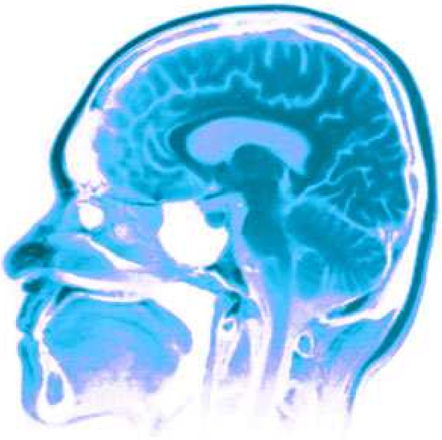
CPSC540



Linear prediction

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Outline of the lecture

This lecture introduces us to the topic of **supervised learning**. Here the data consists of **input**-**output** pairs. Inputs are also often referred to as **covariates**, **predictors** and **features**; while outputs are known as **variates** and **labels**. The goal of the lecture is for you to:

❑ Understand the supervised learning setting.
❑ Understand linear regression (aka **least squares**)
❑ Understand how to apply linear regression models to make predictions.
❑ Learn to derive the least squares estimate by optimization.

Linear supervised learning

❑ Many real processes can be approximated with linear models.

❑ Linear regression often appears as a module of larger systems.

❑ Linear problems can be solved analytically.

❑ Linear prediction provides an introduction to many of the core concepts of machine learning.

We are given a training dataset of n instances of input-ouput pairs $\{\mathbf{x}_{1:n}, \mathbf{y}_{1:n}\}$. Each input $\mathbf{x}_i \in \mathbb{R}^{1\times d}$ is a vector with d attributes. The inputs are also known as predictors or covariates. The output, often referred to as the target, will be assumed to be univariate, $\mathbf{y}_i \in \mathbb{R}$, for now.

$x_{1:n} = \{x_1, x_2, \dots x_n\}$

A typical dataset with $n = 4$ instances and 2 attributes would look like the following table:

$d=2$

	Wind speed	People inside building	Energy requirement
1	100	2	5
2	50	42	25
3	45	31	22
$n=4$	60	35	18

$x_1 = [100 \quad 2]$ $\qquad$ $y_1 = [5]$

Energy demand prediction

Given the training set $\{\mathbf{x}_{1:n}, \mathbf{y}_{1:n}\}$, we would like to learn a model of how the inputs affect the outputs. Given this model and a new value of the input $\mathbf{x}_{n+1}$, we can use the model to make a prediction $\widehat{y}(\mathbf{x}_{n+1})$.

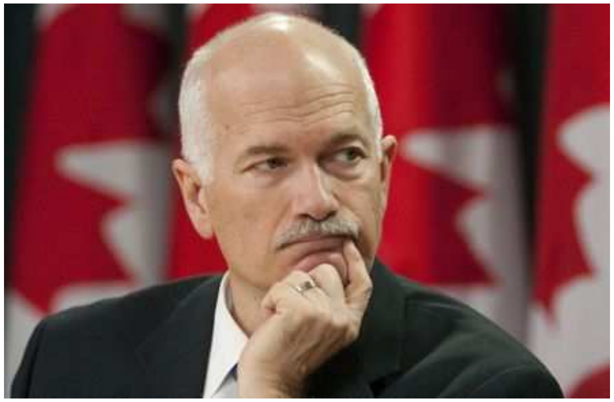
① TRAINING

$\{x_{1:n}, y_{1:n}\} \rightarrow \boxed{\text{Learn}} \rightarrow$ Parameters $\hat{\Theta}$ of a linear model

② Prediction

$x_{n+1}, \hat{\Theta} \rightarrow \boxed{\text{Predict}} \rightarrow \hat{y}_{n+1}$

Prostate cancer example



□ Goal: Predict a prostate-specific antigen (log of lpsa) from a number of clinical measures in men who are about to receive a radical prostatectomy.

□ The inputs are:

- Log cancer volume (lcavol)
- Log prostate weight (lweight)
- Age
- Log of the amount of benign prostatic hyperplasia (lbph)
- Seminal vesicle invasion (svi) - *binary*
- Log of capsular penetration (lcp)
- Gleason score (gleason) – *ordered categorical*
- Percent of Gleason scores 4 or 5 (pgg45)

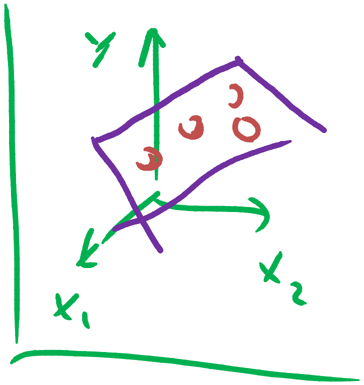
Which inputs are more important?

[Hastie, Tibshirani & Friedman book]

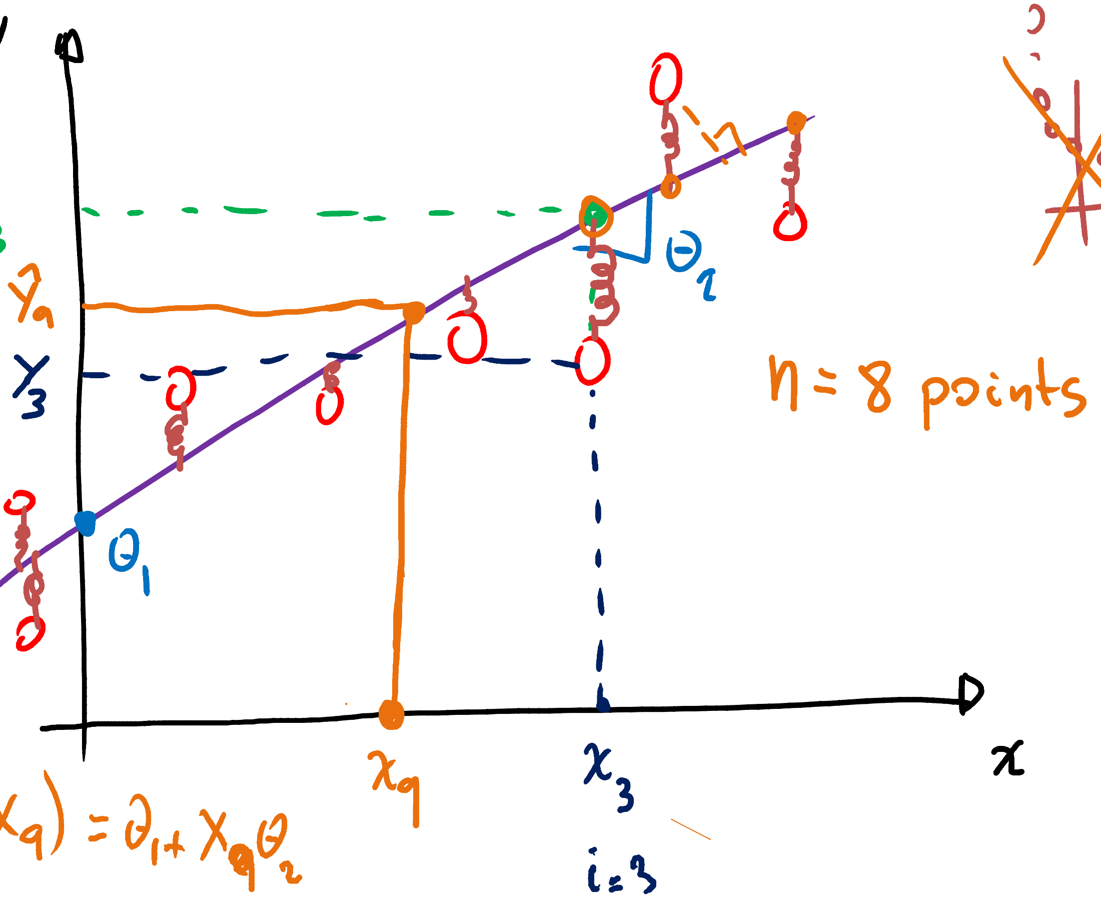
$$\hat{y}(\mathbf{x}_i) = \theta_1 + x_i\theta_2 = \hat{y}_i$$

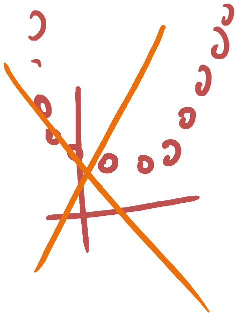
$$J(\boldsymbol{\theta}) = \sum_{i=1}^{n}\underbrace{(y_i - \hat{y}_i)^2} = \sum_{i=1}^{n}(y_i - \theta_1 - x_i\theta_2)^2$$

objective, cost, loss, energy, error function.



$\hat{y}(x_3) = \hat{y}_3$





n = 8 points

o training

o Test

$\hat{y}_q = \hat{y}(x_q) = \theta_1 + x_q\theta_2$

Linear prediction

$$\hat{y}_i = \underbrace{1}_{}\theta_1 + x_i\theta_2$$

$$= x_{i1}\theta_1 + x_{i2}\theta_2$$

In general, the linear model is expressed as follows:

$$\hat{y}_i = \sum_{j=1}^{d} x_{ij}\theta_j,$$

$i = 1, 2, \dots, n$

$j = 1, 2, \dots, d$

where we have assumed that $\underline{x_{i1}} = \underline{1}$ so that θ_1 corresponds to the intercept of the line with the vertical axis. θ_1 is known as the bias or offset.

In matrix form, the expression for the linear model is:

$$\hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta},$$

$$\hat{y}_i = \cancel{x_{11}}^{1}\theta_1 + x_{12}\theta_2 + \dots x_{1d}\theta_d$$

with $\hat{\mathbf{y}} \in \mathbb{R}^{n\times 1}$, $\mathbf{X} \in \mathbb{R}^{n\times d}$ and $\boldsymbol{\theta} \in \mathbb{R}^{d\times 1}$. That is,

$$\begin{bmatrix}\hat{y}_1\\ \vdots\\ \hat{y}_n\end{bmatrix} = \begin{bmatrix}\cancel{x_{11}}^{1} & \cdots & x_{1d}\\ \vdots & \vdots & \vdots\\ \cancel{x_{n1}}^{1} & \cdots & x_{nd}\end{bmatrix}\begin{bmatrix}\theta_1\\ \vdots\\ \theta_d\end{bmatrix} = \begin{bmatrix}\underline{x_1}\\ \underline{x_2}\\ \vdots\\ \underline{x_n}\end{bmatrix}\underline{\theta}$$

Wind speed	People inside building	Energy requirement
100	2	5
50	42	25
45	31	22
60	35	18

For our energy prediction example, we would form the following matrices with $n = 4$ and $d = 3$:

$$\mathbf{y} = \begin{bmatrix} 5 \\ 25 \\ 22 \\ 18 \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & 100 & 2 \\ 1 & 50 & 42 \\ 1 & 45 & 31 \\ 1 & 60 & 35 \end{bmatrix}, \quad \boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}.$$

Suppose that $\boldsymbol{\theta} = \underline{[1 \quad 0 \quad 0.5]}^T$. Then, by multiplying $\mathbf{X}$ times $\boldsymbol{\theta}$, we would get the following predictions on the training set:

$$\widehat{\mathbf{y}} = \begin{bmatrix} 2 \\ 22 \\ 16.5 \\ 18.5 \end{bmatrix} = \begin{bmatrix} 1 & 100 & 2 \\ 1 & 50 & 42 \\ 1 & 45 & 31 \\ 1 & 60 & 35 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0.5 \end{bmatrix}.$$

Predictions on the training set

Linear prediction

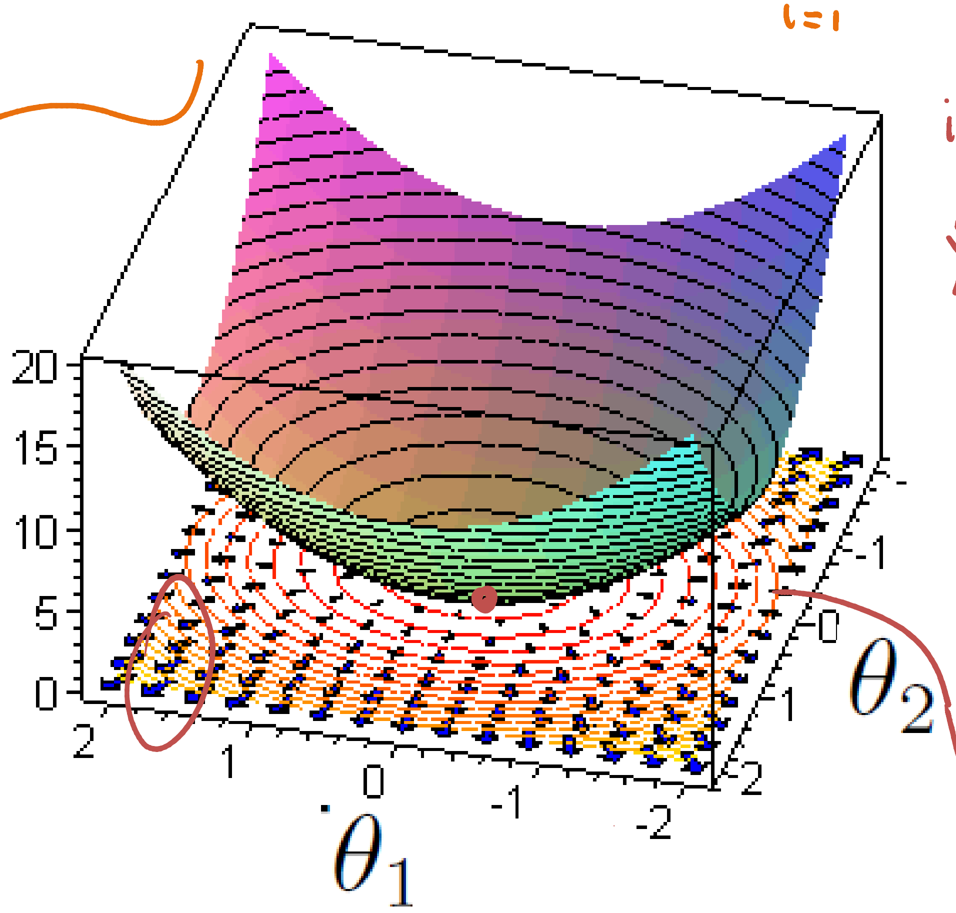
Likewise, for a point that we have never seen before, say $x = \underbrace{[50\ 20]}$, we generate the following prediction:

$$\hat{y}(x) = [1\ \underbrace{50\ 20}] \begin{bmatrix} 1 \\ 0 \\ 0.5 \end{bmatrix} = 1 + 0 + 10 = 11.$$

Optimization approach

Our aim is to mininimise the quadratic cost between the output labels and the model predictions

$$\underbrace{J(\boldsymbol{\theta}) = (\underset{n\times 1}{\mathbf{y}} - \overset{n\times d}{\mathbf{X}}\underset{d\times 1}{\boldsymbol{\theta}})^T}_{1\times 1}(\mathbf{y} - \underbrace{\mathbf{X}\boldsymbol{\theta}}) = \sum_{i=1}^{n}(\underset{1\times 1}{y_i} - \mathbf{x}_i^T \overset{d}{\boldsymbol{\theta}})^2 = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$



in 2D

$\hat{y}_i = 1\theta_1 + x_i\theta_2$

$J(\theta_1, \theta_2)$

contour lines

Optimization approach

$$J(\boldsymbol{\theta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) = \sum_{i=1}^{n}(y_i - \mathbf{x}_i^T\boldsymbol{\theta})^2$$

[Prove]

Optimization: Finding the minimum

$$J(\boldsymbol{\theta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) = \sum_{i=1}^{n}(y_i - \mathbf{x}_i^T\boldsymbol{\theta})^2$$

Suppose $n=3$, $d=2$

$$J(\theta) = (Y_1 - \theta_1 - x_1\theta_2)^2 + (Y_2 - \theta_1 - x_2\theta_2)^2 + (Y_3 - \theta_1 - x_3\theta_2)^2$$

$$= \sum_{i=1}^{3}(Y_i - \theta_1 - x_i\theta_2)^2$$

$$\frac{\partial J(\theta)}{\partial\theta_1} = \sum_{i=1}^{3} 2(Y_i - \theta_1 - x_i\theta_2)(-1) = -2\sum_{i=1}^{3}(Y_i - \theta_1 - x_i\theta_2)$$

Optimization

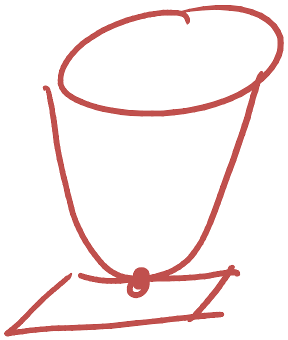
$$J(\boldsymbol{\theta}) = \underbrace{(\overset{n\times 1}{\mathbf{y}} - \overset{n\times d}{\mathbf{X}}\overset{d\times 1}{\boldsymbol{\theta}})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta})}$$

We will need the following results from matrix differentiation:

$\boxed{\frac{\partial \mathbf{A}\theta}{\partial \boldsymbol{\theta}}} = \underline{\mathbf{A}}^T$ and $\frac{\partial \boldsymbol{\theta}^T\mathbf{A}\boldsymbol{\theta}}{\partial \boldsymbol{\theta}} = \underline{2}\mathbf{A}^T\boldsymbol{\theta}$

$$\frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \frac{\partial}{\partial \theta}\left[y^T y + \theta^T \underbrace{X^T X}_{A} \theta - 2\, \overbrace{\underbrace{\overset{1\times n}{y^T} \overset{n\times d}{X}}_{A'} \overset{d\times 1}{\theta}}^{d\times 1} \right]$$

$$= 0 + 2X^TX\theta - 2X^Ty$$



Least squares estimates

$$\cancel{2}X^TX\theta = \cancel{2}X^Ty$$ normal eq.

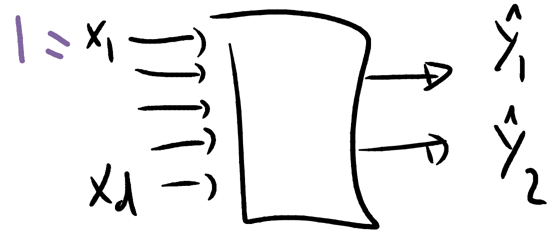
$$\boxed{\hat{\theta} = (X^TX)^{-1}X^Ty}$$ L. S. estimate

$$\hat{y} = X\hat{\theta} = \underbrace{X(X^TX)^{-1}X^T}_{\text{HAT}}y = Hy$$

Multiple outputs

If we have several outputs $\mathbf{y}_i \in \mathbb{R}^c$, our linear regression expression becomes:

eg $c=2$



$$\begin{bmatrix} \hat{y}_{11} & \hat{y}_{12} \\ \vdots & \vdots \\ \hat{y}_{n1} & \hat{y}_{n2} \end{bmatrix} = \begin{bmatrix} 1 & x_{21} & \cdots & x_{1d} \\ 1 & & & \\ 1 & & \ddots & \\ \vdots & & & \\ 1 & & & x_{nd} \end{bmatrix} \begin{bmatrix} \theta_{11} & \theta_{12} \\ \vdots & \vdots \\ \theta_{d1} & \theta_{d2} \end{bmatrix}$$

Next lecture

In the next lecture, we learn to derive the linear regression estimates by maximum likelihood with multivariate Gaussian distributions.

Please go to the Wikipedia page for the multivariate Normal distribution beforehand.