

# Technical report 1

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## Von Mises distribution

Intuitively, the Von Mises distribution[4] is a simple approximation for the normal distribution on a circle (known as the *wrapped normal distribution*). The Von Mises probability density function is defined by the following equation:

$$P(x) = \frac{e^{b \cos(x-a)}}{2\pi I_0(b)}$$

where  $I_0(x)$  is the modified Bessel function of the first kind; the Von Mises cumulative density function has no closed form.

The mean  $\mu = a$  (intuitively, the angle that the distribution clustered around), and the circular variance  $\sigma^2 = 1 - \frac{I_1(b)}{I_0(b)}$  (intuitively,  $b$  is the “concentration” parameter). Therefore, as  $b \rightarrow 0$ , the distribution becomes uniform; as  $b \rightarrow \infty$ , the distribution becomes normal with  $\sigma^2 = 1/b$ .

## Von Mises-Fisher distribution

The Von-Mises Fisher distribution is the generalization of the Von Mises distribution to  $n$ -dimensional hyperspheres. It reduces to the Von-Mises distribution with  $n = 2$ . The probability density function is defined by the following equation:

$$f_p(\mathbf{x}; \boldsymbol{\mu}, \kappa) = C_p(\kappa) \exp(\kappa \boldsymbol{\mu}^T \mathbf{x})$$

where

$$C_p(\kappa) = \frac{\kappa^{p/2-1}}{(2\pi)^p I_{p/2-1}(\kappa)}$$

and intuitively is an approximation for the normal distribution on the hypersphere.

# K-means clustering

$k$ -means clustering is a simple and popular algorithm for the *clustering problem*, the task of grouping a set of observations so that a group is “similar” within itself and “dissimilar” to other groups.  $k$ -means partitions  $n$  observations into  $k$  clusters, with each observation belonging to the nearest mean of the cluster. This problem is NP-hard in general, but there are heuristics which guarantee convergence to a local optimum.

The standard heuristic (known as *Lloyd’s algorithm*) is the following:

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**Algorithm 1** Lloyd’s algorithm for  $k$ -means clustering

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1: generate an initial set of  $k$  means
2: while not converged do
3:   assign all data points to nearest Euclidean-distance mean
4:   calculate new means to as the centroids of the observations in the cluster
5: end while
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There is a choice of initialization method. The *Forgy method* randomly picks  $k$  observations as initial means, while the *Random Partition method* randomly picks a cluster for each observation.

The Lloyd’s algorithm is a heuristic, so it does not guarantee a global optimum. Furthermore, there exists sets of points in which it converges in exponential time. However, it has been shown to have a smoothed polynomial running time, and in practice converges quickly.

## Spherical k-means clustering

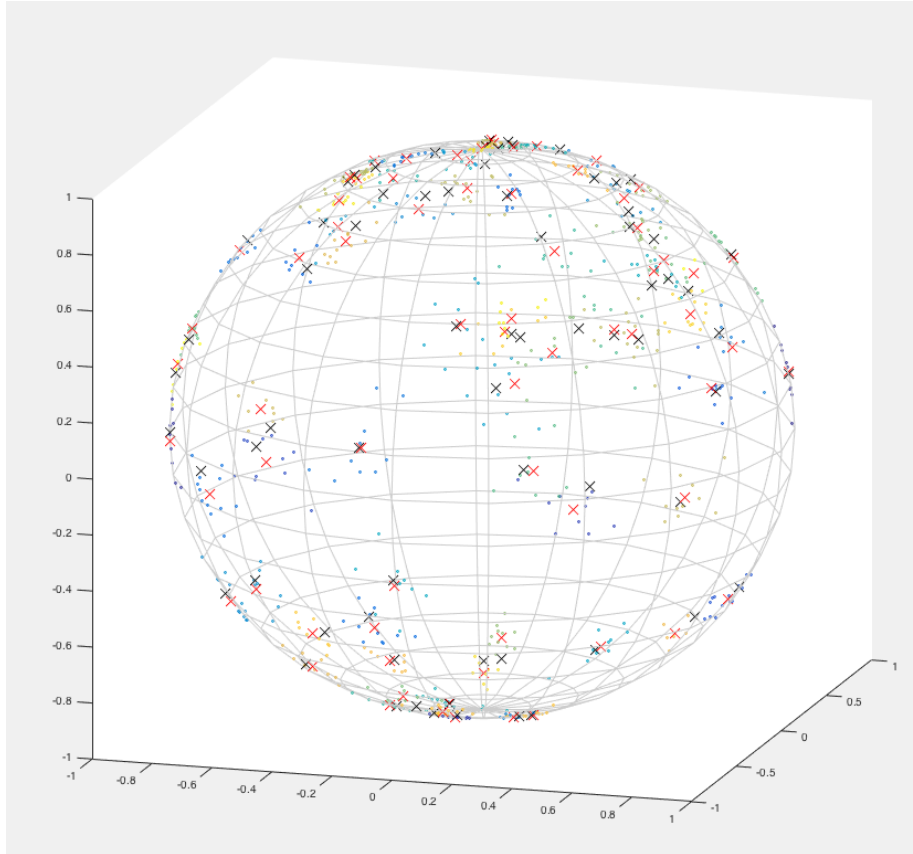
Spherical  $k$ -means clustering the same idea, but with points on a sphere. We investigated a MATLAB implementation by Nguyen[3, 2], which required a mean-and-norm-normalized dataset located on a hypersphere. Important aspects of this implementation include:

- When there exists an empty cluster, the largest cluster is split
- Use the dot product as “negative distance”, which leverages the fact that observations are unit vectors on the hypersphere
- Use the normalized sum of observations as a centroid/mean, which leverages the fact that observations are unit vectors on the hypersphere. Note that this fails on pathological cases where the sum of observations is zero.

## Our investigation

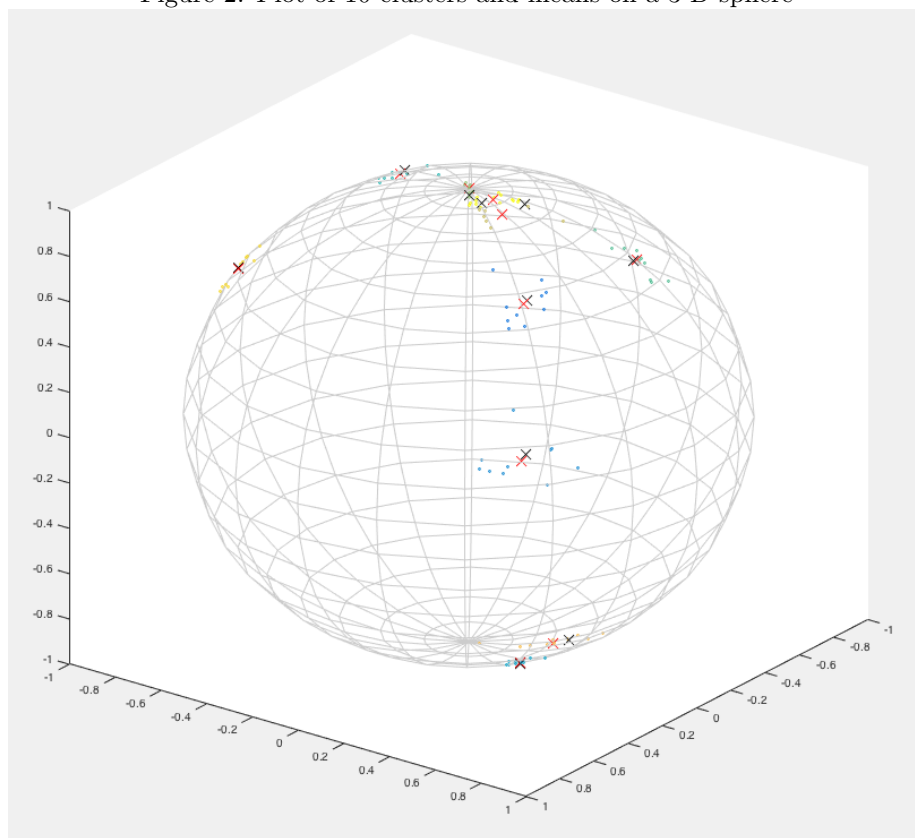
In order to test how well the spherical  $k$ -means clustering algorithm worked, we constructed a random data set using the Von Mises distribution random

Figure 1: Plot of 70 clusters and means on a 3-D sphere



sampling function from the MATLAB Circular Statistics Toolbox[1]. We constructed 70 clusters of 10 points each, using random points on the sphere as means and with  $\kappa = 100$ , and then applied the spherical k-means clustering and visualized the results on the unit three dimensional sphere, color coded for each cluster and with estimated means labeled as red  $X$ 's and true means labeled as black  $X$ 's.

Figure 2: Plot of 10 clusters and means on a 3-D sphere



## References

- [1] Phillip Berens. Matlab central file exchange: Circular statistics toolbox. <http://www.mathworks.com/matlabcentral/fileexchange/10676-circular-statistics-toolbox-directional-statistics->. Accessed: 2016-05-18.
- [2] Vinh Nguyen. Matlab central file exchange: The spherical k-means algorithm. <http://www.mathworks.com/matlabcentral/fileexchange/32987-the-spherical-k-means-algorithm>. Accessed: 2016-05-18.
- [3] Vinh Nguyen. Gene clustering on the unit hypersphere with the spherical k-means algorithm: coping with extremely large number of local optima. In *World Congress in Computer Science, Computer Engineering, and Applied Computing (Hamid R. Arabnia and Youngsong Mun 14 July 2008 to 17 July 2008)*, pages 226–233. CSREA Press, 2008.
- [4] Eric W. Weisstein. von mises distribution. <http://mathworld.wolfram.com/vonMisesDistribution.html>. Accessed: 2016-05-18.