

[KICSV Special AI Lecture]
Mathematics for AI - Theory into Practice

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About Speaker

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- *KFAS-Salzburg Global Leadership Initiative Fellow @ Salzburg Global Seminar*, Salzburg, Austria
- Technology Consultant @ Gerson Lehrman Group (GLG), NY, USA
- *Co-Founder & CTO / Head of Global R&D & Chief Applied Scientist / Senior Fellow @ Gauss Labs, Inc., Palo Alto, CA, USA* 2020 ~ 2023

- Senior Applied Scientist @ Amazon.com, Inc., Vancouver, BC, Canada ~ 2020
- Principal Engineer @ Software R&D Center, DS Division, Samsung, Korea ~ 2017
- Principal Engineer @ Strategic Marketing & Sales Team, Samsung, Korea ~ 2016
- Principal Engineer @ DT Team, DRAM Development Lab, Samsung, Korea ~ 2015
- Senior Engineer @ CAE Team, Samsung, Korea ~ 2012
- PhD - Electrical Engineering @ Stanford University, CA, USA ~ 2004
- Development Engineer @ Vyan, Santa Clara, CA, USA ~ 2001
- MS - Electrical Engineering @ Stanford University, CA, USA ~ 1999
- BS - Electrical & Computer Engineering @ Seoul National University 1994 ~ 1998

Highlight of Career Journey

- BS in EE @ SNU, MS & PhD in EE @ Stanford University
 - *Convex Optimization - Theory, Algorithms & Software*
 - advised by *Prof. Stephen P. Boyd*
- Principal Engineer @ Samsung Semiconductor, Inc.
 - AI & Convex Optimization
 - collaboration with *DRAM/NAND Design/Manufacturing/Test Teams*
- Senior Applied Scientist @ Amazon.com, Inc.
 - e-Commerce AIs - anomaly detection, deep RL, and recommender system
 - Bezos's project - drove *\$200M* in additional sales via Amazon Mobile Shopping App
- *Co-Founder & CTO / Global R&D Head & Chief Applied Scientist @ Gauss Labs, Inc.*
- *Co-Founder & CTO* - AI Technology & Business Development @ Erudio Bio, Inc.

Today

- Machine Learning Prerequisites - 5
 - linear algebra basics, calculus basics, statistics basics
 - discrete random variables, continuous random variables
- Machine Learning Basics - 52
 - optimal estimator, bias & variance, MLE, MAP, Bayesian inference
 - ML - supervised learning, unsupervised learning, reinforcement learning, formulations
 - DL - CNN, RNN
 - DNN training using SGD with backpropagation
- Learning AI - 93
 - tips, some books, online courses, Andrew Ng!
- Appendices - 98
 - LLM
 - Generative AI (genAI) - 128
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ML Prerequisites

Linear Algebra Basics

Scalars, vectors, and matrices

- real number $a \in \mathbf{R}$, called *scalar*
- (ordered) collection of real numbers $(a_1, \dots, a_n) \in \mathbf{R}^n$, called *vector*

$$\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \in \mathbf{R}^n \quad \text{- column vector}$$

$$\begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix} \in \mathbf{R}^{1 \times n} \quad \text{- row vector}$$

- (ordered) collection of 2-dimensional array, called *matrix*

$$\begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,n} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m,1} & A_{m,2} & \cdots & A_{m,n} \end{bmatrix} \in \mathbf{R}^{m \times n}$$

Transposes

- transpose of row vector is column vector & vice versa

$$\begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}^T = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \quad \& \quad \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}^T = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}$$

- transpose of m -by- n matrix is n -by- m matrix

$$\begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,n} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m,1} & A_{m,2} & \cdots & A_{m,n} \end{bmatrix}^T = \begin{bmatrix} A_{1,1} & A_{2,1} & \cdots & A_{m,1} \\ A_{1,2} & A_{2,2} & \cdots & A_{m,2} \\ \vdots & \vdots & \ddots & \vdots \\ A_{1,n} & A_{2,n} & \cdots & A_{m,n} \end{bmatrix} \in \mathbb{R}^{n \times m}$$

Matrix-vector multiplication

- for matrix $A \in \mathbf{R}^{m \times n}$ & vector $b \in \mathbf{R}^n$
 - matrix-vector multiplication Ab defined by

$$Ab = \begin{bmatrix} A_{1,1}b_1 + A_{1,2}b_2 + \cdots + A_{1,n}b_n \\ A_{2,1}b_1 + A_{2,2}b_2 + \cdots + A_{2,n}b_n \\ \vdots \\ A_{m,1}b_1 + A_{m,2}b_2 + \cdots + A_{m,n}b_n \end{bmatrix} \in \mathbf{R}^m$$

in other words

$$(Ab)_i = \sum_{j=1}^n A_{i,j}b_j \quad \text{for } 1 \leq i \leq m$$

- resulting quantity is vector of length m
- number of columns of A *must* equal to length of b

Matrix-matrix multiplication

- for matrices $A \in \mathbf{R}^{m \times n}$ & $B \in \mathbf{R}^{n \times p}$

- matrix-matrix multiplication $AB \in \mathbf{R}^{m \times p}$ defined by

$$(AB)_{i,j} = \sum_{k=1}^n A_{i,k}B_{k,j} \quad \text{for } 1 \leq i \leq m$$

- resulting quantity is m -by- p matrix
 - *order matters* and number of columns of A *must* equal to number of rows of B
- note matrix-vector multiplication is *special case* of matrix-matrix multiplication

Calculus Basics

Functions

- $f : X \rightarrow Y$
 - $X = \text{dom } f$ - domain of f
 - Y - codomain of f
 - $\mathcal{R}(f) = \{f(x) \in Y \mid x \in X\}$ - range of f

Differentiation & derivatives

- for real-valued function $f : \mathbf{R} \rightarrow \mathbf{R}$

- derivative of f at $x \in \mathbf{R}$

$$f'(x) = \frac{d}{dx} f(x) = \lim_{h \rightarrow 0} \frac{f(x + h) - f(x)}{h} \in \mathbf{R}$$

- derivative exists *if and only if* limit exists
 - second derivative of f at $x \in \mathbf{R}$

$$f''(x) = \frac{d^2}{dx^2} f(x) = \lim_{h \rightarrow 0} \frac{f'(x + h) - f'(x)}{h} \in \mathbf{R}$$

- second derivative exists *if and only if* limit exists

Multivariate functions

- $f : \mathbf{R}^n \rightarrow \mathbf{R}$ - real-valued multivariate function

$$f(x) = f\left(\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}\right) = f(x_1, x_2, \dots, x_n) \in \mathbf{R}$$

- examples
 - $f : \mathbf{R}^3 \rightarrow \mathbf{R}$ - linear function

$$f(x) = x_1 + 3x_2 + 2x_3$$

- $f : \mathbf{R}^3 \rightarrow \mathbf{R}$ - convex quadratic function

$$f(x) = x_1^2 + x_1x_2 + 3x_2^2 + 5x_3^2$$

Multivariate vector functions

- $f : \mathbf{R}^n \rightarrow \mathbf{R}^m$ - real-valued multivariate vector function

$$f(x) = \begin{bmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_m(x) \end{bmatrix} \in \mathbf{R}^m$$

where $f_j : \mathbf{R}^n \rightarrow \mathbf{R}$ for $1 \leq j \leq m$

- examples
 - $f : \mathbf{R}^3 \rightarrow \mathbf{R}^2$ - linear function

$$f(x) = \begin{bmatrix} x_1 + 3x_2 + 2x_3 \\ -3x_2 + x_3 \end{bmatrix} \in \mathbf{R}^2$$

- $f : \mathbf{R}^3 \rightarrow \mathbf{R}^3$ - componentwise function

$$f(x) = [\exp(x_1) \quad \exp(x_2) \quad \exp(x_3)]^T \in \mathbf{R}^3$$

Partial derivative & gradient

for $f : \mathbf{R}^n \rightarrow \mathbf{R}$

- i th partial derivative

$$\frac{\partial}{\partial x_i} f(x) = \frac{f(x + he_i) - f(x)}{h} = \frac{f(\dots, x_{i-1}, x_i + h, x_{i+1}, \dots) - f(x)}{h}$$

where $e_i \in \mathbf{R}^n$ is i th unit vector

- gradient is vector of partial derivatives

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix} \in \mathbf{R}^n$$

- we have

$$(\nabla f(x))_i = \frac{\partial}{\partial x_i} f(x) = e_i^T \nabla f(x) \in \mathbf{R}$$

Jacobian

for $f : \mathbf{R}^n \rightarrow \mathbf{R}^m$

- Jacobian matrix

$$Df(x) = \begin{bmatrix} \frac{\partial f_1(x)}{\partial x_1} & \frac{\partial f_1(x)}{\partial x_2} & \dots & \frac{\partial f_1(x)}{\partial x_n} \\ \frac{\partial f_2(x)}{\partial x_1} & \frac{\partial f_2(x)}{\partial x_2} & \dots & \frac{\partial f_2(x)}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m(x)}{\partial x_1} & \frac{\partial f_m(x)}{\partial x_2} & \dots & \frac{\partial f_m(x)}{\partial x_n} \end{bmatrix} \in \mathbf{R}^{m \times n}$$

- equivalently

$$Df(x) = \begin{bmatrix} \nabla f_1(x)^T \\ \nabla f_2(x)^T \\ \vdots \\ \nabla f_m(x)^T \end{bmatrix} \in \mathbf{R}^{m \times n}$$

Chain rule

- for $f : \mathbf{R} \rightarrow \mathbf{R}^m$, $g : \mathbf{R}^m \rightarrow \mathbf{R}$ & $h = g \circ f$, i.e., $h(x) = g(f_1(x), \dots, f_m(x))$, derivative of h at $x \in \mathbf{R}$

$$h'(x) = \sum_{j=1}^m \frac{\partial}{\partial y_j} g(f(x)) f'_j(x) = \sum_{j=1}^m \nabla g(f(x))_j f'_j(x) \in \mathbf{R}$$

- for $f : \mathbf{R}^n \rightarrow \mathbf{R}^m$, $g : \mathbf{R}^m \rightarrow \mathbf{R}^p$ & $h = g \circ f$, Jacobian of h at $x \in \mathbf{R}^n$

$$Dh(x) = Dg(f(x)) Df(x) \in \mathbf{R}^{p \times n}$$

- note $Dg(f(x)) \in \mathbf{R}^{p \times m}$ & $Df(x) \in \mathbf{R}^{m \times n}$
- first is *special case* of second

Statistics Basics

Random experiments & probability law

- *random experiment*
 - outcome varies in unpredictable fashion (even) when experiment is being repeated under same conditions
 - specified by stating experimental procedure and set of one or more measurements or observations
- probability law
 - rule assigning probabilities to events of experiment that belong to event class \mathcal{F}

$$p : \mathcal{F} \rightarrow \mathbf{R}_+$$

- properties (or axioms)
 - for event $A \in \mathcal{F}$, $p(A)$ called *probability* of A
 - for event $A, B \in \mathcal{F}$ with $A \cap B = \emptyset$

$$p(A \cup B) = p(A) + p(B)$$

Conditional probability

- probability of event A given that event B has occurred, called *conditional probability*, denoted by

$$p(A|B)$$

- formula

$$p(A|B) = \frac{p(A \cap B)}{p(B)}$$

- thus

$$p(A \cap B) = p(A|B)p(B) = p(B|A)p(A)$$

- Bayes' theorem

$$p(A|B) = \frac{p(B|A)p(A)}{p(B)}$$

Independence

- for events A & B , when knowledge of occurrence of B does not alter probability of A
 - A said to be *independent* of B
- following statements are equivalent
 - A is independent of B
 - B is independent of A
 - $p(A|B) = p(A)$
 - $p(B|A) = p(B)$
 - $p(A \cap B) = p(A)p(B)$

Random variables

- *discrete* random variable X assumes values from countable set $\{x_1, x_2, \dots\}$
- *continuous* random variable X assumes values from \mathbf{R}
- random *vector* X assumes values from \mathbf{R}^n

PMF, PDF & CDF

- *probability mass function (PMF)* of discrete X

$$p_X(x) = p(X = x)$$

- *probability density function (PDF)* of continuous X

$$\int_a^b p_X(x) = p(a \leq X \leq b)$$

- *cumulative distribution function (CDF)* of (any) X

$$F_X(x) = p(X \leq x)$$

- for discrete X - $F_X(x) = \sum_{x' \leq x} p_X(x')$
- for continuous X - $F_X(x) = \int_{-\infty}^{\bar{x}} p_X(x') dx'$

Expected value, variance & covariance matrix

- expected value

- for discrete X

$$\mathbf{E} X = \sum_x x p_X(x)$$

- for continuous X

$$\mathbf{E} X = \int_{-\infty}^{\infty} x p_X(x) dx$$

- variance for scalar $X \in \mathbf{R}$

$$\mathbf{Var}(X) = \mathbf{E}(X - \mathbf{E} X)^2 = \mathbf{E} X^2 - (\mathbf{E} X)^2$$

- covariance matrix for vector $X \in \mathbf{R}^n$

$$\mathbf{Var}(X) = \mathbf{E}(X - \mathbf{E} X)(X - \mathbf{E} X)^T = \mathbf{E} XX^T - (\mathbf{E} X)(\mathbf{E} X)^T$$

Joint PMF, PDF & CDF

- *joint PMF* of discrete X & Y

$$p_{X,Y}(x, y) = p(X = x, Y = y)$$

- *join PDF* of continuous X & Y

$$\int_c^d \int_a^b p_{X,Y}(x, y) dx dy = p(a \leq X \leq b \ \& \ c \leq Y \leq d)$$

- *joint CDF* of X & Y

$$F_{X,Y}(x, y) = p(X \leq x \ \& \ Y \leq y)$$

Conditional expectation

for two random variables X & Y

- expected value of Y conditioned on X

$$\mathbf{E}(Y|X = x) = \int y p(y|x) dy$$

where

$$p(y|x) = \frac{p_{X,Y}(x,y)}{p_X(x)}$$

- note

$$\mathbf{E}_{X,Y} f(X, Y) = \mathbf{E}_X \mathbf{E}_Y (f(X, Y)|X)$$

because

$$\int \int f(x, y)p(x, y)dxdy = \int \left(\int f(x, y)p(y|x)dy \right) p(x)dx$$

Discrete Random Variables

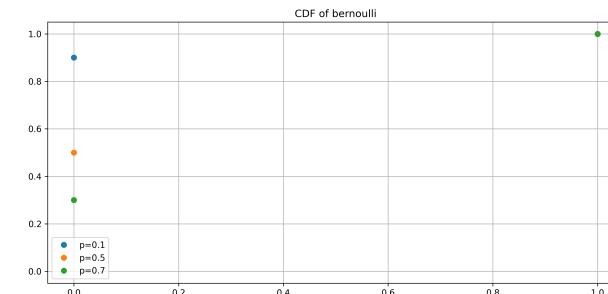
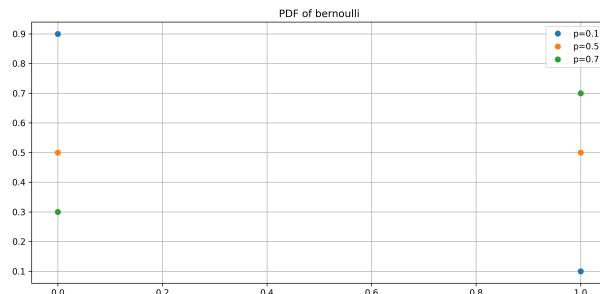
Bernoulli distribution

- model single binary trial with probability p of success (and, hence $(1 - p)$ of failure)
- PMF, mean, variance

$$p(k) = p^k(1-p)^{1-k} = \begin{cases} 1-p & \text{if } k=0 \\ p & \text{if } k=1 \end{cases}$$

$$\mathbf{E}(X) = p \quad \mathbf{Var}(X) = p(1-p)$$

- ML applications - (foundation for)
 - logistic regression, binary classification, modeling click-through rates, A/B testing outcomes



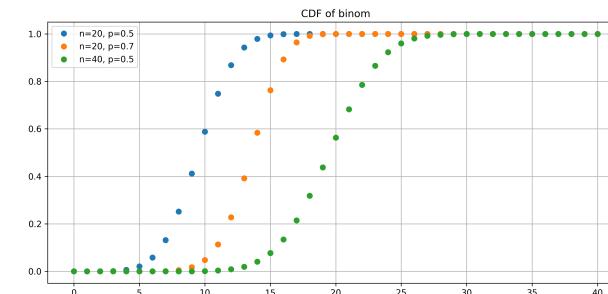
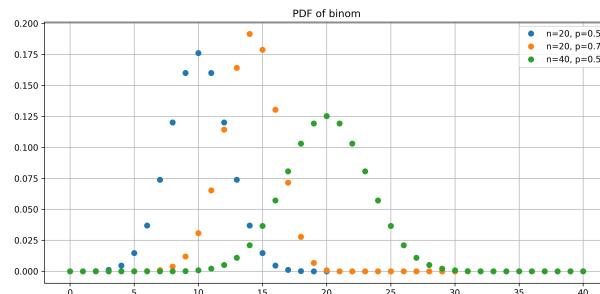
Binomial distribution

- model number of successes in n independent Bernoulli trials with probability p
- PMF, mean, variance

$$p(k) = \binom{n}{k} p^k (n-p)^{1-k} \quad \text{for } 1 \leq k \leq n$$

$$\mathbf{E}(X) = np \quad \mathbf{Var}(X) = np(1-p)$$

- ML applications
 - modeling conversion rates, quality control testing, ensemble voting methods, batch processing success rates



Multinomial distribution

- generalizes binomial distribution to multiple categories with probabilities p_1, \dots, p_k
- PMF, mean, variance

$$p(k) = \frac{n!}{x_1! \cdots x_k!} p_1^{x_1} \cdots p_k^{x_k}$$

$$\mathbf{E}(X_i) = np_i \quad \mathbf{Var}(X_i) = np_i(1 - p_i) \quad \mathbf{Cov}(X_i, X_j) = -np_ip_j$$

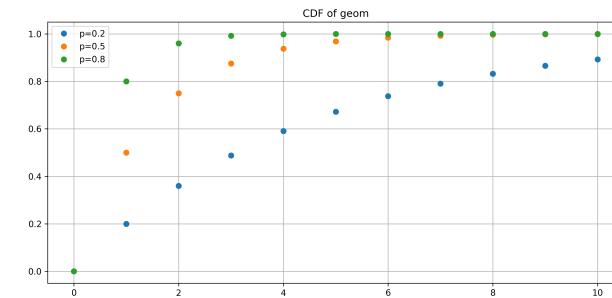
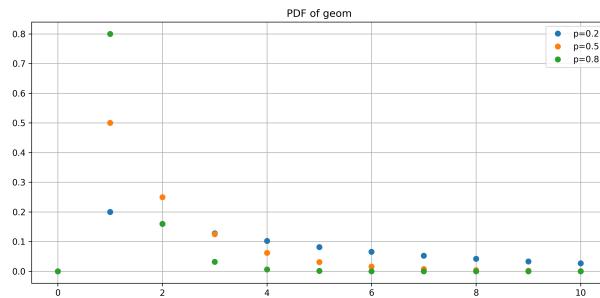
- ML applications
 - multi-class classification, topic modeling, document classification, NLP, recommendation system
 - market basket analysis, survey analysis, election pollings
 - genetics, clinical trials, quality control
- widely used in *Bayesian inference* with Dirichlet priors

Geometric distribution

- model number of trials needed to achieve first success in independent Bernoulli trials
- PMF, mean, variance

$$p(k) = p(1 - p)^{k-1} \quad \mathbf{E}(X) = 1/p \quad \mathbf{Var}(X) = (1 - p)/p^2$$

- ML applications
 - modeling time-to-conversion, failure analysis, reinforcement learning episode lengths, web crawling stopping conditions
- memoryless property $p(X > m + n | X > m) = p(X > n)$

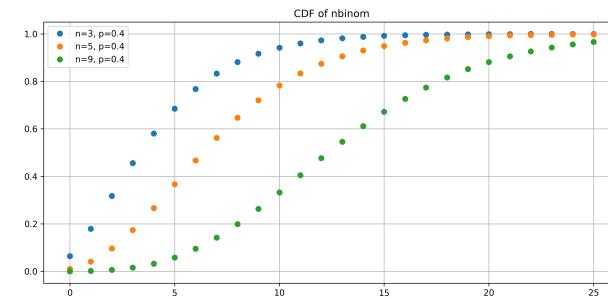
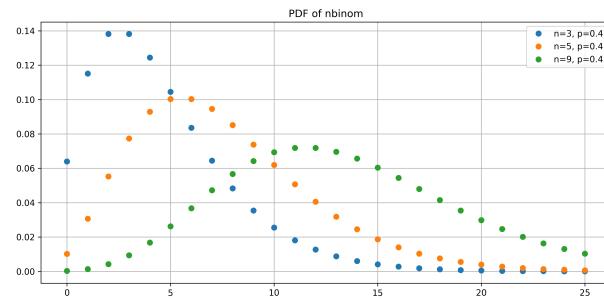


Negative binomial distribution

- model number of trials needed to achieve r successes in independent Bernoulli trials
- PMF, mean, variance

$$p(k) = \binom{k-1}{r-1} p^r (1-p)^{k-r} \quad \mathbf{E}(X) = r/p \quad \mathbf{Var}(X) = r(1-p)/p^2$$

- ML applications
 - modeling overdispersed count data, customer acquisition costs, reliability engineering, text analysis for word frequencies
- *often used when Poisson assumptions are violated due to overdispersion*

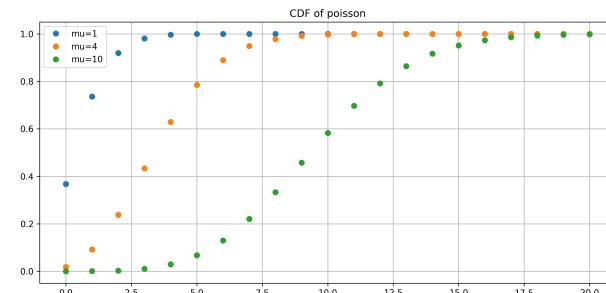
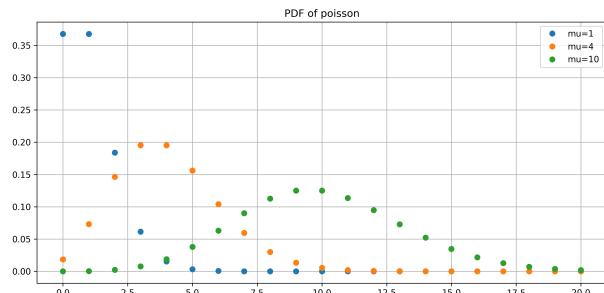


Poisson distribution

- model number of events occurring in fixed interval of time or space
- PMF, mean, variance ($\lambda > 0$)

$$p(k) = e^{-\lambda} \lambda^k / k! \quad \mathbf{E}(X) = \lambda \quad \mathbf{Var}(X) = \lambda$$

- ML applications
 - modeling web traffic, system failures
 - word counts (in NLP), user interactions (in recommendation systems)
- approximates binomial when n is large & p is small with $= np$
- sum of independent Poisson variables is Poisson

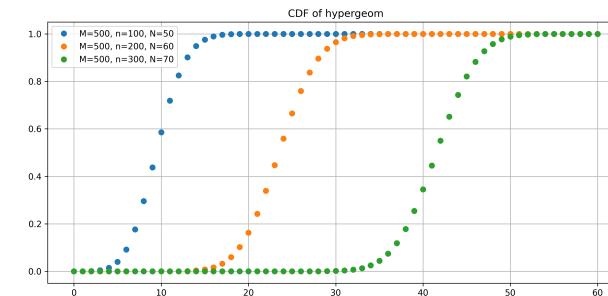
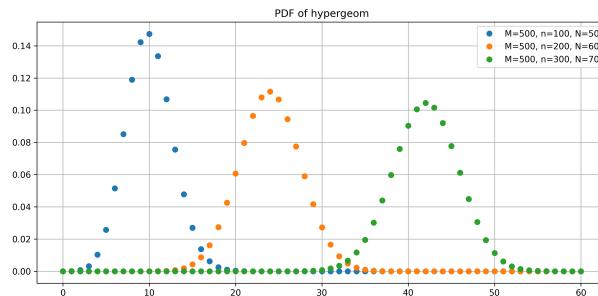


Hypergeometric distribution

- model number of successes in n draws without replacement from finite population of size N containing K successes
- PMF, mean, variance ($N, K \in \mathbf{N}$ with $N > K$)

$$p(k) = \frac{\binom{K}{k} \binom{N-K}{n-k}}{\binom{N}{n}} \quad \mathbf{E}(X) = \frac{nK}{N} \quad \mathbf{Var}(X) = \frac{nK}{N} \cdot \frac{N-K}{N} \cdot \frac{N-n}{N-1}$$

- ML applications
 - sampling without replacement, quality control testing
 - feature selection validation, A/B testing with finite populations



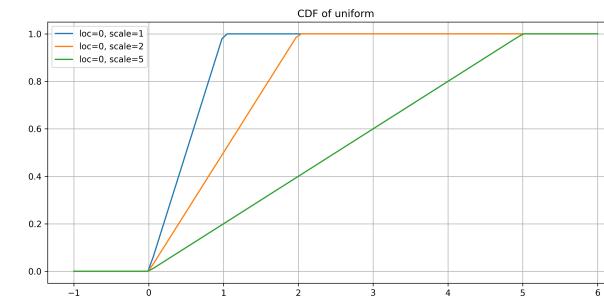
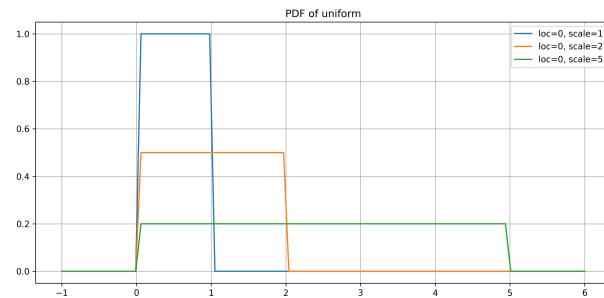
Continuous Random Variables

Uniform distribution

- model equally likely outcomes over continuous interval $[a, b]$ representing complete uncertainty within bounded range
- PDF, mean, variance ($a, b \in \mathbf{R}$ with $b > a$)

$$p(x) = 1/(b - a)I_{[a,b]}(x) \quad \mathbf{E}(X) = (a + b)/2 \quad \mathbf{Var}(X) = (b - a)^2/12$$

- ML applications
 - Monte Carlo sampling, generating baseline distributions for hypothesis testing
- maximum entropy distribution for bounded continuous support
- foundation for pseudo-random number generation and inverse transform sampling

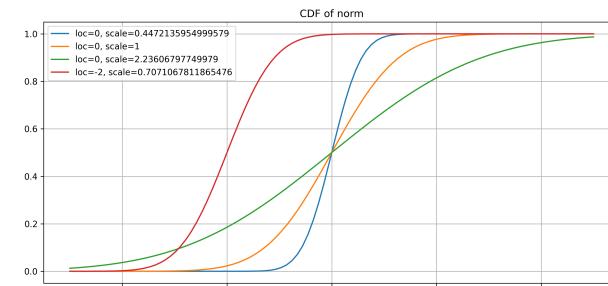
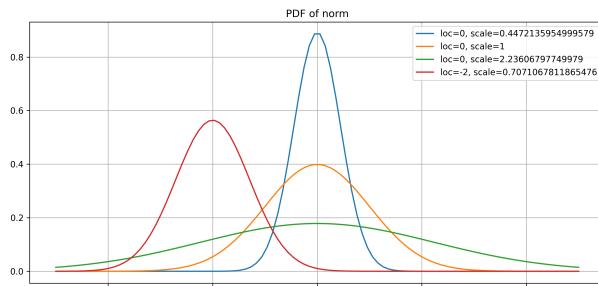


Gaussian distribution

- most important continuous distribution
- model symmetric bell-shaped data arising from many natural processes
- PDF, mean, variance ($\mu \in \mathbf{R}$, $\sigma > 0$)

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-\mu)^2/2\sigma^2} \quad \mathbf{E}(X) = \mu \quad \mathbf{Var}(X) = \sigma^2$$

- ML applications
 - linear regression error terms, NN weight initialization, PCA, noise modeling
- invariant under linear transformations, maximum entropy for given mean and variance

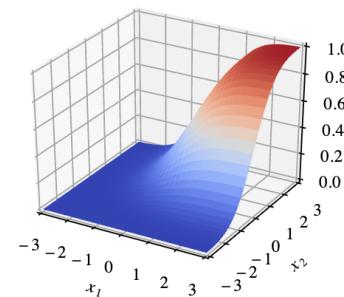
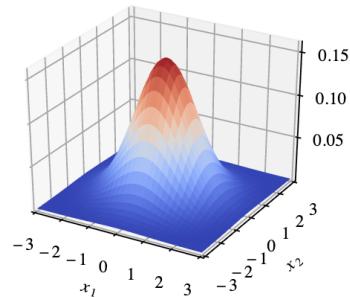


Multivariate Gaussian distribution

- generalize scalar Gaussian to random vector
- PDF, mean, variance ($\mu \in \mathbf{R}^n$, $\Sigma \in \mathbf{S}_{++}^n$)

$$p(x) = \frac{1}{(2\pi)^{n/2} \det(\Sigma)^{1/2}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)} \quad \mathbf{E}(X) = \mu \quad \mathbf{Cov}(X) = \Sigma$$

- ML applications
 - Gaussian mixture, PCA, Kalman filtering, Gaussian processes, latent variable models
- maximum likelihood estimation having closed-form solution, foundation for many Bayesian models

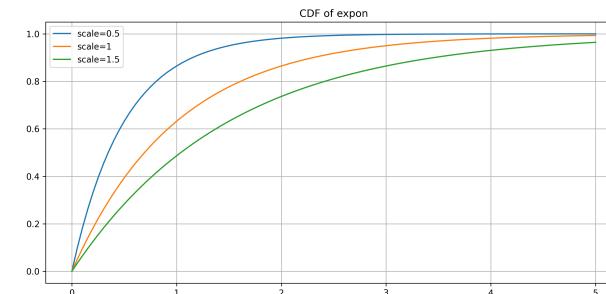
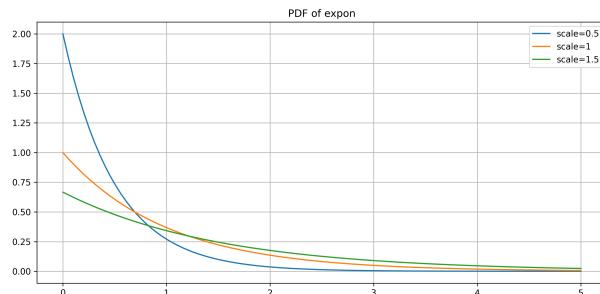


Exponential distribution

- model time between events in Poisson process, representing memoryless waiting times or lifetimes
- PDF, mean, variance ($\lambda > 0$)

$$p(x) = \lambda e^{-\lambda x} I_{[0,\infty)}(x) \quad \mathbf{E}(X) = 1/\lambda \quad \mathbf{Var}(X) = 1/\lambda^2$$

- ML applications
 - system failure times, web session durations, survival analysis
- memoryless property $p(X > s+t | X > s) = p(X > t)$ - only continuous distribution with this property, minimum of exponentials is exponential

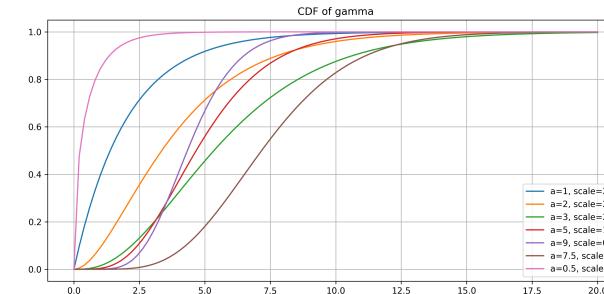
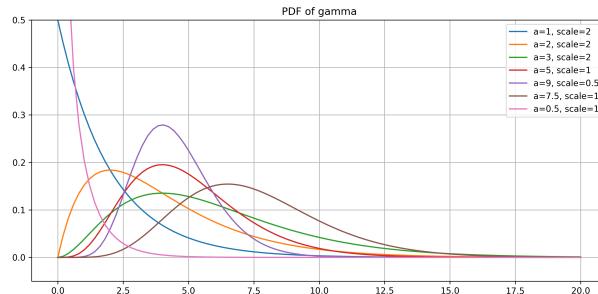


Gamma distribution

- model positive continuous values - generalizing exponential distribution to allow for more flexible shapes, *e.g.*, for waiting times for multiple events
- PDF, mean, variance ($\alpha, \beta > 0$)

$$p(x) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x} I_{[0,\infty)}(x) \quad \mathbf{E}(X) = \alpha/\beta \quad \mathbf{Var}(X) = \alpha/\beta^2$$

- ML applications
 - survival analysis, queuing theory
- exponential is special case when $\alpha = 1$, sum of independent exponentials is gamma, conjugate prior for Poisson and exponential distributions

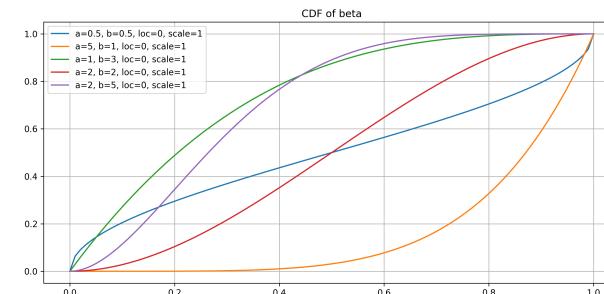
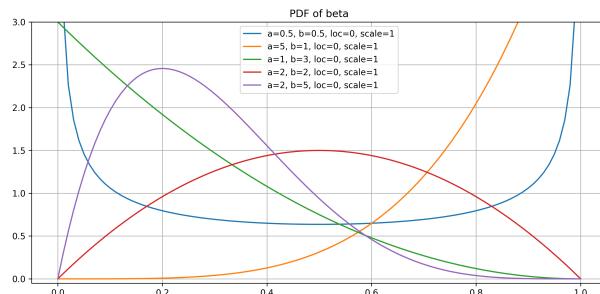


Beta distribution

- model probabilities and proportions, defined on $[0, 1]$ with flexible shapes from uniform to highly skewed
- PDF, mean, variance ($\alpha, \beta > 0$)

$$p(x) = \frac{\Gamma(\alpha, \beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1} (1-x)^{\beta-1} \quad \mathbf{E}(X) = \frac{\alpha}{\alpha + \beta} \quad \mathbf{Var}(X) = \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)}$$

- ML applications
 - modeling success rates, A/B testing, probability calibration
- uniform is special case when $\alpha = \beta = 1$, conjugate prior for Bernoulli & binomial related to Dirichlet distribution

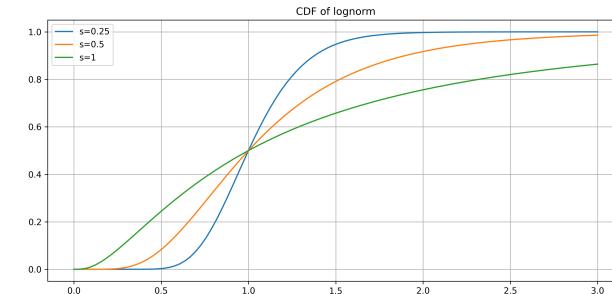
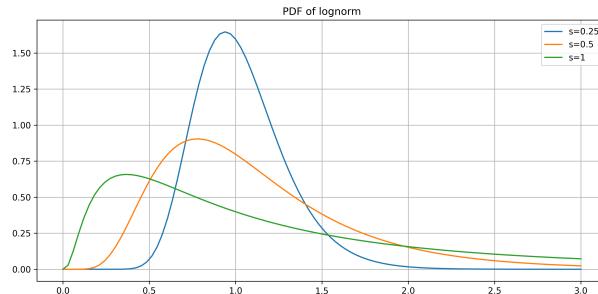


Log-normal distribution

- model positive values where logarithm follows normal distribution, representing multiplicative processes and heavy-tailed phenomena
- PDF, mean, variance ($\mu \in \mathbf{R}$, $\sigma > 0$)

$$p(x) = e^{-(\log x - \mu)^2 / 2\sigma^2} / x\sigma\sqrt{2\pi} \quad \mathbf{E}(X) = e^{\mu + \sigma^2 / 2} \quad \mathbf{Var}(X) = (e^{\sigma^2} - 1)e^{2\mu + \sigma^2}$$

- ML applications
 - modeling income distributions, stock prices, file sizes, network traffic, biological measurements, computational complexity
- heavy right tail, multiplicative central limit theorem

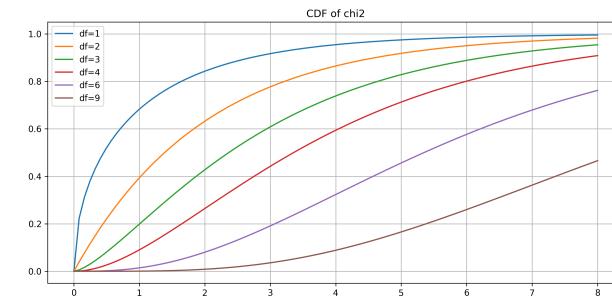
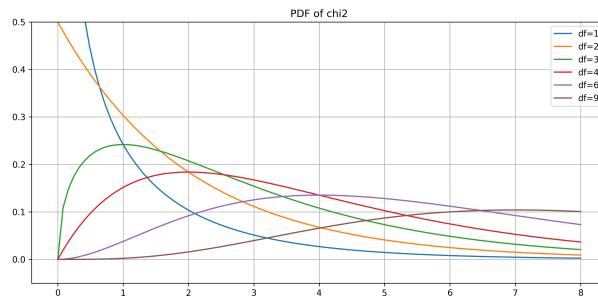


Chi-square distribution

- model sum of squares of independent standard normal random variables, fundamental in statistical testing and confidence intervals
- PDF, mean, variance ($\nu \in \mathbb{N}$ - degree of freedom)

$$p(x) = \frac{1}{2^{\nu/2}\Gamma(\nu/2)}x^{\nu/2-1}e^{-x/2}I_{[0,\infty)}(x) \quad \mathbf{E}(X) = \nu \quad \mathbf{Var}(X) = 2\nu$$

- ML applications
 - goodness-of-fit testing, feature selection, confidence intervals for variance, regularization in NN
- special case of gamma distribution, sum of independent chi-squares is chi-square



Student's t -distribution

- model sum of squares of independent standard normal random variables, fundamental in statistical testing and confidence intervals
- PDF, mean, variance ($\nu > 0$ degrees of freedom - almost always positive integer)

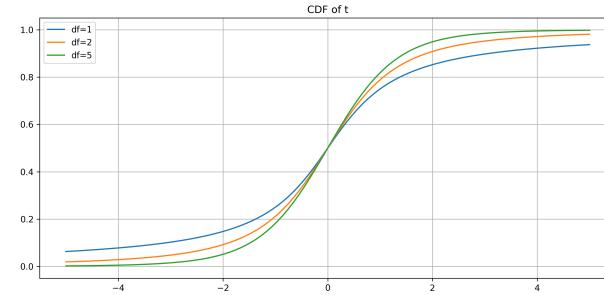
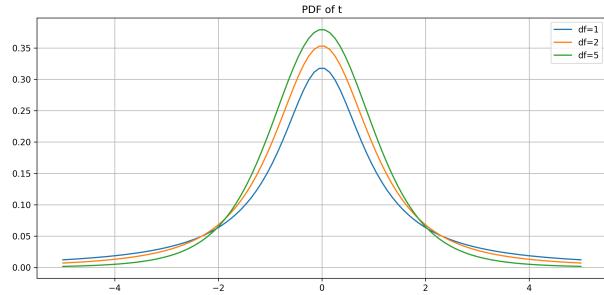
$$p(x) = \frac{\Gamma((\nu + 1)/2)}{\sqrt{\pi\nu}\Gamma(\nu/2)}(1 + x^2/\nu)^{-(\nu+1)/2}$$

$$\mathbf{E}(X) = \begin{cases} 0 & \text{if } \nu > 1 \\ \text{undefined} & \text{otherwise} \end{cases}$$

$$\mathbf{Var}(X) = \begin{cases} \nu/(\nu - 2) & \text{if } \nu > 2 \\ \infty & \text{if } 1 < \nu \leq 2 \\ \text{undefined} & \text{otherwise} \end{cases}$$

- ML applications
 - Bayesian inference, robust regression, confidence intervals with small samples, uncertainty quantification in DL

- heavier tails than normal, approaches standard normal as ν approaches ∞ , symmetric around zero, undefined moments for small ν

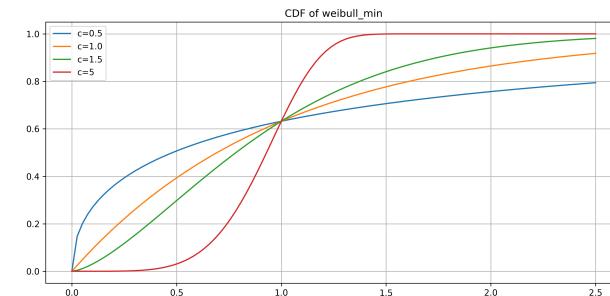
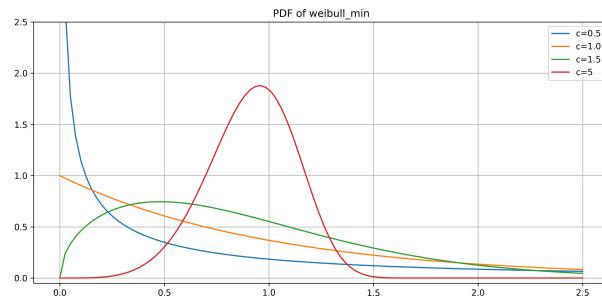


Weibull distribution

- model survival times & failure rates with flexible hazard functions, generalizing exponential distribution for reliability analysis
- PDF, mean, variance ($\lambda, k > 0$)

$$p(x) = (k/\lambda)(x/\lambda)^{k-1} e^{-(x/\lambda)^k} I_{[0,\infty)}(x) \quad \mathbf{E}(X) = \lambda\Gamma(1 + 1/k)$$

- ML applications
 - survival analysis, reliability engineering, wind speed modeling, NN activation functions, extreme value theory
- flexible hazard function, minimum of Weibull variables is Weibull

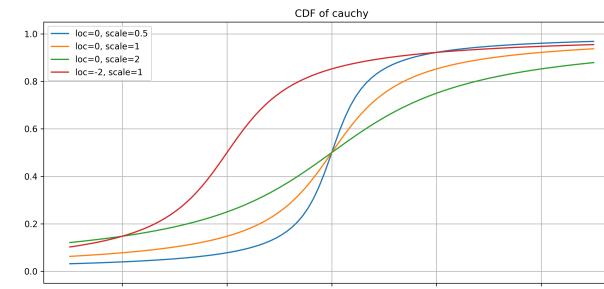
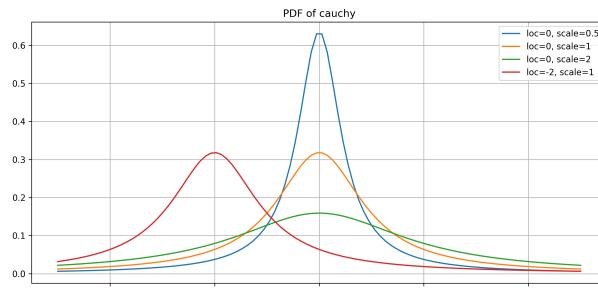


Cauchy distribution

- model heavy-tailed symmetric data with undefined mean and variance, arising in physics and robust statistics
- PDF, mean, variance ($x_0 \in \mathbf{R}$, $\gamma > 0$)

$$p(x) = \frac{1}{\pi\gamma(1 + ((x - x_0)/\gamma)^2)} \quad \mathbf{E}(X) = \text{undefined} \quad \mathbf{Var}(X) = \text{undefined}$$

- ML applications
 - robust statistics, modeling outliers, Bayesian inference with heavy-tailed priors, physics simulations, anomaly detection
- no defined moments, stable distribution, ratio of two independent normals is Cauchy

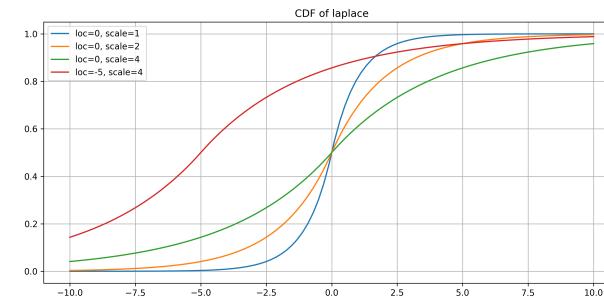
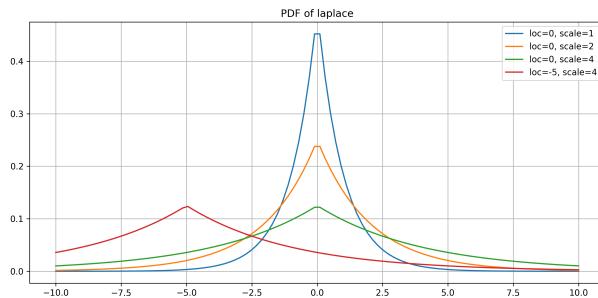


Laplace distribution

- model symmetric data with heavier tails than normal, representing difference between two independent exponential variables
- PDF, mean, variance ($\mu \in \mathbf{R}$, $b > 0$)

$$p(x) = \frac{1}{2b} \exp(-|x - \mu|/b) \quad \mathbf{E}(X) = \mu \quad \mathbf{Var}(X) = 2b^2$$

- ML applications
 - lasso, robust regression, sparse coding, image processing, privacy-preserving ML
- maximum entropy for given mean absolute deviation, related to L1 penalty, robust to outliers (fundamentally more than normal distribution)



Pareto distribution

- model heavy-tailed phenomena following power-law distributions, representing “80-20 rule” and scale-free networks
- PDF, mean, variance ($x_m, \alpha > 0$)

$$p(x) = \alpha x_m^\alpha / x^{\alpha+1}$$

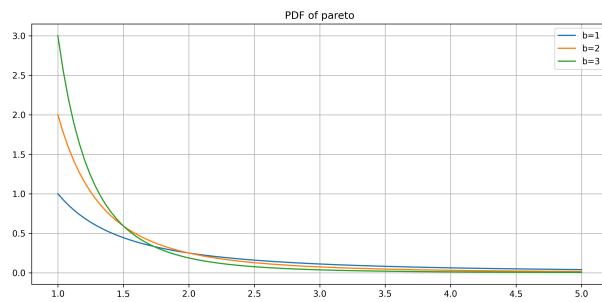
$$\mathbf{E}(X) = \begin{cases} \infty & \text{if } \alpha \leq 1 \\ \alpha x_m / (\alpha - 1) & \text{if } \alpha > 1 \end{cases}$$

$$\mathbf{Var}(X) = \begin{cases} \infty & \text{if } \alpha \leq 2 \\ \alpha x_m^2 / (\alpha - 1)^2 (\alpha - 2) & \text{if } \alpha > 2 \end{cases}$$

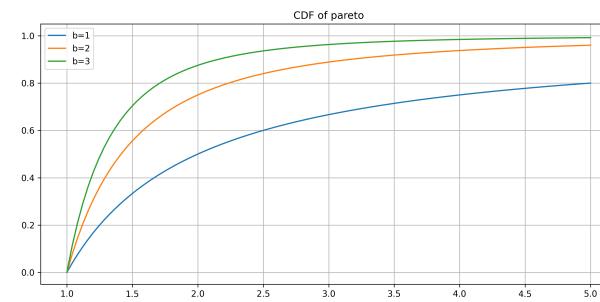
- ML applications
 - model wealth distributions, network degree distributions, web page rankings, file sizes, NLP

- heavy right tail, scale-free property, finite moments only for sufficiently large α , basis for power-law distributions

PDF



CDF



ML Basics

Estimation, Regression, and Inference

The optimal estimator

- estimation problem
 - for two random variables $X \in \mathbf{R}^n$ & $Y \in \mathbf{R}^m$
 - design *estimator or predictor* $g : \mathbf{R}^n \rightarrow \mathbf{R}^m$ to make $g(X)$ *as close as possible* to Y
- when *closeness* measured by mean-square-error (MSE), *the optimal solution* exists

$$g^*(x) = \mathbf{E}(Y|X = x)$$

Proof of optimality

$$\begin{aligned}
 \mathbf{E}_{X,Y}((g(X) - g^*(X))^T(g^*(X) - Y)) &= \mathbf{E}_X \mathbf{E}_Y((g(X) - g^*(X))^T(g^*(X) - Y)|X) \\
 &= \mathbf{E}_X((g(X) - g^*(X))^T \mathbf{E}_Y(g^*(X) - Y)|X) \\
 &= 0
 \end{aligned}$$

hence

$$\begin{aligned}
 \mathbf{E} \|g(X) - Y\|_2^2 &= \mathbf{E} \|g(X) - g^*(X) + g^*(X) - Y\|_2^2 \\
 &= \mathbf{E} \|g(X) - g^*(X)\|_2^2 + \mathbf{E} \|g^*(X) - Y\|_2^2 + 2 \mathbf{E}(g(X) - g^*(X))^T(g^*(X) - Y) \\
 &= \mathbf{E} \|g(X) - g^*(X)\|_2^2 + \mathbf{E} \|g^*(X) - Y\|_2^2 \\
 &\geq \mathbf{E} \|g^*(X) - Y\|_2^2
 \end{aligned}$$

Regression

- in most cases, *not* possible to obtain g^* (unless, e.g., full knowledge of joint PDF)
- regression problem
 - given data set $D = \{(x_1, y_1), \dots, (x_N, y_N)\} \subset \mathbf{R}^n \times \mathbf{R}^m$
 - find $g : \mathbf{R}^n \rightarrow \mathbf{R}^m$ to make $g(X)$ *as close as possible* to Y
- given certain regression method, regressor depends on dataset D

$$g(\cdot; D)$$

Bias & variance

assuming \mathcal{D} is random variable for dataset D

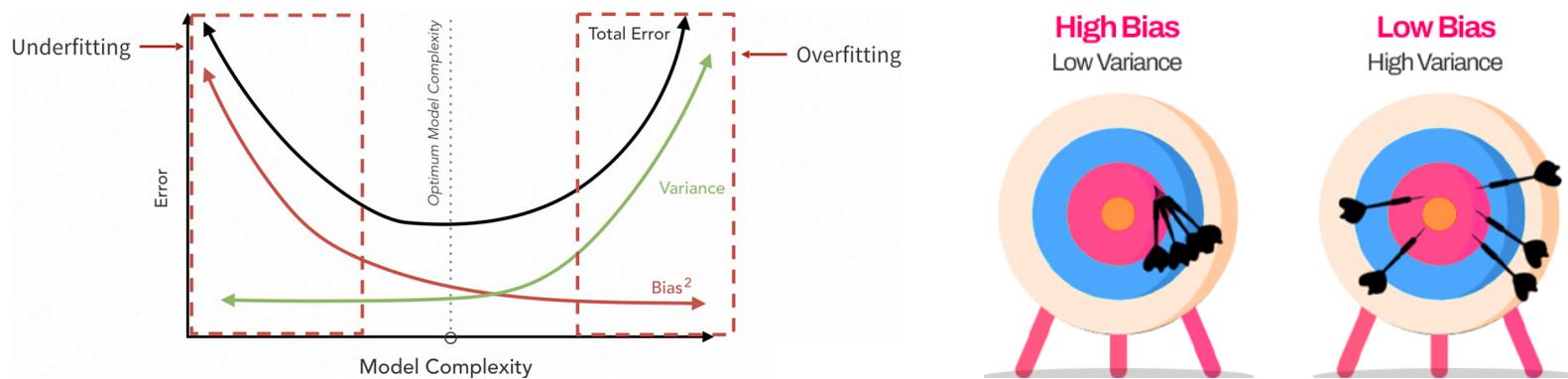
- estimation MSE is

$$\begin{aligned}
 & \mathbf{E}_{X,Y,\mathcal{D}} \|g(X; \mathcal{D}) - Y\|_2^2 \\
 &= \underbrace{\mathbf{E}_{X,\mathcal{D}} \|g(X; \mathcal{D}) - \mathbf{E}_{\mathcal{D}} g(X; \mathcal{D})\|_2^2}_{\text{variance}} + \underbrace{\mathbf{E}_X \|\mathbf{E}_{\mathcal{D}} g(X; \mathcal{D}) - g^*(X)\|_2^2}_{\text{bias}} + \underbrace{\mathbf{E}_{X,Y} \|g^*(X) - Y\|_2^2}_{\text{noise}} \\
 &= \underbrace{\mathbf{E}_{X,\mathcal{D}} \|g(X; \mathcal{D}) - \mathbf{E}_{\mathcal{D}} g(X; \mathcal{D})\|_2^2}_{\text{variance}} + \underbrace{\mathbf{E}_{X,Y} \|\mathbf{E}_{\mathcal{D}} g(X; \mathcal{D}) - Y\|_2^2}_{\text{bias + noise}}
 \end{aligned}$$

- bias & variance
 - *bias* measures how good model is in average
 - *variance* measures how much model varies depending on dataset it is trained on
- *noise* cannot be reduced even with the optimal predictor

Model choice & hyperparameter optimization

- want to choose model or modeling method to make both bias & variance low
 - (too) complex models have low bias, but high variance
 - (too) simple models have low variance, but high bias
- usually solved by *hyperparameter optimization*
 - sometimes called *hyperparameter tuning*



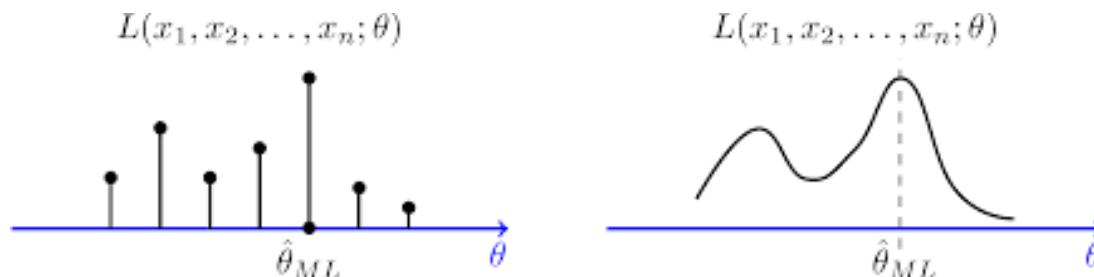
MLE

- maximum likelihood estimation (MLE)
 - assume parameterized distribution of $X \in \mathbb{R}^n$ by $\theta \in \Theta$ - $p(x; \theta)$
 - find θ maximizing *likelihood function*

$$p(x_1, \dots, x_N; \theta) = \prod_{i=1}^N p(x_i; \theta)$$

- MLE solution

$$\hat{\theta}_{\text{MLE}} = \underset{\theta \in \Theta}{\operatorname{argmax}} \prod_{i=1}^N p(x_i; \theta)$$



MAP estimation

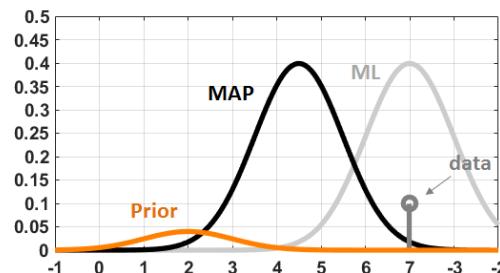
- maximum a posteriori (MAP) estimation
 - assume *prior knowledge* of θ - $p(\theta)$
 - assume parameterized distribution of $X \in \mathbb{R}^n$ by θ - $p(x|\theta)$
 - find θ maximizing *posteriori probability*

$$p(\theta|x_1, \dots, x_N)$$

– Bayes' theorem implies $p(\theta|x_1, \dots, x_N) \propto p(\theta) \prod_{i=1}^N p(x_i|\theta)$

- MAP solution

$$\hat{\theta}_{\text{MAP}} = \underset{\theta \in \Theta}{\operatorname{argmax}} p(\theta) \prod_{i=1}^N p(x_i|\theta)$$



Bayesian inference

- both MLE & MAP estimation are *point estimations*
- Bayesian inference
 - updates *prior distribution* by replacing it with posterior distribution
- conjugate prior
 - if prior can be further parameterized by hyperparameter α and posterior is in same probability distribution family, both prior and posterior called *conjugate distributions*, prior called *conjugate prior*

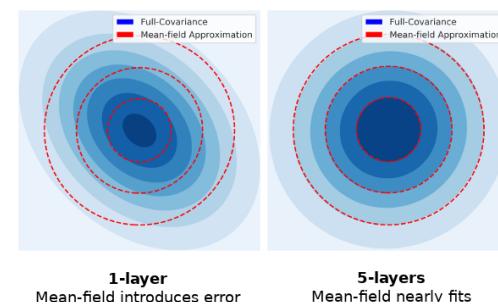
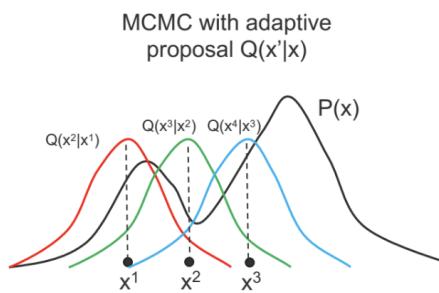
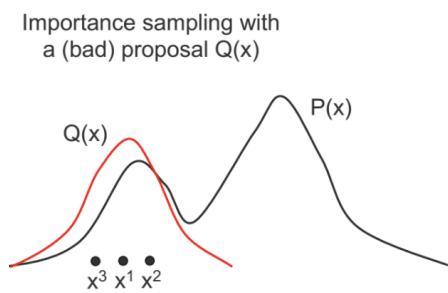
$$p(\theta; \alpha)$$

- in this case, can update hyperparameter α , i.e., find α^+ such that

$$p(\theta; \alpha^+) = p(\theta | x_1, \dots, x_N; \alpha) = \frac{p(\theta; \alpha) \prod_{i=1}^N p(x_i | \theta; \alpha)}{p(x_1, \dots, x_N; \alpha)}$$

Bayesian algorithms & methods

- exact inference methods
 - conjugate priors - *e.g.*, Beta-Binomial, Normal-Normal, *etc.*
- Markov Chain Monte Carlo (MCMC)
 - Metropolis-Hastings algorithm, Gibbs sampling, Hamiltonian Monte Carlo (HMC)
- variational inference (VI)
 - mean field variational Bayes - assuming parameter independence for tractability
 - structured variational inference - maintaining dependencies & inference tractability
 - variational autoencoder (VAE) - NN-based VI for complex distributions

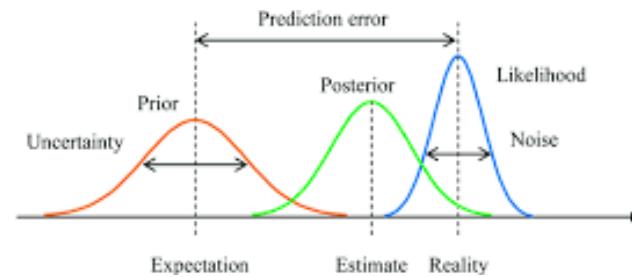


Pros & cons of Bayesian inference

- pros
 - principled uncertainty quantification - providing complete probability distributions
 - incorporates prior knowledge - allowing to formally include domain expertise, *etc.*
 - coherent framework - providing mathematically consistent approach
 - natural sequential learning - easily handles streaming data or online learning scenarios
 - interpretable results - outputs directly interpretable as probabilities
- cons
 - computational complexity - often requiring sophisticated sampling methods
 - prior sensitivity, scalability issues, implementation difficulty, slower inference, model selection challenges

$$p(\theta | \text{data}) = \frac{p(\text{data} | \theta) \cdot p(\theta)}{p(\text{data})}$$

↑ Posterior ↓ Likelihood ↓ Prior
 ↑ Normalization

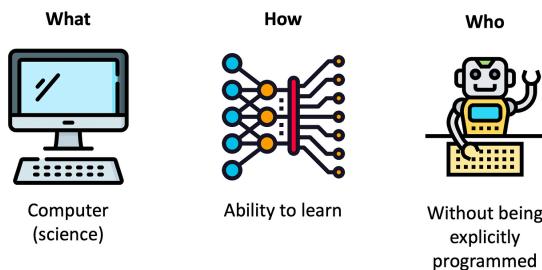


Machine Learning

Machine learning

- ML

- subfield of computer science that
“gives computers the ability to learn without being explicitly programmed.”
- Arthur Samuel (1959)
- *not* magic, still less intelligent than humans for many cases
- *numerically minimizes* certain (mathematical) loss function to (indirectly) solve *some statistically meaningful* problems



Machine learning is the subfield of computer science that gives “computers the ability to learn without being explicitly programmed.”



Arthur Samuel

Two famous quotes and one non-famous quote

- Albert Einstein

The grand aim of all science is to cover the greatest number of empirical facts by logical deduction from the smallest possible number of hypotheses or axioms.

- Alfred North Whitehead

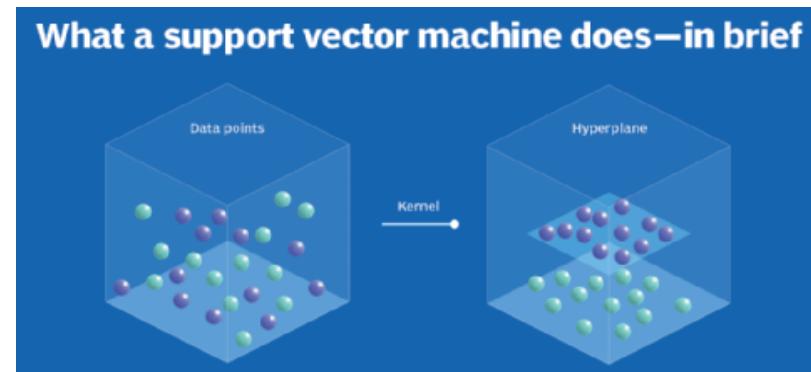
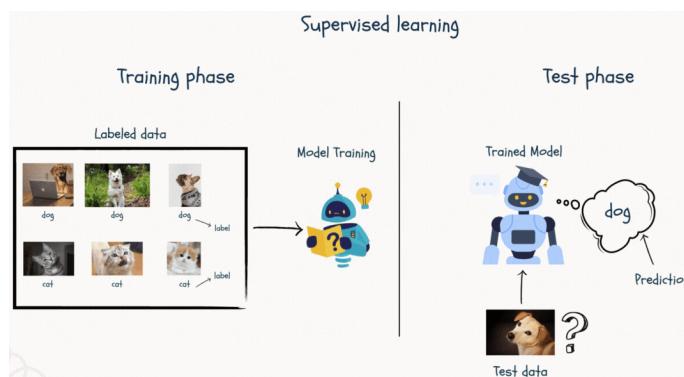
Civilization advances by extending the number of important operations which we can perform without thinking about them. - Operations of thought are like cavalry charges in a battle – they are strictly limited in number, they require fresh horses, and must only be made at decisive moments.

- Demis Hassabis

... biology can be thought of as information processing system, albeit extraordinarily complex and dynamic one ... just as mathematics turned out to be the right description language for physics, biology may turn out to be the perfect type of regime for the application of AI!

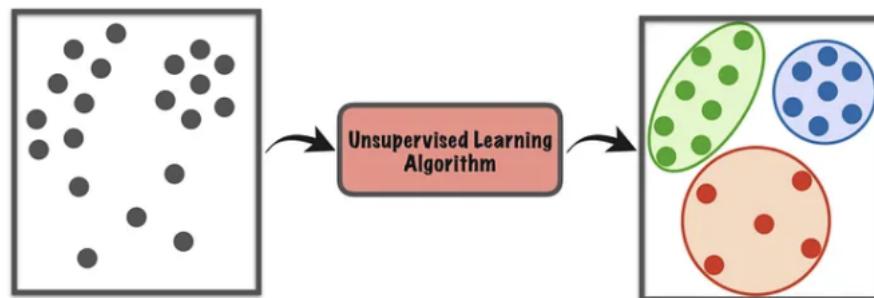
Supervised learning

- most basic and widely used type of ML
- model is trained on dataset where correct output or “label” is provided for each input
- use cases
 - image classification, object detection, semantic segmentation
 - natural language processing (NLP) - text classification, sentiment analysis
 - predictive modeling, medical diagnosis
- algorithms
 - linear regression, logistic regression, decision trees, random forest
 - support vector machine (SVM), k -nearest neighbors (kNN)



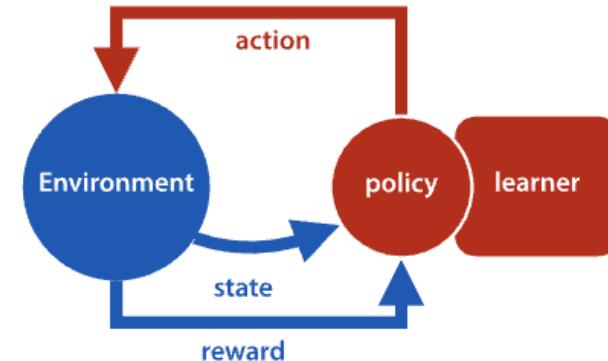
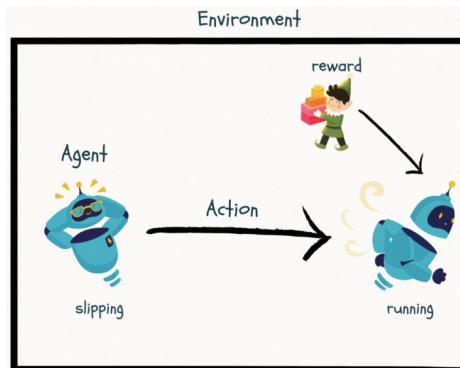
Unsupervised learning

- model is given dataset without any labels or output
- model finds patterns & structure within data on its own
- use cases
 - clustering, dimensionality reduction
 - anomaly detection, generative models
- algorithms
 - k-means clustering, hierarchical clustering, principal component analysis (PCA)
 - t-distributed stochastic neighbor embedding (t-SNE)



Reinforcement learning

- (quite different from supervised & unsupervised learnings)
- model learns from consequences of its actions
 - model receives feedback on its performance; feedback called *reward*
 - uses that information to adjust its actions and improve its performance over time
- use cases
 - robotics, game playing, autonomous vehicles, industrial control
 - healthcare, finance
- algorithms
 - Q-learning, SARSA, DQN, A3C, policy gradient



ML Formulations

Statistical problem formulation

- assume data set $X_m = \{x^{(1)}, \dots, x^{(m)}\}$
 - drawn independently from (true, but unknown) data generating distribution $p_{\text{data}}(x)$
- maximum likelihood estimation (MLE) is to solve

$$\text{maximize } p_{\text{model}}(X; \theta) = \prod_{i=1}^m p_{\text{model}}(x^{(i)}; \theta)$$

where optimization variable is θ

- find *most plausible or likely model* that fits data
- equivalent (but more numerically tractable) formulation

$$\text{maximize } \log p_{\text{model}}(X; \theta) = \sum_{i=1}^m \log p_{\text{model}}(x^{(i)}; \theta)$$

MLE & KL divergence

- in information theory, Kullback-Leibler (KL) divergence defines distance between two probability distributions p & q

$$D_{\text{KL}}(p\|q) = \mathbf{E}_{X \sim p} \log p(X)/q(X) = \int_{x \in \Omega} p(x) \log \frac{p(x)}{q(x)} dx$$

- KL divergence between data distribution p_{data} & model distribution p_{model} can be approximated by Monte Carlo method as

$$D_{\text{KL}}(p_{\text{data}}\|p_{\text{model}}(\theta)) \simeq \frac{1}{m} \sum_{i=1}^m (\log p_{\text{data}}(x^{(i)}) - \log p_{\text{model}}(x^{(i)}; \theta))$$

where $x^{(i)}$ are drawn (of course) according to p_{data}

- hence *minimizing KL divergence is equivalent to solving MLE problem!*

Equivalence of MLE to MSE

- assume model is Gaussian, *i.e.*, $y \sim \mathcal{N}(g_\theta(x), \Sigma)$ ($g_\theta(x) \in \mathbf{R}^p$, $\Sigma \in \mathbf{S}_{++}^p$)

$$p(y|x; \theta) = \frac{1}{\sqrt{2\pi}^p |\Sigma|^{1/2}} \exp \left(-\frac{1}{2} (y - g_\theta(x))^T \Sigma^{-1} (y - g_\theta(x)) \right)$$

- assuming that $\Sigma = \alpha I_p$, log-likelihood becomes

$$\begin{aligned} \sum_{i=1}^m \log p(x^{(i)}, y^{(i)}; \theta) &= \sum_{i=1}^m \log p(y^{(i)}|x^{(i)}; \theta) p(x^{(i)}) \\ &= - \sum_{i=1}^m \|y^{(i)} - g_\theta(x^{(i)})\|_2^2 / 2\alpha - \frac{pm}{2} \log(2\pi\alpha) + \sum_{i=1}^m \log p(x^{(i)}) \end{aligned}$$

- hence *minimizing mean-square-error (MSE) is equivalent to solving MLE problem!*

Numerical optimization problem formulation

- (true) problem to solve

$$\text{minimize } \mathbf{E} l(g_\theta(X), Y)$$

- *impossible* to solve

- basic formulation - surrogate problem to solve

$$\text{minimize } f(\theta) = \frac{1}{m} \sum_{i=1}^m l(g_\theta(x^{(i)}), y^{(i)})$$

- formulation with regularization

$$\text{minimize } f(\theta) = \frac{1}{m} \sum_{i=1}^m l(g_\theta(x^{(i)}), y^{(i)}) + \gamma r(\theta)$$

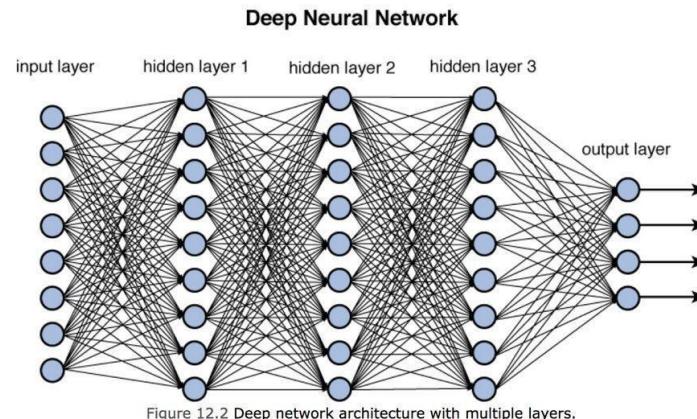
- stochastic gradient descent (SGD)

$$\theta^{(k+1)} = \theta^{(k)} - \alpha_k \nabla f(\theta^{(k)})$$

Deep Learning

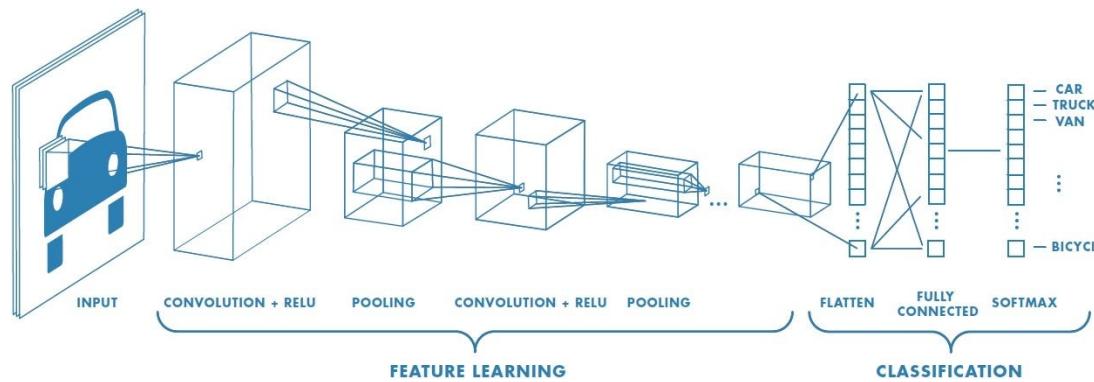
Deep learning (DL)

- machine learning using artificial neural networks with multiple layers for
 - automatically learning hierarchical representations of data
- key components
 - deep neural networks, hidden layers, backpropagation, activation functions
 - hierarchical feature learning, representation learning, end-to-end learning
- key breakthroughs enabling DL
 - massively available data, GPU computing, algorithmic advances



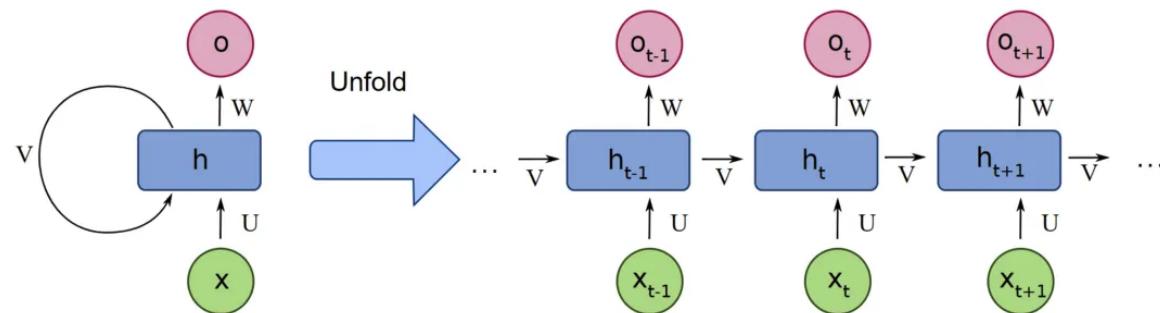
Convolutional neural network (CNN)

- specialized DL learning architecture designed for
 - processing grid-like data such as images
 - where spatial relationships between pixels matter
- key components
 - convolutional layers, pooling layers, activation functions, fully connected layers
- how it works
 - feature extraction, translation invariance, parameter sharing
- why it excels
 - local connectivity, hierarchical learning



Recurrent neural network (RNN)

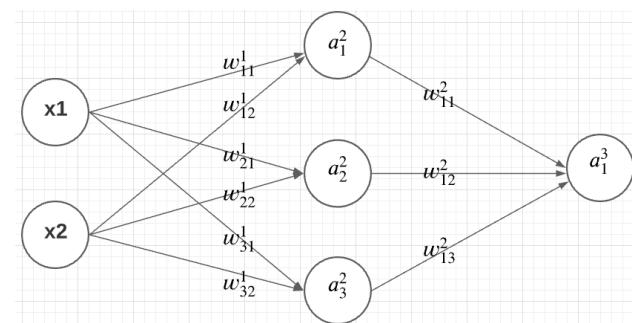
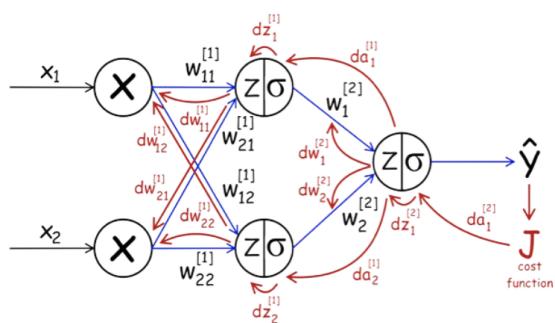
- neural network designed for
 - processing sequential data by maintaining memory of previous inputs
- key components
 - hidden states, recurrent connections, input/output layers, weight sharing
- how it works
 - sequential processing, memory mechanism, temporal dependencies
- why it excels
 - variable length input, context awareness, flexible architecture
- variants - long short-term memory (LSTM), gated recurrent unit (GRU)



Training DNN using SGD

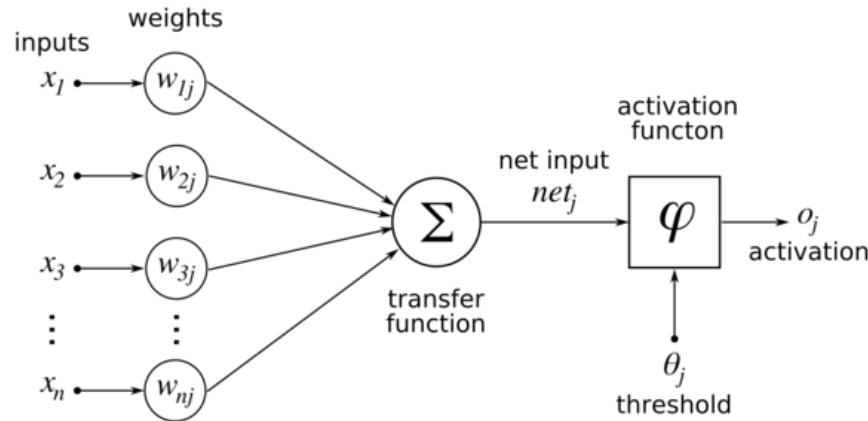
Notations

- p / q - dimension of input / output spaces
- $l : \mathbf{R}^q \times \mathbf{R}^q \rightarrow \mathbf{R}_+$ - loss function
- d - depth of neural network
- n_i ($1 \leq i \leq d$) - number of perceptrons in i th layer
- $z^{[i]} \in \mathbf{R}^{n_i}$ - input to i th layer
- $o^{[i]} \in \mathbf{R}^{n_i}$ - output of i th layer
- $W^{[i]} \in \mathbf{R}^{n_i \times n_{i-1}}$ - weights of connections between $(i-1)$ th and i th layer
- $w^{[i]} \in \mathbf{R}^{n_i \times n_{i-1}}$ - bias weights of i th layer
- $\phi^{[i]} : \mathbf{R}^{n_i} \rightarrow \mathbf{R}^{n_i}$ - activation functions of i th layer

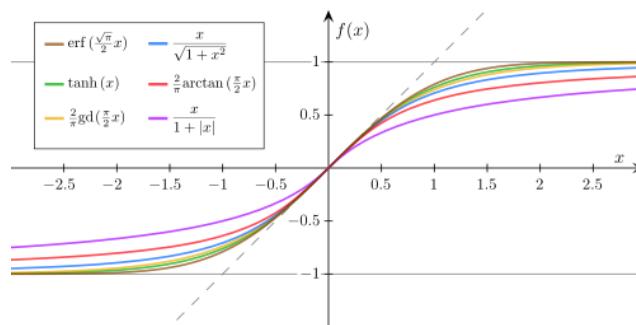


Basic unit & activation function

- basic unit



- activation function



Neural net equations

- modeling function for the (deep) neural network $g_\theta : \mathbf{R}^p \rightarrow \mathbf{R}^q$

$$g_\theta = \phi_\theta^{[d]} \circ \psi_\theta^{[d]} \circ \cdots \circ \phi_\theta^{[1]} \circ \psi_\theta^{[1]}$$

or equivalently

$$g_\theta(x) = \phi_\theta^{[d]}(\psi_\theta^{[d]}(\cdots(\phi_\theta^{[1]}(\psi_\theta^{[1]}(x)))))$$

- for i th layer
 - output via (componentwise) activation function

$$o^{[i]} = \phi^{[i]}(z^{[i]}) \Leftrightarrow o_j^{[i]} = \phi_j^{[i]}(z_j^{[i]}) \quad (1 \leq j \leq n_i)$$

- input via affine transformation $\psi^{[i]} : \mathbf{R}^{n_{i-1}} \rightarrow \mathbf{R}^{n_i}$

$$z^{[i]} = \psi^{[i]}(o^{[i-1]}) = W^{[i]}o^{[i-1]} + w^{[i]}$$

Stochastic gradient descent

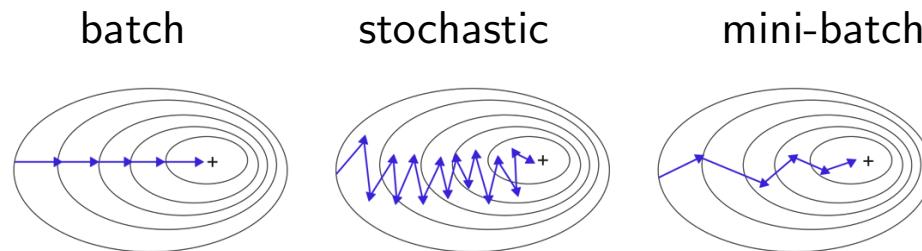
- ML training tries to minimize some loss function - $f(\theta)$ depends on (not only θ , but also) batch of data $(x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)})$

$$\text{minimize } f(\theta)$$

- while exist hundreds of optimization methods solving this problem
 - the only method used widely* is stochastic *gradient descent!*
- (stochastic) gradient descent

$$f(\theta^{k+1}) = f(\theta^k) - \alpha^k \nabla f(\theta^k)$$

- backpropagation* is used to evaluate this (stochastic) *gradient* using *chain rule*



Chain rule

- suppose
 - two functions $f : \mathbf{R}^n \rightarrow \mathbf{R}^m$ & $g : \mathbf{R}^m \rightarrow \mathbf{R}$
 - Jacobian of f - $Df : \mathbf{R}^n \rightarrow \mathbf{R}^{m \times n}$
 - gradient of g - $\nabla g : \mathbf{R}^m \rightarrow \mathbf{R}^m$
- gradient of composite function $h = g \circ f$

$$\nabla h(\theta) = Df(\theta)^T \nabla g(f(\theta)) \in \mathbf{R}^n \quad (\text{using matrix-vector multiplication})$$

in other words

$$\frac{\partial}{\partial \theta_i} h(\theta) = \sum_{j=1}^m \frac{\partial}{\partial \theta_i} f_j(\theta) \nabla_j g(f(\theta)) \quad (\text{scalar version})$$

Loss function & its gradient

- assume cost function of deep neural network is

$$f(\theta) = \frac{1}{m} \sum_{k=1}^m l(g_\theta(x^{(k)}), y^{(k)}) = \frac{1}{m} \sum_{k=1}^m f_k(\theta)$$

where

$$f_k(\theta) = l(g_\theta(x^{(k)}), y^{(k)})$$

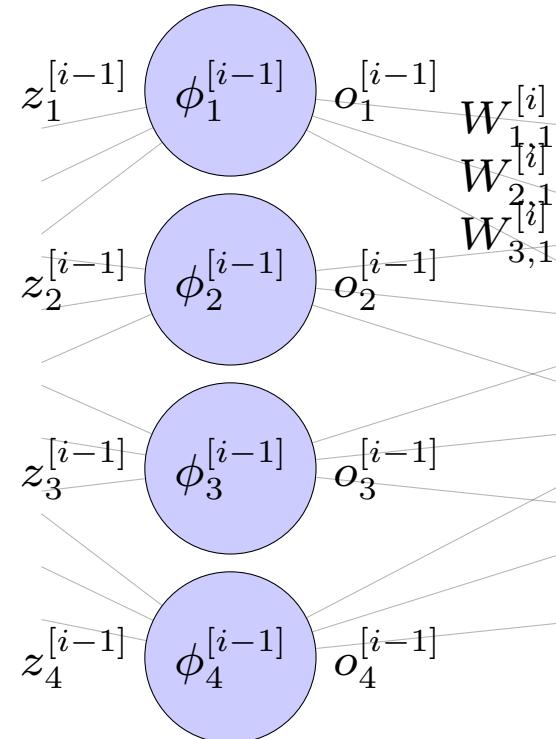
- gradient is

$$m \nabla_\theta f(\theta) = \sum_{k=1}^m \nabla_\theta l(g_\theta(x^{(k)}), y^{(k)}) = \sum_{k=1}^m \nabla_\theta f_k(\theta)$$

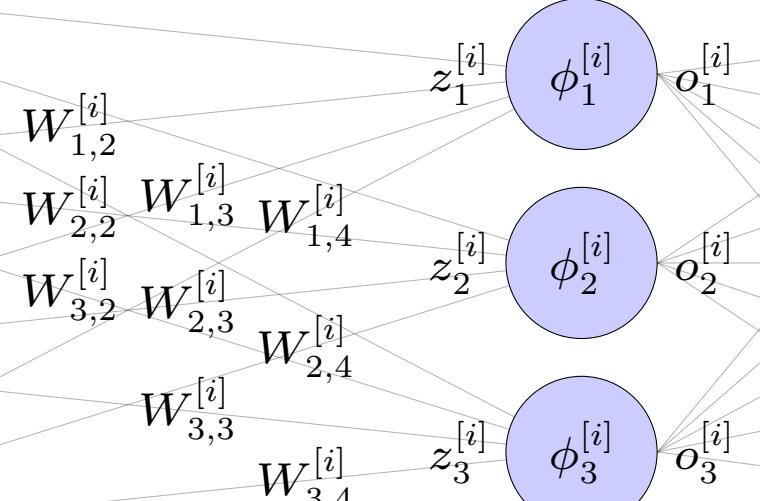
- i.e., evaluate gradient $\nabla_\theta f_k(\theta)$ for each data point $(x^{(k)}, y^{(k)})$

Hidden layers

(i - 1)th hidden layer



ith hidden layer



Backpropagation formula using chain rule

- for each data $(x^{(k)}, y^{(k)})$
 - via activation function

$$\frac{\partial}{\partial z_j^{[i]}} f_k(\theta) = \frac{\partial}{\partial o_j^{[i]}} f_k(\theta) \phi_j^{[i]'}(o_j^{[i]}) \quad \text{for } 1 \leq j \leq n_i \quad (1)$$

where $\phi_j^{[i]'}(o_j^{[i]})$ is derivative of activation function $\phi_j^{[i]}$ evaluated at $o_j^{[i]}$

- via affine transformation

$$\frac{\partial}{\partial W_{j,l}^{[i]}} f_k(\theta) = o_l^{[i-1]} \frac{\partial}{\partial z_j^{[i]}} f_k(\theta) \quad \text{for } 1 \leq j \leq n_i \text{ & } 1 \leq l \leq n_{i-1} \quad (2)$$

$$\frac{\partial}{\partial w_j^{[i]}} f_k(\theta) = \frac{\partial}{\partial z_j^{[i]}} f_k(\theta) \quad \text{for } 1 \leq j \leq n_i \quad (3)$$

$$\frac{\partial}{\partial o_l^{[i-1]}} f_k(\theta) = \sum_{j=1}^{n_i} W_{j,l}^{[i]} \frac{\partial}{\partial z_j^{[i]}} f_k(\theta) \quad \text{for } 1 \leq l \leq n_{i-1} \quad (4)$$

Backpropagation formula using matrix-vector multiplication

- for each data $(x^{(k)}, y^{(k)})$

- via activation function

$$\nabla_{z^{[i]}} f_k(\theta) = D\phi^{[i]} \nabla_{o^{[i]}} f_k(\theta) \quad (5)$$

where $D\phi^{[i]} = \text{diag}(\phi_1^{[i]'}(o_1^{[i]}), \dots, \phi_{n_i}^{[i]'}(o_{n_i}^{[i]}))$ is Jacobian of $\phi^{[i]}$ evaluated at $o^{[i]}$

- via affine transformation

$$\nabla_{W^{[i]}} f_k(\theta) = \nabla_{z^{[i]}} f_k(\theta) o^{[i-1]T} \in \mathbf{R}^{n_i \times n_{i-1}} \quad (6)$$

$$\nabla_{w^{[i]}} f_k(\theta) = \nabla_{z^{[i]}} f_k(\theta) \in \mathbf{R}^{n_i} \quad (7)$$

$$\nabla_{o^{[i-1]}} f_k(\theta) = W^{[i]T} \nabla_{z^{[i]}} f_k(\theta) \in \mathbf{R}^{n_{i-1}} \quad (8)$$

Backpropagation formula using Python numpy package

- for each data $(x^{(k)}, y^{(k)})$
 - via activation function

$$\text{grad_z} = \text{phi_dir} * \text{grad_o} \quad (9)$$

- where grad_z , phi_dir , grad_o are 1d numpy.ndarray of size n_i
- via affine transformation

$$\text{grad_W} = \text{numpy.dot}(\text{grad_z}, \text{val_o.T}) \quad (10)$$

$$\text{grad_w} = \text{grad_z.copy()} \quad (11)$$

$$\text{grad_o_prev} = \text{numpy.dot}(\text{grad_z}, \text{W}) \quad (12)$$

where val_o , grad_w are 1d numpy.ndarray of size n_i , grad_o_prev is 1d numpy.ndarray of size n_{i-1} , grad_W is 2d numpy.ndarray of shape (n_i, n_{i-1})

Gradient evaluation using backpropagation

- forward propagation - evaluate for each $(x^{(k)}, y^{(k)})$

$$g_{\theta}(x^{(k)}) = \phi_{\theta}^{[d]}(\psi_{\theta}^{[d]}(\cdots(\phi_{\theta}^{[1]}(\psi_{\theta}^{[1]}(x^{(k)})))))$$

- *backpropagation - evaluate partial derivatives backward*

- evaluate gradient with respect to output of output layer $o^{[d]} = g_{\theta}(x^{(k)})$

$$\nabla_{o^{[d]}} f_k(\theta) = \nabla_{y_1} l(g_{\theta}(x^{(k)}), y^{(k)})$$

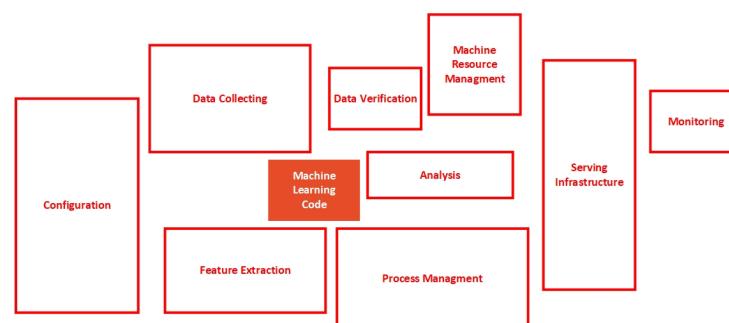
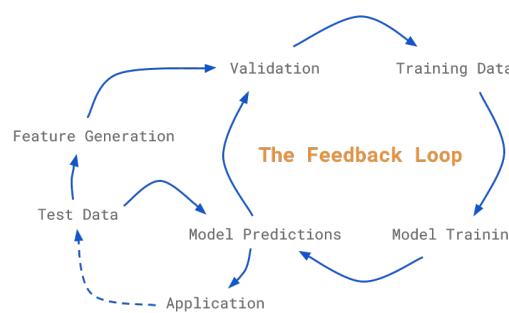
- evaluate gradient with respect to input from that with respect to output using (1), or equivalently, using (5) *i.e.*, evaluate $\nabla_{z^{[i]}} f_k(\theta)$ from $\nabla_{o^{[i]}} f_k(\theta)$
- evaluate gradient with respect to weights, bias, and intput of previous layer using (3), (4), & (2) or equivalently, using (7), (8), & (6) *i.e.*, evaluate $\nabla_{W^{[i]}} f_k(\theta)$, $\nabla_{w^{[i]}} f_k(\theta)$ & $\nabla_{o^{[i-1]}} f_k(\theta)$ from $\nabla_{z^{[i]}} f_k(\theta)$
- repeat back to input layer to evaluate all

$$\nabla_{W^{[1]}} f_k(\theta), \nabla_{w^{[1]}} f_k(\theta), \dots, \nabla_{W^{[d]}} f_k(\theta), \nabla_{w^{[d]}} f_k(\theta)$$

ML in Action

ML in practice

- define business problem - business objective, success metrics, establish baselines (early)
- data collection - data cleaning, validation & exploratory data analysis (EDA)
- feature engineering - based on domain expertise
- train/validation/test split - stratified sampling, chronological splits for time-series
- model selection or/and hyperparameter optimization
- monitoring, retraining & notification
- start simple, iterative fast (fail fast!), validate business impact - *e.g.*, A/B test



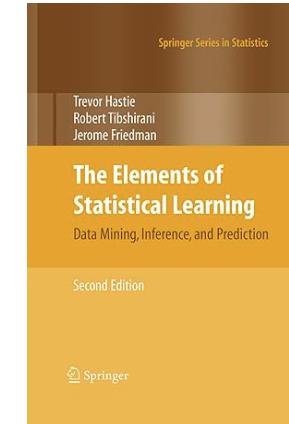
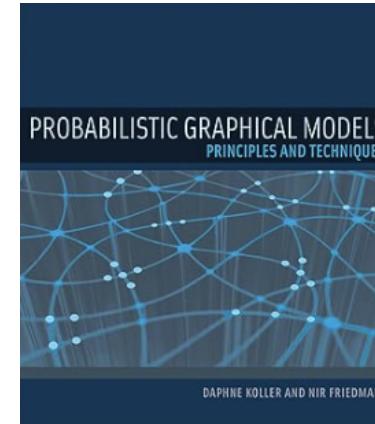
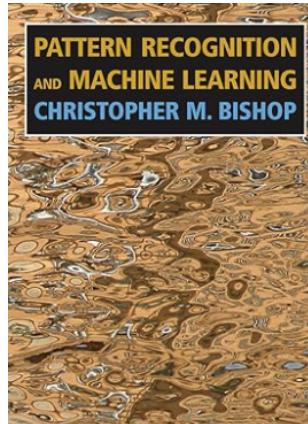
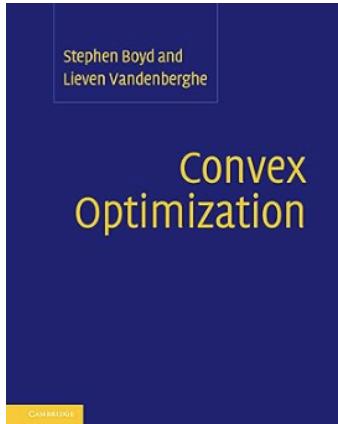
Learning AI

Best ways to learn AI & ML

- first, learn basics - college classes, online courses, (easy) books
 - no need to understand every mathematical details, but should know rough ideas!
- *hands-on is MUST!*
 - learn and practice coding - Python is MUST; do not do (only) R
 - learn git - know how to develop efficiently, plus import others' work
- I think *online courses are blessing to mankind!*
 - *can't* say “you can't do it because I don't have access to good resource or you don't go to good schools” because . . . they are available!
 - getting (expensive) certificates is good idea because . . . otherwise you wouldn't complete it! :) - and can post it on your LinkedIn!
- would be best if your task at work is related to ML
 - however, even if that's not the case or can't be the case, can always do your own personal projects – or contribute to public projects (on github)!

Books

- The Elements of Statistical Learning - Hastie, Tibshirani & Friedman [[HTF01](#)]
- Pattern Recognition and Machine Learning - Christopher M. Bishop [[Bis06](#)]
- Deep Learning - Ian Goodfellow, Yoshua Bengio & Aaron Courville [[GBC16](#)]
- Reinforcement Learning: An Introduction - Richard S. Sutton & Andrew G. Barto [[SB18](#)]
- Machine Learning: A Probabilistic Perspective - Kevin P. Murphy [[Mur12](#)]
- Probabilistic Graphical Models - Daphne Koller & Nir Friedman [[KF09](#)]
- Convex Optimization - Stephen Boyd & Lieven Vandenberghe [[BV04](#)]



Andrew Ng!

- Andrew Ng
 - (co-)founder of “Deep Learning.AI” and “Coursera”, prominent figure in ML & AI
 - his courses highly regarded because well-structured and provide insights
- [latest Andrew Ng courses](#)
 - AI Agents in LangGraph
 - AI Agentic Design Patterns with AutoGen
 - Introduction to On-device AI
 - Multi AI Agent Systems with Crew AI
 - Building Multimodal Search and RAG - contrastive learning, multimodality to RAG
 - Building Agentic RAG with LlamaIndex
 - Quantisation In Depth
 - In Prompt Engineering for Vision Models
 - Getting Started with Mistral - open-source models (Mistral 7B, Mixtral 8x7B)
 - Preprocessing Unstructured Data for LLM

Appendices

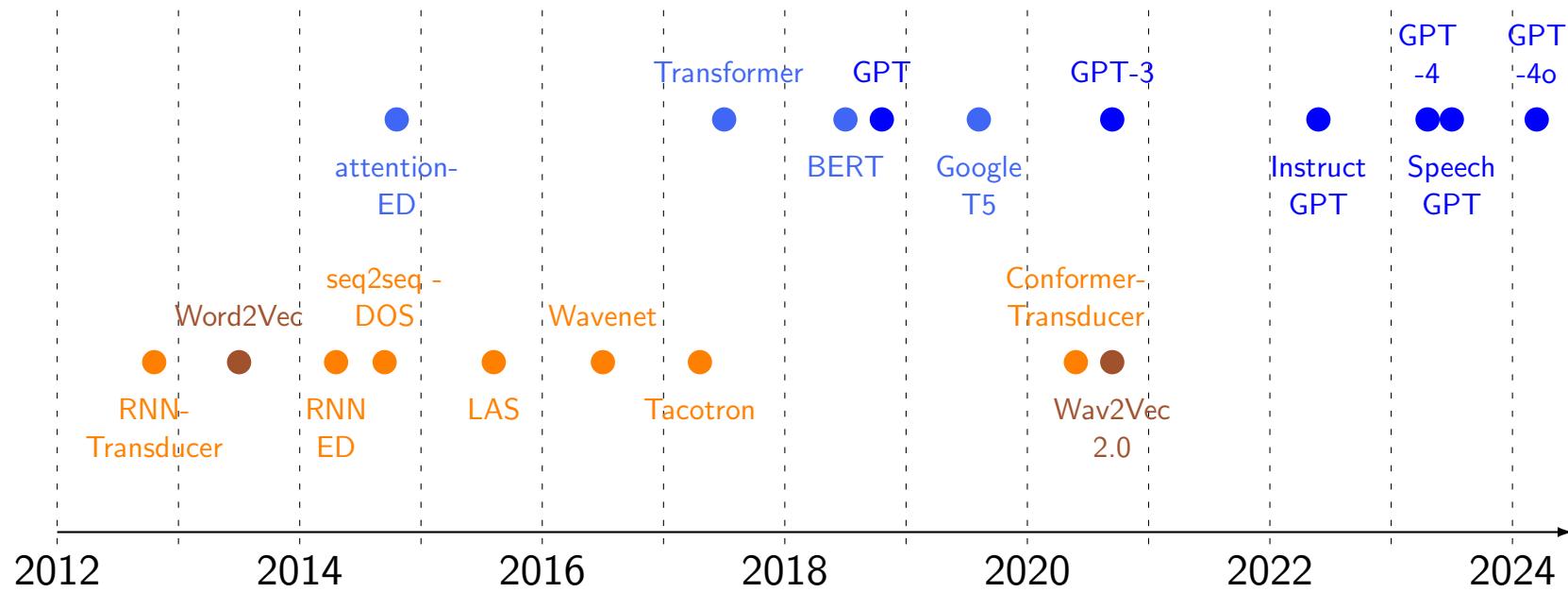
LLM

Language Models

History of language models

- bag of words - first introduced – 1954
- word embedding – 1980
- RNN based models - conceptualized by David Rumelhart – 1986
- LSTM (based on RNN) – 1997
- 380M-sized seq2seq model using LSTMs proposed – 2014
- 130M-sized seq2seq model using gated recurrent units (GRUs) – 2014
- Transformer - Attention is All You Need - A. Vaswani et al. @ Google – 2017
 - 100M-sized encoder-decoder multi-head attention model for machine translation
 - non-recurrent architecture, handle arbitrarily long dependencies
 - parallelizable, *simple* (linear-mapping-based) attention model

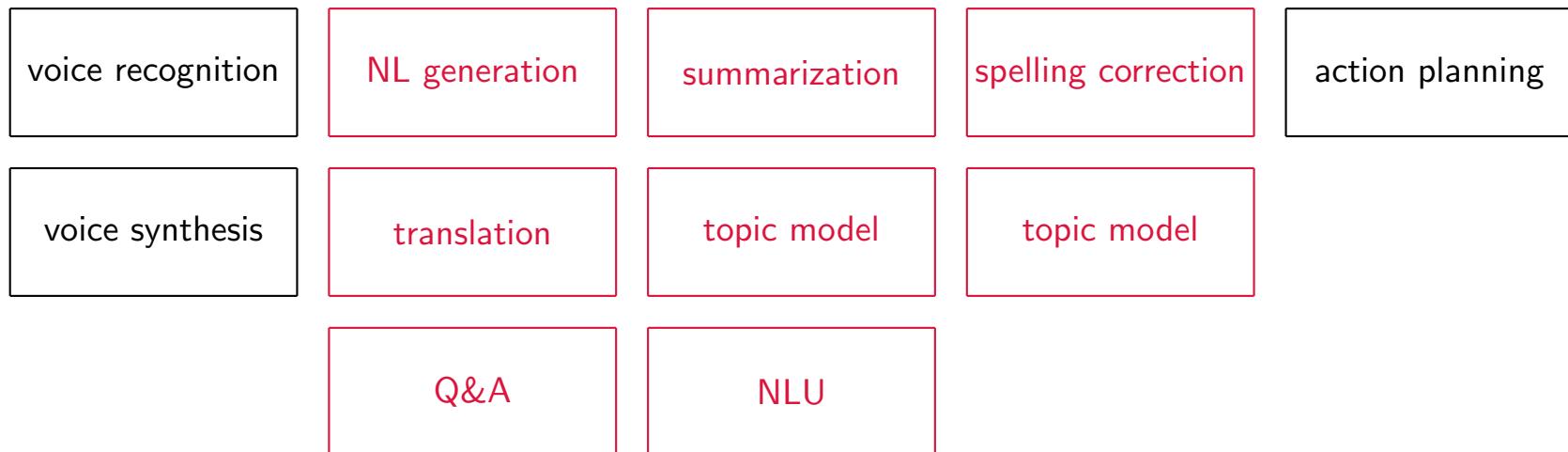
Recent advances in speech & language processing



- LAS: listen, attend, and spell, ED: encoder-decoder, DOS: decoder-only structure

Types of language models

- many of language models have **common requirements** - language representation learning
- can be learned via pre-training *high performing model* and fine-tuning/transfer learning/domain adaptation
- this *high performing model* learning essential language representation *is* (language) foundation model
 - actually, same for other types of learning, e.g., CV



NLP Market

NLP market size

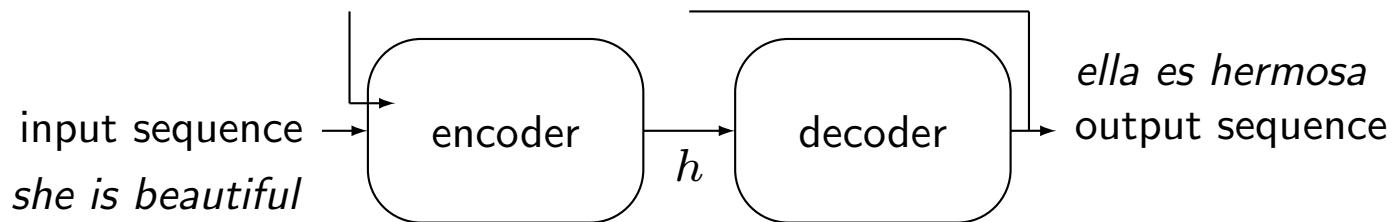
- global NLP market size estimated at USD 16.08B in 2022, is expected to hit USD 413.11B by 2032 - *CAGR of 38.4%*
- in 2022
 - north america NLP market size valued at USD 8.2B
 - high tech and telecom segment accounted revenue share of over 23.1%
 - healthcare segment held a 10% market share
 - (by component) solution segment hit 76% revenue share
 - (deployment mode) on-premise segment generated 56% revenue share
 - (organizational size) large-scale segment contributed highest market share
- source - [Precedence Research](#)



Sequence-to-Sequence Models

Sequence-to-sequence (seq2seq) model

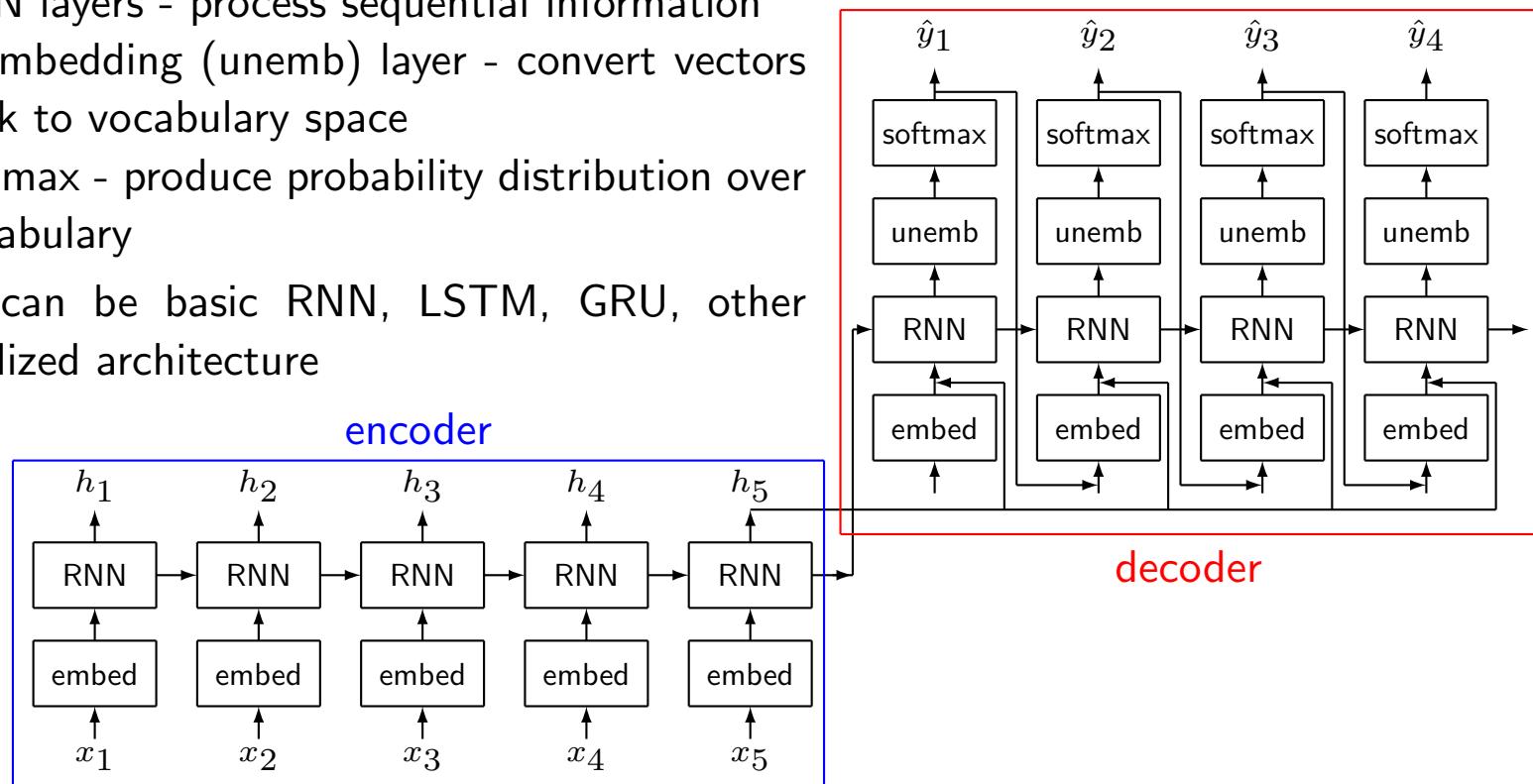
- seq2seq - take sequences as inputs and spit out sequences
- encoder-decoder architecture



- encoder & decoder can be RNN-type models
- $h \in \mathbf{R}^n$ - hidden state - *fixed length* vector
- (try to) condense and store information of input sequence (losslessly) in (fixed-length) hidden states
 - finite hidden state - not flexible enough, *i.e.*, cannot handle arbitrarily large information
 - memory loss for long sequences
 - LSTM was promising fix, but with (inevitable) limits

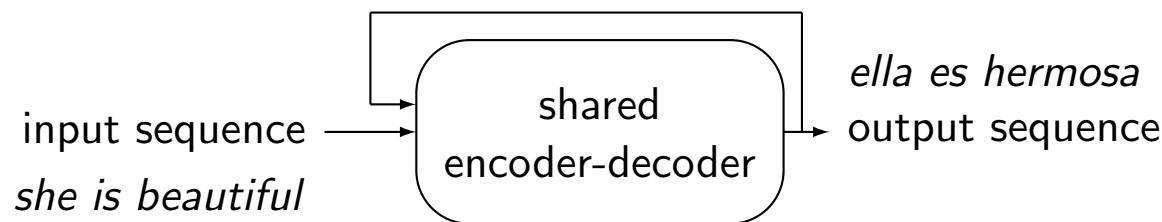
RNN-type encoder-decoder architecture

- components
 - embedding layer - convert input tokens to vector representations
 - RNN layers - process sequential information
 - unembedding (unemb) layer - convert vectors back to vocabulary space
 - softmax - produce probability distribution over vocabulary
- RNN can be basic RNN, LSTM, GRU, other specialized architecture



Shared encoder-decoder model

- single neural network structure can handle both encoding & decoding tasks
 - efficient architecture reducing model complexity
 - allow for better parameter sharing across tasks
- widely used in modern LLMs to process & generate text sequences
 - applications - machine translation, text summarization, question answering
- advantages
 - efficient use of parameters, versatile for multiple NLP tasks



Large Language Models

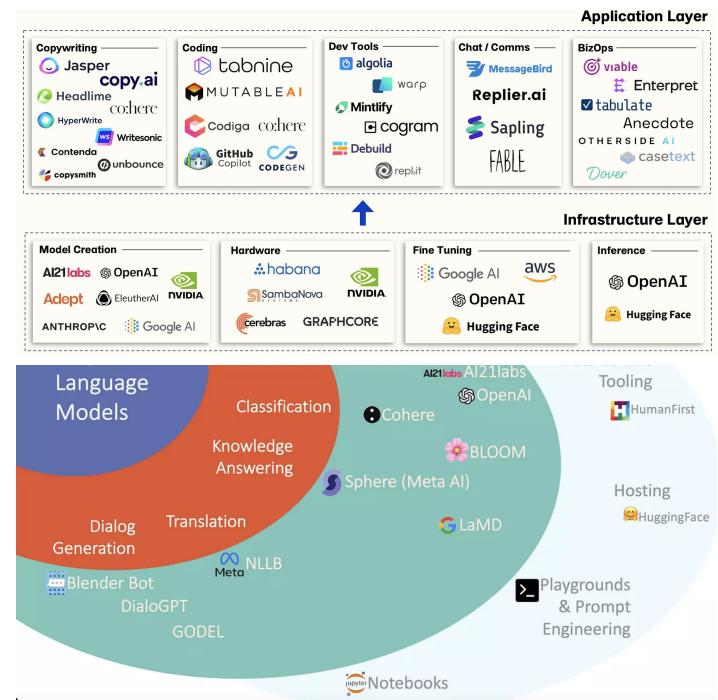
LLM

- LLM
 - type of AI aimed for NLP trained on massive corpus of texts & programming code
 - allow learn statistical relationships between words & phrases, *i.e.*, conditional probabilities
 - *amazing performance shocked everyone - unreasonable effectiveness of data (Halevy et al., 2009)*
- applications
 - conversational AI agent / virtual assistant
 - machine translation / text summarization / content creation / sentiment analysis / question answering
 - code generation
 - market research / legal service / insurance policy / triage hiring candidates
 - + virtually infinite # of applications



LLMs

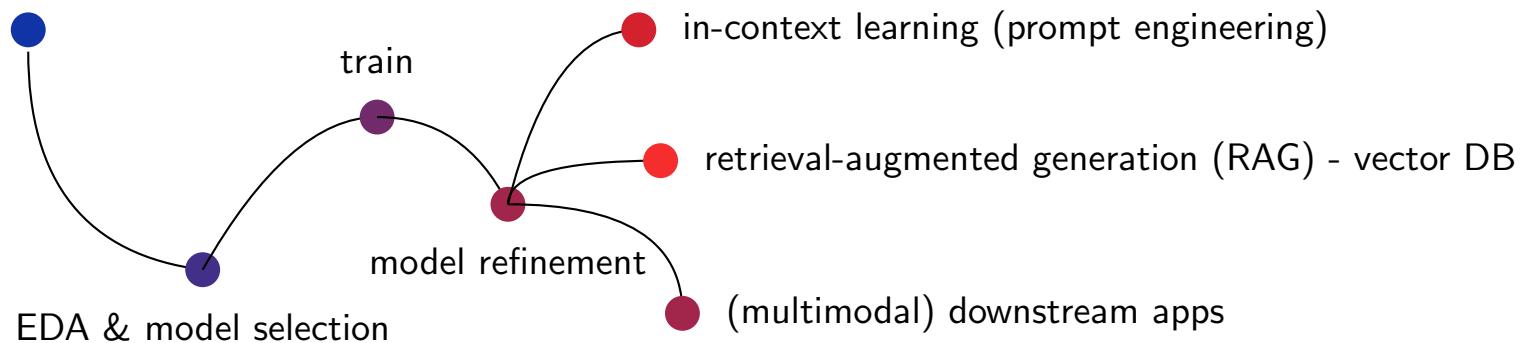
- Foundation Models
 - GPT-x/Chat-GPT - OpenAI, Llama-x - Meta, PaLM-x (Bard) - Google
- # parameters
 - generative pre-trained transformer (GPT) - GPT-1: 117M, GPT-2: 1.5B, GPT-3: 175B, GPT-4: 100T, GPT-4o: 200B
 - large language model Meta AI (Llama) - Llama1: 65B, Llama2: 70B, Llama3: 70B
 - scaling language modeling with pathways (PaLM) - 540B
- burns lots of cash on GPUs!
- applicable to many NLP & genAI applications



LLM building blocks

- data - trained on massive datasets of text & code
 - quality & size critical on performance
- architecture - GPT/Llama/Mistral
 - can make huge difference
- training - self-supervised/supervised learning
- inference - generates outputs
 - in-context learning, prompt engineering

goal and scope of LLM project



Transformer

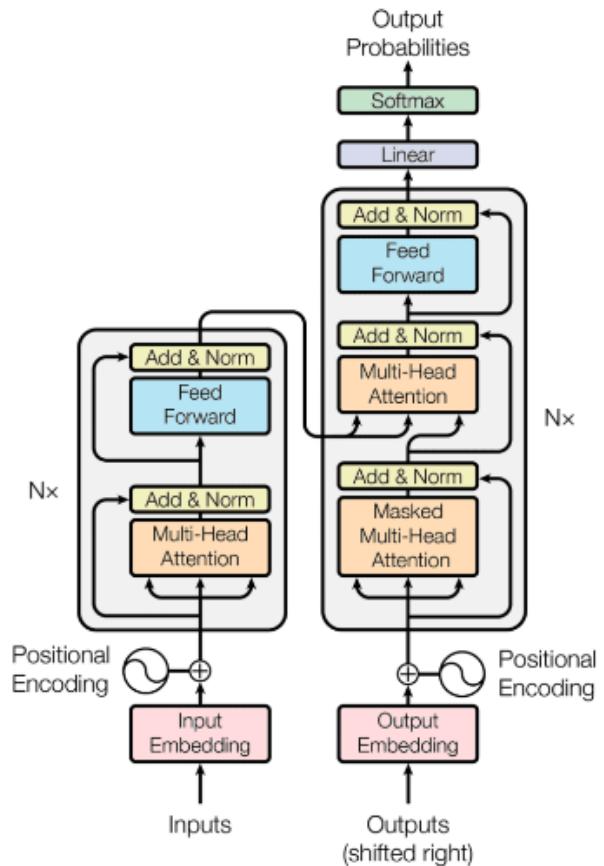
LLM architectural secret (or known) sauce

Transformer - simple parallelizable attention mechanism

A. Vaswani, et al. Attention is All You Need, 2017

Transformer architecture

- encoding-decoding architecture
 - input embedding space → multi-head & mult-layer representation space → output embedding space
- additive positional encoding - information regarding order of words @ input embedding
- multi-layer and multi-head attention followed by addition / normalization & feed forward (FF) layers
- *(relatively simple) attentions*
 - single-head (scaled dot-product) / multi-head attention
 - self attention / encoder-decoder attention
 - masked attention
- benefits
 - *evaluate dependencies between arbitrarily distant words*
 - has recurrent nature w/o recurrent architecture → parallelizable → fast w/ additional cost in computation



Single-head scaled dot-product attention

- values/keys/queries denote value/key/query *vectors*, d_k & d_v are lengths of keys/queries & vectors
- we use *standard* notions for matrices and vectors - not transposed version that (almost) all ML scientists (wrongly) use
- output: weighted-average of values where weights are attentions among tokens
- assume n queries and m key-value pairs

$$Q \in \mathbf{R}^{d_k \times n}, K \in \mathbf{R}^{d_k \times m}, V \in \mathbf{R}^{d_v \times m}$$

- attention! outputs n values (since we have n queries)

$$\text{Attention}(Q, K, V) = V \text{softmax} \left(K^T Q / \sqrt{d_k} \right) \in \mathbf{R}^{d_v \times n}$$

- *much simpler attention mechanism than previous work*
 - attention weights were output of complicated non-linear NN

Single-head - close look at equations

- focus on i th query, $q_i \in \mathbf{R}^{d_k}$, $Q = [\quad - \quad q_i \quad - \quad] \in \mathbf{R}^{d_k \times n}$
- assume m keys and m values, $k_1, \dots, k_m \in \mathbf{R}^{d_k}$ & $v_1, \dots, v_m \in \mathbf{R}^{d_v}$

$$K = [\ k_1 \ \ \cdots \ \ k_m \] \in \mathbf{R}^{d_k \times m}, V = [\ v_1 \ \ \cdots \ \ v_m \] \in \mathbf{R}^{d_v \times m}$$

- then

$$K^T Q / \sqrt{d_k} = \left[\begin{array}{ccc} & & \vdots \\ - & k_j^T q_i / \sqrt{d_k} & - \\ & & \vdots \end{array} \right]$$

e.g., dependency between i th output token and j th input token is

$$a_{ij} = \exp \left(k_j^T q_i / \sqrt{d_k} \right) / \sum_{j=1}^m \exp \left(k_j^T q_i / \sqrt{d_k} \right)$$

- value obtained by i th query, q_i in $\text{Attention}(Q, K, V)$

$$a_{i,1}v_1 + \cdots + a_{i,m}v_m$$

Multi-head attention

- evaluate h single-head attentions (in parallel)
- d_e : dimension for embeddings
- embeddings

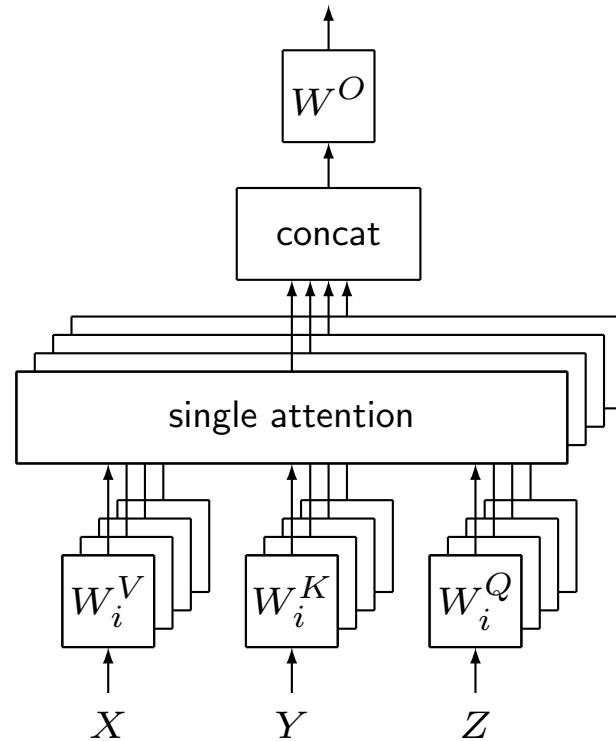
$$X \in \mathbb{R}^{d_e \times m}, Y \in \mathbb{R}^{d_e \times m}, Z \in \mathbb{R}^{d_e \times n}$$

e.g., n : input sequence length & m : output sequence length in machine translation

- h key/query/value weight matrices: $W_i^K, W_i^Q \in \mathbb{R}^{d_k \times d_e}$, $W_i^V \in \mathbb{R}^{d_v \times d_e}$ ($i = 1, \dots, h$)
- linear output layers: $W^O \in \mathbb{R}^{d_e \times hdv}$
- *multi-head attention!*

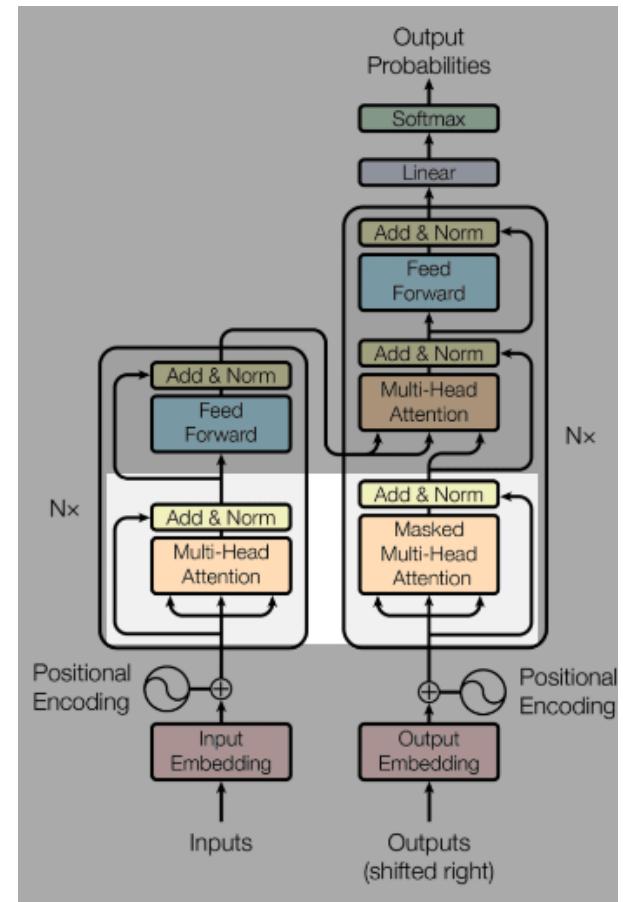
$$W^O \begin{bmatrix} A_1 \\ \vdots \\ A_h \end{bmatrix} \in \mathbb{R}^{d_e \times n},$$

$$A_i = \text{Attention}(W_i^Q Z, W_i^K Y, W_i^V X) \in \mathbb{R}^{d_v \times n}$$



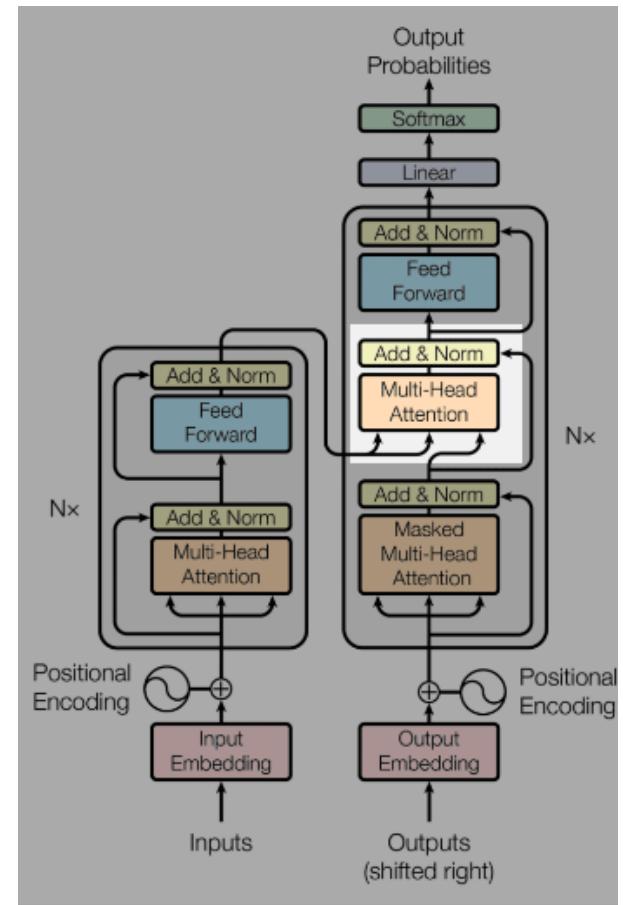
Self attention

- $m = n$
- encoder
 - keys & values & queries (K, V, Q) come from same place (from previous layer)
 - every token attends to every other token in input sequence
- decoder
 - keys & values & queries (K, V, Q) come from same place (from previous layer)
 - every token attends to other tokens up to that position
 - prevent leftward information flow to right to preserve causality
 - assign $-\infty$ for illegal connections in softmax (masking)



Encoder-decoder attention

- m : length of input sequence
- n : length of output sequence
- n queries (Q) come from previous decoder layer
- m keys / m values (K, V) come from output of encoder
- every token in output sequence attends to every token in input sequence

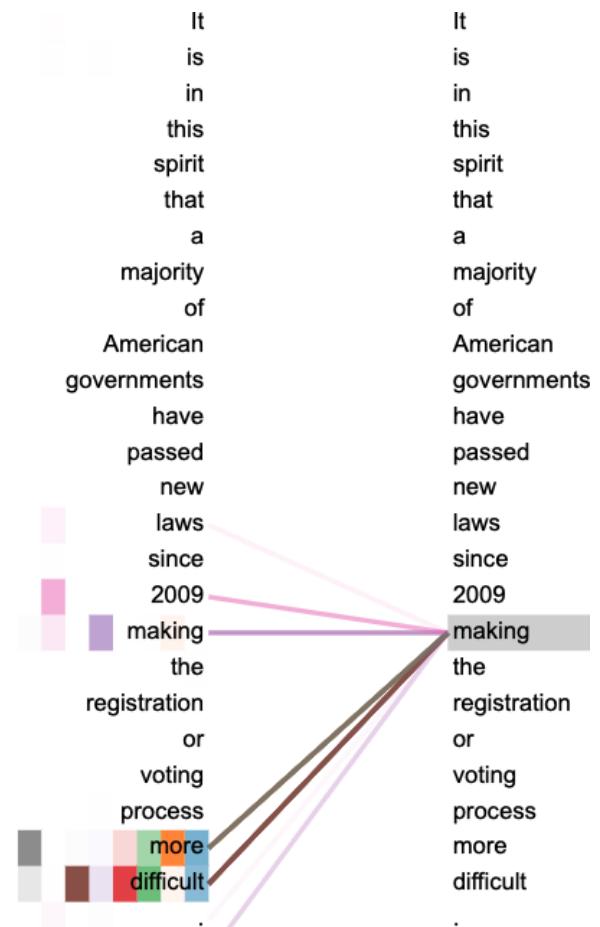


Visualization of self attentions

example sentence

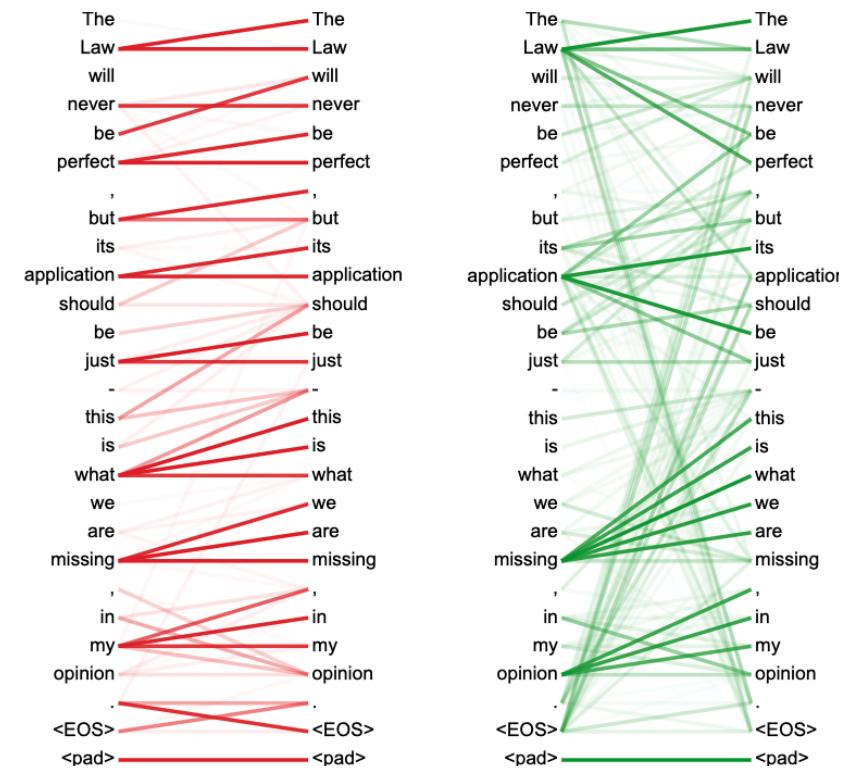
"It is in this spirit that a majority of American governments have passed new laws since 2009 making the registration or voting process more difficult."

- self attention of encoder (of a layer)
 - right figure
 - show dependencies between "making" and other words
 - different columns of colors represent different heads
 - "making" has strong dependency to "2009", "more", and "difficult"

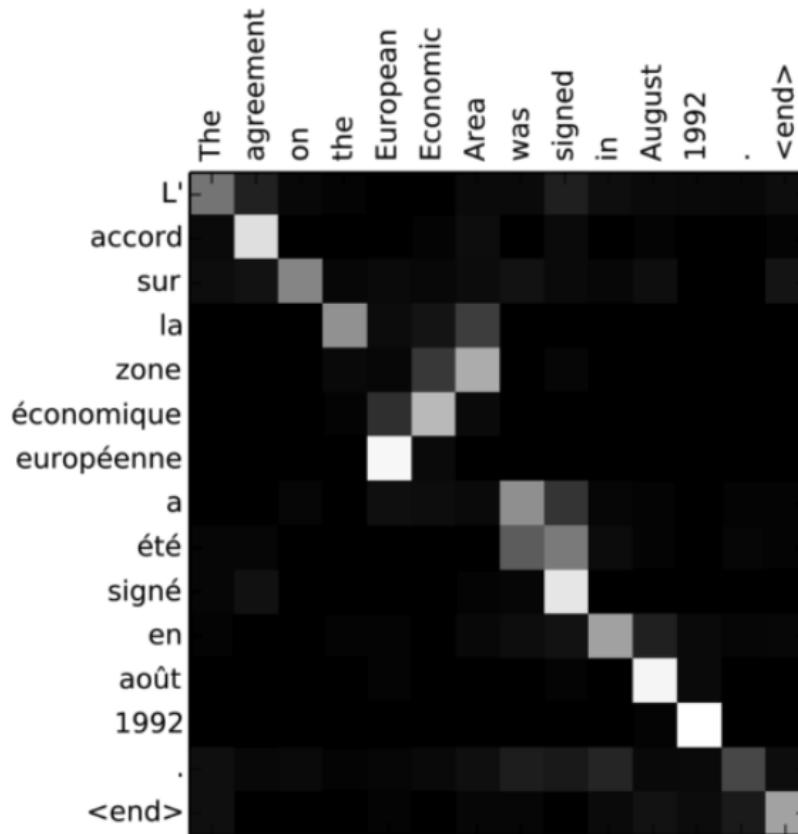


Visualization of multi-head self attentions

- self attentions of encoder for two heads (of a layer)
 - different heads represent different structures
→ advantages of multiple heads
 - multiple heads work together to collectively yield good results
 - dependencies *not* have absolute meanings (like embeddings in collaborative filtering)
 - randomness in resulting dependencies exists due to stochastic nature of ML training



Visualization of encoder-decoder attentions



- machine translation: English → French
 - input sentence: “The agreement on the European Economic Area was signed in August 1992.”
 - output sentence: “L’ accord sur la zone économique européenne a été signé en août 1992.”
- encoder-decoder attention reveals relevance between
 - European ↔ européenne
 - Economic ↔ économique
 - Area ↔ zone

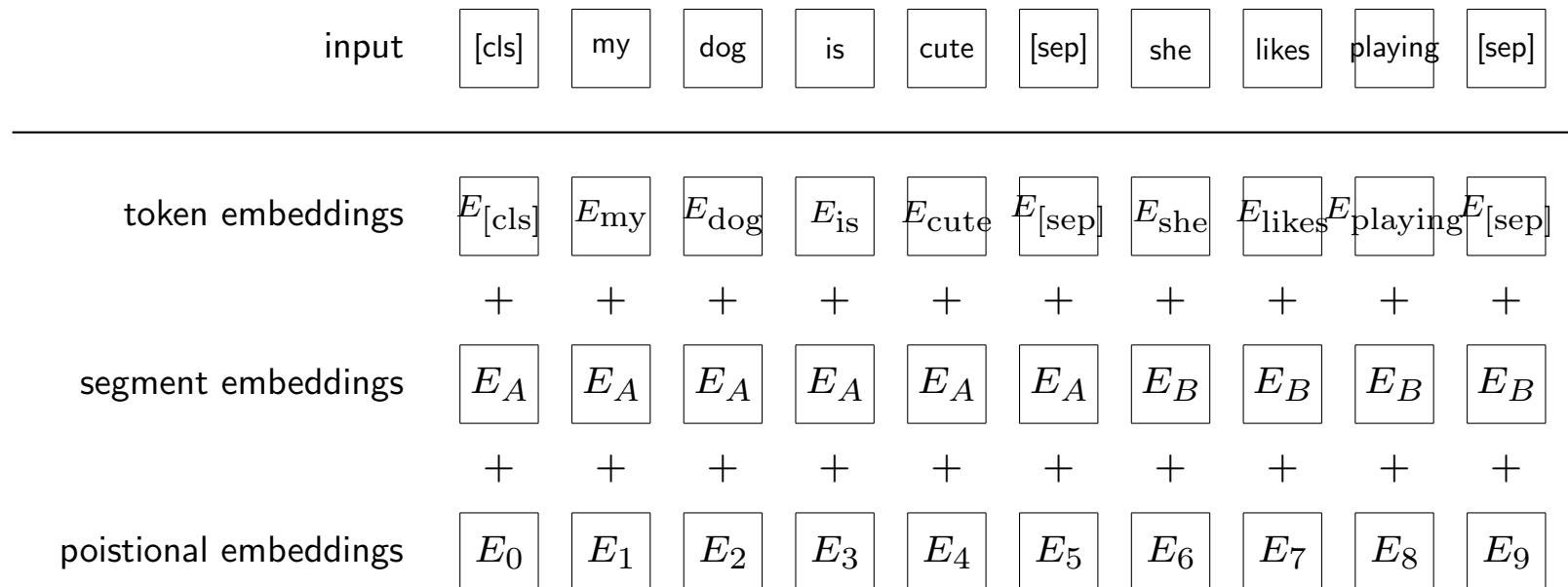
Model complexity

- computational complexity
 - n : sequence length, d : embedding dimension
 - complexity per layer - self-attention: $\mathcal{O}(n^2d)$, recurrent: $\mathcal{O}(1)$
 - sequential operations - self-attention: $\mathcal{O}(1)$, recurrent: $\mathcal{O}(n)$
 - maximum path length - self-attention: $\mathcal{O}(1)$, recurrent: $\mathcal{O}(n)$
- *massive parallel processing, long context windows*
 - makes NVidia more competitive, hence profitable!
 - makes SK Hynix prevail HBM market!

Variants of Transformer

Bidirectional encoder representations from transformers (BERT)

- Bidirectional Encoder Representations from Transformers [DCLT19]
- pre-train deep bidirectional representations from unlabeled text
- fine-tunable for multiple purposes



Challenges in LLMs

- *hallucination - can give entirely plausible outcome that is false*
- data poison attack
- unethical or illegal content generation
- huge resource necessary for both training & inference
- model size - need compact models
- outdated knowledge - can be couple of years old
- lack of reproducibility
- *biases - more on this later . . .*

do not, though, focus on downsides but on *infinite possibilities!*

- it evolves like internet / mobile / electricity
- only “tip of the iceberg” found & released

genAI

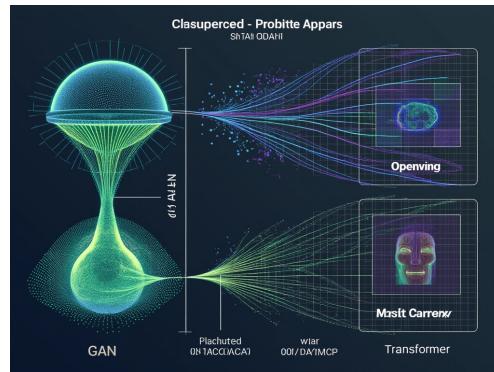
Definition of genAI

Generative AI

- genAI refers to systems capable of producing new (& original) contents based on patterns learned from training data (representation learning)
 - as opposed to discriminative models for, *e.g.*, classification, prediction & regression
 - here content can be text, images, audio, video, *etc.* - what about smell & taste?
- genAI model examples
 - generative adversarial networks (GANs), variational autoencoders (VAEs), diffusion models, Transformers



by Midjourney



by Grok 2 mini



by Generative AI Lab

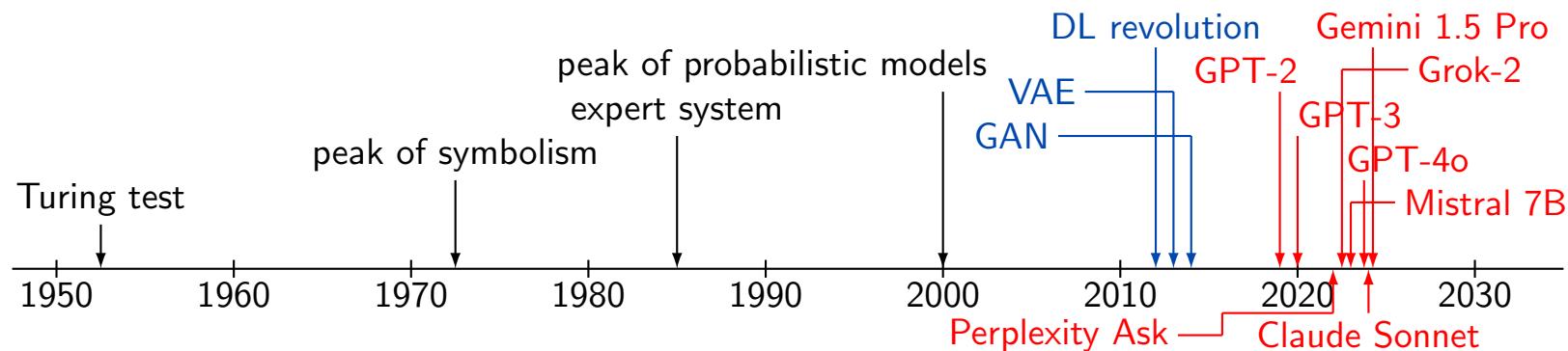
Examples of genAI in action

- text generation
 - Claude, ChatGPT, Mistral, Perplexity, Gemini, Grok
 - conversational agent writing articles, code & even poetry
- image generation
 - DALL-E - creates images based on textual descriptions
 - Stable Diffusion - uses diffusion process to generate high-quality images from text prompts (by denoising random noise)
 - MidJourney - art and visual designs generated through deep learning
- music generation
 - Amper Music - generates unique music compositions
- code generation
 - GitHub Copilot - generates code snippets based on natural language prompts

History of genAI

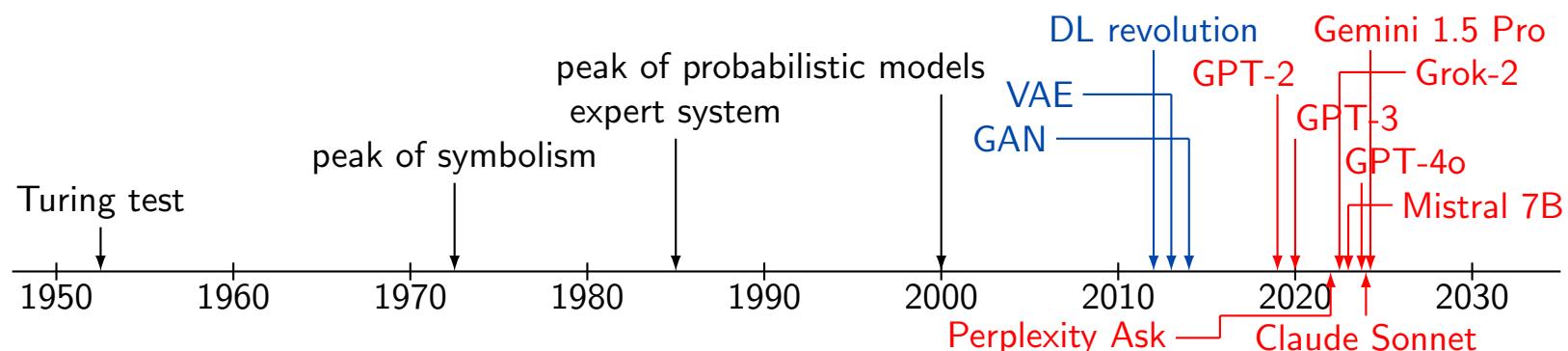
Birth of AI - early foundations & precursor technologies

- 1950s ~ 1970s
 - Alan Turing - concept of “*thinking machine*” & *Turing test* to evaluate machine intelligence (1950s)
 - *symbolists* (as opposed to connectionists) - early AI focused on symbolic reasoning, logic & problem-solving - Dartmouth Conference in 1956 by *John McCarthy, Marvin Minsky, Allen Newell & Herbert A. Simon*
 - precursor technologies - genetic algorithms (GAs), Markov chains & *hidden Markov models (HMMs)* - laying foundation for generative processes (1970s ~)



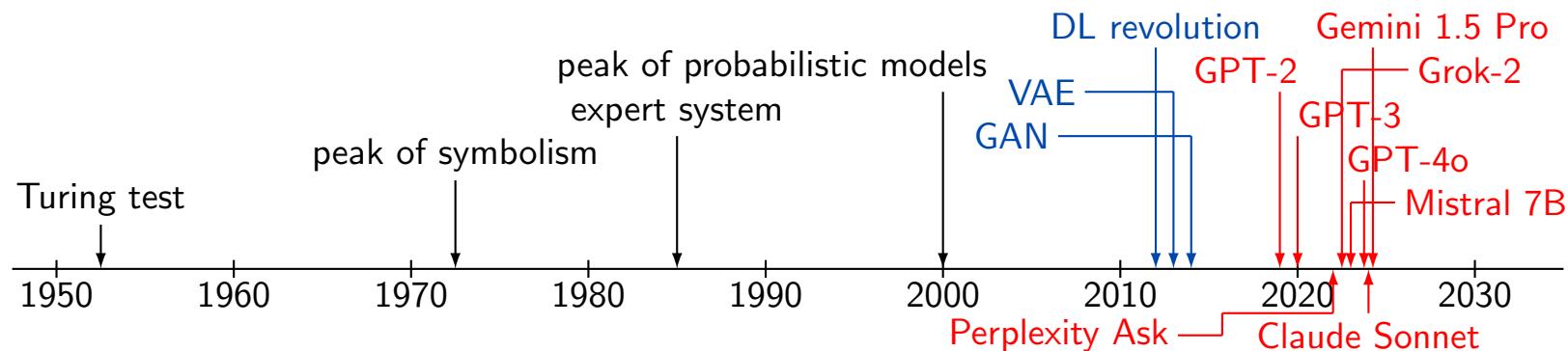
Rule-based systems & probabilistic models

- 1980s ~ early 2000s
 - *expert systems* (1980s) - AI systems designed to mimic human decision-making in specific domains
 - development of neural networks (NN) w/ backpropagation *training multi-layered networks* - setting stage for way more complex generative models
 - *probabilistic models* (including network models, *i.e.*, Bayesian networks) & Markov models - laying groundwork for data generation & pattern prediction



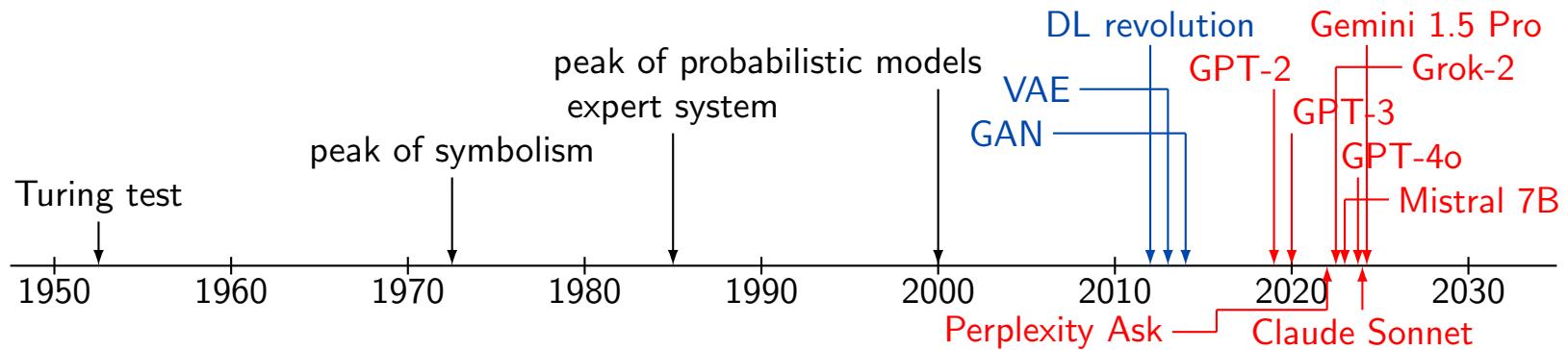
Rise of deep learning & generative models

- 2010s - breakthrough in genAI
 - *deep learning (DL) revolution* - advances in GPU computing and data availability led to the rapid development of deep neural networks.
 - *variational autoencoder (VAE)* (2013) - by Kingma and Welling - learns mappings between input and latent spaces
 - *generative adversarial network (GAN)* (2014) - by Ian Goodfellow - game-changer in generative modeling where two NNs compete each other to create realistic data
 - widely used in image generation & creative tasks



Transformer models & multimodal AI

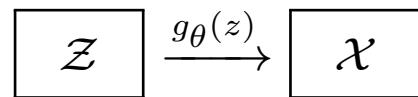
- late 2010s ~ Present
 - Transformer architecture (2017) - by Vaswani et al.
 - *revolutionized NLP*, e.g., LLM & various genAI models
 - GPT series - generative pre-trained transformer
 - GPT-2 (2019) - generating human-like texts - *marking leap in language models*
 - GPT-3 (2020) - 175B params - set *new standards for LLM*
 - multimodal systems - DALL-E & CLIP (2021) - *linking text and visual data*
 - emergence of diffusion models (2020s) - new approach for generating high-quality images - progressively “denoising” random noise (DALL-E 2 & Stable Diffusion)



Mathy Views on genAI

genAI models

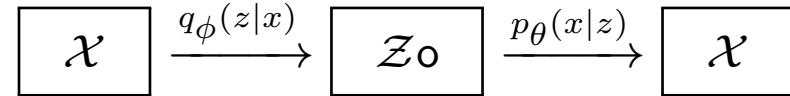
- definition of generative model



- *generate samples in original space, \mathcal{X} , from samples in latent space, \mathcal{Z}*
- g_θ is parameterized model *e.g.*, CNN / RNN / Transformer / diffuction-based model
- training
 - finding θ that minimizes/maximizes some (statistical) loss/merit function so that $\{g_\theta(z)\}_{z \in \mathcal{Z}}$ generates plausible point in \mathcal{X}
- inference
 - random samples z to generated target samples $x = g_\theta(z)$
 - *e.g.*, image, text, voice, music, video

VAE - early genAI model

- variational auto-encoder (VAE) [KW19]



- log-likelihood & ELBO - for any $q_\phi(z|x)$

$$\begin{aligned}
 \log p_\theta(x) &= \mathbf{E}_{z \sim q_\phi(z|x)} \log p_\theta(x) = \mathbf{E}_{z \sim q_\phi(z|x)} \log \frac{p_\theta(x, z)}{q_\phi(z|x)} \cdot \frac{q_\phi(z|x)}{p_\theta(z|x)} \\
 &= \mathcal{L}(\theta, \phi; x) + D_{KL}(q_\phi(z|x) \| p_\theta(z|x)) \geq \mathcal{L}(\theta, \phi; x)
 \end{aligned}$$

- (indirectly) maximize likelihood by maximizing evidence lower bound (ELBO)

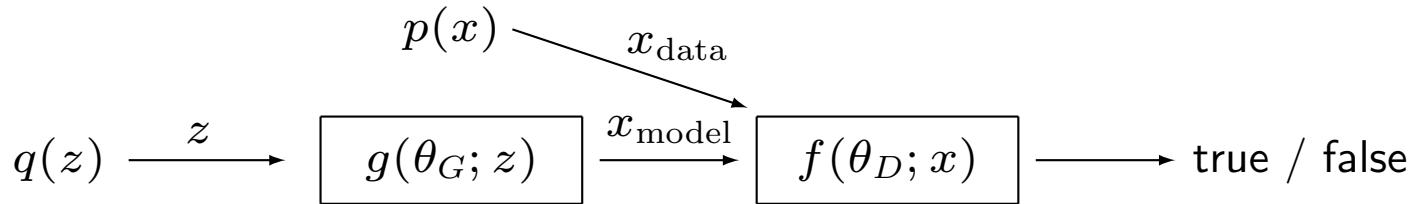
$$\mathcal{L}(\theta, \phi; x) = \mathbf{E}_{z \sim q_\phi(z|x)} \log \frac{p_\theta(x, z)}{q_\phi(z|x)}$$

- generative model

$$p_\theta(x|z)$$

GAN - early genAI model

- generative adversarial networks (GAN) [GPAM⁺14]



- value function

$$V(\theta_D, \theta_G) = \mathbf{E}_{x \sim p(x)} \log f(\theta_D; x)) + \mathbf{E}_{z \sim q(z)} \log(1 - f(\theta_D; g(\theta_G; z)))$$

- modeling via playing min-max game

$$\min_{\theta_G} \max_{\theta_D} V(\theta_D, \theta_G)$$

- generative model

$$g(\theta_G; z)$$

- variants: conditional / cycle / style / Wasserstein GAN

genAI - LLM

- *maximize conditional probability*

$$\underset{\theta}{\text{maximize}} \ d(p_{\theta}(x_t|x_{t-1}, x_{t-2}, \dots), p_{\text{data}}(x_t|x_{t-1}, x_{t-2}, \dots))$$

where $d(\cdot, \cdot)$ distance measure between probability distributions

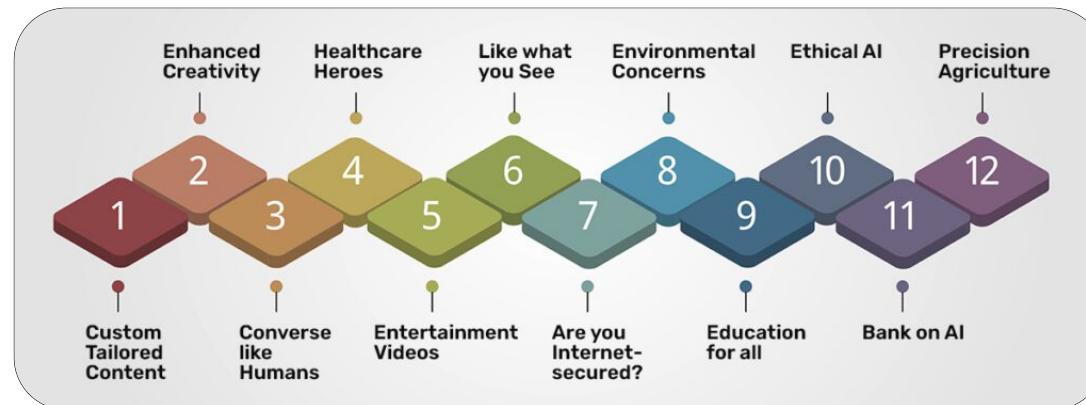
- previous sequence: x_{t-1}, x_{t-2}, \dots
- next token: x_t
- p_{θ} represented by (extremely) complicated model
 - e.g., containing multi-head & multi-layer Transformer architecture inside
- model parameters, e.g., for Llama2

$$\theta \in \mathbf{R}^{70,000,000,000}$$

Current Trend & Future Perspectives

Current trend of genAI

- rapid advancement in language models & multimodal AI capabilities
- rise of AI-assisted creativity & productivity tools
- growing adoption across industries
 - creative industries - design, entertainment, marketing, software development
 - life sciences - healthcare, medical, biotech
- infrastructure & accessibility, *e.g.*, Hugging Face democratizes AI development
- integration with cloud platforms & enterprise-level tools
- increased focus on AI ethics & responsible development



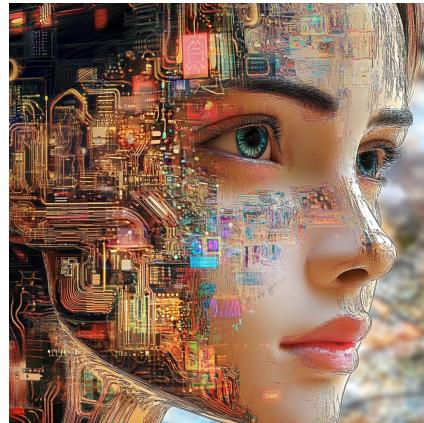
Industry & business impacts

- how genAI is transforming industries
 - creative industries - content creation - advertising, gaming, film
 - life science - enhance research, drug discovery & personalized treatments
 - finance - automating document generation, risk modeling & fraud detection
 - manufacturing & Design - rapid prototyping, 3D modeling & optimization
 - business operations - automate routine tasks to boost productivity



Future perspectives of genAI

- hyper-personalization - highly personalized content for individual users - music, products & services
- AI ethics & governance - concerns over deepfakes, misinformation & bias
- interdisciplinary synergies - integration with other fields such as quantum computing, neuroscience & robotics
- human-AI collaboration - augment human creativity rather than replace it
- energy efficiency - have to figure out how to dramatically reduce power consumption



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Thank You