EECS 127/227A, Fall 2022

Optimization Models in Engineering

Gireeja Ranade, UC Berkeley
Zhiyu An

Contents

1. Linear Algebra

1.a. Least-Squares Problem Statement

Definition 1.1 (Least Squares)
Assume matrix A and vectors $\vec{x}$ and $\vec{b}$. The problem defined by

$$\min_{\vec{x}} \|A\vec{x} - \vec{b}\|^2$$

is a Least Squares Problem (LSP).

Example 1.2
Assume we have two dimensional data set $\vec{x}$ and $\vec{y}$ and we want to formalize a LSP to find a linear correlation between x and y. We first formalize the goal linear correlation as

$$y = mx + c$$

where we want to find the optimal values for m and c to minimize the squared loss across all data points. Summarizing the above equation for all data points gives us

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \\ x_n & 1 \end{bmatrix} \begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Where

$$A = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \\ x_n & 1 \end{bmatrix}, \quad \vec{x} = \begin{bmatrix} m \\ c \end{bmatrix}, \quad \vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

And therefore

$$\min_{\vec{x}} \|A\vec{x} - \vec{b}\|^2 = \min_{m,c} \sum_{i=1}^{n} (y_i - (mx_i + c))^2$$

Theorem 1.3 (Ordinary Least Squares)

Given the column space of the matrix A, for vector $\vec{b}$ not in the said column space, $A\vec{x} - \vec{b} = \vec{e}$ must be orthogonal to the columns of A. (Pythagora's theorem)

Therefore, the dot products of every column of A and $\vec{e}$ must be zero, i.e.

$$\begin{aligned} A^\top(A\vec{x} - \vec{b}) &= 0 \\ A^\top A\vec{x} - A^\top\vec{b} &= 0 \\ A^\top A\vec{x} &= A^\top\vec{b} \\ \vec{x} &= (A^\top A)^{-1}A^\top\vec{b} \end{aligned}$$

We conclude that the solution for Ordinary Least Squares (OLS) is

$$\vec{x}^* = \underset{\vec{x}}{\operatorname{argmin}} \|A\vec{x} - \vec{b}\|^2 = (A^\top A)^{-1}A^\top\vec{b}$$

1.b. Norm

Definition 1.4 (Norm)

A Norm is defined as

$$f : \mathbf{X} \to \mathbb{R}$$

For vector space $\mathbf{X}$.

The norm of x is denoted as $\|x\|$.

For any vector x and y, we have

- $\|x\| \geq 0$ and $\|x\| = 0$ iff $x = \vec{0}$
- $\|x + y\| \leq \|x\| + \|y\|$
- $\|\alpha x\| = |\alpha| * \|x\|$

Definition 1.5 (l-p Norm)

Generally, l-p norm is defined as

$$\|\vec{x}\|_p := \left(\sum |x_i|^p\right)^{\frac{1}{p}}; \quad 1 \leq p < \infty$$

Commonly used norms:

- $\|\vec{x}\|_1 = \sum |x_i|$
- $\|\vec{x}\|_2 = \sqrt{\sum |x_i|^2}$
- $\|\vec{x}\|_\infty = \max |x_i|$

Theorem 1.6 (Cauchy-Schwartz Inequality)

$$< \vec{x}, \vec{y} >= \vec{x}^\top \vec{y} = \|\vec{x}\|_2 \|\vec{y}\|_2 \cos\theta$$

Since $-1 \le \cos\theta \le 1$,

$$< \vec{x}, \vec{y} >= \vec{x}^\top \vec{y} \le \|\vec{x}\|_2 \|\vec{y}\|_2$$

Theorem 1.7 (Holder's Inequality)

For $p, q \ge 1$ s.t. $\frac{1}{p} + \frac{1}{q} = 1$,

$$|\vec{x}^\top \vec{y}| \le \sum_{i=1}^{n} |x_i y_i| \le \|\vec{x}\|_p \|\vec{y}\|_p$$

i.e., Cauchy-Schwartz is a narrowed case of Holder's Inequality.

1.c. Gram-Schimdt

Theorem 1.8 (Gram-Schimdt/QR-decomposition)

Let X be a vector space with basis $\{\vec{a}_1, \vec{a}_2, \dots, \vec{a}_n\}$, which is orthonormal. For any matrix A,

$$A = QR$$

$$\begin{bmatrix}\vec{a}_1, \vec{a}_2, \dots, \vec{a}_n\end{bmatrix} = \begin{bmatrix}\vec{q}_1, \vec{q}_2, \dots, \vec{q}_n\end{bmatrix} \begin{bmatrix} \vec{r}_{11} & \vec{r}_{12} & \cdots & \vec{r}_{1n} \\ 0 & \vec{r}_{22} & \cdots & \vec{r}_{2n} \\ 0 & 0 & \ddots & \vec{r}_{3n} \\ 0 & 0 & 0 & \vec{r}_{nn} \end{bmatrix}$$

Where Q is orthonormal andR is upper-triangular.

Theorem 1.9 (Fundamental Theorem of Linear Algebra)

For matrix $A \in \mathbb{R}^{m*n}$,

$$Null(A) \bigoplus Range(A^\top) = \mathbb{R}^n$$

Where $\oplus$ denotes "direct sum" and $Range(A^\top)$ is the column space of $A^\top$. With the said equation we can also conclude that

$$Range(A) \bigoplus Null(A^\top) = \mathbb{R}^m$$

Theorem 1.10 (orthogonal decomposition theorem)
X a vector space and S a subspace of X. Then for any $\vec{x}$ in X,

$$\vec{x} = \vec{s} + \vec{r}, \quad \vec{s} \in S, \quad \vec{r} \in S^{\perp}$$

Such that

$$S^{\perp} = \{\vec{r} \mid < \vec{r}, \vec{s} > = 0, \quad \forall \vec{s} \in S\}$$

Therefore,

$$\mathbf{X} = S \bigoplus S^{\perp}$$

Example 1.11 (Minimum Norm Problem)
We want to find

$$\min \|\vec{x}\|_2^2$$

subject to $A\vec{x} = \vec{b}$. From FTLA we know that

$$\vec{x} = \vec{y} + \vec{z} \;\; s.t. \;\; \vec{y} \in N(A; \;\; \vec{z} \in R(A^{\top}).$$

And

$$A(\vec{y} + \vec{z}) = 0 + A\vec{z} = \vec{b}$$

Since $\vec{y} \perp \vec{z}$,

$$\|\vec{x}\|_2^2 = \|y\|_2^2 + \|z\|_2^2$$

Consider $\vec{z} = A^{\top}\vec{w}$,

$$\begin{aligned} A\vec{z} &= \vec{b} \\ AA^{\top}\vec{w} &= \vec{b} \\ \vec{w} &= (AA^{\top})^{-1}\vec{b} \end{aligned}$$

Therefore

$$\vec{z} = \min \|\vec{x}\|_2^2 = A^{\top}(AA^{\top})^{-1}\vec{b}$$

1.d. Symmetric Matrices

Definition 1.12

Matrix A is symmetric if $A = A^{\top}$, i.e. $A_{ij} = A_{ji}$.
Set $\mathbb{S}^n$ means the set of symmetric matrices of dimension n.

Theorem 1.13 (Spectral Theorem)
If matrix A $\in \mathbb{S}^{\ltimes}$, then

- All eigenvalues of A are real numbers
- Eigenspaces are orthogonal
- $dim(N(\lambda_i I - A)) = \mu_i$ where μ_i is the algebraic multiplicity of λ_i

This means that A is always diagonalizable. i.e.:

$$A = U \Lambda U^\top$$

where U orthonormal and Λ diagonal. Orthonormal (or, unitary) means that the columns of U are orthogonal and all columns are normalized, i.e.

$$U^{-1} = U^\top$$

Remark 1.14
For a diagonalizable n*n matrix A that has n linearly independent eigenvectors, A can be factorized as

$$A = U \Lambda U^\top$$

Where U orthonormal and Λ is a diagonal matrix consists of the eigenvalues of A such that

$$\Lambda = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_i \end{bmatrix}$$

Therefore it is also called an eigenvalue decomposition.

1.e. Principal Component Analysis

Definition 1.15
For $A \in \mathbb{S}$, its Rayleigh coefficient is defined as

$$R = \frac{\vec{x}^\top A \vec{x}}{\vec{x}^\top \vec{x}}$$

The Rayleigh coefficient can bound the eigenvalues of A such that,

$$\lambda_{min}(A) \leq \frac{\vec{x}^\top A \vec{x}}{\vec{x}^\top \vec{x}} \leq \lambda_{max}(A)$$

PCA is very similar to Singular Value Decomposition (SVD). SVD has more nice properties than PCA.

1.f. Singular Value Decomposition

Theorem 1.16 (SVD)
Let $A \in \mathbb{R}^{m*n}$, the SVD of A is given as

$$A = U\Sigma V^\top$$

Where

$$U \in \mathbb{R}^{m*m}, \;\; \Sigma \in \mathbb{R}^{m*n}, \;\; V \in \mathbb{R}^{n*n}$$

and Σ has real entries in its diagonal (the singular values) and zero's else where. If $Rank(A) = r$, we can rewrite A as

$$A = \sigma_1 \vec{u}_1 \vec{v}_1^\top + \sigma_1 \vec{u}_1 \vec{v}_1^\top + \cdots + \sigma_r \vec{u}_r \vec{v}_r^\top$$

Proof. For $A \in \mathbb{R}^{m*n}$, consider symmetric matrix $A^\top A$ that has eigenvalues $\lambda_1 \cdots \lambda_r > 0$ with corresponding eigenvectors $v_1 \cdots v_r$ and $\lambda_{r+1} \cdots \lambda_n = 0$. Then we know that

$$A^\top A \vec{v}_i = \lambda_i \vec{v}_i$$

Let

$$V = \begin{bmatrix} | & & | \\ \vec{v}_1 & \cdots & \vec{v}_n \\ | & & | \end{bmatrix}$$

Define $\sigma_i = \sqrt{\lambda_i}$, let

$$A\vec{v}_i = \sigma_i \vec{u}_i \;\; i \leq r$$

for some vector $\vec{u}_i$.

Claim. $\vec{u}_i$ are orthonormal.

$$\begin{aligned}
\vec{u}_i^\top \vec{u}_j &= \frac{(A\vec{v}_i)^\top}{\sigma_i} \frac{(A\vec{v}_j)}{\sigma_j} \\
&= \frac{1}{\sigma_i \sigma_j} \vec{v}_i^\top A^\top A \vec{v}_j && A^\top A \vec{v}_j = \lambda_j \vec{v}_j \\
&= \frac{1}{\sigma_i \sigma_j} \vec{v}_i^\top \lambda_j \vec{v}_j \\
&= \frac{\lambda_j}{\sigma_i \sigma_j} \vec{v}_i^\top \vec{v}_j && \vec{v}_i \vec{v}_j \text{ orthonormal} \\
&= \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}
\end{aligned}$$

Therefore $\vec{u}_i$ are orthonormal. Recall that A has rank r, we let

$$V_r = V = \begin{bmatrix} | & & | \\ \vec{v}_1 & \cdots & \vec{v}_r \\ | & & | \end{bmatrix}$$

Hence

$$AV_r = \begin{bmatrix} | & & | \\ \vec{u}_1 & \cdots & \vec{u}_r \\ | & & | \end{bmatrix} \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{bmatrix} = U_r \Sigma_r$$

$$A = U \Sigma V^\top$$

Since V orthonormal and $V^{-1} = V^\top$ ∎

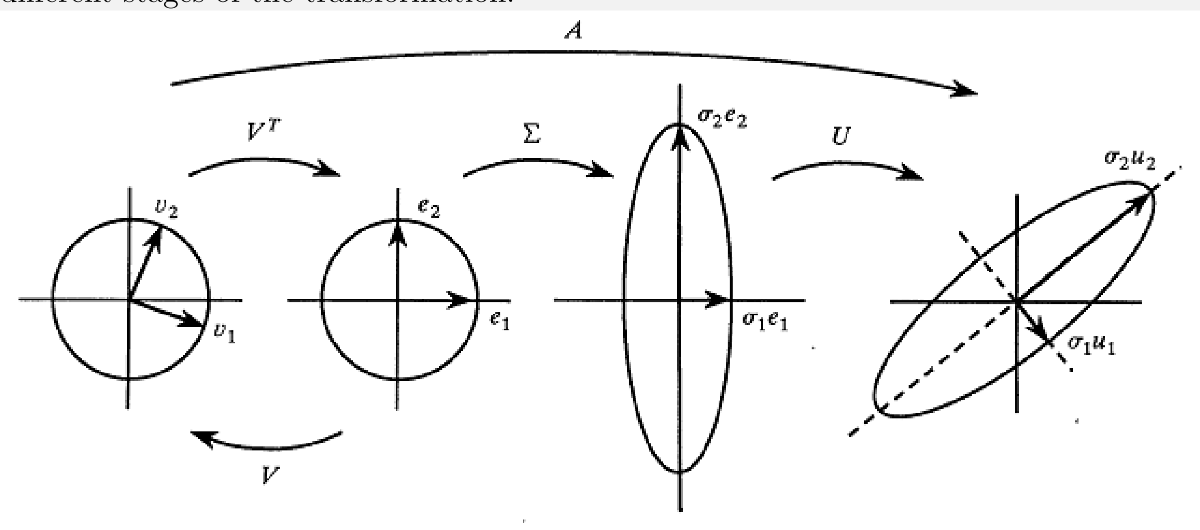
Remark 1.17 (geometric interpretation of SVD)
Consider linear transformation on vector $\vec{x}$ given by matrix A, s.t.

$$A\vec{x} = U\Sigma V^\top \vec{x}$$

SVD helps breaking the transformation into three smaller steps, i.e.

- orthonormal transformation (rotate/reflect) by V,
- scaling by Σ,
- orthonormal transformation by U.

The following illustration is an example of a 2D transformation $A\vec{x}$. It shows the decomposed linear transformation through the unit circles relative to the original unit circle at different stages of the transformation.



1.g. Low-Rank Approximation

Definition 1.18 (matrix norms)
There are two ways to interpret a matrix, either as an operator or as a block of data. Frobenius norm consider the matrix as a block of data.
Frobenius norm of matrix A is defined as

$$\|A\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}^2} = \sqrt{tr(A^\top A)}$$

Frobenius norm is invariant to orthonormal transformations, i.e. given U an orthonormal matrix,

$$\|UA\|_F = \|AU\|_F = \|A\|_F$$

Spectral norm, or l_2 norm, interpret the matrix as an operator and is defined as

$$\|A\|_2 = \max_{\|\vec{x}\|_2=1} \|A\vec{x}\|_2 = \max_{\|\vec{x}\|=1} \sqrt{\vec{x}^\top A^\top A\vec{x}} = \sqrt{\lambda_{max}(A^\top A)} = \sigma_{max}(A^\top A)$$

Intuitively, the spectral norm of a matrix A is the largest scaling that A can do (recall the Σ matrix that is used to scale the unit circle in the three steps of transformation after SVD).

Theorem 1.19 (Eckart-Young-Mirsky Theorem)
$A \in \mathbb{R}^{m*n}$. Do SVD gives us

$$A = U\Sigma V^\top = \sum_{i=1}^{n} \sigma_i \vec{u}_i \vec{v}_i^\top$$

Define

$$A_k = \sum_{i=1}^{k} \sigma_i \vec{u}_i \vec{v}_i^\top$$

We want to find the best k-rank (lower than r) approximation of A, i.e.

$$\underset{B\in\mathbb{R}^{m*n},\ Rank(B)=k}{\operatorname{argmin}} \|A - B\|_F$$

Suprisingly, Eckart-Young-Mirsky Theorem tells us that

$$\underset{B\in\mathbb{R}^{m*n},\ Rank(B)=k}{\operatorname{argmin}} \|A - B\|_F = A_k$$

Moreover,

$$\underset{B\in\mathbb{R}^{m*n},\ Rank(B)=k}{\operatorname{argmin}} \|A - B\|_2 = A_k$$

This theorem relates two completely different norms and is not obvious at all. It shows how fundamental SVD is, such that in any way of looking at a matrix, the decomposition shows up.

Remark 1.20

Eckart-Young-Mirsky Theorem can be used to **compress images**. For an image, the matrix that represents the pixels of the image can be reduced to a lower rank matrix, and hence a smaller set of data, while remains relatively high resolution. The A_k matrix **captures the key features of the image because it keeps k largest singular values and their corresponding vectors that contribute most to the dataset/transformation.**

Definition 1.21 (trace)

The trace of a matrix is defined as

$$trace := \mathbb{R}^{n*n} \to \mathbb{R}$$

$$trace(A) = \sum_{i=1}^{n} a_{ii}$$

Remark 1.22 (Orthonormal transformation invariance of Frobenius norm)

Proof that $\|UA\|_F = \|AU\|_F = \|A\|_F$

Proof. Recall that $\|A\|_F = \sqrt{tr(A^\top A)}$. By definition, for any matrices A and B, we have $tr(AB) = tr(BA)$ Then,

$$\begin{aligned}
\|AU\|_F &= \sqrt{tr((AU)^\top (AU))} \\
&= \sqrt{tr(U^\top A^\top AU)} \\
&= \sqrt{tr(UU^\top A^\top A)} \\
&= \sqrt{tr(A^\top A)} \\
&= \|A\|_F
\end{aligned}$$

■

Remark 1.23 (Frobenius norm is the sqrt of the sum of the squares of the singular values)

$$\begin{aligned}
\|A\|_F = \|U\Sigma V^\top\|_F &= \|\Sigma\|_F \\
&= \sqrt{\sum_{i=1}^{n} \sigma_i^2}
\end{aligned}$$

Proof of Eckart-Young-Mirsky
Goal: B: rank(k), $\|A - B\|_F \geq \|A - A_k\|_F$

Proof.

$$\|A - A_k\|_F = \|\sum_{i=k+1}^{n} \sigma_i \vec{u}_i \vec{v}_i\|_F = \sqrt{\sum_{i=k+1}^{n} \sigma_i^2}$$

Note that the goal is true iff

$$\sum_{i=1}^{n} \sigma_i^2(A - B) \geq \sum_{i=k+1}^{n} \sigma_i^2(A)$$

Further note that the previous statement is true iff:

$$\sigma_i^2(A - B) \geq \sigma_{k+i}^2(A)$$

Let $\sigma_{k+i}(A)$be the k+ith largest singular value of A. Hence

$$\sigma_{k+i}(A) = \sigma_{max}(A - A_k)$$

Denote A-B = C. Then

$$\sigma_i(A - B) = \sigma_i(C) = \|C - C_{i-1}\|_2$$

Since B has rank k,

$$\|B - B_k\|_2 = 0$$

Add it to the previous equation gives us

$$\begin{aligned} \sigma_i(A - B) &= \|C - C_{i-1}\|_2 + \|B - B_k\|_2 \\ &\geq \|C + B - C_{i-1} - B_k\|_2 \\ &\geq \|A - C_{i-1} - B_k\|_2 \end{aligned}$$

Let $D = C_{i-1} + B_k$. Rank(D) $\leq$ i-1+k. Then

$$\sigma_i(A - B) \geq \|A - D\|_2$$

Consider the solution to the optimization problem

$$\operatorname*{argmin}_{D,\, rank(D) \leq i+k-1} \|A - D\|_2 = A_k + i - 1$$

$$\min_{rank(D) \leq i+k-1} \|A - D\|_2 = \sigma_{k+1}(A)$$

Finally, bring the above result back to the previous equation gives us

$$\sigma_i(A - B) \geq \sigma_{k+1}(A)$$

as desired. ∎

2. Vector Calculus

Theorem 2.1 (Taylor's Theorem for Vectors)
For $f(\vec{x}) := \mathbb{R}^n \to \mathbb{R}$, the derivative of f is

$$f(\vec{x}_0 + \Delta\vec{x}) = f(\vec{x}_0) + \nabla f|_{\vec{x}=\vec{x}_0}^\top \Delta\vec{x} + \frac{1}{2!}(\Delta\vec{x})^\top \nabla^2 f|_{\vec{x}=\vec{x}_0} \Delta\vec{x}$$

Where

$$\text{Gradient} = \nabla f|_{\vec{x}=\vec{x}_0}^\top$$
$$\text{Hessian} = \nabla^2 f|_{\vec{x}=\vec{x}_0}$$

And

$$f(\vec{x}_0) + \nabla f|_{\vec{x}=\vec{x}_0}^\top \Delta\vec{x}$$

is the first-order approximation (a hyperplane).

Definition 2.2 (Gradient)
The gradiant $\nabla f(\vec{x})$ captures change according to all components of $\vec{x}$. It is defined as

$$\nabla f(\vec{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} f & \frac{\partial}{\partial x_2} f & \cdots & \frac{\partial}{\partial x_n} f \end{bmatrix}$$

The gradient always has the same dimension as the input vector.

Definition 2.3 (Hessian)
The hessian is a matrix that captures the change according to all gradients. It is defined as

$$\nabla^2 f(\vec{x})_{ij} = \frac{\partial f}{\partial x_i \partial x_j}$$

Hessian is **often** symmetric.

Example 2.4

Let

$$f(\vec{x}) = \|x\|_2^2, \quad f := \mathbb{R}^2 \to \mathbb{R}$$

Then the gradient of this function f is

$$\nabla f(\vec{x}) = \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix} = 2\vec{x}$$

And the hessian is

$$\nabla^2 f(\vec{x}) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

According to taylor theorem,

$$\begin{aligned} f(\vec{x} + \Delta\vec{x}) &= (x_1^2 + x_2^2) + \begin{bmatrix} 2x_1 & 2x_2 \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} \Delta x_1 & \Delta x_2 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix} \\ &= x_1^2 + x_2^2 + 2x_1\Delta x_1 + 2x_2\Delta x_2 + \Delta x_1^2 + \Delta x_2^2 \\ &= (x_1 + \Delta x_1)^2 + (x_2 + \Delta x_2)^2 \end{aligned}$$

Example 2.5

Let

$$f(\vec{x}) = \vec{x}^\top \vec{a} = \sum_{i=1}^{n} x_i a_i$$

Then the gradient of this function f is

$$\nabla f(\vec{x}) = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \vec{a}$$

And the hessian is

$$\nabla^2 f(\vec{x}) = 0$$

Example 2.6

Let

$$f(\vec{x}) = \vec{x}^\top A\vec{x}$$

We can see that

$$\begin{aligned} f(\vec{x}) &= \vec{x}^\top A\vec{x} \\ &= \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix} \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \\ &= \sum_i \sum_j x_i a_{ij} x_j \end{aligned}$$

Since all terms that contain x_i is

$$\sum_{j\neq i} x_i a_{ij} x_j + \sum_{j\neq i} x_j a_{ji} x_i + x_i^2 a_i i$$

We know that

$$\frac{\partial f}{\partial x_i} = \sum_j (a_{ij} + aji) x_j$$

Therefore the gradient of this function f is

$$\nabla f(\vec{x}) = (A + A^\top) \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = (A + A^\top)\vec{x}$$

The hessian is

$$\nabla^2 f(\vec{x}) = A + A^\top$$

Theorem 2.7 (The Main Theorem)

Let $f : \mathbb{R}^n \to \mathbb{R}$ and f is differentiable everywhere. Consider the optimization problem subject to

$$\underset{\vec{x},\, \vec{x}\in\Omega}{\operatorname{argmin}} f(\vec{x})$$

Where Ω is an open set in $\mathbb{R}^n$

Then if $\vec{x}^*$ is an optimal solution, then

$$\frac{df}{dx}(x^*) = 0$$

Note that the converse is not necessarily true.

3. Regression

3.a. Sensitivity

Definition 3.1 (problem statement)
Consider optimization problem

$$A\vec{x} = \vec{y}$$

Under the special case that $A \in \mathbb{R}^{n*n}$ and is invertible. Now we apply a change to y such that $\vec{y} \to \vec{y} + \delta\vec{y}$. Because of this, $\vec{x} \to \vec{x} + \delta\vec{x}$. How big is $\delta\vec{x}$?

Theorem 3.2 (condition number)
The value we are interested in is $\frac{\|\delta\vec{x}\|_2}{\|\vec{x}\|_2}$. To investigate this value, we transform the equation such that

$$\begin{aligned} A(\vec{x} + \delta\vec{x}) &= \vec{y} + \delta\vec{y} \\ A\delta\vec{x} &= \delta\vec{y} \\ \delta\vec{x} &= A^{-1}\delta\vec{y} \\ \|\delta\vec{x}\|_2 &= \|A^{-1}\delta\vec{y}\|_2 \end{aligned}$$

Recall that

$$\|A\|_2 = \max_{\|y\|_2=1} \|A\vec{y}\|_2 = \max_{y} \frac{\|A\vec{y}\|_2}{\|y\|_2} = \sigma_{max}$$

Therefore by the definition of the spectral norm,

$$\|\delta\vec{x}\|_2 = \|A^{-1}\delta\vec{y}\|_2 \le \|A^{-1}\|_2\|\delta\vec{y}\|_2$$

This gives us an upperbound of the solution. To find the lowerbound,

$$\begin{aligned} A\vec{x} &= \vec{y} \\ \|\vec{y}\|_2 &= \|A\vec{x}\|_2 \le \|A\|_2\|\vec{x}\|_2 \\ \|\vec{x}\|_2 &\ge \frac{\|\vec{y}\|_2}{\|A\|_2} \end{aligned}$$

Combining these two inequalities gives

$$\begin{aligned} \frac{\|\delta\vec{x}\|_2}{\|\vec{x}\|_2} &\le \frac{\|A^{-1}\|_2\|\delta\vec{y}\|_2}{\|\vec{y}\|_2/\|A\|_2} \\ &\le \|A\|_2\|A^{-1}\|_2\frac{\|\delta\vec{y}\|_2}{\|\vec{y}\|_2} \\ &\le \left(\frac{\sigma_{max}}{\sigma_{min}}\right)\frac{\|\delta\vec{y}\|_2}{\|\vec{y}\|_2} \end{aligned}$$

The term $\frac{\sigma_{max}}{\sigma_{min}}$ is called the condition number of a matrix. If the condition number is large, a small change in y would cause a large change in x.

3.b. Shift property of eigenvalues

Theorem 3.3 (Shift property of eigenvalues)

Consider matrix A. We add a diagonal matrix to A and change it to $A + \lambda I$. Then for λ_1 and $\vec{v}_1$ be the first eigenpair of A,

$$(A + \lambda I)\vec{v}_1 = A\vec{v}_1 + \lambda\vec{v} = \lambda_1\vec{v}_1 + \lambda\vec{v}_1 = (\lambda_1 + \lambda)\vec{v}$$

The eigenvalue of the new matrix $A + \lambda I$ is shifted by λ, but its eigenvector remain unchanged.

3.c. Ridge Regression

Theorem 3.4 (Ridge regression)

Consider the optimization problem

$$\min_{\vec{x}} \|A\vec{x} - \vec{b}\|^2 + \lambda^2\|\vec{x}\|_2^2$$

Where $\lambda^2\|\vec{x}\|_2^2$ is called the **regularizer**. We have

$$\begin{aligned} f(\vec{x}) &= (A\vec{x} - \vec{b})^\top(A\vec{x} - \vec{b}) + \lambda^2\vec{x}^\top\vec{x} \\ &= \vec{x}^\top A^\top A\vec{x} - \vec{x}^\top A^\top\vec{b} - \vec{b}^\top A\vec{x} + \lambda^2\vec{x}^\top\vec{x} + \vec{b}^\top\vec{b} \end{aligned}$$

The gradient of f is

$$\nabla f(\vec{x}) = 2A^\top A\vec{x} - 2(\vec{b}^\top A)^\top + 2\lambda^2\vec{x}$$

Setting the gradient to zero gives us

$$\begin{aligned} (A^\top A + \lambda^2 I)\vec{x}^* &= A^\top\vec{b} \\ \vec{x}^* &= (A^\top A + \lambda^2 I)^{-1}A^\top\vec{b} \end{aligned}$$

Ridge regression has two interpretations.

- We want to shift the eigenvalues of A to limit the condition number so it is not too large.
- Without the regularizer, the predicted coefficient of the polynomial tend to be really large (10^6-level large). The regularizer integrated the size of x into the minimizing terms and controls the size of the predicted value so that it is not insanely large.

Note: the solution to the ridge regression is **not** the same as the solution to OLS. In general, these two solutions are distinct.

3.d. Tikhonov regularization

Definition 3.5 (Tikhonov regularization)
Consider data $A\vec{x} = \vec{b}$. We decide to add weights W_1 to the data points such that the weights represents the "importance" or "confidence." We then add some new data W_2 to A and a corresponding $\vec{x}_0$ to $\vec{b}$. With the additional information, the original data becomes:

$$W_1 \begin{bmatrix} A \\ W_2 \end{bmatrix} \vec{x} = \begin{bmatrix} \vec{b} \\ \vec{x}_0 \end{bmatrix}$$

where W_1 and W_2 are matrices. The optimization problem becomes:

$$\min_{\vec{x}} \|W_1(A\vec{x} - \vec{b})\|_2^2 + \|W_2(\vec{x} - \vec{x}_0)\|_2^2$$

Such problem is called Tikhonov regression.

3.e. Probablistic perspective

Definition 3.6 (Problem statement)
Consider model

$$y_i = g(x_i) + z_i$$

Where z_i is noise. We have some information about the noise such that

$$z_i \sim N(0, \sigma_i^2) \to f(z_i) = \frac{e^{-z_i^2/2\sigma_i^2}}{\sqrt{2\pi}\sigma_i}$$

This model is our data points. **Assume** the model is linear, i.e. $g(\vec{x}_i) = \vec{x}_i^\top \vec{w}$. In this context, we can call $\vec{w}$ as our "model". We can rewrite the original equation to

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} \cdots & \vec{x}_1^\top & \cdots \\ & \vdots & \\ \cdots & \vec{x}_n^\top & \cdots \end{bmatrix} \vec{w} + \begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix}$$

such that $\vec{y} \approx X\vec{w}$. We could solve this problem by OLS, but OLS does not count into consideration the information we know about the noise and thus gives suboptimal solution. Is there a better way to choose $\vec{w}$?

Theorem 3.7 (Maximum Likelihood estimation)

Goal: find $\vec{w}$ that makes observed data most likely, i.e.

$$\underset{\vec{w}_0}{\text{argmax}}\, f(Y_1 = y_1, \cdots, Y_n = y_n | \vec{w} = \vec{w}_0)$$

Assume z_i i.i.d. Then we can rewrite the original problem into

$$\underset{\vec{w}_0}{\text{argmax}} \prod_{i=1}^{n} f(Y_i = y_i | \vec{w} = \vec{w}_0)$$

Note that

$$\begin{aligned} f(Y_i = y_i | \vec{w} = \vec{w}_0) &= f(\vec{x}_i^\top \vec{w}_0 + z_i = y_i | \vec{w} = \vec{w}_0 \\ &= f(z_i = y_i - \vec{x}_i^\top \vec{w}_0 | \vec{w} = \vec{w}_0) \\ &= \frac{e^{\frac{-(y_i - \vec{x}_i^\top \vec{w}_0)^2}{2\sigma_i^2}}}{\sqrt{2\pi}\sigma_i} \end{aligned}$$

Therefore

$$\begin{aligned} \underset{\vec{w}_0}{\text{argmax}} \prod_{i=1}^{n} f(Y_i = y_i | \vec{w} = \vec{w}_0) &= \underset{\vec{w}_0}{\text{argmax}} \prod_{i=1}^{n} \frac{e^{\frac{-(y_i - \vec{x}_i^\top \vec{w}_0)^2}{2\sigma_i^2}}}{\sqrt{2\pi}\sigma_i} \\ &= \underset{\vec{w}_0}{\text{argmax}} \frac{1}{(\sqrt{2\pi})^n \prod_{i=1}^n \sigma_i} \prod_{i=1}^{n} e^{\frac{-(y_i - \vec{x}_i^\top \vec{w}_0)^2}{2\sigma_i^2}} \\ &= \underset{\vec{w}_0}{\text{argmax}} \frac{1}{(\sqrt{2\pi})^n \prod_{i=1}^n \sigma_i} \exp\left\{-\sum_{i=1}^{n} \frac{-(y_i - \vec{x}_i^\top \vec{w}_0)^2}{2\sigma_i^2}\right\} \\ &= \underset{\vec{w}_0}{\text{argmax}} - \sum_{i=1}^{n} \frac{-(y_i - \vec{x}_i^\top \vec{w}_0)^2}{2\sigma_i^2} \\ &= \underset{\vec{w}_0}{\text{argmin}} \sum_{i=1}^{n} \frac{-(y_i - \vec{x}_i^\top \vec{w}_0)^2}{2\sigma_i^2} \\ &= \underset{\vec{w}_0}{\text{argmin}} \|S(X\vec{w}_0 - \vec{y})\|_2^2 \end{aligned}$$

Where

$$S = \begin{bmatrix} \sqrt{\frac{1}{2\sigma_1^2}} & & \\ & \ddots & \\ & & \sqrt{\frac{1}{2\sigma_n^2}} \end{bmatrix}$$

Theorem 3.8 (Maximum a posteriori estimation (MAP))

Based on the problem stated in MLE, what if we have a prior on $\vec{w}$? Again, we have

$$y_i = g(x_i) + z_i$$

$$z_i \sim N(0, \sigma_i^2) \rightarrow f(z_i) = \frac{e^{-z_i^2/2\sigma_i^2}}{\sqrt{2\pi}\sigma_i}$$

In addition,

$$w_i \sim N(\mu_i, \rho_i^2)$$

i.e.

$$\vec{w} \sim N(\vec{\mu}, \Sigma_{\vec{w}}) \ \ s.t. \ \ \Sigma_{\vec{w}} = \begin{bmatrix} \rho_1^2 & & \\ & \ddots & \\ & & \rho_n^2 \end{bmatrix}$$

Goal: find the most likely $\vec{w}$ given data $y_1, \cdots, y_n$, i.e.

$$\underset{\vec{w}}{\operatorname{argmax}} f(\vec{w}|\vec{Y} = \vec{y})$$

By the Bayes theorem,

$$f(\vec{w}|\vec{Y} = \vec{y}) = \frac{f(\vec{Y} = \vec{y}|\vec{w}) f\vec{w}}{f\vec{Y}}$$

Hence

$$\begin{aligned} \underset{\vec{w}}{\operatorname{argmax}} f(\vec{w}|\vec{Y} = \vec{y}) &= \underset{\vec{w}}{\operatorname{argmax}} f(\vec{Y} = \vec{y}|\vec{w}) f(\vec{w}) \\ &= \underset{\vec{w}}{\operatorname{argmax}} \left(\prod_{i=1}^{n} f(Y = y_i|\vec{w}) \right) f(\vec{w}) \end{aligned}$$

Borrowing the calculation we did in MLE,

$$\begin{aligned} \underset{\vec{w}}{\operatorname{argmax}} f(\vec{w}|\vec{Y} = \vec{y}) &= \underset{\vec{w}}{\operatorname{argmax}} \prod_{i=1}^{n} \frac{\exp\left\{\frac{-(y_i - \vec{x}_i^\top \vec{w}_0)^2}{2\sigma_i^2}\right\}}{\sqrt{2\pi}\sigma_i} \frac{\exp\left\{-(\vec{w}-\vec{\mu})^\top \Sigma_W^{-1} (\vec{w}-\vec{\mu})\right\}}{(\sqrt{2\pi})^n (\prod \rho_i)} \\ &= \underset{\vec{w}}{\operatorname{argmax}} \exp\left\{ \sum_{i=1}^{n} \frac{-(y_i - \vec{x}_i^\top \vec{w}_0)^2}{2\sigma_i^2} - (\vec{w}-\vec{\mu})^\top \Sigma_W^{-1} (\vec{w}-\vec{\mu}) \right\} \\ &= \underset{\vec{w}}{\operatorname{argmax}} \sum_{i=1}^{n} \frac{-(y_i - \vec{x}_i^\top \vec{w}_0)^2}{2\sigma_i^2} - (\vec{w}-\vec{\mu})^\top \Sigma_W^{-1} (\vec{w}-\vec{\mu}) \\ &= \underset{\vec{w}}{\operatorname{argmin}} \sum_{i=1}^{n} \frac{(y_i - \vec{x}_i^\top \vec{w}_0)^2}{2\sigma_i^2} + (\vec{w}-\vec{\mu})^\top \Sigma_W^{-1} (\vec{w}-\vec{\mu}) \\ &= \underset{\vec{w}}{\operatorname{argmin}} \|S(X\vec{w}_0 - \vec{y})\|_2^2 + \|\sqrt{\Sigma_W^{-1}}(\vec{w}-\vec{\mu})\|_2^2 \end{aligned}$$

For example, if some ρ's are large (note that ρ's are the variances of the w's), you do not need to care too much about keeping w and μ close in their values. But if ρ's are small, than differences in values of w and μ are going to have a large impact (Therefore you should put a high weight on keeping w and μ similar).

4. Convexity

4.a. Convex Sets

Definition 4.1 (convex combination)
Consider $\vec{x}_i$,

$$\sum_{i=1}^{n} \lambda_i \vec{x}$$

is a convex combination of $\vec{x}$ if

$$\lambda_i \geq 0 \text{ and } \sum_{i=1}^{n} \lambda_i = 1$$

Definition 4.2 (convex set)
A set C is convex if the line segment joining any two points in the set is contained in the set.

Example 4.3
Consider C a vector space. If C is convex then

$$\theta \vec{x}_i + (1-\theta)\vec{x}_2 \in C \quad \forall \theta$$

if $\vec{x}_1, \vec{x}_2 \in C$ and $\theta \in [0,1]$.

Example 4.4
Let

$$C = \{\vec{x} \mid \vec{a}^\top \vec{x} = b\}$$

Note that C is a hyperplane. It can be rewritten into

$$\begin{aligned} \vec{a}(\vec{x} - \vec{x}_0) &= 0 \\ \vec{a}^\top \vec{x} = \vec{a}^\top \vec{x}_0 &= b \end{aligned}$$

To check wheter C is convex, consider $\vec{x}_1, \vec{x}_2 \in C$ and let

$$\vec{x}_3 = \theta \vec{x}_1 + (1-\theta)\vec{x}_2$$

We know that

$$\vec{a}^\top \vec{x}_3 = \theta \vec{a}^\top \vec{x}_1 + (1-\theta)\vec{a}^\top \vec{x}_2 = b$$

Therefore $\vec{x}_3$ belongs to C and C is convex.

Remark 4.5

A hyperplane (a plane which's dimension is 1 less than the dimension of its ambient space) divides the space into two half spaces. The set

$$\{\vec{x} \mid \vec{a}^\top \vec{x} \geq b\}$$

defines a hyperplane, where $\vec{a}$ is perpendicular to all vectors on this plane. This hyperplane naturally generates a counter part

$$\{\vec{x} \mid \vec{a}^\top \vec{x} \leq b\}$$

Example:

$$P = \{\vec{x} \mid \vec{a}^\top (\vec{x} - \vec{x}_0) \geq 0\} \;\; N = \{\vec{x} \mid \vec{a}^\top (\vec{x} - \vec{x}_0) \leq 0\}$$

devides the space into two parts (P for positive and N for negative).

Example 4.6

Consider

$$P = \{A \mid A \in \mathbb{S}^n, \;\; A \text{ is PSD}\}$$

Recall that A is PSD iff

$$\vec{x}^\top A \vec{x} \geq 0 \;\; \forall \vec{x} \in \mathbb{R}^n$$

Is P convex? Let

$$A_1, \; A_2 \in P \;\; and \;\; A_3 = \theta A_1 + (1 - \theta) A_2$$

Then

$$\begin{aligned} \vec{x}^\top A_3 \vec{x} = \theta(\vec{x}^\top A_1 \vec{x}) + (1 - \theta) \vec{x}^\top A_2 \vec{x} \geq 0 \\ \implies A_3 \in P \end{aligned}$$

Therefore P is convex.

Remark 4.7

Linear transformations always preserve convexity.

Theorem 4.8 (separating hyperplane theorem)

Let C, D be convex sets and $C \cap D = \varnothing$. Then there exists hyperplane $\vec{a}^\top \vec{x} = b$ separating two sets such that

$$\begin{aligned} \forall \vec{x} \in C \;\; \vec{a}^\top \vec{x} \geq b \\ \forall \vec{x} \in D \;\; \vec{a}^\top \vec{x} \leq b \end{aligned}$$

Proof: TODO

4.b. Convex Functions

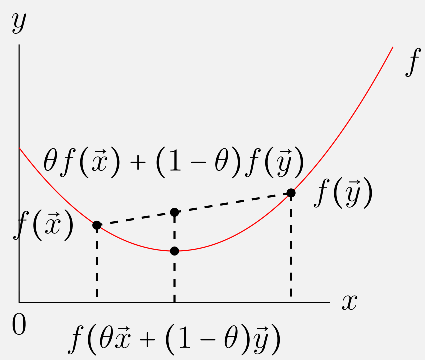
Definition 4.9 (convex functions)
Let

$$f : \mathbb{R}^n \to \mathbb{R}$$

Function f is convex if the domain of f is a convex set and

$$f(\theta\vec{x} + (1-\theta)\vec{y}) \le \theta f(\vec{x}) + (1-\theta)f(\vec{y}) \;\; 0 \le \theta \le 1$$

The above inequality is called **Jensen's Inequality**. Here is an example of a convex function that visualizes the Jensen's Inequality.



If the "cord" is always above the function, the function is **convex**. If the "cord" is always below the function, the function is **concave**.

Theorem 4.10
If a function f is convex, any local minimum is the global minimum.

Definition 4.11 (Epigraph)
The epigraph of a function f is defined as

$$Epi f = \{(x,t) \mid x \in dom f \;\; f(x) \le t\}$$

f is a convex function $\iff$ Epi f is a convex set.

Theorem 4.12 (First-order condition)
Define $f : \mathbb{R}^n \to \mathbb{R}$ a differentiable function. Then f is convex iff

$$f(\vec{y}) \ge f(\vec{x}) + \nabla f(\vec{x})^\top(\vec{y} - \vec{x}) \;\; \forall \vec{x}, \vec{y} \in dom f \;\; 0 \le \theta \le 1$$

Remark 4.13 (Implication of the FOC)
If $\nabla f(\vec{x}_*) = 0$ and f is convex, then

$$f(\vec{y}) \geq f(\vec{x}) + 0(\vec{y} - \vec{x})$$
$$f(\vec{y}) \geq f(\vec{x})$$

For all y in the domain, which means that $\vec{x}_*$ is a global minimum!!

Definition 4.14 (Second-order condition)
Let $f : \mathbb{R}^n \to \mathbb{R}$ who's domain is convex and is twice-differentiable. f is convex iff

$$\nabla^2 f(\vec{x}) \geq 0$$

In another word, $\nabla^2 f(\vec{x})$ is positive semi-definite.

Definition 4.15 (Strict Convexity)
Dom f convex. For all x y in domain, f is strictly convex iff

$$f(\theta\vec{x} + (1-\theta)\vec{y}) < \theta f(\vec{x}) + (1-\theta) f(\vec{y})$$

FOC:
$$f(\vec{y}) > f(\vec{x}) + \nabla f(\vec{x})^\top (\vec{y} - \vec{x}) \quad \forall \vec{x}, \vec{y} \in dom f \quad 0 < \theta < 1$$

SOC:
$$\nabla^2 f(\vec{x}) \succ 0$$

Remark 4.16
If f is a stright line, f is both convex and concave, but not strictly convex.

Definition 4.17 (Strong Convexity)
Dom f convex. For all x y in domain, f is μ-strongly convex iff

$$f(\vec{y}) \geq f(\vec{x}) + \nabla f(\vec{x})^\top (\vec{y} - \vec{x}) + \frac{\mu}{2}\|\vec{y} - \vec{x}\|^2$$

Remark 4.18 (implication of strong convexity)
Recall that by Taylor's theorem, for $f(\vec{x}) := \mathbb{R}^n \to \mathbb{R}$, the derivative of f is

$$f(\vec{y}) \approx f(\vec{x}) + \nabla f^\top(\vec{y} - \vec{x}) + \frac{1}{2}(\vec{y} - \vec{x})^\top \nabla^2 f(\vec{y} - \vec{x})$$

If we let $\mu I = \nabla^2 f$, we have

$$\frac{\mu}{2}\|\vec{y} - \vec{x}\|^2 = \frac{1}{2}(\vec{y} - \vec{x})^\top \mu I(\vec{y} - \vec{x})$$

Thus the implication of strong convexity is that the hessian of f is at least μI.

Remark 4.19
Strong convexity $\implies$ strict convexity $\implies$ convexity

Remark 4.20
For matrices A and B,

$$A \geq B \implies A - B \geq 0$$

5. Gradient Descent

Definition 5.1 (Gradient Descent)

Gradient Descent is an approach to unconstrained optimization problems. The basic idea is to nudge the function in the right direction by a little bit in every step, and after a lot of steps the function will arrive at a local minimum. Formally, for a step size s and a direction $\vec{v}$,

$$f(\vec{x} + s\vec{v}) \approx f(\vec{x}) + s < \nabla f(\vec{x}), \vec{v} >$$

Recall Cauchy-Schwartz, the magnitude of $< \nabla f(\vec{x}), \vec{v} >$ is maximized if $\vec{v}$ is aligned with $\nabla f(\vec{x})$. We want to minimize the inner product while maximize its magnitude so the function steps towards the minimum at the fastest rate, hence we choose

$$\vec{v} = -\nabla f(\vec{x})$$

The formal algorithm for gradiant descent is defined as follows. Let $\vec{x}$ be the parameter of function f. At step k,

$$\vec{x}_{k+1} = \vec{x}_k - \eta \nabla f(\vec{x}_k)$$

Where $\vec{x}_0$ is the initial point and η is the stepsize.

Example 5.2 (GD on LS)

Let $f(\vec{x}) = \|A\vec{x} - \vec{b}\|_2^2$. It has a direct solution of $\vec{x}^* = (A^\top A)^{-1} A^\top \vec{b}$. If A is a n*n matrix, the runtime of computing the direct solution is at least $O(n^3)$ (taking a matrix inverse is approx. $O(n^3)$). It is computationally cheaper to use gradient descent. Thus,

$$\nabla f(\vec{x}) = 2A^\top (A\vec{x} - \vec{b})$$

$$\begin{aligned}
\vec{x}_{k+1} &= \vec{x}_k - \eta \nabla f(\vec{x}_k) \\
&= \vec{x}_k - \eta 2A^\top (A\vec{x} - \vec{b}) \\
\vec{x}_{k+1} &= (I - 2\eta A^\top A)\vec{x}_k + 2\eta A^\top \vec{b}
\end{aligned}$$

Next we need to prove that this algorithm will converge. The following is one of the ways to prove convergence. The difference between optimal value and the k-step value is

$$\begin{aligned}
\vec{x}_{k+1} - (A^\top A)^{-1} A^\top \vec{b} &= (I - 2\eta A^\top A)\vec{x}_k + 2\eta A^\top \vec{b} - (A^\top A)^{-1} A^\top \vec{b} \\
&= (I - 2\eta A^\top A)\vec{x}_k + 2\eta (A^\top A)(A^\top A)^{-1} A^\top \vec{b} - (A^\top A)^{-1} A^\top \vec{b} \\
&= (I - 2\eta A^\top A)\vec{x}_k + (2\eta A^\top A - I)(A^\top A)^{-1} A^\top \vec{b} \\
&= (I - 2\eta A^\top A)(\vec{x}_k - (A^\top A)^{-1} A^\top \vec{b})
\end{aligned}$$

Hence if the absolute values of the eigenvalues of $I - 2\eta A^\top A$ are strictly less than 1, GD converges for LS.