Applied Linear Algebra in Data Analysis

Introduction to Constrained Optimization

Sivakumar Balasubramanian

Department of Bioengineering
Christian Medical College, Bagayam
Vellore 632002

Overdetermined System of linear equations

- For a tall, skinny matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, there is a solution to $\mathbf{A}\mathbf{x} = \mathbf{b}$, only when $\mathbf{b} \in C(\mathbf{A})$.

$$\mathbf{b} = \sum_{i=1}^{n} \mathbf{v}_i a_i = \mathbf{V}\mathbf{a}; \;\; \mathbf{a} \in \mathbb{R}^n, \;\; \mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_n \end{bmatrix} \in \mathbb{R}^{n \times n}$$

- Can we have an approximate solution when $\nexists \mathbf{x}$ such that $\mathbf{A}\mathbf{x} = \mathbf{b}$? Let us define "approximate" solution $\hat{\mathbf{x}}$ as the one that minimizes $\|\mathbf{b} - \mathbf{A}\hat{\mathbf{x}}\|_2^2, \quad \forall \mathbf{x} \in \mathbb{R}^n$. This is the *least squares problem.*

$$\text{Given } \mathbf{A} \text{ and } \mathbf{b}, \text{ choose } \hat{\mathbf{x}} \text{ such that}$$

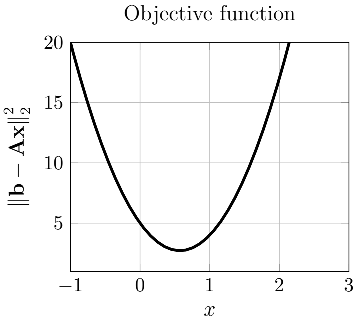
$$\text{minimize} \quad \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2$$

- $\mathbf{A}$ and $\mathbf{b}$ come from the data.
- $\|\mathbf{b} - \mathbf{A}\mathbf{x}\|^2$ is called the objective function.

Least Squares Problem

$$\left.\begin{aligned} 2x &= 1 \\ -1x &= \text{-}2 \\ \sqrt{2}x &= 0 \end{aligned}\right\} \longrightarrow \mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{A} = \begin{bmatrix} 2 \\ -1 \\ \sqrt{2} \end{bmatrix}, \ \mathbf{x} \in \mathbb{R}, \ \mathbf{b} \in \begin{bmatrix} 1 \\ -2 \\ 0 \end{bmatrix}$$

$$\|\mathbf{b} - \mathbf{A}\mathbf{x}\|^2 = (1 - 2x)^2 + (-2 + x)^2 + \left(\sqrt{2}x\right)^2 = 7x^2 - 8x + 5 \geq 0$$



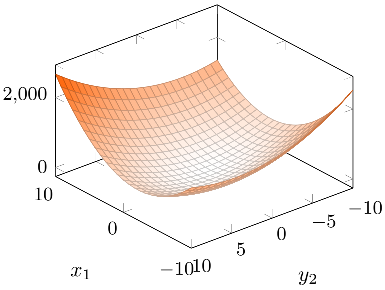
The objective function assumes its minimum value, at $\hat{\mathbf{x}} = \frac{4}{7}$

Least Squares Problem

$$\left.\begin{aligned} 2x_1 - x_2 &= 2 \\ -x_1 + x_2 &= 1 \\ 3x_1 + 2x_2 &= \text{-}1 \end{aligned}\right\} \longrightarrow \mathbf{Ax} = \mathbf{b},\ \ \mathbf{A} = \begin{bmatrix} 2 & -1 \\ -1 & 1 \\ 3 & 2 \end{bmatrix},\ \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix},\ \mathbf{b} \in \begin{bmatrix} 2 \\ 1 \\ -1 \end{bmatrix}$$

$$\|\mathbf{b} - \mathbf{Ax}\|^2 = 14x_1^2 + 6x_2^2 + 6x_2 + 6x_1x_2 + 6 \geq 0$$

$J = 14x_1^2 + 6x_2^2 + 6x_2 + 6x_1x_2 + 6$



The objective function assumes it minimum value at, $\hat{x}_1 = \frac{52}{75}$ and $\hat{x}_2 = \frac{3}{25}$.

Least Squares Methods

- The general solution to this least squares problem can be derived using calculus. Let $f(\mathbf{x}) = \|\mathbf{b} - \mathbf{A}\mathbf{x}\|$

$$\nabla f(\mathbf{x}) = 0 \longrightarrow \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix} = 0$$

Going through the algebra, we end up with the following expression for $\hat{\mathbf{x}}$ that minimizes $f(\mathbf{x})$,

$$\underbrace{\mathbf{A}^T\mathbf{A}\hat{\mathbf{x}} = \mathbf{A}^T\mathbf{b}}_{\text{Normal Equations}}$$

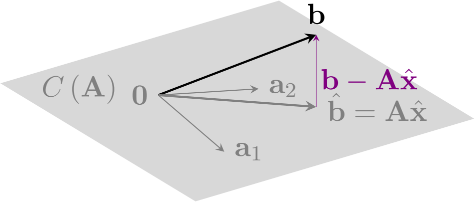
$\mathbf{A}$ is full rank, $\implies$ $\mathbf{A}^T\mathbf{A}$ is invertible.

$$\implies \hat{\mathbf{x}} = \underbrace{\left(\mathbf{A}^T\mathbf{A}\right)^{-1}\mathbf{A}^T}_{\text{Pseudo-inverse}}\mathbf{b} = \mathbf{A}^{\dagger}\mathbf{b}$$

Least Squares Methods

- $\hat{\mathbf{x}}$ is the approximate least squares solution. $\hat{\mathbf{b}} = \mathbf{A}\hat{\mathbf{x}}$, which is in general not equal to $\mathbf{b}$. *When is* $\mathbf{b} = \hat{\mathbf{b}}$*?*

- We know two things about $\hat{\mathbf{b}}$,
  1. $\hat{\mathbf{b}} \in C(\mathbf{A})$: $\hat{\mathbf{b}}$ is the column space of $\mathbf{A}$.
  2. $\left\|\mathbf{b} - \hat{\mathbf{b}}\right\|$ is minimum.



$$\|\mathbf{b} - \mathbf{A}\hat{\mathbf{x}}\|_2^2 \text{ is minimum } \implies (\mathbf{b} - \mathbf{A}\hat{\mathbf{x}}) \perp \mathbf{A}\hat{\mathbf{x}}$$

$$(\mathbf{A}\hat{\mathbf{x}})^T(\mathbf{b} - \mathbf{A}\hat{\mathbf{x}}) = 0 \implies \hat{\mathbf{x}}^T \underbrace{\left(\mathbf{A}^T\mathbf{b} - \mathbf{A}^T\mathbf{A}\hat{\mathbf{x}}\right)}_{\text{Normal Equations}} = 0$$

The least squares approximate solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$ *is the solution solution to the equation* $\mathbf{A}\mathbf{x} = \hat{\mathbf{b}}$*, where* $\hat{\mathbf{b}}$ *is the projection of* $\mathbf{b}$ *onto the column space of* $\mathbf{A}$ $(C(\mathbf{A}))$.

Multi-Objective Least Squares

- There are applications where there is more than one objective that must be optimized,

$$J_1 = \|\mathbf{A}_1\mathbf{x} - \mathbf{b}_1\|^2, \; J_2 = \|\mathbf{A}_2\mathbf{x} - \mathbf{b}_2\|^2, \; \dots \; J_k = \|\mathbf{A}_k\mathbf{x} - \mathbf{b}_k\|^2,$$

  and often these are conflicting objectives.

- We can define a single objective function J that is takes into account the different objective functions.

$$J = \sum_{i=1}^{k} \rho_i J_i, \;\; \rho_i > 0, \;\; \forall 1 \leq i \leq k$$

- The ρ_is indicate the relative weightage given to the individual objectives.

$$J = J_1 + \sum_{i=2}^{k} \rho_i J_i$$

Multi-Objective Least Squares

$$
\begin{aligned}
J &= \rho_1 \left\|\mathbf{A}_1\mathbf{x} - \mathbf{b}_1\right\|^2 + \ldots + \rho_k \left\|\mathbf{A}_k\mathbf{x} - \mathbf{b}_k\right\|^2 \\
&= \left\|\sqrt{\rho_1}\mathbf{A}_1\mathbf{x} - \sqrt{\rho_1}\mathbf{b}_1\right\|^2 + \ldots + \left\|\sqrt{\rho_k}\mathbf{A}_k\mathbf{x} - \sqrt{\rho_k}\mathbf{b}_k\right\|^2
\end{aligned}
$$

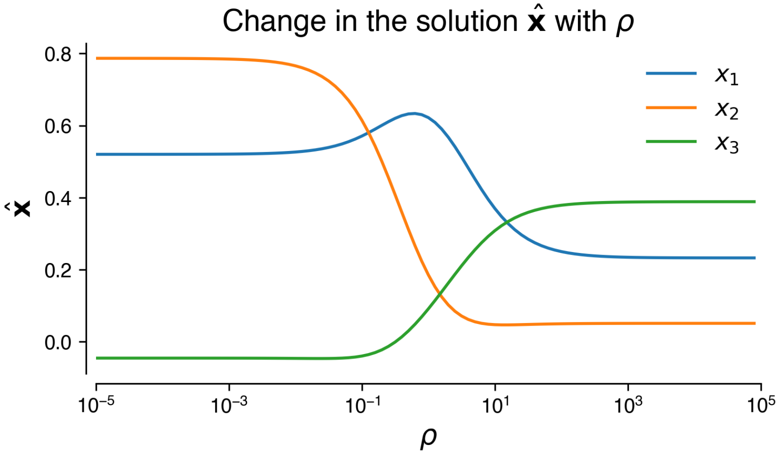
$$
J = \left\| \begin{bmatrix} \sqrt{\rho_1}\mathbf{A}_1 \\ \sqrt{\rho_2}\mathbf{A}_2 \\ \vdots \\ \sqrt{\rho_k}\mathbf{A}_k \end{bmatrix} \mathbf{x} - \begin{bmatrix} \sqrt{\rho_1}\mathbf{b}_1 \\ \sqrt{\rho_2}\mathbf{b}_1 \\ \vdots \\ \sqrt{\rho_k}\mathbf{b}_k \end{bmatrix} \right\|^2 = \left\|\tilde{\mathbf{A}}\mathbf{x} - \tilde{\mathbf{b}}\right\|^2 \implies \hat{x} = \left(\tilde{\mathbf{A}}^T\tilde{\mathbf{A}}\right)^{-1}\tilde{\mathbf{A}}^T\tilde{\mathbf{b}}
$$

The columns of $\tilde{\mathbf{A}}$ are must be independent, which happens if the columns of at least one of the $\mathbf{A}_i$s is independent.
Consider a two objective case, $J = J_1 + \rho J_2$.

$$
\hat{\mathbf{x}} = \begin{cases} \text{argmin}_x \left\|\mathbf{A}_1\mathbf{x} - \mathbf{b}_1\right\|^2 & \rho = 0 \\ \text{argmin}_x \left\|\mathbf{A}_2\mathbf{x} - \mathbf{b}_2\right\|^2 & \rho \to \infty \end{cases}
$$

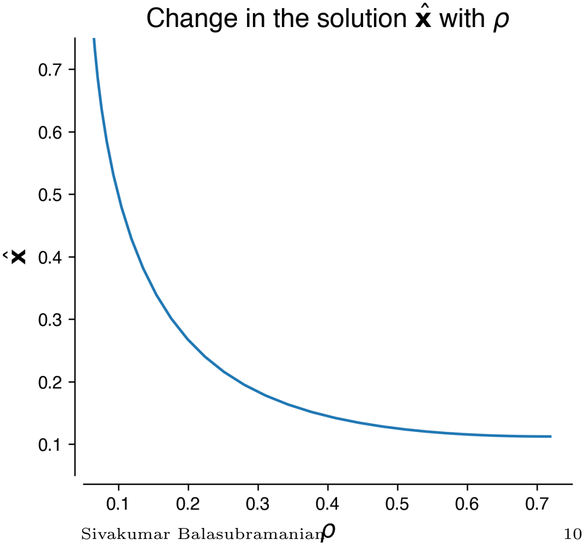
Multi-Objective Least Squares

Consider a problem with the objecrive function, $J(\mathbf{x}) = J_1(\mathbf{x}) + \rho J_2(\mathbf{x})$, where $\mathbf{x} = \mathbb{R}^3$.



Multi-Objective Least Squares

Any solution that lies on this curve is called the *Pareto optimal* solution. There exists no solution $\tilde{\mathbf{x}}$, such that $J_1(\tilde{\mathbf{x}}) \leq J_1(\hat{\mathbf{x}})$ and $J_2(\tilde{\mathbf{x}}) \leq J_2(\hat{\mathbf{x}})$ where, both inqualities hold strictly.



Multi-Objective Least Squares

- Multi-objective least squares methods play an important role in both control and estimation problems.
- Appropriate choice of the objective functions can also help deal with conditions where the columns of A_i are not independent. Consider the following example,

$$J_1 = \|\mathbf{A}_1\mathbf{x} - \mathbf{b}_1\|^2 \quad \text{and} \quad J_2 = \|\mathbf{A}_2\mathbf{x} - \mathbf{b}_2\|^2$$

  where, $\mathbf{A}_1 \in \mathbb{R}^{m_1 \times n}$ and $\mathbf{A}_2 \in \mathbb{R}^{m_2 \times n}$, such that $m_1, m_2 < n$. Thus, the columns of A_1 and A_2 are not independent! However, if $m_1 + m_2 \geq n$, then it is possible that the columns of $\tilde{A}$ are independent.
- This is called **regularized least squares**.
- **Tichonov regularization**: $J = \|\mathbf{A}\mathbf{x} - \mathbf{y}\|^2 + \rho\,\|\mathbf{x}\|^2$, where $\rho > 0$.

$$\tilde{\mathbf{A}} = \begin{bmatrix} \mathbf{A} \\ \sqrt{\rho}\mathbf{I} \end{bmatrix} \implies \hat{\mathbf{x}} = \left(\mathbf{A}^T\mathbf{A} + \rho\mathbf{I}\right)^{-1}\mathbf{A}^T\mathbf{b}$$

Multi-Objective Least Squares

- **Tichonov regularization**: $J = \left\|\mathbf{A}\mathbf{x} - \mathbf{y}\right\|^2 + \rho \left\|\mathbf{x}\right\|^2$, where $\rho > 0$.

$$\tilde{\mathbf{A}} = \begin{bmatrix} \mathbf{A} \\ \sqrt{\rho}\mathbf{I} \end{bmatrix} \implies \hat{\mathbf{x}} = \left(\mathbf{A}^T\mathbf{A} + \rho\mathbf{I}\right)^{-1}\mathbf{A}^T\mathbf{b}$$

- $\hat{\mathbf{x}}$ gives a unique solution in minimizing J, even when $\mathbf{A}$ is not full rank.

- Even when $\mathbf{A}$ is full rank, the regularization term can be used to improve the condition number of the matrix.

Constrained Least Squares

- **Problem**:

$$\begin{aligned} \text{minimize} \quad & \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 \\ \text{subject to} \quad & \mathbf{C}\mathbf{x} = \mathbf{d} \end{aligned}$$

where, $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{b} \in \mathbb{R}^m$, $\mathbf{C} \in \mathbb{R}^{p \times n}$ and $\mathbf{d} \in \mathbb{R}^p$.

- This can be solved using the *method of Lagrange multipliers*. When we do this, we finally arrive the following set of equations, called the *Karush-Kuhn-Tucker* (KKT) equation,

$$2\left(\mathbf{A}^T\mathbf{A}\right)\hat{\mathbf{x}} - 2\mathbf{A}^T\mathbf{b} + \mathbf{C}^T\hat{z} = 0$$

$$\begin{bmatrix} 2\left(\mathbf{A}^T\mathbf{A}\right) & \mathbf{C}^T \\ \mathbf{C} & 0 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{x}} \\ \hat{\mathbf{z}} \end{bmatrix} = \begin{bmatrix} 2\mathbf{A}^T\mathbf{b} \\ \mathbf{d} \end{bmatrix}$$

- The coefficient matrix on the LHS of the KKT equation a square matrix of dimensions $(n+p) \times (n+p)$ is invertible, if and only if, $\begin{bmatrix} \mathbf{A} \\ \mathbf{C} \end{bmatrix}$ is full rank.