CS-UY 4563: Lecture 2
Simple Linear Regression

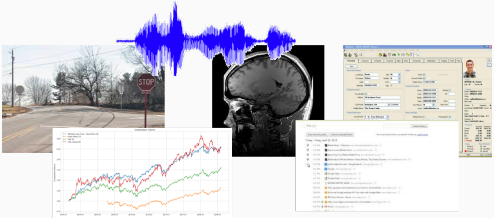
NYU Tandon School of Engineering, Prof. Christopher Musco

COURSE ADMIN

- Please enroll for Piazza. Only about 60% of class has.
- First lab assignment: `lab_housing_partial.ipynb`
    - Due **next Tuesday, 2/4 at 11:59pm**.
    - Go through the simple regression demonstration `demo_auto_mpg.ipynb`.
    - Turn in entire Jupyter Notebook via NYU Classes.
    - At top of notebook list any collaborators you worked with (as many as you like).
    - There will be a corresponding written homework released shortly.

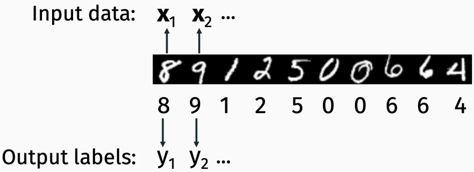
Goal: Develop algorithms to make decisions or predictions based on data.

- **Input:** A single piece of data (an image, audio file, patient healthcare record, MRI scan).



- **Output:** A prediction or decision (this image is a stop sign, this stock will go up 10% next quarter, turn the car right).

Step 1: Collect and label many input/output pairs $(\mathbf{x}_i, y_i)$. For our digit images, we have each $\mathbf{x}_i \in \mathbb{R}^{28\times 28}$ and $y_i \in \{0, 1, \ldots, 9\}$.



This is called the training dataset.

Step 2: Learn from the examples we have.

- Have the computer automatically find some function $f(\mathbf{x})$ such that $f(\mathbf{x}_i) = y_i$ for most $(\mathbf{x}_i, y_i)$ in our training data set (by searching over many possible functions).

In supervised learning every input $\mathbf{x}_i$ in our training dataset comes with a desired output y_i (typically generated by a human, or some other process).

Types of supervised earning:

- **Classification** – predict a discrete class label.
- **Regression** – predict a continuous value.
    - Dependent variable, response variable, target variable, lots of different names for y_i.

Another example of supervised classification: **Face Detection**.

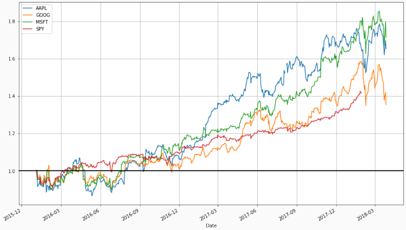
Each input data example $\mathbf{x}_i$ is an image. Each output y_i is 1 if the image contains a face, 0 otherwise.

- Harder than digit recognition, but we now have very reliable methods (used in nearly all digital cameras, phones, etc.)

Other examples of supervised classification:

- Object detection (Input: image, Output: dog or cat)
- Spam detection (Input: email text, Output: spam or not)
- Medical diagnosis (Input: patient data, Output: disease condition or not)
- Credit decision making (Input: financial data, Output: offer loan or not)

Example of supervised regression: **Stock Price Prediction**.



Each input **x** is a vector of metrics about a company (sales volume, PE ratio, earning reports, historical price data).

Each output y_i is the **price of the stock** 3 months in the future.

Other examples of supervised regression:

- Home price prediction (Inputs: square footage, zip code, number of bathrooms, Output: Price)
- Car price prediction (Inputs: make, model, year, miles driven, Output: Price)
- Weather prediction (Inputs: weather data at nearby stations, Output: tomorrows temperature)
- Robotics/Control (Inputs: information about environment and current position at time t, Output: estimate of position at time $t+1$)

Later in the class we will talk about other models:

- **Unsupervised learning** (no labels or response variable)
  - Clustering
  - Representation Learning
- **Reinforcement learning**
  - Game playing

You might also hear about semi-supervised learning or active learning – these categories aren't always cut and dry.

In **supervised learnings** every input $\mathbf{x}_i$ in our training dataset comes with a desired output y_i (typically generated by a human, or some other process).

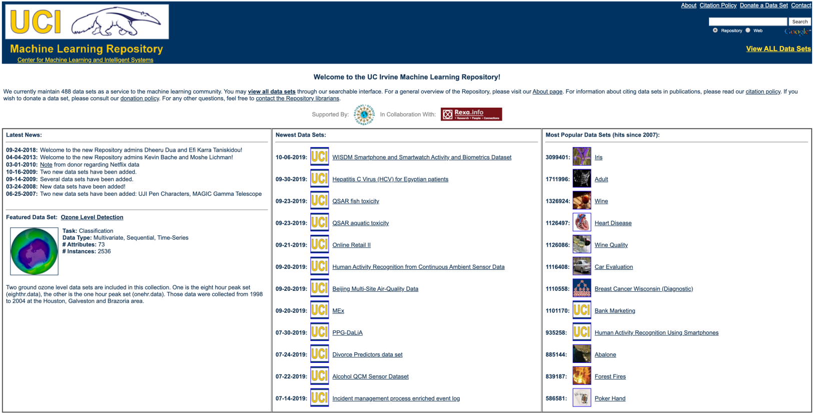
Types of supervised earning:

- **Classification** – predict a discrete class label.
- **Regression** – predict a continuous value.
  - Dependent variable, response variable, target variable, lots of different names for y_i.

Motivating example: Predict the highway miles per gallon (MPG) of a car given quantitative information about its engine. Demo in `demo_auto_mpg.ipynb`.

What factors might matter?

Data set available from the UCI Machine Learning Repository: https://archive.ics.uci.edu/.



This place is a great resource for projects!

PREDICTING MPG

Datasets from UCI (and many other places) comes as tab, space, or comma delimited files.

housing.data   auto-mpg.data

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18.0	8	307.0	130.0	3504.	12.0	70	1	"chevrolet chevelle malibu"
15.0	8	350.0	165.0	3693.	11.5	70	1	"buick skylark 320"
18.0	8	318.0	150.0	3436.	11.0	70	1	"plymouth satellite"
16.0	8	304.0	150.0	3433.	12.0	70	1	"amc rebel sst"
17.0	8	302.0	140.0	3449.	10.5	70	1	"ford torino"
15.0	8	429.0	198.0	4341.	10.0	70	1	"ford galaxie 500"
14.0	8	454.0	220.0	4354.	9.0	70	1	"chevrolet impala"
14.0	8	440.0	215.0	4312.	8.5	70	1	"plymouth fury iii"
14.0	8	455.0	225.0	4425.	10.0	70	1	"pontiac catalina"
15.0	8	390.0	190.0	3850.	8.5	70	1	"amc ambassador dpl"
15.0	8	383.0	170.0	3563.	10.0	70	1	"dodge challenger se"
14.0	8	340.0	160.0	3609.	8.0	70	1	"plymouth 'cuda 340"
15.0	8	400.0	150.0	3761.	9.5	70	1	"chevrolet monte carlo"
14.0	8	455.0	225.0	3086.	10.0	70	1	"buick estate wagon (sw)"
24.0	4	113.0	95.00	2372.	15.0	70	3	"toyota corona mark ii"
22.0	6	198.0	95.00	2833.	15.5	70	1	"plymouth duster"
18.0	6	199.0	97.00	2774.	15.5	70	1	"amc hornet"
21.0	6	200.0	85.00	2587.	16.0	70	1	"ford maverick"
27.0	4	97.00	88.00	2130.	14.5	70	3	"datsun pl510"
26.0	4	97.00	46.00	1835.	20.5	70	2	"volkswagen 1131 deluxe sedan"
25.0	4	110.0	87.00	2672.	17.5	70	2	"peugeot 504"
24.0	4	107.0	90.00	2430.	14.5	70	2	"audi 100 ls"
25.0	4	104.0	95.00	2375.	17.5	70	2	"saab 99e"
26.0	4	121.0	113.0	2234.	12.5	70	2	"bmw 2002"
21.0	6	199.0	90.00	2648.	15.0	70	1	"amc gremlin"
10.0	8	360.0	215.0	4615.	14.0	70	1	"ford f250"

Check dataset description to know what each column means.

housing.data auto-mpg.data ×

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y_1	18.0	8	307.0	130.0	3504.	12.0	70	1	"chevrolet chevelle malibu"	x_1
y_2	15.0	8	350.0	165.0	3693.	11.5	70	1	"buick skylark 320"	x_2
y_3	18.0	8	318.0	150.0	3436.	11.0	70	1	"plymouth satellite"	x_3
	16.0	8	304.0	150.0	3433.	12.0	70	1	"amc rebel sst"	
	17.0	8	302.0	140.0	3449.	10.5	70	1	"ford torino"	
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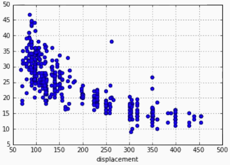
	10.0	8	360.0	215.0	4615.	14.0	70	1	"ford f250"	

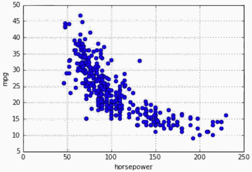
'mpg', 'cylinders','displacement', 'horsepower', 'weight', 'acceleration', 'model year', 'origin', 'car name'

- Use `pandas` for reading data from delimited files. Stores data in a type of table called a "data frame" but this is just a wrapper around a `numpy` array.
- Use `matplotlib` for initial exploration.

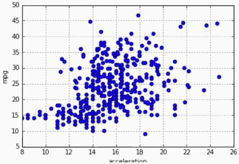
mpg



Displacement

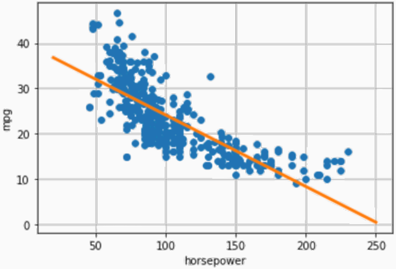


Horsepower



Acceleration

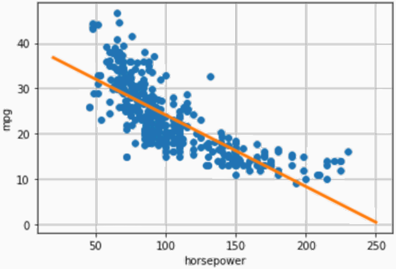
Linear regression from a Machine Learning (not a Statistics) perspective. Our first supervised machine learning model.



Only focus on <u>one predictive variable</u> at a time (e.g. horsepower). This is why it's called <u>simple</u> linear regression.

Dataset:

- $x_1, \ldots, x_n \in \mathbb{R}$ (horsepowers of n cars – this is the predictor/independent variable)
- $y_1, \ldots, y_n \in \mathbb{R}$ (MPG – this is the response/dependent variable)



- **Model** $f_{\boldsymbol{\theta}}(x)$: Class of equations or programs which map input x to predicted output. We want $f_{\boldsymbol{\theta}}(x_i) \approx y_i$ for training inputs.
- **Model Parameters** $\boldsymbol{\theta}$: Vector of numbers. These are numerical nobs which parameterize our class of models.
- **Loss Function** $L(\boldsymbol{\theta})$: Measure of how well a model fits our data. Typically some function of $f_{\boldsymbol{\theta}}(x_1) - y_1, \ldots, f_{\boldsymbol{\theta}}(x_n) - y_n$

Goal: Choose parameters $\boldsymbol{\theta}^*$ which minimize the Loss Function:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$$

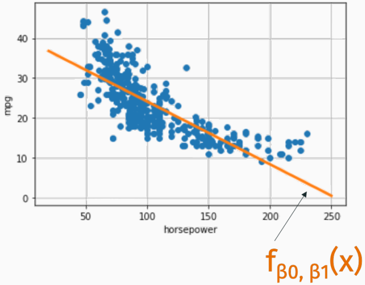
General Supervised Learning

- Model: $f_{\boldsymbol{\theta}}(x)$
- Model Parameters: $\boldsymbol{\theta}$
- Loss Function: $L(\boldsymbol{\theta})$

Linear Regression

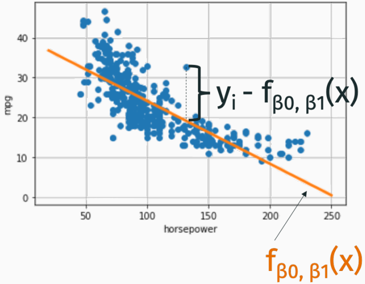
- Model:
- Model Parameters:
- Loss Function:

What is a natural **loss function** for linear regression?



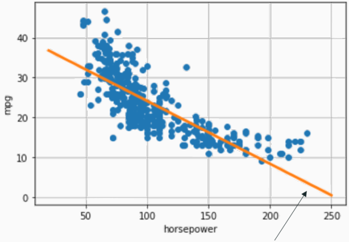
HOW TO MEASURE GOODNESS OF FIT

Typical choices are a function of $y_1 - f_{\beta_0,\beta_1}(x_1), \ldots, y_n - f_{\beta_0,\beta_1}(x_n)$



- ℓ_2/**Squared Loss:** $L(\beta_0, \beta_1) = \sum_{i=1}^{n} [y_i - f_{\beta_0,\beta_1}(x_i)]^2$.
- ℓ_1/**Lease absolute deviations:** $L(\beta_0, \beta_1) = \sum_{i=1}^{n} |y_i - f_{\beta_0,\beta_1}(x_i)|$.
- ℓ_∞ **Loss** $L(\beta_0, \beta_1) = \max_{i \in 1,\ldots,n} |y_i - f_{\beta_0,\beta_1}(x_i)|$.

We're going to start with the Squared Loss/Sum-of-Squares Loss. Also called "Residual Sum-of-Squares (RSS)"



$f_{\beta 0, \beta 1}(x)$

- Relatively robust to outliers.
- Simple to define, leads to simple algorithms for finding β_0, β_1
- Justifications from classical statistics related to assumptions about Gaussian noise. Will discuss later in the course.

General Supervised Learning

- Model: $f_{\boldsymbol{\theta}}(x)$
- Model Parameters: $\boldsymbol{\theta}$
- Loss Function: $L(\boldsymbol{\theta})$

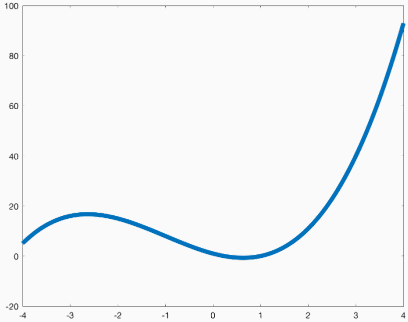
Linear Regression

- Model: $f_{\beta_0,\beta_1}(x) = \beta_0 + \beta_1 \cdot x$
- Model Parameters: β_0, β_1
- Loss Function: $L(\beta_0, \beta_1) = \sum_{i=1}^{n}(y_i - f_{\beta_0,\beta_1}(x_i))^2$

Goal: Choose β_0, β_1 to minimize
$L(\beta_0, \beta_1) = \sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i)^2$.

This is the entire job of any Supervised Learning Algorithm.

Univariate function:



$$x^3 + 3 \cdot x^2 - 5 \cdot x + 1$$

- Find all places where derivative $f'(x) = 0$ and check which has the smallest value.

Multivariate function: $L(\beta_0, \beta_1)$

- Find values of β_0, β_1 where all partial derivatives equal 0.
- $\frac{\partial L}{\partial \beta_0} = 0$ and $\frac{\partial L}{\partial \beta_1} = 0$.

Multivariate function: $L(\beta_0, \beta_1) = \sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i)^2$

- Find values of β_0, β_1 where all partial derivatives equal 0.
- $\frac{\partial L}{\partial \beta_0} = 0$ and $\frac{\partial L}{\partial \beta_1} = 0$.

Some definitions:

- Let $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$. — $\bar{y}$ is the mean of y.
- Let $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$. — $\bar{y}$ is the mean of x.
- Let $\sigma_y^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2$. — σ_y^2 is the variance of y.
- Let $\sigma_x^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$. — σ_x^2 is the variance of x.
- Let $\sigma_{xy} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$. — σ_{xy} is the covariance.

Claim: $L(\beta_0, \beta_1)$ is minimized when:

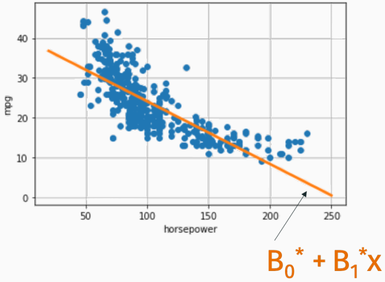
- $\beta_1 = \sigma_{xy}/\sigma_x^2$
- $\beta_0 = \bar{y} - \beta_1\bar{x}$

PROOF

PROOF

Takeaways:

- Minimizing functions is often easy with calculus.
- Tools we will see again: **linearity of derivatives, chain rule**.
- Simple closed form formula for optimal parameters β_0^* and β_1^* for squared-loss!



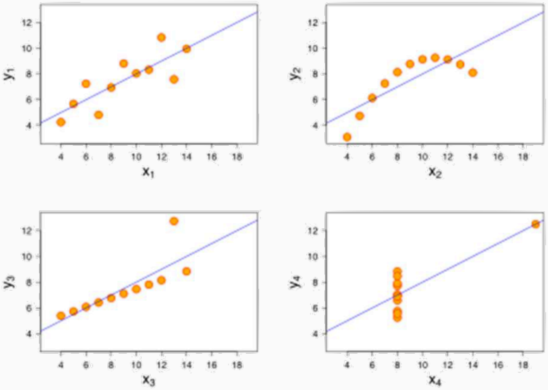
Let $L(\beta_0, \beta_1) = \sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i)^2$.

$$R^2 = 1 - \frac{L(\beta_0, \beta_1)}{n\sigma_y^2}$$

is exactly the R^2 value you may remember from statistics.

The smaller the loss, the closer R^2 is to 1, which means we have a better regression fit.

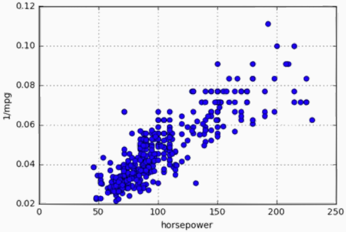
Many reasons you might get a poor regression fit:

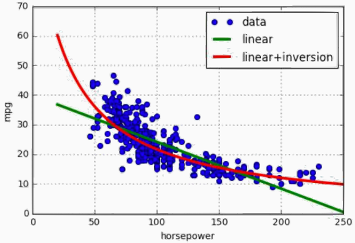


Some of these are fixable!

- Remove outliers, use more robust loss function.
- **Non-linear model transformation.**

Fit the model $\frac{1}{\text{mpg}} \approx \beta_0 + \beta_1 \cdot \text{horsepower}$.





Much better fit, same exact learning algorithm!