Deep Learning

LM Computer Science, Data Science, Cybersecurity
2nd semester - 6 CFU

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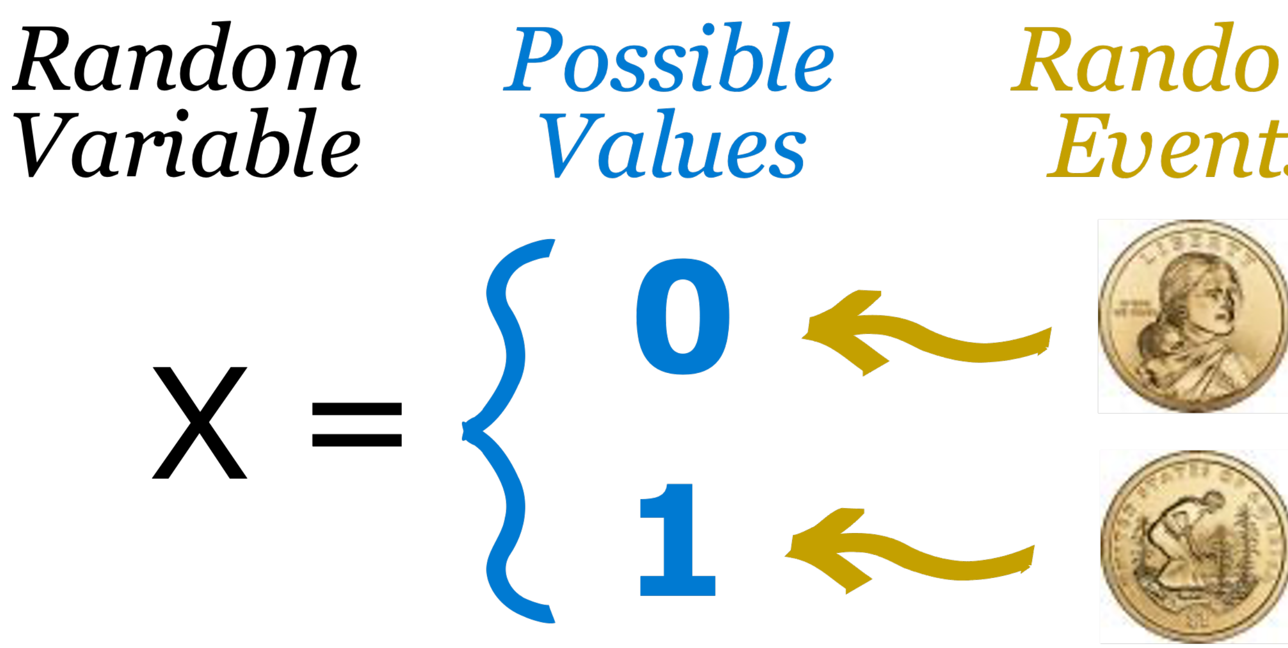
Probability / Information theory

A primer on probability and information theory (chapter 3)

Maximum Likelihood estimation (section 5.5)

Probability

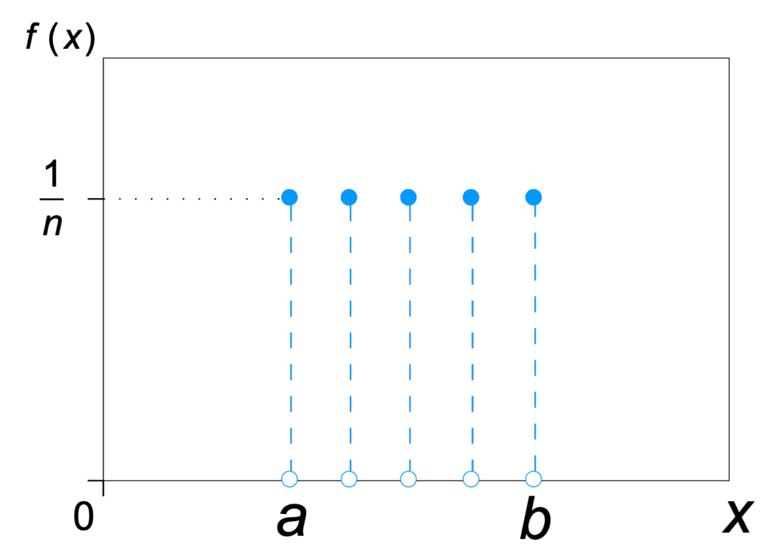
- **Random variable**: a variable that can take different values randomly
- Example: Tossing a coin: we could get Heads or Tails.
  - **Heads=0** and **Tails=1**
  - **In each experiment,** Random Variable x can be either 0 or 1



Probability Distributions

- **Probability Distribution**: A description of how likely a random variable x (or a set of random variables) is to take each of its possible states

- Probability Mass Function (Discrete variables)
  - Domain of P is the set of all possible states of x (k different values)
  - $\forall x \in \mathrm{x}\ 0 \leq P(\mathrm{x} = x) \leq 1$
  - $\sum_{x \in \mathrm{x}} P(x) = 1$



- E.g. Uniform distribution $\forall_{x \in \mathrm{x}}\ P(\mathrm{x} = x) = \frac{1}{k}$

Probability Distributions

- Joint probability distribution: probability distribution over 2 or more variables $P(\mathrm{x}=x, \mathrm{y}=y)$ or $P(x,y)$
    - Example 2 coins: $P(\mathrm{x}=head, \mathrm{y}=tail)$ or $P(head, tail)$
- Marginalization:

$$\forall x \in \mathrm{x}\; P(\mathrm{x}=x) = \sum_{y} P(\mathrm{x}=x, \mathrm{y}=y)$$

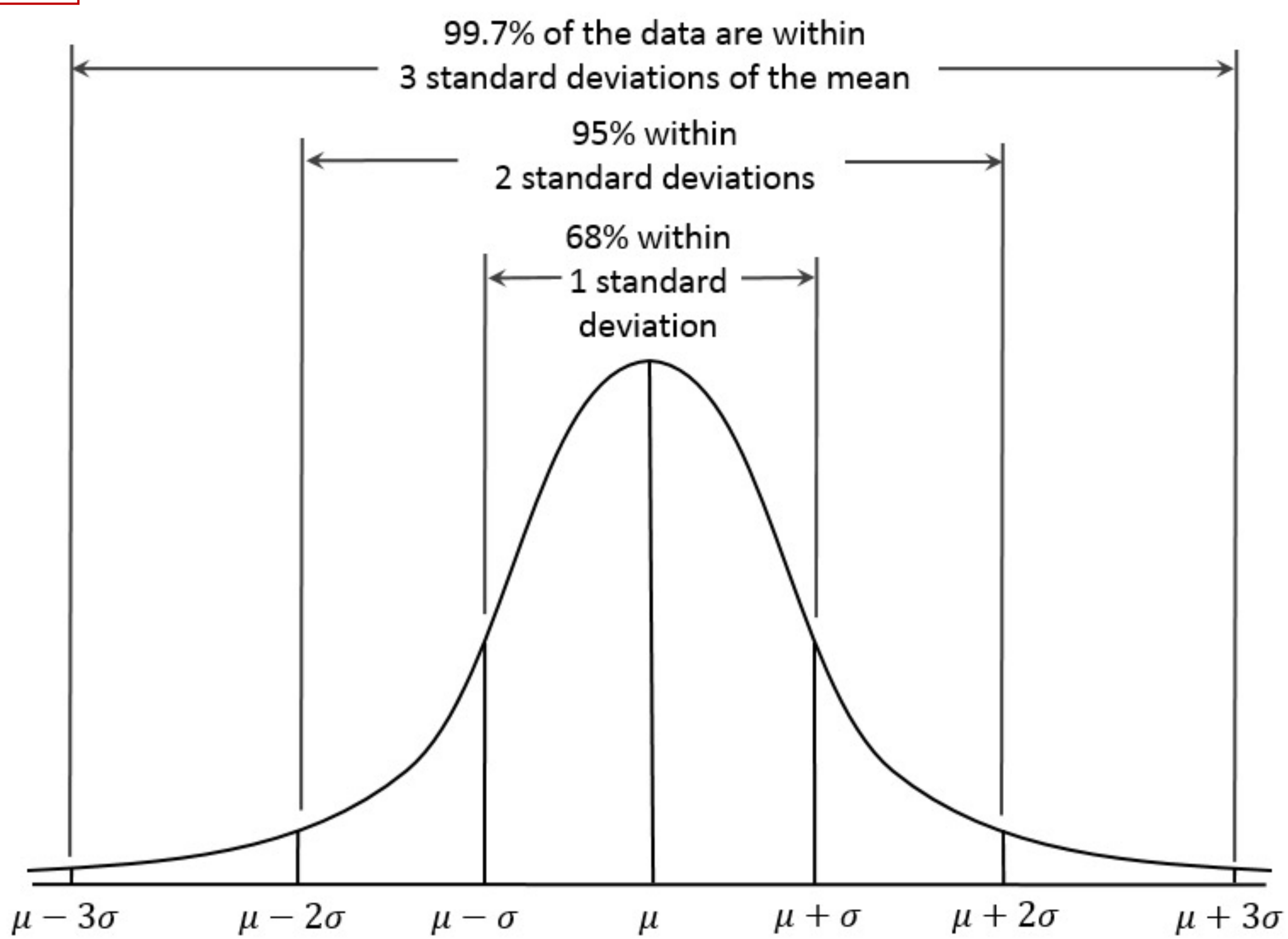
- Continuous variables: Probability distribution is described by a Probability Density Function (PDF)
    - Domain of p is the set of all possible states of x
    - $\forall x \in \mathrm{x}\; P(x) \geq 0$
    - $\int p(x)dx = 1$
- E.g. Gaussian distribution

Gaussian distribution

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

Parametrized by

PDF of Gaussian distribution



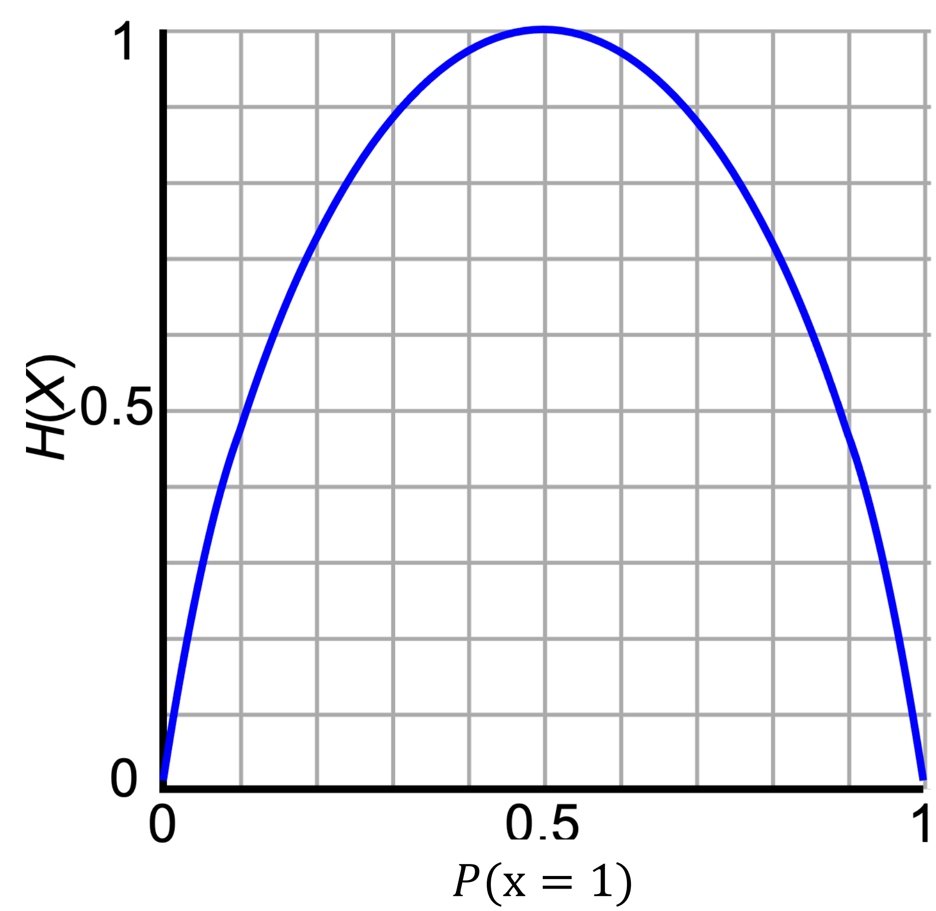
Entropy

- **Shannon Entropy** (discrete variable)

$$H(\mathrm{x}) = -\mathbb{E}_{x \sim P(\mathrm{x})}[\log P(x)]$$

- Expected amount of (self-)**information** in an event drawn from distribution P
- Lower bound on the number of bits needed on average to encode a symbol drawn from that distribution

Entropy H(*X*) of a coin flip, measured in bits, graphed versus the bias of the coin P(*x* = 1), where *x* = 1 represents a result of heads.



Kullback-Leibler divergence and Cross Entropy

- Let's consider two probability distributions $P(x)$ and $Q(x)$

- Measure how different they are

$$D_{KL}(P \parallel Q) = \mathbb{E}_{x \sim P}\left[\log \frac{P(x)}{Q(x)}\right] = \mathbb{E}_{x \sim P}[\log P(x) - \log Q(x)]$$

  - It is not a true distance because it is not symmetric
    - $D_{KL}(P \parallel Q) \neq D_{KL}(Q \parallel P)$

- Cross Entropy

$$H(P, Q) = H(P) + D_{KL}(P \parallel Q) = -\,\mathbb{E}_{x \sim P}[\log Q(x)]$$

Note: minimizing CE of P w.r.t. Q is equivalent to minimize KL divergence between P and Q (if P is given, H(P) and $\mathbb{E}_{x \sim P}[\log P(x)]$ are constants)

Maximum likelihood estimation

- Principled way to derive estimators (models)
- Consider n examples $Tr = \{\boldsymbol{x}^1, \dots, \boldsymbol{x}^n\}$ drawn i.i.d. from $p_{data}(\boldsymbol{x})$

Not known in advance

- Let us consider a family of parametric probability distributions (models) $p_{model}(\boldsymbol{x}; \boldsymbol{\theta})$.
    - $p_{model}(\boldsymbol{x}; \boldsymbol{\theta})$ maps a point $\boldsymbol{x}$ to a real number, estimating $p_{data}(\boldsymbol{x})$
    - Maximum Likelihood estimation for $\boldsymbol{\theta}$ is

$$\boldsymbol{\theta}_{ML} = arg\max_{\boldsymbol{\theta}} p_{model}(Tr; \boldsymbol{\theta}) = arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p_{model}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

Here we do not know $p_{data}(\boldsymbol{x})$, we just know that $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(n)}$ are i.i.d!

Assumption: independence!
$P(x, y) = P(x)P(y)$
If x and y are independent

..A side note on maximum likelihood

- ML is a special case of maximum a posteriori estimation (MAP)
- ML assumes a uniform prior distribution of the hypothesis
- MAP and maximum likelihood approach make predictions using a single point estimate of $\boldsymbol{\theta}$
- the Bayesian approach is to make predictions using a full probability distribution over $\boldsymbol{\theta}$

..A side note on maximum likelihood

Given a new instance x, what is the most probable *classification* ?

- $h_{MAP}(x)$, in general, is not the most probable classification!

Example: let's consider:

- three possibile hypoteses:
$$P(h_1|D) = .4,\ P(h_2|D) = .3,\ P(h_3|D) = .3$$
- given a new instance x,
$$h_1(x) = +,\ h_2(x) = -,\ h_3(x) = -$$
- what is the most probable classification for x?

Maximum likelihood estimation

$$\boldsymbol{\theta}_{ML} = \underset{\boldsymbol{\theta}}{arg\max} \prod_{i=1}^{n} p_{model}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

- Taking the product of many probabilities is numerically unstable.
  - We can apply the $\log$ and the $\underset{\boldsymbol{\theta}}{arg\max}$ does not change (log-likelihood)

$$\boldsymbol{\theta}_{ML} = \log(\underset{\boldsymbol{\theta}}{arg\max} \prod_{i=1}^{n} p_{model}\left(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}\right))$$

$$= \underset{\boldsymbol{\theta}}{arg\max} \sum_{1=1}^{n} \log p_{model}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

Maximum likelihood estimation

$$\boldsymbol{\theta}_{ML} = \underset{\boldsymbol{\theta}}{arg\max} \sum_{1=1}^{n} \log p_{model}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

- We can equivalently divide by n to express ML as an expectation over training data

$$\boldsymbol{\theta}_{ML} = \underset{\boldsymbol{\theta}}{arg\max} \, \mathbb{E}_{\boldsymbol{x}\sim\hat{p}_{data}} [\log p_{model}(x; \boldsymbol{\theta})]$$

- ML minimizes the dissimilarity between $\hat{p}_{data}$ and p_{model}, measured by the KL divergence

ML estimation as KL divergence

- KL divergence between $\hat{p}_{data}$ and p_{model}

$$D_{KL}(\hat{p}_{data} \parallel p_{model}) = \mathbb{E}_{\boldsymbol{x}\sim\hat{p}_{data}}[\log \hat{p}_{data}(\boldsymbol{x}) - \log p_{model}(\boldsymbol{x};\boldsymbol{\theta})]$$

does not depend on the model

- To minimize the KL, we need only to minimize

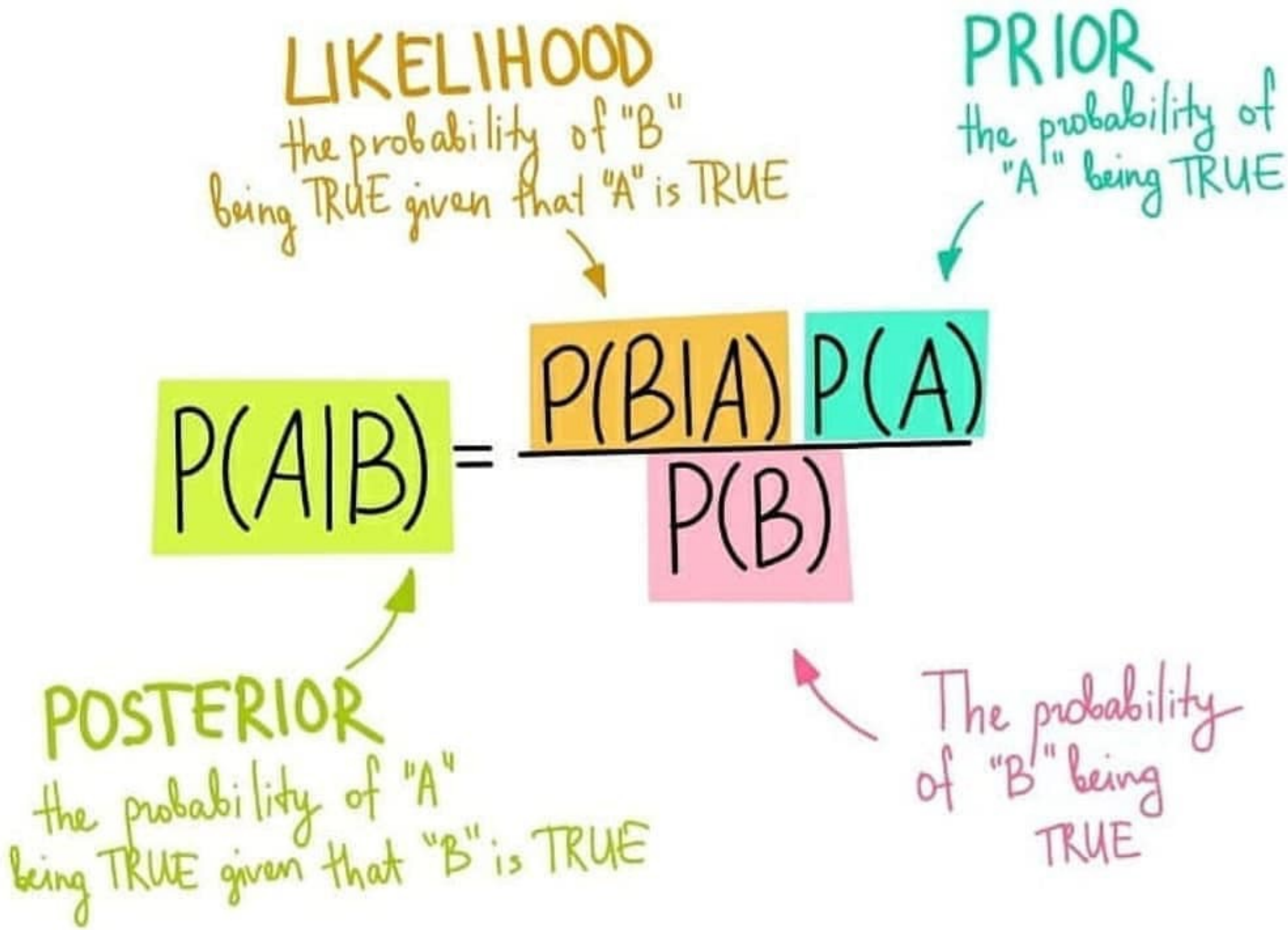
$$\arg\min_{\boldsymbol{\theta}} -\mathbb{E}_{\boldsymbol{x}\sim\hat{p}_{data}}[\log p_{model}(\boldsymbol{x};\boldsymbol{\theta})]$$

- That is the same equation of ML in previous slide

- It also corresponds to minimizing the **cross-entropy** between the two distributions

Conditional Probability

- Probability of an event, given that some other event has happened.



Bayes' rule

Conditional log likelihood

- We can use ML to estimate a **conditional** probability $P(\boldsymbol{y}|\boldsymbol{x};\boldsymbol{\theta})$ to predict $\boldsymbol{y}$ given $\boldsymbol{x}$ (<u>supervised</u> learning)

$$\boldsymbol{\theta}_{\boldsymbol{ML}} = \arg\max_{\boldsymbol{\theta}} P(\boldsymbol{Y}\,|\boldsymbol{X};\boldsymbol{\theta})$$

- If input examples are i.i.d.

$$\boldsymbol{\theta}_{\boldsymbol{ML}} = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log P\left(\boldsymbol{y}^{(i)}\middle|\boldsymbol{x}^{(i)};\boldsymbol{\theta}\right)$$

Warning!

- We will use logarithm properties. Check Algebra cheat sheet if some of the rules applied in the next slide are not clear!

Algebra Cheat Sheet

Basic Properties & Facts

Arithmetic Operations

$ab + ac = a(b+c)$ $\qquad a\left(\frac{b}{c}\right) = \frac{ab}{c}$

$\frac{\left(\frac{a}{b}\right)}{c} = \frac{a}{bc}$ $\qquad \frac{a}{\left(\frac{b}{c}\right)} = \frac{ac}{b}$

$\frac{a}{b} + \frac{c}{d} = \frac{ad+bc}{bd}$ $\qquad \frac{a}{b} - \frac{c}{d} = \frac{ad-bc}{bd}$

$\frac{a-b}{c-d} = \frac{b-a}{d-c}$ $\qquad \frac{a+b}{c} = \frac{a}{c} + \frac{b}{c}$

$\frac{ab+ac}{a} = b+c,\ a \neq 0$ $\qquad \frac{\left(\frac{a}{b}\right)}{\left(\frac{c}{d}\right)} = \frac{ad}{bc}$

Exponent Properties

$a^n a^m = a^{n+m}$ $\qquad \frac{a^n}{a^m} = a^{n-m} = \frac{1}{a^{m-n}}$

$\left(a^n\right)^m = a^{nm}$ $\qquad a^0 = 1,\ \ a \neq 0$

$(ab)^n = a^n b^n$ $\qquad \left(\frac{a}{b}\right)^n = \frac{a^n}{b^n}$

$a^{-n} = \frac{1}{a^n}$ $\qquad \frac{1}{a^{-n}} = a^n$

$\left(\frac{a}{b}\right)^{-n} = \left(\frac{b}{a}\right)^n = \frac{b^n}{a^n}$ $\qquad a^{\frac{n}{m}} = \left(a^{\frac{1}{m}}\right)^n = \left(a^n\right)^{\frac{1}{m}}$

Properties of Radicals

$\sqrt[n]{a} = a^{\frac{1}{n}}$ $\qquad \sqrt[n]{ab} = \sqrt[n]{a}\sqrt[n]{b}$

$\sqrt[m]{\sqrt[n]{a}} = \sqrt[nm]{a}$ $\qquad \sqrt[n]{\frac{a}{b}} = \frac{\sqrt[n]{a}}{\sqrt[n]{b}}$

$\sqrt[n]{a^n} = a$, if n is odd

$\sqrt[n]{a^n} = |a|$, if n is even

Properties of Inequalities

If $a < b$ then $a + c < b + c$ and $a - c < b - c$

If $a < b$ and $c > 0$ then $ac < bc$ and $\frac{a}{c} < \frac{b}{c}$

If $a < b$ and $c < 0$ then $ac > bc$ and $\frac{a}{c} > \frac{b}{c}$

Properties of Absolute Value

$$|a| = \begin{cases} a & \text{if } a \geq 0 \\ -a & \text{if } a < 0 \end{cases}$$

$|a| \geq 0$ $\qquad |-a| = |a|$

$|ab| = |a||b|$ $\qquad \left|\frac{a}{b}\right| = \frac{|a|}{|b|}$

$|a+b| \leq |a| + |b|$ Triangle Inequality

Distance Formula

If $P_1 = (x_1, y_1)$ and $P_2 = (x_2, y_2)$ are two points the distance between them is

$$d(P_1, P_2) = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

Complex Numbers

$i = \sqrt{-1}$ $\qquad i^2 = -1$ $\qquad \sqrt{-a} = i\sqrt{a},\ \ a \geq 0$

$(a+bi) + (c+di) = a + c + (b+d)i$

$(a+bi) - (c+di) = a - c + (b-d)i$

$(a+bi)(c+di) = ac - bd + (ad+bc)i$

$(a+bi)(a-bi) = a^2 + b^2$

$|a+bi| = \sqrt{a^2+b^2}$ Complex Modulus

$\overline{(a+bi)} = a - bi$ Complex Conjugate

$\overline{(a+bi)}(a+bi) = |a+bi|^2$

Logarithms and Log Properties

Definition

$y = \log_b x$ is equivalent to $x = b^y$

Example

$\log_5 125 = 3$ because $5^3 = 125$

Special Logarithms

$\ln x = \log_e x$ natural log

$\log x = \log_{10} x$ common log

where $e = 2.718281828\ldots$

Logarithm Properties

$\log_b b = 1$ $\qquad \log_b 1 = 0$

$\log_b b^x = x$ $\qquad b^{\log_b x} = x$

$\log_b\left(x^r\right) = r\log_b x$

$\log_b(xy) = \log_b x + \log_b y$

$\log_b\left(\frac{x}{y}\right) = \log_b x - \log_b y$

The domain of $\log_b x$ is $x > 0$

Factoring and Solving

Factoring Formulas

$x^2 - a^2 = (x+a)(x-a)$

$x^2 + 2ax + a^2 = (x+a)^2$

$x^2 - 2ax + a^2 = (x-a)^2$

$x^2 + (a+b)x + ab = (x+a)(x+b)$

$x^3 + 3ax^2 + 3a^2x + a^3 = (x+a)^3$

$x^3 - 3ax^2 + 3a^2x - a^3 = (x-a)^3$

$x^3 + a^3 = (x+a)\left(x^2 - ax + a^2\right)$

$x^3 - a^3 = (x-a)\left(x^2 + ax + a^2\right)$

$x^{2n} - a^{2n} = \left(x^n - a^n\right)\left(x^n + a^n\right)$

If n is odd then,

$x^n - a^n = (x-a)\left(x^{n-1} + ax^{n-2} + \cdots + a^{n-1}\right)$

$x^n + a^n$

$= (x+a)\left(x^{n-1} - ax^{n-2} + a^2x^{n-3} - \cdots + a^{n-1}\right)$

Quadratic Formula

Solve $ax^2 + bx + c = 0$, $a \neq 0$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

If $b^2 - 4ac > 0$ - Two real unequal solns.

If $b^2 - 4ac = 0$ - Repeated real solution.

If $b^2 - 4ac < 0$ - Two complex solutions.

Square Root Property

If $x^2 = p$ then $x = \pm\sqrt{p}$

Absolute Value Equations/Inequalities

If b is a positive number

$|p| = b \quad \Rightarrow \quad p = -b$ or $p = b$

$|p| < b \quad \Rightarrow \quad -b < p < b$

$|p| > b \quad \Rightarrow \quad p < -b$ or $p > b$

Completing the Square

Solve $2x^2 - 6x - 10 = 0$

(1) Divide by the coefficient of the x^2

$$x^2 - 3x - 5 = 0$$

(2) Move the constant to the other side.

$$x^2 - 3x = 5$$

(3) Take half the coefficient of x, square it and add it to both sides

$$x^2 - 3x + \left(-\frac{3}{2}\right)^2 = 5 + \left(-\frac{3}{2}\right)^2 = 5 + \frac{9}{4} = \frac{29}{4}$$

(4) Factor the left side

$$\left(x - \frac{3}{2}\right)^2 = \frac{29}{4}$$

(5) Use Square Root Property

$$x - \frac{3}{2} = \pm\sqrt{\frac{29}{4}} = \pm\frac{\sqrt{29}}{2}$$

(6) Solve for x

$$x = \frac{3}{2} \pm \frac{\sqrt{29}}{2}$$

Linear Regression as Maximum Likelihood

- Linear Regression: algorithm that learns to take an input $\boldsymbol{x}$ and produce an output value $\hat{y}$
  - minimize mean squared error, why??

- Let's revisit linear regression from the point of view of maximum likelihood estimation
  - Define a linear regression model that produces a conditional distribution $p(\boldsymbol{y}|\boldsymbol{x}) = \mathcal{N}(y;\ \hat{y}(\boldsymbol{x};\boldsymbol{\theta}), \sigma^2)$
    - output $\hat{y}(\boldsymbol{x};\boldsymbol{\theta})$, the mean of a Gaussian distribution
    - (variance is fixed to some constant)

Linear Regression as Maximum Likelihood

- Examples are assumed to be i.i.d

$$\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p\left(y^{(i)} \middle| \boldsymbol{x}^{(i)}; \boldsymbol{\theta}\right) =$$

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \mathcal{N}\left(y^{(i)}; \hat{y}\left(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}\right), \sigma^2\right) =$$

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log\left(\sqrt{\frac{1}{2\pi\sigma^2}}\; e^{-\frac{1}{2\,\sigma^2}\left(y^{(i)} - \hat{y}^{(i)}\right)^2}\right)$$

Maximise the log likelihood

Gaussian distribution

$\boldsymbol{\theta}$: parameters of the linear regression that computes $\hat{y}^{(i)}$

- $\hat{y}^{(i)}$ is the output of the linear regression $\hat{y}\left(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}\right)$

$$\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log\left(\sqrt{\frac{1}{2\pi\sigma^2}}\, e^{\left(-\frac{1}{2\,\sigma^2}\left(y^{(i)}-\hat{y}^{(i)}\right)^2\right)}\right) =$$

Log product rule

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) + \log e^{\left(-\frac{1}{2\,\sigma^2}\left(y^{(i)}-\hat{y}^{(i)}\right)^2\right)} =$$

Log quotient rule

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log(1) - \log\left(\sqrt{2\pi\sigma^2}\right) + \log e^{\left(-\frac{1}{2\,\sigma^2}\left(y^{(i)}-\hat{y}^{(i)}\right)^2\right)}$$

Log power rule

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \underbrace{\log(1)}_{=0} - \log\left(\sqrt{2\pi\sigma^2}\right) - \frac{1}{2\,\sigma^2}\left(y^{(i)} - \hat{y}^{(i)}\right)^2 \underbrace{\log(e)}_{=1}$$

Log power rule

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} -\frac{1}{2}\log(2\pi\sigma^2) - \frac{1}{2\,\sigma^2}\left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

Algebra

$$= \arg\max_{\boldsymbol{\theta}} -\frac{\boldsymbol{n}}{\mathbf{2}}\log(2\pi\sigma^2) + \sum_{i=1}^{n} -\frac{1}{2}\left(\frac{\left(y^{(i)}-\hat{y}^{(i)}\right)^2}{\sigma^2}\right)$$

$$= \arg\max_{\boldsymbol{\theta}} -\frac{\boldsymbol{n}}{\mathbf{2}}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}\left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

Comparing ML with MSE

$$\theta_{ML} = \arg\max_{\boldsymbol{\theta}} \underbrace{-\frac{\boldsymbol{n}}{\boldsymbol{2}}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}}\sum_{i=1}^{n}\left(y^{(i)} - \hat{y}^{(i)}\right)^2 =$$

Does not depend on $\boldsymbol{\theta}$

$$= \arg\max_{\boldsymbol{\theta}} - \sum_{i=1}^{n}\left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

$$\theta_{MSE} = \arg\min_{\boldsymbol{\theta}} \frac{1}{n}\sum_{i=1}^{n}\left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

maximizing the log-likelihood with respect to θ yields the same estimate of the parameters θ as does minimizing the mean squared error.