## **ISC 5228**

## **Markov Chain Monte Carlo**

**In-class Assignment** 

Due: In 20 minutes

The (Euclidean) distance between two points  $R_i$  and  $R_j$  in 3D is 1

$$R_{ij} = |\mathbf{R}_i - \mathbf{R}_j| = \sqrt{(\mathbf{R}_{i,x} - \mathbf{R}_{j,x})^2 + (\mathbf{R}_{i,y} - \mathbf{R}_{j,y})^2 + (\mathbf{R}_{i,z} - \mathbf{R}_{j,z})^2}$$

I want to find the average distance between two points inside a sphere of unit radius.

- (i) Describe how you would sample  $N \approx 1000$  random points inside the sphere.
- (ii) What are the theoretical maximum and minimum values that  $R_{ij}$  can take?
- (iii) Imagine what the PDF of  $R_{ij}$  might look like?
- (iv) Consider every pair of points in the sample and compute the corresponding distance. What are the maximum, minimum, and average values of  $R_{ij}$  in the sample?<sup>2</sup>
- (v) One way to characterize the error in the estimated average is to compute the standard error. This is given by the standard deviation divided by the square-root of the number of samples.

 $<sup>^{1}</sup>$ In numpy this can be computed using np.linalg.norm(Ri, Rj), where Ri and Rj are arrays with three elements.

<sup>&</sup>lt;sup>2</sup>This part is optional; The true answer is 36/35.