Sketching Algorithms for Big Data

Fall 2017

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1 Low-Rank Approximation and Clustering Via Sketching

We approach solving the problems of low-rank approximation and clustering via a generalization of subspace embeddings called "Projection-Cost Preserving Sketches", or PCP's for short. The material for this lecture comes from a paper by Cohen et al. [1].

1.1 Low-Rank Approximation

Definition 1 (Low-Rank Approximation). Given $A \in \mathbb{R}^{n \times d}$, find $\underset{\text{rank } k \text{ matrix } B}{\operatorname{argmin}} \|A - B\|_F^2$. Or equivalently, find $\underset{\text{rank } k \text{ projection matrix } P}{\operatorname{argmin}} \|A - PA\|_F^2$.

The output P^* of Low-Rank Approximation is a projection onto A's top k singular vectors, i.e.,

$$P^*A = U_k U_k^T A = A_k$$

where U_k is the matrix with the top k singular vectors of A.

This takes $O(nd^2)$ time, and approximate iterative methods take O(nnz(A)k) time, where nnz(A) is the number of nonzero values of A. We want to do better.

Definition 2 (PCP). $\tilde{A} \in \mathbb{R}^{n \times m}$ is an (ε, k) -PCP for A if \forall rank k projections P:

$$(1-\varepsilon)\|A - PA\|_F^2 \le \|\tilde{A} - P\tilde{A}\|_F^2 \le (1+\varepsilon)\|A - PA\|_F^2$$

Ideally we have $m \ll d$.

Now assuming we have \tilde{A} an (ε, k) -PCP for A, let $\tilde{P}^* = \underset{\text{rank } k \text{ projections } P}{\operatorname{argmin}} \|\tilde{A} - P\tilde{A}\|_F^2$. Then

$$\begin{split} \|A - \tilde{P}^*A\|_F^2 &\leq \frac{1}{1 - \varepsilon} \|\tilde{A} - \tilde{P}^*\tilde{A}\|_F^2 \\ &\leq \frac{1}{1 - \varepsilon} \|\tilde{A} - P^*\tilde{A}\|_F^2 \\ &\leq \frac{1 + \varepsilon}{1 - \varepsilon} \|A - P^*A\|_F^2 \end{split}$$

For small ε we have $\frac{1+\varepsilon}{1-\varepsilon} = 1 + O(\varepsilon)$.

The run time using PCP is now $O(nm^2)$.

Theorem 3. We can compute an (ε, k) -PCP for A in $nnz(A) + \tilde{O}(nk^2/\varepsilon^2)$ time with $m \approx k/\varepsilon^2$.

This would make the total run time $O(nnz(A)) + \tilde{O}(nk^2/\varepsilon^4)$. Before proving this theorem, we show another application of PCPs.

1.2 Constrained Low-Rank Approximation Problem

Definition 4 (Constrained Low-Rank Approximation Problem). Let $T \subseteq$ all rank k projection matrices. Then find $\underset{P \in T}{\operatorname{argmin}} \|A - PA\|_F^2$.

Claim 5. If \tilde{A} is an (ε, k) -PCP for A, and $\tilde{P} \leq \gamma \min_{P \in T} \|\tilde{A} - P\tilde{A}\|_F^2$, then

$$\|A - \tilde{P}A\|_F^2 \le (1 + O(\varepsilon))\gamma \min_{P \in T} \|A - PA\|_F^2$$

This follows from the same reasoning as before.

Definition 6 (k-means clustering). Given $a_1, ..., a_n \in \mathbb{R}^d$, which we can represent as the rows of $A \in \mathbb{R}^{n \times d}$,

$$\min_{\text{partitions into } k \text{ sets } C = \{C_1, \dots, C_k\}} \sum_{i=1}^{\kappa} \sum_{j \in C_i} \|a_j - \mu(C_i)\|_2^2$$

where $\mu(C_i) = \frac{1}{|C_i|} \sum_{j \in C_i} a_j$ is the centroid.

We now show that k-means is constrained low-rank approximation. Let

$$f(C, A) = \sum_{j \in C_i} \|a_j - \mu(C_i)\|_2^2.$$

Then we will show

$$f(C, A) = ||A - P_C A||_F^2$$

for some rank k projection matrix P_C .

We have $P_C = Z_C^T Z_C$, where Z_C is a cluster indicator matrix, i.e., $Z_C \in \mathbb{R}^{k \times n}$ and

$$(Z_C)_{ij} = \begin{cases} \frac{1}{\sqrt{|C_i|}} & \text{if } a_j \in C_i \\ 0 & \text{otherwise.} \end{cases}$$

Note Z_C is an orthogonal matrix and $Z_C Z_C^T = I$, which implies P_C is a projection. So we get $||A - Z_C^T Z_C A||_F^2$.

After showing these applications, we now show how to get a PCP sketch.

2 Projection-Cost Preserving Sketches

2.1 Subspace Embeddings

Definition 7 (Subspace Embedding). Given $A \in \mathbb{R}^{n \times d}$, S is an ε -subspace embedding if $\forall x \in \mathbb{R}^n$, $\|x^T A S\|_2^2 \in (1 \pm \varepsilon) \|x^T A\|_2^2$.

Observation 8. If S is a subspace embedding, it is an (ε, k) -PCP for any k.

Let $Y \in \mathbb{R}^{n \times n}, Y = I - P$.

Then PCP is equivalent to

$$\|Y\tilde{A}\|_{F}^{2} = \sum_{i=1}^{n} \|y_{i}^{T}\tilde{A}\|_{2}^{2} \in (1 \pm \varepsilon) \|YA\|_{F}^{2}$$

Then set $\tilde{A} = AS$. We get

$$\|YAS\|_{F}^{2} = \sum_{i=1}^{n} \|y_{i}^{T}AS\|_{2}^{2} \in (1 \pm \varepsilon) \sum_{i=1}^{n} \|y_{i}^{T}A\|_{2}^{2} = (1 \pm \varepsilon)\|YA\|_{F}^{2}$$

S works but is too expensive. Typically $S \in \mathbb{R}^{d \times m}$ where $m = \Theta(d/\varepsilon^2)$. We want $m = \Theta(k/\varepsilon^2)$.

2.2 Smaller m

Theorem 9. $S \in \mathbb{R}^{d \times m}$, where $S_{ij} = \pm \frac{1}{\sqrt{m}}$ independently at random. Then if $m = O(k \log(1/\delta)\varepsilon^{-2})$, then $\tilde{A} = AS$ is (ε, k) -PCP with probability $1 - \delta$.

That is, letting Y = I - P for any rank k projection P, we want the PCP guarantee:

$$|||YA||_F^2 - ||YAS||_F^2| \le \varepsilon ||YA||_F^2$$

Write $A = A_k + A_{\overline{k}}$, where A_k is A projected onto its top k singular vectors (what we care about) and $A_{\overline{k}}$ is the rest (noise).

Then our expression becomes

$$|||Y(A_k + A_{\overline{k}})||_F^2 - ||Y(A_k + A_{\overline{k}})S||_F^2|$$

Now using the fact that $||M||_F^2 = \operatorname{tr}(MM^T)$:

$$\operatorname{tr}(YA_{k}A_{k}^{T}Y) + \operatorname{tr}(YA_{\overline{k}}A_{\overline{k}}^{T}Y) + 2\operatorname{tr}(YA_{k}A_{\overline{k}}^{T}Y) - \operatorname{tr}(YA_{k}SS^{T}A_{k}^{T}Y) - \operatorname{tr}(YA_{\overline{k}}SS^{T}A_{\overline{k}}^{T}Y) - 2\operatorname{tr}(YA_{k}SS^{T}A_{\overline{k}}^{T}Y) - \operatorname{tr}(YA_{k}SS^{T}A_{\overline{k}}^{T}Y) - \operatorname{tr}(YA_{k}SS^{T}A_{\overline{k}}^{T}$$

Note that $\operatorname{tr}(YA_kA_{\overline{k}}^TY) = 0$ since $A_k, A_{\overline{k}}$ are orthogonal.

2.3 Head Terms (Subspace Embedding)

We show

$$|\operatorname{tr}(YA_kA_k^TY) - \operatorname{tr}(YA_kSS^TA_k^TY)| \le \varepsilon ||YA||_H^2$$

Note the left hand side is

$$|||YA_k||_F^2 - ||YA_kS||_F^2| \le \varepsilon ||YA||_F^2$$

 A_k is rank k, so since $m \approx k/\varepsilon^2$, S is an ε -subspace embedding for A_k , i.e., $\forall x, \|x^T A_k S\|_2^2 \in (1 \pm \varepsilon) \|x^T A_k\|_2^2$.

2.4 Tail Term (Approximate Matrix Multiplication)

We bound

$$|\operatorname{tr}(YA_{\overline{k}}A_{\overline{k}}^{T}Y) - \operatorname{tr}(YA_{\overline{k}}SS^{T}A_{\overline{k}}^{T}Y)|$$

Recall Y = I - P.

$$||(I-P)A_{\overline{k}}||_F^2 = ||A_{\overline{k}}||_F^2 - ||PA_{\overline{k}}||_F^2$$

So we get

$$\|A_{\overline{k}}\|_{F}^{2} - \|PA_{\overline{k}}\|_{F}^{2} - \|A_{\overline{k}}S\|_{F}^{2} + \|PA_{\overline{k}}S\|_{F}^{2}$$
$$\|A_{\overline{k}}\|_{F}^{2} - \|A_{\overline{k}}S\|_{F}^{2} \leq c\|A_{\overline{k}}\|_{F}^{2} \leq$$

If $m > \log(1/\delta)\varepsilon^{-2}$, then $|||A_{\overline{k}}||_F^2 - ||A_{\overline{k}}S||_F^2| \le \varepsilon ||A_{\overline{k}}||_F^2 \le \varepsilon ||(I-P)A||_F^2$ for any P. Now

$$\begin{split} &|\|PA_{\overline{k}}\|_F^2 - \|PA_{\overline{k}}S\|_F^2| \\ &= |\operatorname{tr}(P[A_{\overline{k}}A_{\overline{k}}^T - A_{\overline{k}}SS^TA_{\overline{k}}^T]P)| \end{split}$$

Let $M = A_{\overline{k}}A_{\overline{k}}^T - A_{\overline{k}}SS^TA_{\overline{k}}^T$ and let $\lambda_1 > \ldots > \lambda_k > 0$ be its first k eigenvalues. Then we get

$$= \sum_{i=1}^{k} \lambda_i(M) |$$

$$\leq \sum_{i=1}^{k} |\lambda_i(M)|$$

$$\leq \sqrt{k} \sqrt{\sum_{i=1}^{k} \lambda_i^2(M)}$$

$$\leq \sqrt{k} \|PMP\|_F$$

$$\leq \sqrt{k} \|M\|_F$$

Recall (Approximate Matrix Multiplication) that for any C, D,

$$\|CD - CSS^TD\| \le \frac{1}{\sqrt{m}} \|C\|_F \|D\|_F$$

where m is the number of columns in S.

Here, we take $C = D = A_{\overline{k}}$. Then we get

$$\leq \sqrt{k} \frac{\varepsilon}{\sqrt{k}} \|A_{\overline{k}}\|_F^2$$
$$\leq \varepsilon \|A_{\overline{k}}\|_F^2$$
$$\leq \varepsilon \|(I-P)A\|_F^2$$

for any P.

2.5 Cross Term

We show

$$|\operatorname{tr}(YA_kSS^TA_{\overline{k}}^TY)|$$

is small. Set $C = AA^T$ and let C^+ be the pseudoinverse of C. Then this becomes

$$\begin{aligned} |\operatorname{tr}(YCC^{+}A_{k}SS^{T}A_{\overline{k}}^{T}Y)| \\ &= |\operatorname{tr}(Y^{2}CC^{+}A_{k}SS^{T}A_{\overline{k}}^{T})| \\ &= |\operatorname{tr}(YCC^{+}A_{k}SS^{T}A_{\overline{k}}^{T})| \\ &= |\operatorname{tr}((YCC^{+/2})(C^{+/2}A_{k}SS^{T}A_{\overline{k}}^{T})| \\ &\leq \sqrt{\operatorname{tr}(YCC^{+/2}C^{+/2}CY)}\sqrt{\operatorname{tr}(A_{\overline{k}}SS^{T}A_{k}^{T}C^{+/2}C^{+/2}A_{k}SS^{T}A_{\overline{k}}^{T})} \end{aligned}$$

where the last inequality comes from Cauchy-Schwarz. Then the first part can be bounded by

$$\sqrt{\operatorname{tr}(YCC^{+/2}C^{+/2}CY)}$$
$$= \sqrt{\operatorname{tr}(YCY)}$$
$$= \sqrt{\operatorname{tr}(YAA^{T}Y)}$$
$$= ||YA||_{F}$$

Using SVD, we get $A_k = V_k \Sigma_k V_k^T$, so

$$\begin{split} &\sqrt{\operatorname{tr}(A_{\overline{k}}SS^TA_k^TC^{+/2}C^{+/2}A_kSS^TA_{\overline{k}}^T)} \\ &= \sqrt{\operatorname{tr}(A_{\overline{k}}SS^TV_k\Sigma_kU_k^TU\Sigma^{-2}U^TU_k\Sigma_kV_k^TSS^TA_{\overline{k}}^T)} \\ &= \sqrt{\operatorname{tr}(A_{\overline{k}}SS^TV_kV_k^TSS^TA_{\overline{k}}^T)} \\ &= \|A_{\overline{k}}SS^TV_k\|_F \\ &\leq \frac{1}{\sqrt{m}}\|A_{\overline{k}}\|_F\|V_k\|_F \\ &\leq \frac{\varepsilon}{\sqrt{k}}\|(I-P)A\|_F\sqrt{k} \\ &= \varepsilon\|(I-P)A\|_F \end{split}$$

again for any P.

References

 Michael Cohen, Sam Elder, Cameron Musco, Christopher Musco, Madalina Persu. Dimensionality Reduction for k-Means Clustering and Low Rank Approximation. In Proceedings of the Forty-Seventh Annual ACM on Symposium on Theory of Computing, pages 163–172. ACM, 2015.