf{R}_j e_0$:

\[
p(e_{i}|e_{i}, \cdots, e_{i_{n-1}}) = p(\mathbf{R}_j e_{i}|e_{i}, \cdots, e_{i_{n-1}})
\]
This identity allows to relate the elements of $Q_n^{(i)}$ to those of $Q_n^{(0)}$.

As an example, consider a 2-dimensional square lattice. There are $z = 4$ unit vectors $e_k$ (with the convention $e_{k+z} = e_k$), and the transformations $R_j$ can be defined as $R_j = R_0^j$ where $R_0$ is a $90^\circ$-rotation. Moreover, we have $R_j e_k = e_{k+j}$. This yields

$$p(e_k | e_i, e_{i_1}, \ldots, e_{i_{n-1}}) = p(e_{k-i} | e_0, e_{i_1-i}, \ldots, e_{i_{n-1}-i})$$

(10)

Defining $\sigma'_i = \sum_{j=1}^{n-1} (|i_j - i| \mod z) z^{n-j-2}$, this identity can be transformed to relate matrix elements of $Q_n^{(i)}$ to those of $Q_n^{(0)}$, namely

$$Q_n^{(i)} \sigma'_{i,k} = Q_n^{(0)} \sigma'_{i,(k-i) \mod z}$$

Finally, note that because the matrix $E(q)$ is a diagonal matrix, the structure of the matrix $P_n E(q)$ will be similar as the one of $P_0$.

**Appendix B - Computational cost**

In the formalism proposed in this paper, the MFPT is found by a matrix inversion. In particular, one inversion must be performed per each possible value of $q$. Given that the computational cost of the inversion of a matrix of size $n \times n$ is proportional to $n^3$, the scaling of our computational method should as $t_{CPU} \sim L^d z^{3n}$. For large values of $n$, this might become particularly expensive. This can be dealt with by rewriting the problem in a different way and using an approximate method for the matrix inversion.

As explained in the main text, the MFPT can be written as a dot product $p_n \cdot \langle t_n \rangle$, with $p_n = M^{-1}_n v_n$ and $\langle t_n \rangle = \sum_{q \neq 0} (I - P_n E_n(q))^{-1} u_n$. Let us now write this as

$$\langle T_n \rangle = \sum_i p_{ni} \langle t_{ni} \rangle$$

$$= \sum_{q \neq 0} \sum_i \sum_{j,k} \left[(I - P_n E_n(q))^{-1}\right]_{ij} (M^{-1}_n)_{kj} u_{nj} v_{nk}$$

$$= \sum_{q \neq 0} \sum_{j,k} u_{nj} v_{nk} \sum_i \left[(I - P_n E_n(q))^{-1}\right]_{ij} (M^{-1}_n)_{jk}$$

By noting $H_n(q) = M^T_n (I - P_n E_n(q))$ we obtain

$$\langle T_n \rangle = \sum_{q \neq 0} \sum_{j,k} u_{nj} v_{nk} (H_n(q))^{-1}_{jk}$$

Now, we use $u_{nj} = 1$ for any $j$, and $v_{nk} = \delta_{k,z^{n-1}}$ and find

$$\langle T_n \rangle = \sum_{q \neq 0} \sum_{j} (H_n(q))^{-1}_{j,z^{n-1}}$$

The MFPT is therefore equal to the sum of the elements of the last column of the inverse of $H_n$. If the matrix size $z^n$ is not too large, the matrix can be entirely inverted without much effort. However, this procedure becomes very expensive for large matrices. As one only needs one column of the matrix $H^{-1}_n$, one could use approximate methods to estimate specific matrix elements. This is what Bai et al. proposed in ref. [?], in which the authors provide an algorithm to come up with upper an lower bounds for specific elements of matrix inverses without having to invert the matrix entirely.

**Appendix C - Minimization algorithm**

In order to find the optimal algorithm for an $n$-step search process, we have applied a coordinate-descent minimization procedure with constraint. In our formalism, the MFPT $T$ is a function of the conditional probabilities $p(e_k | e_i, \ldots, e_{i_{n-1}})$. Because of rotational symmetry, there are $N = z^n$ different such coefficients. In addition, it holds $\sum_{k=0}^{z-1} p(e_k | e_i, \ldots, e_{i_{n-1}}) = 1$, which consists in a set of constraints. Let us now order all these coefficients in a vector $x = \{x_0, \ldots, x_{N-1}\}$, and minimize the function $T(x)$ following algorithm[??]. This procedure is repeated many times, always starting from a different initial guess in order to distinguish local minima from the global minimum.
Initialize $x$ randomly, ensuring $\forall j \in [0, N - 1], \sum_{i=j}^{(j+1)z-1} x_i = 1$;

while $\Delta T > \epsilon$ do

$\chi \leftarrow \text{random permutation of } [0, N - 1]$;

for $i \in [0, N - 1]$ do

$j \leftarrow \chi_i$;

$k_0 \leftarrow z \left\lfloor \frac{j}{z} \right\rfloor$;

choose randomly $k \in [k_0; k_0 + z] \setminus \{j\}$;

$s \leftarrow \sum_{k'=k_0}^{k_0+z} x_{k'} - x_j - x_k$;

$x_j \leftarrow \text{argmin}_y T(x_0, \ldots, x_{j-1}, y, x_{j+1}, \ldots, x_{k-1}, 1 - y - s, x_{k+1}, \ldots, x_{N-1})$;

$\Delta T = |T_0 - T(x)|$;

$T_0 \leftarrow T(x)$;

end for

end while

Algorithm 1: Random-order coordinate-descent with constraint