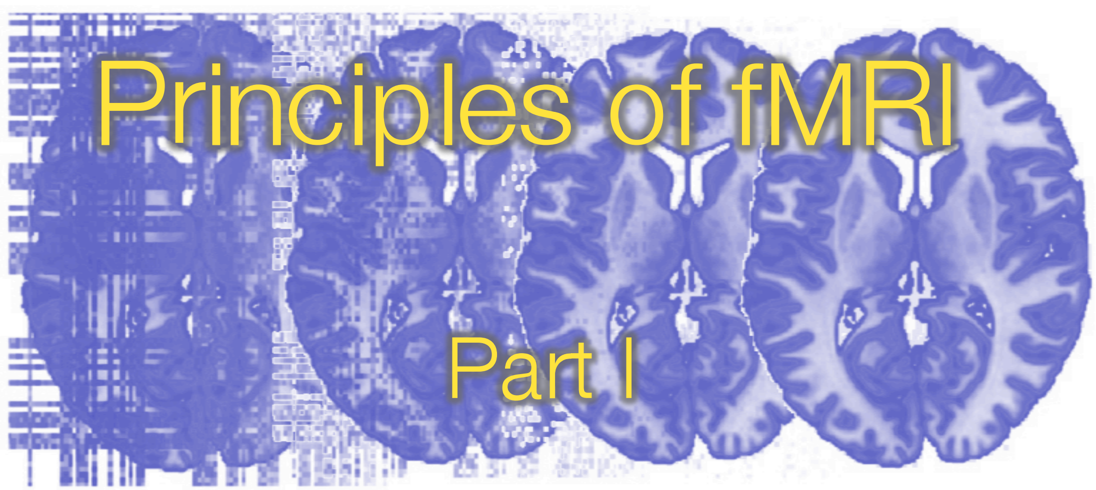
Principles of fMRI

Part I



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GLM Estimation

GLM

A standard GLM can be written:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \qquad \boldsymbol{\varepsilon} \sim N(\mathbf{0}, \mathbf{V})$$

where

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & X_{11} & \cdots & X_{1p} \\ 1 & X_{21} & \cdots & X_{2p} \\ \vdots & \vdots & & \vdots \\ 1 & X_{n1} & \cdots & X_{np} \end{bmatrix} \times \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

fMRI Data

Design matrix

Regression coefficients

Noise

V is the covariance matrix whose format depends on the noise model.

Problem Formulation

- Assume the model:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \qquad \boldsymbol{\varepsilon} \sim N(\mathbf{0}, \mathbf{I}\sigma^2)$$

- The matrices X and Y are assumed to be known, and the noise is assumed to be uncorrelated.

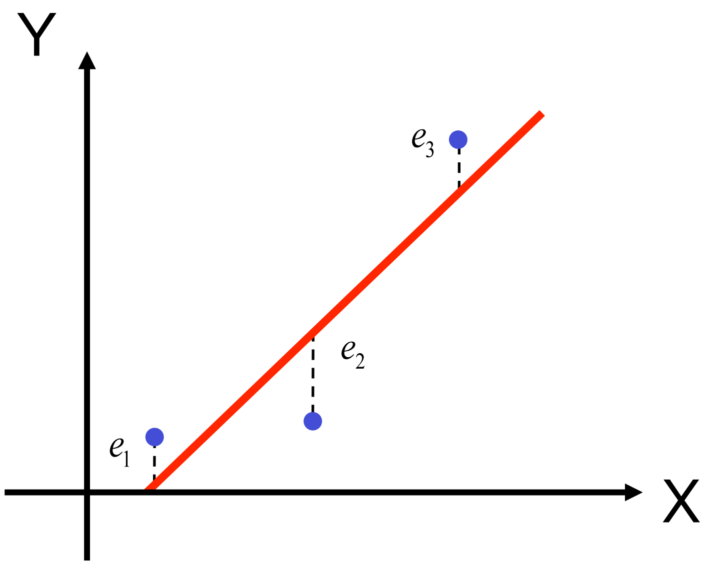
- Our goal is to find the value of $\boldsymbol{\beta}$ that minimizes:

$$(\mathbf{Y} - \mathbf{X}\beta)^T(\mathbf{Y} - \mathbf{X}\beta)$$

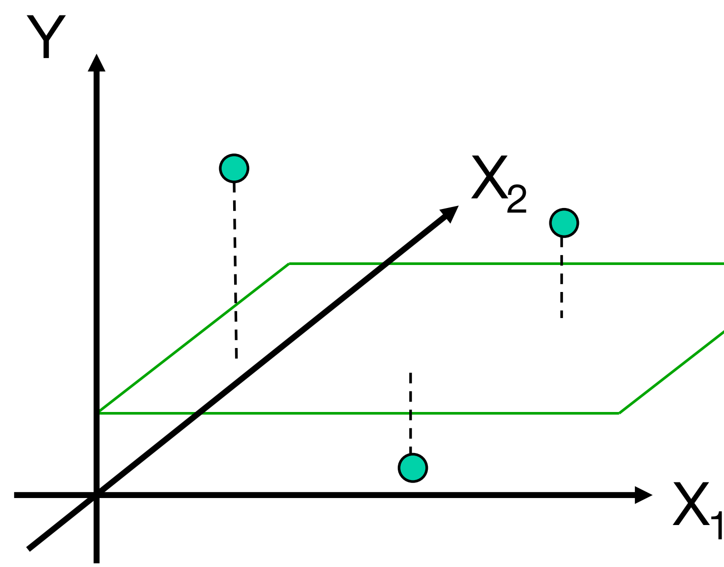
Sums of squared errors (SSE)

Least Squares Estimation

One explanatory variable X.



Two explanatory variables X_1 and X_2.



Least Squares Estimation

- The least squares criterion:

$$Q = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})$$

- Taking the derivative with respect to $\boldsymbol{\beta}$ and setting it to 0 gives us the normal equations:

$$\mathbf{X}'\mathbf{X}\hat{\beta} = \mathbf{X}'\mathbf{Y}$$

- The ordinary least squares (OLS) estimators are given by

$$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

OLS Solution

- Ordinary least squares solution:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

- Properties:

$$E\left(\hat{\beta}\right) = \beta \qquad\qquad Var(\hat{\beta}) = \sigma^2\left(\mathbf{X}^T\mathbf{X}\right)^{-1}$$

- Any other unbiased estimator of $\boldsymbol{\beta}$ will have a larger variance than the OLS solution.
  - Best linear unbiased estimator (BLUE)

Estimation

- If $\boldsymbol{\varepsilon}$ is i.i.d., then Ordinary Least Square (OLS) estimate is optimal

model | estimate

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \longrightarrow \hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

- If Var($\boldsymbol{\varepsilon}$) =$\mathbf{V}\sigma^2 \neq \mathbf{I}\sigma^2$, then Generalized Least Squares (GLS) estimate is optimal

model | estimate

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \longrightarrow \hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{Y}$$

Residuals

model

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \quad \longrightarrow$$

estimate

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{Y}$$

fitted values

$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\beta}$$

residuals

$$\mathbf{r} = \mathbf{Y} - \hat{\mathbf{Y}}$$

$$= (\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1})\mathbf{Y}$$

$$= \mathbf{RY}$$

Estimating the Variance

- Even if we assume $\boldsymbol{\varepsilon}$ is i.i.d., we still need to estimate the residual variance, σ^2.

- Our estimate:

$$\hat{\sigma}^2 = \frac{\mathbf{r}^T\mathbf{r}}{tr(\mathbf{RV})}$$

- For OLS:

$$\hat{\sigma}^2 = \frac{\mathbf{r}^T\mathbf{r}}{N - p}$$

- Estimating $\mathbf{V} \neq \mathbf{I}$ more difficult.

A geometric interpretation of the GLM

Principles of fMRI Part I

Think of y as a vector in a space with one dimension per observation

Minimize sum of squared errors (Q):

$$Q = (\mathbf{Y} - \mathbf{X\beta})'(\mathbf{Y} - \mathbf{X\beta})$$

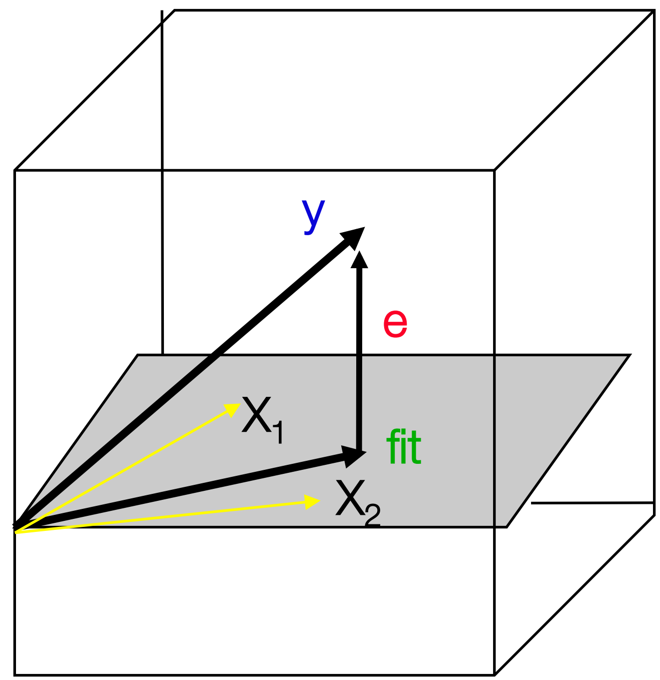
Solve for beta:
Project data (y) onto subspace of X

$$\hat{\beta} = (X^T X)^{-1} X^T y$$

Projection matrix

$$\hat{\beta} = (X)^{-} y$$

(pseudoinverse of X) * y



End of Module

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