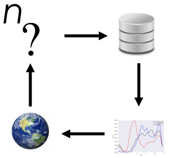
Data Science 100

Lecture 13:
Modeling and Estimation



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2018 updates - Fernando Perez, fernando.perez@berkele.edu

Recap … so far we have covered

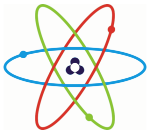
- **Data collection**: Surveys, sampling, administrative data
- **Data cleaning and manipulation**: Pandas, text & regexes.
- **Exploratory Data Analysis**
  - Joining and grouping data
  - Structure, Granularity, Temporality, Faithfulness and Scope
  - Basic exploratory data visualization
- **Data Visualization:**
  - Kinds of visualizations and the use of size, area, and color
  - Data transformations using Tukey Mosteller bulge diagram
- **An introduction to database systems and SQL**

Today –
Models & Estimation

What is a model?

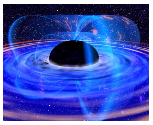
What is a model?

A model is an an ***idealized*** *representation of a system*



Atoms don't actually work like this…

Proteins are far more complex



We haven't really seen one of these.

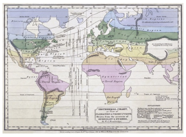
> *"Essentially,*
> *all models are wrong,*
> *but some are useful."*

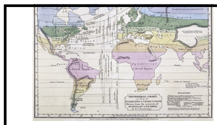
George Box
Statistician
1919-2013

Why do we build models?

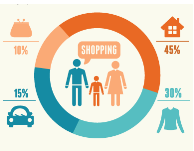
Why do we build models?

- Models enable us to make **accurate predictions**



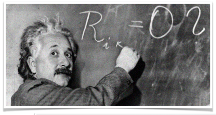


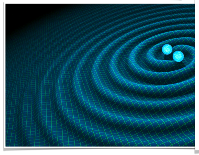
- **Provide insight** into complex phenomena



WORLD BANK

A few types of models: “physical” or “mechanistic”





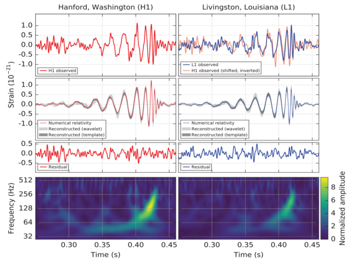
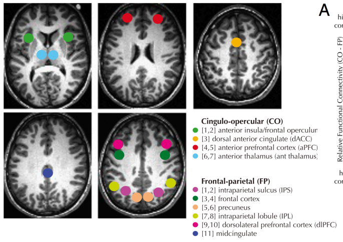
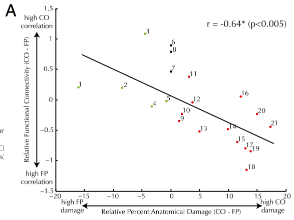


FIG. 1. The gravitational-wave event GW150914 observed by the LIGO Hanford (H1, left column panels) and Livingston (L1, right column panels) detectors. Times are shown relative to September 14, 2015 at 09:50:45 UTC. For visualization, all time series are filtered with a 35–350 Hz bandpass filter to suppress large fluctuations outside the detectors' most sensitive frequency band, and band-reject

Models: Statistical correlations (A)

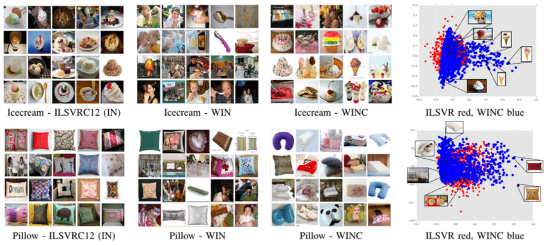
A ROI coordinates from Dosenbach et al, 2007


Cingulo-opercular (CO)
● [1,2] anterior insula/frontal operculum
● [3] dorsal anterior cingulate (dACC)
● [4,5] anterior prefrontal cortex (aPFC)
● [6,7] anterior thalamus (ant thalamus)
Frontal-parietal (FP)
● [1,2] intraparietal sulcus (IPS)
● [3,4] frontal cortex
● [5,6] precuneus
● [7,8] intraparietal lobule (IPL)
● [9,10] dorsolateral prefrontal cortex (dlPFC)
● [11] midcingulate



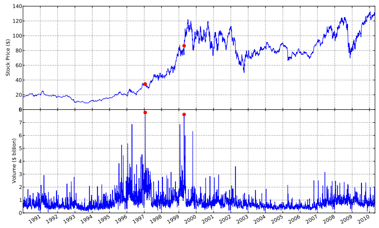
Nomura et al, PNAS 2010

Models: statistical correlations (B)



Massouh et al. IROS 2017

Models: statistical correlations (C)



Pérez et al. CISE 2007

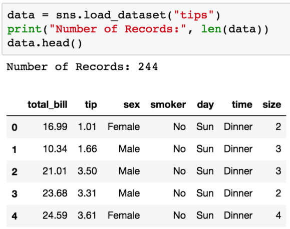
Models and the World

- **Data Generation Process:** the real-world phenomena from which the data is collected
  - **Example:** *everyday there are some number of clouds and it rains or doesn't*
  - We don't' know or can't compute this, could be stochastic or adversarial
- **Model:** a theory of the data generation process
  - **Example:** *if there are more than X clouds then it will rain*
  - How do we pick this model? EDA? Art?
  - May not reflect reality … "all models are wrong …"
- **Estimated Model:** an instantiation of the model
  - **Example:** *If there are more than 42 clouds then it will rain*
  - How do we estimate it?
  - What makes the estimate "good"?

Example – Restaurant Tips

Follow along with the notebook …

Step 1: Understanding the Data (EDA)



```
data = sns.load_dataset("tips")
print("Number of Records:", len(data))
data.head()
```

```
Number of Records: 244
```

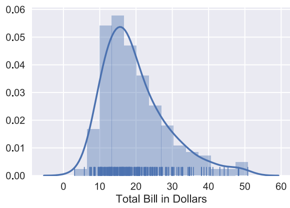
	total_bill	tip	sex	smoker	day	time	size
0	16.99	1.01	Female	No	Sun	Dinner	2
1	10.34	1.66	Male	No	Sun	Dinner	3
2	21.01	3.50	Male	No	Sun	Dinner	3
3	23.68	3.31	Male	No	Sun	Dinner	2
4	24.59	3.61	Female	No	Sun	Dinner	4

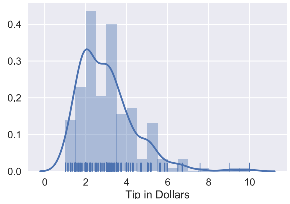
Collected by a single waiter over a month

Why?

- **Predict** which tables will tip the highest
- **Understand** relationship between tables and tips

Understanding the Tips





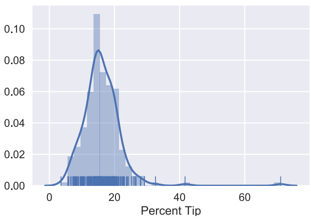
Observations:
- Right skewed
- Mode around $15
- Mean around $20
- No large bills

Observations:
- Right skewed
- Mean around 3
- Possibly bimodal? → Explanations?
- Large outliers → Explanations?

Derived Variable: Percent Tip

$$\texttt{pct\_tip} = \frac{\texttt{tip}}{\texttt{total\_bill}} * 100$$

- Natural representation of tips
  - Why? Tradition in US is to tip %
- Issues in the plot?
  - Outliers
  - Explanation?
    - Small bills … bad data?
  - Transformations?
    - Remove outliers



Step 1: Define the Model

START SIMPLE!!

Start with a ***Simple Model***: Constant

$$\text{percentage tip} = \theta^*$$

* Means true parameter determined by universe

- **Rationale:** There is a percent tip θ^* that all customers pay
  - Correct?
    - *No! We have different percentage tips in our data*
    - *Why? Maybe people make mistakes calculating their bills?*
  - Useful?
    - Perhaps. A good estimate θ^* could allow us to predict future tips …
- The **parameter** θ^* is determined by the universe
  - we generally don't get to see θ^* …
  - we will need to develop a procedure to **estimate θ^* from the data**

How do we estimate the parameter θ^*

- Guess a number using **prior knowledge**: 15%
- **Use the data!** How?
- Estimate the value θ^* *as:*
  - the percent tip from a **randomly selected** receipt
  - the **mode** of the distribution observed
  - the **mean** of the percent tips observed
  - the **median** of the percent tips observed
- Which is the best? How do I define best?
  - Depends on our goals …

Defining an the Objective (Goal)

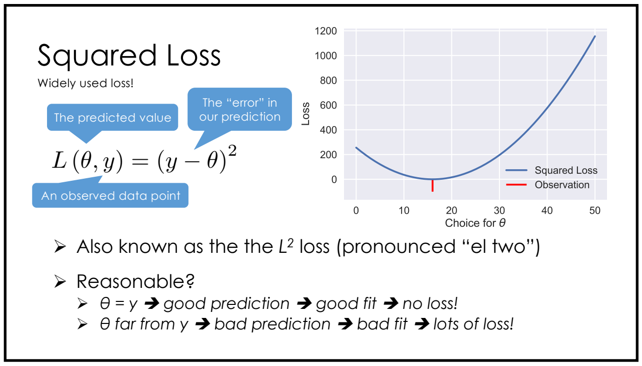
- **Ideal Goal:** estimate a value for θ^* such that the model makes good predictions about the future.
  - **Great goal!** Problem?
    - We don't know the future. How will we know if our estimate is good?
  - There is hope! … we will return to this goal … *in the future* ☺
- **Simpler Goal:** estimate a value for θ^* such that the model ***"fits"*** the data
  - What does it mean to *"fit"* the data?
  - We can define a **loss function** that measures the error in our model on the data

Step 2: Define the Loss

"Take the Loss"

Loss Functions

- **Loss function**: a function that characterizes the cost, error, or loss resulting from a particular choice of model or model parameters.
- *Many definitions* of loss functions and the choice of loss function affects the **accuracy** and **computational cost of estimation**.
- The choice of loss function **depends on the estimation task**
  - quantitative (e.g., tip) or qualitative variable (e.g., political affiliation)
  - Do we care about the outliers?
  - Are all errors equally costly? (e.g., false negative on cancer test)



Squared Loss

Widely used loss!

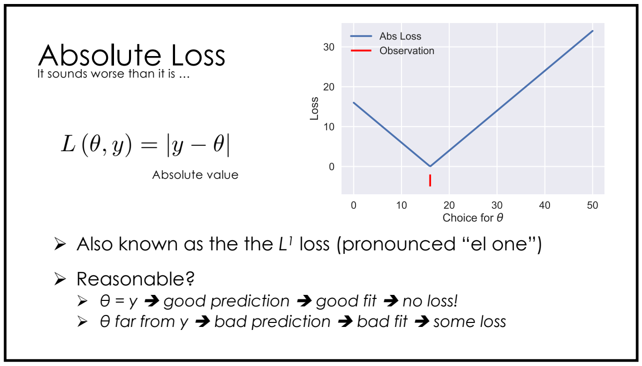
The predicted value

The "error" in our prediction

$$L(\theta, y) = (y - \theta)^2$$

An observed data point

- ➢ Also known as the the L^2 loss (pronounced "el two")
- ➢ Reasonable?
  - ➢ *θ = y ➔ good prediction ➔ good fit ➔ no loss!*
  - ➢ *θ far from y ➔ bad prediction ➔ bad fit ➔ lots of loss!*



Absolute Loss

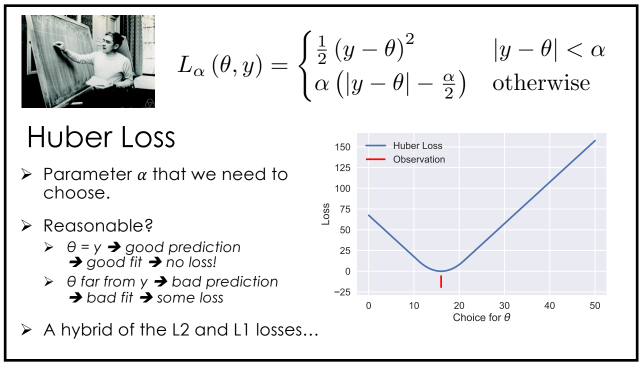
It sounds worse than it is …

$$L(\theta, y) = |y - \theta|$$

Absolute value

- ➢ Also known as the the L^1 loss (pronounced "el one")
- ➢ Reasonable?
  - ➢ *θ = y ➔ good prediction ➔ good fit ➔ no loss!*
  - ➢ *θ far from y ➔ bad prediction ➔ bad fit ➔ some loss*

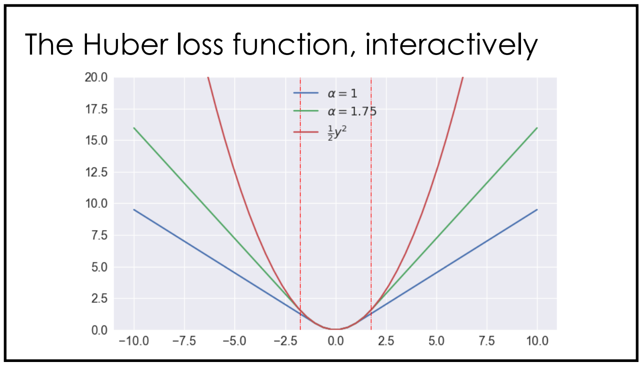
Can you think of another Loss Function?



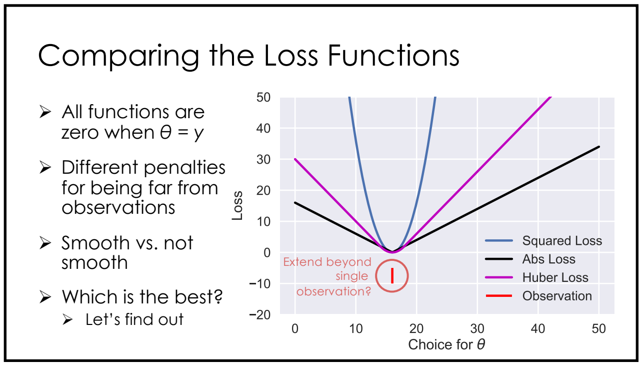
$$L_\alpha(\theta, y) = \begin{cases} \frac{1}{2}(y - \theta)^2 & |y - \theta| < \alpha \\ \alpha\left(|y - \theta| - \frac{\alpha}{2}\right) & \text{otherwise} \end{cases}$$

Huber Loss

- ➢ Parameter α that we need to choose.
- ➢ Reasonable?
  - ➢ *θ = y ➔ good prediction ➔ good fit ➔ no loss!*
  - ➢ *θ far from y ➔ bad prediction ➔ bad fit ➔ some loss*
- ➢ A hybrid of the L2 and L1 losses…



The Huber loss function, interactively



Comparing the Loss Functions

- ➢ All functions are zero when θ = y
- ➢ Different penalties for being far from observations
- ➢ Smooth vs. not smooth
- ➢ Which is the best?
  - ➢ Let's find out

Extend beyond single observation?

Average Loss

- A natural way to define the loss on our entire dataset is to compute the average of the loss on each record.

$$L\left(\theta, \mathcal{D}\right) = \frac{1}{n}\sum_{i=1}^{n} L(\theta, y_i)$$

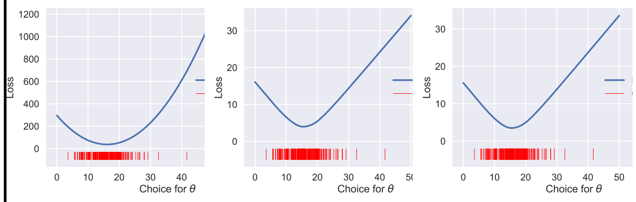
The set of n data points

- In some cases we might take a weighted average (when?)
  - Some records might be more important or reliable
- What does the average loss look like?

Double Jeopardy

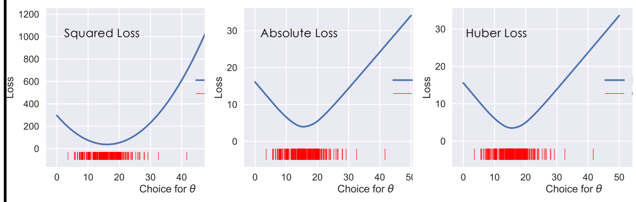
Name that Loss!

Name that loss



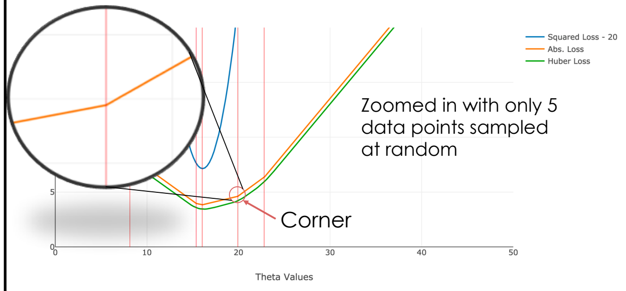
(a) (b) (c)

Name that loss



(a) (b) (c)

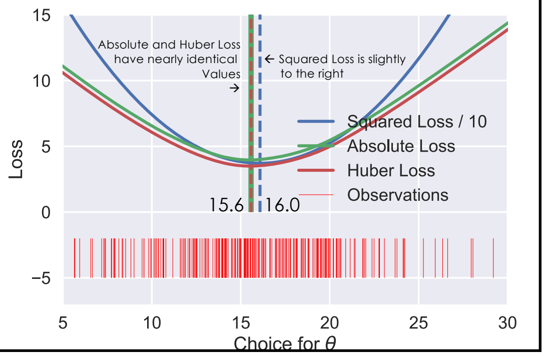
Difference between Huber and L1



Zoomed in with only 5 data points sampled at random

Corner

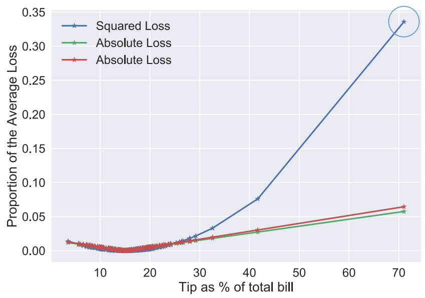
Different Minimizers



Absolute and Huber Loss have nearly identical Values →

← Squared Loss is slightly to the right

Sensitivity to Outliers



34% of loss due to a **single point**

Small fraction of loss on outliers…

Recap on Loss Functions

- **Loss functions:** *a mechanism to measure how well a particular instance of a model fits a given dataset*
- **Squared Loss:** *sensitive to outliers but a smooth function*
- **Absolute Loss:** *less sensitive to outliers but not smooth*
- **Huber Loss:** less sensitive to outliers and smooth but has an extra parameter to deal with
- Why is smoothness an issue → Optimization! …

Summary of Model Estimation (so far…)

1. **Define the Model:** simplified representation of the world
   - Use domain knowledge but … ***keep it simple!***
   - Introduce **parameters** for the unknown quantities
2. **Define the Loss Function:** measures how well a particular instance of the model "fits" the data
   - We introduced L^2, L^1, and Huber losses for each record
   - Take the average loss over the entire dataset
3. **Minimize the Loss Function:** find the parameter values that minimize the loss on the data
   - So far we have done this graphically
   - Now we will **minimize the loss analytically**

Step 3: Minimize the Loss

A Brief Review of Calculus

Minimizing a Function

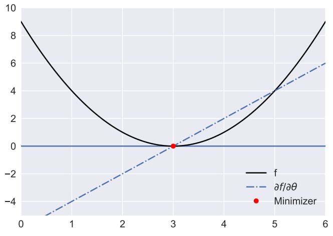
- Suppose we want to minimize:

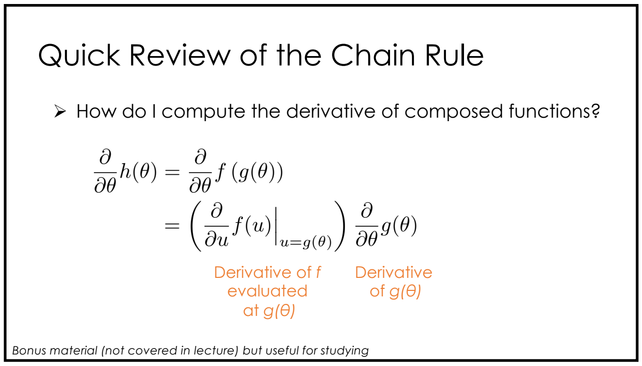
$$f(\theta) = (\theta - 3)^2$$

- Solve for derivative = 0:

$$\frac{\partial}{\partial \theta} f(\theta) = 2(\theta - 3) = 0$$

- Procedure:
  1. take derivative
  2. Set equal to zero
  3. Solve for parameters





Quick Review of the Chain Rule

- How do I compute the derivative of composed functions?

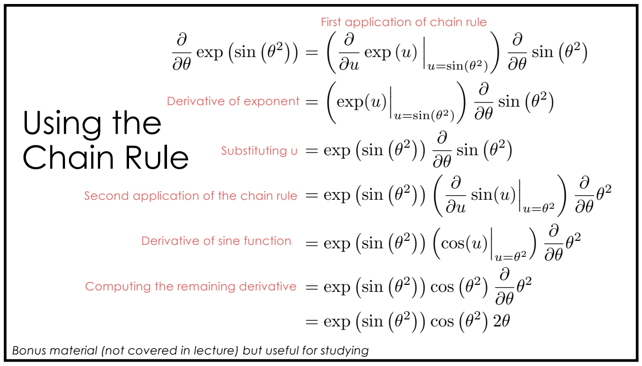
$$\frac{\partial}{\partial\theta}h(\theta) = \frac{\partial}{\partial\theta}f\left(g(\theta)\right)$$

$$= \left(\frac{\partial}{\partial u}f(u)\Big|_{u=g(\theta)}\right)\frac{\partial}{\partial\theta}g(\theta)$$

Derivative of *f* evaluated at *g(θ)*

Derivative of *g(θ)*

Bonus material (not covered in lecture) but useful for studying



Using the Chain Rule

First application of chain rule

$$\frac{\partial}{\partial\theta}\exp\left(\sin\left(\theta^2\right)\right) = \left(\frac{\partial}{\partial u}\exp\left(u\right)\Big|_{u=\sin(\theta^2)}\right)\frac{\partial}{\partial\theta}\sin\left(\theta^2\right)$$

Derivative of exponent $= \left(\exp(u)\Big|_{u=\sin(\theta^2)}\right)\frac{\partial}{\partial\theta}\sin\left(\theta^2\right)$

Substituting u $= \exp\left(\sin\left(\theta^2\right)\right)\frac{\partial}{\partial\theta}\sin\left(\theta^2\right)$

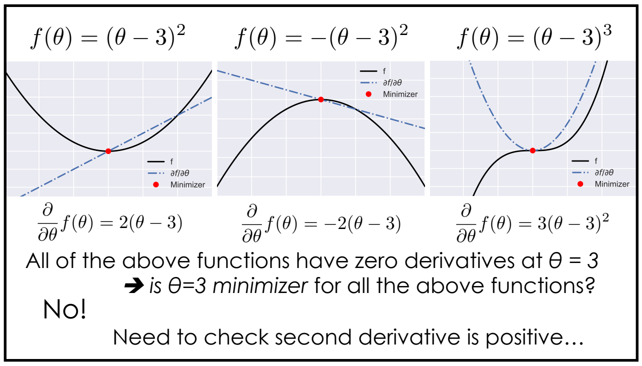
Second application of the chain rule $= \exp\left(\sin\left(\theta^2\right)\right)\left(\frac{\partial}{\partial u}\sin(u)\Big|_{u=\theta^2}\right)\frac{\partial}{\partial\theta}\theta^2$

Derivative of sine function $= \exp\left(\sin\left(\theta^2\right)\right)\left(\cos(u)\Big|_{u=\theta^2}\right)\frac{\partial}{\partial\theta}\theta^2$

Computing the remaining derivative $= \exp\left(\sin\left(\theta^2\right)\right)\cos\left(\theta^2\right)\frac{\partial}{\partial\theta}\theta^2$

$$= \exp\left(\sin\left(\theta^2\right)\right)\cos\left(\theta^2\right)2\theta$$

Bonus material (not covered in lecture) but useful for studying



$f(\theta) = (\theta-3)^2$ $\quad$ $f(\theta) = -(\theta-3)^2$ $\quad$ $f(\theta) = (\theta-3)^3$

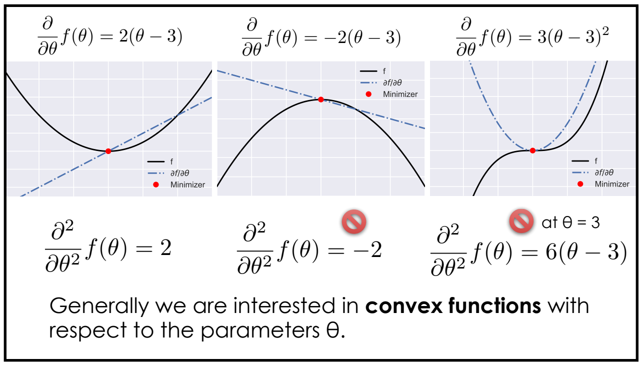
$\frac{\partial}{\partial\theta}f(\theta) = 2(\theta-3)$ $\quad$ $\frac{\partial}{\partial\theta}f(\theta) = -2(\theta-3)$ $\quad$ $\frac{\partial}{\partial\theta}f(\theta) = 3(\theta-3)^2$

All of the above functions have zero derivatives at *θ = 3*

➔ *is θ=3 minimizer* for all the above functions?

No!

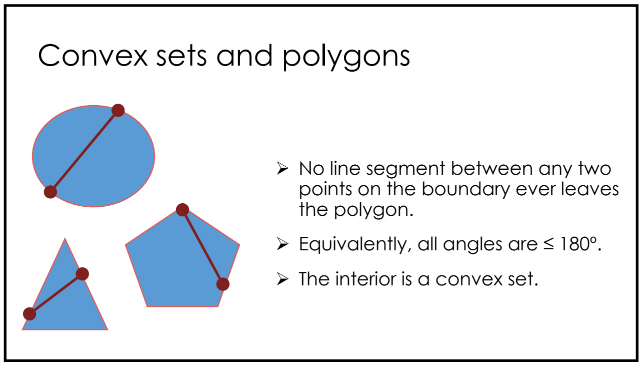
Need to check second derivative is positive…



$\frac{\partial}{\partial\theta}f(\theta) = 2(\theta-3)$ $\quad$ $\frac{\partial}{\partial\theta}f(\theta) = -2(\theta-3)$ $\quad$ $\frac{\partial}{\partial\theta}f(\theta) = 3(\theta-3)^2$

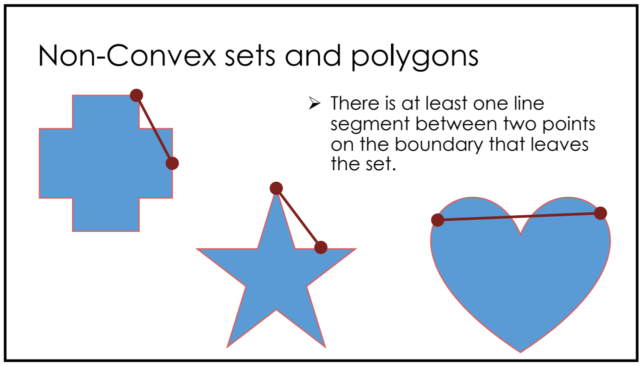
$\frac{\partial^2}{\partial\theta^2}f(\theta) = 2$ $\quad$ 🚫 $\frac{\partial^2}{\partial\theta^2}f(\theta) = -2$ $\quad$ 🚫 at θ = 3 $\frac{\partial^2}{\partial\theta^2}f(\theta) = 6(\theta-3)$

Generally we are interested in **convex functions** with respect to the parameters θ.



Convex sets and polygons

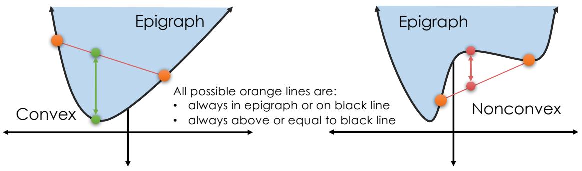
- No line segment between any two points on the boundary ever leaves the polygon.
- Equivalently, all angles are ≤ 180°.
- The interior is a convex set.



Non-Convex sets and polygons

- There is at least one line segment between two points on the boundary that leaves the set.

Formal Definition of Convex Functions

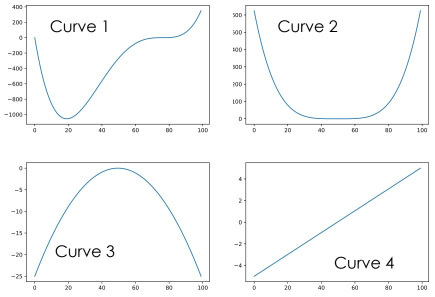


All possible orange lines are:
- always in epigraph or on black line
- always above or equal to black line

➢ A function f is convex if and only if:

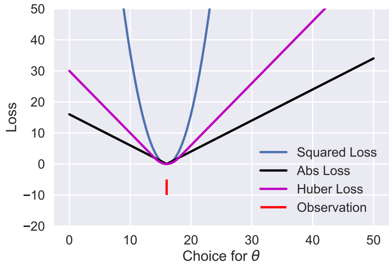
$$tf(a) + (1-t)f(b) \geq f\left(ta + (1-t)b\right)$$
$$\forall a, \; \forall b, \; t \in [0,1]$$

http://bit.ly/ds100-sp18-cvx



Convex or Not Convex

Are our previous loss functions convex?

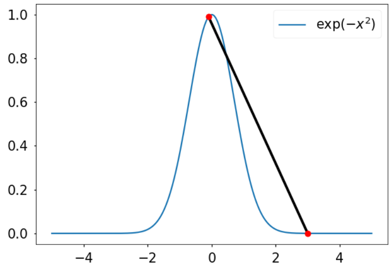


Yes!

Average Loss? Yes!

(Sum of convex functions is convex)

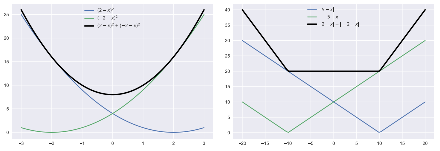
Is a Gaussian convex?



Sum of Convex Functions is Convex

➢ In class professor Gonzalez was asked: *"Are you sure that the sum of convex functions is convex?"*
  - ➢ The answer is yes! Always!
    - ➢ Professor Gonzalez should have had a proof ready! ☹ It's Easy!

➢ Proposed counter examples … (not entirely obvious)



Bonus material (not covered in lecture) but useful for studying

Formal Proof

➢ Suppose you have two convex functions f and g:

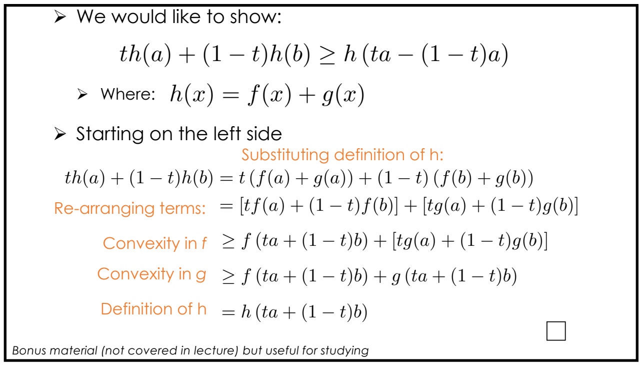
$$tf(a) + (1-t)f(b) \geq f\left(ta - (1-t)a\right)$$
$$tg(a) + (1-t)g(b) \geq g\left(ta - (1-t)a\right)$$
$$\forall a, \; \forall b, \; t \in [0,1]$$

➢ We would like to show:

$$th(a) + (1-t)h(b) \geq h\left(ta - (1-t)a\right)$$

➢ Where: $h(x) = f(x) + g(x)$

Bonus material (not covered in lecture) but useful for studying



- We would like to show:

$$th(a) + (1-t)h(b) \geq h\left(ta - (1-t)a\right)$$

  - Where: $h(x) = f(x) + g(x)$

- Starting on the left side

Substituting definition of h:

$$th(a) + (1-t)h(b) = t\left(f(a) + g(a)\right) + (1-t)\left(f(b) + g(b)\right)$$

Re-arranging terms: $= [tf(a) + (1-t)f(b)] + [tg(a) + (1-t)g(b)]$

Convexity in f $\geq f\left(ta + (1-t)b\right) + [tg(a) + (1-t)g(b)]$

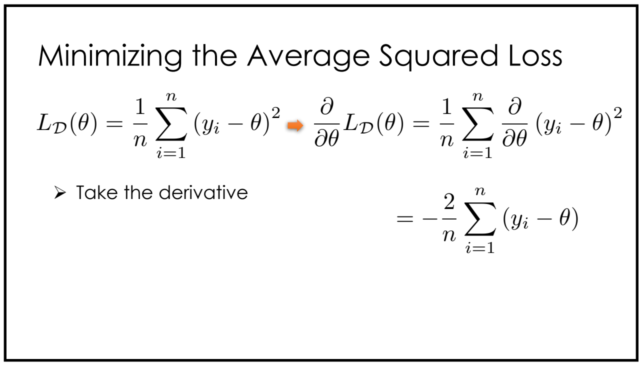
Convexity in g $\geq f\left(ta + (1-t)b\right) + g\left(ta + (1-t)b\right)$

Definition of h $= h\left(ta + (1-t)b\right)$

□

Bonus material (not covered in lecture) but useful for studying

Minimizing the Average Squared Loss

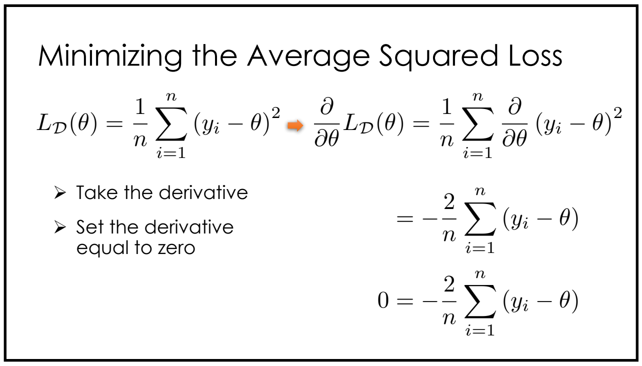


Minimizing the Average Squared Loss

$$L_{\mathcal{D}}(\theta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \theta)^2 \Rightarrow \frac{\partial}{\partial\theta}L_{\mathcal{D}}(\theta) = \frac{1}{n}\sum_{i=1}^{n}\frac{\partial}{\partial\theta}(y_i - \theta)^2$$

- Take the derivative

$$= -\frac{2}{n}\sum_{i=1}^{n}(y_i - \theta)$$



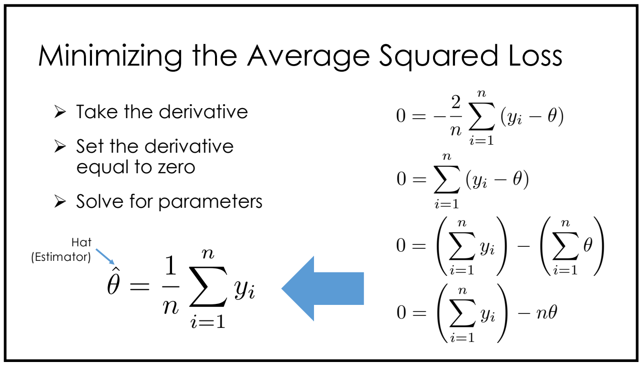
Minimizing the Average Squared Loss

$$L_{\mathcal{D}}(\theta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \theta)^2 \Rightarrow \frac{\partial}{\partial\theta}L_{\mathcal{D}}(\theta) = \frac{1}{n}\sum_{i=1}^{n}\frac{\partial}{\partial\theta}(y_i - \theta)^2$$

- Take the derivative
- Set the derivative equal to zero

$$= -\frac{2}{n}\sum_{i=1}^{n}(y_i - \theta)$$

$$0 = -\frac{2}{n}\sum_{i=1}^{n}(y_i - \theta)$$



Minimizing the Average Squared Loss

- Take the derivative
- Set the derivative equal to zero
- Solve for parameters

$$0 = -\frac{2}{n}\sum_{i=1}^{n}(y_i - \theta)$$

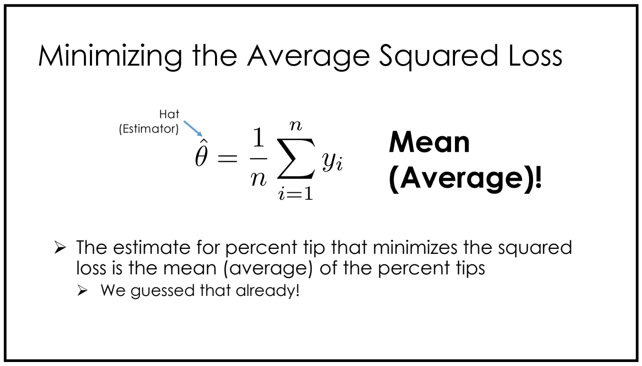
$$0 = \sum_{i=1}^{n}(y_i - \theta)$$

$$0 = \left(\sum_{i=1}^{n} y_i\right) - \left(\sum_{i=1}^{n}\theta\right)$$

$$0 = \left(\sum_{i=1}^{n} y_i\right) - n\theta$$

Hat (Estimator)

$$\hat{\theta} = \frac{1}{n}\sum_{i=1}^{n} y_i \quad ⬅$$



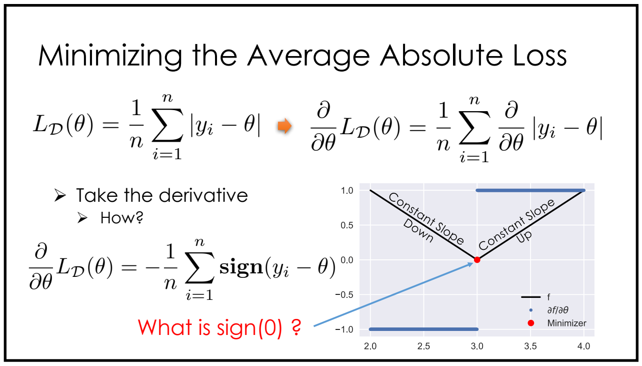
Minimizing the Average Squared Loss

Hat (Estimator)

$$\hat{\theta} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

Mean (Average)!

- The estimate for percent tip that minimizes the squared loss is the mean (average) of the percent tips
  - We guessed that already!



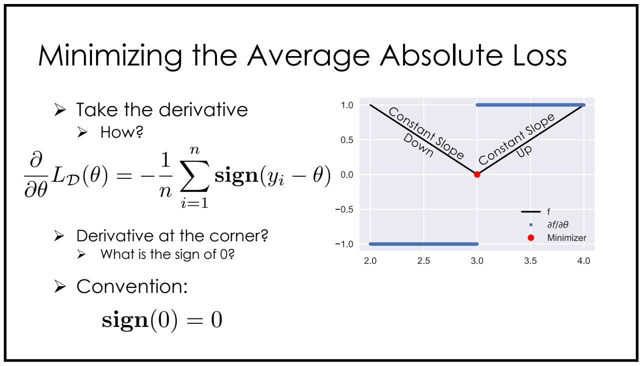
Minimizing the Average Absolute Loss

$$L_{\mathcal{D}}(\theta) = \frac{1}{n}\sum_{i=1}^{n} |y_i-\theta| \quad ➡ \quad \frac{\partial}{\partial\theta}L_{\mathcal{D}}(\theta) = \frac{1}{n}\sum_{i=1}^{n} \frac{\partial}{\partial\theta}|y_i-\theta|$$

- Take the derivative
  - How?

$$\frac{\partial}{\partial\theta}L_{\mathcal{D}}(\theta) = -\frac{1}{n}\sum_{i=1}^{n} \mathbf{sign}(y_i-\theta)$$

What is sign(0) ?



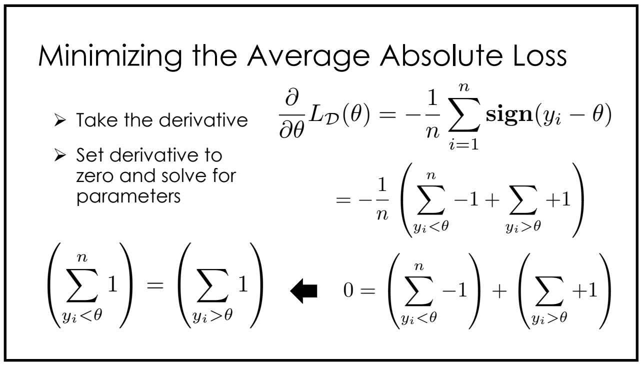
Minimizing the Average Absolute Loss

- Take the derivative
  - How?

$$\frac{\partial}{\partial\theta}L_{\mathcal{D}}(\theta) = -\frac{1}{n}\sum_{i=1}^{n} \mathbf{sign}(y_i-\theta)$$

- Derivative at the corner?
  - What is the sign of 0?
- Convention:

$$\mathbf{sign}(0) = 0$$



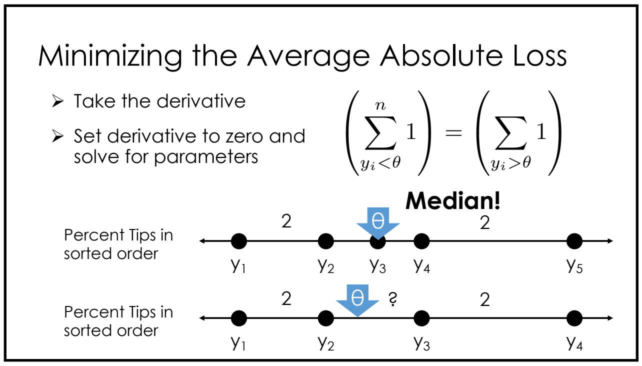
Minimizing the Average Absolute Loss

- Take the derivative
- Set derivative to zero and solve for parameters

$$\frac{\partial}{\partial\theta}L_{\mathcal{D}}(\theta) = -\frac{1}{n}\sum_{i=1}^{n} \mathbf{sign}(y_i-\theta)$$

$$= -\frac{1}{n}\left(\sum_{y_i<\theta}^{n} -1 + \sum_{y_i>\theta} +1\right)$$

$$\left(\sum_{y_i<\theta}^{n} 1\right) = \left(\sum_{y_i>\theta} 1\right) \quad ⬅ \quad 0 = \left(\sum_{y_i<\theta}^{n} -1\right) + \left(\sum_{y_i>\theta} +1\right)$$



Minimizing the Average Absolute Loss

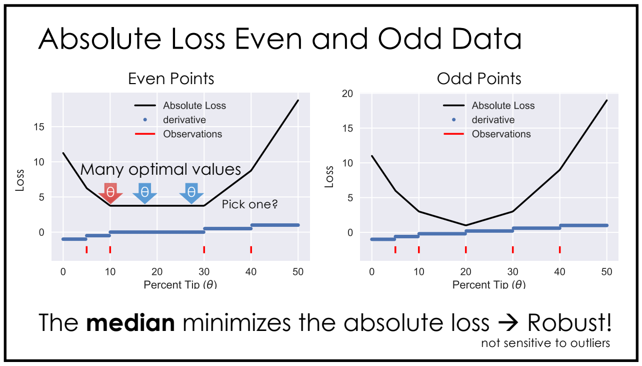
- Take the derivative
- Set derivative to zero and solve for parameters

$$\left(\sum_{y_i<\theta}^{n} 1\right) = \left(\sum_{y_i>\theta} 1\right)$$

Median!

Percent Tips in sorted order

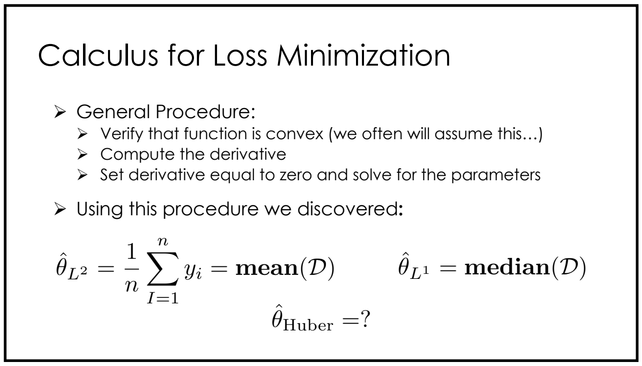
Percent Tips in sorted order



Absolute Loss Even and Odd Data

The **median** minimizes the absolute loss → Robust!

not sensitive to outliers



Calculus for Loss Minimization

- General Procedure:
  - Verify that function is convex (we often will assume this…)
  - Compute the derivative
  - Set derivative equal to zero and solve for the parameters
- Using this procedure we discovered:

$$\hat{\theta}_{L^2} = \frac{1}{n}\sum_{I=1}^{n} y_i = \mathbf{mean}(\mathcal{D}) \qquad \hat{\theta}_{L^1} = \mathbf{median}(\mathcal{D})$$

$$\hat{\theta}_{\text{Huber}} = ?$$

Minimizing the Average Huber Loss

$$L_\alpha(\theta, y) = \begin{cases} \frac{1}{2}(y-\theta)^2 & |y-\theta| < \alpha \\ \alpha\left(|y-\theta| - \frac{\alpha}{2}\right) & \text{otherwise}\end{cases}$$

- Take the derivative of the average Huber Loss

$$\frac{\partial}{\partial\theta} L_\mathcal{D}(\theta) = \frac{1}{n}\sum_{i=1}^{n} \begin{cases} -(y_i-\theta) & |y_i-\theta|<\alpha \\ -\alpha\,\mathbf{sign}(y_i-\theta) & \text{otherwise}\end{cases}$$

Minimizing the Average Huber Loss

$$L_\alpha(\theta, y) = \begin{cases} \frac{1}{2}(y-\theta)^2 & |y-\theta| < \alpha \\ \alpha\left(|y-\theta| - \frac{\alpha}{2}\right) & \text{otherwise}\end{cases}$$

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Minimizing the Average Huber Loss

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$$\frac{\partial}{\partial\theta} L_\mathcal{D}(\theta) = \frac{1}{n}\sum_{i=1}^{n} \begin{cases} -(y_i-\theta) & |y_i-\theta|<\alpha \\ -\alpha\,\mathbf{sign}(y_i-\theta) & \text{otherwise}\end{cases}$$

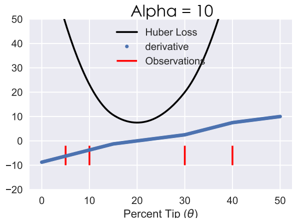
- Set derivative equal to zero:

$$\left(\sum_{\theta\ge y_i+\alpha}\alpha\right) - \left(\sum_{\theta\le y_i-\alpha}\alpha\right) - \left(\sum_{|y_i-\theta|<\alpha}(y_i-\theta)\right) = 0$$

- Solution?
- No simple analytic solution …
  - We can still plot the derivative

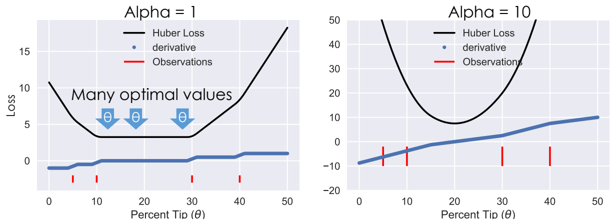
Visualizing the Derivative of the Huber Loss

$$L_\alpha(\theta, y) = \begin{cases} \frac{1}{2}(y-\theta)^2 & |y-\theta| < \alpha \\ \alpha\left(|y-\theta| - \frac{\alpha}{2}\right) & \text{otherwise}\end{cases}$$



- Large ***α*** ➔ unique optimum like squared loss

Visualizing the Derivative of the Huber Loss



- Derivative is continuous
- Small $\boldsymbol{\alpha}$ ➔many optima

- Large $\boldsymbol{\alpha}$ ➔ unique optimum like squared loss

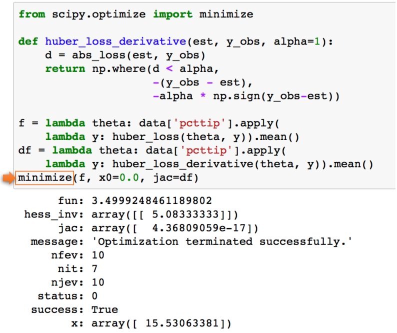
Numerical Optimization

Minimizing the Huber Loss **Numerically**

Often we will use numerical optimization methods

The following are **helpful properties** when using numerical optimization methods:

- **convex** loss function
- **smooth** loss function
- analytic **derivative**



```
from scipy.optimize import minimize

def huber_loss_derivative(est, y_obs, alpha=1):
    d = abs_loss(est, y_obs)
    return np.where(d < alpha,
                    -(y_obs - est),
                    -alpha * np.sign(y_obs-est))

f = lambda theta: data['pcttip'].apply(
    lambda y: huber_loss(theta, y)).mean()
df = lambda theta: data['pcttip'].apply(
    lambda y: huber_loss_derivative(theta, y)).mean()
minimize(f, x0=0.0, jac=df)
```

```
      fun: 3.4999248461189802
 hess_inv: array([[ 5.08333333]])
      jac: array([  4.36809059e-17])
  message: 'Optimization terminated successfully.'
     nfev: 10
      nit: 7
     njev: 10
   status: 0
  success: True
        x: array([ 15.53063381])
```

Summary of Model Estimation

1. **Define the Model:** simplified representation of the world
   - Use domain knowledge but … ***keep it simple!***
   - Introduce **parameters** for the unknown quantities
2. **Define the Loss Function:** measures how well a particular instance of the model "fits" the data
   - We introduced L^2, L^1, and Huber losses for each record
   - Take the average loss over the entire dataset
3. **Minimize the Loss Function:** find the parameter values that minimize the loss on the data
   - We did this graphically
   - Minimize the loss analytically using calculus
   - Minimize the loss numerically

Improving the Model

Going beyond the simple model

$$\text{percentage tip} = \theta^*$$

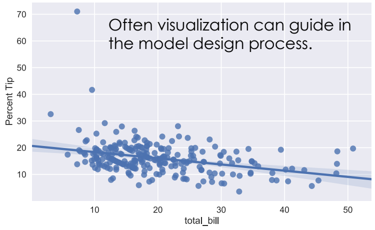
- How could we improve upon this model?
- Things to consider when improving the model
  - **Related factors** to the quantity of interest
    - Examples: quality of service, table size, time of day, total bill
    - Do we have data for these factors?
  - The **form of the relationship** to the quantity of interest
    - Linear relationships, step functions, etc …
  - Goals for improving the model
    - Improve **prediction accuracy** → more complex models
    - Provide **understanding** → simpler models
  - Is my model "identifiable" (is it possible to estimate the parameters?)
    - *percent tip* = $\theta_1^* + \theta_2^*$ ← many identical parameterizations

$$\texttt{percentage tip} = \theta_1^* + \theta_2^* * \texttt{total bill}$$

Rationale:
Larger bills result in larger tips and people tend to to be more careful or stingy on big tips.

Parameter Interpretation:

- θ$_1$: Base tip percentage
- θ$_2$: Reduction/increase in tip for an increase in total bill.



Often visualization can guide in the model design process.

Estimating the model parameters:

$$\texttt{percentage tip} = \theta_1^* + \theta_2^* * \texttt{total bill}$$

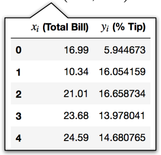
- Write the loss (e.g., average squared loss)

$$L_{\mathcal{D}}(\theta_1, \theta_2) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (\theta_1 + \theta_2 x_i)\right)^2$$

% Tip

Total Bill

n



	x_i **(Total Bill)**	y_i **(% Tip)**
0	16.99	5.944673
1	10.34	16.054159
2	21.01	16.658734
3	23.68	13.978041
4	24.59	14.680765

$$L_{\mathcal{D}}(\theta_1, \theta_2) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (\theta_1 + \theta_2 x_i)\right)^2$$

- Take the derivative(s):

$$\begin{aligned}\frac{\partial}{\partial \theta_1} L_{\mathcal{D}}(\theta_1, \theta_2) &= \frac{1}{n}\sum_{i=1}^{n}\frac{\partial}{\partial \theta_1}\left(y_i - (\theta_1 + \theta_2 x_i)\right)^2 \\ &= -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - (\theta_1 + \theta_2 x_i)\right)\end{aligned}$$

$$L_{\mathcal{D}}(\theta_1, \theta_2) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (\theta_1 + \theta_2 x_i)\right)^2$$

- Take the derivative(s):

$$\begin{aligned}\frac{\partial}{\partial \theta_1} L_{\mathcal{D}}(\theta_1, \theta_2) &= -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - (\theta_1 + \theta_2 x_i)\right) \\ \frac{\partial}{\partial \theta_2} L_{\mathcal{D}}(\theta_1, \theta_2) &= -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - (\theta_1 + \theta_2 x_i)\right)\frac{\partial}{\partial \theta_2}\theta_2 x_i \\ &= -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - (\theta_1 + \theta_2 x_i)\right) x_i\end{aligned}$$

$$L_{\mathcal{D}}(\theta_1, \theta_2) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - (\theta_1 + \theta_2 x_i)\right)^2$$

- Take the derivative(s):

$$\begin{aligned}\frac{\partial}{\partial \theta_1} L_{\mathcal{D}}(\theta_1, \theta_2) &= -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - (\theta_1 + \theta_2 x_i)\right) \\ \frac{\partial}{\partial \theta_2} L_{\mathcal{D}}(\theta_1, \theta_2) &= -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - (\theta_1 + \theta_2 x_i)\right) x_i\end{aligned}$$

- Set derivatives equal to zero and solve for parameters

Solving for θ$_1$

Breaking apart the sum

$$\begin{aligned}0 &= -\frac{2}{n}\sum_{i=1}^{n}\left(y_i - (\theta_1 + \theta_2 x_i)\right) \\ &= -\frac{2}{n}\left(\left(\sum_{i=1}^{n} y_i\right) - n\theta_1 - \theta_2\sum_{i=1}^{n} x_i\right)\end{aligned}$$

Rearranging Terms

$$\sum_{i=1}^{n} y_i = n\theta_1 + \theta_2\sum_{i=1}^{n} x_i$$

Solving for θ$_1$

$$\sum_{i=1}^{n} y_i = n\theta_1 + \theta_2 \sum_{i=1}^{n} x_i \xrightarrow{\text{Divide by n}} \frac{1}{n}\sum_{i=1}^{n} y_i = \theta_1 + \theta_2 \frac{1}{n}\sum_{i=1}^{n} x_i$$

- Define the average of x and y:

$$\bar{x} := \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\bar{y} := \frac{1}{n}\sum_{i=1}^{n} y_i$$

$$\bar{y} = \theta_1 + \theta_2 \bar{x}$$

$$\theta_1 = \bar{y} - \theta_2 \bar{x}$$

Solving for θ$_2$

Scratch $\boxed{\theta_1 = \bar{y} - \theta_2 \bar{x}}$

$$\frac{\partial}{\partial \theta_2} L_{\mathcal{D}}(\theta_1, \theta_2) = -\frac{2}{n}\sum_{i=1}^{n} \left(y_i - (\theta_1 + \theta_2 x_i)\right) x_i$$

Distributing the x$_i$ term

Breaking apart the sum

$$= -\frac{2}{n}\sum_{i=1}^{n} \left(y_i x_i - \theta_1 x_i - \theta_2 x_i^2\right)$$

$$= -\frac{2}{n}\left(\left(\sum_{i=1}^{n} y_i x_i\right) - \left(\theta_1 \sum_{i=1}^{n} x_i\right) - \theta_2 \sum_{i=1}^{n} x_i^2\right)$$

Solving for θ$_2$

Scratch $\boxed{\theta_1 = \bar{y} - \theta_2 \bar{x}}$

$$0 = -\frac{2}{n}\left(\left(\sum_{i=1}^{n} y_i x_i\right) - \left(\theta_1 \sum_{i=1}^{n} x_i\right) - \theta_2 \sum_{i=1}^{n} x_i^2\right)$$

Rearranging Terms

$$\sum_{i=1}^{n} y_i x_i = \theta_1 \sum_{i=1}^{n} x_i + \theta_2 \sum_{i=1}^{n} x_i^2$$

Divide by n

$$\frac{1}{n}\sum_{i=1}^{n} y_i x_i = \theta_1 \frac{1}{n}\sum_{i=1}^{n} x_i + \theta_2 \frac{1}{n}\sum_{i=1}^{n} x_i^2$$

Solving for θ$_2$

Scratch $\boxed{\theta_1 = \bar{y} - \theta_2 \bar{x}}$

$$\frac{1}{n}\sum_{i=1}^{n} y_i x_i = \theta_1 \frac{1}{n}\sum_{i=1}^{n} x_i + \theta_2 \frac{1}{n}\sum_{i=1}^{n} x_i^2$$

$$\bar{x} := \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\overline{xy} := \frac{1}{n}\sum_{i=1}^{n} x_i y_i$$

$$\overline{x^2} := \frac{1}{n}\sum_{i=1}^{n} x_i^2$$

$$\overline{xy} = \theta_1 \bar{x} + \theta_2 \overline{x^2}$$

System of Linear Equations

$$\theta_1 = \bar{y} - \theta_2 \bar{x}$$

$$\overline{xy} = \theta_1 \bar{x} + \theta_2 \overline{x^2}$$

- Substituting θ$_1$ and solving for θ$_2$

$$\overline{xy} = (\bar{y} - \theta_2 \bar{x})\,\bar{x} + \theta_2 \overline{x^2}$$

$$= \bar{y}\bar{x} - \theta_2 \bar{x}^2 + \theta_2 \overline{x^2}$$

$$= \bar{y}\bar{x} + \theta_2 \left(\overline{x^2} - \bar{x}^2\right)$$

solving for θ$_2$

$$\theta_2 = \frac{\overline{xy} - \bar{y}\bar{x}}{\overline{x^2} - \bar{x}^2} = \frac{\frac{1}{n}\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\frac{1}{n}\sum_{I=1}^{n} (x_i - \bar{x})^2}$$

Algebra…

Denominator Derivation

Skipped in Class

- Completing the squares:

$$\sum_{i=1}^{n} (x_i^2 - \bar{x}x_i) = \sum_{i=1}^{n} (x_i^2 - \bar{x}x_i + \bar{x}^2 - \bar{x}x_i - \bar{x}^2 + \bar{x}x_i)$$

$$= \sum_{i=1}^{n} (x_i^2 - 2\bar{x}x_i + \bar{x}^2 - \bar{x}^2 + \bar{x}x_i)$$

$$= \sum_{i=1}^{n} \left((x_i - \bar{x})^2 - \bar{x}^2 + \bar{x}x_i\right)$$

$$= \sum_{i=1}^{n} (x_i - \bar{x})^2 - n\bar{x}^2 + \bar{x}\sum_{i=1}^{n} x_i$$

$$= \sum_{i=1}^{n} (x_i - \bar{x})^2 - n\bar{x}^2 + \bar{x}n\bar{x}$$

$$= \sum_{i=1}^{n} (x_i - \bar{x})^2$$

- Completing the squares:

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

Numerator Derivation

Skipped in Class

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

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

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

$$= \sum_{i=1}^{n}(y_i - \bar{y})(x_i - \bar{x})$$

Summary so far …

- **Step 1:** Define the model with unknown parameters

$$\texttt{percentage tip} = \theta_1^* + \theta_2^* * \texttt{total bill}$$

- **Step 2:** Write the loss (we selected an average squared loss)

$$L_{\mathcal{D}}(\theta_1, \theta_2) = \frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_1 + \theta_2 x_i))^2$$

- **Step3:** Minimize the loss
  - Analytically (using calculus)
  - Numerically (using optimization algorithms)

$$L_{\mathcal{D}}(\theta_1, \theta_2) = \frac{1}{n}\sum_{i=1}^{n}(y_i - (\theta_1 + \theta_2 x_i))^2$$

- **Step3:** Minimize the loss
  - Analytically (using calculus)
  - Numerically (using optimization algorithms)

$$\frac{\partial}{\partial \theta_1} L_{\mathcal{D}}(\theta_1, \theta_2) = -\frac{2}{n}\sum_{i=1}^{n}(y_i - (\theta_1 + \theta_2 x_i))$$

$$\frac{\partial}{\partial \theta_2} L_{\mathcal{D}}(\theta_1, \theta_2) = -\frac{2}{n}\sum_{i=1}^{n}(y_i - (\theta_1 + \theta_2 x_i))\, x_i$$

- Set derivatives equal to zero and solve for parameter values

$$\theta_1 = \bar{y} - \theta_2\bar{x}$$

$$\theta_2 = \frac{\overline{xy} - \bar{y}\bar{x}}{\overline{x^2} - \bar{x}^2} = \frac{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\frac{1}{n}\sum_{I=1}^{n}(x_i - \bar{x})^2}$$

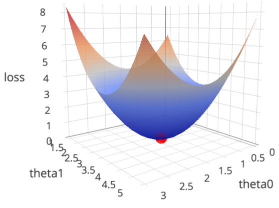
- Is this a local minimum?

$$\frac{\partial^2}{\partial \theta_1^2} L_{\mathcal{D}}(\theta_1, \theta_2) = -\frac{2}{n}\sum_{i=1}^{n}\frac{\partial}{\partial \theta_1}(y_i - (\theta_1 + \theta_2 x_i)) = -\frac{2}{n}\sum_{i=1}^{n} -1 = 2$$

$$\frac{\partial^2}{\partial \theta_2^2} L_{\mathcal{D}}(\theta_1, \theta_2) = -\frac{2}{n}\sum_{i=1}^{n}\frac{\partial}{\partial \theta_2}(y_i - (\theta_1 + \theta_2 x_i)) = \frac{2}{n}\sum_{i=1}^{n} x_i^2 \; > 0$$

Visualizing the **Higher Dimensional** Loss

- What does the loss look like?
- Go to notebook …



“Improving” the Model (more…)

$$\texttt{percentage tip} = \theta_1^* + \theta_2^* * \texttt{is Male} + \theta_3^* * \texttt{is Smoker} + \theta_4^* * \texttt{table size}$$

Rational:
Each term encodes a potential factor that could affect the percentage tip.

***Possible* Parameter Interpretation:**

- θ_1: base tip percentage paid by female non-smokers without accounting for table size.
- θ_2: tip change associated with male patrons ...

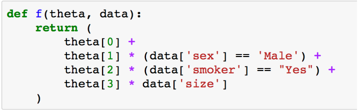
Maybe difficult to estimate … what if all smokers are male?

Difficult
to
Plot

Go to Notebook

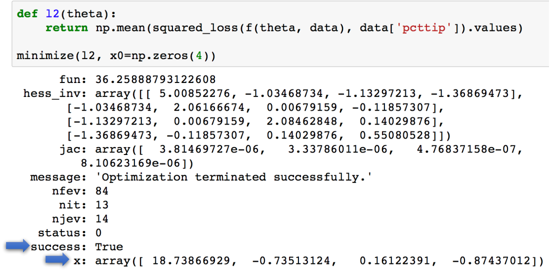
Define the model

- Use python to define the function



```
def f(theta, data):
    return (
        theta[0] +
        theta[1] * (data['sex'] == 'Male') +
        theta[2] * (data['smoker'] == "Yes") +
        theta[3] * data['size']
    )
```

Define and Minimize the Loss

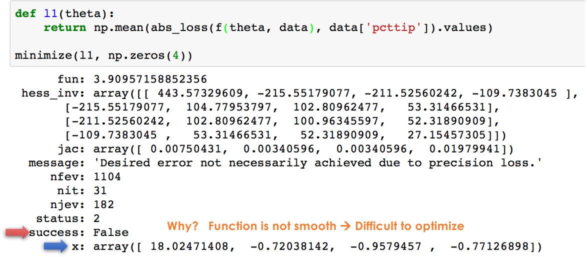


```
def l2(theta):
    return np.mean(squared_loss(f(theta, data), data['pcttip']).values)

minimize(l2, x0=np.zeros(4))
```

```
      fun: 36.25888793122608
 hess_inv: array([[ 5.00852276, -1.03468734, -1.13297213, -1.36869473],
       [-1.03468734,  2.06166674,  0.00679159, -0.11857307],
       [-1.13297213,  0.00679159,  2.08462848,  0.14029876],
       [-1.36869473, -0.11857307,  0.14029876,  0.55080528]])
      jac: array([  3.81469727e-06,   3.33786011e-06,   4.76837158e-07,
         8.10623169e-06])
  message: 'Optimization terminated successfully.'
     nfev: 84
      nit: 13
     njev: 14
   status: 0
  success: True
        x: array([ 18.73866929,  -0.73513124,   0.16122391,  -0.87437012])
```

Define and Minimize the Loss



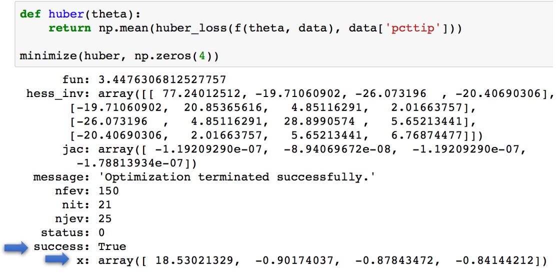
```
def l1(theta):
    return np.mean(abs_loss(f(theta, data), data['pcttip']).values)

minimize(l1, np.zeros(4))
```

```
      fun: 3.90957158852356
 hess_inv: array([[ 443.57329609, -215.55179077, -211.52560242, -109.7383045 ],
       [-215.55179077,  104.77953797,  102.80962477,   53.31466531],
       [-211.52560242,  102.80962477,  100.96345597,   52.31890909],
       [-109.7383045 ,   53.31466531,   52.31890909,   27.15457305]])
      jac: array([ 0.00750431,  0.00340596,  0.00340596,  0.01979941])
  message: 'Desired error not necessarily achieved due to precision loss.'
     nfev: 1104
      nit: 31
     njev: 182
   status: 2
  success: False
        x: array([ 18.02471408,  -0.72038142,  -0.9579457 ,  -0.77126898])
```

Why? Function is not smooth → Difficult to optimize

Define and Minimize the Loss



```
def huber(theta):
    return np.mean(huber_loss(f(theta, data), data['pcttip']))

minimize(huber, np.zeros(4))
```

```
      fun: 3.4476306812527757
 hess_inv: array([[ 77.24012512, -19.71060902, -26.073196  , -20.40690306],
       [-19.71060902,  20.85365616,   4.85116291,   2.01663757],
       [-26.073196  ,   4.85116291,  28.8990574 ,   5.65213441],
       [-20.40690306,   2.01663757,   5.65213441,   6.76874477]])
      jac: array([ -1.19209290e-07,  -8.94069672e-08,  -1.19209290e-07,
        -1.78813934e-07])
  message: 'Optimization terminated successfully.'
     nfev: 150
      nit: 21
     njev: 25
   status: 0
  success: True
        x: array([ 18.53021329,  -0.90174037,  -0.87843472,  -0.84144212])
```