

Notes on Sketching for Low Rank Approximation

1 Low rank approximation of a matrix

Let A be an $m \times n$ matrix over reals. In practice, it is often the case that both m and n are very large. For example, consider a customer-product buying matrix A , where, the row indices $i = 1, 2, \dots, m$ correspond to ids given to customers and the column indices $j = 1, 2, \dots, n$ correspond to product ids. Typically A_{ij} denotes the number of times customer i purchased product j (or, A_{ij} denotes the number of units of product j purchased by customer i , etc.). Such matrices typically can be quite sparse and/or have “lot of noise”. For example, consider the matrix

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \epsilon_1 & 0 \\ 0 & 0 & \epsilon_2 \end{bmatrix}$$

where, we assume that $|\epsilon_1|, |\epsilon_2| \ll 1$. So A has full rank, although it seems to be reasonably well approximated by the rank 1 matrix

$$\hat{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

This is often quantified by answering the following questions:

1. What is $\|A - \hat{A}\|_F$? or,
2. What is $\|A - \hat{A}\|_2$?

In this example, it is easy to see that $\|A - \hat{A}\|_F = (\epsilon_1^2 + \epsilon_2^2)^{1/2}$ and $\|A - \hat{A}\|_2 = \max(|\epsilon_1|, |\epsilon_2|)$. The low rank approximation question is posed as follows.

Let A be an $m \times n$ matrix. The best rank- k approximation matrix with respect to Frobenius (resp. 2-norm) for A is a matrix $\hat{A} \in \mathbb{R}^{m \times n}$ satisfying the following condition:

$$\|A - \hat{A}\|_F = \min_{\text{rank}(X) \leq k} \|A - X\|_F .$$

The notation $\text{argmin}_{X \in S} \phi(X)$ is often used to return a value of $X^* \in S$ in the feasible space S that attains the minimum value $\min\{\phi(X) \mid X \in S\}$. That is, $\phi(X^*) = \min\{\phi(X) \mid X \in S\}$. In this notation,

$$\hat{A} = \text{argmin}_{\text{rank}(X) \leq k} \|A - X\|_F .$$

Analogously, a similar definition for the best rank- k approximation may be formulated with respect to the 2-norm of a matrix. This defines \hat{A} to be a matrix that minimizes the $\|A - X\|_2$, among all matrices $X \in \mathbb{R}^{m \times n}$ such that $\text{rank}(X) \leq k$. That is,

$$\|A - \hat{A}\|_2 = \min_{\text{rank}(X) \leq k} \|A - X\|_2, \text{ or, } \hat{A} = \text{argmin}_{\text{rank}(X) \leq k} \|A - X\|_2 .$$

The Eckart-Young Theorem. We now state the famous and widely applicable Eckart-Young Theorem. We first state a few notations used by this theorem. Let $A \in \mathbb{R}^{m \times n}$ be a given matrix and let $A = U\Sigma V^T$ be the classical SVD of A . Let $\text{rank}(A) = r$. In this notation, we assume that the corresponding left singular vectors in U and right singular vectors in V are arranged so that the sequential diagonal entries of Σ are ordered in a non-increasing order, that is,

$$\sigma_1 = \Sigma_{11} \geq \sigma_2 = \Sigma_{22} \geq \cdots \geq \sigma_r = \Sigma_{rr} .$$

All other entries in the matrix Σ are zeros. For $1 \leq k \leq r$, the Eckart-Young theorem's statement defines the notation A_k to denote the matrix

$$A_k = U\Sigma_k V^T = U \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_k \\ & & & & 0 \end{bmatrix} V^T$$

where, Σ_k has only the first k -diagonal entries $\sigma_1, \sigma_2, \dots, \sigma_k$ in sequence, and all other entries including all remaining diagonal entries set to zero. Another way of viewing A and the A_k 's are the sum of single rank matrices.

$$A = U\Sigma V^T = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \cdots + \sigma_r u_r v_r^T$$

where, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$. A_k is the sum of the first k terms in the above summation, that is,

$$A_k = U\Sigma_k V^T = \sigma_1 u_1 v_1^T + \cdots + \sigma_k u_k v_k^T .$$

It follows that

$$\begin{aligned} A - A_k &= U(\Sigma - \Sigma_k)V^T \\ &= \sigma_{k+1} u_{k+1} v_{k+1}^T + \cdots + \sigma_r u_r v_r^T \\ &= U \begin{bmatrix} 0 & & & \\ & \ddots & & \\ & & \sigma_{k+1} & \\ & & & \ddots \\ & & & & \sigma_r \end{bmatrix} V^T . \end{aligned}$$

$\Sigma - \Sigma_k$ has top k diagonal entries as zeros, followed by the diagonal entries $\sigma_{k+1}, \dots, \sigma_r$. All other entries of $\Sigma - \Sigma_k$ are zeros.

It follows that

1. $\|A - A_k\|_2 = \sigma_{k+1}$
2. $\|A - A_k\|_F = (\sigma_{k+1}^2 + \cdots + \sigma_r^2)^{1/2}$

We now state the Eckart-Young Theorem.

Theorem 1. *Eckart-Young Theorem*

1. $\|A - A_k\|_F = \min_{\text{rank}(X) \leq k} \|A - X\|_F, \quad A_k = \text{argmin}_{\text{rank}(X) \leq k} \|A - X\|_F .$
2. $\|A - A_k\|_2 = \min_{\text{rank}(X) \leq k} \|A - X\|_2, \quad A_k = \text{argmin}_{\text{rank}(X) \leq k} \|A - X\|_2 .$

The Eckart-Young theorem states that the best rank- k or less approximation matrix for A is A_k , for both Frobenius norm and 2-norm.

There are varied advantages of approximating A by a low rank A_k , for example,

1. Space complexity of storing the approximation is less $O((m+n)k)$ real numbers.
2. Data is more interpretable and has less noise, etc.. High rank can be because of noise.

2 Low rank approximation

The best rank- k approximation of a matrix A by A_k is universally obtained by using the Eckart-Young theorem. This requires the computation of the SVD of A . Typically this requires time $O(\min(mn^2, m^2n))$. In this section, we consider the problem of using sketching to obtain low rank approximation of a matrix A more efficiently than that given above, while obtaining bounds on how much sub-optimal it can get as compared to A_k (for rank- k approximation).

2.1 Motivation

Consider as a first step the linear regression problem

$$\min_X \|A_k X - A\|_F .$$

First, we note that by the Eckart-Young's theorem, $X = I_n$ is clearly an optimal solution, since, $A_k X$ has rank at most $\text{rank}(A_k) = k$. Therefore,

$$\|A_k \cdot I - A\|_F \geq \min_X \|A_k X - A\|_F \geq \min_{\text{rank}(Y) \leq k} \|Y - A\|_F = \|A_k - A\|_F$$

since, $Y = A_k$ is an optimal solution to the latter problem above, by Eckart-Young theorem.

Suppose we write the matrix of right singular vectors V as

$$V = [v_1 \ v_2 \ \dots, v_n] = [V_k \ V_k^\perp]$$

where, $V_k = [v_1 \ \dots \ v_k]$ and $V_k^\perp = [v_{k+1} \ \dots \ v_n]$. Note that the optimal solution to the linear regression problem $\min_X \|A_k X - A\|_F$ is

$$X^* = A_k^- A = V \Sigma_k^- U^T U \Sigma V^T = V \Sigma_k^- \Sigma V^T = [V_k \ V_k^\perp] \begin{bmatrix} I_k & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_k^T \\ (V_k^\perp)^T \end{bmatrix} = [V_k \ V_k^\perp] \begin{bmatrix} V_k^T \\ 0 \end{bmatrix} = V_k V_k^T$$

Further,

$$\|X^*\|_F = \|V_k V_k^T\|_F = \|V_k\|_F = \sqrt{k} .$$

Above, it was suggested that $X = I$ is an optimal solution to $\min_X \|A_k X - A\|_F$? Below, we try to connect the dots (if any left unspecified). Suppose we write the left singular vector matrix U as

$$U = \begin{bmatrix} u_1 & u_2 & \cdots & u_m \end{bmatrix} = \begin{bmatrix} U_k & U_k^\perp \end{bmatrix}$$

where, $U_k = \begin{bmatrix} u_1 & \cdots & u_k \end{bmatrix}$ and $U_k^\perp = \begin{bmatrix} u_{k+1} & \cdots & u_m \end{bmatrix}$. Then,

$$A_k X^* = (U_k \Sigma_k V_k^T)(V_k V_k^T) = U_k \Sigma_k V_k^T = A_k \text{ .}$$

In other words, the optimal solution value to $\min_X \|A_k X - A\|_F$ is $\|A_k - A\|$. The solution to the problem

$$\operatorname{argmin}_X \|X\|_F \text{ subject to } \|A_k X - A\|_F = \|A_k - A\|_F$$

is X^* , based on linear regression. The general solution to $A_k X = A_k$ is $X = V_k V_k^T + (V_k^\perp) Y$, where, $Y \in \mathbb{R}^{(n-k) \times n}$ is any matrix. In particular, a solution is $Y = (V_k^\perp)^T$, which gives $X = V_k V_k^T + V_k^\perp (V_k^\perp)^T = I_n$. Further, the general solution $X = V_k V_k^T + (V_k^\perp)^T Y$ has Frobenius norm

$$\begin{aligned} \|X\|_F^2 &= \|V_k V_k^T + V_k^\perp Y\|_F^2 \\ &= \|V_k V_k^T\|_F^2 + \|V_k^\perp Y\|_F^2 + 2 \operatorname{tr} V_k V_k^T V_k^\perp Y \\ &= \|V_k^T\|_F^2 + \|Y\|_F^2 \\ &= k + \|Y\|_F^2 \end{aligned}$$

since, step 3 follows from $V_k^T V_k^\perp = 0_{k \times (n-k)}$.

With this detour, we now return to our problem $\min_X \|A_k X - A\|_F$.

Affine subspace embeddings

Suppose we consider solving the problem $\min_X \|A_k X - A\|_F$ approximately using affine subspace embeddings. Let S be a random matrix drawn from a distribution \mathcal{D} such that S approximately preserves the norms of vectors in the affine subspace $A_k X - A$, that is,

$$\|SA_k X - SA\|_F \in (1 \pm \epsilon) \|A_k X - A\|_F, \quad \text{for all } X \in \mathbb{R}^{n \times n} \text{ .}$$

It would then follow that

$$\min_X \|SA_k X - SA\|_F \leq (1 + \epsilon) \min_X \|A_k X - A\|_F = (1 + \epsilon) \|A_k - A\|_F \text{ .}$$

The solution

$$\operatorname{argmin}_X \|SA_k X - SA\|_F \text{ is } \hat{X} = (SA_k)^- SA$$

and therefore, by affine subspace embedding norm preservation properties,

$$(1 - \epsilon) \|A_k \hat{X} - A\|_F \leq \|SA_k \hat{X} - SA\|_F \leq (1 + \epsilon) \|A_k - A\|_F \text{ .}$$

Since, $\hat{X} = (SA_k)^- SA$, substituting in the above,

$$\|A_k (SA_k)^- SA - A\|_F \leq \left(\frac{1 + \epsilon}{1 - \epsilon} \right) \|A_k - A\|_F = (1 + 3\epsilon) \|A_k - A\|_F$$

for $\epsilon \leq \frac{1}{9}$.

Note that $A_k(SA_k)^-SA$ is a matrix with rank at most k (since it has A_k as a factor) and whose rowspace is a subspace of the row space of SA .

Conclusion. Consider a solution to the problem

$$\min_{\text{rank}(X) \leq k} \|XSA - A\|_F .$$

Then,

$$\min_{\text{rank}(X) \leq k} \|XSA - A\|_F \leq \|A_k(SA_k)^-SA - A\|_F \leq (1 + 3\epsilon)\|A_k - A\|_F$$

where, the first inequality follows by setting $X = A_k(SA_k)^-SA$ and the last inequality follows from the previous paragraph. Further, since $\text{rank}(XSA) \leq \text{rank}(X) \leq k$,

$$\min_{\text{rank}(X) \leq k} \|XSA - A\|_F \geq \min_{\text{rank}(Y) \leq k} \|Y - A\|_F = \|A_k - A\|_F .$$

Putting the two equations together, we have,

$$\|A_k - A\|_F \leq \min_{\text{rank}(X) \leq k} \|XSA - A\|_F \leq (1 + 3\epsilon)\|A_k - A\|_F .$$

So, we now turn towards trying to solve the optimization problem $\min_{\text{rank}(X) \leq k} \|XSA - A\|_F$.

2.2 How to solve $\|XSA - A\|_F$ subject to $\text{rank}(X) \leq k$

Let us consider how to solve the problem

$$\min_{\text{rank}(X) \leq k} \|XSA - A\|_F$$

and the problems encountered in doing so. Let X^* denote the least Frobenius solution to the regression problem $\min_X \|XSA - A\|_F$. Then, by linear regression,

$$X^* = A(SA)^- \quad \text{and} \quad X^*SA = A(SA)^-SA .$$

In particular,

$$X^*SA - A = A(SA)^-SA - A = -A(I - (SA)^-SA)$$

has a row space that lies in the orthogonal complement to the row space of SA . (For this discussion, keep S fixed. In other words, the discussion is conditional on S).

$$\begin{aligned} \|XSA - A\|_F^2 &= \|(X - X^*)SA + X^*SA - A\|_F^2 \\ &= \|(X - X^*)SA\|_F^2 + \|X^*SA - A\|_F^2 \end{aligned}$$

since, $(X - X^*)SA$ has a rowspace which is a subspace of the row space of SA and $X^*SA - A$ has a row space in the orthogonal complement space of SA of \mathbb{R}^n . Therefore,

$$\min_{\text{rank}(X) \leq k} \|XSA - A\|_F^2 = \|X^*SA - A\|_F^2 + \min_{\text{rank}(X) \leq k} \|(X - X^*)SA\|_F^2$$

since, $\|X^*SA - A\|_F$ is not a function of X .

We may use the Eckart-Young theorem for the following problem.

$$\min_{\text{rank}(X) \leq k} \|XSA - X^*SA\|_F = \min_{\text{rank}(X) \leq k} \|XSA - A(SA)^-SA\|_F$$

Let $SA = U\Sigma V^T$ in SVD form. Then, letting $Y = XU\Sigma$,

$$\begin{aligned} \min_{\text{rank}(X) \leq k} \|XSA - A(SA)^-SA\|_F &= \min_{\text{rank}(X) \leq k} \|XU\Sigma V^T - A(SA)^-U\Sigma V^T\|_F \\ &= \min_{\text{rank}(X) \leq k} \|XU\Sigma - A(SA)^-U\Sigma\|_F \\ &= \min_{\text{rank}(Y) \leq k} \|Y - A(SA)^-U\Sigma\|_F . \end{aligned}$$

The minimization step has optimal solution $Y^* = [A(SA)^-U\Sigma]_k$ by the Eckart-Young theorem. The final solution $X^* = Y^*\Sigma^{-1}U^T$.

The problem that arises is how to find the SVD of $A(SA)^-U\Sigma$ more efficiently, since it is an $m \times n$ matrix.

2.3 Solving Affine Embedding

Consider the problem considered in the subsection above, namely,

$$\min_{\text{rank}(X) \leq k} \|XSA - A\|_F .$$

Conditioned on S , we can consider an embedding R such that it approximately preserves norms for the affine embedding:

$$\|XSAR - AR\|_F \in (1 \pm \epsilon)\|XSA - A\|_F, \quad \text{for all } X \in \mathbb{R}^{m \times k}.$$

Following the steps in the previous subsection, and letting $\hat{X} = AR(SAR)^-$ we have,

$$\min_{\text{rank}(X) \leq k} \|XSAR - AR\|_F^2 = \|X^*SAR - AR\|_F^2 + \min_{\text{rank}(X) \leq k} \|XSAR - X^*SAR\|_F^2 .$$

Letting $SAR = U\Sigma V^T$, we have,

$$\|XSAR - X^*SAR\|_F = \|(X - X^*)U\Sigma V^T\|_F = \|(X - X^*)U\Sigma\|_F .$$

Therefore,

$$\begin{aligned} \min_{\text{rank}(X) \leq k} \|XSAR - X^*SAR\|_F &= \min_{\text{rank}(X) \leq k} \|XU\Sigma - AR(SAR)^-U\Sigma\|_F \\ &= \min_{\text{rank}(Y) \leq k} \|Y - AR(SAR)^-U\Sigma\|_F . \end{aligned}$$

The solution is obtained by letting $Y^* = [AR(SAR)^-U\Sigma]_k$ and obtaining

$$X^* = Y^*\Sigma^{-1}U^T = Y^*(\Sigma_k)^{-1}U_k^T .$$

Since $\text{rank}(Y^*) \leq k$, $\text{rank}(X^*) \leq k$.