Lecture 3
Multiple Linear Regression

EE-UY 4563/EL-GY 9123: INTRODUCTION TO MACHINE LEARNING

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(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:
  - Go through Lecture 2 (Simple Linear Regression) 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

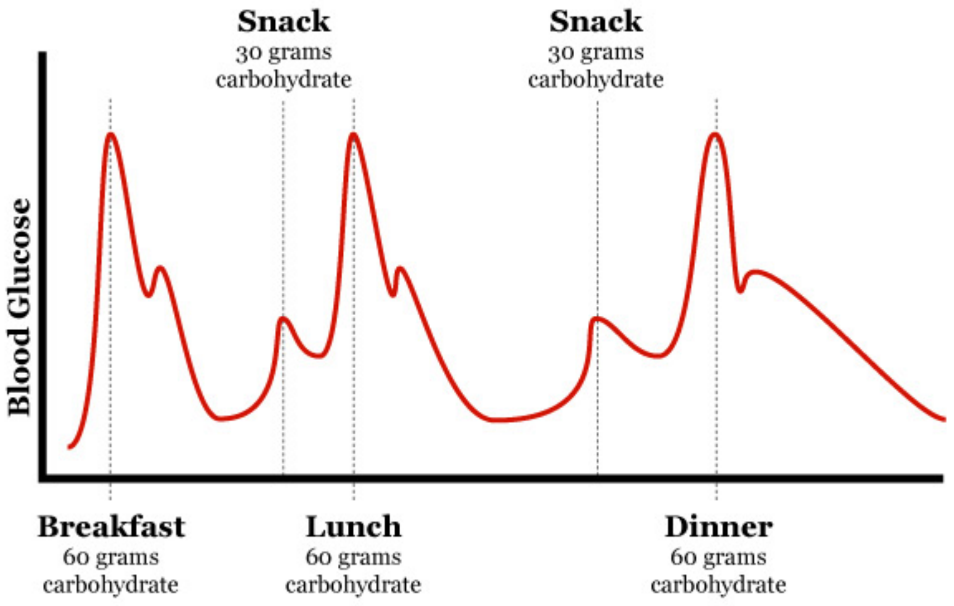
- Graduate students:
  - You can skip Lecture 2 and start this after Lecture 1
  - But, useful to read Lecture 2 and the corresponding demo on your own time.
  - Will not review basic linear algebra in class. You should review this on your own.

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), a
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

About Citation Policy

UCI

Machine Learning Repository

Center for Machine Learning and Intelligent Systems

Diabetes Data Set

Download: Data Folder, Data Set Description

Abstract: This diabetes dataset is from AIM '94

Data Set Characteristics:	Multivariate, Time-Series	**Number of Instances:**	N/A	**Area:**	Life
Attribute Characteristics:	Categorical, Integer	**Number of Attributes:**	20	**Date Donated**	N/A
Associated Tasks:	N/A	**Missing Values?**	N/A	**Number of Web Hits:**	161379

Demo on GitHub

- All code is available in github:
  https://github.com/sdrangan/introml/blob/master/unit02_mult_lin_reg/demo02_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

```
from sklearn import datasets, linear_model, preprocessing

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

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

```
num samples=442  num attributes=10
```

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

Matrix Representation of Data

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

$$X = \overbrace{\begin{bmatrix} x_{11} & \cdots & x_{1k} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nk} \end{bmatrix}}^{\text{Attributes}}$$

Target vector

$$y = \left.\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}\right\} \text{Samples}$$

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

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Multiple Variable Linear Model

- Vector of features: $\boldsymbol{x}^{\boldsymbol{T}} = [x_1, \dots, x_k]$
  - k features (also known as predictors or independent variable attributes)
- Single target variable y
- Linear model:

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

  - $p = k + 1$ terms in the model
  - $\hat{y}$ = predicted value
- Data for training
  - Samples are $(\boldsymbol{x}_i, y_i)$, i=1,2,…,n.
  - Each sample has a vector of features: $\boldsymbol{x}_i{}^{\boldsymbol{T}} = [x_{i1}, \dots, x_{ik}]$ and scalar target y_i
  - How to learn the best coefficients $\boldsymbol{\beta}^{T} = [\beta_0, \beta_1, \dots, \beta_k]$ 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
  - Coefficient β_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):
  - Matrix vector multiply: Ax
  - Transpose: A^T
  - Matrix multiply: AB
  - Solution to linear equations: Solve for u: $x = Bu$
  - Matrix inverse: B^{-1}

Matrix Form of Linear Regression

- Predicted value for i-th sample:

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

- Define feature matrix and regression vector:

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

  - Feature matrix is data matrix + column of 1's

- Then, predicted vector for all training samples is: $\hat{\boldsymbol{y}} = A\,\boldsymbol{\beta}$
- Given a new sample with feature vector $\boldsymbol{x}$, the predicted value is $\hat{y}(\boldsymbol{x}) = [1\ \ \boldsymbol{x}^T]\,\boldsymbol{\beta}$

Slopes and Intercept

- Model $\hat{y} = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k$

- Divide coefficients into two parts: $\boldsymbol{\beta}^{\boldsymbol{T}} = [\beta_0, \boldsymbol{\beta}_{1:k}{}^T]$
  - β_0 : Intercept
  - $\boldsymbol{\beta}_{1:k}{}^T = [\beta_1, \dots, \beta_k]$: Slope coefficients

- Then, can rewrite model as: $\hat{y}(\boldsymbol{x}) = \beta_0 + \boldsymbol{\beta}_{1:k}^T \boldsymbol{x}$

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Least Squares Model Fitting

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

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

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

Finding Parameters via Optimization
A general ML recipe

General ML problem | **Multiple linear regression**

- Pick a model with parameters → Linear model: $\hat{y} = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k$
- Get data → Data: $(\boldsymbol{x}_i, y_i), i = 1,2, \ldots, n$
- Pick a loss function → Loss function:
  - Measures goodness of fit model to data
  - Function of the parameters

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

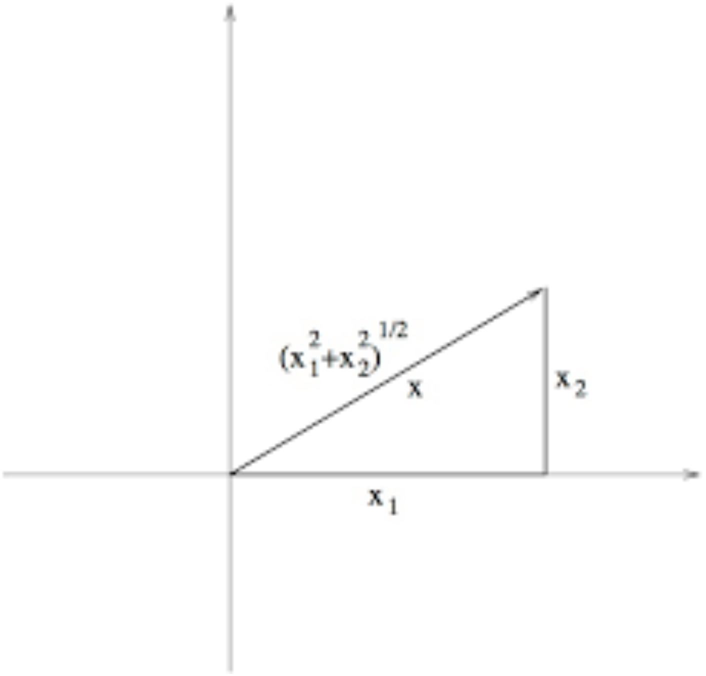
- Find parameters that minimizes loss → Select $\boldsymbol{\beta} = (\beta_0, \ldots, \beta_k)$ to minimize $RSS(\boldsymbol{\beta})$

RSS as a Vector Norm

- RSS is given by sum:

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

- Define norm of a vector:
  - $\|\boldsymbol{x}\| = (x_1^2 + \cdots + x_r^2)^{1/2}$
  - Standard Euclidean norm.
  - Sometimes called ℓ-2 norm. ℓ is for Lebesque



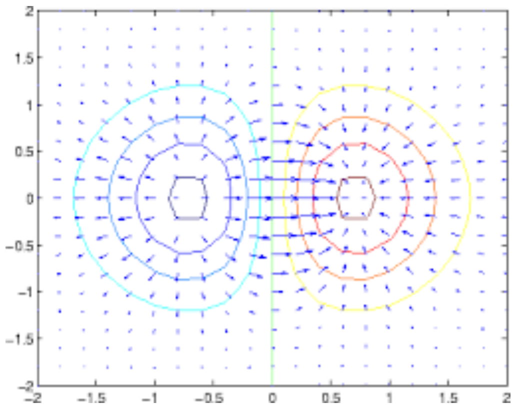
- Write RSS in vector form:

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

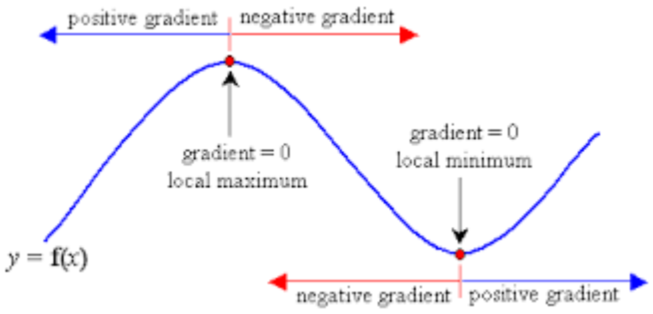
Gradients and Multi-Variable Functions

- Consider scalar valued function of a vector: $f(\boldsymbol{x}) = f(x_1, \dots, x_n)$
- Gradient is the column vector:

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



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



Least Squares Solution

- Consider cost function of the RSS:

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

  - Vector $\boldsymbol{\beta}$ that minimizes RSS called the least-squares solution

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

LS Solution via Auto-Correlation Functions

- Each data sample has a linear feature vector:

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

- Define sample auto-correlation matrix and cross-correlation vector:
  - $R_{AA} = \frac{1}{n} A^T A,\ R_{AA}(\ell, m) = \frac{1}{n} \sum_{i=1}^{n} A_{i\ell} A_{im}$ (correlation of feature ℓ and feature m)
  - $R_{Ay} = \frac{1}{n} A^T y,\ R_{yA}(\ell) = \frac{1}{n} \sum_{i=1}^{n} A_{i\ell} y_i$ (correlation of feature ℓ and target)

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

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:

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

  - $R^2 \in [0,1]$ always
  - $R^2 \approx 1 \Rightarrow$ 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
- Residual sum of squares: $\mathrm{RSS} = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$
- RSS per sample: $\mathrm{RSS}/_{n}$
- Normalized RSS:

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

Applying Linear Regression on Mean Removed Data

- Why do we need the intercept term?
  - To compensate the mean difference between x_j and y
  - Can show that mean of predicted y = mean of y
- Alternative approach: predict mean-removed y from mean-removed **x**
  - First compute mean from data: $\bar{y}\,, \bar{\boldsymbol{x}}^{\boldsymbol{T}} = [\bar{x}_1, \cdots, \bar{x}_k]$
  - Mean-removed data: $\tilde{\boldsymbol{y}} = \boldsymbol{y} - \mathbf{1}\,\bar{y}, \tilde{X} = X - \mathbf{1}\,\bar{\boldsymbol{x}}^{T}$, **1**: a nx1 vector consisting of n ones
  - Predict $\tilde{\boldsymbol{y}}$ from $\tilde{X}$ using linear regression, without the intercept term
    - $\breve{\boldsymbol{y}} = \tilde{\boldsymbol{X}}\tilde{\boldsymbol{\beta}}$
  - Least squares solution for $\tilde{\boldsymbol{y}} = \tilde{\boldsymbol{X}}\tilde{\boldsymbol{\beta}}$ is $\tilde{\boldsymbol{\beta}}= \left(\tilde{X}^T\tilde{X}\right)^{-1}\tilde{X}^T\,\tilde{\boldsymbol{y}}$
  - To estimate actual y for a given feature vector **x**, we add the mean back, yielding
  - $\hat{y} = \breve{y}+ \bar{y}= \tilde{\boldsymbol{x}}^T\tilde{\boldsymbol{\beta}} +\bar{y}=(\boldsymbol{x}^T - \bar{\boldsymbol{x}}^T)\,\tilde{\boldsymbol{\beta}} + \bar{y} = \boldsymbol{x}^T\tilde{\boldsymbol{\beta}} + \beta_0$, $\beta_0=\bar{y} - \bar{\boldsymbol{x}}^T\,\tilde{\boldsymbol{\beta}}$

Solution in terms of Sample Mean, Covariance and Cross-Covariance Matrices

- Sample mean: $\bar{y} = \sum_{i=1}^{n} y_i$, $\bar{x}_j = \sum_{i=1}^{n} x_{i,j}$, $\bar{\boldsymbol{x}}^T = [\bar{x}_1, \cdots, \bar{x}_k]$
- Sample covariance matrix and cross-covariance vector:
  - $S_{xx}(\ell, m) = \frac{1}{n}\sum_{i=1}^{n}(x_{i\ell} - \bar{x}_\ell)(x_{im} - \bar{x}_m)$, $S_{xx} = \frac{1}{n}\tilde{X}^T\tilde{X}$
  - $S_{xy}(\ell) = \frac{1}{n}\sum_{i=1}^{n}(x_{i\ell} - \bar{x}_\ell)(y_i - \bar{y})$, $S_{xy} = \frac{1}{n}\tilde{X}^T\tilde{\boldsymbol{y}}$
- Write parameters as $\boldsymbol{\beta}^{\boldsymbol{T}} = [\beta_0, \boldsymbol{\beta}_{1:k}]$
  - ${\boldsymbol{\beta}_{1:k}}^T = [\beta_1, \dots, \beta_k]$ coefficients for the features (=$\tilde{\boldsymbol{\beta}}$)
  - β_0 = constant term
- From previous derivation, given a sample feature $\boldsymbol{x}$, the optimal predictor is
  - $y = {\boldsymbol{\beta}^{1:k}}^T \boldsymbol{x} + \beta_0$, $\boldsymbol{\beta}_{1:k} = S_{xx}^{-1} S_{xy}$, $\beta_0 = \bar{y} - \boldsymbol{\beta}_{1:k}^T \bar{\boldsymbol{x}}$
  - It can be shown that the solution is the same as the original one with the intersect term

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- ❑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

```
ones = np.ones((ns_train,1))
A = np.hstack((ones,X_tr))
```

```
out = np.linalg.lstsq(A,y_tr)
beta = out[0]
```

- 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 $\beta = P A^T y$
  - 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)
```

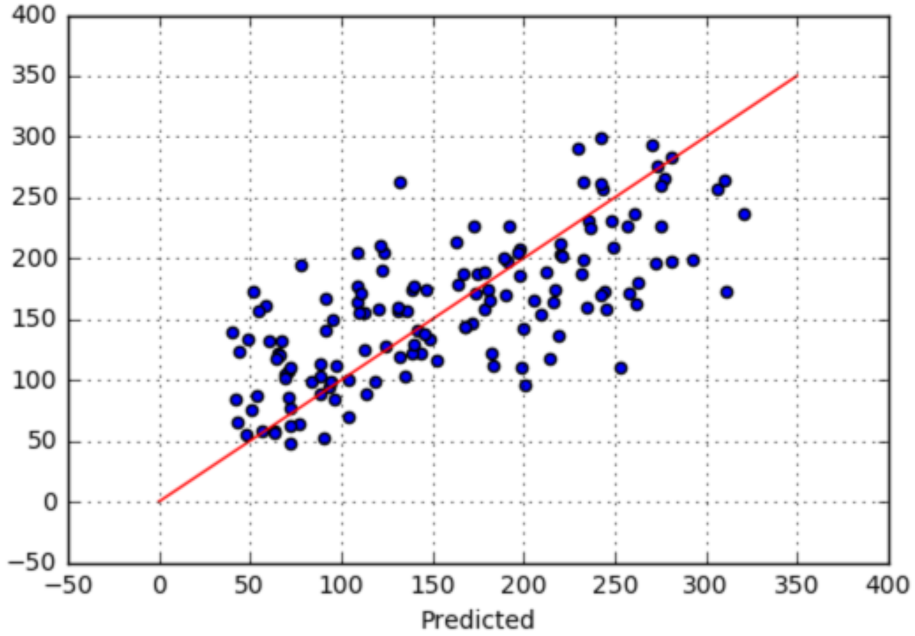
```
X_test = X[ns_train:,:]
y_test = y[ns_train:]
y_test_pred = regr.predict(X_test)
RSS_test = np.mean((y_test_pred-y_test)**2)/(np.std(y_test)**2)
Rsq_test = 1-RSS_test
print("RSS per sample = {0:f}".format(RSS_test))
print("R^2 =            {0:f}".format(Rsq_test))
```

```
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 s

```
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



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Simple vs. Multiple Regression

- Simple linear regression: One predictor (feature)
  - Scalar predictor x
  - Linear model: $\hat{y} = \beta_0 + \beta_1 x$
  - Can only account for one variable

- Multiple linear regression: Multiple predictors (features)
  - Vector predictor $\boldsymbol{x} = (x_1, \dots, x_k)$
  - Linear model: $\hat{y} = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k$
  - Can account for multiple predictors
  - Turns into simple linear regression when $k = 1$

Comparison to Single Variable Models

- We could compute models for each variable separately:

$$
\begin{aligned}
y &= a_1 + b_1 x_1 \\
y &= a_2 + b_2 x_2 \\
&\vdots
\end{aligned}
$$

- 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
  - What does C tell you that A and B do not?

Special Case: Single Variable

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

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

- Obtain single variable solutions for coefficients (after some algebra):

$$\beta_1 = \frac{s_{xy}}{s_x^2}, \qquad \beta_0 = \bar{y} - \beta_1 \bar{x}, \qquad R^2 = \frac{s_{xy}^2}{s_x^2 s_y^2}$$

Simple Linear Regression for Diabetes Data

```
ym = np.mean(y)
syy = np.mean((y-ym)**2)
Rsq = np.zeros(natt)
for k in range(natt):
    xm = np.mean(X[:,k])
    sxy = np.mean((X[:,k]-xm)*(y-ym))
    sxx = np.mean((X[:,k]-xm)**2)
    Rsq[k] = (sxy)**2/sxx/syy

    print("{0:2d}  Rsq={1:f}".format(k,Rsq[k]))
```

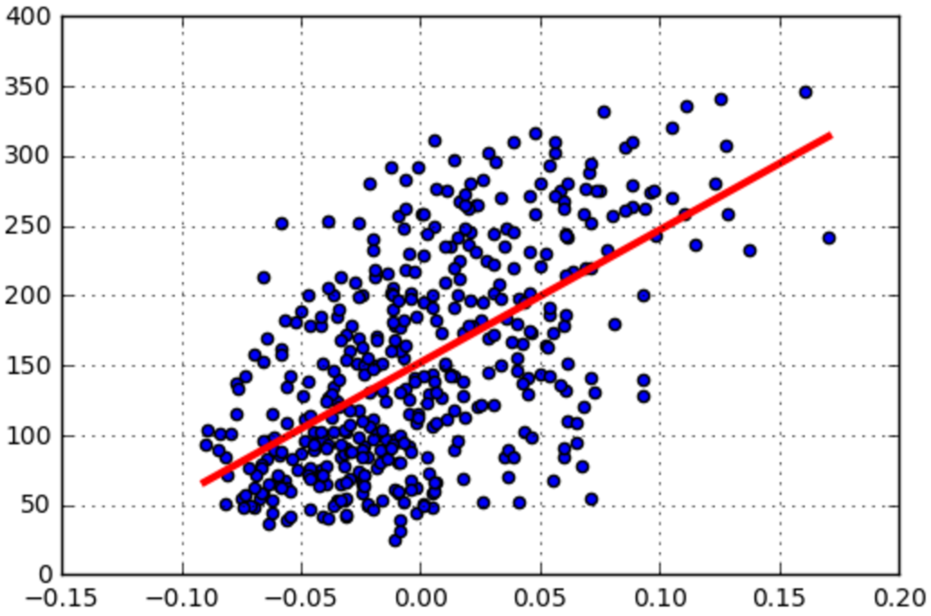
```
 0  Rsq=0.035302
 1  Rsq=0.001854
 2  Rsq=0.343924
 3  Rsq=0.194908
 4  Rsq=0.044954
 5  Rsq=0.030295
 6  Rsq=0.155859
 7  Rsq=0.185290
 8  Rsq=0.320224
 9  Rsq=0.146294
```

Best individual variable

- Try a fit of each variable individually
- Compute R_k^2 coefficient for each variable
- Use formula on previous slide
- "Best" individual variable is a poor fit
  - $R_k^2 \approx 0.34$

Scatter Plot

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

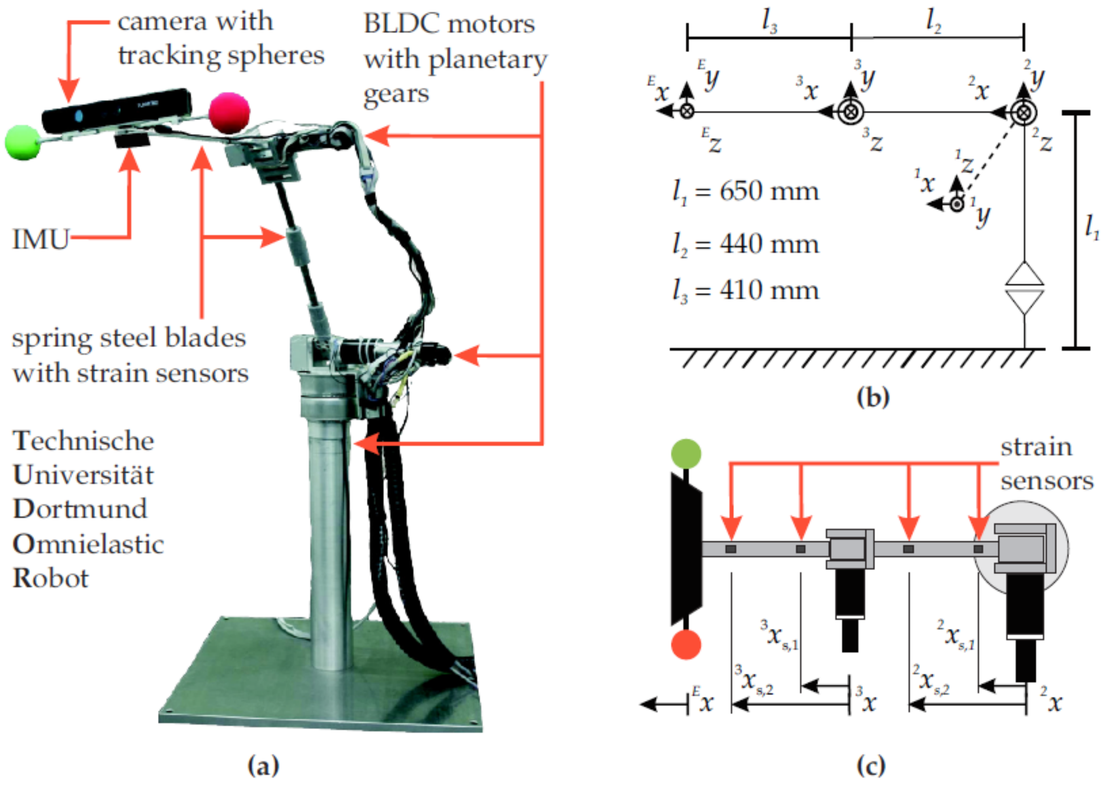



```python
# Find the index of the single variable with the best R^2
imax = np.argmax(Rsq)

# 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()
```

Go through the demo for this unit

- Results with simple regression
- Results with multiple variable regression
  - Using built-in sklearn linear regression model
  - Manually computing the solution

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.tu-dortmund.de/cms/en/research/robotics/TUDOR_engl/index.html

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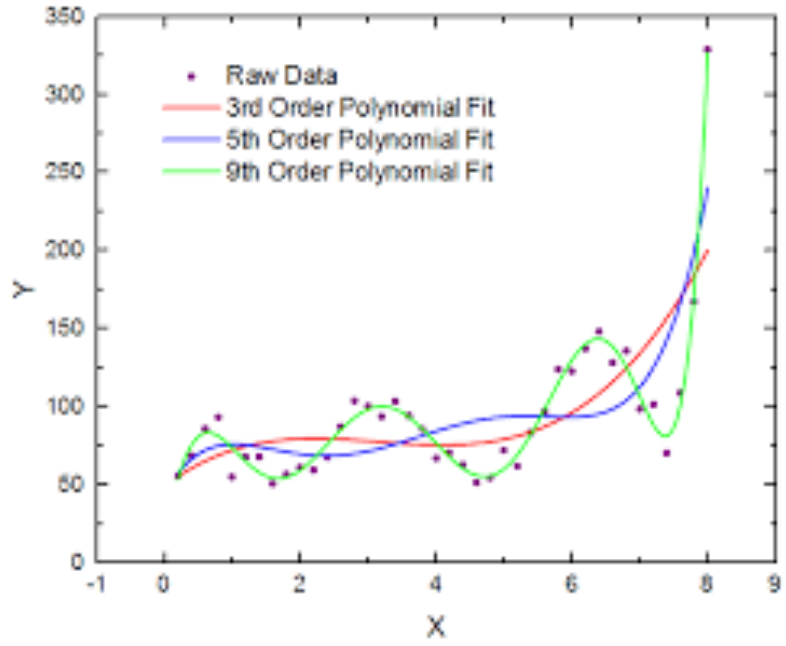
Polynomial Fitting

- 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 $(x_i, y_i), i = 1, \dots, n$
- 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 : $x, x^2, \dots, x^d$
- Form feature matrix and coefficient vector

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

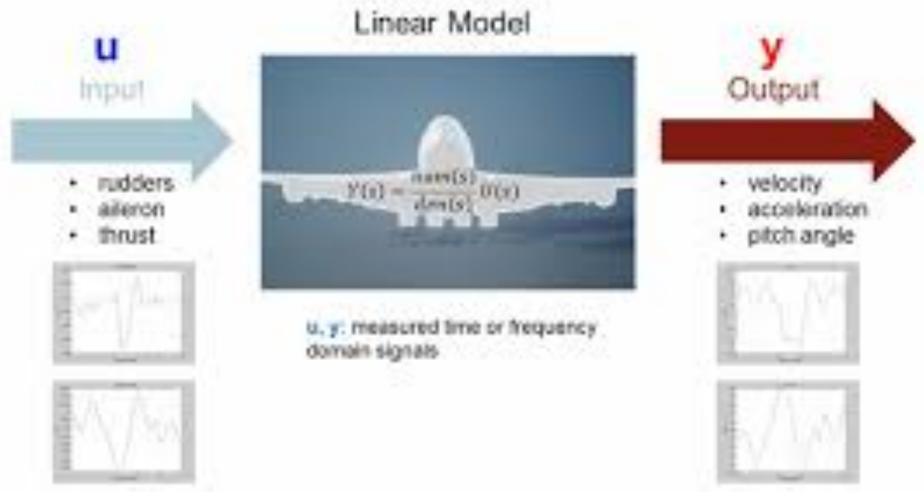
  - $p = d + 1$ transformed features from 1 original feature
- Will discuss model order selection in next year
- Extensions to other nonlinear transforms



Learning Linear Systems

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

  How do we determine $\beta = (a_1, \cdots, a_m, b_0, \cdots, b_n)^T$
- Can be solved using linear regression!
- 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

- Suppose that one feature x_j is a categorical variable
  - Example: We want to predict the price of a car, given its model x_1 and interior space x_2 . There could be 3 different models of a car
  - Arbitrarily assign an index to each possible car model may give unreasonable results
- One-hot coding example:
  - With 3 possible categories, represent x_1 using 3 binary features (u_1, u_2, u_3),
    - Ford=[1 0 0], BMW=[0 1 0], GM=[0 0 1]
  - Model: $y = \beta_0 + \beta_1 u_1 + \beta_2 u_2 + \beta_3 u_3 + \beta_4 x_2$
  - 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: $y = \beta_0 + \beta_3 + \beta_4 x_2$
  - Hot encoding allows different intercepts (or mean values) for different categories!

Model	u_1	u_2	u_3
Ford	0	0	0
BMW	1	0	0
GM	0	1	0

What you should know from this unit?

- ❑Formulate a machine learning model as a multiple linear regression model.
  - Identify prediction vector and target for the problem.
  - May need to transform original predictors (features).
- ❑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
  - Gradient calculation for a function of multiple variables
- ❑Manipulate 2D arrays in python (indexing, stacking, computing shapes, …)
- ❑Compute the LS solution using python linear algebra and machine learning packages