walkr

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Abstract The `walkr` package samples points using random walks from the intersection of the N simplex with M hyperplanes. Mathematically, the sampling space is all vectors x that satisfy $Ax = b$, $\sum x = 1$, and $x_i \geq 0$. The sampling algorithms implemented are hit-and-run and Dikin walk, both of which are MCMC (Monte-Carlo Markov Chain) random walks. `walkr` also provide tools to examine and visualize the convergence properties of the random walks.

Introduction

Consider all possible vectors x that satisfy the underdetermined matrix equation $Ax = b$, such that every component of x is ≥ 0 and sum to 1. How do we generate a diverse sample of such x's? The `walkr` package uses MCMC (Monte-Carlo Markov Chain) random walks to generate such a sample.

`walkr` contains two MCMC random walks. Our first random walk is hit-and-run. Hit-and-run is a widely used MCMC sampling method that guarantees uniform sampling asympotically, but mixes slower and slower as the dimensions of A increase. Our second random walk is the Dikin Walk. Dikin Walk generates a nearly uniform sample and exhibits much stronger mixing.

`walkr` also provides statistical diagnostics of the mixing and convergence properties of a MCMC random walk.

Mathematical Background of Sampling Space

In this section, we go through the mathematical background of the space from which we are sampling – the intersection of the N-simplex and hyperplanes. The reader does not need to read this section in order to use our package or understand the sampling algorithms. However, this section should provide the reader a better sense of what the sample space is geometrically and mathematically.

1) $\mathbf{Ax = b}$ represent a system of M linear equations with N variables ($M \ll N$). Hence, A is a $M \times N$ matrix (M variables and N constraints), x is a $N \times 1$ vector, and b is a $M \times 1$ vector. Every row in A represents a hyperplane in $\mathbb{R}^N$.

2) The N-dimensional unit simplex (N-Simplex) is described by:

$$x_1 + x_2 + x_3 + ... + x_N = 1$$
$$x_i \geq 0$$

Sampling space: simple 3D case

Let's begin with the simplest case – one linear constraint in 3 dimensional space.

$$x_1 + x_3 = 0.5$$

We can express this in terms of matrix equation $Ax = b$, where:

$$A = \begin{bmatrix} 1 & 0 & 1 \end{bmatrix}, \quad b = 0.5, \quad x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

In addition, we require the solution space to be intersected with the 3D simplex:

$$\sum x_i = 1$$
$$x_i \geq 0$$

In the following graph, we draw the intersection of the two. The orange equilateral triangle represents the 3D simplex, and the blue rectangle represents the plane $w_1 + w_3 = 0.5$. The intersection of the hyperplane (blue) with the simplex (orange) is the red line segment, which is our sampling space.

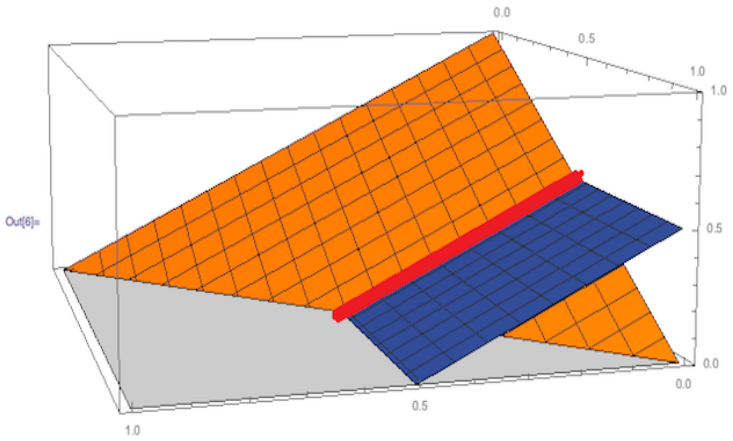


Figure 1: The sampling space is the line segment (red), which is the intersection of the 3D simplex (orange) and a hyperplane (blue)

Matrix Representation of Multiple Hyperplanes

Every hyperplane is described by one linear equation. Thus, a system of linear equations is the intersection of hyperplanes. In general, if we have M linear equations and N variables, then $Ax = b$ would look like:

$$A_{M\times N} = \underbrace{\left[\begin{array}{c} \cdots \end{array}\right]}_{\text{N columns (variables)}} \Big\} \text{M rows (constraints)}$$

Again, b is a $M \times 1$ vector, and x is a $N \times 1$ vector.

4D space

Just like how the 3D simplex is a 2D surface living in 3D space, the 4D simplex (i.e. $x_1 + x_2 + x_3 + x_4 = 1$, $x_i \geq 0$) could be viewed as a 3D object. Specifically, the 4D simplex is the following tetradhedron when viewed from 3D space, with verticies $(1,0,0,0)$, $(0,1,0,0)$, $(0,0,1,0)$, and $(0,0,0,1)$.

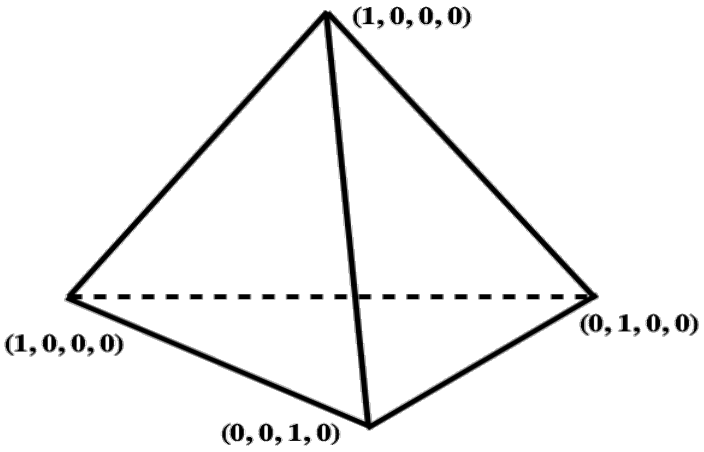


Figure 2: 4D Simplex Can Live in 3D Space

Now imagine the intersection of the 4D simplex with one hyperplane in 4D (1 equation, or 1 row in $Ax = b$). For a specific A and b, we demonstrate the intersection in the figure below. The resulting shape is a trapezoid in 4D space.

$$A = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 22 & 2 & 2 & 37 \end{bmatrix}, \quad b = \begin{bmatrix} 1 \\ 16 \end{bmatrix}$$

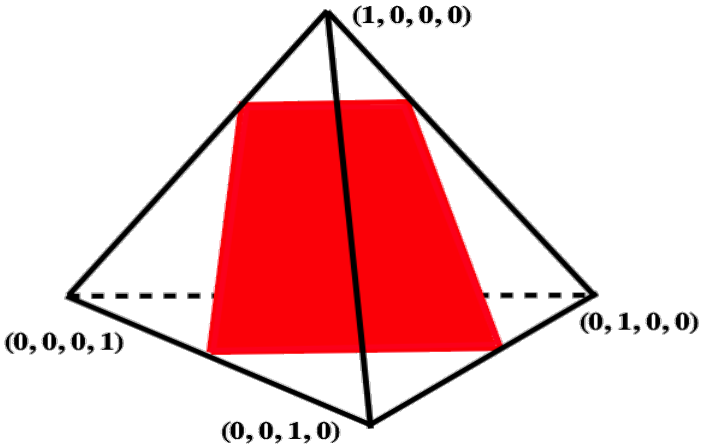


Figure 3: Intersection of a 4D Simplex and a Hyperplane

In higher dimensions, the same logic applies. Each row in $Ax = b$ is a hyperplane living in $\mathbb{R}^N$ (given N variables). Thus, geometrically, our sampling space is: **the intersection of hyperplanes with the N-simplex**.

From $Ax = b$ and the N-simplex to $Ax \leq b$

Our sampling space is bounded (i.e. has finite volume in $\mathbb{R}^N$). More formally, our sampling space is known as a **convex-polytope** in $\mathbb{R}^N$. Convex-polytopes are commonly described in the literature by a generic $Ax \leq b$. Here, we present a simple linear transformation which transforms the intersection of $Ax = b$ and the N-simplex to the form $Ax \leq b$.

First, note that the equality part of the simplex constraint ($\sum x = 1$) could be added as an extra row in $Ax = b$

$$A = \begin{bmatrix} & ..... & \\ & ..... & \\ & ..... & \\ 1 & 1 & ..... & 1 & 1 \end{bmatrix}, \quad b = \begin{bmatrix} ... \\ ... \\ ... \\ 1 \end{bmatrix}$$

Second, to find the complete solution to the new $Ax = b$ (i.e. the set of all possible x's that satisfy $Ax = b$), we must find the Null Space of A(all x's that satisfy $Ax = 0$), then add on any particular solution to $Ax = b$ (This procedure can be found in any Linear Algebra textbook).

Mathematically, if the original A was $M \times N$, then after adding on the extra row from the simplex, the basis vectors, each with N components, which span the Null Space of our new A will be:

$$\left\{ v_1, \quad v_2, \quad v_3, \quad ..... \quad , \quad v_{N-(M+1)} \right\}$$

Using any particular solution, $v_{particular}$, the complete solution to the new $Ax = b$ will be

$$\left\{ v_{particular} + \alpha_1 v_1 + \alpha_2 v_2 + \alpha_3 v_3 + ... + \alpha_{N-(M+1)} v_{N-(M+1)} \quad | \quad \alpha_i \in \mathbb{R} \right\}$$

Lastly, we tag on the $x_i \geq 0$ constraints, and with some algebraic manipulations:

$$v_{particular} + \alpha_1 v_1 + \alpha_2 v_2 + \alpha_3 v_3 + ... + \alpha_{N-(M+1)} v_{N-(M+1)} \quad \geq \begin{bmatrix} 0 \\ 0 \\ ... \\ ... \\ ... \\ 0 \end{bmatrix}$$

$$\alpha_1 v_1 + \alpha_2 v_2 + \alpha_3 v_3 + ... + \alpha_{N-(M+1)} v_{N-(M+1)} \quad \geq -v_{particular}$$

$$V\alpha \geq -v_{particular}, \quad \text{where:} \quad V = \begin{bmatrix} v_1 & v_2 & ... & v_{N-(M+1)} \end{bmatrix}, \quad \alpha = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ ... \\ \alpha_{N-(M+1)} \end{bmatrix}$$

And finally, we arrive at the form $Ax \leq b$.

$$-V\alpha \leq v_{particular}$$

We have performed a **transformation** from "x-space" (coordinates described by $x_1, x_2, ...$) to "α-space" (coordinates described by $\alpha_1, \alpha_2, ...$). The geometric object described is still the same convex polytope. In fact, `walkr` internally performs this transformation, samples the α's, maps them back to "x-space, and then returns the sampled points.

The user need not be concerned with this transformation affecting the uniformity or mixing properties of our MCMC sampling algorithms. This is because the transformation above is an affine transformation, which preserves uniformity. Simply put, sampling in either space is equivalent.

Having understood that the intersection of $Ax = b$ with the unit-simplex is a convex polytope, we are ready to dive into the core of `walkr` – MCMC random walks.

Random Walk: How to pick starting points?

MCMC random walks need a starting point, x_0, in the interior of the convex polytope. `walkr` generates such starting points using linear programming. Specifically, the `lsei` function of `limSolve` finds x which:

$$\begin{aligned} \text{minimizes} \quad & |Cx - d|^2 \\ \text{subject to} \quad & Ax \leq b \end{aligned}$$

Thus, we randomly generate C and d obtaining x which satisfy $Ax \leq b$. We discovered that the x's generated this way fall randomly on the boundaries of our convex polytope, due to the minimizing property of linear programming. Thus, we repeat this for say, 10 times, and then take an average of the x's generated. This averaged point is x_0, our starting point.

Random Walk: Hit-and-run

The hit-and-run algorithm is as follows:

1. Set starting point x_0 as current point
2. Randomly generate a direction $\vec{d}$. If we are in N dimensions, then d will be a vector of N components. Specifically, d is a uniformly generated unit vector on the N dimensional unit-sphere
3. Find the chord S through x_0 along the directions $\vec{d}$ and $-\vec{d}$. We find end points s_1 and s_2 of the chord by going through the rows of $Ax_0 \leq b$ one by one, setting the inequality to equality (so we hit the surface). Then, parametrize the chord along x_0 by $s_1 + t(s_2 - s_1)$, where $t \in [0,1]$
4. Pick a random point x_1 along the chord S by generating t from `Uniform[0,1]`
5. Set x_1 as current point
6. Repeat algorithm until number of desired points sampled

Here is a picture of the hit-and-run algorithm:

Random Walk: Dikin Walk

Preliminary Definitions

Recall, our sampling space is a convex polytope. We call this convex polytope K, which can be described in the form $Ax \leq b$.

For the definitions below, let a_i represent a row in A, x_i, b_i represent the i^{th} element of x and b. Also recall that A is a $M \times N$ matrix.

Log Barrier Function ϕ:

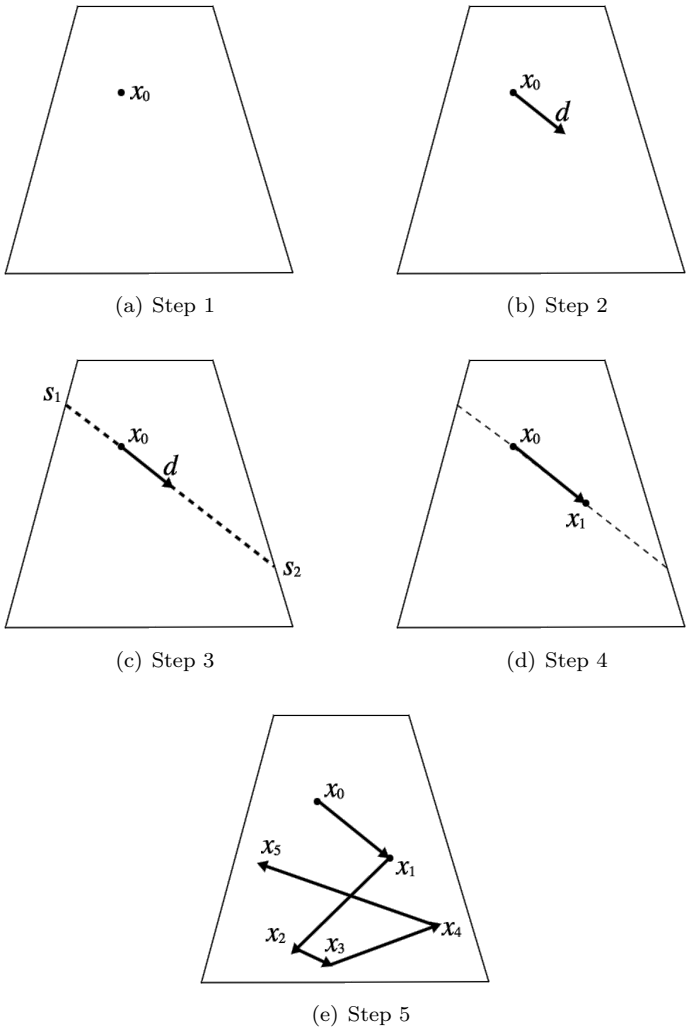
$$\phi(x) = \sum -\log(b_i - a_i^T x)$$

We can compute and simplify the Hessian of the Log Barrier:

Hessian of Log Barrier H_x:

$$H_x = \nabla^2 \phi(x) = ... = A^T D^2 A \quad , \quad \text{where:}$$
$$D = diag(\frac{1}{b_i - a_i^T x})$$

Note: H_x is a $N \times N$ linear operator. D is a $M \times M$ diagonal matrix.



(a) Step 1 (b) Step 2

(c) Step 3 (d) Step 4

(e) Step 5

Figure 4: The hit-and-run algorithm begins with an interior point x_0 (Step 1). A random direction is selected (Step 2), and the chord along that direction is calculated (Step 3). Then, we pick a random point along that chord and move there as our new point (Step 4). The algorithm is repeated to sample many points (Step 5)

Definition - Dikin Ellipsoid $D^r_{x_0}$

$D^r_{x_0}$, the Dikin Ellipsoid centered at x_0 with radius r is defined as:

$$D^r_{x_0} = \{y \mid (y-x)^T H_{x_0}(y-x) \leq r^2\}$$

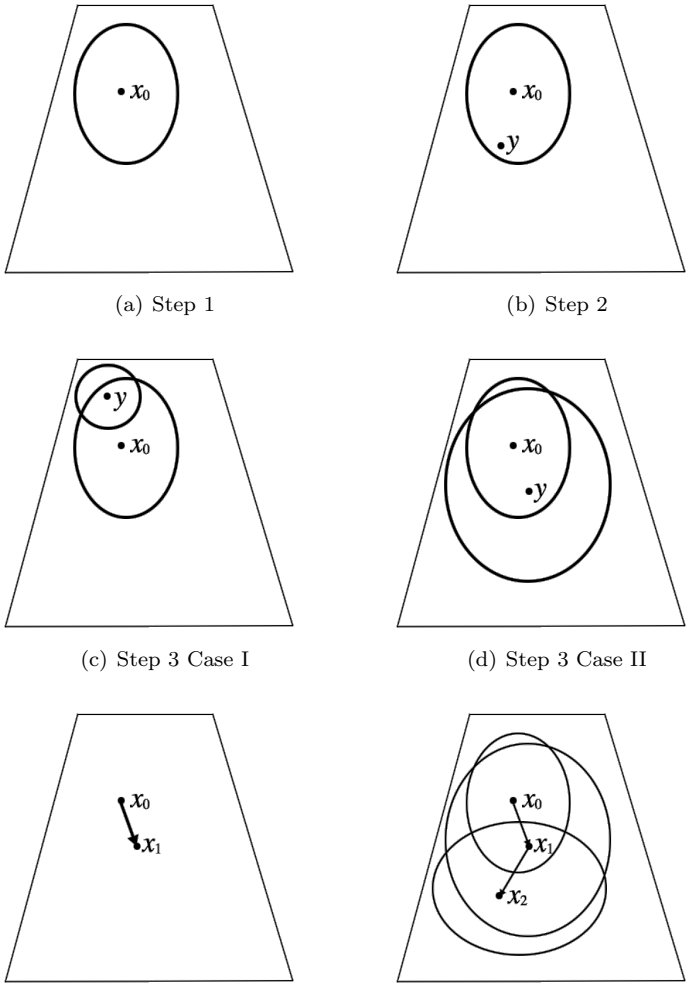
The shape of the Dikin Ellipsoid with radius r is a function of A, b, and its center x_0. Thus, throughout the convex polytope K, the Dikin Ellipsoid changes shape depending on where the center x_0 is.

Algorithm `Dikin`

1. Begin with a point $x_0 \in K$. This starting point must be in the polytope.
2. Construct D_{x_0}, the Dikin Ellipsoid centered at x_0
3. Pick a random point y from D_{x_0}
4. If $x_0 \notin D_y$, then reject y (be careful, this condition is counter-intuitive)
5. If $x_0 \in D_y$, then accept y with probability $\min(1, \sqrt{\frac{det(H_y)}{det(H_{x_0})}})$ (the big picture is that the ratio of the determinants are equal to the ratio of volumes of the ellipsoids centered at x_0 and

y. Thus, the geometric argument would be that this way the Dikin walk can avoid extreme corners of the region)

6. repeat until obtained number of desired points



(a) Step 1 (b) Step 2

(c) Step 3 Case I (d) Step 3 Case II

(e) Step 4 (f) Step 5

Figure 5: The Dikin Walk begins by constructing the Dikin Ellipsoid at the starting point x_0 (Step 1). An uniformly random point y is generated in the Dikin Ellipsoid centered at x_0 (Step 2). If point x_0 is not in the Dikin Ellipsoid centered at y, then reject y (Step 3 Case I). If point x_0 is contained in the Dikin Ellipsoid centered at y, then accept y with probability $\min(1, \sqrt{\frac{det(H_y)}{det(H_{x_0})}})$ (Step 3 Case II). Once we've successfully accepted y, we set y as our new point, x_1 (Step 4). Algorithm repeats (Step 5)

How to pick a random point uniformly from a Dikin Ellipsoid?

Let's say, we now have D_x^r, the Dikin Ellipsoid centered at x with radius r.

1. generate ζ from the n dimensional Standard Gaussian (i.e. `zeta = rnorm(n,0,1)`)
2. normalize ζ to be on the n dimensional ball with radius r, that is:
$$\zeta = < x_1, x_2, ..., x_n > \rightarrow < \frac{rx_1}{\sqrt{x_1^2+x_2^2+...+x_n^2}}, \frac{rx_2}{\sqrt{x_1^2+x_2^2+...+x_n^2}}, ..., \frac{rx_n}{\sqrt{x_1^2+x_2^2+...+x_n^2}} >$$
3. Solve for d in the matrix equation $H_x d = A^T D\zeta$ (note, as long as x_0 is not on the boundary of our polytope K, H_x will be non-singular, thus, d will always be unique)
4. $y = x_0 + d$ is our randomly sampled point from D_x^r

Important Theorem

In algorithm `Dikin`, what if the point y we accept is outside of our polytope K? Luckily, there is no need to worry about that because of the following theorem:

Theorem – If $x_0 \in K$, then $D^1_{x_0} \subseteq K$. That is, if our starting point x_0 is in our polytope K, then the Dikin Ellipsoid centered at x_0 with radius 1 will always be contained in K.

Thus, if we set $r = 1$ (or $r \leq 1$), then our algorithm will guarantee to sample points only within the polytope K.

These points need elaboration and editing

The shape of the Dikin Ellipsoid is a function of A, b, and x_0. In other words, if we think in terms of running a MCMC chain within our polytope K, the Dikin Ellipsoid is able to reshape itself accordingly as it surveys through the polytope.

Although there are still two rejection components to the algorithm (see above), the rejection rate is much lower than expected because of this theorem.

Dikin versus Hitandrun

	`hit-and-run`	`Dikin Walk`
Uniform Sampling	Yes, needs $O(N^3)$ points, where N is the dimension of the polytope	No, concentrates in the interior
Mixing	$O(\frac{N^2R^2}{r^2})$ *, slows down substantially as dimension of polytope increases and polytope becomes "skinnier"	$O(MN)$, where A is $M \times N$; much stronger mixing.
Cost of One Step	$O(MN)$	$O(MN^2)$, in practice, one step of Dikin is much more costly than hit-and-run
Rejection Sampling	No	Yes (see probability formula and $x \notin D_y$), but rejection rate not high

*R is the radius of the smallest ball that contains the polytope K. r is the radius of the largest ball that is contained within the polytope K. Thus, $\frac{R}{r}$ increases as the polytope is "skinnier".

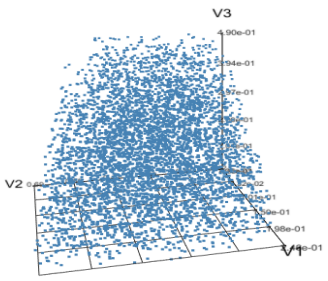


Figure 6: Dikin concentrates at the center

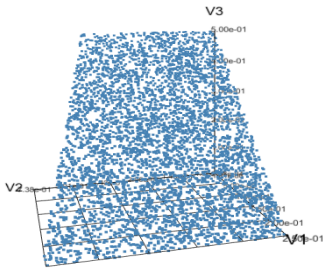


Figure 7: Hit-and-run samples the space thoroughly

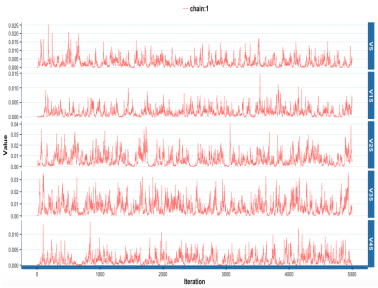


Figure 8: Dikin mixes stronger

Figure 9: Hit-and-run mixes slower

Using `walkr` to sample points

`walkr` has one main function `walkr` which makes it very easy for the user to sample points.

For example, define A and b as follows:

```
> A <- matrix(c(1, 0, 1, 0, 1), ncol = 3)
> b <- 0.5
```

Then, the sampling could be simply ran with `walkr`:

```
> ## n is the number of points sampled
> ## method is the sampling method
>
> hitandrun <- walkr(A = A, b = b, n = 1000, method = "hit-and-run")
> dikin <- walkr(A = A, b = b, n = 1000, method = "dikin")
> optimized_dikin <- walkr(A = A, b = b, n = 1000, method = "optimized-dikin")
> ## see some of the sampled points
>
> hitandrun[ , 10:15]
> dikin[ , 10:15]
> optimized_dikin[ , 10:15]
```

To see the difference in performance between Dikin in R and Optimized Dikin using Rcpp:

```
> A <- matrix(c(1,0,1,0,1), ncol = 5)
> b <- 0.5
> unoptimized <- function() {walkr(A = A, b = b, n = 5000, method = "dikin")}
> optimized <- function() {walkr(A = A, b = b, n = 5000, method = "optimized-dikin")}
> microbenchmark(
+
+   unoptimized(),
+   optimized(),
+   times = 20
+ )
>
```

Using `walkr` to examine MCMC random walks

We could visualize/diagnose the MCMC chains by:

```
> vis_sampling(hitandrun, chains = 1)
> optimized_dikin(hitandrun, chains = 1)
```

Conclusion

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