1 Least Squares

PVK 2019: MAD

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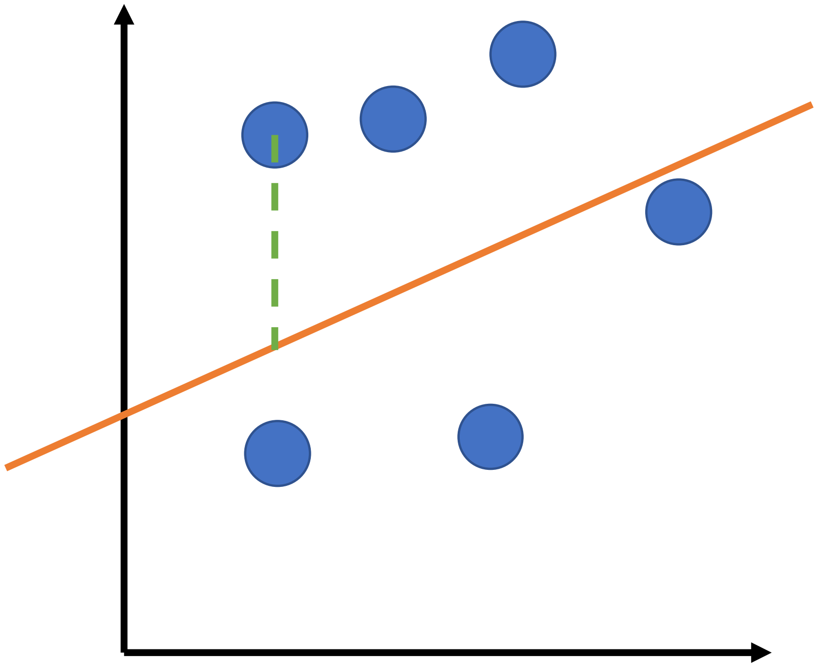
Theory

Setup

- Dataset in 1D $D_1 = \{(x_1, y_1), \dots, (x_N, y_N)\}$
- Dataset in nD $D_n = \{(\overrightarrow{x_1}, y_1), \dots, (\overrightarrow{x_N}, y_N)\}$
- Datavector $\vec{x} = [x_1, \dots, x_N]^T$
- Feature $\overrightarrow{x_i} = \left[x_1^i, \dots, x_n^i\right]^T$
- Datamatrix $X = [\overrightarrow{x_1}, \dots, \overrightarrow{x_N}]^T$
- Labelvector $\vec{y} = [y_1, \dots, y_N]^T$
- Weight/ Parameter w
- Weightvector $\vec{w} = [w_1, \dots, w_K]^2$
- 2-Norm $\|\cdot\|_2$

LLS in 1D



- Datapoint
- LLS fit „prediction“
- Error

LLS in 1D cont.

- Problem formulation:

$$\vec{x}w \approx \vec{y}$$

- Error between LHS and RHS:

$$e = \vec{x}w - \vec{y}$$

- Minimize the squared error to obtain optimal weight:

$$w^* = \arg\min_{w} e^2 = \arg\min_{w} ||\vec{x}w - \vec{y}||_2^2$$

LLS in 1D cont. Example

- Compute the closed form solution to $w^* = \arg\min_{w} \|\vec{x}w - \vec{y}\|_2^2$.

LLS in 1D cont. Example

- Given:
  - $D_1 = \{(0,0),(1,1.5),(2,2.2)\}$

- Task:
  - Set up all vectors
  - Compute the LLS solution manually; Solve $\arg\min_w \|\vec{x}w - \vec{y}\|_2^2$ (don‘t plug in)
  - Predict a the label for $x = 10$

LLS in KD

- Problem formulation:

$$X\vec{w} = \vec{y}$$

- Error between LHS and RHS:

$$e = X\vec{w} - \vec{y}$$

- Minimize the squared error to obtain optimal weight:

$$\vec{w}^* = \arg\min_{\vec{w}} e^2 = \arg\min_{\vec{w}} \|X\vec{w} - \vec{y}\|_2^2$$

LLS in KD cont.

- Closed form solution to $\vec{w}^* \arg\min_{\vec{w}} \|X\vec{w} - \vec{y}\|_2^2$:

$$\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$$

- Also called “normal equation”

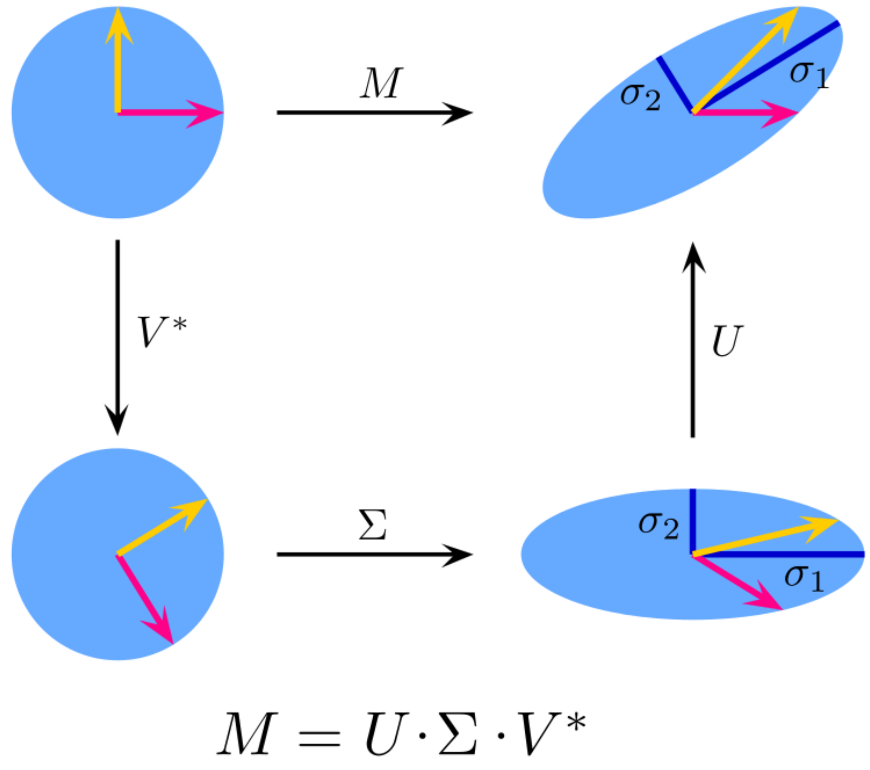
LLS in KD cont. Example

- Given:
  - $D_1 = \{(1,\ 1), (2,\ 3), (3,\ 5)\}$
  - Proposed model: $w_1 + w_2 \cdot x + w_3 \cdot x^2 = y$

- Task:
  - Set up all vectors and matrices, $X\vec{w} = \vec{y}$
  - Compute the solution $\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$ (use a computer)
  - Predict a the label for $\vec{x} = 5$

SVD

- U, V: Orthogonal matrices
- Σ: non-squared diagonal Matrix
- Decomposition:
$$M = U\Sigma V^T$$
- Inverse:
$$\mathrm{M}^{-1} = \mathrm{V}\Sigma^{-1}\mathrm{U}^{\mathrm{T}}$$
- Note: $diag^{-1}(\sigma_i\ ) = diag\left(\frac{1}{\sigma_i}\right)$



Pseudo inverse

- Remember SVD:

$$M^{-1} = V\Sigma^{-1}U^T$$

- If $\sigma_i = 0 \iff M$ is singular
- If M is non-square the inv. doesn't exist
- Define the pseudo inverse:
  - Transpose Σ
  - Reciprocal of non-zero singular values
  - Zeros remain in Σ
  - $M^+ = V\Sigma^+U^T$

$$\Sigma^+ = \begin{bmatrix} \frac{1}{\sigma_1} & & & & & \\ & \ddots & & & & \\ & & \frac{1}{\sigma_r} & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{bmatrix}$$

LLS with large condition number

- Condition number of a system $A\vec{x} = \vec{b}$:

$$\kappa(A) = \|A\| \cdot \|A^{-1}\| = \frac{\sigma_{max}(A)}{\sigma_{min}(A)}$$

- Describes the impact of numerical error:

$$\|\vec{x}_{true} - \vec{x}_{num}\| \sim \kappa \cdot \left\|\vec{b}_{true} - A\vec{x}_{num}\right\|$$

- Problem is “well” conditioned if κ not too large: **Use normal equation**
- Problem is “ill” conditioned if is large: **Use pseudo inverse**

Exercises

Exercise 1

- Given:
  - $D_2 = \{([1,1]^T,\ 1), ([1,2]^T,\ 3), ([2,4]^T,\ 5)\}$
  - Proposed model: $w_1 + w_2 \cdot x_1 + w_3 \cdot x_2^2 = y$

- Task:
  - Set up all vectors and matrices, $X\vec{w} = \vec{y}$ (how to incorporate w_1 and x_2^2 ?)
  - Compute the solution $\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$ (use a computer)
  - Predict a the label for $\vec{x} = [10, 10]^T$

Exercise 2

- Given:
  - Dataset D_1
  - Proposed model: $w_1 \exp(w_2 x + w_3 x^2) = y$

- Task:
  - Set up the LLS formulation

Exercise 3

- Given:
  - $D_{3,x} = \{[1,\ 0,\ 0], [0,\ 2,\ 0], [0, 0, ½]\}$
- Task:
  - Compute the conditional number
  - Is the problem well conditioned?

Homework

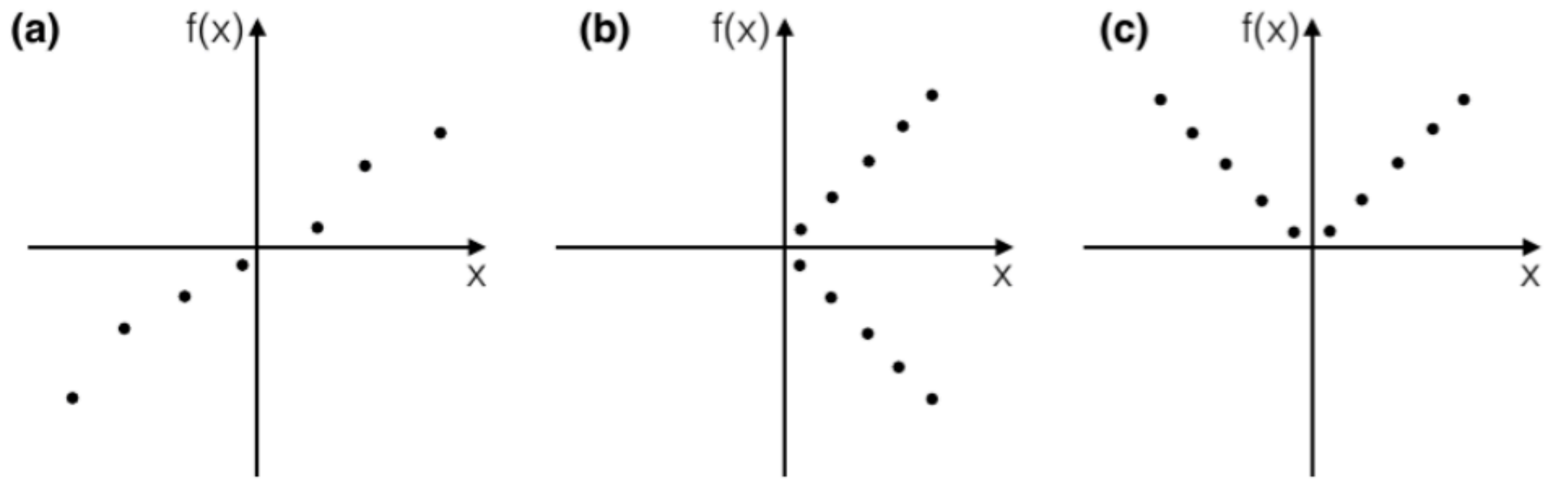
HW 1

- Compute the closed form solution to $\arg\min_{\vec{w}} \|X\vec{w} - \vec{y}\|_2^2$

- Tipps:
  - $\|\vec{x}\|_2^2 = \vec{x}^T\vec{x}$
  - $(A + B)^T = A^T + B^T$
  - $(AB)^T = B^T A^T$
  - $\frac{d}{dx} A\vec{x} = A^T$
  - $\frac{d}{dx} \vec{x}^T A = A$
  - $\frac{d}{dx} \vec{x}^T\vec{x} = 2\vec{x}$
  - $\frac{d}{dx} \vec{x}^T A\vec{x} = A\vec{x} + A^T\vec{x}$

HW 2

- Draw an approximate fit of a LLS fit of(1) a degree 1 polynomial and (2) a degree 2 polynomial



HW 3

- Assume we have perfectly generated data from $x_i + \widetilde{w}_1 = y_i$ if $i = 1, \dots, N\ i \neq j$; and **one** “outlier” $x_j + \widetilde{w}_1 + \epsilon_j = y_j$
- Write down the LLS solution (find $x + w_1 = y$) for the above problem, the solution should only depend on $\widetilde{w}_1$, ϵ_j, and N

HW 4

- Given the dataset $D_3 = \left\{([1,\ 0,\ 0], 2), \left(\left[0,\ \frac{1}{2},\ 0\right], 5\right)\right\}$
  - Compute the rank – is a pseudo-inverse required?
  - Decompose the matrix as $X = U\Sigma V^T$ (Tipp: U and V are identities – what dimensions?)
  - Write down the pseudo inverse
  - Compute $\vec{w}^*$