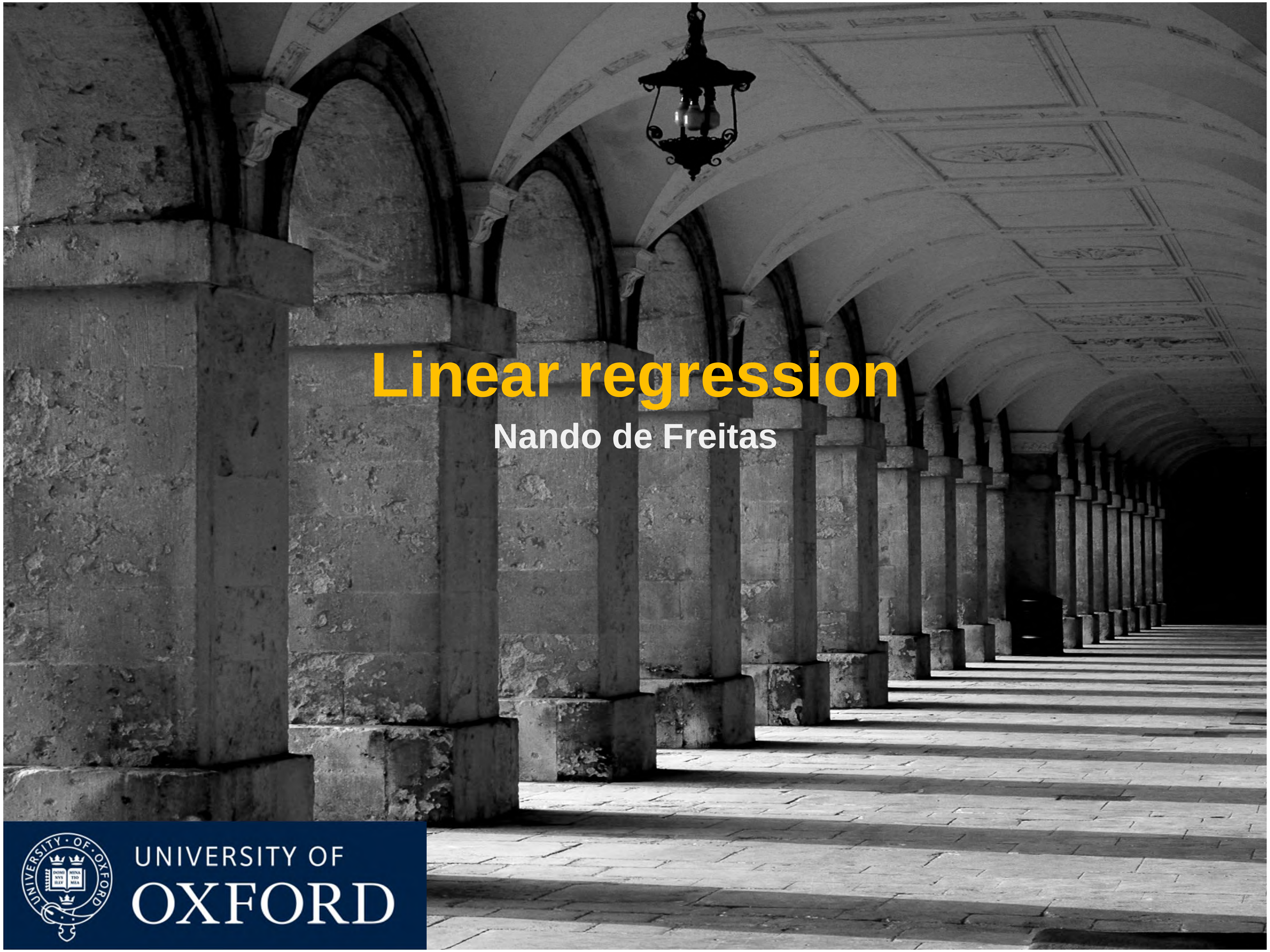

Linear regression

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Outline

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, targets and labels. The goal of the lecture is for you to:

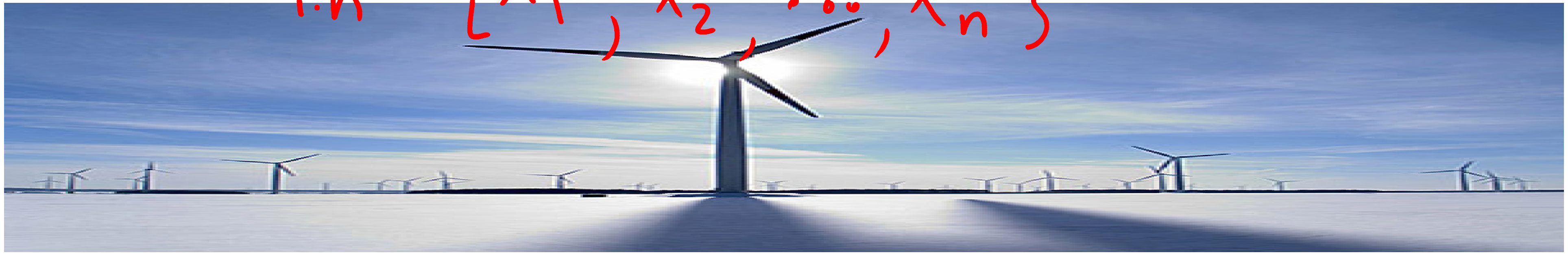
- ❑ Understand the supervised learning setting.
- ❑ Understand linear regression (aka least squares)
- ❑ Understand how to apply linear regression models to make predictions.
- ❑ Learn to derive the least squares estimate.

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, $\underbrace{\mathbf{y}_i \in \mathbb{R}}$, for now.

$X_{1:n} = \{X_1, X_2, \ldots, X_n\}$



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

	Wind speed	People inside building		Energy requirement	
X_1	100	2	Y_1	5	
	50	42		25	
X_3	45	31		22	Y_3
	60	35		18	

$d=2$

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
learning

DATA

$$\begin{tikzcd} \{x_{1:n}, y_{1:n}\} \arrow[r] & \boxed{\text{Learner}} \arrow[r] & \Theta \end{tikzcd}$$

model parameters

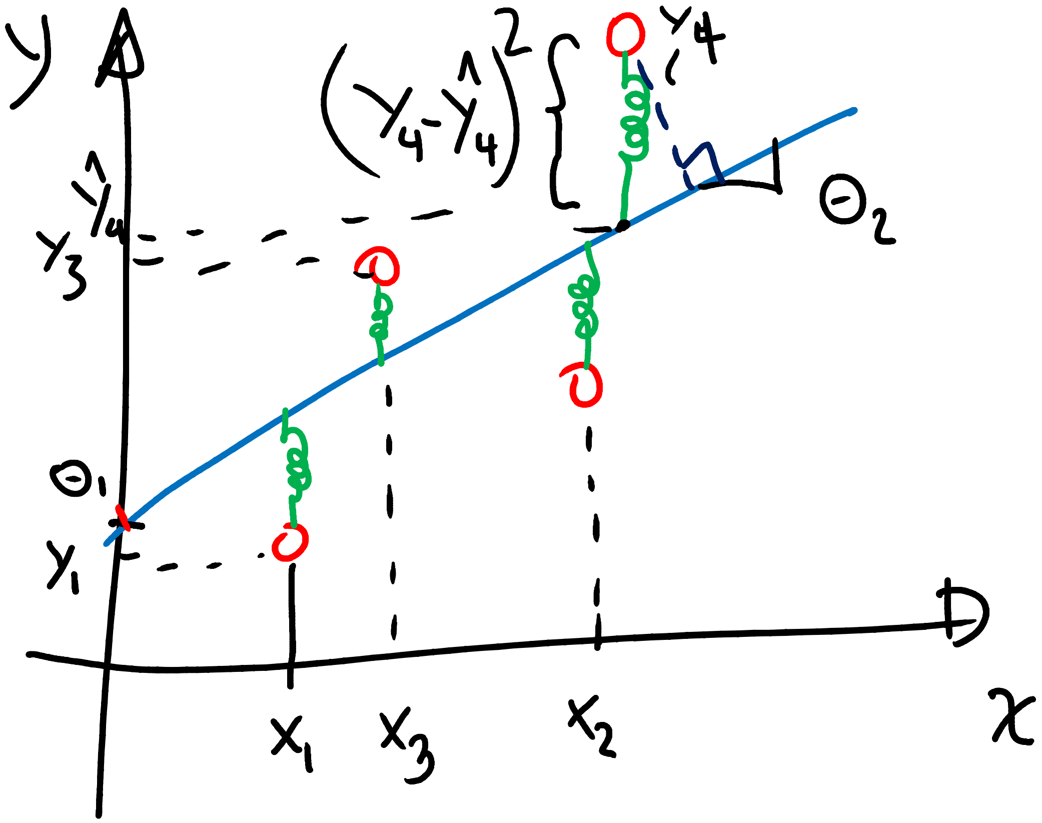
② TESTING
prediction

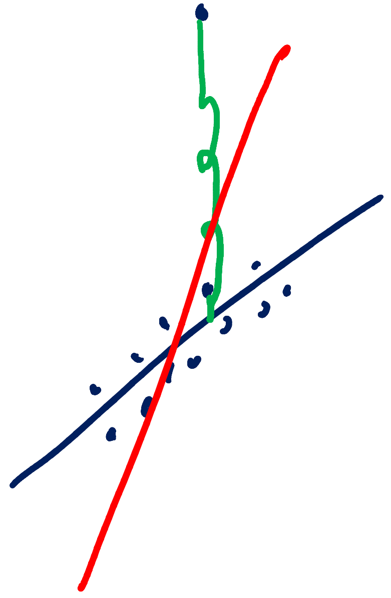
$$\begin{tikzcd} x_{n+1}, \Theta \arrow[r] & \boxed{\text{Predictor}} \arrow[r] & \hat{y}_{n+1} \end{tikzcd}$$

$$\hat{y}(\mathbf{x}_i) = 1\theta_1 + x_i\theta_2$$

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

Objective function
Energy
Loss





Linear prediction

In general, the linear model is expressed as follows:

$$\underline{\widehat{y}_i = \sum_{j=1}^{d} x_{ij}\theta_j}, \quad = \underline{\overset{1}{\cancel{x}}_{i1}\theta_1 + x_{i2}\theta_2 + \cdots + x_{id}\theta_d}$$

where we have assumed that $x_{i1} = 1$ 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:

$$\boxed{\widehat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta},}$$

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

$$i \begin{bmatrix} \widehat{y}_1 \\ \vdots \\ \widehat{y}_n \end{bmatrix} = \begin{bmatrix} x_{11} & \cdots & x_{1d} \\ \vdots & \vdots & \vdots \\ x_{n1} & \cdots & x_{nd} \end{bmatrix} \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}.$$

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

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

Linear prediction on test data

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

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

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

$$\underline{x} = (x_1 \quad x_2)^T \qquad \underline{y} = (y_1 \quad y_2)^T \qquad \underline{x}^T \underline{y} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$= x_1 y_1 + x_2 y_2$$

$$= \sum_i x_i y_i$$

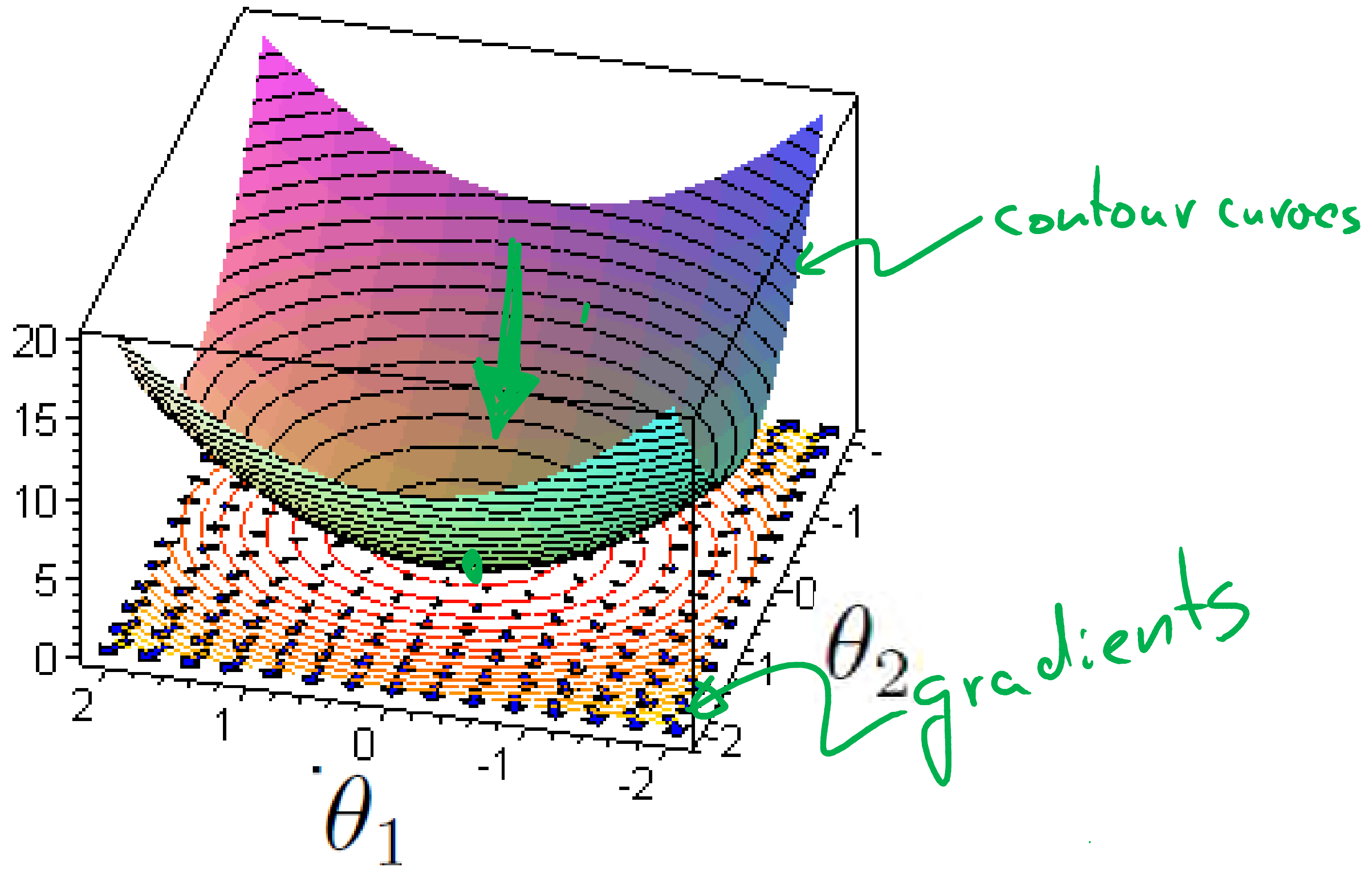
$$\overbrace{\left(\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} - \begin{bmatrix} x_1^T \\ x_2^T \\ x_n^T \end{bmatrix} [\theta] \right)}$$

Optimization approach

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

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

$\underline{\Theta \in \mathbb{R}^2}$



Finding the solution by differentiation

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

$$\left.\begin{array}{l} \dfrac{dJ(\theta)}{d\theta_1} \longrightarrow g(\theta_1, \theta_2) \\[2em] \dfrac{dJ(\theta)}{d\theta_2} \longrightarrow g_2(\theta_1\ \theta_2) \end{array}\right\} \text{Normal Eqns.}$$

Least squares Wiki

Finding the solution by differentiation

$$J(\boldsymbol{\theta}) = (\underbrace{\mathbf{y}}_{}^{n\times 1} - \overset{n\times d \; d\times 1}{\mathbf{X}\boldsymbol{\theta}})^T(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \qquad X = \begin{bmatrix} x_1^T \\ x_2^T \end{bmatrix}$$

We will need the following results from matrix differentiation:

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

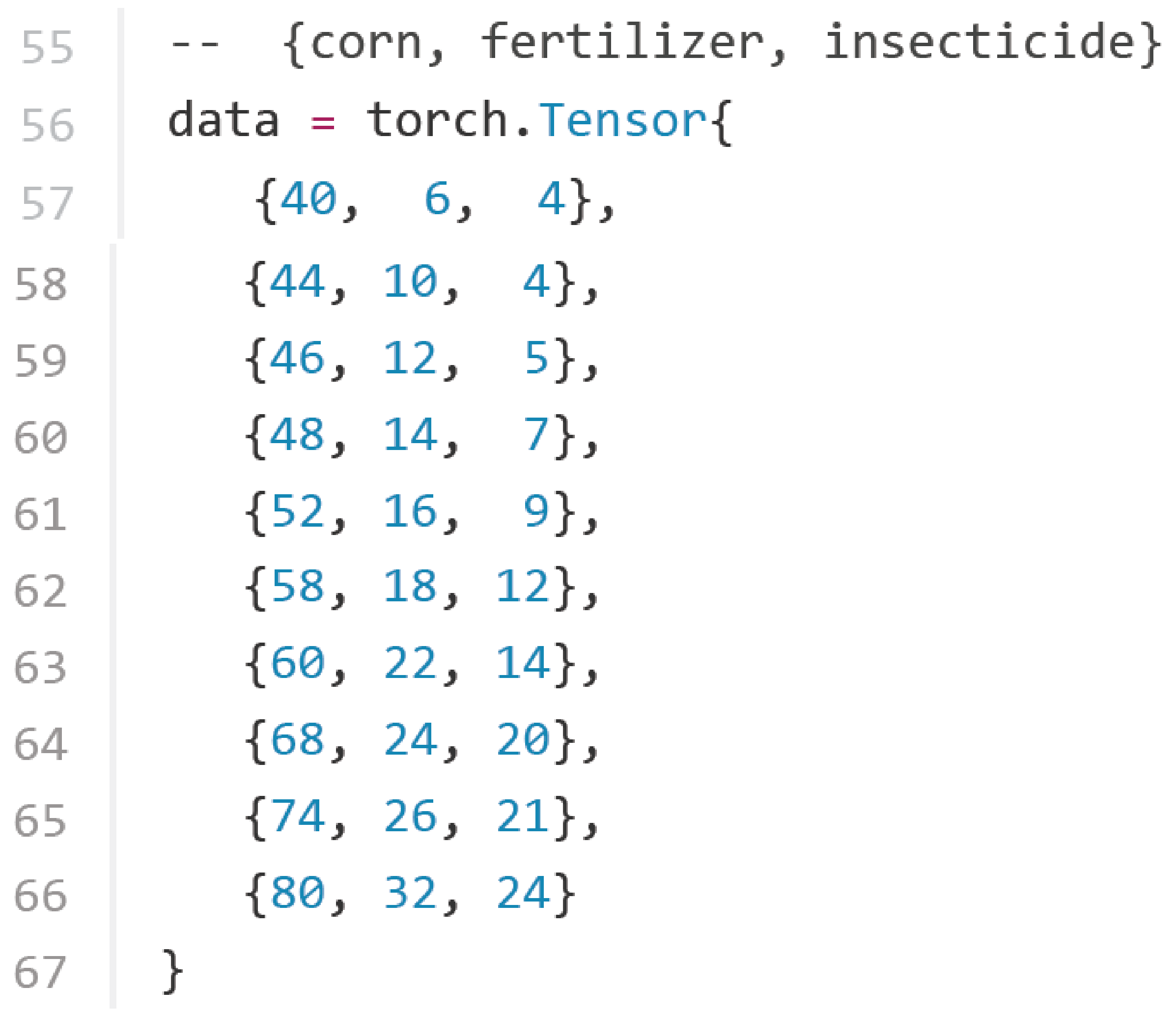
$$\frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \frac{\partial}{\partial \theta}\left(y^T y - \underline{2 y^T X \theta} + \theta^T X^T X \theta \right)$$

$$= 0 - 2X^T y + X^T X \theta \xrightarrow{\text{equals}} 0$$

$$\theta = \underline{(X^T X)^{-1} X^T y}$$

Torch: Data

Torch 7

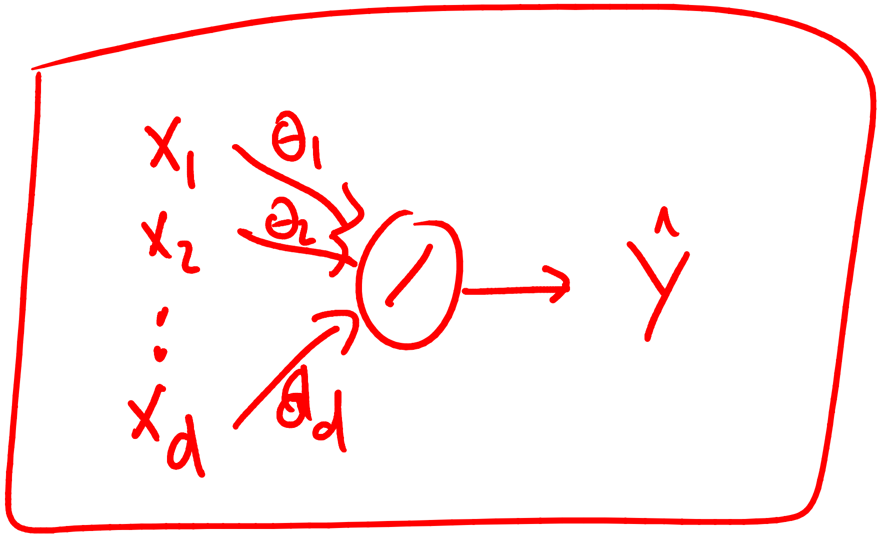


```
--  {corn, fertilizer, insecticide}
data = torch.Tensor{
    {40,  6,  4},
    {44, 10,  4},
    {46, 12,  5},
    {48, 14,  7},
    {52, 16,  9},
    {58, 18, 12},
    {60, 22, 14},
    {68, 24, 20},
    {74, 26, 21},
    {80, 32, 24}
}
```

http://torch.cogbits.com/doc/tutorials_supervised/
https://github.com/torch/demos/blob/master/linear-regression/example-linear-regression.lua

Torch: Model

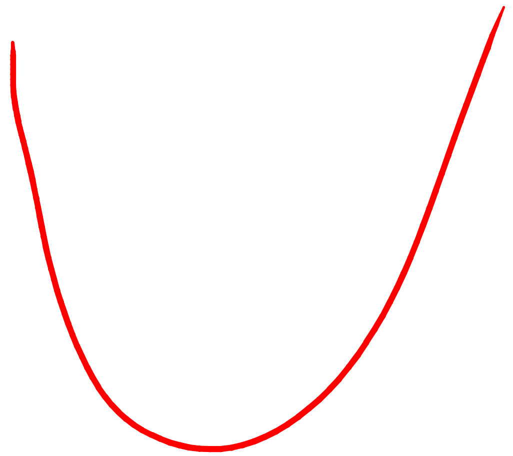
```lua
model = nn.Sequential()
ninputs = 2; noutputs = 1
model:add(nn.Linear(ninputs, noutputs))
```



http://torch.cogbits.com/doc/tutorials_supervised/
https://github.com/torch/demos/blob/master/linear-regression/example-linear-regression.lua

Torch: Loss / objective

```lua
criterion = nn.MSECriterion()
```



http://torch.cogbits.com/doc/tutorials_supervised/
https://github.com/torch/demos/blob/master/linear-regression/example-linear-regression.lua

Torch: Compute parameters

http://torch.cogbits.com/doc/tutorials_supervised/
https://github.com/torch/demos/blob/master/linear-regression/example-linear-regression.lua

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 or, even better, read Chapter 4 of Kevin Murphy’s book and attempt the first three questions of the exercise sheet.