Data Mining: Homework 3

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Problem 2

We will now study some questions of k-means on 1 dimension.

1. Recall that in the k-means problem we want to minimize the total squared ℓ_2 distance between each point and the center to which it is assigned to:

$$\sum_{i=1}^{k} \sum_{x \in C_i} \|\mathbf{x} - \boldsymbol{\mu}_i\|^2$$

where C_i is the set of points that belong to the ith cluster, $\boldsymbol{\mu}_i$ the mean of the points in the ith cluster, and

$$\|\mathbf{x}\|^2 = \sum_{j=1}^{d} x_j^2$$

if $\mathbf{x} = (x_1, x_2, ..., x_d)$.

In class, we said that in general the k-means problem is NP-hard. However, for $d = 1$ the problem is polynomial. Design an algorithm that solves the k-means problem in time polynomial in the number of points n and the number of clusters k, for $d = 1$.

(**Hint**: Can you solve the problem for k clusters if you assume that you can solve it for fewer than k clusters?)

Solution: Let $X \subset \mathbb{R}, |X| = n$ be the set of points we want to cluster, denote by $\mathbf{x} = (x_1, x_2, ..., x_n)$ the sequence of elements in X sorted by value and let $\mathbf{x}[i : j] = (x_i, x_{i+1}, ..., x_{j-1})$. The problem of k-means for $d = 1$ can be rewritten as finding $k - 1$ indices $i_1, i_2, ..., i_{k-1}$ that minimize

$$\phi_k(\mathbf{x}) = \sum_{j=0}^{k-1} \phi(\mathbf{x}[i_j : i_{j+1}]), \qquad \text{with } i_0 = 1,\ i_k = n$$

where $\phi(\mathbf{y}), \mathbf{y} = (y_1, y_2, ..., y_m)$ is the contribute to the k-means cost of a sequence of points, i.e.

$$\phi(\mathbf{y}) = \sum_{i=1}^{m} |y_i - \mu(\mathbf{y})|^2$$
$$\mu(\mathbf{y}) = \frac{\sum_{i=1}^{m} y_i}{m}.$$

Note that this is equivalent to finding k partitions that minimize the cost however we reduce the set of possible partitions to

$$\mathcal{P}(X) = \{P = (P_1, P_2, ..., P_k) | x_i \in P_o \wedge x_j \in P_o \wedge x_i < x_l < x_j \implies x_l \in P_o\}$$

i.e. intervals of the $\mathbb{R}$ space.
Lemma 1. *Let $P = (P_1, P_2, ..., P_k)$ be the optimal solution to the k-means problem for set $X = \{x_1, x_2, ..., x_n\}$ and let $x_i \in P_o$ and $x_j \in P_o$ with $x_i \neq x_j$. For any $x \in X$ such that $x_i < x < x_j$ then $x \in P_o$.*

Proof. Assume by contradiction $x \in P_p \neq P_o$. Given that P is optimal then

$$|x - \mu(P_p)|^2 < |x - \mu(P_o)|^2$$

Without loss of generality assume $x \geq \mu(P_o)$ then we have the following cases:

(a) $\mu(P_o) < \mu(P_p) < x$: this would cotradict the hypothesis since by attaching x_j to P_p would lower the cost which by hyp was optimal.

(b) $x < \mu(P_p) < x + |x - \mu(P_o)|$ again assigning x_j to P_p would lower the cost contradicting the optimality hypothesis.

The same holds for $x \leq \mu(P_o)$ with x_i. □

The Lemma above shows that restricting the partitions to intervals leads to an optimal solution therefore the formulation above is correct. Now we can solve the problem by performing an exhaustive search over the possible values of i_js.

Assume we know the optimal cost $\phi^*_{h-1}(\mathbf{x}[1:m])$, $\forall m$: $h-1 < m \leq n$ for some $h-1 < k$. Then

$$\phi^*_h(\mathbf{x}[1:m]) = \min_{l=h}^{m} \phi^*_{h-1}(\mathbf{x}[1:l]) + \phi(\mathbf{x}[l:m]).$$

i.e. if we know the optimal clustering of size $h-1$ for all prefixes of the points, we can derive the optimal clustering of size h.

This is possible since minimizing $\phi_h(\mathbf{y})$ is equivalent to minimizing each $\phi(\mathbf{y}[i_j, i_{j+1}])$ and once we know $\phi^*_{h-1}(\mathbf{y}[1:m]) = \min_m \phi_{h-1}(\mathbf{y}[1:m])$ for each m, what is left to choose is to which of the m corresponds i_{h-1} (the starting index of the last cluster) which minimizes the cost.

We can compute a matrix M where $M_{h,m} = \phi^*_h(\mathbf{x}[1:m])$ computed as shown by the formula above except for the first row which is simply $\phi^*_1(\mathbf{x}[1:m]) = \phi(\mathbf{x}[1:m])$ and another matrix S keeping for each $M_{h,m}$ the index of the column in the previous row which minimized the cost in order to reconstruct the solution.

$$M = \begin{bmatrix} \phi^*_1(\mathbf{x}[1:1]) & \phi^*_1(\mathbf{x}[1:2]) & \phi^*_1(\mathbf{x}[1:3]) & \dots & \phi^*_1(\mathbf{x}[1:n]) & \phi^*_1(\mathbf{x}[1:n+1]) \\ \perp & \phi^*_2(\mathbf{x}[1:2]) & \phi^*_2(\mathbf{x}[1:3]) & \dots & \phi^*_2(\mathbf{x}[1:n]) & \phi^*_2(\mathbf{x}[1:n+1]) \\ \perp & \perp & \phi^*_3(\mathbf{x}[1:3]) & \dots & \phi^*_3(\mathbf{x}[1:n]) & \phi^*_3(\mathbf{x}[1:n+1]) \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \perp & \perp & \perp & \dots & \phi^*_k(\mathbf{x}[1:n]) & \phi^*_k(\mathbf{x}[1:n+1]) \end{bmatrix}$$
$$S_{h,m} = \arg\min_{l=h}^{m} \phi^*_{h-1}(\mathbf{x}[1:l]) + \phi(\mathbf{x}[l:m])$$

Thus in order to solve the problem we need to compute the S matrix and then find the indices by calling with parameters k, n the following function:
Indices$(k', n') \triangleq$ **if** $k > 1$: $\{S_{k',n'}\} \cup$ Indices$(k'-1, S_{k',n'} - 1)$ **else**: $\emptyset$.

Cost analysis: In order to compute the optimal indices as shown above the full S matrix is needed therefore the cost in terms of space is in $O(kn)$. The computation time of the algorithm is in $O(kn^3)$ since the time for computing each cell of the matrix is in $O(n^2)$. The latter cost can be reduced to be in $O(n)$ obtaining a computation time in $O(kn^2)$ observing that $\phi(\mathbf{x}[l:m])$ can be computed once in a given row using any online algorithm for the Total Sum of Squares (or Corrected Sum of Squares). We overlooked the cost of sorting the points since it does not affect the computation time in Big-O notation.

2. We are given a set P of n points in $\mathbb{R}$. For simplicity, assume that $\mu(P) = 0$, that is, $\sum_{x \in P} x = 0$. Let $\|P\|^2 = \sum_{x \in P} x^2$ be the optimal 1-means cost. Show that by adding carefully $O(1/\epsilon)$ centers, we can make the k-means cost at most $\epsilon \cdot \sum_{x \in P} x^2$.

   Hint: First show that by adding 2 centers at locations $-\ell$ and ℓ, for an appropriate value of ℓ, the cost decreases by a factor of 3/4.

   Solution: Assume we add $1/2\epsilon$ pairs of *symmetric* centers $\ell_1, \ell_2, ..., \ell_{1/2\epsilon}$ and $-\ell_1, -\ell_2, ..., -\ell_{1/2\epsilon}$ with $\ell_{i-1} \leq \ell_i$ and $\ell_i \geq 0, \forall i$ and denote by P_i^+ the set of points assigned to center ℓ_i and P_i^- the ones assigned to $-\ell_i$. Also let P_0 be the set of points assigned to center 0. Then we can write the cost as

$$\begin{aligned}
\phi &= \sum_{x \in P_0} x^2 + \sum_{i=1}^{1/2\epsilon} \sum_{x \in P_i^+} (x - \ell_i)^2 + \sum_{i=1}^{1/2\epsilon} \sum_{x \in P_i^-} (x + \ell_i)^2 \\
&= \sum_{x \in P_0} x^2 + \sum_{i=1}^{1/2\epsilon} \sum_{x \in P_i^+} (x^2 - 2x\ell_i + \ell_i^2) + \sum_{i=1}^{1/2\epsilon} \sum_{x \in P_i^-} (x^2 + 2x\ell_i + \ell_i^2) \\
&= \sum_{x \in P} x^2 + \sum_{i=1}^{1/2\epsilon} \sum_{x \in P_i^+} (-2x\ell_i + \ell_i^2) + \sum_{i=1}^{1/2\epsilon} \sum_{x \in P_i^-} (2x\ell_i + \ell_i^2) \\
&= \|P\|^2 + \sum_{i=1}^{1/2\epsilon} \sum_{x \in P_i^+} (-2x\ell_i + \ell_i^2) + \sum_{i=1}^{1/2\epsilon} \sum_{x \in P_i^-} (2x\ell_i + \ell_i^2).
\end{aligned}$$

   We can observe that $\forall x \in P_i \wedge 1 \leq i < 1/2\epsilon$ holds $|x| \geq \frac{\ell_{i+1} + \ell_i}{2}$ and for $i = 1/2\epsilon$, $|x| \geq \frac{l_i}{2}$ i.e. the points belonging to a center i should be closer to center i than $i+1$ (preceding center). Given that in the sums above $\forall x \in P_i^+ \rightarrow -2x\ell_i \leq 0$ and $\forall x \in P_i^- \rightarrow 2x\ell_i \leq 0$ we can write

$$\begin{aligned}
\phi &= \|P\|^2 + \sum_{i=1}^{1/2\epsilon} \sum_{x \in P_i^+} (-2x\ell_i + \ell_i^2) + \sum_{i=1}^{1/2\epsilon} \sum_{x \in P_i^-} (2x\ell_i + \ell_i^2) \\
&\leq \|P\|^2 + \sum_{i=1}^{1/2\epsilon - 1} \sum_{x \in P_i^+} (-2\left(\frac{\ell_{i+1} + \ell_i}{2}\right)\ell_i + \ell_i^2) + \sum_{i=1}^{1/2\epsilon - 1} \sum_{x \in P_i^-} (2\left(-\frac{\ell_{i+1} + \ell_i}{2}\right)\ell_i + \ell_i^2) \\
&= \|P\|^2 - 2\sum_{i=1}^{1/2\epsilon - 1} \sum_{x \in P_i^+} (\ell_i \ell_{i+1}) \\
&\leq \|P\|^2 - 2\sum_{i=1}^{1/2\epsilon - 1} (\ell_i \ell_{i+1}) \\
&= \|P\|^2 - \frac{\epsilon - 1}{2\epsilon - 1} \|P\|^2 \sum_{i=1}^{1/2\epsilon - 1} \frac{1}{i(i+1)} \qquad \text{if } \ell_i = \frac{1}{i\sqrt{2}} (\|P\|^2)^{\frac{1}{2}} \frac{\epsilon - 1}{2\epsilon - 1} \\
&= \epsilon \|P\|^2
\end{aligned}$$