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

A and b represent the system of equations that we have above. Specifically, A is a $M \times N$ matrix (M variables and N constraints), and b is a $M \times 1$ vector.

Mathematical Background of Sampling Space

In this section, we go through the mathematical background needed to understand the space from which we are sampling – the intersection of the N simplex and hyperplanes. Specifically, we go through a few examples as well as some linear algebra tricks. The reader does not need to read this section in order to use our package or understand our sampling algorithms. However, this section should help the reader understand better what the sample space is both geometrically and mathematically.

Definition: The N-dimensional unit 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.

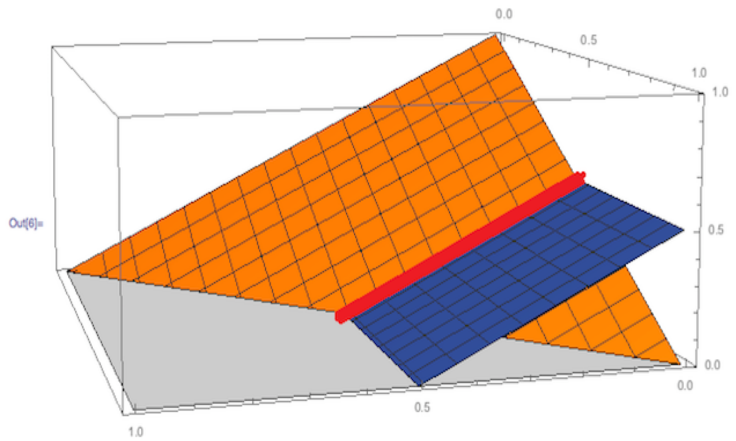

Figure 1: Intersection (red line) of Simplex and 2D hyperplane living in 3D space

Matrix Representation of 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:

$$A_{M\times N} = \underbrace{\begin{bmatrix} & & \\ & \cdots & \\ & & \end{bmatrix}}_{\text{N columns (variables)}} \left.\vphantom{\begin{bmatrix} \\ \\ \\ \end{bmatrix}}\right\}\text{M rows (constraints)}$$

$$b = b_{M\times 1}, \quad x = x_{N\times 1}$$

Going from $Ax = b$ and the unit-simplex to $Ax \leq b$

Our sampling space is represented by equalities $Ax = b$, $\sum x = 1$, and non-negativity constraint $x_i \geq 0$. Because of the inequality, our sampling space is bounded (i.e. has finite volume in $\mathbb{R}^N$). More formally, our sampling space known as a **convex-polytope** in $\mathbb{R}^N$, which could be described by a generic $Ax \leq b$. Here, we describe a transformation which takes us from the intersection of $Ax = b$ and the unit-simplex to a large matrix inequality of the form $Ax \leq b$.

First, note that the equality part of the simplex constraint could be added as an extra row in $Ax = b$

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

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 Basis of A, the set of all possible x's that satisfy $Ax = 0$, then add on a particular solution to $Ax = b$.

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

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

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

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

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

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

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

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

And finally, we obtain the mathematical description of our sampling space in the form $Ax \leq b$.

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

Note that we have performed a **transformation** from "x-space" (coordinates described by $x_1, x_2, ..., x_N$) to "α-space" (coordinates described by $\alpha_1, \alpha_2, ...$). However, the geometric object described is still the same one. In fact, in `walkr`, when the user inputs A and b for $Ax = b$, the package internally performs this transformation, samples the α's, maps them back to "x-space, and then returns the sampled points.

The reader 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.

Random Walks

Now that we've understood

Starting Points

MCMC algorithms need a starting point, x_0, in the interior of the convex polytope.

Hit-and-run

Dikin Walk

Using `walkr`

Examining/Visualizing Results

Conclusion

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