Mathematical Tools for Neural and Cognitive Science

Fall semester, 2018

Section 2: Least Squares

Least Squares (outline)

- Standard regression: Fit data with weighted sum of regressors. Solution via calculus, orthogonality, SVD
- Choosing regressors, overfitting
- Robustness: weighted regression, iterative outlier trimming, robust error functions, iterative re-weighting
- Constrained regression: linear, quadratic constraints
- Total Least Squares (TLS) regression, and Principle Components Analysis (PCA)















... or linear algebra:

$$\min_{\beta} \sum_{n} (y_n - \beta x_n)^2 = \min_{\beta} ||\vec{y} - \beta \vec{x}||^2$$













$$\begin{split} \min_{\vec{\beta}} ||\vec{y} - X\vec{\beta}||^2 &= \min_{\vec{\beta}} ||\vec{y} - USV^T\vec{\beta}||^2 \\ &= \min_{\vec{\beta}} ||U^T\vec{y} - SV^T\vec{\beta}||^2 \\ &= \min_{\vec{\beta}^*} ||\vec{y}^* - S\vec{\beta}^*||^2 \\ &\text{where } \vec{y}^* = U^T\vec{y}, \quad \vec{\beta}^* = V^T\vec{\beta} \end{split}$$

Solution: $\beta_{\text{opt},k}^* = y_k^*/s_k, \quad \text{for each } k$
or $\vec{\beta}_{\text{opt}}^* = S^{\#}\vec{y}^*$
[on board: transformations, elliptical geometry]

































Constrained Least Squares

Linear constraint:

$$\min_{\vec{\beta}} ||\vec{y} - X\vec{\beta}||^2, \quad \text{where } \vec{c} \cdot \vec{\beta} = \alpha$$

Quadratic constraint:

 $\min_{\vec{\beta}} ||\vec{y} - X\vec{\beta}||^2, \quad \text{where } ||C\vec{\beta}||^2 = 1$

Both can be solved exactly using linear algebra (SVD)... [on board, with geometry]

















