

A PROOFS AND DERIVATIONS

PROOF 1. (**Proposition ??**) For any two sub-matrix : $X_1, X_2 \in R^{N \times 1}$, regardless of row or column sub-matrix of the original matrix. Note for any matrix X_S with column = 1, $(X_S^T X_S)^{-1} = \|X_S\|^2 = \text{Vol}(X_S)^2$. Considering the pseudo-inverse is denoted as: $X_S^+ := (X_S^T X_S)^{-1} X_S^T$, the bias variation is:

$$\begin{aligned}
 \text{bias}_2^2 - \text{bias}_1^2 &= \|X^+ - X_2^+\|^2 - \|X^+ - X_1^+\|^2 \\
 &= \|X^+\|^2 - 2 \langle X^+, X_2^+ \rangle + \|X_2^+\|^2 - \|X^+\|^2 + 2 \langle X^+, X_1^+ \rangle - \|X_1^+\|^2 \\
 &= \|X^+\|^2 - 2 \|X_2^+\|^2 + \|X_2^+\|^2 - \|X^+\|^2 + 2 \|X_1^+\|^2 - \|X_1^+\|^2 \\
 &= \|X_1^+\|^2 - \|X_2^+\|^2 = \frac{1}{\|X_1\|^4} \|X_1^T\|^2 - \frac{1}{\|X_2\|^4} \|X_2^T\|^2 \\
 &== \frac{1}{\|X_1\|^2} - \frac{1}{\|X_2\|^2} = \frac{1}{\text{Vol}(X_1)^2} - \frac{1}{\text{Vol}(X_2)^2}
 \end{aligned} \tag{1}$$

Since the $\text{Vol}(X)$ is constant under $\text{column} = 1$, a larger volume yields a smaller bias is proved. Combined with the relation $\text{variation}_1 - \text{variation}_2 = \text{bias}_2 - \text{bias}_1$, a larger volume yields a larger parameter variation is apparent.

PROOF 2. (**Proposition ??**) The proposition ?? is expanded by substituting $X^+ = G^{-1} X^T$, where $G := X^T X$ is the left Gram matrix.

$$\begin{aligned}
 \text{bias}_2^2 - \text{bias}_1^2 &:= \|X^+ - X_2^+\|^2 - \|X^+ - X_1^+\|^2 \\
 &= \|X^+\|^2 - 2 \langle X^+, X_2^+ \rangle + \|X_2^+\|^2 - \|X^+\|^2 + 2 \langle X^+, X_1^+ \rangle - \|X_1^+\|^2 \\
 &= \|X_2^+\|^2 - \|X_1^+\|^2 + 2 \langle X^+, X_1^+ - X_2^+ \rangle \\
 &= \|G_2^{-1} X_2^T\|^2 - \|G_1^{-1} X_1^T\|^2 + 2 \langle G^{-1} X^T, G_1^{-1} X_1^T - G_2^{-1} X_2^T \rangle
 \end{aligned} \tag{2}$$

Inspired by the work of Xu et al.[?], G^{-1} can be expanded by Sylvester's matrix theorem.

THEORY 1. (**Sylvester's Matrix Theorem**). Given a diagonalizable square matrix X , any analytic function $f()$ can be expanded,

$$f(X) = \sum_{l=1}^k f(\lambda_l) X_l, \tag{3}$$

where λ_l is the l -th distinct eigenvalue of X and X_l is the Frobenius covariant as follows:

$$X_l := \prod_{j=1, j \neq l}^k \frac{1}{\lambda_l - \lambda_j} (X - \lambda_j I). \tag{4}$$

COROLLARY 1. Supposing $f()$ is a inverse function, then,

$$f(X) = X^{-1} = \sum_{l=1}^k \frac{1}{\lambda_l} X_l \tag{5}$$

For G is diagonalizable matrix, G^{-1} can be written as follows by above corollary.

$$G^{-1} = \sum_{l=1}^k \frac{1}{\lambda_l} G_l = \prod_{j=1, j \neq l}^k \frac{1}{\lambda_l - \lambda_j} \prod_{j=1, j \neq l}^k (G - \lambda_j I) \tag{6}$$

Denoting $p_l = \prod_{j=1, j \neq l}^k \frac{1}{\lambda_l - \lambda_j}$ and expanding the products, we have:

$$\frac{1}{p_l} = \underbrace{\Lambda \sum_{g=1}^k (-1)^{g+1} \lambda_l^{k-g} \left[\sum_{\mathcal{H} \subseteq \{1, \dots, k\} \setminus \{l\}, |\mathcal{H}|=g-1} \left(\prod_{h \in \{1, \dots, k\} \setminus \mathcal{H}} \frac{1}{\lambda_h} \right) \right]}_{\sigma_l}, \tag{7}$$

where $\Lambda = \prod_{i=1}^k \lambda_i = |\mathbf{G}|$. The Equation 6 can be rewritten as:

$$\begin{aligned} \mathbf{G}^{-1} &= \frac{1}{|\mathbf{G}|} \frac{1}{\sigma_l} \underbrace{\prod_{j=1, j \neq l}^k (\mathbf{G} - \lambda_j \mathbf{I})}_{\mathbf{Q}} \\ &= \frac{1}{\text{Vol}(\mathbf{X})^2} \frac{1}{\sigma_l} \underbrace{\prod_{j=1, j \neq l}^k (\mathbf{G} - \lambda_j \mathbf{I})}_{\mathbf{Q}} \end{aligned} \quad (8)$$

Substituting $\mathbf{G}^{-1}(\mathbf{G}_1^{-1}, \mathbf{G}_2^{-1})$ in Equation 2 by above result, the Equation 2 can be rewritten as:

$$\text{bias}_2^2 - \text{bias}_1^2 = \frac{\|Q_2 X_2^T\|^2}{\text{Vol}(X_2)^4} - \frac{\|Q_1 X_1^T\|^2}{\text{Vol}(X_1)^4} + 2 \left\langle \frac{Q_X X^T}{\text{Vol}(X)^2}, \frac{Q_1 X_1^T}{\text{Vol}(X_1)^2} - \frac{Q_2 X_2^T}{\text{Vol}(X_2)^2} \right\rangle \quad (9)$$

LEMMA 1. For any matrix $X = [X_1^T, X_2^T]^T \in R^{N \times M}$ and $X_1^T, X_2^T \in R^{\frac{N}{2} \times M}$ are submatrices in row, there exists $\text{Vol}(X) \gg \max(\text{Vol}(X_1), \text{Vol}(X_2))$ when $N \rightarrow \infty$. The relation is same for column submatrices.

LEMMA 2. For a invertible matrix A and any column vector u and v , then there exists:

$$\det(A + uv^T) = \det(A) (1 + v^T A^{-1} u) \quad (10)$$

PROOF 3. (**Lemma 1**) Considering a matrix $\bar{X} = [X^T, x^T]^T$, where $X^T \in R^{n \times m}$ is a submatrix, $x^T \in R^{1 \times m}$ is a row vector. The square volume of \bar{X} can be written as:

$$\begin{aligned} \text{Vol}(\bar{X})^2 &= |\bar{X}^T \bar{X}| = \left| \begin{bmatrix} X^T & x^T \end{bmatrix} \begin{bmatrix} X \\ x \end{bmatrix} \right| \\ &= |X^T X + x^T x| = \sigma_1 |X^T X|. \end{aligned} \quad (11)$$

According to the property of transposed matrix product (Lemma 2), the constant coefficient $\sigma = 1 + x(X^T X)^{-1} x^T$ is greater than 1. Considering another submatrix $X' = [x_1^T, \dots, x_n^T]^T$ and adding its row vectors in matrix X row by row, the square volume changing is written as:

$$\begin{aligned} \text{Vol}([X^T, X'^T]^T) &= \text{Vol}([X^T, x_1^T, \dots, x_n^T]^T) \\ &= \sigma_n \text{Vol}([X^T, x_1^T, \dots, x_{n-1}^T]^T) = \dots = \prod_{i=1}^n \sigma_i \text{Vol}(X), \end{aligned} \quad (12)$$

where $\sigma_i = 1 + x_i(X^T X)^{-1} x_i^T$. For each sigma is greater than 1, $\prod_{i=1}^n \sigma_i \rightarrow \infty$ when $n \rightarrow \infty$. Above all, **Lemma 1** is proved taking X_1 and X_2 as a new addition submatrix, respectively. Same conclusions can be applied in column submatrices.

PROOF 4. (**Proposition ??**) Considering a replication-involving dataset $X_{rep} = \begin{bmatrix} X^T, \underbrace{X_S^T, \dots, X_S^T}_d \end{bmatrix}^T$, where $X_S^T \in R$ is row vector and is replicated for d times. According to Equation 12, the square volume of X_{rep} is written as:

$$\text{Vol}(X_{rep})^2 = (1 + X_S(X^T X)^{-1} X_S^T)^d |X^T X| \quad (13)$$

For $(1 + X_S(X^T X)^{-1} X_S^T) > 1$, the exponential increasing of volume under replication is proved. When $\lim_{d \rightarrow \infty} \text{Vol}(X_{rep}) = \infty$ is hold. The same result can be applied in X_S in a submatrices form in row/column.

PROOF 5. (**Proposition ??**) Considering a replication-involving matrix $X_{rep} = \text{replicate}(X, c)$, the inflation is written as:

$$\text{inflation} = \frac{\text{clusterRV}(X_{rep})}{\text{clusterRV}(X)} = \frac{\text{Vol}(\tilde{X}_{rep}) \prod_{i \in K} \rho_{rep,i}}{\text{Vol}(\tilde{X}) \prod_{i \in K} \rho_i} \quad (14)$$

Due to direct copying, the clusters in X_{rep} and X are with similar shapes and similar cluster centers, thus, $\text{Vol}(\tilde{X}_{rep}) \approx \text{Vol}(\tilde{X})$.

Following summation formula of geometric progression,

$$1 \leq \rho_{rep,i} := \sum_{p=0}^{\phi_{rep,i}} \alpha^p = \frac{1 - \alpha^{(\phi_{rep,i}+1)}}{1 - \alpha} \leq \frac{1}{1 - \alpha} \quad (15)$$

$$1 \leq \rho_i := \sum_{p=0}^{\phi_i} \alpha^p = \frac{1 - \alpha^{(\phi_i+1)}}{1 - \alpha} \leq \frac{1}{1 - \alpha} \quad (16)$$

Thus,

$$(1 - \alpha)^K \leq \text{inflation} \leq (1 - \alpha)^{-K} \quad (17)$$

PROOF 6. (**Proposition ??**) When $\alpha = 1/\beta N$, the following inequality relation exists:

$$1 \leq \rho_{rep,i} = \sum_{p=0}^{\phi_{rep,i}} \frac{1}{\beta N} \alpha^p \leq \frac{1}{1 - \frac{1}{\beta N}} = 1 + \frac{1}{\beta N - 1} \quad (18)$$

$$1 \leq \rho_i = \sum_{p=0}^{\phi_i} \frac{1}{\beta N} \alpha^p \leq \frac{1}{1 - \frac{1}{\beta N}} = 1 + \frac{1}{\beta N - 1} \quad (19)$$

Combined with Equation 14,

$$\left(1 + \frac{1}{\beta N - 1}\right)^{-K} \leq \text{inflation} \leq \left(1 + \frac{1}{\beta N - 1}\right)^K \quad (20)$$

When $N \rightarrow \infty$, the following limit theorem is exist.

$$\lim_{n \rightarrow \infty} \left(1 + \frac{1}{\beta N - 1}\right)^{-K} = \lim_{n \rightarrow \infty} \left(1 + \frac{1}{\beta N - 1}\right)^K = 1 \quad (21)$$

Thus, $\text{inflation} \rightarrow 1$ is hold under $N \rightarrow \infty$.

PROOF 7. (**Proposition ??**) Taking the scenario where the dataset X is clustered to K partitions as an example. The matrix of cluster centers is denoted as \tilde{X} . For a balanced dataset, each clusters $C_i, i = 1, \dots, K$ is supposed to contain D data points. Then, we have

$$\begin{aligned} \text{Vol}(X_1) &= \left| \left[(\tilde{X}_1 + \Gamma_1)^T, \dots, (\tilde{X}_1 + \Gamma_D)^T \right]^T \begin{bmatrix} \tilde{X}_1 + \Gamma_1 \\ \vdots \\ \tilde{X}_1 + \Gamma_1 \end{bmatrix} \right| \\ &= \left| \sum_{i=1}^D (\tilde{X}_1 + \Gamma_1)^T (X_1 + \Gamma_1) \right| \end{aligned} \quad (22)$$

where \tilde{X}_1 is the matrix of cluster centers and $\Gamma_i = \begin{bmatrix} C_{0,i} - \tilde{X}_0 \\ \vdots \\ C_{K,i} - \tilde{X}_K \end{bmatrix}$ denotes the relative distance of i -th data points in each clusters to its cluster's center. Each cluster center generated by k -Means is:

$$\tilde{X}_k = \frac{\sum_{i=1}^D \delta_{ik} x_i}{\sum_{i=1}^D \delta_{ik}}. \quad (23)$$

where δ_{ik} is a cluster indicator variable with $\delta_{ik} = 1$ if x_i in k -th cluster. As the number of data points increases, the distance vectors of the points to cluster center are cancel each other out,

$$\sum_{i=0}^D \Gamma_D \rightarrow \vec{0}. \quad (24)$$

Thus, the Equation 22 can be rewritten as:

$$\text{Vol}(X_1) = \left| \sum_{i=1}^D (\tilde{X}_1)^T (X_1) + \sum_{i=1}^D (\tilde{\Gamma}_i)^T (\Gamma_i) \right|, \quad (25)$$

In the same way to get

$$\text{Vol}(X_2) = \left| \sum_{i=1}^D (\tilde{X}_2)^T (X_2) + \sum_{i=1}^D (\tilde{\Upsilon}_i)^T (\Upsilon_i) \right| \quad (26)$$

Applying determinant property,

$$\begin{aligned} \frac{\text{Vol}(X_1)}{\text{Vol}(X_2)} &= \frac{\left| D \cdot (\tilde{X}_1)^T (X_1) + \sum_{i=1}^D (\Gamma_i)^T (\Gamma_i) \right|}{\left| D \cdot (\tilde{X}_2)^T (X_2) + \sum_{i=1}^D (\Upsilon_i)^T (\Upsilon_i) \right|} \\ &= \frac{\left| (\tilde{X}_1)^T (X_1) + \frac{1}{D} \sum_{i=1}^D (\Gamma_i)^T (\Gamma_i) \right|}{\left| (\tilde{X}_2)^T (X_2) + \frac{1}{D} \sum_{i=1}^D (\Upsilon_i)^T (\Upsilon_i) \right|} \end{aligned} \quad (27)$$

When $N \rightarrow \infty$, Equation 21 has proved the following relation,

$$\frac{RV(\tilde{X}_1)}{RV(\tilde{X}_2)} = \frac{Vol(\tilde{X}_1) \prod_{i \in K} \rho_{1,i}}{Vol(\tilde{X}_2) \prod_{i \in K} \rho_{2,i}} \rightarrow \frac{Vol(\tilde{X}_1)}{Vol(\tilde{X}_2)} \quad (28)$$

Combined Equation 28 with Equation 27, $RV(\tilde{X}_1)/RV(\tilde{X}_2)]/[V(X_1)/V(X_2) \rightarrow 1$ under $N \rightarrow \infty$ is hold.

DEFINITION 1. (Unbounded subset-sum problem) Given a set of positive integers $\{k_0, \dots, k_n\}$, an unbounded subset-sum problem is defined as to find the non-negative integers α_i so that $\sum_{i=1}^n \alpha_i k_i = K$, for we can achieve K by k_i for any times, it's known that unbounded subset-sum problem is NP-hard.

LEMMA 3. Let $v_i = p_i, i = 1, \dots, n, p_{n+1} = K + \Delta$ when $v_{n+1} = K$ and $\Delta \in (0, 1)$, a subadditive and monotone function $p(x)$ interpolating on the points (v_i, p_i) exist if and only if unbounded subset sum $\sum_{i=1}^n \alpha_i v_i = K$ not exists.

PROOF 8. (Lemma 3) If $\sum_{i=1}^n \alpha_i p_i = K$ exists, then we have:

$$K + \Delta = p(K) = p\left(\sum_{i=1}^n \alpha_i v_i\right) \leq \sum_{i=1}^n \alpha_i p_i \stackrel{v_i=p_i}{=} K \quad (29)$$

$K + \Delta = K$ is a contradiction so that if $\sum_{i=1}^n \alpha_i v_i = K$ exists, a subadditive and monotone function $p(x)$ interpolating on the $n + 1$ points (v_i, p_i) is not exist.

Conversely, in the next, we prove if $\sum_{i=1}^n \alpha_i p_i = K$ not exists, we can construct a subadditive and monotone function $p(x)$ that interpolates the $(n + 1)$ points. First, we introduce a function (x) to reflect the smallest possible unbounded subset sum at x . (x) at least constrains an unbounded subset sum contains x , thus $(x) \geq x$. Then, we define a function $p(x) = \min((x), K + \Delta)$ and our goal is to prove such $p(x)$ is satisfied subadditive, monotone and interpolating on the $n + 1$ points (v_i, p_i) . It is apparent that $p(x)$ is monotone. Since a set containing x -self is a minimum unbounded subset sum, we have $v_i = p_i \leq K + \Delta$. For we have assumed that $\sum_{i=1}^n \alpha_i p_i = K$ is not exist, thus $(v_{i+1}) \geq K + 1$. Then the $p(x)$ can be written as:

$$p(x) = \begin{cases} \mu(x), & \mu(x) \leq K \\ K + \Delta, & \mu(x) \geq K + 1 \end{cases} \quad (30)$$

If $\mu(x) \geq K + 1$, then $p(x + y) \leq K + \Delta = p(x) \leq p(x) + p(y)$. The relation is also holds when $\mu(y) \geq K + 1$. When both $\mu(x) \leq K$ and $\mu(y) \leq K$, we have $p(x) = (x) = \sum_{i=1}^n \alpha_i v_i$ and $p(y) = (y) = \sum_{i=1}^n \beta_i v_i$. Then, $x + y \leq p(x) + p(y) = \sum_{i=1}^n (\alpha_i + \beta_i) v_i$. According to the definition of (x) , $p(x + y) = (x + y) = \min(x + y, \sum_{i=1}^n \gamma_i) \leq \sum_{i=1}^n (\alpha_i + \beta_i) v_i = p(x) + p(y)$.

Above all, we have proved Lemma 3). However, the unbounded subset-sum problem is NP-hard, whether the sufficient and necessary conditions that unbounded subset sum $\sum_{i=1}^n \alpha_i v_i = K$ not existing in Lemma 3) is a co-NP hard problem.

PROOF 9. (Proposition ??) For the pricing function p satisfies $p(x)/x \geq p(y)/y$ when $x \leq y$, then, it must have:

$$\begin{aligned} \frac{p(x+y)}{x+y} &\leq \min\left(\frac{p(x)}{x}, \frac{p(y)}{y}\right) \Rightarrow \\ p(x+y) &\leq \min\left(p(x) + \underbrace{\frac{yp(x)}{x}}_{\geq p(y)}, p(y) + \underbrace{\frac{xp(y)}{y}}_{\geq p(x)}\right) \\ &\leq p(x) + p(y) \end{aligned} \quad (31)$$

Constraint $p(x)/x \geq p(y)/y, x \leq y$ representing a subspace of sub-additivity constraint is proved.