# Linear Regression

Aarti Singh

Machine Learning 10-701
Mar 20, 2023

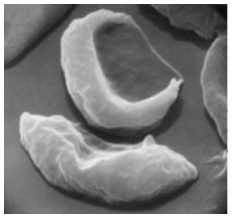
# Supervised Learning Tasks

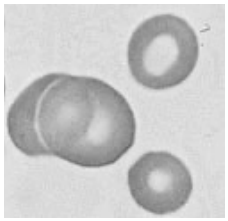
## Classification

X = Document

Sports
Science
News

Y = Topic



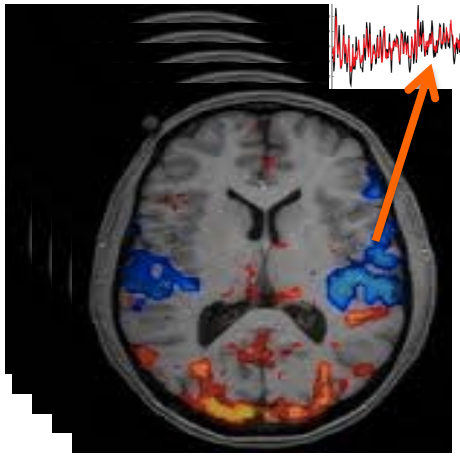


X = Cell Image

Anemic cell
Healthy cell

Y = Diagnosis

## Regression

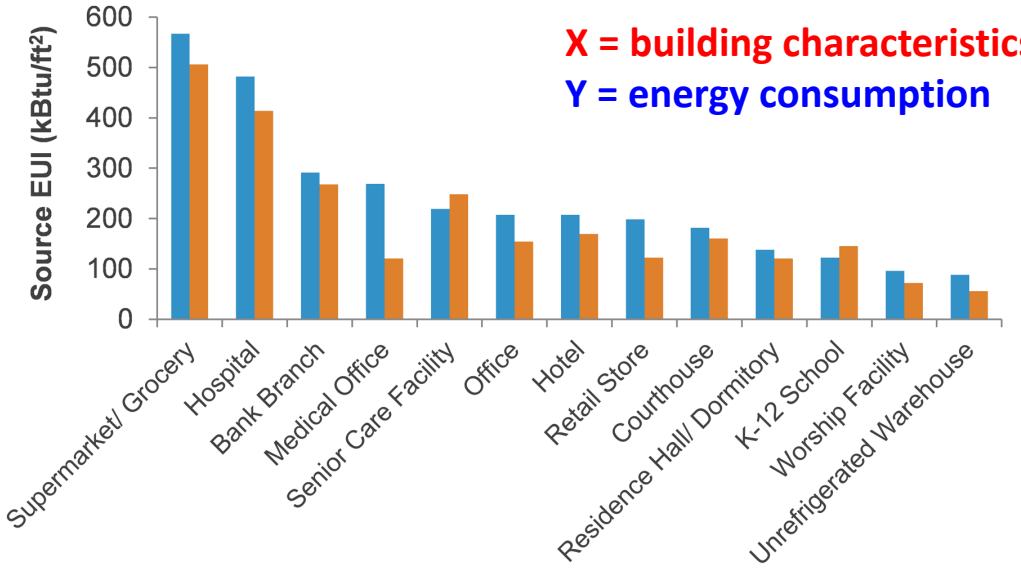


X = Brain Scan

Y = Age of a subject

# Regression Tasks

Estimating Energy Usage




energystar.gov

Estimating Contamination

# Mean Squared Error (MSE) Minimization

Optimal predictor: $$f^* = \arg\min_f \mathbb{E}[(f(X) - Y)^2]$$

# Mean Squared Error (MSE) Minimization

Optimal predictor: $$f^* = \arg\min_f \mathbb{E}[(f(X) - Y)^2]$$

Empirical Minimizer: $$\widehat{f}_n = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (f(X_i) - Y_i)^2$$

**Empirical mean**

Law of Large Numbers:

$$\frac{1}{n} \sum_{i=1}^{n} [\text{loss}(Y_i, f(X_i))] \xrightarrow{n \to \infty} \mathbb{E}_{XY} [\text{loss}(Y, f(X))]$$

# Restrict class of predictors

Optimal predictor: $$f^* = \arg\min_f \mathbb{E}[(f(X) - Y)^2]$$

Empirical Minimizer: $$\widehat{f}_n = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (f(X_i) - Y_i)^2$$

**Class of predictors**

- Why?

$\mathcal{F}$ - Class of Linear functions
- Class of Polynomial functions
- Class of nonlinear functions

# Linear Regression

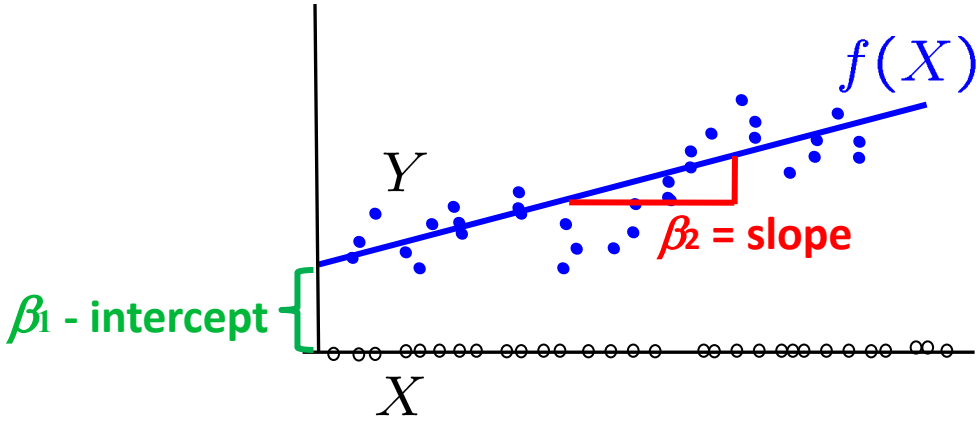
$$\hat{f}_n^L = \arg\min_{f \in \mathcal{F}_L} \frac{1}{n} \sum_{i=1}^{n} (f(X_i) - Y_i)^2$$

Least Squares Estimator

$\mathcal{F}_L$ - Class of Linear functions

Uni-variate case:

$$f(X) = \beta_1 + \beta_2 X$$




Multi-variate case:

$$f(X) = f(X^{(1)}, \ldots, X^{(p)}) = \beta_1 X^{(1)} + \beta_2 X^{(2)} + \cdots + \beta_p X^{(p)}$$

($X^{(1)} = 1$)

$$= X\beta \qquad \text{where} \quad X = [X^{(1)} \ldots X^{(p)}], \quad \beta = [\beta_1 \ldots \beta_p]^T$$

# Linear Regression (Matrix-vector form)

$$\widehat{f}_n^L = \arg\min_{f \in \mathcal{F}_L} \frac{1}{n} \sum_{i=1}^{n} (f(X_i) - Y_i)^2 \qquad f(X_i) = X_i \beta$$

$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n} \sum_{i=1}^{n} (X_i \beta - Y_i)^2 \qquad \widehat{f}_n^L(X) = X\widehat{\beta}$$

$$= \arg\min_{\beta} \frac{1}{n} (\mathbf{A}\beta - \mathbf{Y})^T (\mathbf{A}\beta - \mathbf{Y})$$

$$\mathbf{A} = \begin{bmatrix} X_1 \\ \vdots \\ X_n \end{bmatrix} = \begin{bmatrix} X_1^{(1)} & \dots & X_1^{(p)} \\ \vdots & \ddots & \vdots \\ X_n^{(1)} & \dots & X_n^{(p)} \end{bmatrix} \qquad \mathbf{Y} = \begin{bmatrix} \mathbf{Y}_1 \\ \vdots \\ \mathbf{Y}_n \end{bmatrix}$$

# Linear Regression

$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n}(\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) = \arg\min_{\beta} J(\beta)$$

$$J(\beta) = (\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y})$$

- Poll

Is the objective convex in $\beta$?

A) Convex, quadratic in $\beta$
B) Non-convex, A may not be positive semi definite
C) Depends on conditioning (ratio of max:min eigenvalues) of $A^TA$
D) Convex, $A^TA$ is positive semi definite

# Linear Regression

$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n}(\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) = \arg\min_{\beta} J(\beta)$$

$$J(\beta) = (\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y})$$

$$\left.\frac{\partial J(\beta)}{\partial \beta}\right|_{\widehat{\beta}} = 0$$

# Linear regression solution satisfies Normal Equations

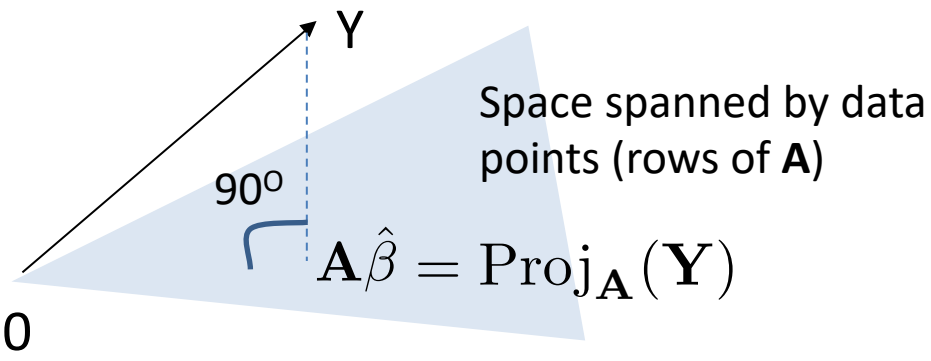
$$(\mathbf{A}^T\mathbf{A})\hat{\beta} = \mathbf{A}^T\mathbf{Y}$$

p x p  p x1  p x1

If $(\mathbf{A}^T\mathbf{A})$ is invertible,

$$\hat{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{Y} \qquad \hat{f}_n^L(X) = X\hat{\beta}$$

Predicted labels for training points $\mathbf{A}\hat{\beta} = \mathrm{Proj}_{\mathbf{A}}(\mathbf{Y})$



# Linear regression solution satisfies Normal Equations

$$(\mathbf{A}^T\mathbf{A})\hat{\beta} = \mathbf{A}^T\mathbf{Y}$$

p x p  p x1  p x1

If $(\mathbf{A}^T\mathbf{A})$ is invertible,

$$\hat{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{Y} \qquad \hat{f}_n^L(X) = X\hat{\beta}$$

Later: When is $(\mathbf{A}^T\mathbf{A})$ invertible ?

Now: What if $(\mathbf{A}^T\mathbf{A})$ is invertible but expensive (p very large)?

# Gradient Descent

Even when $(\mathbf{A}^T\mathbf{A})$ is invertible, might be computationally expensive if **A** is huge.

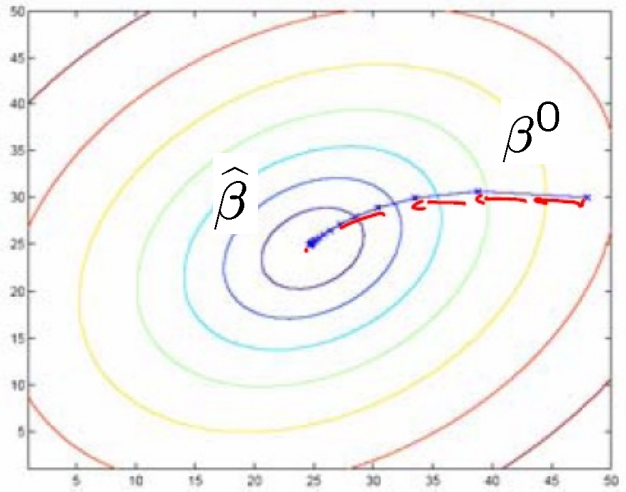
$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n}(\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) = \arg\min_{\beta} J(\beta)$$

**Since J(β) is convex, move along negative of gradient**

Initialize: $\beta^0$

step size

Update:
$$\beta^{t+1} = \beta^t - \frac{\alpha}{2}\frac{\partial J(\beta)}{\partial \beta}\Big|_t$$
$$= \beta^t - \alpha\, \mathbf{A}^T(\underbrace{\mathbf{A}\beta^t - Y}_{0 \text{ if } \widehat{\beta} = \beta^t})$$




Stop: when some criterion met e.g. fixed # iterations, or $\frac{\partial J(\beta)}{\partial \beta}\Big|_{\beta^t} < \varepsilon$.

# Least Square solution satisfies Normal Equations

$$\left.\frac{\partial J(\beta)}{\partial \beta}\right|_{\widehat{\beta}} = 0 \qquad \text{gives} \qquad (\mathbf{A}^T\mathbf{A})\widehat{\beta} = \mathbf{A}^T\mathbf{Y}$$

p x p  p x1  p x1

If $(\mathbf{A}^T\mathbf{A})$ is invertible,

1) If dimension p not too large, analytical solution:

$$\widehat{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{Y} \qquad \widehat{f}_n^L(X) = X\widehat{\beta}$$

2) If dimension p is large, computing inverse is expensive $O(p^3)$
Gradient descent since objective is convex ($\mathbf{A}^T\mathbf{A} \succeq 0$)

$$\begin{aligned}\beta^{t+1} &= \beta^t - \frac{\alpha}{2}\left.\frac{\partial J(\beta)}{\partial \beta}\right|_t \\ &= \beta^t - \alpha\ \mathbf{A}^T(\mathbf{A}\beta^t - Y)\end{aligned}$$

# Linear regression solution satisfies Normal Equations

$$(\mathbf{A}^T\mathbf{A})\hat{\beta} = \mathbf{A}^T\mathbf{Y}$$

p x p  p x1  p x1

When is $(\mathbf{A}^T\mathbf{A})$ invertible ?

Recall: Full rank matrices are invertible. What is rank of $(\mathbf{A}^T\mathbf{A})$ ?