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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

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

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 $\{\vec{a}_1, \vec{a}_2, \ldots, \vec{a}_n\}$, which is orthonormal. For any matrix A,

$$A = QR$$

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

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

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

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 $\vec{z} = A^{\intercal}\vec{w}$,

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

Therefore

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

1.d. Symmetric Matrices

Definition 1.12

Matrix A is symmetric if $A = A^{\intercal}$, 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 $V^{-1} = V^\top$ ■

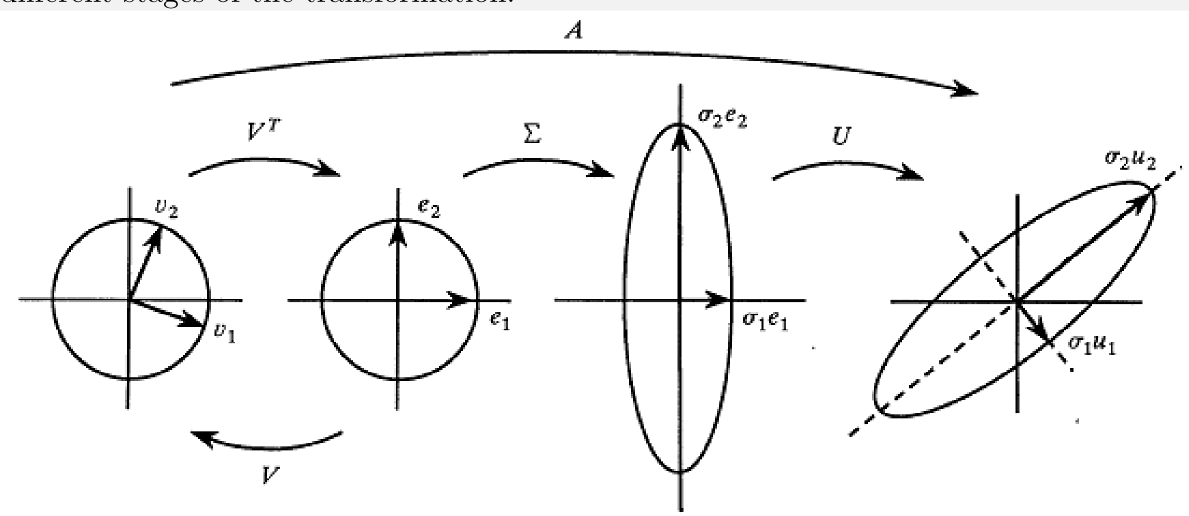
Remark 1.17 (geometric interpretation of SVD)
Consider linear transformation on vector $\vec{x}$ given by matrix A, s.t.

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

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) ≤ i-1+k. Then

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

Consider the solution to the optimization problem

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

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

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.

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

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

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

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

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

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

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

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

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.

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

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

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

Borrowing the calculation we did in MLE,

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

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

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

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

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

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

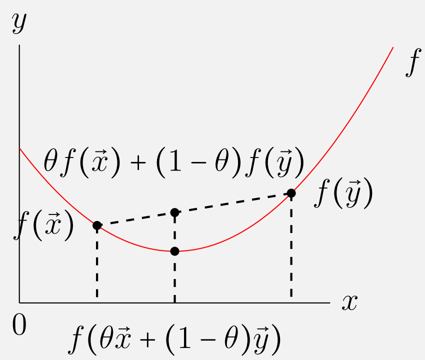
Definition 4.9 (convex functions)
Let

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

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!!

Theorem 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:

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

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,

$$A \succeq B \implies A - B \succeq 0$$

5. Gradient Descent

5.a. Introduction to 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.

Example 5.3 (GD on LS continued)

Since we showed in the previous part that

$$\vec{x}_{k+1} - (A^\intercal A)^{-1} A^\intercal \vec{b} = (I - 2\eta A^\intercal A)^{k+1} (\vec{x}_k - (A^\intercal A)^{-1} A^\intercal \vec{b})$$

Where η (step size) is a parameter of choice and we want to make sure the absolute values of the eigenvalues of $(I - 2\eta A^\intercal A)$ is strictly less than 1, we should choose an appropriate η such that the algorithm converges.

5.b. Gradient Descent for μ-strongly convex L-smooth functions

Definition 5.4 (Bounds of convex functions)

Recall the definition of μ-strongly convex: Dom f convex. For all x y in domain, f is μ-strongly convex iff

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

Intuitively, this means that there exists a quadratic function under f such that this quadratic function is the lower-bound of f, hence the gradient of f is changing fast enough. On the other hand, **L-smooth** means that there exists a quadratic function such that f is upper-bounded by this function, hence the gradient of f is not changing too fast. Formally,

$$f(\vec{y}) \leq f(\vec{x}) + \nabla f(\vec{x})^\intercal (\vec{y} - \vec{x}) + \frac{L}{2} \|\vec{y} - \vec{x}\|_2^2$$

Theorem 5.5

Let $f : \mathbb{R}^n \to \mathbb{R}$ and define optimization problem

$$\min_{\vec{x} \in \mathbb{R}^n} f(\vec{x})$$

Let $\vec{x}_*$ be the optimal solution to the above problem. Then for GD approach

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

I can choose an η such that

$$\|\vec{x}_{t+1} - \vec{x}_*\|_2^2 \leq (C)^{t+1} \|\vec{x}_0 - \vec{x}_*\|_2^2$$

Lemma 5.6

Let f L-smooth, then

$$\|\nabla f(\vec{x})\|_2^2 \leq 2L(f(\vec{x}) - f(\vec{x}_*))$$

Proof. Since $f(\vec{x}_*)$ minimum, we have

$$f(\vec{x}_*) \leq f(\vec{x})$$

And

$$f(\vec{x}_*) \leq f(\vec{x} - \frac{\nabla f(\vec{x})}{L})$$

Recall the definition of L-smooth:

$$f(\vec{y}) \leq f(\vec{x}) + \nabla f(\vec{x})^\top (\vec{y} - \vec{x}) + \frac{L}{2} \|\vec{y} - \vec{x}\|_2^2$$

We choose $f(\vec{y}) = f(\vec{x} - \frac{\nabla f(\vec{x})}{L})$, then

$$\begin{aligned} f(\vec{x} - \frac{\nabla f(\vec{x})}{L}) &\leq f(\vec{x}) + \nabla f(\vec{x})^\top (-\frac{\nabla f(\vec{x})}{L}) + \frac{L}{2} \| - \frac{\nabla f(\vec{x})}{L} \|_2^2 \\ &\leq f(\vec{x}) - \frac{1}{L} \|\nabla f(\vec{x})\|^2 + \frac{1}{2L} \|\nabla f(\vec{x})\|_2^2 \\ &\leq f(\vec{x}) + \frac{1}{2L} \|\nabla f(\vec{x})\|_2^2 \end{aligned}$$

Since $f(\vec{x}_*) \leq f(\vec{x} - \frac{\nabla f(\vec{x})}{L})$,

$$f(\vec{x}_*) \leq f(\vec{x}) + \frac{1}{2L} \|\nabla f(\vec{x})\|_2^2$$

■

Lemma 5.7

If f μ-strongly convex,

$$\nabla f(\vec{x})^\top (\vec{x}_* - \vec{x}) \geq f(\vec{x}) - f(\vec{x}_*) + \frac{\mu}{2} \|\vec{x}_* - \vec{x}\|_2^2$$

Proof. Recall the definition of μ-strong convexity: Dom f convex. For all x y in domain, f is μ-strongly convex iff

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

Let $\vec{y} = \vec{x}_*$. We have

$$\begin{aligned} f(\vec{x}_*) &\geq f(\vec{x}) + \nabla f(\vec{x})^\top (\vec{x}_* - \vec{x}) + \frac{\mu}{2} \|\vec{x}_* - \vec{x}\|^2 \\ f(\vec{x}_*) - f(\vec{x}) - \frac{\mu}{2} \|\vec{x}_* - \vec{x}\|_2^2 &\geq \nabla f(\vec{x})^\top (\vec{x}_* - \vec{x}) \\ -f(\vec{x}_*) + f(\vec{x}) + \frac{\mu}{2} \|\vec{x}_* - \vec{x}\|_2^2 &\leq \nabla f(\vec{x})^\top (\vec{x}_* - \vec{x}) \end{aligned}$$

■

Proof of Main Theorem (Theorem 5.5): TODO

5.c. Introduction to Stochastic Gradient Descent

Definition 5.8

Let $f : \mathbb{R}^n \to \mathbb{R}$ and define optimization problem

$$\min_{\vec{x} \in \mathbb{R}^n} f(\vec{x})$$

Assume the function f is of the following form:

$$f(\vec{x}) = \sum_{i=1}^{m} \frac{1}{m} f_i(\vec{x})$$

E.g. for least squares problem

$$\frac{1}{2m} \|A\vec{x} - \vec{b}\|_2^2 = \frac{1}{2m} \sum_{i=1}^{m} (\vec{a}_i^\top \vec{x} - \vec{b}_i)^2$$

For

$$A = \begin{bmatrix} \cdots & \vec{a}_1^\top & \cdots \\ & \vdots & \\ \cdots & \vec{a}_n^\top & \cdots \end{bmatrix}$$

To calculate the solution of such problem using gradient descent would cost too much computation time (order n time complexity to calculate n losses). Thus instead of computing all of the losses, we choose one component of the gradient in each step.

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

This works because

$$\begin{aligned} \mathbb{E}[\nabla f_i(\vec{x}_k)] &= \frac{1}{m} \sum_{i=1}^{m} f_i(\vec{x}) \\ &= \nabla f(\vec{x}_k) \end{aligned}$$

We usually let η be time-dependent.

Example 5.9

Consider optimization problem

$$f(\vec{x}) = \frac{1}{m}\sum_{i=1}^{m} \|\vec{x} - \vec{p}_i\|_2^2$$

We use SGD to solve this problem. Let step size $\eta = \frac{1}{t}$ and $\vec{x}_0 = 0$, then

$$\nabla f(\vec{x}) = \frac{1}{2}2(\vec{x} - \vec{p}_i) = \vec{x} - \vec{p}_i$$

The $\vec{x}$ in each step goes like

$$\begin{aligned}
\vec{x}_0 &= 0 \\
\vec{x}_1 &= \vec{x}_0 - \frac{1}{1}(\vec{x}_0 - \vec{p}_1) = \vec{p}_1 \\
\vec{x}_2 &= \vec{x}_1 - \frac{1}{2}(\vec{x}_1 - \vec{p}_2) = \frac{\vec{p}_1 + \vec{p}_2}{2} \\
\vec{x}_3 &= \vec{x}_2 - \frac{1}{3}(\vec{x}_2 - \vec{p}_3) = \frac{\vec{p}_1 + \vec{p}_2 + \vec{p}_3}{3}
\end{aligned}$$

The future terms of GD can be projected to

$$\vec{x}_i = \frac{\sum_{j=1}^{i} p_j}{i}$$

5.d. Projected Gradient Descent

Definition 5.10 (projected gradient descent)

Differ from ordinary gradient descent, projected gradient descent solves for the general GD problem where $\vec{x}$ is constrained. Formally, we want to solve the problem

$$\min_{\vec{x}} f(\vec{x}) \ , \ \vec{x} \in C$$

Such that

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

And

$$\prod_C(\vec{y}) = \operatorname*{argmin}_{\vec{\delta} \in C} \|\vec{y}_{k+1} - \vec{\delta}\|_2^2$$

However, this could still be computationally expensive, therefore is replaced by Conditional Gradient Descent in the next subsection.

5.e. Conditional Gradient Descent

Definition 5.11 (conditional gradient descent/Frank–Wolfe algorithm)
Let γ_k be a predetermined sequence. Define

$$\vec{y}_k = \underset{\vec{y} \in C}{\operatorname{argmin}} \nabla f(\vec{x}_k)^\top \vec{y}$$

And

$$\begin{aligned}\vec{x}_{k+1} &= (1 - \gamma_k)\vec{x}_k + \gamma_k \vec{y}_k \\ &= \vec{x}_k + \gamma_k(\vec{y}_k - \vec{x}_k)\end{aligned}$$

Both Frank-Wolfe and PGD are generally computationally expensive, but Frank-Wolfe is sometimes cheaper. Frank-Wolfe also has a nice sparse property but it is out of scope for this class.

6. Duality

Remark 6.1

Gradient Descent works for unconstrained optimization problem on convex functions. It has challenges that the function should be differentiable and convex, and at the same time GD is computationally expensive.

Duality is a technique that transforms every problem to a convex form (the dual form). It does not necessarily give us the solution to the original problem, but it will always give a bound.

Theorem 6.2 (Lagrangian)

Optimization problem

$$p^* = \min f_0(\vec{x})$$

Under the constrains

$$\begin{aligned} f_i(\vec{x}) &\leq 0, \quad \forall i \;\; 1 \leq i \leq m \\ h_i(\vec{x}) &= 0, \quad \forall i \;\; 1 \leq i \leq p \end{aligned}$$

The problem defined above is called a **primal problem**. Define **Lagrangian**:

$$L(\vec{x}, \vec{\lambda}, \vec{\nu}) = f_0(\vec{x}) + \sum_{i=1}^{m} \lambda_i f_i(\vec{x}) + \sum_{i=1}^{p} \nu_i h_i(\vec{x}) \quad \forall \lambda_i \geq 0$$

Note that it is an **affine** function of λ and ν, which means that it is **both convex and concave**. Now, define new problem

$$\min_{\lambda \geq 0} L(\vec{x}, \vec{\lambda}, \vec{\nu}) := g(\vec{\lambda}, \vec{\nu})$$

Over all $\vec{x}$. Examine g. Properties of g include

1. g is a function of only $\vec{\lambda}, \vec{\nu}$.
2. L is an affine function of $\vec{\lambda}, \vec{\nu}$.
3. By 1 and 2, g is a concave function of $\vec{\lambda}, \vec{\nu}$.
4. It turns out, **g**$(\vec{\lambda}, \vec{\nu})$ **is a lower bound on the primal optimal** p^*.

Proof of property No. 4: TODO

Example 6.3

Let $A \in \mathbb{R}^{m*n}$, $m < n$. Problem

$$\min \vec{x}^\top \vec{x} = \vec{p}^*$$

Under the constrain

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

Since there is no inequality constains, the lagrangian of this problem does not have λ.

$$L(\vec{x}, \vec{\nu}) = \vec{x}^\top \vec{x} + \nu^\top (A\vec{x} - \vec{b})$$

$$g(\vec{\nu}) = \min_{\vec{x}} L(\vec{x}, \vec{\nu})$$

To solve for g, we do

$$\nabla_{\vec{x}} L(\vec{x}, \vec{\nu}) = 2\vec{x} + A^\top \vec{\nu}$$

Set gradient to zero,

$$\vec{x} = -\frac{1}{2} A^\top \vec{\nu}$$

Is the point where L is minimized. g at this point is

$$\begin{aligned} g(\vec{\nu}) = L(-\frac{1}{2}A^\top \vec{\nu}, \vec{\nu}) &= (-\frac{1}{2}A^\top \vec{\nu})^\top (-\frac{1}{2}A^\top \vec{\nu}) + \vec{\nu}^\top (-\frac{1}{2}AA^\top \vec{\nu} - \vec{b}) \\ &= \frac{1}{4}\vec{\nu}^\top AA^\top \vec{\nu} + \vec{\nu}^\top (-AA^\top \vec{\nu} - \vec{b}) \\ &= -\frac{1}{4}\vec{\nu}^\top AA^\top \vec{\nu} - \vec{\nu}^\top \vec{b} \end{aligned}$$

Which is the lower bound of p^*. What is the max lower bound? In another word, we want to find

$$\max_{\vec{\nu}} g(\vec{\nu})$$

Definition 6.4 (Dual)

Continuing the definition of lagrangian, we want to find the tightest lower bound of p^*, formally

$$\max_{\vec{\lambda} \geq 0} g(\vec{\lambda}, \vec{\nu}) = d^*$$

Over $\vec{\nu}$, this problem is the **DUAL Problem**. It is a maximization problem of a concave function under linear constrains, thus a **convex program**.