# Lecture 3 Multiple Linear Regression

EE-UY 4563/EL-GY 9123: INTRODUCTION TO MACHINE LEARNING PROF. SUNDEEP RANGAN
(WITH MODIFICATION BY YAO WANG)





# Learning Objectives

- ☐ Formulate a machine learning model as a multiple linear regression model.
  - Identify prediction vector and target for the problem.
- ☐ Write the regression model in matrix form. Write the feature matrix
- □ Compute the least-squares solution for the regression coefficients on training data.
- ☐ Derive the least-squares formula from minimization of the RSS
- ☐ Manipulate 2D arrays in python (indexing, stacking, computing shapes, ...)
- □ Compute the LS solution using python linear algebra and machine learning packages





# Pre-Requisites for this Lecture

#### ☐ Undergraduate students:

- We will cover Lecture 2 (Simple Linear Regression) in class first
- Some of the material in this lecture is a duplicate of Lecture 2
- I will go through this lecture more slowly, esp. for the linear algebra

#### ☐ Graduate students:

- We will can skip Lecture 2 and start this lecture directly after Lecture 1
- But, useful to read Lecture 2 and the corresponding demo on your own time.
- Will not review basic linear algebra in class. You should review this on your own.





### Outline

Motivating Example: Understanding glucose levels in diabetes patients

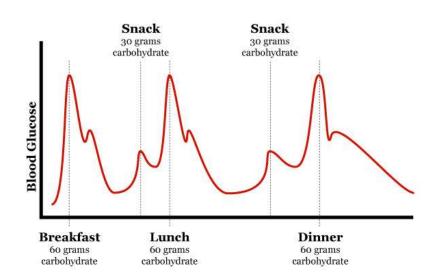
- ☐ Multiple variable linear models
- ☐ Least squares solutions
- ☐ Computing the solutions in python
- ☐ Special case: Simple linear regression
- **□** Extensions





# Example: Blood Glucose Level

- ☐ Diabetes patients must monitor glucose level
- ■What causes blood glucose levels to rise and fall?
- ☐ Many factors
- ☐ We know mechanisms qualitatively
- ☐But, quantitative models are difficult to obtain
  - Hard to derive from first principles
  - Difficult to model physiological process precisely
- □ Can machine learning help?





# Data from AIM 94 Experiment

#### Data Set Information:

Diabetes patient records were obtained from two sources: ar clock to timestamp events, whereas the paper records only p assigned to breakfast (08:00), lunch (12:00), dinner (18:00), records have more realistic time stamps.

Diabetes files consist of four fields per record. Each field is s

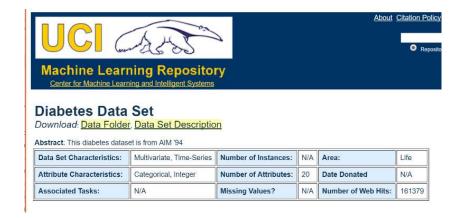
File Names and format:

- (1) Date in MM-DD-YYYY format
- (2) Time in XX:YY format
- (3) Code
- (4) Value

The Code field is deciphered as follows:

- 33 = Regular insulin dose
- 34 = NPH insulin dose
- 35 = UltraLente insulin dose
- 48 = Unspecified blood glucose measurement
- 57 = Unspecified blood glucose measurement
- 58 = Pre-breakfast blood glucose measurement
- 59 = Post-breakfast blood glucose measurement
- 60 = Pre-lunch blood glucose measurement
- 61 = Post-lunch blood glucose measurement
- 62 = Pre-supper blood glucose measurement
- 63 = Post-supper blood glucose measurement

- □ Data collected as series of events
  - Eating
  - Exercise
  - Insulin dosage
- ☐ Target variable glucose level monitored







### Demo on GitHub

#### □All code is available in github:

https://github.com/sdrangan/introml/blob/master/unit03 mult lin reg/demo2 glucose.ipynb

### Demo: Predicting Glucose Levels using Mulitple Linear Regression

In this demo, you will learn how to:

- Fit multiple linear regression models using python's sklearn pachage.
- · Split data into training and test.
- · Manipulating and visualizing multivariable arrays.

We first load the packages as usual.

```
import numpy as np
import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline
```

#### **Diabetes Data Example**

To illustrate the concepts, we load the well-known diabetes data set. This dataset is included in the sklearn.da can be loaded as follows.

```
from sklearn import datasets, linear model, preprocessing
```





# Loading the Data

```
# Load the diabetes dataset
diabetes = datasets.load_diabetes()
X = diabetes.data
y = diabetes.target
```

#### ■Sklearn package:

- Many methods for machine learning
- Datasets
- Will use throughout this class
- ☐ Diabetes dataset is one example

```
nsamp, natt = X.shape
print("num samples={0:d} num attributes={1:d}".format(nsamp,natt))
num samples=442 num attributes=10
```





# Matrix Representation of Data

- ☐ Data is a matrix
- $\square n$  samples:
  - One sample per row
- $\square k$  features / attributes / predictors:
  - One feature per column

$$X = \begin{bmatrix} x_{11} & \cdots & x_{1k} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nk} \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

**Attributes** 

Target vector

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \qquad \text{Samples}$$

- ☐ This example:
  - $y_i$  = blood glucose measurement of i-th sample
  - $\circ x_{i,j}$ : j-th feature of i-th sample
  - $x_i^T = [x_{i,1}, x_{i,2}, ..., x_{i,k}]$ : feature or predictor vector
  - i-th sample contains  $x_i, y_i$

### Outline

- ☐ Motivating Example: Understanding glucose levels in diabetes patients
- Multiple variable linear models
- ☐ Least squares solutions
- ☐ Computing the solutions in python
- ☐ Special case: Simple linear regression
- **□** Extensions





# Multiple Variable Linear Model

- $\square$  Vector of features:  $x = [x_1, ..., x_k]$ 
  - k features (also known as predictors or independent variable attributes)
- $\square$  Single target variable y
- Linear model:

$$y \approx \hat{y} = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k$$

- p = k + 1 terms in the model
- $\hat{y}$  = predicted value
- ☐ Data for training
  - Samples are  $(x_i, y_i)$ , i=1,2,...,n.
  - $\circ$  Each sample has a vector of features:  $\mathbf{x}_i = [x_{i1}, ..., x_{ik}]$  and scalar target  $y_i$
- $\square$  Problem: Learn the best coefficients  $\pmb{\beta} = [\beta_0, \beta_1, ..., \beta_k]$  from the training data





# Why Use a Linear Model?

- ☐ Many natural phenomena have linear relationship
- ☐ Predictor has small variation
  - Suppose y = f(x)
  - If variation of x is small around some value  $x_0$ , then

$$y \approx f(x_0) + f'(x_0)(x - x_0) = \beta_0 + \beta_1 x$$

$$\beta_0 = f(x_0) - f'(x_0)x_0, \qquad \beta_1 = f'(x_0)$$

- ☐ Gaussian random variables:
  - If two variables are jointly Gaussian, the optimal predictor of one from the other is linear predictor
- ☐ Simple to compute
- ☐ Easy to interpret relation
  - $\circ$  Coefficient  $\beta_j$  indicates the importance of feature j for the target.





### **Matrix Review**

#### **□**Consider

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}, \qquad B = \begin{bmatrix} 2 & 0 \\ 3 & 2 \end{bmatrix}, \qquad x = \begin{bmatrix} 2 \\ 3 \end{bmatrix},$$

- □Compute (computations on the board):
  - $\circ$  Matrix vector multiply: Ax
  - $\circ$  Transpose:  $A^T$
  - Matrix multiply: *AB*
  - Solution to linear equations: Solve for u: x = Bu
  - $\circ$  Matrix inverse:  $B^{-1}$





# Matrix Form of Linear Regression

 $\square$  Predicted value for *i*-th sample:

$$\hat{y}_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_k x_{ik}$$

☐ Define feature matrix and regression vector:

$$A = \begin{bmatrix} 1 & \chi_{11} & \cdots & \chi_{1k} \\ \vdots & \vdots & \cdots & \vdots \\ 1 & \chi_{n1} & \cdots & \chi_{nk} \end{bmatrix}, \qquad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} \qquad p = k+1 \text{ linear features}$$

- Feature matrix is data matrix + column of 1's
- $\Box$ Then, predicted vector for all training samples is:  $\hat{y} = A \beta$
- $\Box$  Given a new sample with feature vector x, the predicted value is  $\hat{y}(x) = [1, x^T] \beta$



# Slopes and Intercept

- □ Sometimes use notation:  $\hat{y} = b + w_1 x_1 + \cdots + w_k x_k$
- □Components have two components:
  - $b = \beta_0$ : Bias or intercept
  - $\mathbf{w} = \boldsymbol{\beta}_{1:k} = [\beta_1, ..., \beta_k]$ : Weights or slope vector
- $oxed{\Box}$  Can write with inner product:  $\hat{y}(x) = \beta_0 + oldsymbol{\beta}_{1:k} \cdot x = b + w \cdot x$
- □Inner product:
  - $\circ \mathbf{w} \cdot \mathbf{x} = \sum_{j=1}^k w_j x_j$
  - Will use alternate notation:  $\mathbf{w}^T \mathbf{x} = \langle \mathbf{w}, \mathbf{x} \rangle$



### Arrays and Vector in Python and MATLAB

☐ There are some key differences between MATLAB and Python that you need to get used to

#### **□**MATLAB

- All arrays are at least 2 dimensions
- Vectors are  $1 \times N$  (row vectors) or  $N \times 1$  (column) vectors
- Matrix vector multiplication syntax depends if vector is on left or right: x'\*A or A\*x

#### ■Python:

- Arrays can have 1, 2, 3, ... dimension
- Vectors can be 1D arrays; matrices are generally 2D arrays
- Vectors that are 1D arrays are neither row not column vectors
- If x is 1D and A is 2D, then left and right multiplication are the same: x.dot(A) and A.dot(x)
- $\Box$  Lecture notes: We will generally treat x and  $x^T$  the same.
  - Can write  $x = (x_1, ..., x_N)$  and still multiply by a matrix on left or right





### Outline

- ☐ Motivating Example: Understanding glucose levels in diabetes patients
- ☐ Multiple variable linear models
- Least squares solutions
  - ☐ Computing the solutions in python
  - ☐ Special case: Simple linear regression
  - **□** Extensions



# Least Squares Model Fitting

- □ How do we select parameters  $\beta = (\beta_0, ..., \beta_k)$ ?
- $\Box \text{ Define } \hat{y}_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_k x_{ik}$ 
  - Predicted value on sample i for parameters  $\boldsymbol{\beta} = (\beta_0, ..., \beta_k)$
- □ Define average residual sum of squares:

RSS(
$$\beta$$
): =  $\sum_{i=1}^{n} (y_i - \hat{y}_i)^2$ 

- $\circ$  Note that  $\hat{y}_i$  is implicitly a function of  $\boldsymbol{\beta} = (\beta_0, ..., \beta_k)$
- Also called the sum of squared residuals (SSR) and sum of squared errors (SSE)
- $\square$  Least squares solution: Find  $\beta$  to minimize RSS.
  - Geometrically, minimizes squared distances of samples to regression line

# Finding Parameters via Optimization A general ML recipe

#### General ML problem

☐ Pick a model with parameters

☐Get data

☐ Pick a loss function

- Measures goodness of fit model to data
- Function of the parameters

#### Multiple linear regression

Linear model:  $\hat{y} = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k$ 

Data:  $(x_i, y_i), i = 1, 2, ..., n$ 

Loss function:

$$RSS(\beta_0, ..., \beta_k) \coloneqq \sum (y_i - \hat{y}_i)^2$$

 $\square$  Find parameters that minimizes loss  $\longrightarrow$  Select  $\beta = (\beta_0, ..., \beta_k)$  to minimize  $RSS(\beta)$ 



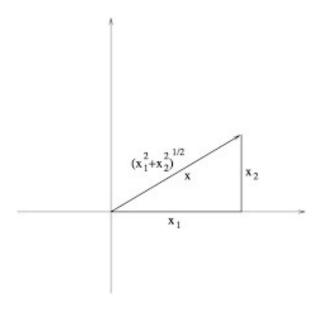
### RSS as a Vector Norm

☐RSS is given by sum:

$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

- □ Define norm of a vector:
  - $||x|| = (x_1^2 + \dots + x_r^2)^{1/2}$
  - Standard Euclidean norm.
  - $^{\circ}$  Sometimes called  $\ell$ -2 norm.  $\ell$  is for Lebesque
- ■Write RSS in vector form:

$$RSS = \|\boldsymbol{y} - \widehat{\boldsymbol{y}}\|^2$$

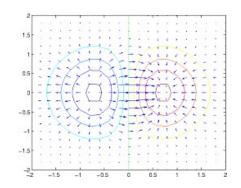


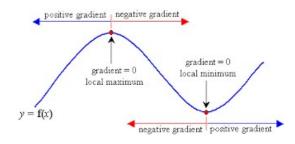
### Gradients and Multi-Variable Functions

- $\square$  Consider scalar valued function of a vector:  $f(x) = f(x_1, ..., x_n)$
- ☐ Gradient is the column vector:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \partial f(\mathbf{x}) / \partial x_1 \\ \vdots \\ \partial f(\mathbf{x}) / \partial x_n \end{bmatrix}$$

- $\Box \text{Ex: } f(x_1, x_2) = x_1 \sin x_2 + x_1^2 x_2.$ 
  - Compute  $\nabla f(x)$ . Solution on board
- ☐ Represents direction of maximum increase
- $\square$  At a local minima or maxima:  $\nabla f(x) = 0$ 
  - $\circ$  Solve n equations and n unknowns





# Least Squares Solution

□ Consider cost function of the RSS:

RSS = 
$$\sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$
,  $\hat{y}_i = \sum_{j=0}^{p} A_{ij} \beta_j$ 

- $\circ$  Vector  $\boldsymbol{\beta}$  that minimizes RSS called the least-squares solution
- Compute partial derivatives via chain rule:  $\frac{\partial RSS}{\partial \beta_j} = 2\sum_{i=1}^n (y_i \hat{y}_i) A_{ij}, j = 1, 2, ..., k$
- $\square$  Matrix form: RSS =  $||A\boldsymbol{\beta} \boldsymbol{y}||^2$ ,  $\nabla RSS = 2A^T(\boldsymbol{y} A\boldsymbol{\beta})$
- □ Solution:  $A^T(y A\beta) = 0 \rightarrow \beta = (A^TA)^{-1}A^Ty$  (least squares solution of equation  $A\beta = y$ )
- $\square \text{Minimum RSS: } RSS = \mathbf{y}^T [I A(A^T A)^{-1} A^T] \mathbf{y}$ 
  - Proof on the board





### LS Solution via Auto-Correlation Functions

☐ Each data sample has a linear feature vector:

$$A_i = (A_{i0}, \dots, A_{ik}) = (1, x_{i1}, \dots, x_{ik})$$

☐ Define sample auto-correlation matrix and cross-correlation vector:

- $R_{AA} = \frac{1}{n}A^TA$ ,  $R_{AA}(\ell,m) = \frac{1}{n}\sum_{i=1}^n A_{i\ell}A_{im}$  (correlation of feature  $\ell$  and feature m)
- $R_{Ay} = \frac{1}{n}A^Ty$ ,  $R_{yA}(\ell) = \frac{1}{n}\sum_{i=1}^n A_{i\ell}y_i$  (correlation of feature  $\ell$  and target)

 $\Box$  Least squares solution is:  $\beta = R_{AA}^{-1}R_{Ay}$ 





### R^2: Goodness of Fit

Define target sample mean and variance: 
$$\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i, \qquad s_y^2 = \frac{1}{n} \sum_{i=1}^{n} (y_i - \bar{y})^2$$

□ Consider minimum prediction error per sample

$$\frac{RSS}{n} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

■ Multiple variable coefficient of determination:

$$R^2 = 1 - \frac{RSS/n}{s_v^2} = 1 - \frac{\text{avg error with linear model}}{\text{avg error with } prediction by mean}$$

- $R^2 \in [0,1]$  always
- $\circ R^2 \approx 1 \Rightarrow$  linear model provides a good fit
- $R^2 \approx 0 \Rightarrow$  linear model provides a poor fit



### **Notation**

- ☐Often, RSS is quoted in some relative form
- ☐ We will use the following terminology
  - Note: these are not standard
- $\square$  Residual sum of squares: RSS =  $\sum_{i=1}^{n} (y_i \hat{y}_i)^2$
- $\square$ RSS per sample:  $\frac{RSS}{n}$
- ■Normalized RSS:

$$\frac{RSS/n}{s_y^2} = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$



### Mean Removed Form of the LS Solution

- □Often useful to remove mean from data before fitting
- Sample mean:  $\bar{y} = \frac{1}{N} \sum_{i=1}^{N} y_i$ ,  $\bar{x}_i = \frac{1}{N} \sum_{i=1}^{N} x_{ij}$ ,  $\bar{x} = [\bar{x}_1, \dots, \bar{x}_k]$
- $\square$  Defined mean removed data:  $\tilde{X}_{ij} = x_{ij} \bar{x}_i$ ,  $\tilde{y}_i = y_i \bar{y}$
- □ Sample covariance matrix and cross-covariance vector:

$$S_{xx}(\ell,m) = \frac{1}{N} \sum_{i=1}^{N} (x_{i\ell} - \bar{x}_{\ell})(x_{im} - \bar{x}_{m}), \quad S_{xx} = \frac{1}{N} \widetilde{X}^{T} \widetilde{X}$$

$$S_{xy}(\ell) = \frac{1}{N} \sum_{i=1}^{N} (x_{i\ell} - \bar{x}_{\ell}) (y_i - \bar{y}), \quad S_{xy} = \frac{1}{N} \widetilde{X}^T \widetilde{y}$$

☐ Mean-Removed form of the least squares solution:

$$\hat{y} = \boldsymbol{\beta}_{1:k} \cdot \boldsymbol{x} + \beta_0, \qquad \boldsymbol{\beta}_{1:k} = S_{xx}^{-1} S_{xy}, \qquad \beta_0 = \bar{y} - \boldsymbol{\beta}_{1:k} \cdot \bar{\boldsymbol{x}}$$

$$\boldsymbol{\beta}_{1:k} = S_{xx}^{-1} S_{xy},$$

$$\beta_0 = \bar{y} - \boldsymbol{\beta}_{1:k} \cdot \overline{\boldsymbol{x}}$$

Proof: On board





# Outline

- ☐ Motivating Example: Understanding glucose levels in diabetes patients
- ☐ Multiple variable linear models
- ☐ Least squares solutions
- Computing the solutions in python
- ☐ Special case: Simple linear regression
- **□** Extensions



# Fitting Using sklearn

```
ns_train = 300
ns_test = nsamp - ns_train
X_tr = X[:ns_train,:]
y_tr = y[:ns_train]
```

- ☐ Return to diabetes data example
- □ All code in demo
- ☐ Divide data into two portions:
  - Training data: First 300 samples
  - Test data: Remaining 142 samples
- ☐ Train model on training data.
- ☐ Test model (i.e. measure RSS) on test data
- ☐ Reason for splitting data discussed next lecture.





# Manually Computing the Solution

- Use numpy linear algebra routine to solve  $\beta = (A^T A)^{-1} A^T y$
- **□**Common mistake:
  - Compute matrix inverse  $P = (A^T A)^{-1}$ ,
  - Then compute  $\beta = PA^Ty$
  - Full matrix inverse is VERY slow. Not needed.
  - Can directly solve linear system:  $A \beta = y$
  - Numpy has routines to solve this directly



# Calling the sklearn Linear Regression method

```
regr = linear_model.LinearRegression()
regr.fit(X_tr,y_tr)
```

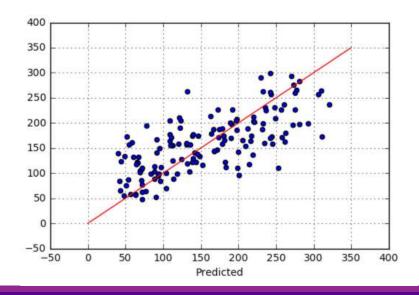
```
X_test = X[ns_train:,:]
y_test = y[ns_train:]
y_test_pred = regr.predict(X_test)
RSS_test = np.mean((y_test_pred-y_test)**2)/(np.std(y_test)**2)
Rsq_test = 1-RSS_test
print("RSS per sample = {0:f}".format(RSS_test))
print("R^2 = {0:f}".format(Rsq_test))
```

RSS per sample = 0.492801 R^2 = 0.507199

We see that the model predicts new samples almost as well as it did the training  $\boldsymbol{\epsilon}$ 

```
plt.scatter(y_test,y_test_pred)
plt.plot([0,350],[0,350],'r')
plt.xlabel('Actual')
plt.xlabel('Predicted')
plt.grid()
```

- ☐ Construct a linear regression object
- ☐Run it on the training data
- ☐ Predict values on the test data







# Outline

- ☐ Motivating Example: Understanding glucose levels in diabetes patients
- ☐ Multiple variable linear models
- ☐ Least squares solutions
- ☐ Computing the solutions in python
- Special case: Simple linear regression
  - **□** Extensions





# Simple vs. Multiple Regression

- ☐ Simple linear regression: One predictor (feature)
  - $\circ$  Scalar predictor x
  - Linear model:  $\hat{y} = \beta_0 + \beta_1 x$
  - Can only account for one variable
- ☐ Multiple linear regression: Multiple predictors (features)
  - $\circ$  Vector predictor  $\mathbf{x} = (x_1, \dots, x_k)$
  - Linear model:  $\hat{y} = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k$
  - Can account for multiple predictors
  - $\circ\,$  Turns into simple linear regression when k=1



# Comparison to Single Variable Models

■We could compute models for each variable separately:

$$y = a_1 + b_1 x_1$$
  
 $y = a_2 + b_2 x_2$   
:

- ☐ But, doesn't provide a way to account for joint effects
- □ Example: Consider three linear models to predicting longevity:
  - A: Longevity vs. some factor in diet (e.g. amount of fiber consumed)
  - B: Longevity vs. exercise
  - C: Longevity vs. diet AND exercise
  - $\,^\circ\,$  What does C tell you that A and B do not?



# Special Case: Single Variable

- $\square$ Suppose k=1 predictor.
- ☐ Feature matrix and coefficient vector:

$$A = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}, \qquad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

LS soln: 
$$\beta = \left(\frac{1}{N}A^{T}A\right)^{-1}\left(\frac{1}{N}A^{T}y\right) = P^{-1}r$$

$$P = \begin{bmatrix} 1 & \bar{x} \\ \bar{x} & \bar{x}^{2} \end{bmatrix}, \qquad r = \begin{bmatrix} \bar{y} \\ \bar{x}y \end{bmatrix}$$



### Simple Linear Regression for Diabetes Data

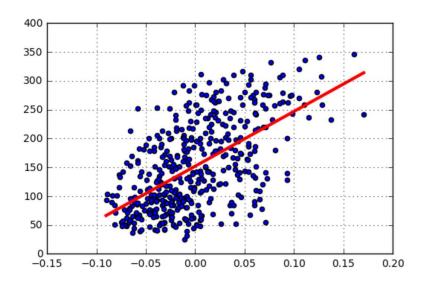
```
☐ Try a fit of each variable individually
ym = np.mean(y)
syy = np.mean((y-ym)**2)
Rsq = np.zeros(natt)
                                                    \square Compute R_k^2 coefficient for each variable
for k in range(natt):
   xm = np.mean(X[:,k])
   sxy = np.mean((X[:,k]-xm)*(y-ym))
                                                    ☐ Use formula on previous slide
   sxx = np.mean((X[:,k]-xm)**2)
   Rsq[k] = (sxy)**2/sxx/syy
                                                    "Best" individual variable is a poor fit
   print("{0:2d} Rsq={1:f}".format(k,Rsq[k]))
                                                      R_k^2 \approx 0.34
0 Rsq=0.035302
1 Rsq=0.001854
                                    Best individual variable
 2 Rsq=0.343924 <
 3 Rsq=0.194908
4 Rsq=0.044954
 5 Rsq=0.030295
 6 Rsq=0.155859
7 Rsq=0.185290
8 Rsq=0.320224
```

9 Rsq=0.146294



### Scatter Plot

- ☐ No one variable explains glucose well
- ☐ Multiple linear regression is much better



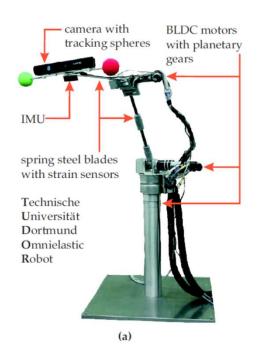
```
# Find the index of the single variable with the best R^2
imax = np.argmax(Rsq)

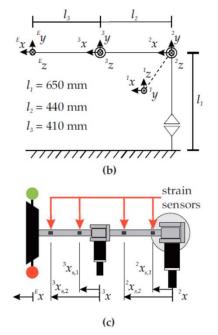
# Regression line over the range of x values
xmin = np.min(X[:,imax])
xmax = np.max(X[:,imax])
ymin = beta0[imax] + beta1[imax]*xmin
ymax = beta0[imax] + beta1[imax]*xmax
plt.plot([xmin,xmax], [ymin,ymax], 'r-', linewidth=3)

# Scatter plot of points
plt.scatter(X[:,imax],y)
plt.grid()
```



### Lab: Robot Calibration





- ☐ Predict the current draw
  - Needed to predict power consumption
- ☐ Predictors:
  - Joint angles, velocity and acceleration
  - Strain gauge readings (measure of load)
- ☐ Full website at TU Dortmund, Germany
  - http://www.rst.e-technik.tudortmund.de/cms/en/research/robotics/T UDOR\_engl/index.html

### Outline

- ☐ Motivating Example: Understanding glucose levels in diabetes patients
- ☐ Multiple variable linear models
- ☐ Least squares solutions
- □Computing in python

Extensions



# Polynomial Fitting

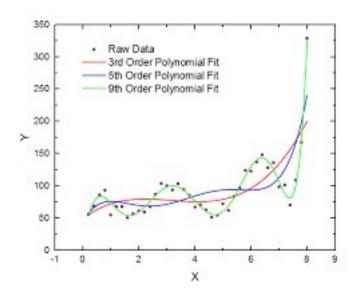
□Suppose y only depends on a single variable x, and we want to model y as a polynomial function of x

• 
$$y \approx \beta_0 + \beta_1 x + \cdots + \beta_d x^d$$

- □Given data  $(x_i, y_i)$ , i = 1, ..., n
- Using only  $x_i$ , we can only fit a linear model  $y \approx \beta_0 + \beta_1 x$
- ☐ How do we fit a model with degree d>1?
- □Generate multiple transformed features from  $x: x, x^2,..., x^d$
- ☐ Form feature matrix and coefficient vector

$$\mathbf{A} = \begin{bmatrix} 1 & x_1 & \cdots & x_1^d \\ \vdots & \vdots & \cdots & \vdots \\ 1 & x_n & \cdots & x_n^d \end{bmatrix}, \qquad \beta = \begin{bmatrix} \beta_0 \\ \vdots \\ \beta_d \end{bmatrix}$$

- p = d + 1 transformed features from 1 original feature
- □Will discuss model order selection in next year
- □Extensions to other nonlinear transforms

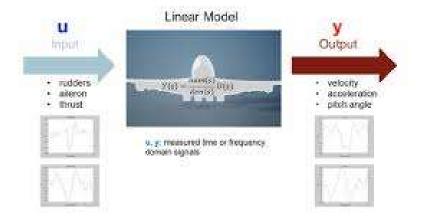


# Learning Linear Systems

- $\Box \text{Linear system: } y_k = a_1 y_{k-1} + \dots + a_m y_{k-m} + b_0 x_k + \dots + b_n x_{k-n} + w_k$
- $\Box \text{Transfer function: } H(z) = \frac{b_0 + \dots + b_n z^{-n}}{1 a_1 z^{-1} \dots a_m z^{-m}}$
- ☐Given input sequence and output sequence for T samples,

How do we determine  $\beta = (a_1, \dots, a_m, b_0, \dots, b_n)^T$ 

- □Can be solved using linear regression!
- $\square$ Write  $y = A\beta + w$  and define A, y
  - See homework problem
- Many applications
  - Learning dynamics in robots / mechanical systems
  - Modeling responses in neural systems
  - Stock market time series
  - Speech modeling. Fit a model each 25 ms.



# One Hot Coding

- $\square$  Suppose that one feature  $x_i$  is a categorical variable
- $\square$ Ex: Predict the price of a car, y, given model  $x_1$  and interior space  $x_2$ 
  - Suppose there are 3 different models of a car (Ford, BMW, GM)
  - Bad idea: Arbitrarily assign an index to each possible car model
  - Can give unreasonable relations

#### □One-hot coding example:

- With 3 possible categories, represent  $x_1$  using 2 binary features  $(u_1, u_2)$
- Model:  $y = \beta_0 + \beta_1 u_1 + \beta_2 u_2 + \beta_4 x_2$
- Essentially obtain 3 different models:
  - Ford:  $y = \beta_0 + \beta_1 + \beta_4 x_2$
  - BMW:  $y = \beta_0 + \beta_2 + \beta_4 x_2$
  - GM:  $y = \beta_0 + \beta_4 x_2$
- Allows different intercepts (or mean values) for different categories!
- $\circ$  In general, if there are K categories, we need K-1 variables
- Constant offset term  $\beta_0$  term used for all models

Model	$u_1$	$u_2$
Ford	1	0
BMW	0	1
GM	0	0