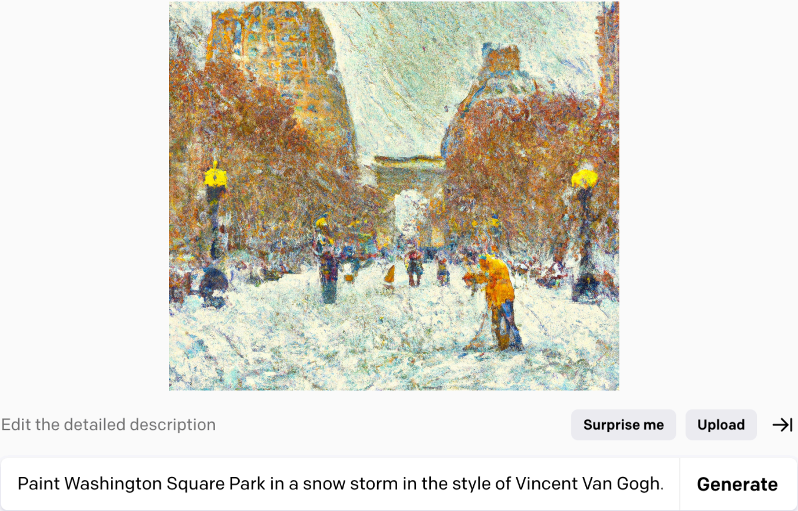
CS-GY 6923: Lecture 1
Introduction to Machine Learning

NYU Tandon School of Engineering, Prof. Christopher Musco

ARTIFICIAL INTELLIGENCE IS HAVING A MOMENT

Who has tried ChatGPT? DALLE? Imagen?



Paint Washington Square Park in a snow storm in the style of Vincent Van Gogh.

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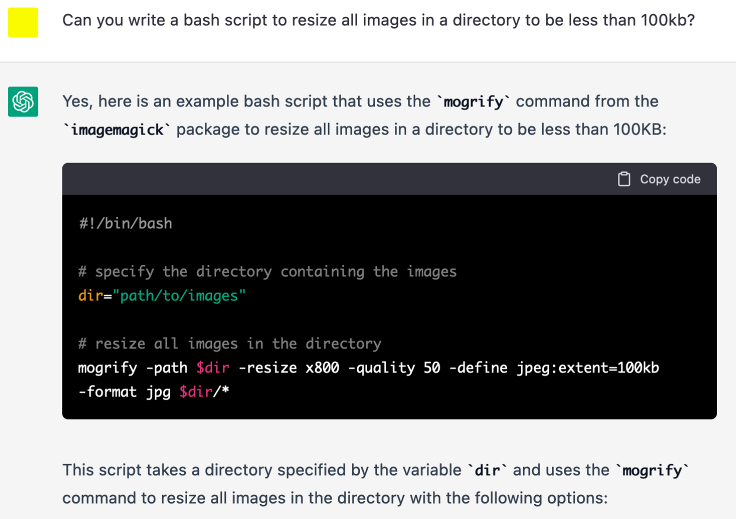


Can you write a bash script to resize all images in a directory to be less than 100kb?

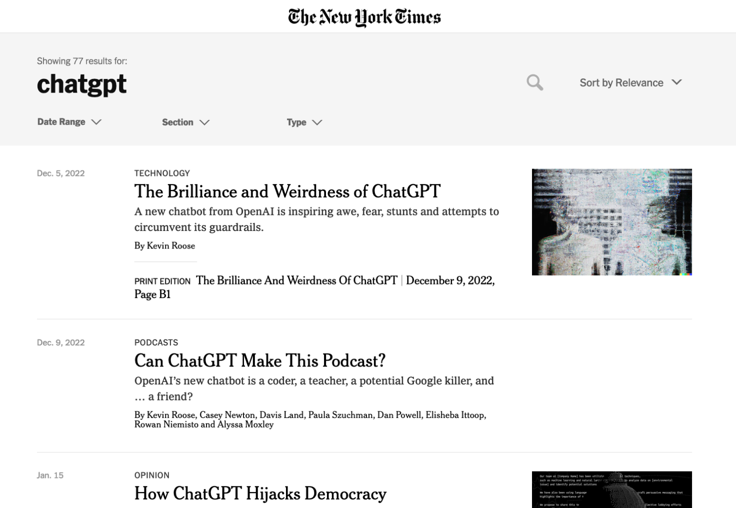
Yes, here is an example bash script that uses the `mogrify` command from the `imagemagick` package to resize all images in a directory to be less than 100KB:

```
#!/bin/bash

# specify the directory containing the images
dir="path/to/images"

# resize all images in the directory
mogrify -path $dir -resize x800 -quality 50 -define jpeg:extent=100kb
-format jpg $dir/*
```

This script takes a directory specified by the variable `dir` and uses the `mogrify` command to resize all images in the directory with the following options:

ARTIFICIAL INTELLIGENCE IS HAVING A MOMENT

May look back on 2015-now as a the dawn of true artificial intelligence.



The New York Times

Showing 77 results for:

chatgpt

Dec. 5, 2022

TECHNOLOGY

The Brilliance and Weirdness of ChatGPT

A new chatbot from OpenAI is inspiring awe, fear, stunts and attempts to circumvent its guardrails.

By Kevin Roose

PRINT EDITION The Brilliance And Weirdness Of ChatGPT | December 9, 2022, Page B1

Dec. 9, 2022

PODCASTS

Can ChatGPT Make This Podcast?

OpenAI's new chatbot is a coder, a teacher, a potential Google killer, and … a friend?

By Kevin Roose, Casey Newton, Davis Land, Paula Szuchman, Dan Powell, Elisheba Ittoop, Rowan Niemisto and Alyssa Moxley

Jan. 15

OPINION

How ChatGPT Hijacks Democracy

ARTIFICIAL INTELLIGENCE IS HAVING A MOMENT

Other developments in recent years:

- Human-level image classification and understanding.
- Near perfect machine translation.
- Human level game play in very complex games (Go, Starcraft).
- Machine learning as a central tool in science.

What technologies have caught people's eye?

GOAL OF THIS CLASS

Give you a foundation to understand the main ideas in modern machine learning.

GOAL OF THIS CLASS

We will do so through a combination of:

- Hands on implementation.
  - Demos and take-home labs using `Python` and `Jupyter notebooks`. 20% of grade
  - We will use `Google Colab` as the primary programming environment.
- Theoretical exploration.
  - Written problem sets. 20%
  - Midterm and final exam. 25% of grade each.

COURSE OBJECTIVES

Goals of theoretical component:

1. Build experience with the most important mathematical tools used in machine learning, including probability, statistics, and linear algebra. This experience will prepare you for more advanced coursework in ML, or research.
2. Be able to understand contemporary research in machine learning, including papers from NeurIPS, ICML, ICLR, and other major machine learning venues.
3. Learn how theoretical analysis can help explain the performance of machine learning algorithms and lead to the design of entirely new methods.

COURSE OBJECTIVES

Goals of hands-on component:

1. Reinforce theory learned in class, and make sure you understand algorithms described by implementing them.
2. Learn how to view and formulate real world problems in the language of machine learning.
3. Gain experience applying the most popular and successful machine learning algorithms to thse problems.

MORE ADVANCED CLASSES AT TANDON

- CS-GY 6953: **Deep Learning** (Prof. Chinmay Hegde)
- ECE-GY 7143: **Advanced Machine Learning** (Prof. Anna Chromanska)
- CS-GY 6763: **Algorithmic Machine Learning and Data Science** (me)
- Keep your eyes out for special topics courses.

SOMETHING A BIT DIFFERENT

Given recent progress, we will run this semester of the course as a special semester focused on generative machine learning.

- Still cover all the basics.
- Add material in each section on background for topics like text and image generation, style transfer, etc.

BASIC INFORMATION

All class information can be found at:

`www.chrismusco.com/machinelearning2023_grad`

TWO MOST IMPORTANT THINGS FROM SYLLABUS

1. Make sure you are signed into and follow EdStem, which will be used for all classroom communication (no email). Now integrated into Brightspace.
2. Don't hesitate to ask me or the TAs for help.[1]

Aarshvi Gajjar

Atsushi Shimizu

Teal Witter

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[1] Fill out office hours poll on Ed!

CLASS PARTICIPATION

Class participation accounts for 10% of your grade. It's easy to get a perfect score:

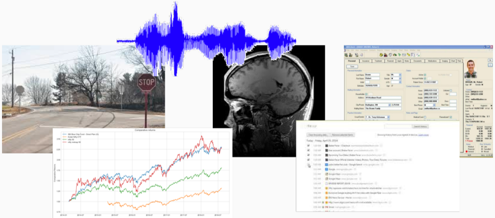
- Ask and answer questions in lecture.
- Post questions or responses to other students on Ed. Or other things you find interesting.
- Participate in professor or TA office hours.

THE PREDICTION PROBLEM

BASIC GOAL

Goal: Develop algorithms to make predictions based on data.

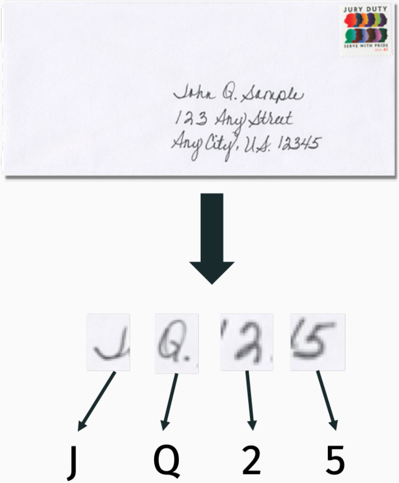
- **Input:** A single piece of data (an image, audio file, patient healthcare record, MRI scan).



- **Output:** A prediction (this image is a stop sign, this stock will go up 10% next quarter, this song is in French).

CLASSIC EXAMPLE

Optical character recognition (OCR): Decide if a handwritten character is an $a, b, \ldots, z, 0, 1, \ldots, 9, \ldots$.



CLASSIC EXAMPLE

Optical character recognition (OCR): Decide if a handwritten character is an $a, b, \ldots, z, 0, 1, \ldots, 9, \ldots$.

Applications:

- Automatic mail sorting.
- Text search in handwritten documents.
- Digitizing scanned books.
- License plate detection for tolls.
- Etc.

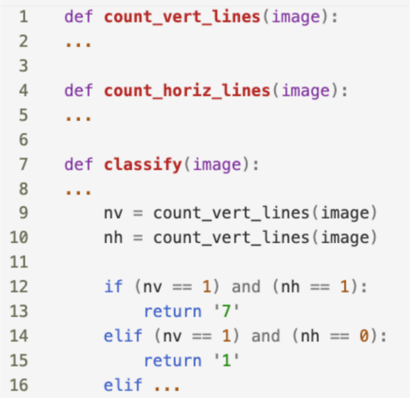
EXPERT SYSTEMS

How would you write an **code** to distinguish these digits?

Suppose you just want to distinguish <u>between a 1 and a 7</u>.

1s vs. 7s algorithm

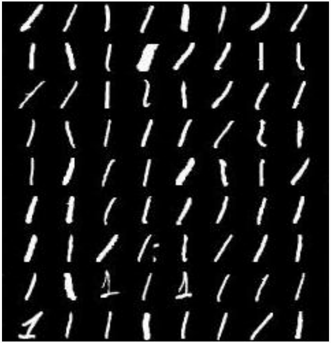
Reasonable approach: A number which contains one vertical line is a 1, if it contains one vertical and one horizontal line, it's a 7.

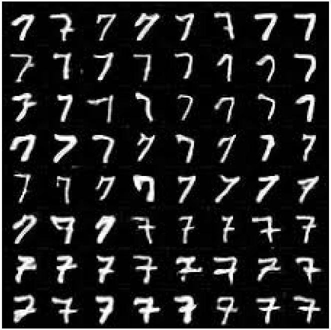


```
def count_vert_lines(image):
...

def count_horiz_lines(image):
...

def classify(image):
...
    nv = count_vert_lines(image)
    nh = count_vert_lines(image)

    if (nv == 1) and (nh == 1):
        return '7'
    elif (nv == 1) and (nh == 0):
        return '1'
    elif ...
```

1S VS. 7S ALGORITHM

This rule breaks down in practice:





Even fixes/modifications of the rule tend to be brittle... Maybe you could get 80% accuracy, but not nearly good enough.

CHALLENGE OF EXPERT SYSTEMS

Rule based systems, also called Expert Systems were the dominant approach to artificial intelligence in the 1970s and 1980s.

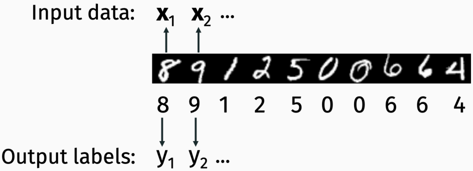
Major limitation: While human's are very good at many tasks,

- It's often hard to encode why humans make decisions in simple programmable logic.
- We think in abstract concepts with no mathematical definitions (how exactly do you define a line? how do you define a curve? straight line?)

A DIFFERENT APPROACH: SUPERVISED MACHINE LEARNING

Focus on what humans do well: solving the task at hand!

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 $y_i \in \{0, 1, \ldots, 9\}$.



Input data: $\mathbf{x}_1$ $\mathbf{x}_2$ ...

8 9 1 2 5 0 0 6 6 4

Output labels: y_1 y_2 ...

This is called the training dataset.

A DIFFERENT APPROACH: MACHINE LEARNING

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).

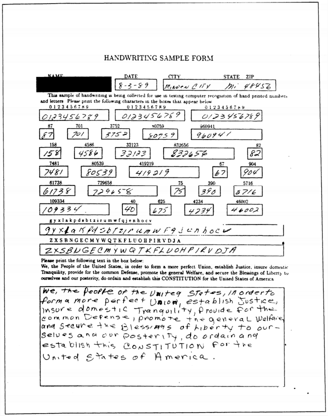
Think of f as any crazy equation, or an arbitrary program:

$$f(\mathbf{x}) = 10 \cdot x[1,1] - 6 \cdot x[3,45] \cdot x[9,99] + 5 \cdot \text{mean}(\mathbf{x}) + \ldots$$

This approach of learning a function from labeled data is called supervised learning.

SUPERVISED LEARNING FOR OCR

National Institute for Standards and Technology collected a huge amount of handwritten digit data from census workers and high school students in the early 90s:



HANDWRITING SAMPLE FORM

NAME	DATE	CITY	STATE ZIP
[redacted]	8-3-89	Minden City	MI 48456

This sample of handwriting is being collected for use in testing computer recognition of hand printed numbers and letters. Please print the following characters in the boxes that appear below

0123456789	0123456789	0123456789		
0123456789	0123456789	0123456789		
87	701	3752	80759	960941
87	701	3752	80759	960941
158	4586	32123	832656	82
158	4586	32123	832656	82
7481	80539	419219	67	904
7481	80539	419219	67	904
61738	729658	75	390	5716
61738	729658	75	390	5716
109334	40	625	4234	46002
109334	40	675	4234	46002

gyxlakpdsbtzirumwfqjenhocv

gyxlakpdsbtzirumwfqjenhocv

ZXSBNGECMYWQTKFLUOHPIRVDJA

ZXSBNGECMYWQTKFLUOHPIRVDJA

Please print the following text in the box below:
We, the People of the United States, in order to form a more perfect Union, establish Justice, insure domestic Tranquility, provide for the common Defense, promote the general Welfare, and secure the Blessings of Liberty to ourselves and our posterity, do ordain and establish this CONSTITUTION for the United States of America

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form a more perfect Union, establish Justice,
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common Defense, promote the general Welfare,
and secure the Blessings of Liberty to our-
selves and our posterity, do ordain and
establish this CONSTITUTION for the
United States of America.

This is called the NIST dataset, and was used to create the famous MNIST handwritten digit dataset.

MACHINE LEARNING

Since the 1990s machine learning have overtaken expert systems as the dominant approach to artificial intelligence.

- Current methods achieve .17% error rate for OCR on benchmark datasets (MNIST).[2]
- Very successful on other problems as well. The big break through for supervised learning in the 2010s was image classification.

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[2] Not because of overfitting! See: *Cold Case: The Lost MNIST Digits* by Chhavi Yadav + Léon Bottou.

CENTRAL QUESTIONS IN SUPERVISED MACHINE LEARNING

Once we have the basic supervised machine learning setup, many very difficult questions remain:

- How do we parameterize a class of functions f to search?
- How do we efficiently find a good function in the class?
- How do we ensure that an $f(\mathbf{x})$ which works well on our training data will generalize to perform well on future data?
- How do we deal with imperfect data (noise, outliers, incorrect training labels)?

MACHINE LEARNING

Recall that in the supervised learning setup 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.

SUPERVISED LEARNING

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 essentially perfect methods (used in nearly all digital cameras, phones, etc.)

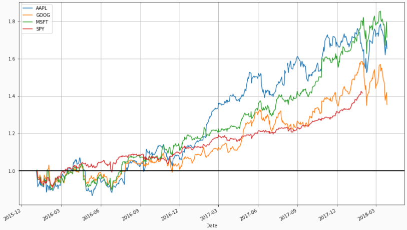
SUPERVISED LEARNING

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)

SUPERVISED LEARNING

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.

SUPERVISED LEARNING

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 $t+1$)

OTHER TYPES OF LEARNING

Later in the class we will talk about other frameworks:

- **Unsupervised learning** (no labels or response variable)
  - Important for representation learning and generative ML.
- **Semi-supervised learning, self-supervised learning**.

Focus less in this class on:

- **Reinforcement learning**
  - Game playing
- **Active-learning.**
  - The learning algorithms can request labels.

SUPERVISED LEARNING

Types of supervised learning:

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

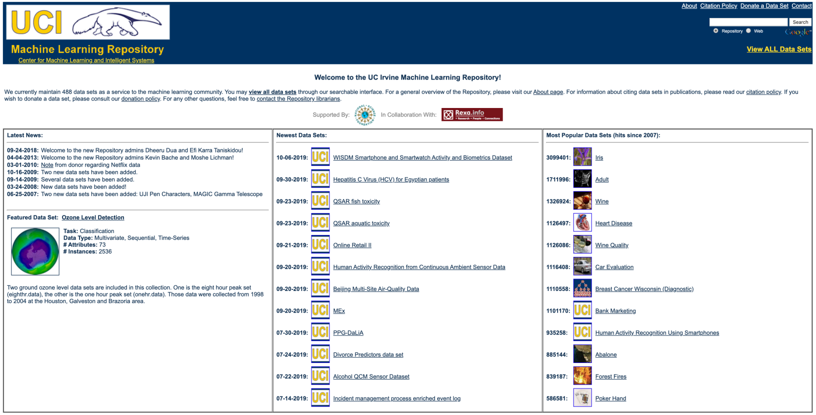
PREDICTING MPG

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?

PREDICTING MPG

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



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Machine Learning Repository
Center for Machine Learning and Intelligent Systems
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View ALL Data Sets

Welcome to the UC Irvine Machine Learning Repository!

We currently maintain 488 data sets as a service to the machine learning community. You may **view all data sets** through our searchable interface. For a general overview of the Repository, please visit our About page. For information about citing data sets in publications, please read our citation policy. If you wish to donate a data set, please consult our donation policy. For any other questions, feel free to contact the Repository librarians.

Supported By: In Collaboration With: Rexa.info

Latest News:

09-24-2018: Welcome to the new Repository admins Dheeru Dua and Efi Karra Taniskidou!
04-04-2013: Welcome to the new Repository admins Kevin Bache and Moshe Lichman!
03-01-2010: Note from donor regarding Netflix data
10-16-2009: Two new data sets have been added.
09-14-2009: Several data sets have been added.
03-24-2008: New data sets have been added!
06-25-2007: Two new data sets have been added: UJI Pen Characters, MAGIC Gamma Telescope

Featured Data Set: **Ozone Level Detection**

Task: Classification
Data Type: Multivariate, Sequential, Time-Series
# Attributes: 73
# Instances: 2536

Two ground ozone level data sets are included in this collection. One is the eight hour peak set (eighthr.data), the other is the one hour peak set (onehr.data). Those data were collected from 1998 to 2004 at the Houston, Galveston and Brazoria area.

Newest Data Sets:

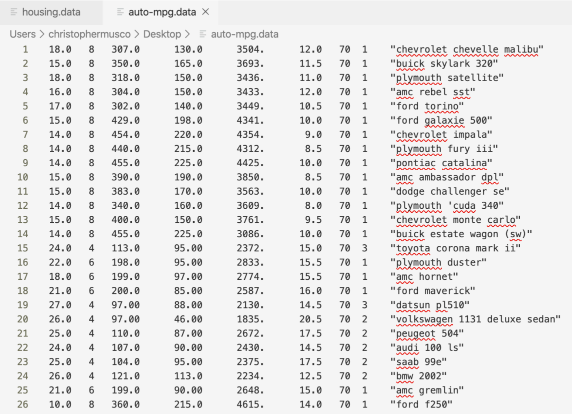
10-06-2019: WISDM Smartphone and Smartwatch Activity and Biometrics Dataset
09-30-2019: Hepatitis C Virus (HCV) for Egyptian patients
09-23-2019: QSAR fish toxicity
09-23-2019: QSAR aquatic toxicity
09-21-2019: Online Retail II
09-20-2019: Human Activity Recognition from Continuous Ambient Sensor Data
09-20-2019: Beijing Multi-Site Air-Quality Data
09-20-2019: MEx
07-30-2019: PPG-DaLiA
07-24-2019: Divorce Predictors data set
07-22-2019: Alcohol QCM Sensor Dataset
07-14-2019: Incident management process enriched event log

Most Popular Data Sets (hits since 2007):

3099401: Iris
1711996: Adult
1326924: Wine
1126497: Heart Disease
1126086: Wine Quality
1116408: Car Evaluation
1110558: Breast Cancer Wisconsin (Diagnostic)
1101170: Bank Marketing
935258: Human Activity Recognition Using Smartphones
885144: Abalone
839187: Forest Fires
586581: Poker Hand

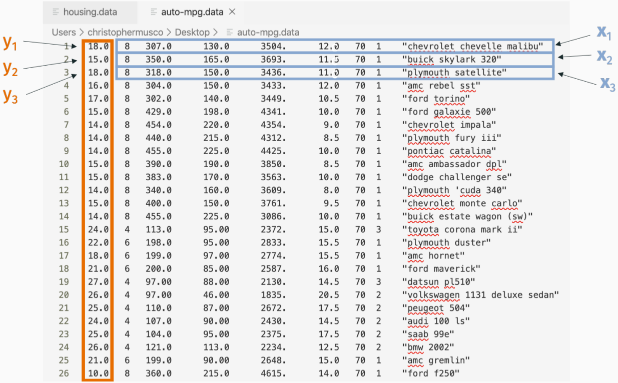
PREDICTING MPG

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



```
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.



```
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15.0   8   390.0      190.0      3850.       8.5   70  1    "amc ambassador dpl"
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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"
```
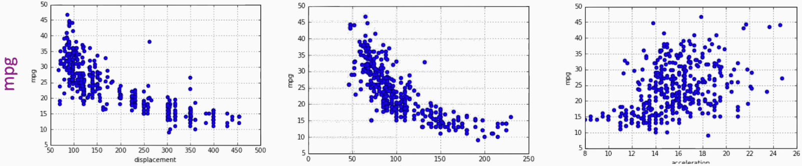

’mpg’, ’cylinders’,’displacement’, ’horsepower’, ’weight’, ’acceleration’, ’model year’, ’origin’, ’car name’

LIBRARIES FOR INITIAL DATA READING

- 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.

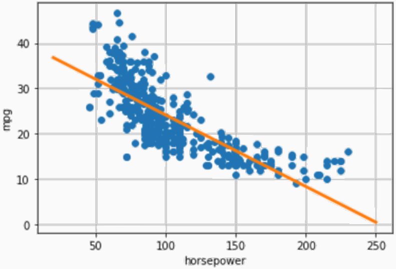


Displacement Horsepower Acceleration

SIMPLE LINEAR REGRESSION

SIMPLE LINEAR REGRESSION

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

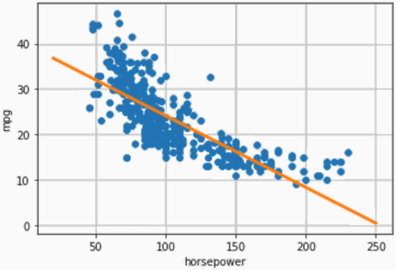


Only focus on <u>one predictive variable</u> at a time (e.g. horsepower). This is why it's called <u>simple</u> linear regression.

SIMPLE 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)



SUPERVISED LEARNING DEFINITIONS

- **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 knobs which parameterize our class of models.
- **Loss Function $L(\boldsymbol{\theta})$:** Measure of how well a model fits our data. Often some function of $f_{\boldsymbol{\theta}}(x_1) - y_1, \ldots, f_{\boldsymbol{\theta}}(x_n) - y_n$

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

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

Choosing $\boldsymbol{\theta}^*$ based on minimizing the empirical error on our training data is called Empirical Risk Minimization. It is by far the most common approach to solving supervised learning problems.

General Supervised Learning

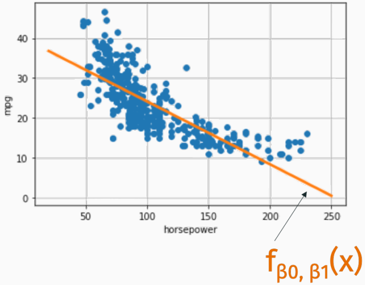
- Model: $f_{\boldsymbol{\theta}}(x)$
- Model Parameters: $\boldsymbol{\theta}$
- Loss Function: $L(\boldsymbol{\theta})$

Linear Regression

- Model:
- Model Parameters:
- Loss Function:

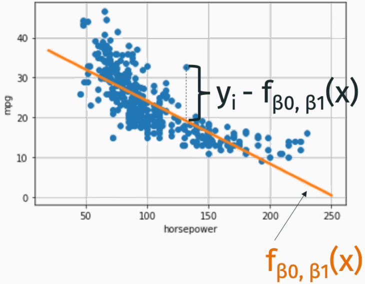
HOW TO MEASURE GOODNESS OF FIT

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



HOW TO MEASURE GOODNESS OF FIT

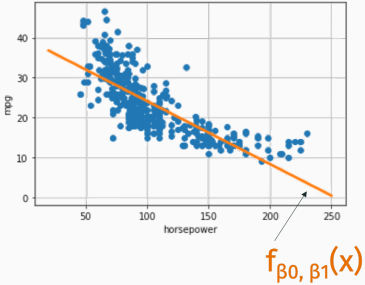
Typical choices are a function of $y_1 - f_{\beta_0,\beta_1}(x_1), \ldots, y_n - f_{\beta_0,\beta_1}(x_n)$



- 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** $L(\beta_0, \beta_1) = \max_{i \in 1,\ldots,n} |y_i - f_{\beta_0,\beta_1}(x_i)|$.

HOW TO MEASURE GOODNESS OF FIT

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



- Relatively robust to outliers.
- Simple to define, leads to simple algorithms for finding β_0, β_1
- Theoretically justified 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

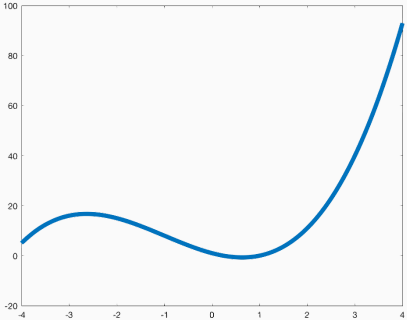
- Model: $f_{\beta_0,\beta_1}(x) = \beta_0 + \beta_1 \cdot x$
- Model Parameters: β_0, β_1
- Loss Function: $L(\beta_0, \beta_1) = \sum_{i=1}^{n}(y_i - f_{\beta_0,\beta_1}(x_i))^2$

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.

FUNCTION MINIMIZATION

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.

FUNCTION MINIMIZATION

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 $\frac{\partial L}{\partial \beta_1} = 0$.

MINIMIZING SQUARED LOSS FOR REGRESSION

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

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

PROOF

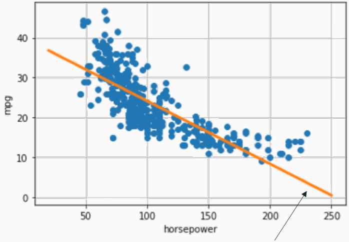
Loss function after substitution:

$$\tilde{L}(\beta_1) = \sum_{i=1}^{n}(y_i - \bar{y} + \beta_1\bar{x} - \beta_1 x_i)^2$$

MINIMIZING SQUARED LOSS FOR REGRESSION

Takeaways:

- Minimizing functions exactly is sometimes easy with calculus, but not always! We will learn much more general tools (like gradient descent).
- Simple closed form formula for optimal parameters β_0^* and β_1^* for squared-loss!



$B_0^* + B_1^*x$

A FEW COMMENTS

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

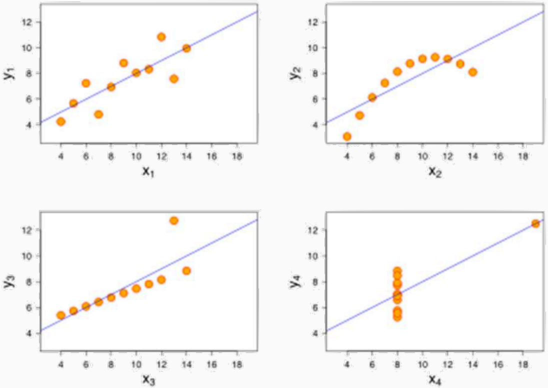
$$R^2 = 1 - \frac{L(\beta_0, \beta_1)}{n\sigma_y^2}$$

is exactly the R^2 value (“coefficient of determination”) you may remember from statistics.

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

A FEW COMMENTS

Many reasons you might get a poor regression fit:

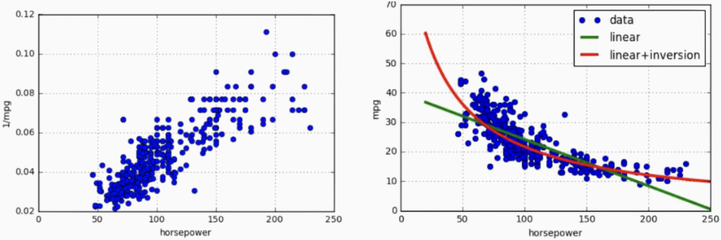


A FEW COMMENTS

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!

MULTIPLE LINEAR REGRESSION

MORE COMMON GOAL

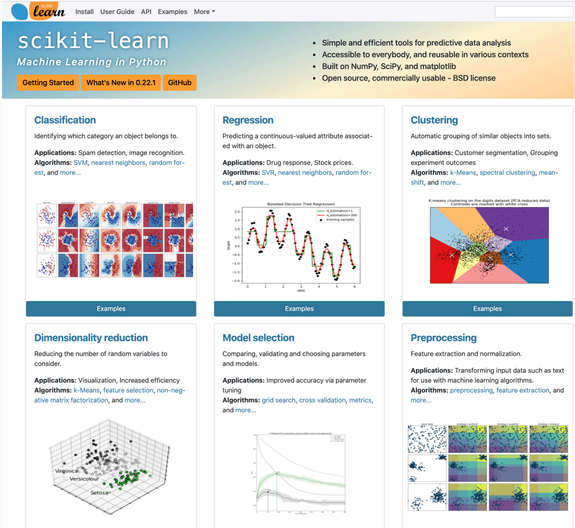
Predict target y using multiple features, simultaneously.

Motivating example: Predict diabetes progression in patients after 1 year based on health metrics. (Measured via numerical score.)

Features: Age, sex, average blood pressure, six blood serum measurements (e.g. cholesterol, lipid levels, iron, etc.)

Demo in `demo_diabetes.ipynb`.

Introducing **Scikit Learn**.



scikit-learn

Machine Learning in Python

- Simple and efficient tools for predictive data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

Classification

Identifying which category an object belongs to.

Applications: Spam detection, image recognition.
Algorithms: SVM, nearest neighbors, random forest, and more...

Regression

Predicting a continuous-valued attribute associated with an object.

Applications: Drug response, Stock prices.
Algorithms: SVR, nearest neighbors, random forest, and more...

Clustering

Automatic grouping of similar objects into sets.

Applications: Customer segmentation, Grouping experiment outcomes
Algorithms: k-Means, spectral clustering, mean-shift, and more...

Dimensionality reduction

Reducing the number of random variables to consider.

Applications: Visualization, Increased efficiency
Algorithms: k-Means, feature selection, non-negative matrix factorization, and more...

Model selection

Comparing, validating and choosing parameters and models.

Applications: Improved accuracy via parameter tuning
Algorithms: grid search, cross validation, metrics, and more...

Preprocessing

Feature extraction and normalization.

Applications: Transforming input data such as text for use with machine learning algorithms.
Algorithms: preprocessing, feature extraction, and more...

SCIKIT LEARN

Pros:

- One of the most popular “traditional” ML libraries.
- Many built in models for regression, classification, dimensionality reduction, etc.
- Easy to use, works with ‘numpy‘, ‘scipy‘, other libraries we use.
- Great for rapid prototyping, testing models.

Cons:

- Everything is very “black-box”: difficult to debug, understand why models aren’t working, speed up code, etc.

SCIKIT LEARN

Modules used:

- `datasets` module contains a number of pre-loaded datasets. Saves time over downloading and importing with `pandas`.
- `linear_model` can be used to solve Multiple Linear Regression. A bit overkill for this simple model, but gives you an idea of `sklearn`'s general structure.

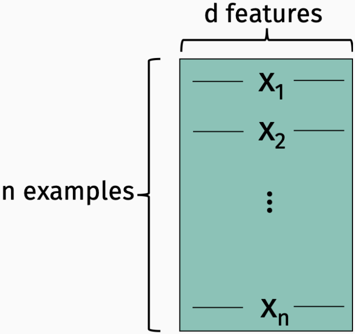
THE DATA MATRIX

Target variable:

- Scalars $y_1, \ldots, y_n$ for n data examples (a.k.a. samples).

Predictor variables:

- d dimensional vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$ for n data examples and d features



LINEAR ALGEBRA REVIEW

Now it the time to review your linear algebra!

Notation:

- Let $\mathbf{X}$ be an $n \times d$ matrix. Written $\mathbf{X} \in \mathbb{R}^{n\times d}$.
- $\mathbf{x}_i$ is the ith row of the matrix.
- $\mathbf{x}^{(j)}$ is the jth column.
- x_{ij} is the i, j entry.
- For a vector $\mathbf{y}$, y_i is the ith entry.
- $\mathbf{X}^T$ is the matrix transpose.
- $\mathbf{y}^T$ is a vector transpose.

LINEAR ALGEBRA REVIEW

Things to remember:

- Matrix multiplication. If I multiply $\mathbf{X} \in \mathbb{R}^{n\times d}$ by $\mathbf{Y} \in \mathbb{R}^{d\times k}$ I get $\mathbf{XY} = \mathbf{Z} \in \mathbb{R}^{n\times k}$.
- Inner product/dot product. $\langle \mathbf{y}, \mathbf{z}\rangle = \sum_{i=1}^{n} y_i z_i$.
- $\langle \mathbf{y}, \mathbf{z}\rangle = \mathbf{y}^T\mathbf{z} = \mathbf{z}^T\mathbf{y}$.
- Euclidean norm: $\|\mathbf{y}\|_2 = \sqrt{\mathbf{y}^T\mathbf{y}}$.
- $(\mathbf{XY})^T = \mathbf{Y}^T\mathbf{X}^T$.

Things to remember:

- Identity matrix is denoted as $\mathbf{I}$.
- "Most" square matrices have an inverse: i.e. if $\mathbf{Z} \in \mathbb{R}^{n \times n}$, there is a matrix $\mathbf{Z}^{-1}$ such that $\mathbf{Z}^{-1}\mathbf{Z} = \mathbf{Z}\mathbf{Z}^{-1} = \mathbf{I}$.
- Let $\mathbf{D} = \text{diag}(\mathbf{d})$ be a diagonal matrix containing the entries in $\mathbf{d}$.
- $\mathbf{XD}$ scales the columns of $\mathbf{X}$. $\mathbf{DX}$ scales the rows.

LINEAR ALGEBRA REVIEW

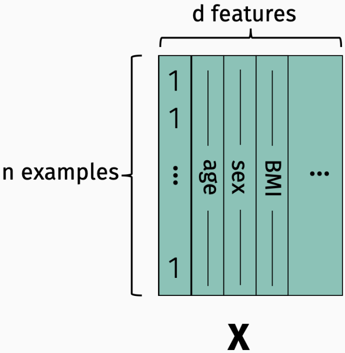
You also need to be comfortable working with matrices in `numpy` . Go through the `demo_numpy_matrices.ipynb` slowly.

Target variable:

- Scalars $y_1, \ldots, y_n$ for n data examples (a.k.a. samples).

Predictor variables:

- d dimensional vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$ for n data examples and d features



MULTIPLE LINEAR REGRESSION

Data matrix indexing:

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1d} \\ x_{21} & x_{22} & \dots & x_{2d} \\ x_{31} & x_{32} & \dots & x_{3d} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nd} \end{bmatrix}$$

Multiple Linear Regression Model:

$$\text{Predict} \qquad y_i \approx \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_d x_{id}$$

The rate at which diabetes progresses depends on many factors, with each factor having a different magnitude effect.

MULTIPLE LINEAR REGRESSION

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1d} \\ x_{21} & x_{22} & \dots & x_{2d} \\ x_{31} & x_{32} & \dots & x_{3d} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nd} \end{bmatrix} = \begin{bmatrix} 1 & x_{12} & \dots & x_{1d} \\ 1 & x_{22} & \dots & x_{2d} \\ 1 & x_{32} & \dots & x_{3d} \\ \vdots & \vdots & & \vdots \\ 1 & x_{n2} & \dots & x_{nd} \end{bmatrix}$$

Multiple Linear Regression Model:

Predict $$y_i \approx \boldsymbol{\beta_1} + \beta_2 x_{i2} + \ldots + \beta_d x_{id}$$

In this case, β_1 serves as the “intercept” parameter.

MULTIPLE LINEAR REGRESSION

Use as much linear algebra notation as possible!

- Model Parameters:

- Model:

- Loss Function:

Linear Least-Squares Regression.

- Model Parameters:

$$\boldsymbol{\beta} = [\beta_1, \beta_2, \ldots, \beta_d]$$

- Model:

$$f_{\boldsymbol{\beta}}(\mathsf{x}) = \langle \mathsf{x}, \boldsymbol{\beta} \rangle$$

- Loss Function:

$$\begin{aligned} L(\boldsymbol{\beta}) &= \sum_{i=1}^{n} |y_i - \langle \mathsf{x}_i, \boldsymbol{\beta} \rangle|^2 \\ &= \|\mathsf{y} - \mathsf{X}\beta\|_2^2 \end{aligned}$$

LINEAR ALGEBRAIC FORM OF LOSS FUNCTION

LOSS MINIMIZATION

Machine learning goal: minimize the loss function $L(\boldsymbol{\beta}) : \mathbb{R}^d \rightarrow \mathbb{R}$.

Find optimum by determining for which $\boldsymbol{\beta} = [\beta_1, \ldots, \beta_d]$ all partial derivatives are 0. I.e. when do we have:

$$\begin{bmatrix} \frac{\partial L}{\partial \beta_1} \\ \frac{\partial L}{\partial \beta_2} \\ \vdots \\ \frac{\partial L}{\partial \beta_d} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \ldots \\ 0 \end{bmatrix}$$

THE ALL IMPORTANT GRADIENT

For any function $L(\boldsymbol{\beta}) : \mathbb{R}^d \to \mathbb{R}$, the gradient $\nabla L()\boldsymbol{\beta})$ is a function from $\mathbb{R}^d \to \mathbb{R}^d$ defined:

$$\nabla L(\boldsymbol{\beta}) = \begin{bmatrix} \frac{\partial L}{\partial \beta_1} \\ \frac{\partial L}{\partial \beta_2} \\ \vdots \\ \frac{\partial L}{\partial \beta_d} \end{bmatrix}$$

The gradient of the loss function is a central tool in machine learning. We will use it again and again.

GRADIENT

Loss function:

$$L(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2$$

Gradient:

$$-2 \cdot \mathbf{X}^T(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Find optimum by determining for which $\boldsymbol{\beta} = [\beta_1, \ldots, \beta_d]$ the gradient is 0. I.e. when do we have:

$$\nabla L(\beta) = \begin{bmatrix} \frac{\partial L}{\partial \beta_1} \\ \frac{\partial L}{\partial \beta_2} \\ \vdots \\ \frac{\partial L}{\partial \beta_d} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

LOSS MINIMIZATION

Goal: minimize the loss function $L(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2$.

$$\begin{aligned} \nabla L(\boldsymbol{\beta}) &= -2 \cdot \mathbf{X}^T(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \\ &= 2\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} - 2\mathbf{X}^T\mathbf{y} = \mathbf{0} \end{aligned}$$

Solve for optimal $\boldsymbol{\beta}^*$:

$$\begin{aligned} \mathbf{X}^T\mathbf{X}\boldsymbol{\beta}^* &= \mathbf{X}^T\mathbf{y} \\ \boldsymbol{\beta}^* &= \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y} \end{aligned}$$

MULTIPLE LINEAR REGRESSION SOLUTION

Need to compute $\beta^* = \arg\min_{\beta} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}$.

- Main cost is computing $(\mathbf{X}^T\mathbf{X})^{-1}$ which takes $O(nd^2)$ time.
- Can solve slightly faster using the method `numpy.linalg.lstsq`, which is running an algorithm based on QR decomposition.
- For larger problems, can solve much faster using an *iterative methods* like `scipy.sparse.linalg.lsqr`.

Will learn more about iterative methods when we study Gradient Descent.

GRADIENT WARMUP

Function:

$$f(\mathbf{z}) = \mathbf{a}^T\mathbf{z} \text{ for some fixed vector } \mathbf{a} \in \mathbb{R}^d$$

Gradient:

Function:

$$f(\mathbf{z}) = \|\mathbf{z}\|_2^2$$

Gradient:

GRADIENT

Loss function:

$$L(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2$$

GRADIENT

Loss function:

$$L(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2$$

TEST YOUR INTUITION

Model: $f_{\boldsymbol{\beta}}(\mathbf{x}) = \sum_{i=1}^{d} \beta_1 x_i$

Example from book: What is the sign of β_1 when we run a simple linear regression using the following predictors for number of sales in a particular market as a function of:

- Amount of TV advertising in that market:
- Amount of print advertising in that market:

INTERACTING VARIABLES

What is the sign of the corresponding β's when we run a multiple linear regression using the following predictors together:

- Amount of TV advertising in that market: Positive
- Amount of print advertising in that market: Negative, close to zero

Can you explain this? Try to think of your own example of a regression problem where this phenomenon might show up.

DEALING WITH CATEGORICAL VARIABLES

The sex variable in the diabetes problem was binary. We encoded it as 2 numbers – e.g. (0,1), (-1,1), (1,2).

Suppose we go back to the MPG prediction problem. What if we had a categorical predictor variable for car make with more than 2 options: e.g. Ford, BMW, Honda. **How would you encode as a numerical column?**

$$\begin{bmatrix} \texttt{ford} \\ \texttt{ford} \\ \texttt{honda} \\ \texttt{bmw} \\ \texttt{honda} \\ \texttt{ford} \end{bmatrix} \rightarrow \begin{bmatrix} \quad \\ \\ \\ \\ \\ \\ \end{bmatrix}$$

ONE HOT ENCODING

Better approach: One Hot Encoding.

$$\begin{bmatrix} \texttt{ford} \\ \texttt{ford} \\ \texttt{honda} \\ \texttt{bmw} \\ \texttt{honda} \\ \texttt{ford} \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

- Create a separate feature for every category, which is 1 when the variable is in that category, zero otherwise.
- Not too hard to do by hand, but you can also use library functions like `sklearn.preprocessing.OneHotEncoder`.

Avoids adding inadvertent linear relationships.