

# Numerical Optimization

## Unit 7: Least Square Problems

Che-Rung Lee

Department of Computer Science  
National Tsing Hua University

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# Linear least squares

- Given samplings  $\vec{a}_1, \vec{a}_2, \dots, \vec{a}_m \in \mathbb{R}^n$  for observations  $b_1, b_2, \dots, b_m \in \mathbb{R}^1$ , the linear least square method wants to find  $\vec{x} = (x_1, x_2, \dots, x_n)^T \in \mathbb{R}^n$  s.t.  $F(\vec{x}) = \sum_{i=1}^m (\vec{a}_i^T \vec{x} - b_i)^2$  is minimized.

- Let  $A = \begin{pmatrix} \vec{a}_1^T \\ \vec{a}_2^T \\ \vdots \\ \vec{a}_m^T \end{pmatrix} \in \mathbb{R}^{m \times n}$ ,  $\vec{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix} \in \mathbb{R}^m$ .

- Let  $F(\vec{x}) = \|A\vec{x} - \vec{b}\|^2 = (A\vec{x} - \vec{b})^T (A\vec{x} - \vec{b})$ . The problem can be written as

$$\min_{\vec{x}} F(\vec{x})$$

# Normal equation

- The optimal condition of linear least squares is  $\nabla F = 0$ ,

$$\nabla F(\vec{x}) = 2A^T(A\vec{x} - \vec{b}) = 0.$$

- The equation

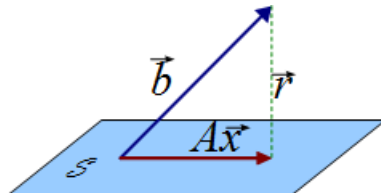
$$A^T A \vec{x} = A^T \vec{b}, \tag{1}$$

is called the *normal equation*.

- Matrix  $A^T A$  is symmetric positive semi-definite. (why?)
- If  $A^T A$  is SPD, we can solve (1) by the Cholesky decomposition.
- If  $A^T A$  is ill-conditioned, solving (1) directly is not numerically stable.
- How to solve (1) if  $A^T A$  is singular or ill-conditioned?
- A best way to solve the normal equation is by the QR method.

# Geometrical interpretation of linear least square

- The problem  $\min_{\vec{x}} \|A\vec{x} - \vec{b}\|^2$  is to find a linear combination of  $A$ 's column vectors which is closet to  $\vec{b}$ .
- Let  $\mathcal{S}$  be the subspace spanned by  $A$ 's column vectors.
- If  $\vec{b}$  is in  $\mathcal{S}$ , then there exists  $\vec{x} \in \mathcal{S}$  s.t.  $A\vec{x} = \vec{b}$ .
- If  $\vec{b}$  is not in  $\mathcal{S}$ , then  $A\vec{x}$  is  $\vec{b}$ 's projection on  $\mathcal{S}$ . (why?)



- Moreover,  $\|\vec{r}\| = \min_{\vec{x}} \|A\vec{x} - \vec{b}\|$ .

# Geometrical interpretation

- The vector  $\vec{r}$  is orthogonal to all the column vectors in  $A = [\vec{a}_1 \ \vec{a}_2 \ \dots \ \vec{a}_n]$ , which means

$$A^T \vec{r} = \begin{bmatrix} \vec{a}_1^T \vec{r} \\ \vec{a}_2^T \vec{r} \\ \vdots \\ \vec{a}_n^T \vec{r} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \Rightarrow A^T (A\vec{x} - \vec{b}) = 0 \Rightarrow A^T A\vec{x} = A^T \vec{b}.$$

which is the normal equation again.

- The column vectors of  $Q_1$  form an orthogonal basis of  $\mathcal{S}$ . The vector that  $\vec{b}$  projected to  $\mathcal{S}$  is  $Q_1 Q_1^T \vec{b}$ , where  $Q_1^T \vec{b}$  is the coordinates of the projected vector in the  $Q_1$  coordinate system.

# QR method

The QR method for linear least square problem for  $m \geq n$ .

## Algorithm 1: QR method

- 1 Compute  $A$ 's QR decomposition:

$$AP = Q_1 \begin{bmatrix} R_{k \times k} & T_{k \times (n-k)} \end{bmatrix}, \quad (2)$$

where  $Q_1$  is an  $m \times k$  matrix,  $Q_1^T Q_1 = I$ ,  $R$  is full ranked upper triangular, and  $P$  is an  $n \times n$  permutation matrix.

- 2 The inverse of  $P$  is  $P^T$ , so

$$A = Q_1 \begin{bmatrix} R_{k \times k} & T_{k \times (n-k)} \end{bmatrix} P^T. \quad (3)$$

- 3 The optimal solution  $\vec{x}^* = P \begin{bmatrix} R^{-1} Q_1^T \vec{b} \\ \vec{0}_{n-k} \end{bmatrix}$ .

# Matrix rank and orthogonal matrix

- Rank of a matrix: the number of linearly independent rows or columns of a matrix.
- Let  $Q_2$  be the orthogonal complement of  $Q_1$ , and  $Q = [Q_1 \ Q_2]$ . The matrix  $Q$  is an  $m \times m$  orthogonal matrix, which means  $Q^T Q = I$ , and  $Q^{-1} = Q^T$ . It implies  $Q_1^T Q_1 = I_k$ ,  $Q_2^T Q_2 = I_{m-k}$ ,  $Q_1^T Q_2 = 0_{k \times (m-k)}$ , and  $Q_2^T Q_1 = 0_{(m-k) \times k}$ .
- From the normal equation  $A^T A \vec{x} = A^T \vec{b}$  and (3), we have

$$P \begin{bmatrix} R^T \\ T^T \end{bmatrix} Q_1^T Q_1 \begin{bmatrix} R & T \end{bmatrix} P^T \vec{x} = P \begin{bmatrix} R^T \\ T^T \end{bmatrix} Q_1^T \vec{b}$$

Let  $P^T \vec{x}^T = [\vec{x}_1^T \ \vec{x}_2^T]$  where  $\vec{x}_1 \in \mathbb{R}^k$  and  $\vec{x}_2 \in \mathbb{R}^{n-k}$ . It becomes

$$\begin{bmatrix} R^T R & R^T T \\ T^T R & T^T T \end{bmatrix} \begin{bmatrix} \vec{x}_1 \\ \vec{x}_2 \end{bmatrix} = \begin{bmatrix} R^T Q_1^T \vec{b} \\ T^T Q_1^T \vec{b} \end{bmatrix} \quad (4)$$

# Algebraic derivation

Let  $Q = [Q_1 \ Q_2]$  be a full orthogonal matrix, where  $Q_1$  and  $Q_2$  are defined as in the QR method.

$$\begin{aligned}\|\vec{r}\|^2 &= \|A\vec{x} - \vec{b}\|^2 = \|Q^T(A\vec{x} - \vec{b})\|^2 \\ &= \|Q_1^T(A\vec{x} - \vec{b})\|^2 + \|Q_2^T(A\vec{x} - \vec{b})\|^2 \\ &= \|Q_1^T A\vec{x} - Q_1^T \vec{b}\|^2 + \|Q_2^T \vec{b}\|^2.\end{aligned}$$

- We can control  $\vec{x}$  and make the first term 0, but we cannot do anything about the second term.
- The first equation from (4) shows  $R\vec{x}_1 + T\vec{x}_2 = Q_1^T \vec{b}$ . One of the solution is to set  $\vec{x}_1 = R^{-1}Q_1^T \vec{b}$  and  $\vec{x}_2 = \vec{0}$ , which gives us a solution

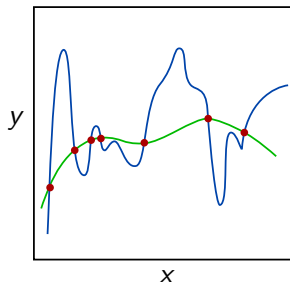
$$\vec{x}^* = P \begin{bmatrix} \vec{x}_1 \\ \vec{x}_2 \end{bmatrix} = P \begin{bmatrix} R^{-1}Q_1^T \vec{b} \\ \vec{0}_{n-k} \end{bmatrix}.$$

- The solution  $\vec{x}^*$  is not unique, but  $A\vec{x}^* = Q_1 Q_1^T \vec{b}$  is unique.



# Overfitting problem and regularization

- The solution of a least square problem may generate a model that fits the given data well, but loses the generality. Such problem is called overfitting.
- Regularization is the process of adding information to prevent overfitting.



Two commonly used regularizations:

- 1  $\ell_2$  regularization (ridge regression, Tikhonov regularization):

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

- 2  $\ell_1$  regularization (LASSO: Least Absolute Shrinkage and Selection Operator):

$$\min_{\vec{x}} \|A\vec{x} - \vec{y}\|^2 + \lambda \|\vec{x}\|_1$$

- The objective of the ridge regression is

$$\begin{aligned} J(\vec{x}) &= \|A\vec{x} - \vec{y}\|^2 + \lambda \|\vec{x}\|_2^2 \\ &= (A\vec{x} - \vec{y})^T (A\vec{x} - \vec{y}) + \lambda \vec{x}^T \vec{x} \\ &= \vec{x}^T (A^T A + \lambda I) \vec{x} - 2\vec{y}^T A\vec{x} + \vec{y}^T \vec{y} \end{aligned}$$

- Since  $A^T A$  is symmetric positive semi-definite and  $\lambda > 0$ ,  $J$  is a convex function, which has a unique minimum point at  $\nabla J = 0$ .

$$\nabla J = 2(A^T A + \lambda I)\vec{x} - 2A^T \vec{y} = 0$$

$$\vec{x}^* = (A^T A + \lambda I)^{-1} A^T \vec{y}.$$

- This is just like the modified Newton method using shift.

- The objective of LASSO is

$$J(\vec{x}) = \|A\vec{x} - \vec{y}\|^2 + \lambda \|\vec{x}\|_1,$$

where  $\|\vec{x}\|_1 = |x_1| + |x_2| + \cdots + |x_n|$ .

- Since the absolute function is non-differentiable, it cannot be solved directly. However, we can reformulate it as a constrained optimization problem.

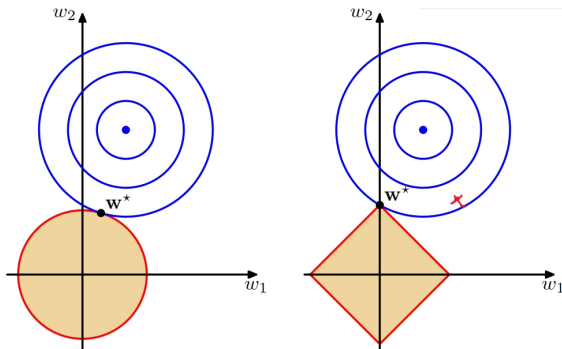
$$\min_{\vec{x}, s} \|A\vec{x} - \vec{y}\|^2 + \lambda \sum_{i=1}^n s_i$$

$$\begin{aligned} \text{s.t.} \quad & x_i \leq s_i \quad \text{for } i = 1, 2, \dots, n \\ & -x_i \leq s_i \quad \text{for } i = 1, 2, \dots, n \\ & s_i \geq 0 \end{aligned}$$

- We will learn how to solve this constrained optimization problem later.

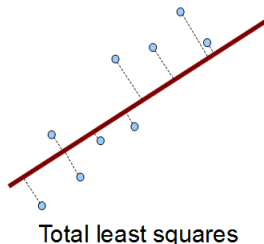
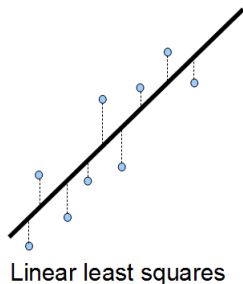
# Comparison of those two regularization methods

- $\ell_2$  regularization pushes all the element in  $\vec{x}$  toward 0, but not exactly zero.
- $\ell_1$  regularization makes the solution  $\vec{x}$  sparse (many zeros) because of the natural of 1-norm.



# Errors in observations and sampling points

- In the linear least square problems, we assume that the samplings,  $\vec{a}_1, \vec{a}_2, \dots, \vec{a}_m$ , have no bias and the only error comes from the observations  $b_1, b_2, \dots, b_m$ . What if the error is contributed by sampling and observations?
- The two dimensional problem: Suppose the sampling points are at  $\vec{x}_1, \vec{x}_2, \dots, \vec{x}_m$ , and the observations are  $y_1, y_2, \dots, y_m$ .



# Total least square problem for 2D

- Total least square: find a line  $ax + by + c = 0$  such that the summation of the distance of all points  $(x_1, y_1), (x_2, y_2), \dots, (x_m, y_m)$  to this line is minimized.
- We need to find  $a, b, c$ . To make solution unique, we let  $\sqrt{a^2 + b^2} = 1$ .
- How to compute the distance from a point to a line?
  - The distance of a point  $(x_i, y_i)$  to the line  $ax + by + c = 0$  is  $|ax_i + by_i + c|$ . (why?)
- Therefore, the total least squares can be formulated as

$$\min_{a,b,c} \sum_{i=1}^m (ax_i + by_i + c)^2,$$

where  $a^2 + b^2 = 1$ .

# How to solve?

- Let  $F(a, b, c) = \sum_{i=1}^m (ax_i + by_i + c)^2$ . You may want to solve this problem by solving  $\nabla F = 0$ .

$$\nabla F = \begin{pmatrix} \partial F / \partial a \\ \partial F / \partial b \\ \partial F / \partial c \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^m 2x_i(ax_i + by_i + c) \\ \sum_{i=1}^m 2y_i(ax_i + by_i + c) \\ \sum_{i=1}^m 2(ax_i + by_i + c) \end{pmatrix}$$

- But this is not correct, since it has a constraint  $a^2 + b^2 = 1$ .
- Fortunately, the condition  $\partial F / \partial c = 0$  is still held.
  - Let  $\bar{x} = \frac{1}{m} \sum_{i=1}^m x_i$  and  $\bar{y} = \frac{1}{m} \sum_{i=1}^m y_i$ .  $(\bar{a}, \bar{b})$  is the centroid of data.
  - $(\bar{a}, \bar{b})$  must be on the solution line. (why?)
  - If we shift all the points to make  $(\bar{a}, \bar{b}) = (0, 0)$ , then the line equation becomes  $ax + by = 0$ .

# The two dimensional problem example

- Let  $\tilde{x}_i = x_i - \bar{x}$  and  $\tilde{y}_i = y_i - \bar{y}$ . The problem becomes

$$\min_{a,b} \sum_{i=1}^m (a\tilde{x}_i + b\tilde{y}_i)^2 \text{ s.t. } a^2 + b^2 = 1$$

- Let matrix  $A = \begin{pmatrix} x_1 - \bar{x} & y_1 - \bar{y} \\ x_2 - \bar{x} & y_2 - \bar{y} \\ \vdots & \vdots \\ x_m - \bar{x} & y_m - \bar{y} \end{pmatrix}$ , and  $\vec{x} = \begin{pmatrix} a \\ b \end{pmatrix}$ .
- The problem can be expressed as

$$\min_{\vec{x}, \|\vec{x}\|=1} \vec{x}^T A^T A \vec{x}.$$

- In statistics, the matrix  $A^T A$  is the **covariance matrix** of data  $\{(x_i, y_i)\}_{i=1 \dots m}$ .



# How to solve that?

- For the constrained optimization problem, the optimality condition is  $\nabla f(\vec{x}) = \lambda \nabla c(\vec{x})$ , where  $c(\vec{x}) = 0$  is the constraint and  $\lambda$  is some scalar.
- Therefore, the optimal solution  $\vec{x}^*$  must satisfy

$$A^T A \vec{x}^* = \lambda \vec{x}^*.$$

- The above equation says the solution is an eigenvector of  $A^T A$ , but which one?
- A faster way is using the singular value decomposition (SVD)

# Singular value decomposition (SVD)

## Theorem (Existence of SVD)

If  $A$  is a real  $m \times n$  matrix, there exist orthogonal matrix  $U \in \mathbb{R}^{m \times m}$  and  $V \in \mathbb{R}^{n \times n}$  such that

$$U^T A V = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_p)$$

where  $p = \min(m, n)$  and  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_p \geq 0$ .

## Theorem (min-max of SVD)

If  $A$  is a real  $m \times n$  matrix with singular values  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_p$ ,  $p = \min(m, n)$ , then for  $k = 1, 2, \dots, p$ ,

$$\sigma_k = \max_{\dim(S)=p-k+1} \min_{\vec{x} \in S} \frac{\|A\vec{x}\|}{\|\vec{x}\|}.$$

# General form of least squares

- Let  $f(\vec{x}) = \frac{1}{2} \sum_{j=1}^m r_j^2(\vec{x})$ , in which  $r_j(\vec{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$  is a smooth function, and  $m \geq n$ .
- Each  $r_j = \phi(\vec{x}_j) - y_j$  is called a “residual”, where function  $\phi(\vec{x})$  is called the model function and  $y_j$  is an observation obtained at the sampling point  $\vec{x}_j$ .
- The least square problem is to solve

$$\min_{\vec{x}} f(\vec{x})$$

- If  $\phi$  is nonlinear, the problem is called nonlinear least squares.

# Vector function form

- Define a vector function  $\vec{r}(\vec{x}) = \mathbb{R}^n \rightarrow \mathbb{R}^m$ .

$$\vec{r}(\vec{x}) = \begin{pmatrix} r_1(\vec{x}) \\ r_2(\vec{x}) \\ \vdots \\ r_m(\vec{x}) \end{pmatrix}.$$

- The Jacobian  $J(\vec{x})$  of  $\vec{r}(\vec{x})$  is an  $m \times n$  matrix

$$J(\vec{x}) = \begin{bmatrix} \nabla \vec{r}_1^T(\vec{x}) \\ \nabla \vec{r}_2^T(\vec{x}) \\ \vdots \\ \nabla \vec{r}_m^T(\vec{x}) \end{bmatrix} = \begin{bmatrix} \partial r_1 / \partial x_1 & \partial r_1 / \partial x_2 & \dots & \partial r_1 / \partial x_n \\ \partial r_2 / \partial x_1 & \partial r_2 / \partial x_2 & \dots & \partial r_2 / \partial x_n \\ \vdots & \vdots & \ddots & \vdots \\ \partial r_m / \partial x_1 & \partial r_m / \partial x_2 & \dots & \partial r_m / \partial x_n \end{bmatrix}$$

# Nonlinear least square problems

- From the above definition,  $f(\vec{x}) = \frac{1}{2} \vec{r}^T \vec{r}$ .
- The gradient of  $f(\vec{x})$  is

$$\nabla f(\vec{x}) = \sum_{j=1}^m r_j(\vec{x}) \nabla r_j(\vec{x}) = J(\vec{x})^T \vec{r}(\vec{x})$$

- The Hessian of  $f(\vec{x})$  is

$$\begin{aligned} \nabla^2 f(\vec{x}) &= \sum_{j=1}^m \nabla r_j(\vec{x}) \nabla r_j(\vec{x})^T + \sum_{j=1}^m r_j(\vec{x}) \nabla^2 r_j(\vec{x}) \\ &= J(\vec{x})^T J(\vec{x}) + \sum_{j=1}^m r_j(\vec{x}) \nabla^2 r_j(\vec{x}) \end{aligned}$$

- If  $\phi$  is linear,  $J(\vec{x}) = A$ ,  $\vec{r}(\vec{x}) = A\vec{x} - \vec{b}$ , and  $\nabla^2 f(\vec{x}) = A^T A$ .

# Solve nonlinear least squares

We will present two algorithms to solve nonlinear least squares

- The Gauss–Newton method
- The Levenberg–Marquardt method.

## The Gauss–Newton method

- Assume the residuals  $r_j(\vec{x})$  are small, and we can approximate  $\nabla^2 f(\vec{x}) \approx J^T J$ .
- Use Newton's method to compute the search direction  $\vec{p} = -H^{-1}\vec{g}$ .
- It goes back to the linear least square method normal equation

$$(J^T J)\vec{p} = -J^T \vec{r}.$$

# The Levenberg-Marquardt method

- It is under the trust-region framework. (See note 3.)
- The model is quadratic

$$m_k(\vec{p}) = \frac{1}{2} \|\vec{r}_k\|^2 + \vec{p}^T J_k^T \vec{r}_k + \frac{1}{2} \vec{p}^T J_k^T J_k \vec{p}$$

$$\min_{\vec{p}} \frac{1}{2} \|J_k \vec{p} + \vec{r}_k\|^2 \text{ s.t. } \|\vec{p}\| \leq \Delta_k$$

- We will learn how to solve this kind of constrained problem in the rest of semester. Here are some clues.
  - If  $\vec{z} = -(J_k^T J_k)^{-1} (J_k^T \vec{r}_k)$  and  $\|\vec{z}\| < \Delta_k$ ,  $\vec{p} = \vec{z}$ .
  - Otherwise, there exists an  $\lambda$  s.t.  $(J_k^T J_k + \lambda I) \vec{p} = -J_k^T \vec{r}_k$  and  $\|\vec{p}\| = \Delta_k$ . The remaining problem is how to find  $\lambda_k$ .

## Other variations

### Weighted least square problem

For a diagonal matrix  $W$ , the weighted least squares is to solve

$$\min_{\vec{x}} \|W(A\vec{x} - \vec{b})\|^2.$$

### Lorentzian functions

- The square function is sensitive to outliers. Use Lorentzian function

$$L(\vec{r}) = \log(1 + \vec{r}^T \vec{r} / \sigma).$$

- The problem becomes  $\min_{\vec{x}} L(A\vec{x} - \vec{b})$ .

### Constrained least squares

$$\min_{\vec{x}} \|A\vec{x} - \vec{b}\|^2 \text{ s.t. } \|B\vec{x} + \vec{d}\| \leq \alpha.$$