4. Regularized least squares

- Regularized least squares
- Tikhonov regularization

Regularized least squares

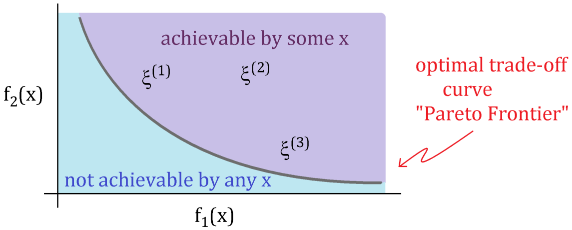
Multi-objective least-squares

Many problems need to balance competing objectives, e.g.

- make $f_1(x) = \|Ax - b\|_2^2$ small
- make $f_2(x) = \|Fx - g\|_2^2$ small

Can make $f_1(x)$ or $f_2(x)$ small, but not both.

Example: $\xi^{(i)} = \big(f_1(x^{(i)}), f_2(x^{(i)})\big)$

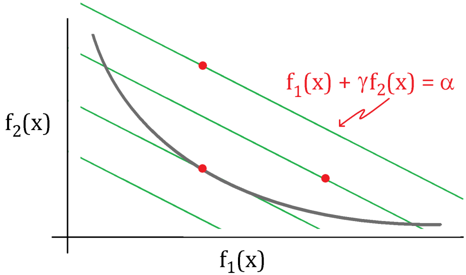


Weighted-sum objective

- Weighted-sum objective gives a Pareto optimal solution:

$$f_1(x) + \gamma f_2(x) = \|Ax - b\|^2 + \lambda \|Fx - g\|^2$$

- parameter $\gamma \geq 0$ defines relative weight between objectives
- points where $f_1(x) + \gamma f_2(x) = \alpha$ correspond to a line with slop $-\gamma$



Example: Signal denoising

- Suppose we observe noisy measurements of a signal:

$$b = \hat{x} + w \quad \text{with} \quad \hat{x} \in \mathbf{R}^n \quad \text{signal,} \quad w \in \mathbf{R}^n \quad \text{noise}$$

- Naive least squares fits noise perfectly

$$\underset{x \in \mathbf{R}^n}{\text{minimize}} \quad \tfrac{1}{2}\|x - b\|^2$$

- Suppose we have prior information that the signal is "smooth"
- Then we might balance fit against smoothness

$$\underset{x \in \mathbf{R}^n}{\text{minimize}} \quad \underbrace{\tfrac{1}{2}\|x - b\|^2}_{f_1(x)} \; + \; \underbrace{\tfrac{1}{2}\gamma \sum_{i=1}^{n-1} (x_i - x_{i+1})^2}_{f_2(x)}$$

where $f_2(x)$ "encourages" smoothness of the solution x

Example: Signal denoising

- Define the finite difference matrix

$$D = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \end{bmatrix} \in \mathbf{R}^{n-1 \times n}$$

  so that $\sum_{i=1}^{n-1} (x_i - x_{i+1})^2 = \|Dx\|^2$

- Resulting least-squares objective:

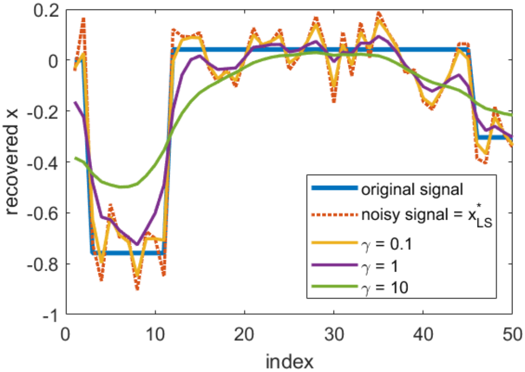
$$\|x - b\|_2^2 + \gamma \|Dx\|^2 = \left\| \begin{bmatrix} I \\ \sqrt{\gamma} D \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|^2$$

- Normal equations

$$(I + \gamma D^T D)x = b$$

Example: Signal denoising

Demo



In homework, will discover a much better penalty function

Regularized least squares (aka Tikhonov)

- General form

$$\underset{x}{\text{minimize}} \quad \frac{1}{2}\|Ax - b\|^2 + \frac{\gamma}{2}\|Dx\|^2, \quad \gamma \geq 0$$

  - $\|Dx\|_2^2$ is the **regularization penalty term**
  - $\gamma \geq 0$ is the **regularization parameter**

- Equivalent expression for objective

$$\frac{1}{2}\|A - b\|_2^2 + \gamma\|Dx\|^2 = \left\| \begin{bmatrix} A \\ \sqrt{\gamma}D \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|^2$$

- Normal equations

$$(A^T A + \gamma D^T D)x = A^T b$$