Indian Institute of Information Technology, Allahabad

Introduction to Machine Learning

Maximum Likelihood Estimation

By

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Your first consulting job

- Client: I have special coin, if I flip it, what's the probability it will be ***heads***?

- You (a machine learner): I need to collect data.

H H

- You (a frequentist): The probability is:

100% heads!

Your first consulting job

- Client: Uhhhh…. You sure about that? I just got a tails.

- You (a machine learner): I need to collect **more data**.
  - *flips coin 5 times, get HHTHT

- You: The probability is: 60% Heads, 40% Tails!

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- Client: ***Why should I believe you?***

- You (a machine learner): Let's do some math!

Coin – Bernoulli Distribution

- **Data:** sequence *D= (HHTHT…)*, **k heads** out of **n flips**
- **Hypothesis:** P(Heads) = θ, P(Tails) = 1-θ
    - Flips are i.i.d.:
        - Independent events
        - Identically distributed according to Bernoulli distribution

$$P(\mathcal{D}|\theta) =$$

$= P(HHTHT \mid \theta)$

$= P(H)P(H)P(T)P(H)P(T)$ # by independence

$= \theta^k (1-\theta)^{n-k}$

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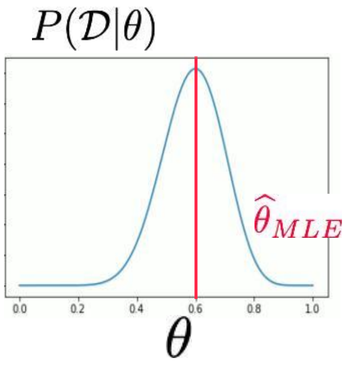
- **Likelihood:**

$$P(\mathcal{D}|\theta) = \theta^k (1-\theta)^{n-k}$$ # likelihood

- **Maximum likelihood estimation (MLE):** Choose θ that maximizes the probability of observed data:

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} \; P(\mathcal{D}|\theta)$$



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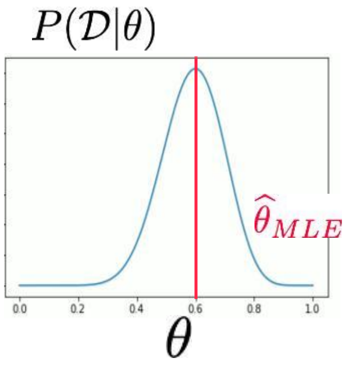
$$\begin{aligned}\widehat{\theta}_{MLE} &= \arg\max_{\theta} \; P(\mathcal{D}|\theta) \\ &= \arg\max_{\theta} \; \log P(\mathcal{D}|\theta)\end{aligned}$$



Why take the log?

- Easier to work with

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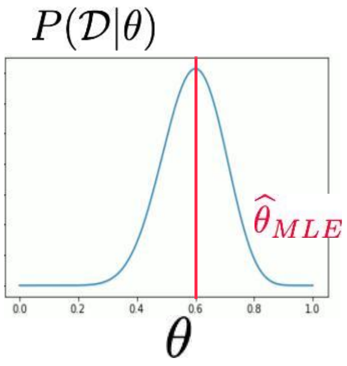
Why take the log?

- Easier to work with



MLE: Your first learning algorithm

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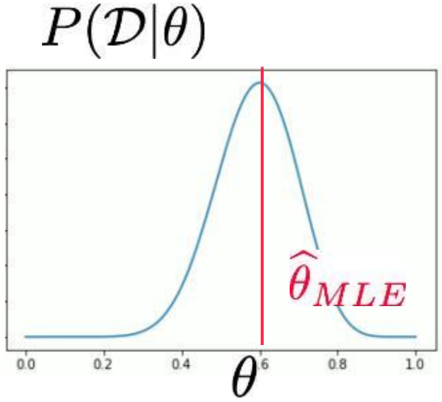

- How do we find θ that maximizes likelihood?

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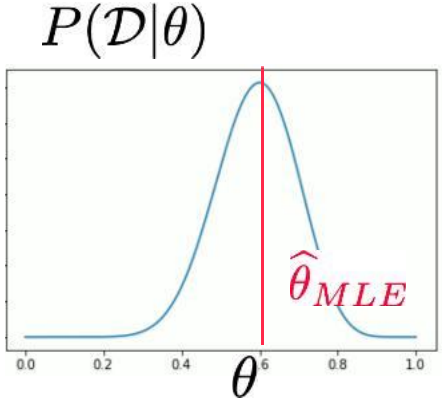

- How do we find θ that maximizes likelihood?
- Use the fact that derivative is zero at maxima (also at minima)
- Set derivative to zero, and find θ satisfying:

$$\boxed{\frac{d}{d\theta} \log P(\mathcal{D}|\theta) = 0}$$ # MLE

MLE: Your first learning algorithm

- First manipulate the log likelihood to make it easy to work with:

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} \ \log P(\mathcal{D}|\theta)$$

$$= \arg\max_{\theta} \ \log \theta^k (1-\theta)^{n-k}$$

$$= \arg\max_{\theta} \ k\log\theta + (n-k)\log(1-\theta)$$

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for your formula sheet

$$\frac{d}{dx}\log x = \frac{1}{x}$$

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$$\frac{d}{dx}\log x = \frac{1}{x}$$

$$k - k\theta = n\theta - k\theta$$

$$\boxed{\hat{\theta}_{\mathrm{MLE}} = \frac{k}{n}}$$

our example:

$$\hat{\theta}_{\mathrm{MLE}} = \frac{3}{5} = 60\%$$

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How good is MLE? Well, it's unbiased

- We treat MLE $\widehat{\theta}_{\mathrm{MLE}}$ is a random variable, where there is a ground truth parameter ϑ^* that generates the data

$\mathscr{D} = (HHTTH\ldots)$ of a fixed size n

$$\hat{\theta}_{\mathrm{MLE}} = \frac{k}{n}$$ # random variable

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- We treat MLE $\widehat{\theta}_{\mathrm{MLE}}$ as a random variable, where there is a ground truth parameter ϑ^* that generates the data
  $\mathscr{D} = (HHTTH\ldots)$ of a fixed size n

  $$\hat{\theta}_{\mathrm{MLE}} = \frac{k}{n}$$ # random variable

- What can we say about this random variable $\widehat{\theta}_{\mathrm{MLE}}$?
- First good property of MLE for Binomial: **unbiased**
  - Definition: **bias** of our MLE is

"true predictor"

$$\mathrm{Bias}(\widehat{\theta}_{\mathrm{MLE}}) := \mathbb{E}_{\mathscr{D}\sim P_{\theta^*}}[\hat{\theta}_{\mathrm{MLE}}] - \theta^* = E\left[\frac{k}{n}\right] - \theta^*$$

Unbiased means bias = 0

$$= \frac{\theta^* \cancel{n}}{\cancel{n}} - \theta^* = 0$$

- Expectation describes how the estimator behaves on average

How many flips do I need?

- Consider running many experiments with $\theta^* = \frac{3}{5}$, and observe many instances of the random variable

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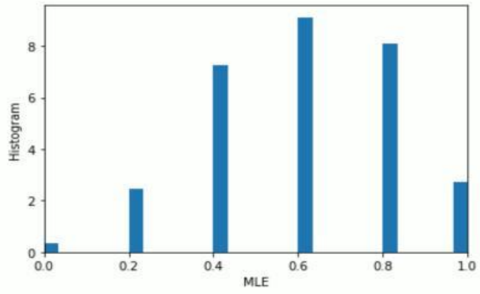

- Client: I flipped the coin 5 times and got 2 heads.

$$\widehat{\theta}_{MLE} =$$

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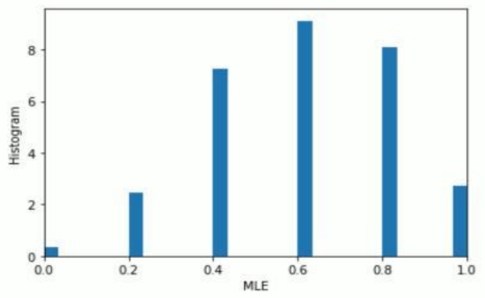

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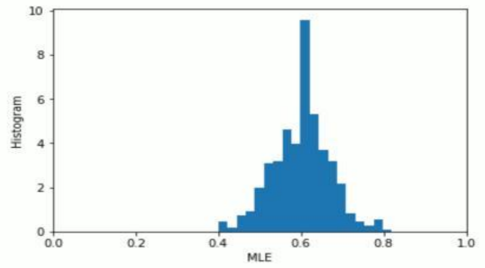

- Client: I flipped the coin 50 times and got 30 heads

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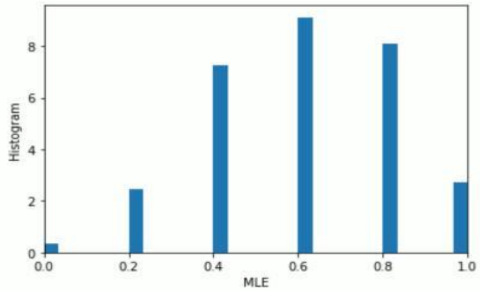

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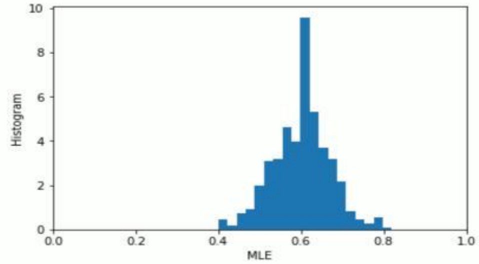


- Client: I flipped the coin 50 times and got 30 heads

$$\widehat{\theta}_{MLE} =$$

- Client: they are both unbiased, which one is right? Why?
- Variance goes down with larger *n*

$$\sqrt{\mathrm{Var}(\widehat{\theta}_{\mathrm{MLE}})} = \sqrt{\frac{\theta^*(1-\theta^*)}{n}}$$

Fundamental machine learning truth

- More data -> better performance
  - “The Bitter Lesson”
    - https://www.cs.utexas.edu/~eunsol/courses/data/bitter_lesson.pdf

Maximum Likelihood Estimation

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

Likelihood function $L_n(\theta) = \prod_{i=1}^{n} f(X_i;\theta)$

Log-Likelihood function $l_n(\theta) = \log(L_n(\theta)) = \sum_{i=1}^{n} \log(f(X_i;\theta))$

Maximum Likelihood Estimator (MLE) $\widehat{\theta}_{MLE} = \arg\max_{\theta} L_n(\theta)$

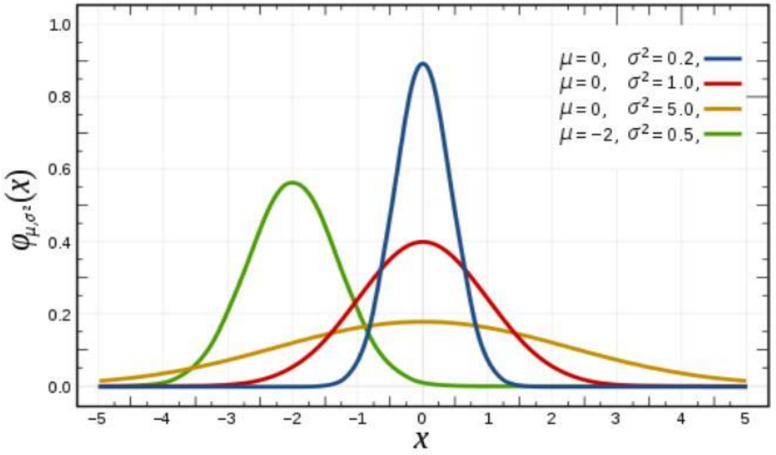
What about continuous variables?

- Client: What if I am measuring a continuous variable?
- You: Let me tell you about Gaussians…

$$P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

PDF of Gaussian

(good candidate for formula sheet)



Given a set of i.i.d. samples from a Gaussian, fit what parameters?

$\theta = [\mu, \sigma]$

Some properties of Gaussians

- Affine transformation (multiplying by scalar and adding a constant)
  - $X \sim N(\mu,\sigma^2)$
  - $Y = aX + b \quad \rightarrow \quad Y \sim N(a\mu+b, a^2\sigma^2)$

- Sum of Gaussians
  - $X \sim N(\mu_X,\sigma^2_X)$
  - $Y \sim N(\mu_Y,\sigma^2_Y)$
  - $Z = X+Y \quad \rightarrow \quad Z \sim N(\mu_X+\mu_Y, \sigma^2_X+\sigma^2_Y)$

MLE for Gaussian

- Prob. of i.i.d. samples D=$\{x_1,\ldots,x_n\}$:

$$P(\mathcal{D}|\mu,\sigma) = P(x_1,\ldots,x_n|\mu,\sigma)$$

MLE for Gaussian

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Likelihood: $$= \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^n \prod_{i=1}^{n} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

Wait, why can I just multiply all samples together?

→ By i.i.d. assumption

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- Log-likelihood of data:

LL: $$\log P(\mathcal{D}|\mu,\sigma) = -n\log(\sigma\sqrt{2\pi}) - \sum_{i=1}^{n}\frac{(x_i-\mu)^2}{2\sigma^2}$$

- What is $\widehat{\theta}_{MLE}$ for $\theta = (\mu,\sigma^2)$? Draw a picture!

MLE for Gaussian

Generate $\mathcal{D} = \{x_1, \ldots, x_n\}$, where

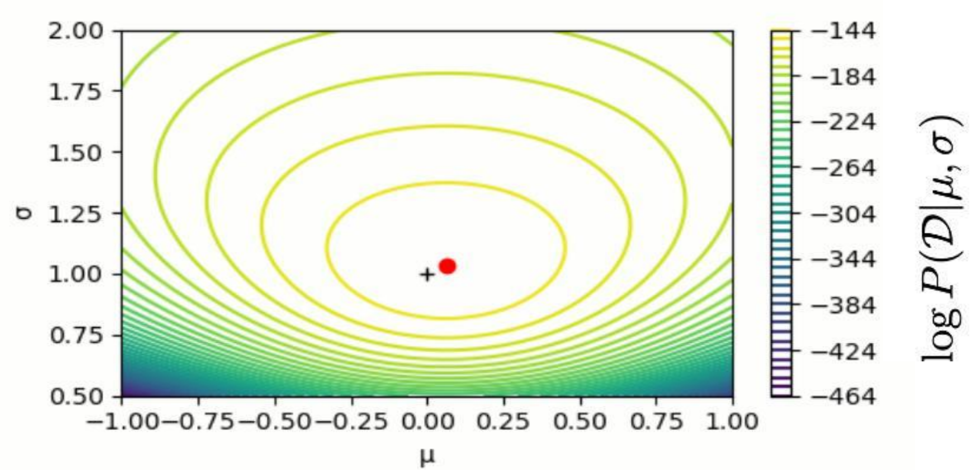
$$n = 100$$

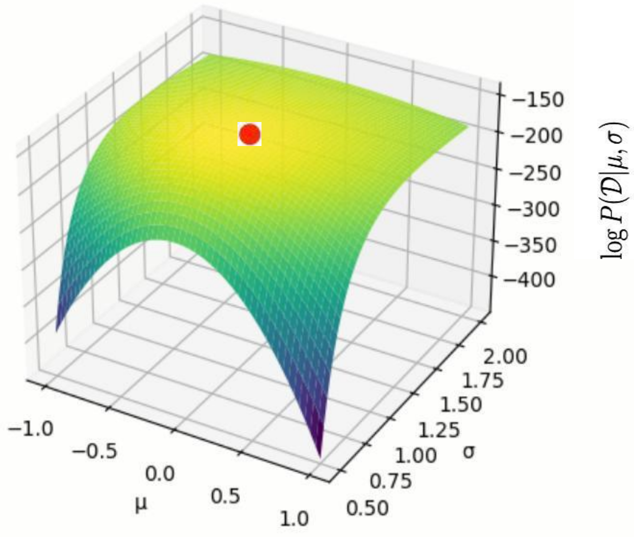
$$x_i \sim \mathcal{N}(\mu, \sigma^2)$$

$$\mu = 0$$

$$\sigma^2 = 1$$

$$\log P(\mathcal{D}|\mu, \sigma) = -n \log(\sigma\sqrt{2\pi}) - \sum_{i=1}^{n} \frac{(x_i - \mu)^2}{2\sigma^2}$$





+ $(\mu_{True}, \sigma_{True})$

● $(\hat{\mu}_{MLE}, \hat{\sigma}_{MLE})$

MLE for Mean of a Gaussian

- What's MLE for mean? Set **partial derivative** to zero.

$$\frac{\partial}{\partial \mu} \log P(\mathcal{D} \mid \mu, \sigma) = \frac{\partial}{\partial \mu}\left[-n \log(\sigma\sqrt{2\pi}) - \sum_{i=1}^{n} \frac{(x_i - \mu)^2}{2\sigma^2}\right]$$

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$$= \cancel{-}\sum_{i=1}^{n} \frac{\cancel{-}\cancel{2}(x_i - \mu)}{\cancel{2}\sigma^2}$$

$$= \frac{-n\mu + \sum_{i=1}^{n} x_i}{\sigma^2} = 0$$

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$$\boxed{\hat{\mu}_{\mathrm{MLE}} = \frac{1}{n}\sum_{i=1}^{n} x_i}$$

empirical mean!

MLE for Variance

- Again, set partial derivative to zero:

$$\frac{\partial}{\partial \sigma} \log P(\mathcal{D} \mid \mu, \sigma) = \frac{\partial}{\partial \sigma} \left[-n \log(\sigma \sqrt{2\pi}) - \sum_{i=1}^{n} \frac{(x_i - \mu)^2}{2\sigma^2} \right]$$

MLE for Variance

reminders for formulas:

$$\frac{d}{dx}\log x = \frac{1}{x} \qquad \frac{d}{dx}\frac{1}{x^2} = \frac{d}{dx}x^{-2} = -2x^{-3}$$

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$$= \frac{-n}{\sigma} + \sum_{i=1}^{n}\frac{\cancel{2}(x_i-\mu)^2}{\cancel{2}\sigma^3}$$

$$= \frac{-n\sigma^2 + \sum_{i=1}^{n}(x_i-\mu)^2}{\cancel{\sigma^3}} = 0$$

$$\boxed{= \sigma^2_{\mathrm{MLE}} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu}_{\mathrm{MLE}})^2}$$

Learning Gaussian parameters

- MLE:

$$\widehat{\mu}_{MLE} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\widehat{\sigma^2}_{MLE} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \widehat{\mu}_{MLE})^2$$

- MLE for the variance of a Gaussian is biased

$$\mathbb{E}[\widehat{\sigma^2}_{MLE}] \neq \sigma^2$$

- Unbiased variance estimator:

$$\widehat{\sigma^2}_{unbiased} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \widehat{\mu}_{MLE})^2$$

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Maximum Likelihood Estimator (MLE) $\widehat{\theta}_{MLE} = \arg\max_{\theta} L_n(\theta)$

Under benign assumptions, as the number of observations $n \to \infty$ we have $\hat{\theta}_{MLE} \to \theta_*$

The MLE is a "recipe" that begins with a *model* for data $f(x;\theta)$

Recap

- Learning is…
  - Collect some data
    - E.g., coin flips
  - Choose a hypothesis class or model
    - E.g., Bernoulli
  - Choose a loss function
    - E.g., data likelihood
  - Choose an optimization procedure
    - E.g., set derivative to zero to obtain MLE

Applications Preview

Maximum Likelihood Estimation

Why is it useful to recover the “true” parameters θ_* of a probabilistic model?

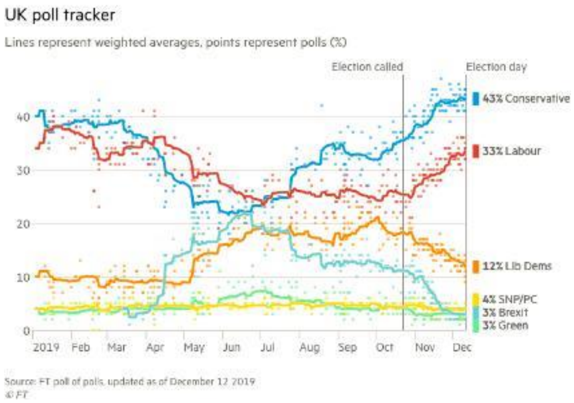
- **Estimation** of the parameters θ_* is the goal
- Help **interpret** or summarize large datasets
- Make **predictions** about future data
- **Generate** new data $X \sim f(\,\cdot\,; \hat{\theta}_{\text{MLE}})$

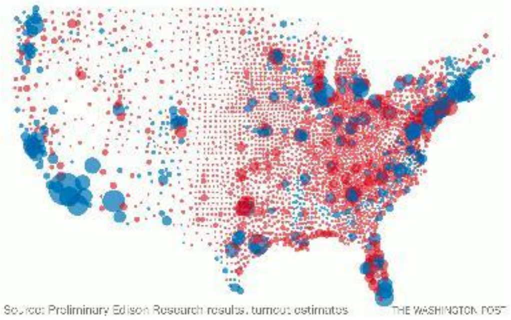
Estimation

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

Opinion polls
How does the greater population feel about an issue?
Correct for over-sampling?

- θ_* is "true" average opinion
- $X_1, X_2, \ldots$ are sample calls





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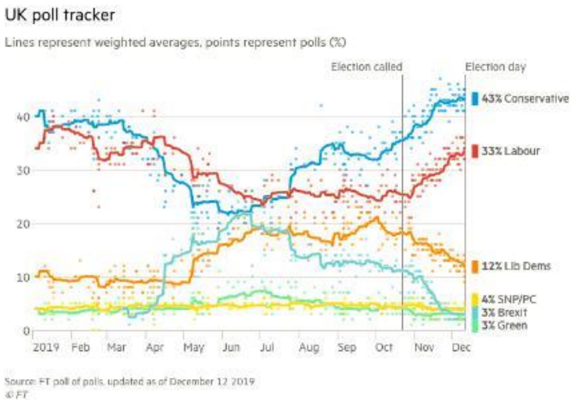
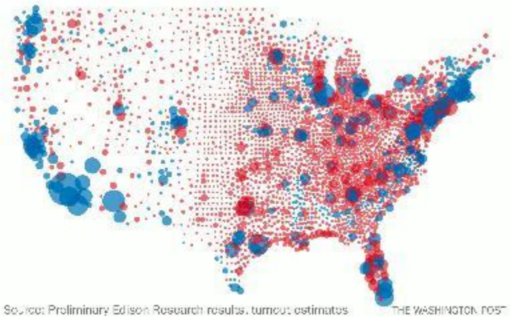




A/B testing
How do we figure out which ad results in more click-through?

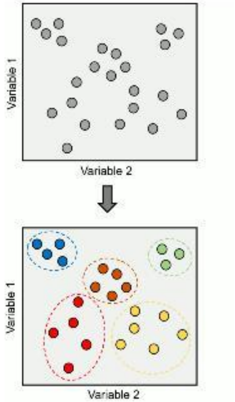
- θ_* are the "true" average rates
- $X_1, X_2, \ldots$ are binary "clicks"

Interpret

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

Customer segmentation / clustering
Can we identify distinct groups of customers by their behavior?

- θ_* describes "center" of distinct groups
- $X_1, X_2, \ldots$ are individual customers

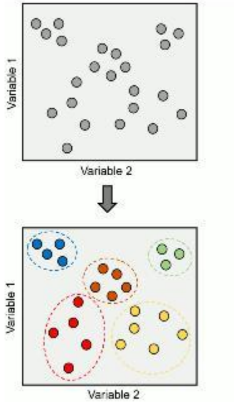


Interpret

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

Customer segmentation / clustering
Can we identify distinct groups of customers by their behavior?

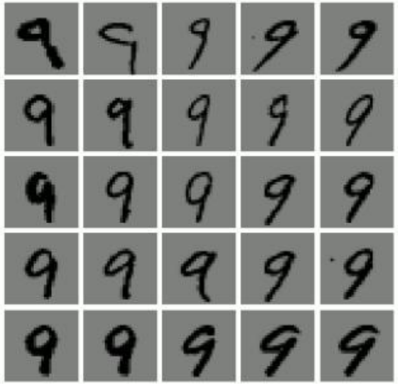
- θ_* describes "center" of distinct groups
- $X_1, X_2, \ldots$ are individual customers



Data exploration

What are the degrees of freedom of the dataset?

- θ_* describes the principle directions of variation
- $X_1, X_2, \ldots$ are the individual images



Predict

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

Content recommendation
Can we predict how much someone will like a movie based on past ratings?

- θ_* describes user's preferences
- $X_1, X_2, \ldots$ are (movie, rating) pairs

Predict

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

Content recommendation
Can we predict how much someone will like a movie based on past ratings?

- θ_* describes user's preferences
- $X_1, X_2, \ldots$ are (movie, rating) pairs

Object recognition / classification
Identify a flower given just its picture?

- θ_* describes the characteristics of each kind of flower
- $X_1, X_2, \ldots$ are the (image, label) pairs

(a) (b) (c)

Figure 1.1: Three types of Iris flowers: Setosa, Versicolor and Virginica. Used with kind permission of Dennis Kramb and SIGNA.

index	sl	sw	pl	pw	label
0	5.1	3.5	1.4	0.2	Setosa
1	4.9	3.0	1.4	0.2	Setosa
	...				
50	7.0	3.2	4.7	1.4	Versicolor
	...				
149	5.9	3.0	5.1	1.8	Virginica

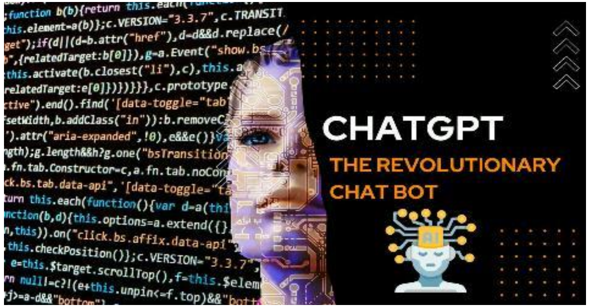
Generate

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

Text generation
Can AI generate text that could have been written like a human?

- θ_* describes language structure
- $X_1, X_2, \ldots$ are text snippets found online

"Kaia the dog wasn't a natural pick to go to mars. No one could have predicted she would…"



MLE!

https://chat.openai.com/chat

Generate

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

Text generation
Can AI generate text that could have been written like a human?

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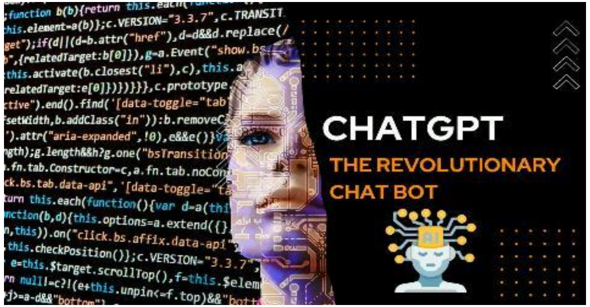

MLE!

https://chat.openai.com/chat

Image to text generation
Can AI generate an image from a prompt?

- θ_* describes the coupled structure of images and text
- $X_1, X_2, \ldots$ are the (image, caption) pairs found online

"dog talking on cell phone under water, oil painting"

https://labs.openai.com/

Acknowledgement

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THANK YOU