Parametric Models: from data to models

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Machine Learning 10-701
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Recall: Model-based ML

- Learning: From data to model
  - A model thus is a summary of the data
  - But also a story of how the data was generated
  - Could thus be used to describe how future data can be generated
  - **E.g. given (symptoms, diseases) data, a model explains how symptoms and diseases are related**

- Inference: From model to knowledge
  - Given the model, how can we answer questions relevant to us
  - **E.g. given (symptom, disease) model, given some symptoms, what is the disease?**

Model Learning: Data to Model

- What are some general principles in going from data to model?
- What are the guarantees of these methods?

LET US CONSIDER THE EXAMPLE OF A SIMPLE MODEL

Your first consulting job

- A billionaire from the suburbs of Seattle asks you a question:
  - He says: I have a coin, if I flip it, what's the probability it will fall with the head up?
  - You say: Please flip it a few times:

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  - You say: Please flip it a few times:

  - You say: The probability is: **3/5**
  - **He says: Why???**
  - You say: Because… frequency of heads in all flips

Questions

- Why frequency of heads?

- How good is this estimation?
  - Would you be willing to bet money on your guess of the probability?
  - Why not?

Model

- First we need a model that would capture the experimental data
- What is the experimental data?
- Coin Flips

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Model

- A model for coin flips
  - Bernoulli Distribution
- X is a random variable with Bernoulli distribution when:
  - X takes values in $\{0,1\}$
  - $P(X = 1) = p$
  - $P(X = 0) = 1 - p$
  - Where p in $[0,1]$

Model

- X is a random variable with Bernoulli distribution when:
  - X takes values in {0,1}
  - $P(X = 1) = p$
  - $P(X = 0) = 1 - p$
  - Where p in [0,1]
- X = 1 i.e. heads with probability p, and X = 0 i.e. tails with probability 1 – p
  - Coin with probability of flipping heads = p
- And we draw **independent** samples that are **identically distributed** from same distribution
  - flip the same coin multiple times

Bernoulli distribution

Data, D = 

- P(Heads) = θ, P(Tails) = 1-θ

- Flips are **i.i.d.**:
  - **Independent** events
  - **Identically distributed** according to Bernoulli distribution

<u>Choose θ that maximizes the probability of observed data</u>

Probability of one coin flip

Let's say we observe a coin flip $X \in \{0, 1\}$.

The probability of this coin flip,
given a Bernoulli distribution with parameter p:

$$p^X (1-p)^{1-X}.$$

Equal to p when $X = 1$, and equal to $(1-p)$ when $X = 0$.

Probability of Multiple Coin Flips

$$\text{Probability of Data} = \mathbb{P}(X_1, X_2, \ldots, X_n; \theta)$$

Probability of Multiple Coin Flips

$$\begin{aligned}\text{Probability of Data} &= \mathbb{P}(X_1, X_2, \ldots, X_n; \theta) \\ &= P(X_1)\, P(X_2) \ldots P(X_n)\end{aligned}$$

…Independence of samples

Probability of Multiple Coin Flips

$$\begin{aligned}\text{Probability of Data} &= \mathbb{P}(X_1, X_2, \ldots, X_n; \theta) \\ &= P(X_1)\, P(X_2) \ldots P(X_n) \\ &= \prod_{i=1}^{n} P(X_i)\end{aligned}$$

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\end{aligned}
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…probability of a Bernoulli sample

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$$\ldots\ p^a\, p^b = p^{a+b}$$

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&= p^{\sum_{i=1}^{n} X_i}\, (1-p)^{n-\sum_{i=1}^{n} X_i} \\
&= p^{n_h}\, (1-p)^{n-n_h}.
\end{aligned}
$$

where n_h is the number of heads,
n is the total number of coin flips

Maximum Likelihood Estimator (MLE)

The MLE solution is then given by solving the following problem:

$$\begin{aligned}\widehat{p} &= \arg\max_{p} \mathbb{P}(X_1, \ldots, X_n; p) \\ &= \arg\max_{p} \left\{ p^{n_h} (1-p)^{n-n_h} \right\}\end{aligned}$$

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&= \arg\max_p \left\{n_h \log p + (n - n_h) \log(1-p)\right\}
\end{aligned}$$

…argmax_x f(x) = argmax_x log f(x)

MLE for coin flips

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$$\widehat{p} = \arg\max_p \{n_h \log p + (n - n_h)\ \log(1 - p)\}$$

$$\implies \frac{n_h}{\widehat{p}} - \frac{n - n_h}{1 - \widehat{p}} = 0$$

$$\implies \widehat{p} = \frac{n_h}{n}.$$

Maximum Likelihood Estimation

Choose θ that maximizes the probability of observed data

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

MLE of probability of head:

$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$ **= 3/5**

"Frequency of heads"

How many flips do I need?

$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

- Billionaire says: I flipped 3 heads and 2 tails.
- You say: θ = 3/5, it is the MLE!
- He says: What if I flipped 30 heads and 20 tails?
- You say: Same answer, it is the MLE!
- **He says: If you get the same answer, would you prefer to flip 5 times or 50 times?**
- You say: Hmm… The more the merrier???
- He says: Is this why I am paying you the big bucks???

KEY QUESTION: HOW GOOD IS THE MLE (OR ANY OTHER ESTIMATOR)?

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…since the sample mean converges to E(X) = p

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…linearity of expectation:
E(a X + b Y) = a E(X) + b E(Y)

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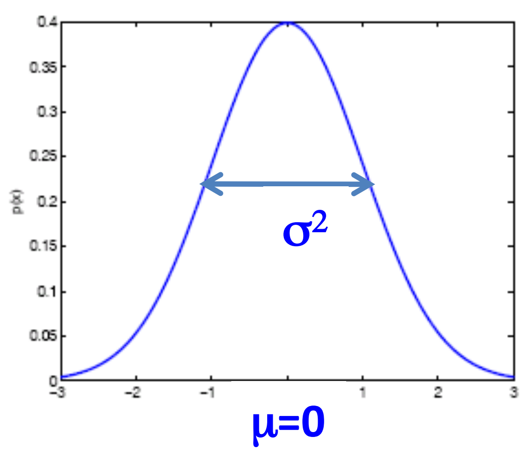
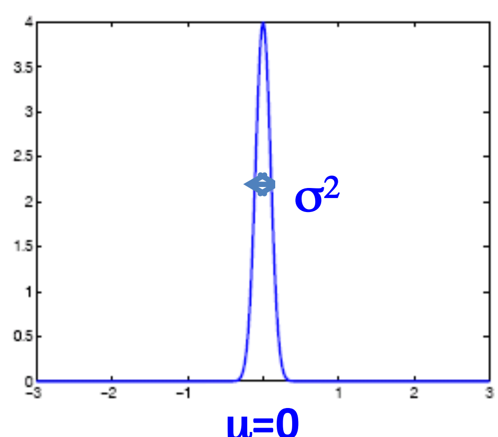
&= \mathbb{E}X_1 \\
&= p.
\end{aligned}$$

What about continuous variables?

- Billionaire says: If I am measuring a continuous variable, what can you do for me?
- **You say: Let me tell you about Gaussians…**

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





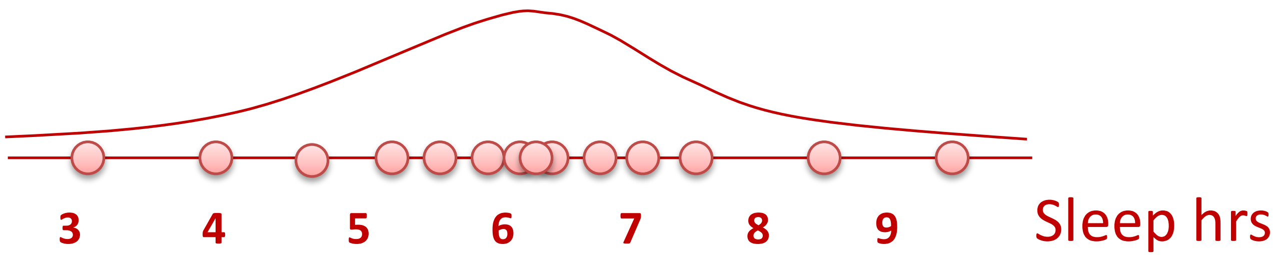
Properties of Gaussians

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

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

Gaussian distribution

Data, D =



- Parameters: μ – mean, σ^2 - variance
- Sleep hrs are **i.i.d.**:
  - **Independent** events
  - **Identically distributed** according to Gaussian distribution

MLE for Gaussian mean and variance

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

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

Note: MLE for the variance of a Gaussian is **biased**

- Expected result of estimation is **not** true parameter!
- Unbiased variance estimator:

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

MLE for parametric models

Data: $X_1, X_2, \ldots, X_n$.

Model: $P(X;\theta)$ with parameters θ.

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Assumption: Data drawn $i.i.d$ from distribution $P(X; \theta^*)$ for some unknown θ^*.

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R. A. Fisher

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Likelihood Function: $L(\theta) := \prod_{i=1}^{n} P(X_i; \theta)$
The probability of seeing data $X_1, X_2, \ldots, X_n$ assuming parameters were θ.

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i.e. pick the θ that would maximize the probability of having seen the data that we do see

Unbiasedness

An estimator $\widehat{\theta}(X_1, \ldots, X_n)$ where $X_i \sim P(X; \theta^*)$ is unbiased if

$$\mathbb{E}(\widehat{\theta}) = \theta^*.$$

MLE is "asymptotically" unbiased i.e. there are some error terms that go to zero as a function of n, the number of samples

Consistency

An estimator $\widehat{\theta}(X_1, \ldots, X_n)$ where $X_i \sim P(X; \theta^*)$ is consistent if $\widehat{\theta} \to \theta^*$ in probability as $n \to \infty$.

MLE is consistent under some mild regularity conditions on the model, and when the model size is fixed.

How many flips?

- But recall the Billionaire's question:
  - How many flips would you prefer: 5 or 50?
  - How many flips would you need to be willing to bet money on your answer?
- Unbiasedness and Consistency do not answer this question
- We need convergence rates for our estimator

Simple bound (Hoeffding's inequality)

- For $n = \alpha_H + \alpha_T$, and $\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$

- Let θ^* be the true parameter, for any $\varepsilon>0$:

$$P(|\widehat{\theta} - \theta^*| \geq \epsilon) \leq 2e^{-2n\epsilon^2}$$

PAC Learning

- PAC: Probably Approximate Correct
- Billionaire says: I want to know the coin parameter θ, within ε = 0.1, with probability at least 1-δ = 0.95. How many flips?

$$P(|\ \widehat{\theta} - \theta^* \ | \geq \epsilon) \ \leq \ 2e^{-2n\epsilon^2}$$

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Suffice to have n large enough for RHS to be less than \delta

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$$\begin{aligned} 2e^{-2n\epsilon^2} &< \delta \\ -2n\epsilon^2 &< \ln(\delta/2) \\ 2n\epsilon^2 &> \ln(2/\delta) \\ n &> \frac{\ln(2/\delta)}{2\epsilon^2} \end{aligned}$$

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Sample complexity

$$n \geq \frac{\ln(2/\delta)}{2\epsilon^2}$$

From data to model

- Well-studied question in Statistics
  - Estimators e.g. MLE
  - Guarantees (consistency, unbiasedness, rates)
- What has Machine Learning contributed to this statistical question:
  - Specific kinds of guarantees e.g. sample complexity
  - New tools to derive guarantees (VC Dimension, etc.)
  - Computational Issues

Computational Issues

- MLE

$$\max_\theta \prod_{i=1}^{n} P(X_i;\theta)$$

$$\max_\theta \frac{1}{n} \sum_{i=1}^{n} \log P(X_i;\theta)$$

Computational Issues

- When number of parameters, or number of samples n is large, computing the MLE is a **large-scale optimization problem**
- Well-studied problem in optimization/operations research
- Machine Learning has contributed considerably via:
  - Better understanding of optimization problems that arise from statistical estimators such as MLE (in contrast to general optimization problems)