k-means

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Last Lecture..

Truncated SVD solves the

Rank-r Matrix Factorization Problem

The Rank-r Matrix Factorization Problem

Given: a data matrix $D \in \mathbb{R}^{n \times d}$ and a rank $r < \min\{n, d\}$.

Find: matrices $X \in \mathbb{R}^{d \times r}$ and $Y \in \mathbb{R}^{n \times r}$ whose product approximates the data matrix:

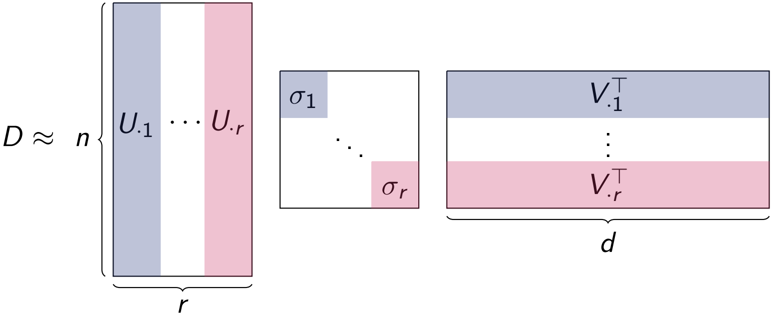
$$\min_{X,Y} \|D - YX^\top\|^2 \qquad \text{s.t. } X \in \mathbb{R}^{d \times r}, Y \in \mathbb{R}^{n \times r}$$

Solution: Let $D = U\Sigma V^\top$ be the SVD of D. Choose $X \in \mathbb{R}^{d \times r}$ and $Y \in \mathbb{R}^{n \times r}$ such that

$$YX^\top = U_{\cdot\mathcal{R}} \Sigma_{\mathcal{R}\mathcal{R}} V_{\cdot\mathcal{R}}^\top$$

Truncated SVD

The approximation $D \approx U_{\cdot\mathcal{R}}\Sigma_{\mathcal{R}\mathcal{R}}V_{\cdot\mathcal{R}}^\top$ is called truncated SVD.



Truncated SVD

Theorem (MF is Nonconvex)

The rank-r matrix factorization problem, defined for a matrix $D \in \mathbb{R}^{n\times d}$ and a rank $r < \min\{n, d\}$ as

$$\min_{X,Y} \|D - YX^\top\|^2 \qquad s.t.\ X \in \mathbb{R}^{d\times r}, Y \in \mathbb{R}^{n\times r}$$

is a nonconvex optimization problem.

Matrix Completion for Recommender Systems

Movies

Users		*A*	*B*	*C*	*D*
	1	★★★★★	?	★★☆☆☆	★☆☆☆☆
	2	?	★☆☆☆☆	★★★★★	?
	3	★★★★★	★☆☆☆☆	★★★★★	★★☆☆☆
	4	★★★★★	?	★★★★★	★★★☆☆
	5	★★★★★	★★★★★	?	?
	6	?	★★★★☆	★★★★★	★★★☆☆

Can we fill the ? with the rating which would be given by the user if (s)he had seen the movie?

SVD in the Scope of Movie Recommender Systems

$$\begin{pmatrix} 5 & \mu & 1 & 1 \\ \mu & 1 & 5 & \mu \\ 2 & 1 & 5 & 3 \\ 4 & \mu & 4 & 2 \\ 5 & 5 & \mu & 1 \\ \mu & 1 & 5 & 3 \end{pmatrix} \approx \begin{pmatrix} -0.3 & 0.5 \\ -0.4 & -0.4 \\ -0.4 & -0.4 \\ -0.4 & 0.1 \\ -0.5 & 0.5 \\ -0.4 & -0.4 \end{pmatrix} \begin{pmatrix} -9.0 & -5.8 & -9.5 & -5.3 \\ 2.6 & 3.3 & -3.3 & -2.2 \end{pmatrix}$$

Every user's preferences are approximated by a linear combination of the rows in the second matrix:

$$\begin{aligned} \begin{pmatrix} 5 & \mu & 1 & 1 \end{pmatrix} \approx & -0.3 \cdot \begin{pmatrix} -9.0 & -5.8 & -9.5 & -5.3 \end{pmatrix} \\ & + 0.5 \cdot \begin{pmatrix} 2.6 & 3.3 & -3.3 & -2.2 \end{pmatrix} \end{aligned}$$

Today: k-means

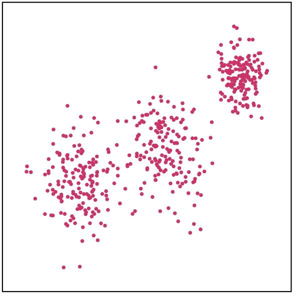
1

Informal Problem Description

Clustering Means to Group Data Points According to a Similarity Criterion

Question: what are clusters in a deck of cards?

Clustering is a Task with Multiple Valid Outcomes



1. How many clusters do we have?
2. Do they overlap?
3. How are clusters characterized?

Cluster models differ according to the answers to these questions.

2

Derive the Formal Problem Definition

The Cluster Model of k-means

1. How many clusters do we have? Let the user decide..
2. Do they overlap? No. Every point belongs to exactly one cluster

   $$\mathcal{C}_s \cap \mathcal{C}_t = \emptyset,\ \mathcal{C}_1 \cup \ldots \cup \mathcal{C}_r = \{1, \ldots, n\}$$

   That is, $\{\mathcal{C}_1, \ldots, \mathcal{C}_r\}$ is a partition of $\{1, \ldots, n\}$. We denote the set of all partitions from $\{1, \ldots, n\}$ with $\mathcal{P}_n$.
3. How are clusters characterized? Points within a cluster are close in average:

   $$\frac{1}{|\mathcal{C}_s|} \sum_{i,j \in \mathcal{C}_s} \|D_{i\cdot} - D_{j\cdot}\|^2 \text{ is small.}$$

The k-means Objective

Given: a data matrix $D \in \mathbb{R}^{n \times d}$ and the number of clusters r.

Find: clusters $\{\mathcal{C}_1, \ldots, \mathcal{C}_r\} \in \mathcal{P}_n$ which create a partition of $\{1, \ldots, n\}$, minimizing the distance between points within clusters (within cluster scatter):

$$\min_{\{\mathcal{C}_1,\ldots,\mathcal{C}_r\} \in \mathcal{P}_n} Dist(\mathcal{C}_1, \ldots, \mathcal{C}_r) = \sum_{s=1}^{r} \frac{1}{|\mathcal{C}_s|} \sum_{j,i \in \mathcal{C}_s} \|D_{j\cdot} - D_{i\cdot}\|^2 \tag{1}$$

3

Optimization

Ok, we have here now one problem:

The standard optimization methods relying on gradients do not apply, this is a discrete optimization problem.

How can we optimize the objective of k-means when the gradients are not defined?

Transform the objective to get a better idea.

Minimizing the Within Cluster Distance Means Minimizing the Distance of Points to their Centroid

Theorem (k-means centroid objective)

The k- means objective in Eq. (1) is equivalent to

$$\min \sum_{s=1}^{r} \sum_{i \in \mathcal{C}_s} \|D_{i\cdot} - X_{\cdot s}^\top\|^2 \qquad s.t.\ X_{\cdot s} = \frac{1}{|\mathcal{C}_s|} \sum_{i \in \mathcal{C}_s} D_{i\cdot}^\top,$$
$$\{\mathcal{C}_1, \ldots, \mathcal{C}_r\} \in \mathcal{P}_n$$

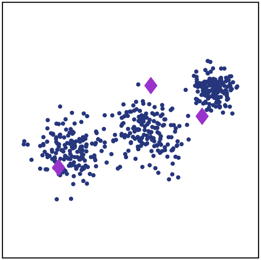
$X_{\cdot s}$ is the centroid (the arithmetic mean position) of all points assigned to cluster $\mathcal{C}_s$.

Does this notion of centroids deliver more easily solvable sub-problems?

Maybe it's more easy to compute the centroids given the clusters and vice versa instead of computing clusters and centroids simultaneously?

Minimizing the Distance of Points to their Centroids

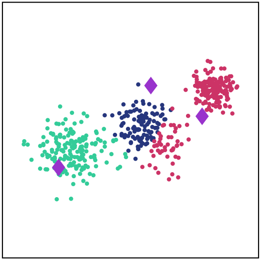
Let us start with some randomly sampled centroids (the purple diamonds).



Question: how do we assign points to clusters?

Minimizing the Distance of Points to their Centroids

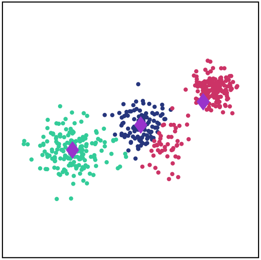
We assign every point to the cluster with the closest centroid.



Problem: now the centroids are not actually centroids of all points in one cluster!

Minimizing the Distance of Points to their Centroids

We update the centroids.



Observation: now we can again decrease the objective function by assigning the points to their closest centroid!

Congratulations!

You just came up with the algorithm for k-means on your own.

Lloyds k-means Algorithm

function K-MEANS(r, D)
  $X \leftarrow$ INITCENTROIDS(D, r) ▷ centroid initialization
  while not converged **do**
    for $s \in \{1, \dots, r\}$ **do**
      $\mathcal{C}_s \leftarrow \left\{ i \middle| s = \arg\min_{1 \le t \le r} \left\{ \|X_{\cdot t} - D_{i\cdot}^\top\|^2 \right\}, 1 \le i \le n \right\}$
    end for
    for $s \in \{1, \dots, r\}$ **do**
      $X_{\cdot s} \leftarrow \frac{1}{|\mathcal{C}_s|} \sum_{i \in \mathcal{C}_s} D_{i\cdot}^\top$ ▷ centroid update
    end for
  end while
  return $\{\mathcal{C}_1, \dots, \mathcal{C}_r\}$
end function

Cool, we have now a algorithm for the discrete optimization problem of k-means.

How good is this algorithm?

Does it converge? Is it just a heuristic or can we derive some quality guarantees of the result?

These questions can all be answered under the more general framework of matrix factorization.

Indicating Clusters by a Binary Matrix

Let $Y \in \{0,1\}^{n \times r}$ such that $Y_{is} = 1$ if and only if $i \in \mathcal{C}_s$.

Every point belongs to exactly one cluster if and only if

$$|Y_{i\cdot}| = 1 \text{ for all } i \in \{1, \ldots, n\},$$

We denote with $\mathbb{1}^{n \times r}$ the set of all binary matrices which indicate a partition of n points into r sets:

$$\mathbb{1}^{n \times r} = \{Y \in \{0,1\}^{n \times r} \mid |Y_{i\cdot}| = 1 \text{ for } i \in \{1, \ldots, n\}\}$$

The Centroid Matrix

Given a cluster indicator matrix $Y \in \mathbb{1}^{n\times r}$, the sth centroid is

$$X_{\cdot s} = \frac{1}{|\mathcal{C}_s|} \sum_{i\in\mathcal{C}_s} D_{i\cdot}^\top = \frac{1}{|Y_{\cdot s}|} \sum_{i=1}^{n} Y_{is} D_{i\cdot}^\top = \frac{1}{|Y_{\cdot s}|} D^\top Y_{\cdot s}.$$

We can compute the matrix X which gathers all centroids column-wise by

$$X = D^\top Y \begin{pmatrix} \frac{1}{|Y_{\cdot 1}|} & & 0 \\ & \ddots & \\ 0 & & \frac{1}{|Y_{\cdot r}|} \end{pmatrix} = D^\top Y (Y^\top Y)^{-1}.$$

k-means is Matrix Factorization

Theorem (k-means MF objective)

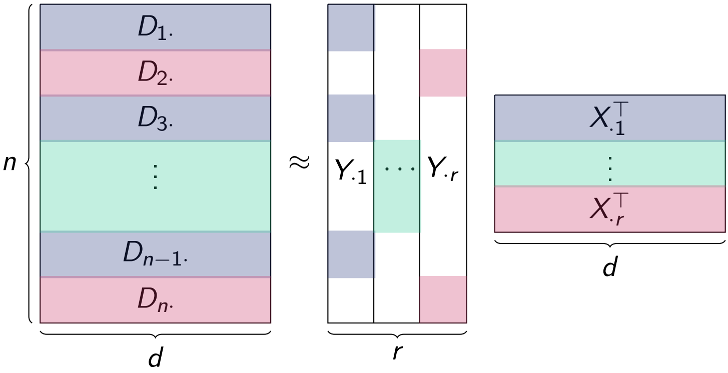
The k- means objective in Eq. (1) is equivalent to

$$\min_Y RSS(X, Y) = \|D - YX^\top\|^2 \qquad s.t. \;\; Y \in \mathbb{1}^{n \times r},$$
$$X = D^\top Y(Y^\top Y)^{-1}$$

The matrix Y indicates the cluster assignments.

The matrix X gathers the centroids of all clusters column-wise.

The k-means Decomposition Scheme



Example: k-means for Movie Recommender Systems

$$\begin{pmatrix} 5 & \mu & 1 & 1 \\ \mu & 1 & 5 & \mu \\ 2 & 1 & 5 & 3 \\ 4 & \mu & 4 & 2 \\ 5 & 5 & \mu & 1 \\ \mu & 1 & 5 & 3 \end{pmatrix} \approx \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 4.7 & 3.7 & 2.7 & 1.3 \\ 2.3 & 1.0 & 5.0 & 3.0 \end{pmatrix}$$

Every user's preferences are approximated by a linear combination of the rows in the second matrix:

$$\begin{pmatrix} 5 & \mu & 1 & 1 \end{pmatrix} \approx 1 \cdot \begin{pmatrix} 4.7 & 3.7 & 2.7 & 1.3 \end{pmatrix} + 0 \cdot \begin{pmatrix} 2.3 & 1.0 & 5.0 & 3.0 \end{pmatrix}$$

Ok, so *k*-means is an instance of the rank-*r* matrix factorization problem.

Can we also characterize the global minimizers of k-means like we did it for the rank-r matrix factorization problem with truncated SVD?

Unfortunately not.

However, we can characterize the global minimizers of the objective when we fix one of the factor matrices.

Centroids are Part of the Solution

Theorem (Centroids as minimizers of an optimization problem)

Given $D \in \mathbb{R}^{n\times d}$ and $Y \in \mathbb{1}^{n\times r}$, the minimizer of the optimization problem

$$\min_X \|D - YX^\top\|^2 \qquad s.t.\ X \in \mathbb{R}^{d\times r} \tag{2}$$

is given by the centroid matrix $X = D^\top Y(Y^\top Y)^{-1}$.

Proof (sketch): Show that the objective in Eq. (2) is convex. The minimizer is then given by the stationary point:

$$\begin{aligned} \nabla_X \|D - YX^\top\|^2 &= -2(D - YX^\top)^\top Y = 0 \\ &\Leftrightarrow D^\top Y(Y^\top Y)^{-1} = X \end{aligned}$$

Nearest Centroid Clusters are another Part of the Solution

Theorem (Nearest centroid clusters as minimizers)

Given $D \in \mathbb{R}^{n\times d}$ and $X \in \mathbb{R}^{d\times r}$, the minimizer of the optimization problem

$$\min_Y \|D - YX^\top\|^2 \qquad s.t.\ \ Y \in \mathbb{1}^{n\times r}$$

is the matrix, assigning every point to the nearest centroid:

$$Y_{is} = \begin{cases} 1 & \text{if } s = \arg\min_{1\leq t\leq r}\left\{\|X_{\cdot t} - D_{i\cdot}\|^2\right\} \\ 0 & \text{otherwise} \end{cases}$$

Proof (sketch): Follows from the k-means centroid objective:

$$\min_Y \sum_{s=1}^{r}\sum_{i=1}^{n} Y_{is}\|D_{i\cdot} - X_{\cdot s}^\top\|^2.$$

Lloyds' Algorithm Performs Block-Coordinate Descent

Lloyds' algorithm actually performs an alternating minimization, also called block coordinate descent:

$$X_{k+1} \leftarrow \arg\min_{X \in \mathbb{R}^{d \times r}} \|D - Y_k X^\top\|^2$$

$$Y_{k+1} \leftarrow \arg\min_{Y \in \mathbb{1}^{n \times r}} \|D - Y X_{k+1}^\top\|^2$$

The sequence $\{(X_k, Y_k)\}$ converges, since we decrease the objective function value in every step:

$$RSS(X_0, Y_0) > RSS(X_1, Y_1) > RSS(X_2, Y_2) > \ldots \geq 0.$$

Some Notes about *k*-means Optimization

The *k*-means problem is NP-hard. (SVD is polynomially solvable!)

k-means poses a nonconvex optimization problem, and every feasible cluster indicator matrix and the corresponding centroids are one local minimum.

Hence, finding a good initialization is important! (HW).

The Most Important Slide of this Lecture

Theorem (Equivalent k-means objectives)

The following objectives are equivalent

$$\min_{Y} \sum_{s=1}^{r}\sum_{i=1}^{n} Y_{is}\|D_{i\cdot} - X_{\cdot s}^\top\|^2 \qquad s.t.\ X \in \mathbb{R}^{d\times r}, Y \in \mathbb{1}^{n\times r}$$

$$\min_{Y} \|D - YX^\top\|^2 \qquad s.t.\ X = D^\top Y(Y^\top Y)^{-1}, Y \in \mathbb{1}^{n\times r}$$

$$\min_{Y,X} \|D - YX^\top\|^2 \qquad s.t.\ X \in \mathbb{R}^{d\times r}, Y \in \mathbb{1}^{n\times r}$$

The k-means algorithm (Lloyds' algorithm) performs **block coordinate descent.**