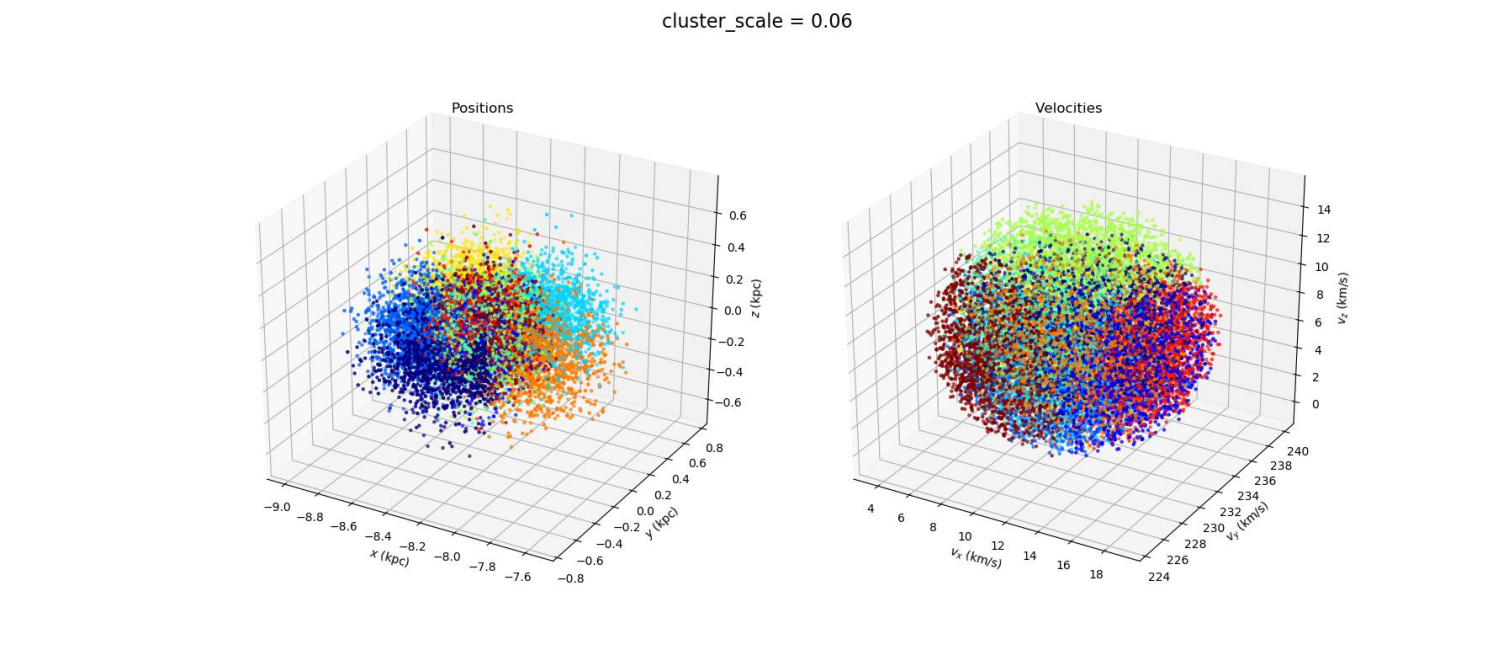
KMeans Clustering in 6 Dimensions to sample phase space

By: Michael Poon, Mathew Bub

June 2018

‘clustering technique to reduce 6D dataset’



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Overview: Gaia DR2 RV (6D) -> main program -> 3D or 4D subspace?

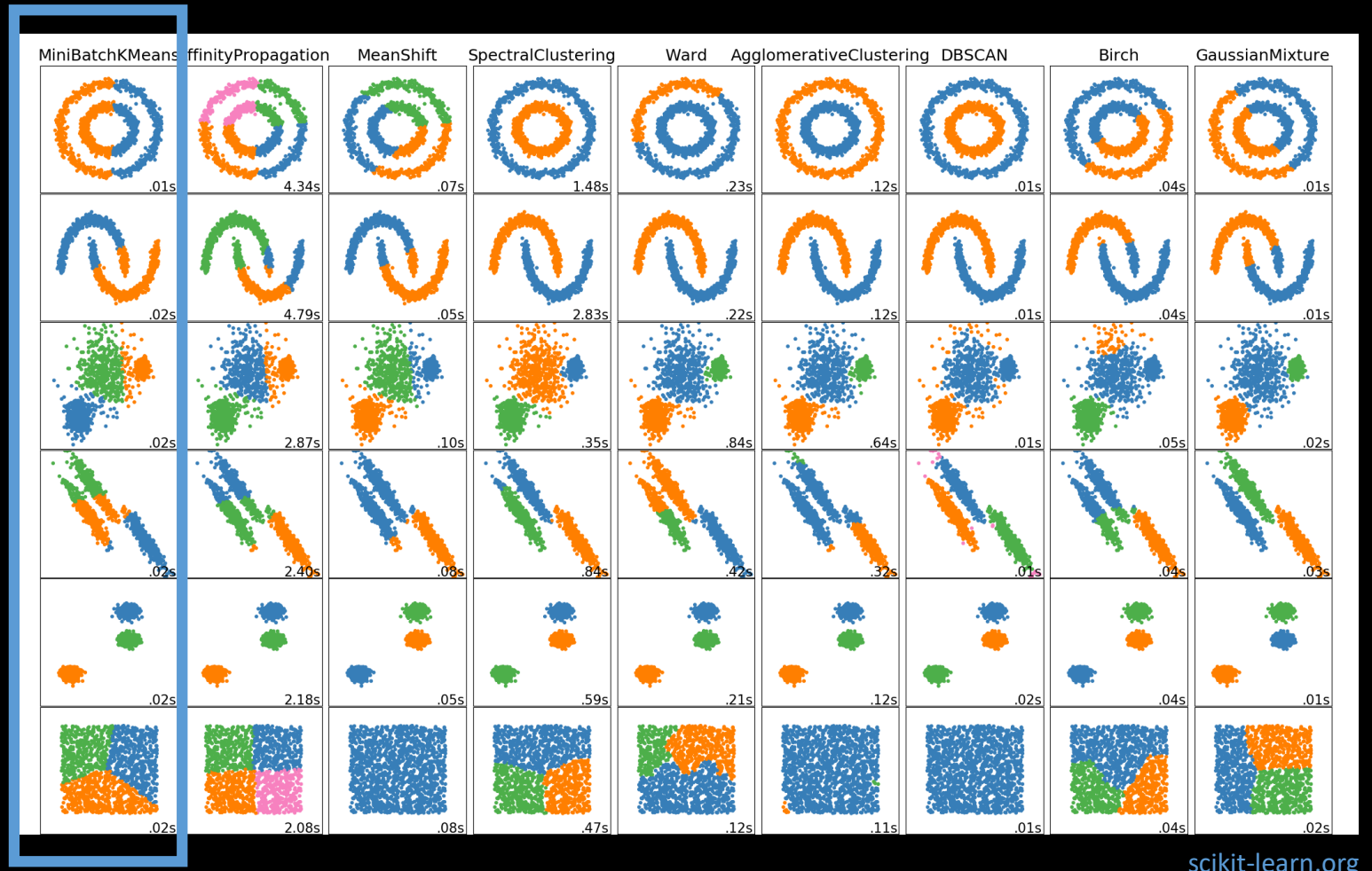
Due to constraints from: Conserved (1) Energy, (2) Ang. Momentum, (3?) *Mystery*

Problem: main program bottleneck, reduce dataset to a reasonable sample

GOAL:
Want a reduction: 7,224,631 Stars -> quality cuts -> KMeans Clustering -> 100,000? Cluster Centers

What is KMeans Clustering?

-unsupervised (no “correct” solution) machine learning technique



scikit-learn.org

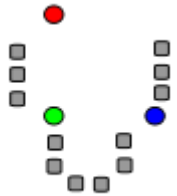
Clusters how we want it to, and runs (relatively) fast:
Linear in Big O: O(kN), k - #iterations, N - #datapoints

How Does KMeans Work?

Voronoi Tessellation:

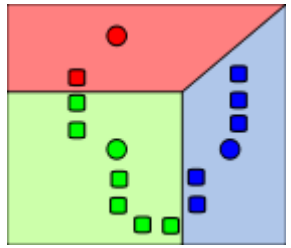
KMeans Clustering:

1. Random Initialization

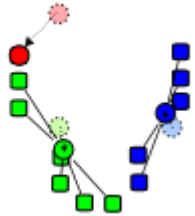


Circles are not datapoints, they are randomly put

2. Voronoi Tessellation



3. Adjust “random” points



to cluster centroid

wikipedia.org/wiki/K-means_clustering

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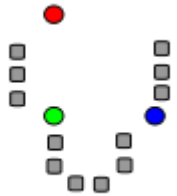

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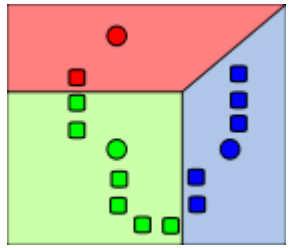

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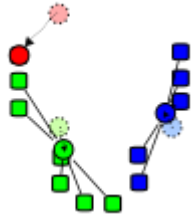

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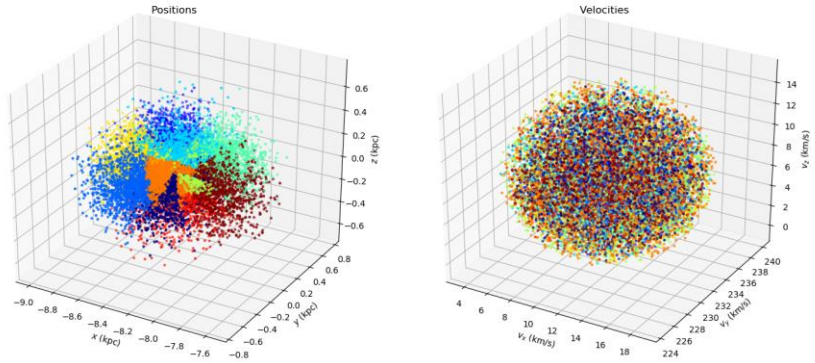
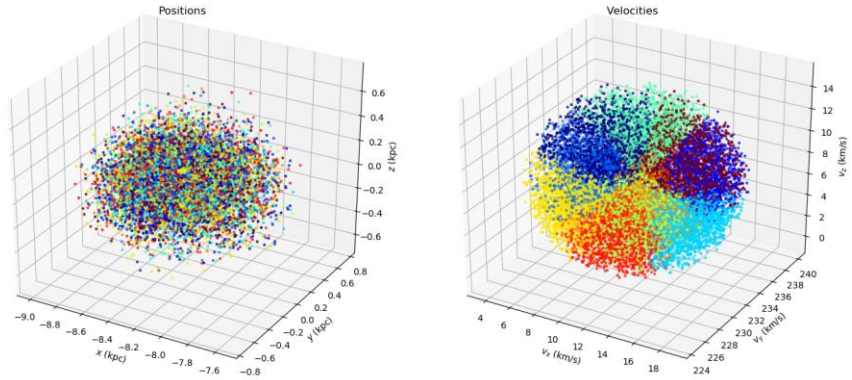
Preliminary Results:

#stars: 15,000

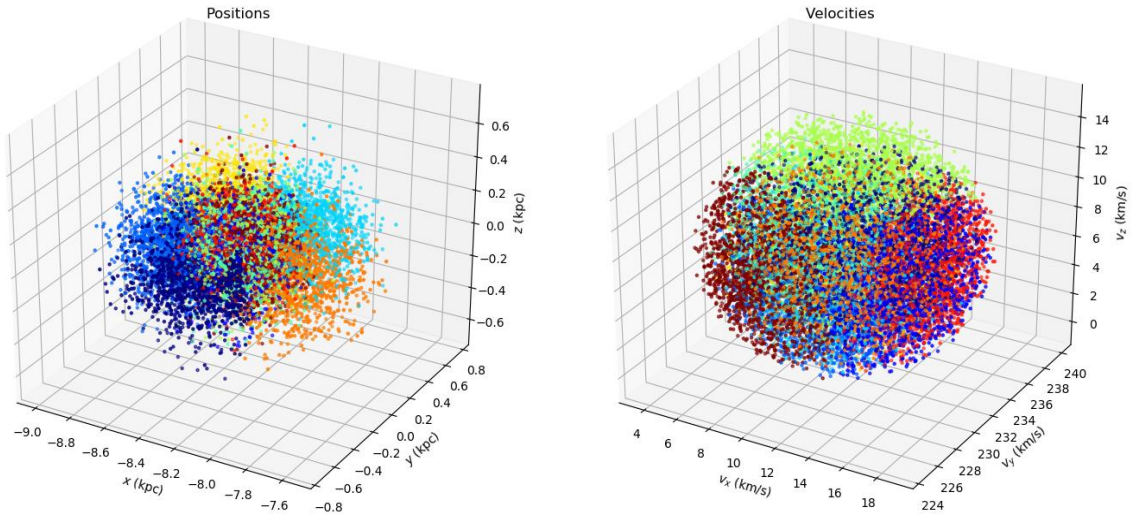
cluster_scale = 0.01



cluster_scale = 0.20



cluster_scale = 0.06



Discuss:

Reason for cluster_scale (Normalization)

Consequences to cluster_scale

Alternatives: Standard Dev. / Interq. Range

Next Steps:

Runtime Table (KMeans MiniBatch):

Sample size	Dimensions (x, y, z, vx, vy, vz)	# of Clusters	Runtime
1009373	2D (x, y)	1000	13.8s
6376803	2D (x, y)	1000	1min 2s
1009373	2D (x, y)	10000	2min 55s
36745	3D (x, y, z)	10000	2min 48s
1009373	3D (x, y, z)	10000	4min 23s

What sample size should we start with? Or use all?

How many clusters should we make?

KMeans vs. KMeans MiniBatch?