

HW 1 for CSCI 5525

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1 Problem 1

1.1 a

Show that $\langle A, B \rangle = \text{tr}(A^T B)$ and so $\|M\|_F = \sqrt{\text{tr}(M^T M)}$

PROOF:

$\because \langle A, B \rangle = \sum_{ij} a_{ij} b_{ij}$ and A and B have same size.

$\therefore \langle A, B \rangle = \sum_j \mathbf{a}_j^T \mathbf{b}_j$, where \mathbf{a}_j and \mathbf{b}_j are column vector of A and B respectively.

$\because A^T B = [\mathbf{a}_1, \dots, \mathbf{a}_j]^T [\mathbf{b}_1, \dots, \mathbf{b}_j]$ and $\text{tr}(M) = \sum_i m_{ii}$.

$$\therefore A^T B = \begin{bmatrix} \mathbf{a}_1^T \mathbf{b}_1 & \dots & \dots & \dots & \dots \\ \dots & \mathbf{a}_2^T \mathbf{b}_2 & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \mathbf{a}_j^T \mathbf{b}_j \end{bmatrix}$$

$\therefore \text{tr}(A^T B) = \sum_j \mathbf{a}_j^T \mathbf{b}_j = \langle A, B \rangle$ and $\text{tr}(M^T M) = \langle M, M \rangle$

Summarizing:

$$\langle A, B \rangle = \text{tr}(A^T B) \quad (1)$$

$$\|M\|_F = \sqrt{\text{tr}(M^T M)} \quad (2)$$

1.2 b

Show that $\text{tr}(A^T B) = \text{tr}(B^T A)$

PROOF:

$\because \langle A, B \rangle = \text{tr}(A^T B)$ and $\langle A, B \rangle = \langle B, A \rangle$

$\therefore \text{tr}(A^T B) = \langle A, B \rangle = \langle B, A \rangle = \text{tr}(B^T A)$

Summarizing:

$$\text{tr}(A^T B) = \text{tr}(B^T A) \quad (3)$$

1.3 c

Assume A and B have the same size. In general, AB^T and $B^T A$ have different sizes, but $\text{tr}(AB^T) = \text{tr}(B^T A)$. Show it.

PROOF:

$\therefore \text{tr}(AB^\top) = \langle A^\top, B^\top \rangle = \sum_{ji} a_{ji} b_{ji}$, where a_{ji} and b_{ji} are (j, i) -th element of A^\top and B^\top respectively.

$\therefore \text{tr}(B^\top A) = \langle A, B \rangle = \sum_{ij} a_{ij} b_{ij}$, where a_{ij} and b_{ij} are (i, j) -th element of A and B respectively.

$\therefore \text{tr}(AB^\top) = \text{tr}(B^\top A)$

Summarizing:

$$\text{tr}(AB^\top) = \text{tr}(B^\top A) \quad (4)$$

1.4 d

Show that $\text{tr}(M_1 M_2 M_3) = \text{tr}(M_3 M_1 M_2) = \text{tr}(M_2 M_3 M_1)$, assuming that the sizes of M_1 , M_2 and M_3 are compatible with all the matrix multiplications. This is known as the *cyclic property* of matrix traces. (Hint: think of (c))

PROOF:

Provided that $M_1 M_2 = A$, $M_3 = B^\top$, according to the [Eq. \(4\)](#):

$$\text{tr}(M_1 M_2 M_3) = \text{tr}(AB^\top) = \text{tr}(B^\top A) = \text{tr}(M_3 M_1 M_2)$$

Similarly,

$$\text{tr}(M_3 M_1 M_2) = \text{tr}(M_2 M_3 M_1)$$

Summarizing:

$$\text{tr}(M_1 M_2 M_3) = \text{tr}(M_3 M_1 M_2) = \text{tr}(M_2 M_3 M_1) \quad (5)$$

1.5 e

For any matrices A, B, C, D of compatible sizes, we always have $\langle ACB, D \rangle = \langle CB, A^\top D \rangle = \langle AC, DB^\top \rangle$, i.e., we can always move the **leading** matrix of one side of the inner product to the other side as **leading matrix once transposed** (if these matrices are complex-valued, should be conjugate transposed), and similarly the **trailing** matrix to the other side as **trailing matrix once transposed**. Why? (Hint: think of the above results and also try to remember this important property that will be useful for calculation later)

PROOF:

In terms of the [Eq. \(1\)](#):

$$\langle ACB, D \rangle = \langle D, ACB \rangle = \text{tr}(D^\top ACB)$$

Provided that $D^\top A = M_1$ and $CB = M_2$. In terms of the [Eq. \(1\)](#):

$$\text{tr}(D^\top ACB) = \text{tr}(M_1 M_2) = \langle M_1^\top, M_2 \rangle = \langle A^\top D, CB \rangle = \langle CB, A^\top D \rangle$$

Similarly, in terms of the Eq. (5):

$$\langle ACB, D \rangle = \langle D, ACB \rangle = \text{tr}(D^T ACB) = \text{tr}(BD^T AC) = \langle DB^T, AC \rangle$$

Summarizing:

$$\langle ACB, D \rangle = \langle CB, A^T D \rangle = \langle AC, DB^T \rangle \quad (6)$$

1.6 f

For M , let's perform a *compact* SVD (if not sure, check up Wikipedia! https://en.wikipedia.org/wiki/Singular_value_decomposition#Compact_SVD) to obtain $M = U\Sigma V^T$, so that U and V are orthonormal (not necessarily square) matrices, i.e., $U^T U = I$ and $V^T V = I$. Use the cyclic property of trace and that $\|M\|_F = \sqrt{\text{tr}(M^T M)}$ to show that

$$\|M\|_F = \sqrt{\sum_{i=1}^r \sigma_i^2},$$

assuming the rank of M is r . Here σ_i 's are the singular values of M .

PROOF:

since $M = U\Sigma V^T$, $\|M\|_F = \sqrt{\text{tr}(M^T M)}$, $U^T U = I$ and $V^T V = I$ so,

$$\|M\|_F = \sqrt{\text{tr}(V\Sigma U^T U \Sigma V^T)} = \sqrt{\text{tr}(V\Sigma \Sigma V^T)} = \sqrt{\text{tr}(V^T V \Sigma \Sigma)} = \sqrt{\text{tr}(\Sigma_r \Sigma_r)} = \sqrt{\sum_{i=1}^r \sigma_i^2}$$

2 Problem 2

2.1 a

Let A be a square matrix. Deriving the gradient and Hessian of the quadratic function $f(x) = x^T A x + b^T x$. Please include your calculation details. (Hint: note that Hessian must be a symmetric matrix.)

SOLUTION:

$$\begin{aligned} f(x + \sigma) &= (x + \sigma)^T A (x + \sigma) + b^T (x + \sigma) \\ &= (x^T + \sigma^T) (Ax + A\sigma) + b^T x + b^T \sigma \\ &= x^T Ax + x^T A\sigma + \sigma^T Ax + \sigma^T A\sigma + b^T x + b^T \sigma \\ &= f(x) + \sigma^T Ax + x^T A\sigma + b^T \sigma + \sigma^T A\sigma \end{aligned} \quad (7)$$

$\because \sigma^T Ax$ is a scalar

$$\therefore \sigma^T Ax = (\sigma^T Ax)^T = x^T A^T \sigma$$

$$\begin{aligned} f(x + \sigma) &= f(x) + (x^T A^T + x^T A + b^T) \sigma + \sigma^T A\sigma \\ &= f(x) + \langle Ax + A^T x + b, \sigma \rangle + \langle \sigma, A\sigma \rangle \end{aligned} \quad (8)$$

Consequently,

$$\nabla f(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{A}^\top \mathbf{x} + \mathbf{b}$$

$$\nabla^2 f(\mathbf{x}) = 2\mathbf{A}$$

2.2 b

Let $p(\mathbf{x}; \beta) = \frac{e^{\beta^\top \mathbf{x}}}{1 + e^{\beta^\top \mathbf{x}}}$. The log-likelihood for logistic regression with two classes is (assuming N samples of the form (\mathbf{x}_i, y_i))

$$\begin{aligned} f(\beta) &= \sum_{i=1}^N [y_i \log p(\mathbf{x}_i; \beta) + (1 - y_i) \log (1 - p(\mathbf{x}_i; \beta))] \\ &= \sum_{i=1}^N [y_i \beta^\top \mathbf{x}_i - \log (1 + e^{\beta^\top \mathbf{x}_i})]. \end{aligned}$$

Derive the gradient and Hessian of $f(\beta)$. Please include your calculation details. (1/12) For logistic regression, we are going to maximize $f(\beta)$, which is equivalent to minimize $-f(\beta)$. Does the minimization problem has a unique minimizer or not?

SOLUTION:

denote $f(\beta)$ as matrix form,

$$\begin{aligned} f(\beta) &= \sum_{i=1}^N [y_i \beta^\top \mathbf{x}_i - \log (1 + e^{\beta^\top \mathbf{x}_i})] \\ &= \mathbf{y}^\top \mathbf{X}\beta - \mathbf{1}^\top \log (\mathbf{1} + e^{\mathbf{X}\beta}) \end{aligned} \tag{9}$$

where $\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_N^\top \end{bmatrix}$, $\mathbf{y} = [y_1, \dots, y_N]^\top$, $\mathbf{1} = [1, \dots, 1]$.

Since $f(\beta)$ map vector to scalar, $df = \sum_i \frac{\partial f}{\partial \beta_i} d\beta_i = \left(\frac{\partial f}{\partial \beta} \right)^\top d\beta = \nabla_\beta f^\top d\beta$

$$\begin{aligned} df &= \mathbf{y}^\top \mathbf{X} d\beta - \frac{\mathbf{1}^\top (e^{\mathbf{X}\beta} \circ d\mathbf{X}\beta)}{\mathbf{1} + e^{\mathbf{X}\beta}} \\ &= \mathbf{y}^\top \mathbf{X} d\beta - \frac{(e^{\mathbf{X}\beta})^\top d\mathbf{X}\beta}{\mathbf{1} + e^{\mathbf{X}\beta}} \end{aligned} \tag{10}$$

Let $\sigma(a) = \frac{e^a}{1+e^a}$, $\sigma'(a) = \frac{e^a}{(1+e^a)^2}$,

$$\begin{aligned}
df &= \mathbf{y}^\top \mathbf{X} d\boldsymbol{\beta} - \frac{\mathbf{1}^\top (e^{\mathbf{X}\boldsymbol{\beta}} \circ d\mathbf{X}\boldsymbol{\beta})}{\mathbf{1} + e^{\mathbf{X}\boldsymbol{\beta}}} \\
&= \mathbf{y}^\top \mathbf{X} d\boldsymbol{\beta} - \frac{(e^{\mathbf{X}\boldsymbol{\beta}})^\top \mathbf{X} d\boldsymbol{\beta}}{\mathbf{1} + e^{\mathbf{X}\boldsymbol{\beta}}} \\
&= \mathbf{y}^\top \mathbf{X} d\boldsymbol{\beta} - \sigma(\mathbf{X}\boldsymbol{\beta})^\top \mathbf{X} d\boldsymbol{\beta} \\
&= (\mathbf{y}^\top - \sigma(\mathbf{X}\boldsymbol{\beta})^\top) \mathbf{X} d\boldsymbol{\beta}
\end{aligned} \tag{11}$$

So $\nabla f = \mathbf{X}^\top (\mathbf{y} - \sigma(\mathbf{X}\boldsymbol{\beta}))$. $\nabla^2 f = \frac{\partial^2 f}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}^\top}$, so,

$$\begin{aligned}
d\nabla f &= d(\mathbf{X}^\top (\mathbf{y} - \sigma(\mathbf{X}\boldsymbol{\beta}))) \\
&= -\mathbf{X}^\top d\sigma(\mathbf{X}\boldsymbol{\beta}) \\
&= -\mathbf{X}^\top (\sigma'(\mathbf{X}\boldsymbol{\beta}) \circ d\mathbf{X}\boldsymbol{\beta}) \\
&= -\mathbf{X}^\top \text{diag}(\sigma'(\mathbf{X}\boldsymbol{\beta})) \mathbf{X} d\boldsymbol{\beta}
\end{aligned} \tag{12}$$

Similarly,

$$\nabla^2 f = -\mathbf{X}^\top \text{diag}(\sigma'(\mathbf{X}\boldsymbol{\beta})) \mathbf{X}, \text{ where } \sigma'(\mathbf{X}\boldsymbol{\beta}) = \frac{e^{\mathbf{X}\boldsymbol{\beta}}}{(1+e^{\mathbf{X}\boldsymbol{\beta}})^2}$$

Consequently,

$$\begin{aligned}
\nabla f &= \mathbf{X}^\top (\mathbf{y} - \sigma(\mathbf{X}\boldsymbol{\beta})), \\
\nabla^2 f &= -\mathbf{X}^\top \text{diag}(\sigma'(\mathbf{X}\boldsymbol{\beta})) \mathbf{X}
\end{aligned}$$

$$\text{where } \sigma(\mathbf{X}\boldsymbol{\beta}) = \frac{e^{\mathbf{X}\boldsymbol{\beta}}}{1+e^{\mathbf{X}\boldsymbol{\beta}}}, \sigma'(\mathbf{X}\boldsymbol{\beta}) = \frac{e^{\mathbf{X}\boldsymbol{\beta}}}{(1+e^{\mathbf{X}\boldsymbol{\beta}})^2}.$$

Also,

$$\begin{aligned}
\nabla^2 f &= \mathbf{X}^\top \text{diag}(\sigma'(\mathbf{X}\boldsymbol{\beta})) \mathbf{X} \\
&= \begin{bmatrix} \sum_i^N \lambda_i x_{i,1}^2 & \cdots & \cdots \\ \cdots & \cdots & \cdots \\ \cdots & \cdots & \sum_i^N \lambda_i x_{i,M}^2 \end{bmatrix}
\end{aligned} \tag{13}$$

Where λ_i is diagonal entries of $\text{diag}(\sigma'(\mathbf{X}\boldsymbol{\beta}))$, and M is the number of column vector of \mathbf{X} . As $\sigma'(a) > 0$, diagonal entries of $\nabla^2 f$ more than 0. So, $\nabla^2 f$ is positive definite.

Therefore, only one unique minimizer exists.

2.3 c

Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ with $m \leq n$, then given a $\mathbf{y} \in \mathbb{R}^m$, the least-squares problem $\min_{\mathbf{x}} \|\mathbf{y} - \mathbf{Ax}\|_2^2$ has infinitely many solutions. Now let's say we want a solution with a small ℓ_2 norm, then it is reasonable to put a penalty on the ℓ_2 norm:

$$\min_{\mathbf{x}} \|\mathbf{y} - \mathbf{Ax}\|_2^2 + \lambda \|\mathbf{x}\|_2^2$$

with a chosen $\lambda > 0$. This is *ridge regression*. Now we know that for an unconstrained first-order differentiable function $g(\mathbf{x})$, any of its local minimizer \mathbf{x}_* must satisfy the *first-order optimality condition*: $\nabla g(\mathbf{x}_*) = \mathbf{0}$. Use this to derive \mathbf{x}_* (1/12). Is the \mathbf{x}_* unique? Why?

SOLUTION:

$$\begin{aligned} g(\mathbf{x} + \boldsymbol{\sigma}) &= \|\mathbf{y} - \mathbf{A}(\mathbf{x} + \boldsymbol{\sigma})\|_2^2 + \lambda \|\mathbf{x} + \boldsymbol{\sigma}\|_2^2 \\ &= \|\mathbf{y} - \mathbf{Ax}\|_2^2 + \lambda \|\mathbf{x}\|_2^2 + \lambda \|\boldsymbol{\sigma}\|_2^2 + 2\lambda \langle \mathbf{x}, \boldsymbol{\sigma} \rangle - 2 \langle \mathbf{A}^\top (\mathbf{y} - \mathbf{Ax}), \boldsymbol{\sigma} \rangle + \|\mathbf{A}\boldsymbol{\sigma}\|_2^2 \\ &= g(\mathbf{x}) + \boldsymbol{\sigma}^\top (\lambda \mathbf{I} + \mathbf{A}^\top \mathbf{A}) \boldsymbol{\sigma} + 2(\lambda \mathbf{x}^\top - (\mathbf{y} - \mathbf{Ax})^\top \mathbf{A}) \boldsymbol{\sigma} \\ &= g(\mathbf{x}) + 2 \langle \lambda \mathbf{x} - \mathbf{A}^\top (\mathbf{y} - \mathbf{Ax}), \boldsymbol{\sigma} \rangle + \langle \boldsymbol{\sigma}, (\lambda \mathbf{I} + \mathbf{A}^\top \mathbf{A}) \boldsymbol{\sigma} \rangle \end{aligned} \quad (14)$$

So,

$$\nabla g = 2(\lambda \mathbf{x} - \mathbf{A}^\top \mathbf{y} + \mathbf{A}^\top \mathbf{Ax})$$

$$\nabla^2 g = 2(\lambda \mathbf{I} + \mathbf{A}^\top \mathbf{A})$$

Let $\nabla g(\mathbf{x}_*) = 0$,

$$\mathbf{x}_* = (\lambda \mathbf{I} + \mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{y}$$

$\mathbf{A}^\top \mathbf{A}$ is positive definite in that its diagonal entries are all positive. Hence, $\nabla^2 g = 2(\lambda \mathbf{I} + \mathbf{A}^\top \mathbf{A})$ is positive definite as well, which indicates \mathbf{x}_* is unique.

3 Problem 3

The solution for this problem has been finished in the [Colab](#), and I will upload this notebook *HW1_CS5525_YangyangLi.ipynb* as well. Feel free to check that.

Have a good day!