A Guide to Data Science

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This is a brief introduction to data science. Data science can be seen as an extension of statistics.

- All sciences are, in the abstract, mathematics.
- All judgments are, in their rationale, statistics. by C.P. Rao

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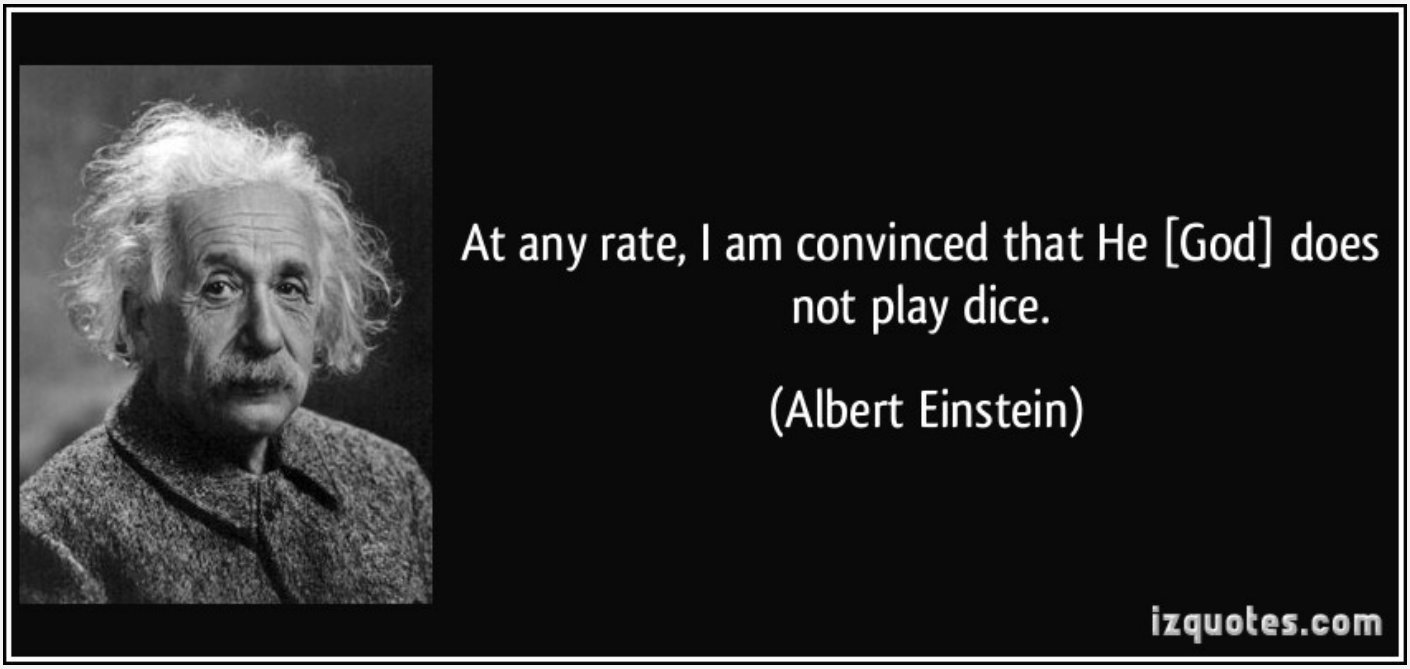
On Chomsky and the Two Cultures of Statistical Learning or Statistical Modeling: The Two Cultures (with comments and a rejoinder by the author) provides more discussion of statistical model or data science.

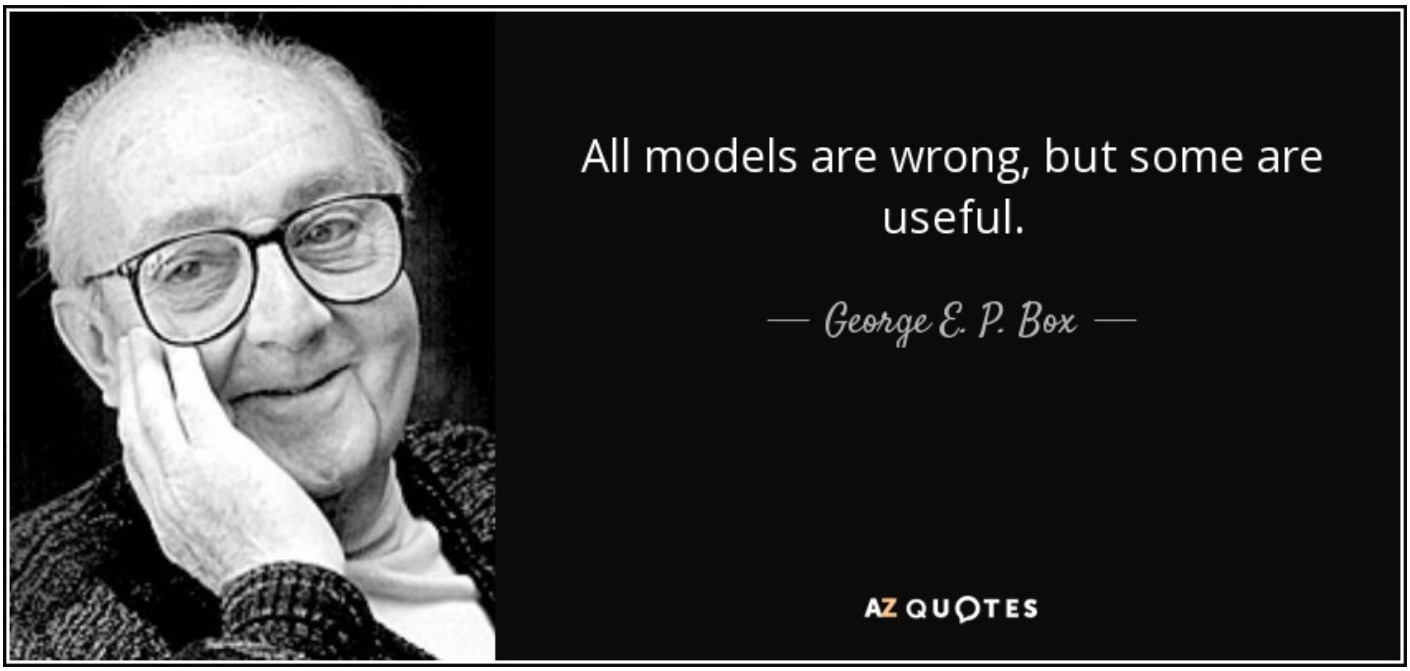
Statistical Foundation

"Statistics, in a nutshell, is a discipline that studies the best ways of dealing with randomness, or more precisely and broadly, variation", Professor Xiao-Li Meng said.

On mathematical model

On mathematical model





On mathematical model

"The sciences do not try to explain, they hardly even try to interpret, they mainly make models. By a model is meant a mathematical construct which, with the addition of certain verbal interpretations, describes observed phenomena. The justification of such a mathematical construct is solely and precisely that it is expected to work—that is, correctly to describe phenomena from a reasonably wide area."

John von Neumann

Basic Probability

Probability theory is regarded as the theoretical foundation of statistics,
which provides the ideal models to measure the stochastic phenomenon, randomness, chance or luck.
It is the distribution theory bridging probability and statistics.
The project seeing theory is a brief introduction to statistics and probability theory and also a .pdf file.

Random Variable

Random variable is to represent the stochastic event, where stochastic event is the event that may or may not happen with some known results.

Definition: A random variable is a mapping

$$X : \Omega \to \mathbb{R}$$

that assigns a real number $X(\omega)$ to each outcome ω.

- Ω *is the sample space.*

- *ω in Ω are called sample outcomes or realization.*
- *Subsets of Ω are called Event.*

Probability

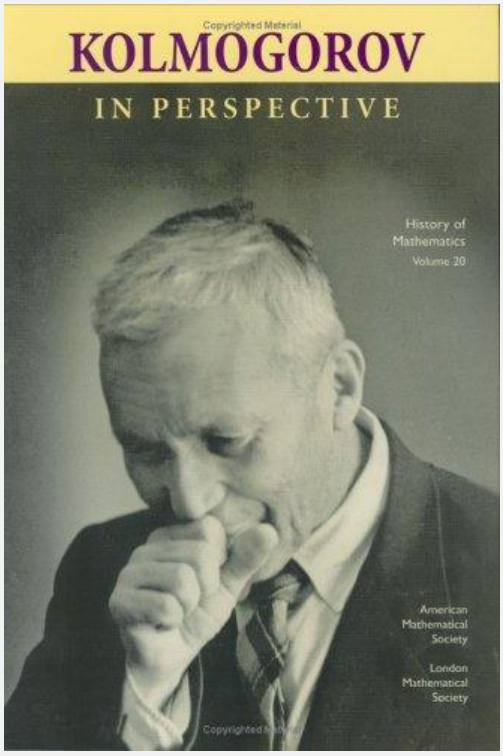
Probability is the mathematical measure to likelihood or chance.

> *Definition A function P is called probability function with respect to the known sample space Ω and all the event $\forall \omega \in \Omega$ if*

Properties	***Conditions***	***Interpretation***
Nonnegative	$P(\omega) \geq 0 \forall \omega \in \Omega$	*Impossible = 0*
Normalized	$P(\Omega) = 1$	*Something must happen*
Additive	*If $\omega_1, \omega_2, \cdots \in \Omega$ are disjoint, then* $P(\bigcup_{i=1}^{\infty} \omega_i) = \sum_{i=1}^{\infty} P(\omega_i)$	*Do your own business*

These properties are called **Kolmogorov axioms**[1].

1	2	3

1	2	3
		

- A biography;
- Kolmogorov website;
- https://www.wikiwand.com/en/Probability_theory

Discrete Distribution

Random variable or event is countable or listed, then we can list the probability of every event.
If so, we can compute the probability of a random variable less than the given value. For example, $P(X \leq 10) = \sum_{i=1}^{10} P(X = i)$ if the random variable X only takes positive integers.

What is more, there is a link of discrete distribution or more [2].

Probability Mass Function

The probability mass function (pmf in short) of a discrete random variable X is defined as

> *Definition: The probability mass function of a discrete random variable X is defined as*
>
> $$f_X(x) = P_X(X = x)$$
>
> *for all x.*

The left subindex X is to point out that the probability is with respect to the random variable X and it can omit if no confusion.

Continuous Distribution

If random variables may take on a continuous range of values, it is hard or valueless to compute the probability of a given value. It is usually to find the cumulative distribution function.

Cumulative Distribution function

> *Definition: A function $F(x)$ is called cumulative distribution function (CDF in short) if*
>
> - $\lim_{x\to-\infty} F(x) = 0$ *and* $\lim_{x\to\infty} F(x) = 1$ *;*
> - *The function $F(x)$ is monotone increasing function with x;*
> - $\lim_{x\to x_0^+} F(x) = F(x_0)$ *for all* x_0.

In probability, $\forall x$, $F(x) = P(X \leq x)$ for some random variable X.

For example, if the random variable X has the cumulative distribution function (CDF)

$$F_X(x) = \begin{cases} x, & x \in [0,1] \\ 1, & x \in (1,\infty) \\ 0, & \text{otherwise} \end{cases},$$

we say the random variable X is uniformly distributed in $[0,1]$.

We can see this link as reference[3].

Probability Density Function

The probability density function can be seen as the counterpart of pmf.
For the continuous random variable X, its CDF $F_X(x)$ is not required to be differentiable.
But if so, we can compute the derivative of the CDF $F_X(x)$: $\frac{\mathrm{d}F_X(x)}{\mathrm{d}x} = f_X(x)$.

> *Definition: We call the function $f_X(x)$ is the probability density function with respect to the continuous random variable X if*

$$F_X(x) = \int_{-\infty}^{x} f_X(t)\mathrm{d}t$$

for all x, where $F_X(x)$ is the probability cumulative function of the random variable X.

For example, the random variable X uniformly distributed in $[0, 1]$ has the probability density function

$$f_X(x) = \begin{cases} 1, & x \in [0,1] \\ 0, & \text{otherwise} \end{cases}.$$

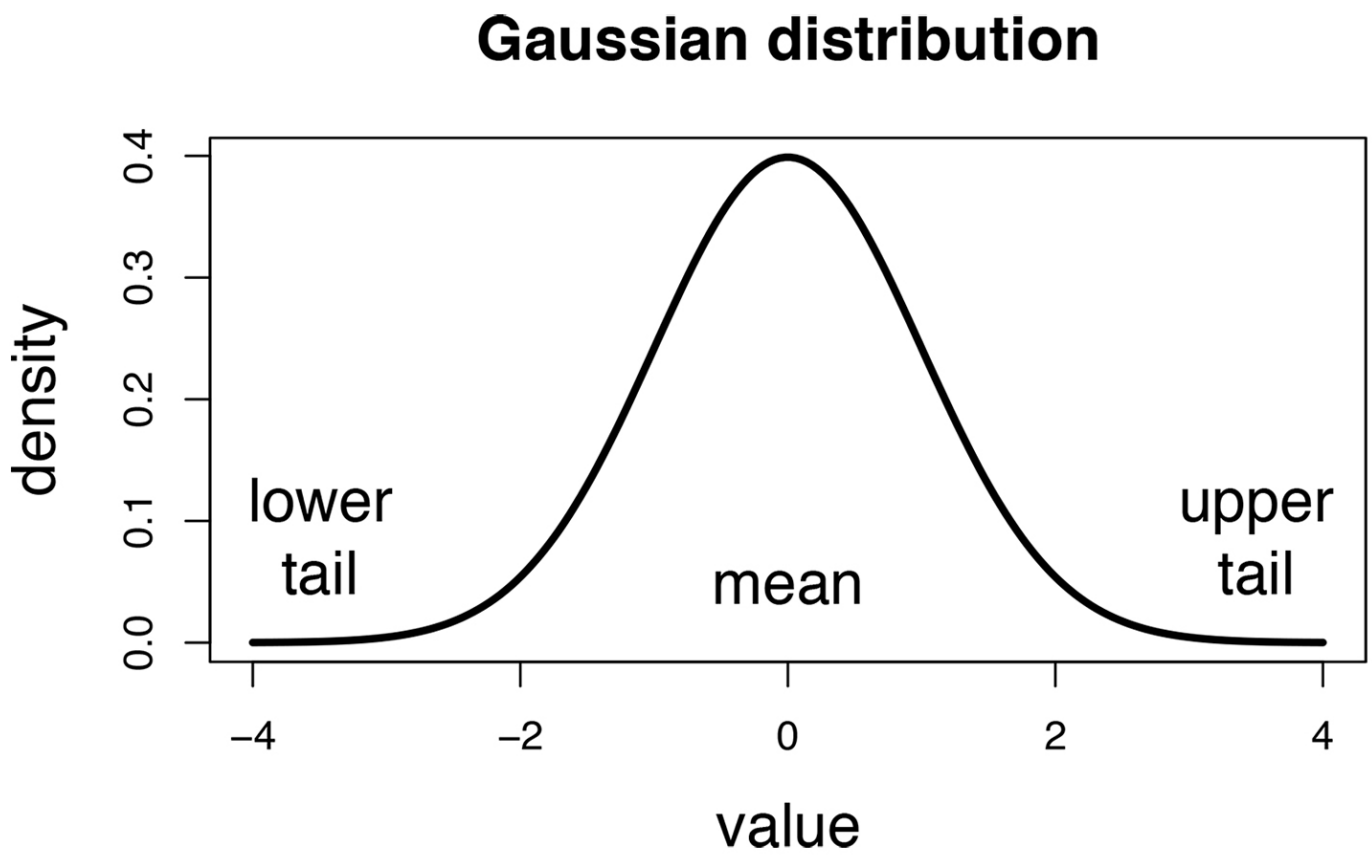
Thus the probability of event A can be written as $\int_{x \in A} f_X(x) \mathrm{d}x$.
PS: *NOT* all random variables have the probability density function.

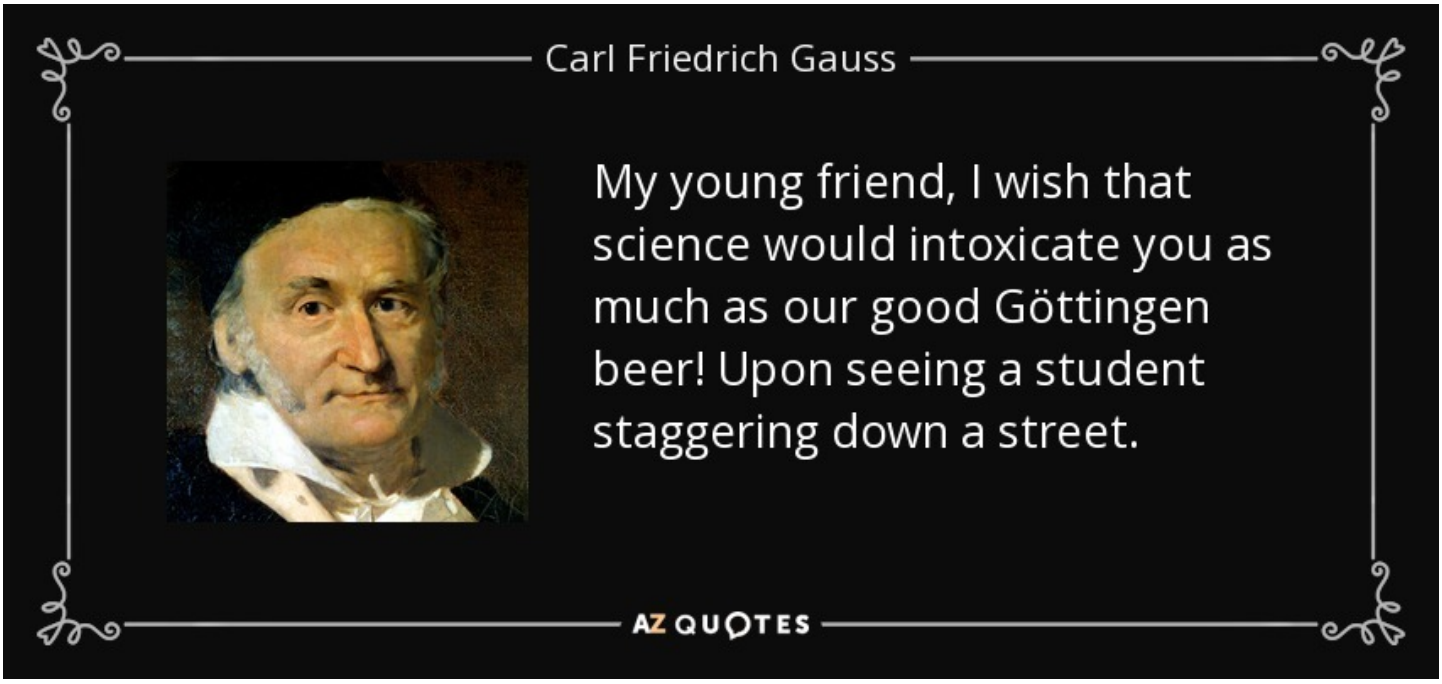
> *Definition: If the pdf f_X is positive in the set $\mathbf{S}$, we call the set $\mathbf{S}$ is the support set or support of the distribution.*

One common probability - normal or Gaussian distribution - is often given in the pdf:

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

where σ^2 is given positive and finite, μ is given and finite. And its support is $(-\infty, \infty)$.





Carl Friedrich Gauss

Power-law Distributions

The density function of a power law distribution is in the form of

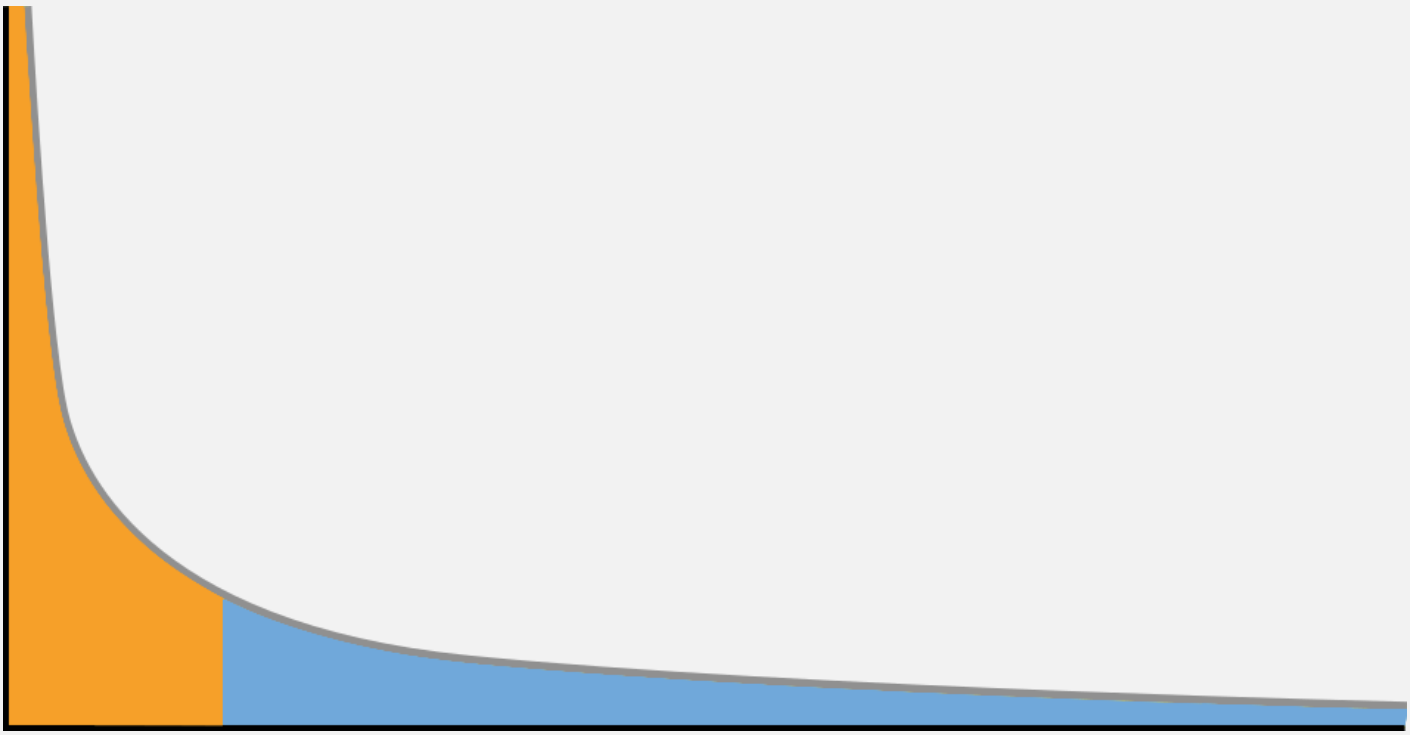
$$f_X(x) = x^{-\alpha}, x \in [1, \infty)$$

where α is real. It is also called Pareto-type distribution.

The power law can be used to describe a phenomenon where a small number of items is clustered at the top of a distribution (or at the bottom), taking up 95% of the resources. In other words, it implies a small amount of occurrences is common, while larger occurrences are rare.

Pareto Distribution

Pareto Distribution



https://www.wikiwand.com/en/Power_law.

http://www.wikiwand.com/en/Pareto_distribution

Every probability distribution is an ideal mathematical model that describes some real event.
Here is a field guide to continuous distribution.

See more content in wikipedia. [4]

Link between discrete and continuous distributions

This is the link between discrete and continuous distributions in Wikipedia.

It is possible to represent certain discrete random variables as well as random variables involving both a continuous and a discrete part with a generalized probability density function, by using the Dirac delta function. For example, let us consider a binary discrete random variable having the Rademacher distribution — that is, taking −1 or 1 for values, with probability ½ each. The density of probability associated with this variable is:

$$f(t) = \frac{1}{2}(\delta(t+1) + \delta(t-1)).$$

More generally, if a discrete variable can take *n* different values among real numbers, then the associated probability density function is:

$$f(t) = \sum_{i=1}^{n} p_i \, \delta(t - x_i)$$

where $x_1, \cdots, x_n$ are the discrete values accessible to the variable and $p_1, \cdots, p_n$ are the probabilities associated with these values.

This substantially unifies the treatment of discrete and continuous probability distributions. For instance, the above expression allows for determining statistical characteristics of such a discrete variable (such as its mean, its variance and its kurtosis), starting from the formulas given for a continuous distribution of the probability.

Bivariate Distribution

The cumulative probability function and probability density function are really functions with some required properties. We wonder the bivariate functions in probability theory.

> *Definition: The joint distribution function $F : \mathbb{R}^2 \to [0, 1]$, where X and Y are discrete variables, is given by*
>
> $$F_{(X,Y)}(x, y) = P(X \leq x, Y \leq y).$$

Their joint mass function $f : \mathbb{R}^2 \to [0, 1]$ is given by

$$f_{(X,Y)}(x, y) = P(X = x, Y = y).$$

> *Definition: The joint distribution function $F_{(X,Y)} : \mathbb{R}^2 \to [0, 1]$, where X and > Y are continuous variables, is given by $F_{(X,Y)}(x, y) = P(X \leq x, Y \leq y)$. And their joint density > function if $f_{X,Y}(x, y)$ satisfies that*
>
> $$F_{(X,Y)}(x, y) = \int_{v=-\infty}^{y} \int_{u=-\infty}^{x} f_{(X,Y)}(u, v) \mathrm{d}u \mathrm{d}v$$
>
> *for each $x, y \in \mathbb{R}$.*

The marginal distribution

> *Definition: The marginal distributed of X and Y are*
>
> -
>
> $$F_X(x) = P(X \leq x) = F_{(X,Y)}(x, \infty) \quad \text{and} \quad F_Y(y) = P(X \leq x) = F_{(X,Y)}(\propto$$

for discrete random variables;

- $$F_X(x) = \int_{-\infty}^{x} (\int_{\mathbb{R}} f_{(X,Y)}(u,y)\mathrm{d}y)\mathrm{d}u \quad \text{and} \quad F_Y(y) = \int_{-\infty}^{y} (\int_{\mathbb{R}} f_{(X,Y)}(x,v)\mathrm{d}v$$

for continuous random variables and the marginal probability density function is

$$f_X(x) = \int_{\mathbb{R}} f_{(X,Y)}(x,y)\mathrm{d}y, \quad f_Y(y) = \int_{\mathbb{R}} f_{(X,Y)}(x,y)\mathrm{d}x.$$

Definition: Two random variables X and Y are called as identically distributed if $P(x \in A) = P(y \in A)$ for any $A \subset \mathbb{R}$.

Representation of Random Variable

The random variable is nearly no sense without its probability distribution. We can choose the CDF or pdf to depict the probability, which depends on the case.

We know that a function of random variable is also a random variable.
For example, supposing that X is a random variable, the function $g(X) = e^X$ is a random variable as well as $g(X) = \ln(X)$.

The function of random variable must have its distribution.
We can take it to generate more distributions.

*Theorem Suppose that X is with the cumulative distribution function CDF $F_X(x)$ and $Y = F_X(X)$, then Y is **uniformly** distributed in the interval $[0,1]$.*

Let X and Y be two different random variables, $Z = X + Y$ or $Z = X \cdot Y$ are typical functions of random variables, especially X is discrete while Y is continuous.
More on the Wikipedia page random variable

Mixture Representation

Let $P_1, P_2, \cdots, P_n$ be probability distribution and $\sum_{i=1}^{n} \lambda_i = 1, \lambda_i > 0 \quad \forall i \in \{1, 2, \cdots, n\}$, we can get

$$P = \sum_{i=1}^{n} \lambda_i P_i$$

is also a probability distribution.
If X is distributed in P, i.e.$X \sim P$, its probability is computed as

$$P(X = x) = \sum_{i=1}^{n} \lambda_i P_i(X = x)$$

for discrete random variable or

$$P(X \leq x) = \sum_{i=1}^{n} \lambda_i P_i(X \leq x)$$

for continuous random variable.

> *Definition: A random variable X is said to have a mixture distribution if the distribution of X depends on a quantity that also has a distribution.*

Sometimes, it is quite difficult if we directly generate a random vector $X \sim f_X(x)$, but the augmented vector $(X, Z)^\top \sim f_{(X,Z)}(x, z)$ is relatively easy to generate such as Box-Muller algorithm.
And we can represent $f_X(x)$ as the marginal probability distribution of $f_{(X,Y)}(x, y)$ in integral form

$$\int_{\mathbb{R}} f_{(X,Z)}(x, z)\mathrm{d}z.$$

It is **Khintchine's (1938) theorem** that shows how to mix the distributions.

Thanks to Professor Tian Guoliang(Gary) in SUSTech, who brought me to computational statistics.[5]

- http://rspa.royalsocietypublishing.org/content/466/2119/2079
- A discussion on unimodal distribution
- Mixture model

More information on probability can be founded in The Probability web.

Bayes' Theorem

Bayes theorem is the foundation of Bayesian statistics in honor of the statistician Thomas Bayes [6].

Conditional Probability

If the set A is the subset of B, i.e. $A \subset B$, we know that if $x \in A$, $x \in B$.
We can say if A happened, the event B must have happened. However, if B happened, what is probability when A happened? It should be larger than the probability of A when B did not happened and it is also larger than the probability of A when the events including B happened. We know that $A \bigcap B = A$ when A is the subset of B.

> *Definition: Supposing $A, B \in \Omega$ and $P(B) > 0$, the conditional probability of A given B(denoted as $P(A|B)$) is*
>
> $$P(A|B) = \frac{P(A \bigcap B)}{P(B)}.$$

The **vertical bar** $|$ means that the right one is given or known and is parameter rather than variable.

Here is a visual explanation.

> *Definition: If $P(A \bigcap B) = P(A)P(B)$, we call the event A and B are statistically independent.*

From the definition of conditional probability, it is obvious that:

- $P(B) = \frac{P(A \bigcap B)}{P(A|B)}$
- $P(A \bigcap B) = P(A|B)P(B)$;
- $P(A \bigcap B) = P(B|A)P(A)$.

Thus

- $P(A|B)P(B) = P(B|A)P(A)$,
- $P(A|B) = \frac{P(B|A)P(A)}{P(B)} = P(B|A)\frac{P(A)}{P(B)}$,
- $P(B) = \frac{P(B|A)P(A)}{P(A|B} = \frac{P(B|A)}{P(A|B)}P(A)$

> *Definition: The conditional distribution function of Y given $X = x$ is the function $F_{Y|X}(y|x)$ given by*
>
> $$F_{Y|X}(y|x) = \int_{-\infty}^{x} \frac{f_{(X,Y)}(x,v)}{f_X(x)}\mathrm{d}v = \frac{\int_{-\infty}^{x} f_{(X,Y)}(x,v)\mathrm{d}v}{f_X(x)}$$
>
> *for the support of $f_X(x)$ and the conditional probability density function of $F_{Y|X}$, written $f_{Y|X}(y|x)$, is given by*

$$f_{Y|X}(y|x) = \frac{f_{(X,Y)}(x,y)}{f_X(x)}$$

for any x such that $f_X(x) > 0$.

Definition: If X and Y are non-generate and jointly continuous random variables with density $f_{X,Y}(x,y)$ then, if B has positive measure,

$$P(X \in A|Y \in B) = \frac{\int_{y\in B}\int_{x\in A} f_{X,Y}(x,y)\mathrm{d}x\mathrm{d}y}{\int_{y\in B}\int_{x\in \mathbb{R}} f_{X,Y}(x,y)\mathrm{d}x\mathrm{d}y}.$$

(Chain Rule of Probability)

$$P(x^{(1)},\cdots,x^{(n)}) = P(x^{(1)})\prod_{i=2}^{n} P(x^i|x^{(1),\cdots,x^{(i-1)}})$$

More content are in wikipedia.

Definition: The event A and B are conditionally independent given C if and only if

$$P(A\bigcap B|C) = P(A|C)P(B|C).$$

There are more on joint distribution:

- https://www.wikiwand.com/en/Joint_probability_distribution
- https://www.wikiwand.com/en/Copula_(probability_theory)
- http://brenocon.com/totvar/

Total Probability Theorem

This is the total probability theorem in Wikipedia.

(Total Probability Theorem) Supposing the events $A_1, A_2, \cdots$ are disjoint in the sample space Ω and $\bigcup_{i=1}^{\infty} A_i = \Omega$, B is any subset of Ω, we have

$$P(B) = \sum_{i=1}^{\infty} P(B \bigcap A_i) = \sum_{i=1}^{\infty} P(B|A_i)P(A_i).$$

- For the discrete random variable, the total probability theorem tells that any event can be decomposed to the basic event in the event space.
- For the continuous random variable, this theorems means that $\int_{\mathbb{B}} f_X(x)\mathrm{d}x = \sum_{i=1}^{\infty} \int_{\mathbb{B} \bigcap \mathbb{A}_i} f_X(x)\mathrm{d}x$.

Bayes' Theorem

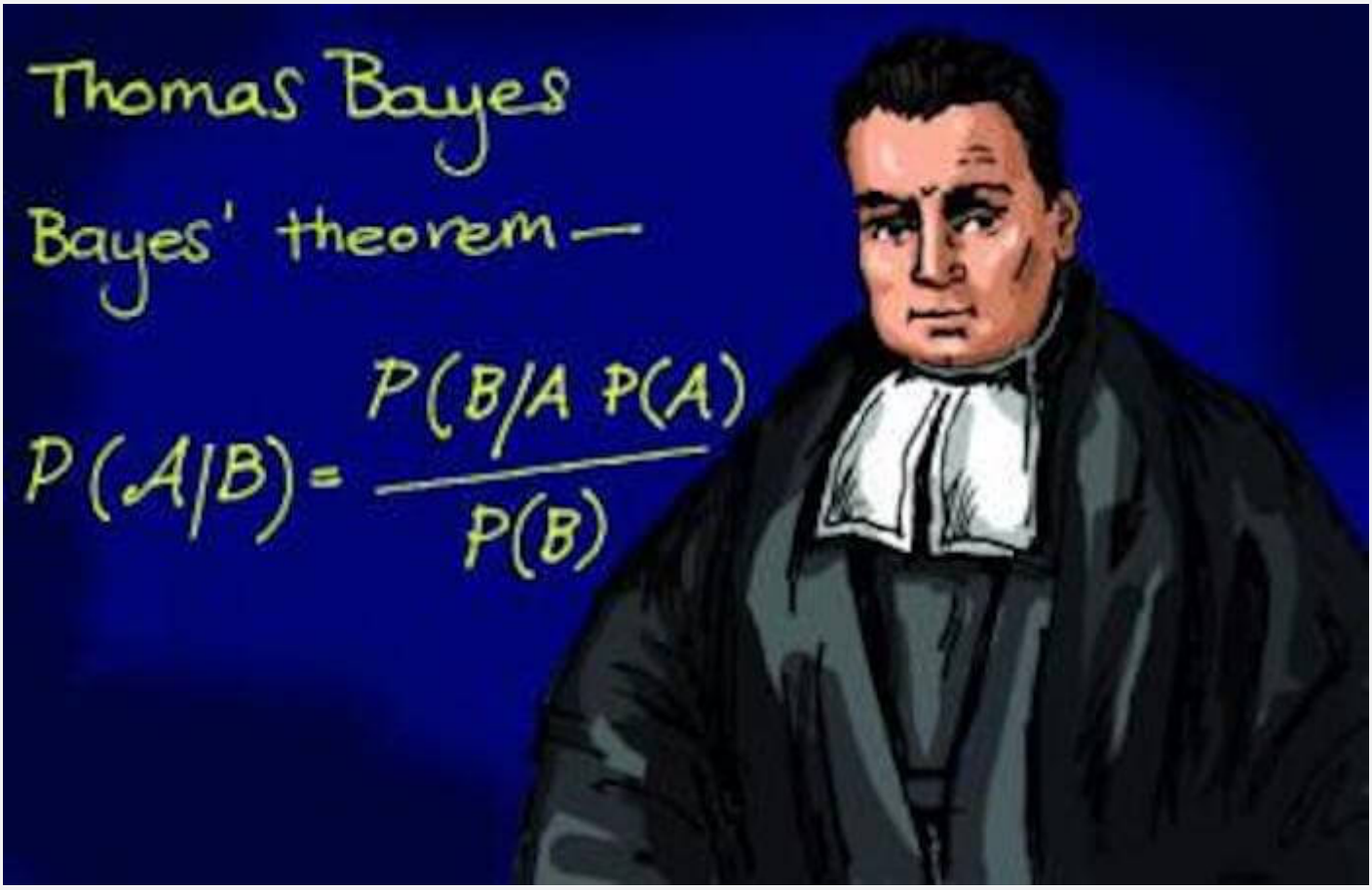
> *(Bayes' Theorem) Supposing the events $A_1, A_2, \cdots$ are disjoint in the sample space Ω and $\bigcup_{i=1}^{\infty} A_i = \Omega$, B is any subset of Ω, we have*

$$P(A_i|B) = \frac{P(B|A_i)P(A_i)}{\sum_{i=1}^{\infty} P(B|A_i)P(A_i)} = \frac{P(B|A_i)P(A_i)}{P(B)}.$$

- The probability $P(A_i)$ is called prior probability of event A_i and the conditional probability $P(A_i|B)$ is called posterior probability of the event A_i in Bayesian statistics.
- For any A_i, $P(A_i|B) \propto P(B|A_i)P(A_i)$ and $P(B)$ is the normalization constant as the sum of $P(B|A_i)P(A_i)$.

Thomas Bayes, 1702-1761

Thomas Bayes, 1702-1761



There are some related links:

- Bayesian probability inWikipedia.
- .pdf file on a history of Bayes' theorem.
- a visual explanation.
- an intuitive explanation.
- online courses and more.
- Count Bayesie

Inverse Bayes' Formula

The joint pdf of the random variables X and Y can be expressed as

$$f_{(x,y)}(x,y) = f_{X|Y}(x|y)f_Y(y) = f_{Y|X}(y|x)f_X(x).$$

in **some proper conditions**.
Thus we get by division

$$f_Y(y) = \frac{f_{Y|X}(y|x)f_X(x)}{f_{X|Y}(x|y)}. \qquad (1)$$

Integrating this identity with respect to y on support of $f_Y(y)$, we immediately have the **point-wise formula** as shown below

$$f_X(x) = \{\int_{f_{X|Y}(x|y)\neq 0} \frac{f_{Y|X}(y|x)}{f_{X|Y}(x|y)}\mathrm{d}y\}^{-1}. \tag{2}$$

Now substitute (2) into (1), we obtain the dual form of IBF for $f_Y(y)$ and hence by symmetry we obtain the **function-wise formula** of $f_Y(y)$ at y_0 as shown in (3), or the sampling formula in (4) when the normalizing constant is omitted.

$$f_X(x) = \{\int_{f_{Y|X}(y|X)\neq 0} \frac{f_{X|Y}(x|y_0)}{f_{Y|X}(y_0|x)}\mathrm{d}x\}^{-1}\frac{f_{X|Y}(x|y_0)}{f_{Y|X}(y_0|x)} \tag{3}$$

$$\propto \frac{f_{X|Y}(x|y_0)}{f_{Y|X}(y_0|x)} \tag{4}$$

The Inventor of IBF

- http://web.hku.hk/~kaing/Background.pdf
- http://101.96.10.64/web.hku.hk/~kaing/Section1_3.pdf
- http://web.hku.hk/~kaing/HKSSinterview.pdf
- http://web.hku.hk/~kaing/HKSStalk.pdf|

Professor Tian taught me this part.[5:1]

- http://reliawiki.org/index.php/Life_Data_Analysis_Reference_Book
- http://camdavidsonpilon.github.io/Probabilistic-Programming-and-Bayesian-Methods-for-Hackers/

What determines a distribution?

The cumulative density function (CDF) or probability density function(pdf) is roughly equal to random variable, i.e. one random variable is always attached with CDF or pdf. However, what we observed is not the variable itself but its realization or

sample.

- In theory, what properties do some CDFs or pdfs hold? For example, are they all integrable?
- In practice, the basic question is how to determine the CDF or pdf if we only observed some samples?

Expectation, Variance and Entropy

Expectation and variance are two important factors that characterize the random variable.

The expectation of a discrete random variable is defined as the weighted sum.

> *Definition: For a discrete random variable X, of which the range is $x_1, \cdots, x_\infty$, its (mathematical)* ***expectation*** *$\mathbb{E}(X)$ is defined as $\mathbb{E}(X) = \sum_{i=1}^{\infty} x_i P(X = x_i)$.*

The expectation of a discrete random variable is a weighted sum. Average is one special expectation with equiprob, i.e. $P(X = x_1) = P(X = x_2) = \cdots = P(X = x_i) = \cdots \forall i$.

The expectation of a continuous random variable is defined as one special integration.

> *Definition: For a continuous random variable X with the pdf $f(x)$, if the integration $\int_{-\infty}^{\infty} |x| f(x) \mathrm{d}x$ exists, the value $\int_{-\infty}^{\infty} x f(x) \mathrm{d}x$ is called the (mathematical)* ***expectation*** *of X, which is often denoted as $\mathbb{E}(X)$.*

Note that NOT all random variables have expectation. For example, standard Cauchy distribution

$$f_X(x) = \frac{1}{\pi(1 + x^2)}$$

is undefined.

The expectation is the center of the probability density function in many cases. What is more,

$$\arg\max_b \mathbb{E}(X - b)^2 = \mathbb{E}(X)$$

which implies that $\mathbb{E}(X)$ is the most likeliest to appear in expectation.

> *Definition: Now suppose that X is a random vector $X = (X_1, \cdots, X_d)$, where X_j, $j = 1, \cdots, d$, is real-valued. Then $\mathbb{E}(X)$ is simply the vector*
>
> $$(\mathbb{E}(X_1), \cdots, \mathbb{E}(X_d))$$

where $\mathbb{E}(X_i) = \int_{\mathbb{R}} x_i f_{X_i} \mathrm{d}x_i \forall i \in \{1, 2, \cdots, d\}$ and $f_{X_i}(x_i)$ is the marginal probability density function of X_i.

Definition: If the random variable has finite expectation $\mathbb{E}(X)$, then the expectation of $(X - \mathbb{E}(X))^2$ is called the variance of X (denoted as $Var(X)$), i.e. $\sum_{i=1}^{\infty}(x_i - \mathbb{E}(X))^2 P(X = x_i)$ for discrete random variable and $\int_{-\infty}^{\infty}(x - \mathbb{E}(X))^2 f_X(x)\mathrm{d}x$ for continuous random variable.

It is obvious that

$$Var(X) = \int_{\mathbb{R}} (x - \mathbb{E}(X))^2 f_X(x)\mathrm{d}x = \int_{\mathbb{X}} (x - \mathbb{E}(X))^2 f_X(x)\mathrm{d}x$$

where the set $\mathbb{X}$ is the support of X.

Definition: In general, let X be a random variable with pdf $f_X(x)$, the expectation of the random variable $g(X)$ is equal to the integration $\int_{\mathbb{R}} g(x) f_X(x)\mathrm{d}x$ if it exists.

In analysis, the expectation of a random variable is the integration of some functions.

Definition: The conditional expectation of Y given X can be defined as

$$\Psi(X) = \mathbb{E}(Y|X) = \int_{\mathbb{R}} y f_{Y|X}(y|x)\mathrm{d}y.$$

It is a **parameter-dependent integral**, where the parameter x can be considered as fixed constant. See the content in Calculus II.

Tower rule Let X be random variable on a sample space Ω, let the events $A_1, A_2, \cdots$ are disjoint in the sample space Ω and $\bigcup_{i=1}^{\infty} A_i = \Omega$, B is any subset of Ω, $\mathbb{E}(X) = \sum_{i=1}^{\infty} \mathbb{E}(X|A_i)P(A_i)$. In general, the conditional expectation $\Psi(X) = \mathbb{E}(Y|X)$ satisfies $\mathbb{E}(\Psi(X)) = \mathbb{E}(Y)$.

The probability of an event can be expressed as the expectation, i.e.

Probability as Integration

$$P(x \in A) = \int_{\mathbb{R}} \mathbb{I}_A f_X(x) \mathrm{d}x$$

where

$$\mathbb{I}_A = \begin{cases} 1, & \text{if } x \in A \\ 0, & \text{otherwise} \end{cases}.$$

It is called as the indictor function of A.

Definition: The Shannon entropy is defined as

- $$H = -\sum_{i=1}^{\infty} P(X = x_i) \ln P(X = x_i)$$

  for the discrete random variable X with the range $\{x_1, \cdots, x_n\}$ with the convention $P(X = x) = 0$ that $P(X = x) \ln \frac{1}{P(X = x)} = 0$ and

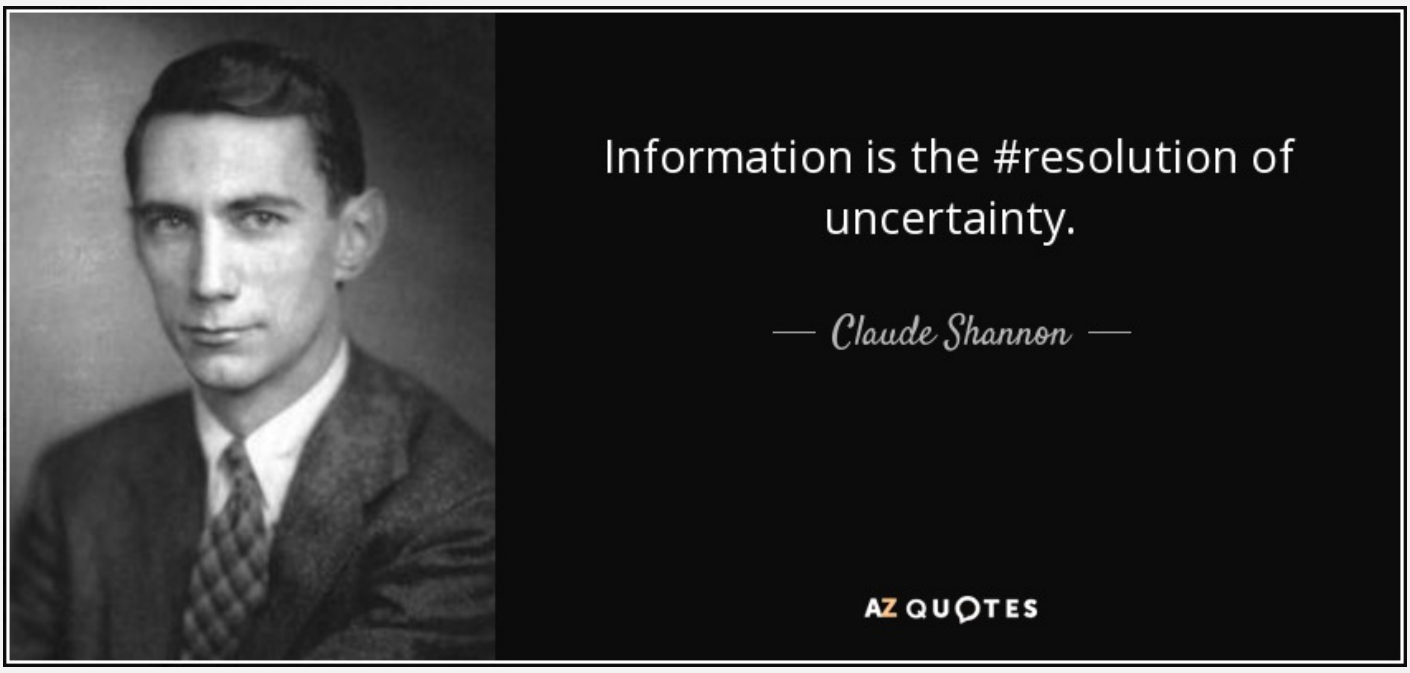
- $$H = \int_{\mathbb{X}} \ln(\frac{1}{f_X(x)}) f_X(x) \mathrm{d}x$$

  for the continuous random variable X with the support $\mathbb{X}$.

The Shannon entropy is often related to *finite* state discrete random variable, i.e. $n < \infty$ and the value of random variable is not involved in its entropy.

Claude Elwood Shannon, 1916-2001

Claude Elwood Shannon, 1916-2001



Visual information

Moment and Moment Generating Function

In calculus, we know that some proper functions can be extended as a Taylor series in a interval.

Moment is a specific quantitative measure of the shape of a function.

> *Definition: The n-th moment of a real-valued continuous function $f_X(x)$ of a real variable about a value c is*

$$\mu_n = \int_{x\in\mathbb{R}} (x-c)^n f_X(x)\mathrm{d}x.$$

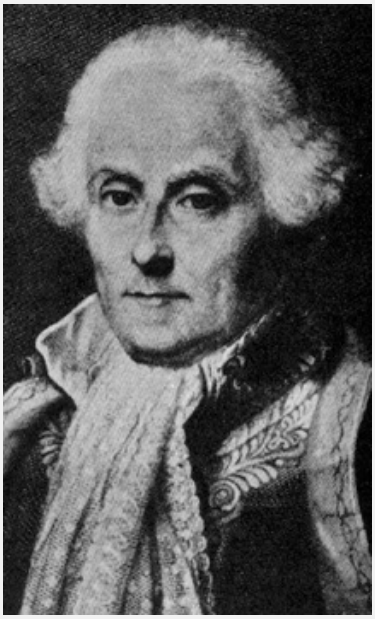
And the constant c always take the expectation $\mathbb{E}(X)$ or 0.

> *Definition: Moment generating function of a random variable X is the expectation of the random variable of e^{tX}, i.e.*

Moment generating function

$M_X(t) = \int_{\mathbb{R}} e^{tx} f_X(x)\mathrm{d}x$ for continuous random variable
$M_X(t) = \sum_{i=1}^{\infty} e^{tx_i} P(x = x_i)$ for discrete random variable

It is Laplace transformation applied to probability density function. And it is also related with cumulants.

Pierre-Simon Laplace	French	1749-1827
		

More pictures

Sampling Methods

There are some related links in web:

- **Random number generation**.
- **List of Random number generating**.
- **Pseudorandom number generator**.
- **Non-uniform pseudo-random variate generation**.
- **Sampling methods**.
- **MCMC**.
- **Visualizing MCMC**.

Sampling from Discrete Distribution

> *(Inverse transform technique) Let F be a probability cumulative function of a random variable taking non-negative integer values, and let U be uniformly distributed on interval $[0, 1]$. The random variable given by $X = k$ if and only if $F(k-1) < U < F(k)$ has the distribution function F.*

Sampling from Categorical Distribution

> *The **categorical distribution** (also called a **generalized Bernoulli distribution**, **multinoulli distribution**) is a discrete probability distribution that describes the possible results of a random variable that can take on one of K possible categories, with the probability of each category separately specified.*

The category can be represented as one-hot vector, i.e. the vector $(1, 0, \cdots, 0)$ is referred as the first category and the others are as similar as it. This representation is of some advantages:

1. Each category is identified by its position and equal to each other in norm;
2. The one-hot vectors can not be compared as the real number in value;
3. The probability mass function of the *K* categories distribution can be written in a compact form - $P(\mathrm{X}) = [p_1, p_2, \cdots, p_K] \cdot \mathrm{X}^T$,
   where
   - The probability $p_i \geq 0, \forall i \in [1, \cdots, K]$ and $\sum_{i=1}^{K} p_i = 1$;
   - The random variable X is one-hot vector and X^T is the transpose of X.

Sampling it by inverse transform sampling:

1. Pick a uniformly distributed number between 0 and 1.
2. Locate the greatest number in the CDF whose value is less than or equal to the number just chosen., i.e. $F^{-1}(u) = inf\{x : F(x) \leq u\}$.
3. Return the category corresponding to this CDF value.
   See more on Categorical distribution.

The categorical variable cannot be ordered, how to compute the CDF?

Sampling from Continuous Distribution

Direct Methods

> *(Inverse transform technique) Let F be a probability cumulative function of a continuous random variable, and let U be uniformly distributed on interval $[0, 1]$. The random variable $X = F^{-1}(U)$ has the distribution function F.*

Khintchine's (1938) theorem: Suppose the random variable X with density given by

$$f_X(x) = \int_x^{\infty} z^{-1} f_Z(z) \mathrm{d}z \tag{0}$$

or This mixture can be represented equivalently by

$$Z \sim f_Z(z), z > 0 \qquad \text{and} \tag{1}$$
$$X|(Z = z) \sim Uinf(0, z). \tag{2}$$

Hence $\frac{X}{Z}|(Z = z) = \frac{X}{z}|(Z = z) \sim Unif(0, 1)$ not depending on z, so that

$$\frac{X}{Z}|(Z = z) = \frac{X}{z}|(Z = z) \sim Unif(0, 1)$$
$$\frac{X}{Z} \overset{d}{=} U \sim Unif(0, 1)$$
$$X = ZU \tag{3}$$

and U and Z are mutually independent.

If $\nabla f_X(x)$ exists and $f_X(\infty) = 0$, we can obtain the following equation by Newton-Leibiniz's theorem

$$f_X(x) = -\int_x \nabla f_X(z)\mathrm{d}z \tag{4}$$

and comparing (4) and (0), it is obvious: $\nabla f_X(z) = -z^{-1} f_Z(z)$.

See more information on On Khintchine's Theorem and Its Place in Random Variate Generation and Reciprocal symmetry, unimodality and Khintchine's theorem.

Rejection sampling

The rejection sampling is to draw samples from a distribution with the help of a proposal distribution.

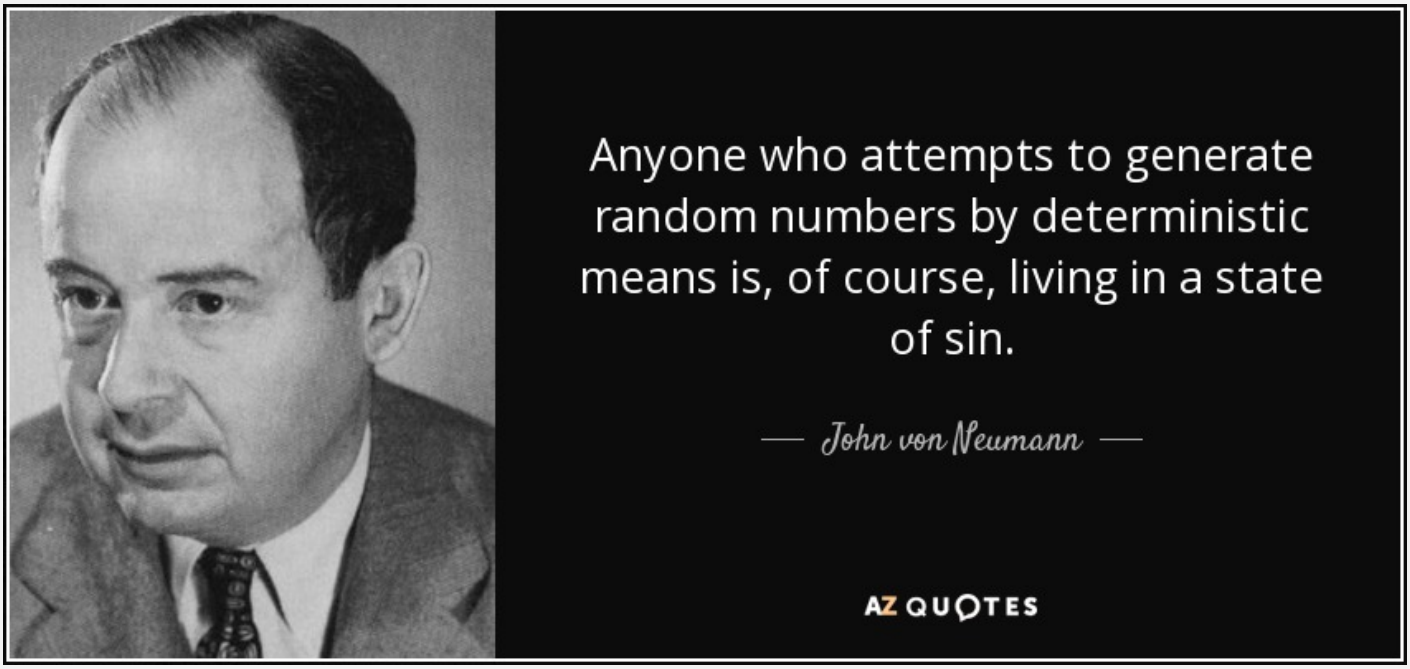
The algorithm (used by John von Neumann and dating back to Buffon and his needle) to obtain a sample from distribution X with density f using samples from distribution Y with density g is as follows:

- Obtain a sample y from distribution Y and a sample u from $\mathrm{Unif}(0, 1)$(the uniform distribution over the unit interval).
- Check whether or not $u < f(y)/Mg(y)$.
    - If this holds, accept y as a sample drawn from f;
    - if not, reject the value of y and return to the sampling step.

The algorithm will take an average of M iterations to obtain a sample.
Ziggural algorithm is an application of rejection sampling to draw samples from Gaussian distribution.

John von Neumann, 1903-1957

John von Neumann, 1903-1957



Sampling-importance-resampling

It is also called SIR method in short. As name shown, it consists of two steps: sampling and importance sampling.
The SIR method generates an approximate i.i.d. sample of size m from the target density
$f(x), x \in \mathbb{X} \subset \mathbb{R}^n$..

The SIR without replacement is as following:

1. Draw $X^{(1)}, X^{(2)}, \cdots, X^{(J)}$ independently from the proposal density $g(\cdot)$.
2. Select a subset $\{X^{(k_i)}\}_{i=1}^m$ from $\{X^{(i)}\}_{i=1}^J$ via resampling without replacement from the discrete distribution $\{\omega_i\}_{i=1}^J$
    - where $w_i = \frac{f(X^{(i)})}{g(X^{(i)})}$ and $\omega_i = \frac{w_i}{\sum_{i=1}^n w_i}$.

The Conditional Sampling Method

The conditional sampling method due to the prominent Rosenblatt
transformation is particularly available when the joint distribution of a d vector is very difficult to generate but one marginal distribution and $d-1$ univariate conditional distributions are easy to simulate.

It is based on the chain rule of probability:

$$f(x) = f(x_d) \prod_{i=1}^{d-1} f_k(x_k | x_{k+1}, x_{k+2}, \cdots, x_d)$$

where $x = (x_1, x_2, \cdots, x_d)$ and $f(x)$ is the probability density function.

To generate X from $f(x)$, we only need to generate x_d from the marginal
density $f_d(x_d)$, then to generate x_k sequentially from the conditional density

$f_k(x_k|x_{k+1}, x_{k+2}, \cdots, x_d)$.

The Vertical Density Representation Method

Law of Large Number

The law of large number provides theoretical guarantee to estimate the expectation of distributions from the samples.

> *(Strong law of large numbers): Let $X_1, X_2, \ldots$ be a sequence of independently identically distributed (i.i.d.) random variables (r.v.s) with expectation μ. Consider the sum*
>
> $$\bar{X}_N = X_1 + X_2 + \cdots + X_N.$$
>
> *Then as $N \to \infty$,*
>
> $$P(\lim_{N\to\infty} \bar{X}_N = \mu) = 1$$
>
> *i.e.*
>
> $$\bar{X}_N \overset{a.s.}{\to} \mu.$$
>
> *See more on Wikipedia.*

Central Limit Theorem

> *Lindeberg–Lévy CLT. Suppose $X_1, X_2, \cdots$ is a sequence of i.i.d. random variables with $E[X_i] = \mu$ and $Var[X_i] = \sigma^2 < \infty$. Then as n approaches infinity, the random variables $\sqrt{n}(\bar{X}_n - \mu)$ converge in distribution to a normal $N(0, \sigma^2)$:*
>
> $$\sqrt{n}(\bar{X}_n - \mu) \overset{d}{\to} N(0, \sigma^2).$$
>
> *The Wikipedia page has more information.*

https://www.datasciencecentral.com/profiles/blogs/new-perspective-on-central-limit-theorem-and-related-stats-topics

Multivariate Normal Distribution

Definition: A random variable $\mathcal{X} = (\mathcal{X}_1, \mathcal{X}_2, \cdots, \mathcal{X}_n)^{\mathcal{T}}$ is multivariate normal if any linear combination of the random variable $X_1, X_2, \cdots, X_n$ is normally distributed, i.e.

$$a_1 X_1 + a_2 X_2 + \cdots + a_n X_n = \vec{a}^T \mathcal{X} \sim \mathcal{N}(\mu, \sigma^2)$$

where $\vec{a} = (a_1, a_2, \cdots, a_n)^T$ and $\mu < \infty$, $0 < \sigma^2 < \infty$.

If $\mathcal{X}$ is multivariate normal, it also has a *mean* vector μ such that

$$\mu = (\mathbb{E}(X_1), \mathbb{E}(X_2), \cdots, \mathbb{E}(X_n))$$

where $\mathbb{E}(X)$ is the expectation(or mean) of the random variable. The random vector $\mathcal{X}$ also has a *covariance matrix* Σ satisfying

$$\Sigma_{ij} = Cov(X_i, X_j)$$

where $Cov(X_i, X_j) = \mathbb{E}[(X_i - \mathbb{E}(X_i))(X_j - \mathbb{E}(X_j))]$ is the covariance of the random variables X_i and X_j.

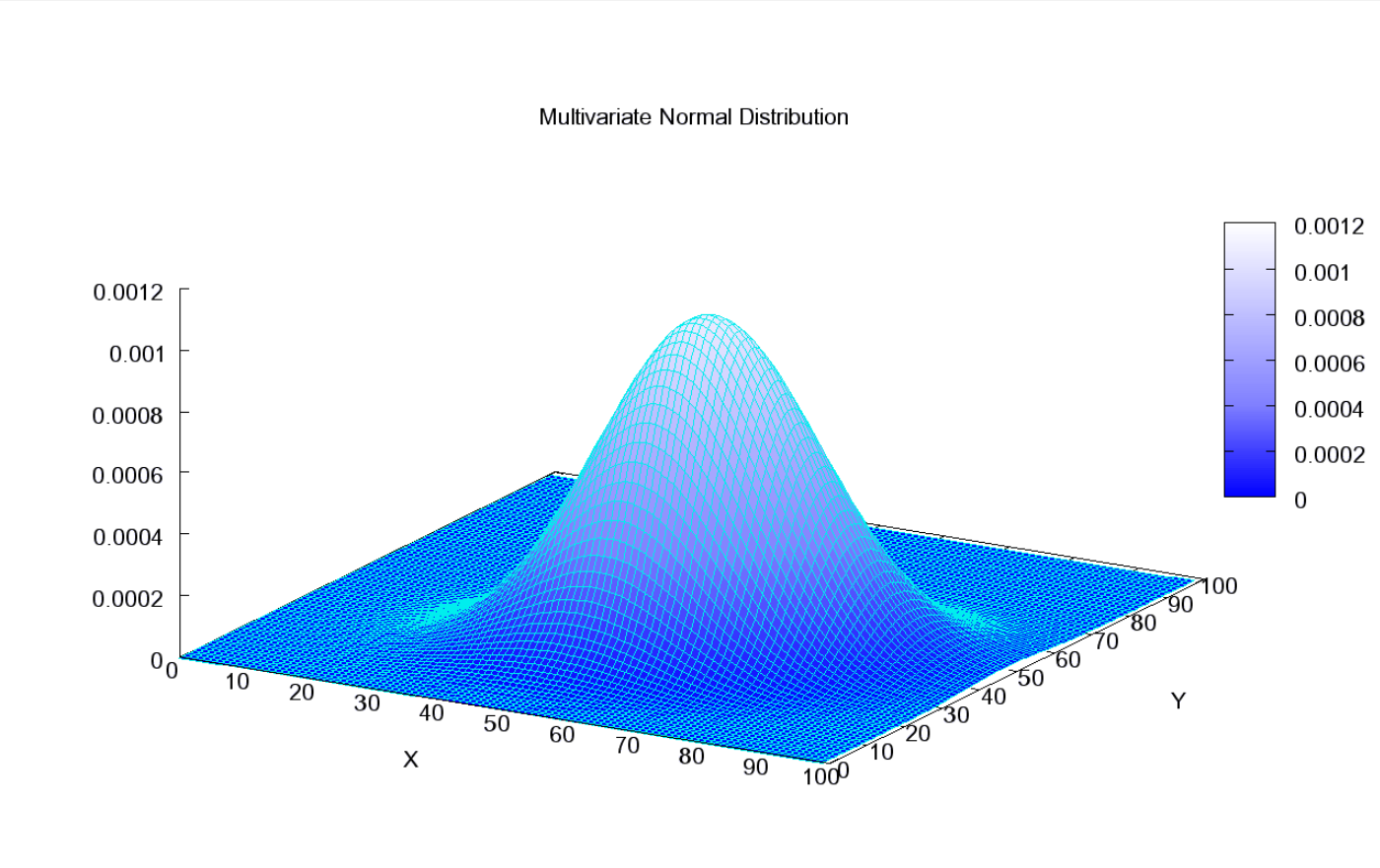
The probability density function of a multivariate normal random vector $\mathcal{X}$ is given by

$$p(\vec{x}|\mu, \Sigma) = \frac{1}{(2\pi)^{\frac{n}{2}} |\Sigma|^{\frac{1}{2}}} exp(-(\vec{x} - \mu)^T \Sigma^{-1} (\vec{x} - \mu))$$

where $exp(x) = e^x$ and $\vec{x}$ is a realization of $\mathcal{X}$, $|\cdot|$ is determinant.
Because $\mathcal{X}$ is completely defined by μ and Σ, it is convenient to write

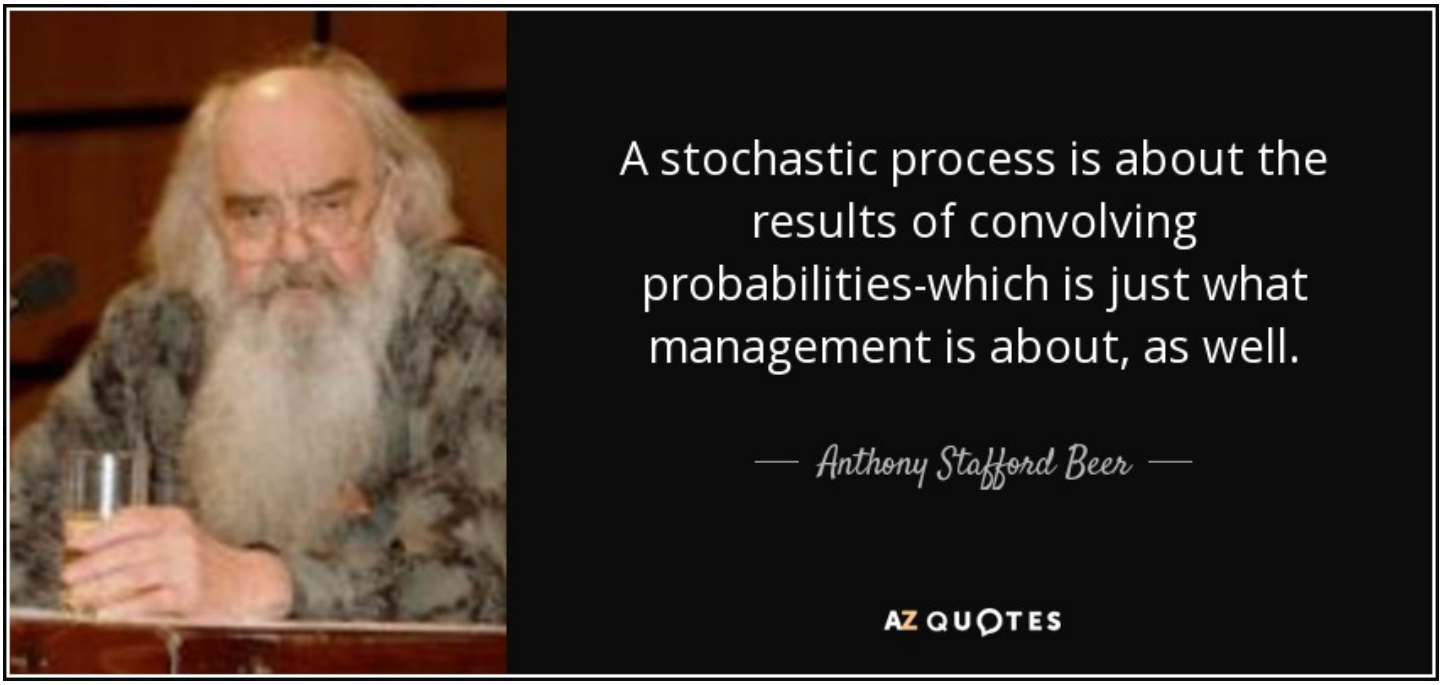
$$\mathcal{X} \sim \mathcal{N}(\mu, \Sigma).$$

- https://brilliant.org/wiki/multivariate-normal-distribution/
- https://www.wikiwand.com/en/Multivariate_normal_distribution



Stochastic Processes

Stochastic processes focus on the independent random variables.
For more information see the Wikipedia page.



Poisson Process

Poisson process is named after the statistician **Siméon Denis Poisson**.

> *Definition:The homogeneous Poisson point process, when considered on the positive half-line, can be defined as a counting process, a type of stochastic process, which can be denoted as* $\{N(t), t \geq 0\}$*. A counting process represents the total number of occurrences or events that have happened up to and including time* t*. A counting process is a Poisson counting process with rate* $\lambda > 0$ *if it has the following three properties:*

- $N(0) = 0$;
- has independent increments, i.e. $N(t) - N(t - \tau)$ and $N(t + \tau) - N(t)$ are independent for $0 \leq \tau \leq t$; and
- the number of events (or points) in any interval of length t is a Poisson random variable with parameter (or mean) λt.

Siméon Denis Poisson

Poisson distribution

It is a discrete distribution with the pmf:

$$P(X = k) = e^{-\lambda}\frac{\lambda^k}{k!}, k \in \{0, 1, \cdots\},$$

where $k!$ is the factorial of k, i.e. $k! = k \times (k-1) \times (k-2) \cdots \times 2 \times 1$.
See more in Wikipedia page.

Markov Chain

Markov chain is a simple stochastic process in honor of **Andrey (Andrei) Andreyevich Marko**.

> *Definition: The process X is a **Markov** chain if it satisfies the Markov condition:*
>
> $$P(X_n = x_n | X_1 = x_1, \cdots, X_{n-1} = x_{n-1}) = P(X_n = x_n | X_{n-1} = x_{n-1})$$
>
> *for all $n \geq 1$.*

People introduced to Markov chains through a typical course on stochastic processes have usually only seen examples where the state space is finite or countable. If the state space is finite, written $\{x_1, \cdots, x_n\}$, then the initial distribution can be associated with a vector $\lambda = (\lambda_1, \cdots, \lambda_n)$ defined by

$$P(X = x_i) = \lambda_i \quad i = 1, \cdots, n,$$

and the transition probabilities can be associated with a matrix P having elements p_{ij} defined by

$$P(X_{n+1} = x_i | X_n = x_j) = p_{ij} \quad i = 1, \cdots, n, \text{and } j = 1, \cdots, n.$$

When the state space is countably infinite, we can think of an infinite vector and matrix. But most Markov chains of interest in **MCMC** have uncountable state space, and then we cannot think of the initial distribution as a vector or the transition probability distribution as a matrix. We must think of them as an unconditional probability distribution and a conditional probability distribution.

Stationarity

A stochastic process is stationary if for every positive integer k the distribution of the k-tuple

$$(X_{n+1}, X_{n+2}, \cdots, X_{n+k})$$

does not depend on n. A Markov chain is stationary if it is a stationary stochastic process. In a Markov chain, the conditional distribution of $(X_{n+2}, \cdots, X_{n+k})$ given X_{n+1} does not depend on n. It follows that a Markov chain is stationary if and only if the marginal distribution of X_n does not depend on n.

An initial distribution is said to be **stationary** or **invariant** or **equilibrium** for some transition probability distribution if the Markov chain specified by this initial distribution and transition probability distribution is stationary. We also indicate this by saying that the transition probability distribution **preserves** the initial distribution.

Stationarity implies stationary transition probabilities, but not vice versa.

Reversibility

A transition probability distribution is reversible with respect to an initial distribution if, for the Markov chain $X_1, X_2, \cdots$ they specify, the distribution of pairs (X_i, X_{i+1}) is exchangeable.

A Markov chain is reversible if its transition probability is reversible with respect to its initial distribution. Reversibility implies stationarity, but not vice versa. A reversible Markov chain has the same laws running forward or backward in time, that is, for any i and k the distributions of $(X_{i+1}, \cdots, X_{i+k})$ and $(X_{i+k}, \cdots, X_{i+1})$ are the same.

Andrey (Andrei) Andreyevich Markov,1856-1922

А. А. Марков (1886).

his short biography in .pdf file format

http://arogozhnikov.github.io/2016/12/19/markov_chain_monte_carlo.html

Markov Chain Monte Carlo

1. http://www.mcmchandbook.net/
2. http://www.cs.princeton.edu/courses/archive/spr06/cos598C/papers/AndrieuFreitasDoucetJordan2003.pdf
3. https://math.uchicago.edu/~shmuel/Network-course-readings/MCMCRev.pdf
4. https://skymind.ai/wiki/markov-chain-monte-carlo
5. https://chi-feng.github.io/mcmc-demo/app.html#HamiltonianMC,banana
6. http://probability.ca/jeff/ftpdir/lannotes.4.pdf
7. https://www.seas.harvard.edu/courses/cs281/papers/andrieu-defreitas-doucet-jordan-2002.pdf

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- https://www.seas.harvard.edu/courses/cs281/papers/neal-1998.pdf
- http://www.mcmchandbook.net/HandbookChapter1.pdf
- https://www.seas.harvard.edu/courses/cs281/papers/roberts-rosenthal-2003.pdf
- Hamiltonian Monte Carlo 1
- Roadmap of HMM
- PyMC2
- https://cosx.org/2013/01/lda-math-mcmc-and-gibbs-sampling

Importance sampling

Let $\vec{X}$ be a random vector, and we wan to compute the integration or the expectation

$$\mu = \mathbb{E}(f(\vec{X})) = \int_{\mathbb{R}} f(\vec{X})p(X)\mathrm{d}X,$$

where $p(X)$ is the probability density function of $\vec{X}$.
We can rewrite the expectation

$$\mu = \int_{\mathbb{R}} \frac{f(\vec{X})p(X)}{q(X)}q(X)\mathrm{d}X = \mathbb{E}_q(\frac{f(\vec{X})p(X)}{q(X)}),$$

where $q(X)$ is another probability density function and $q(X) = 0$ implies $f(\vec{X})p(X) = 0$.

The algorithm of importance sampling is as following:

1. Generate samples $\vec{X}_1, \vec{X}_2, \cdots, \vec{X}_n$ from the distribution $q(X)$;
2. Compute the estimator $\hat{\mu}_q = \frac{1}{n}\sum_{i=1}^{n} \frac{f(\vec{X_i})p(\vec{X_i})}{q(\vec{X_i})}$

See more in

- Wikipedia page.
- Stanford statweb

Statistical Estimation

It is based on the assumption that the data are independently identically distributed (IID).

> *Definition: Any function of sample $W(X_1, X_2, \cdots, X_n)$ is called a point estimator.*

$Note$: A point estimator is a random variable or statistic.

The Method of Moments Estimator

The moments method is to estimate the moments of probability distribution function via sample moments.

The nth sample moment is defined as

$$\hat{\mu}_n = \frac{1}{L}\sum_{i=1}^{L} X_i^n$$

The method of moments estimator $\hat{\theta}_L$ is defined to be the value of θ such that

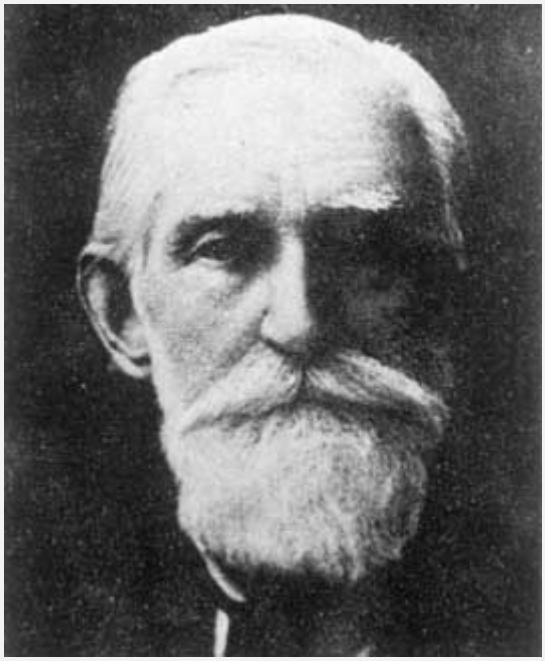
$$\mu_j(\hat{\theta}_L) = \hat{\mu}_j, \forall j \in \{1, 2, \cdots, k\}.$$

By solving the above system of equations for $\hat{theta}$ in the term of $\hat{\mu}_j$, we will obtain the method of moments estimator.

See more on Wikipedia.

Pafnuty Chebyshev,1821-1894

Pafnuty Chebyshev,1821-1894



Some details on his biography

Maximum Likelihood Estimation

Maximum likelihood estimation is a method to estimate the parameters of statistical independent identical distributed samples. It is based on the belief that **what we observed is what is most likely to happen. Let us start with an example.**

Supposing $X_1, X_2, \cdots, X_n \overset{i.i.d.}{\sim} \mathrm{N}(\mu, \sigma^2)$, we can get the joint distribution of their samples $\{x_1, x_2, \cdots, x_n\}$:

$$L(\theta|x_1, \cdots, x_n) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}.$$

The independency of the random variables can directly infer their joint probability is the product of each probability.

We want to find the optimal parameters $\hat{\mu}, \hat{\sigma}^2$ of the probability density function:

$$\arg\max_{\theta} L(\theta|x_1, \cdots, x_n) = \arg\max_{\theta} \ell(\theta|x_1, \cdots, x_n)$$

where the log-likelihood function $\ell(\theta|x_1, \cdots, x_n)$ is defined as the logarithm of likelihood function, i.e.

$$\arg\max_{\mu,\sigma^2} \ell(\mu, \sigma^2|x_1, x_2, \cdots, x_n) = \arg\max_{\mu,\sigma^2} \sum_{i=1}^{n} -\frac{(x_i-\mu)^2}{2\sigma^2} - n\log\sqrt{2\pi\sigma^2}.$$

Setting $\frac{\partial \ell}{\partial \mu} = 0$ and $\frac{\partial \ell}{\partial \sigma^2} = 0$, we can get $\hat{\mu} = \bar{x} = \frac{\sum_{i=1}^{n} x_i}{n}$ and $\hat{\sigma}^2 = \frac{\sum_{i=1}^{n}(x_i-\mu)^2}{\bar{x}}$ as their maximum likelihood estimation.

> *Definition: For each sample point X, let $\hat{\theta}(X)$ be a parameter value at which $L(\theta|X)$ attains its maximum as a function of X, with X held fixed. A maximum likelihood estimator (MLE) of the parameter θ based on a sample X is $\hat{\theta}(X)$.*

We can see more in the Wikipedia page.

http://www.notenoughthoughts.net/posts/normal-log-likelihood-gradient.html

Bayesian Estimation of Parameters

Bayesian inference is usually carried out in the following way[7].

---

1. *We choose a probability density function $f(\theta)$ - called the **prior distribution** - that express our degrees of beliefs on a parameter of interest θ before we see any data.*
2. *We choose a statistical model $f(x|\theta)$ that reflects our beliefs about x given θ.*
3. *After observing data $X_1, X_2, \cdots, X_n$, we update our beliefs and form the **posterior** distribution $f(\theta|X_1, X_2, \cdots, X_n)$.*

For example, the Bayesian version of maximum likelihood estimation will find the parameters θ that maximizes the posterior $f(\theta|X)f(\theta)$ where $f(\theta|X)$ is the likelihood function of samples, i.e. $f(\theta|X) = L(\theta|X_1, \ldots, X_n)$. The Bayesian estimator is

$$\hat{\theta} = \arg\max_\theta f(\theta|X)f(\theta).$$

More related links on *Bayesian methods*:

- https://github.com/Hulalazz/BayesianLearning
- http://www.cs.columbia.edu/~scohen/bayesian/
- [CS598jhm Advanced NLP (Bayesian Methods)]https://courses.engr.illinois.edu/cs598jhm/sp2013/index.html
- https://onlinecourses.science.psu.edu/stat414/node/241/
- https://www.countbayesie.com/blog/2016/5/1/a-guide-to-bayesian-statistics
- https://www.statlect.com/fundamentals-of-statistics/normal-distribution-Bayesian-estimation
- http://www.cnblogs.com/bayesianML/
- https://www.wikiwand.com/en/Bayes_estimator

Confidence Interval Estimation

The pivot quantity is the core.

> *Definition: A* $1-\alpha$ *confidence interval for a parameter* θ *an interval* $C_n=(a,b)$ *where* $a=a(X_1,\cdots,X_n)$ *and* $b=b(X_1,\cdots,X_n)$ *are functions of the data* $\{X_1,\cdots,X_n\}$ *such that*
>
> $$P_\theta(\theta\in C_n)\geq 1-\theta.$$

Note: C_n is random and θ isfixed! If θ is a vector then we use a confidence set (such a sphere or an ellipse) instead of an interval.

An interpretation is this[7:1].

> *On day 1, you collect data and construct a 95 percent confidence interval for a parameter* θ_1*. On day 2, you collect new data and construct a 95 per cent confidence interval for an unrelated parameter* θ_2*. On day 3, you collect new data and construct a 95 percent confidence interval for an unrelated parameter* θ_3*. You continue this way constructing confidence intervals for a sequence of unrelated parameters* $\theta_2,\theta_2,\cdots$*. Then 95 percent your intervals will trap the true parameter value. There is no need to introduce the idea of repeating the same experiment over and over.*

See the thereby links for more information:

- The Fallacy of Placing Confidence in Confidence Intervals;
- BS704_Confidence_Intervals;
- Wikipedia page;
- http://www.stat.yale.edu/Courses/1997-98/101/confint.htm

Goodness of Fit

- https://www.wikiwand.com/en/Goodness_of_fit
- https://onlinecourses.science.psu.edu/stat504/node/60/

Thanks to Professor Tian Guoliang(Gary) again.[8]

Numerical Optimization

IN A Few Useful Things to Know about Machine Learning, Pedro Domingos put up a relation:
$LEARNING=REPRESENTATION+EVALUATION+OPTIMIZATION$.

- Representation as the core of the note is the general (mathematical) **model** that computer can handle.

- Evaluation is **criteria**. An evaluation function (also called objective function, cost function or scoring function) is needed to distinguish good classifiers from bad ones.
- Optimization is to aimed to find the parameters taht optimizes the evaluation function, i.e.

$$\arg\min_{\theta} f(\theta) = \{\theta^* | f(\theta^*) = \min f(\theta)\} \text{ or } \arg\max_{\theta} f(\theta) = \{\theta^* | f(\theta^*) = \max f(\theta)\}.$$

The objective function to be minimized is also called cost function.

Evaluation is always attached with optimization; the evavluation which cannot be optimized is not a good evaluation in machine learning.

- https://www.wikiwand.com/en/Mathematical_optimization
- https://web.stanford.edu/~boyd/cvxbook/bv_cvxbook.pdf
- http://www.cs.cmu.edu/~pradeepr/convexopt/

Gradient Descent and More

Each iteration of a line search method computes a search direction p^k and then decides how far to move along that direction. The iteration is given by

$$x^{k+1} = x^k + \alpha_k p^k \qquad \text{(Line search)}$$

where the positive scalar α^k is called the step length. The success of a line search method depends on effective choices of both the direction p^k and the step length α_k.

$Note$: we use the notation x^k and α_k to represent the kth iteration of the vector variables x and kth step length, respectively.
Most line search algorithms require pk to be a descent direction—one for which $\langle p^k, \nabla f_k \rangle < 0$ — because this property guarantees that the function f can be reduced along this direction, where ∇f_k is the gradient of objective function f at the kth iteration point x_k i.e. $\nabla f_k = \nabla f(x^k)$.

Gradient descent and its variants are to find the local solution of the unconstrained optimization problem:

$$\min f(x)$$

where $x \in \mathbb{R}^n$.

Its iterative procedure is:

$$x^{k+1} = x^k - \alpha_k \nabla_x f(x^k)$$

where x^k is the kth iterative result, $\alpha_k \in \{\alpha | f(x^{k+1}) < f(x^k)\}$ and particularly $\alpha_k = \arg\min_\alpha f(x^k - \alpha \nabla_x f(x^k))$.

Some variants of gradient descent methods are not line search method.
For example, the **heavy ball method**:

$$x^{k+1} = x^k - \alpha_k \nabla_x f(x^k) + \rho_k (x^k - x^{k-1})$$

where the momentum coefficient $\rho_k \in [0, 1]$ generally and the step length α_k cannot be determined by line search.

Nesterov accelerated gradient method:

$$\begin{aligned} x^k &= y^k - \alpha^{k+1} \nabla_x f(y^k) && \text{Descent} \\ y^{k+1} &= x^k + \rho^k (x^k - x^{k-1}) && \text{Momentum} \end{aligned}$$

where the momentum coefficient $\rho_k \in [0, 1]$ generally.

Inventor of Nesterov accelerated Gradient

- https://www.wikiwand.com/en/Gradient_descent
- http://wiki.fast.ai/index.php/Gradient_Descent
- https://blogs.princeton.edu/imabandit/2013/04/01/acceleratedgradientdescent/
- https://blogs.princeton.edu/imabandit/2015/06/30/revisiting-nesterovs-acceleration/
- http://awibisono.github.io/2016/06/20/accelerated-gradient-descent.html

- https://jlmelville.github.io/mize/nesterov.html
- https://smartech.gatech.edu/handle/1853/60525
- https://zhuanlan.zhihu.com/p/41263068
- https://zhuanlan.zhihu.com/p/35692553
- https://zhuanlan.zhihu.com/p/35323828

Mirror Gradient Method

It is often called **mirror descent**.
It can be regarded as non-Euclidean generalization of **projected gradient descent** to solve some constrained optimization problems.

Projected Gradient Descent

Projected gradient descent is aimed to solve convex optimization problem with explicit constraints, i.e.

$$\arg\min_{x\in\mathbb{S}} f(x)$$

where $\mathbb{S}\subset\mathbb{R}^n$.
It has two steps:

$$\begin{aligned} z^{k+1} &= x^k - \alpha_k \nabla_x f(x^k) && \text{Gradient descent} \\ x^{k+1} &= Proj_{\mathbb{S}}(z^{k+1}) = \arg\min_{x\in\mathbb{S}} \|x - z^{k+1}\|^2 && \text{Projection} \end{aligned}$$

Mirror descent

Mirror descent can be regarded as the non-Euclidean generalization via replacing the ℓ_2 norm or Euclidean distance in projected gradient descent by Bregman divergence.

Bregman divergence is induced by convex smooth function f:

$$B(x,y) = f(x) - f(y) - \langle \nabla f(y), x - y\rangle$$

where $\langle\cdot,\cdot\rangle$ is inner product.
Especially, when f is quadratic function, the Bregman divergence induced by f is

$$B(x,y) = x^2 - y^2 - \langle 2y, x-y\rangle = x^2 + y^2 - 2xy = (x-y)^2$$

i.e. the Euclidean distance.

It is given by:

$$\begin{aligned} z^{k+1} &= x^k - \alpha_k \nabla_x f(x^k) && \text{Gradient descent} \\ x^{k+1} &= \arg\min_{x \in \mathbb{S}} B(x, z^{k+1}) && \text{Bregman projection} \end{aligned}.$$

One special method is called **entropic mirror descent** when $f = e^x$ and $\mathbb{S}$ is simplex.

See more on the following link list.

- http://users.cecs.anu.edu.au/~xzhang/teaching/bregman.pdf
- https://zhuanlan.zhihu.com/p/34299990
- https://blogs.princeton.edu/imabandit/2013/04/16/orf523-mirror-descent-part-iii/
- https://blogs.princeton.edu/imabandit/2013/04/18/orf523-mirror-descent-part-iiii/
- https://www.stat.berkeley.edu/~bartlett/courses/2014fall-cs294stat260/lectures/mirror-descent-notes.pdf

Variable Metric Methods

Newton's Method

NEWTON'S METHOD and QUASI-NEWTON METHODS are classified to variable metric methods.

It is also to find the solution of unconstrained optimization problems, i.e.

$$\min f(x)$$

where $x \in \mathbb{R}^n$.

Newton's method is given by

$$x^{k+1} = x^k - \alpha^{k+1} H^{-1}(x^k) \nabla_x f(x^k)$$

where $H^{-1}(x^k)$ is inverse of the Hessian matrix of the function $f(x)$ at the point x^k.
It is called **Newton–Raphson algorithm** in statistics.
Especially when the log-likelihood function $\ell(\theta)$ is well-behaved,
a natural candidate for finding the MLE is the **Newton–Raphson algorithm** with quadratic convergence rate.

The Fisher Scoring Algorithm

In maximum likelihood estimation, the objective function is the log-likelihood function, i.e.

$$\ell(\theta) = \sum_{i=1}^{n} \log P(x_i|\theta)$$

where $P(x_i|\theta)$ is the probability of realization $X_i = x_i$ with the unknown parameter θ.
However, when the sample random variable $\{X_i\}_{i=1}^n$ are not observed or realized, it is best to replace negative Hessian matrix (i.e. $-\frac{\partial^2 \ell(\theta)}{\partial\theta\partial\theta^T}$) of the likelihood function with the **observed information matrix**:

$$J(\theta) = \mathbb{E}(-\frac{\partial^2 \ell(\theta)}{\partial\theta\partial\theta^T}) = -\int \frac{\partial^2 \ell(\theta)}{\partial\theta\partial\theta^T} f(x_1, \cdots, x_n|\theta) \mathrm{d}x_1 \cdots \mathrm{d}x_n$$

where $f(x_1, \cdots, x_n|\theta)$ is the joint probability density function of $X_1, \cdots, X_n$ with unknown parameter θ.

And the **Fisher scoring algorithm** is given by

$$\theta^{k+1} = \theta^k + \alpha_k J^{-1}(\theta^k) \nabla_\theta \ell(\theta^k)$$

where $J^{-1}(\theta^k)$ is the inverse of observed information matrix at the point θ^k.

See http://www.stats.ox.ac.uk/~steffen/teaching/bs2HT9/scoring.pdf or https://wiseodd.github.io/techblog/2018/03/11/fisher-information/.

Fisher scoring algorithm is regarded as an example of **Natural Gradient Descent** in information geometry such as https://wiseodd.github.io/techblog/2018/03/14/natural-gradient/ and https://www.zhihu.com/question/266846405.

Quasi-Newton Methods

Quasi-Newton methods, like steepest descent, require only the gradient of the objective function to be supplied at each iterate.
By measuring the changes in gradients, they construct a model of the objective function that is good enough to produce superlinear convergence.
The improvement over steepest descent is dramatic, especially on difficult problems. Moreover, since second derivatives are not required, quasi-Newton methods are sometimes more efficient than Newton's method.[9]

In optimization, quasi-Newton methods (a special case of **variable-metric methods**) are algorithms for finding local maxima and minima of functions. Quasi-Newton methods are based on Newton's method to find the stationary point of a function, where the gradient is 0.
In quasi-Newton methods the Hessian matrix does not need to be computed. The Hessian is updated by analyzing successive gradient vectors instead. Quasi-Newton methods are a generalization of the secant method to find the root of the first derivative for multidimensional problems. In multiple dimensions the secant equation is under-determined, and quasi-Newton methods differ in how they constrain the solution, typically by adding a simple low-rank update to the current estimate of the Hessian.
One of the chief advantages of quasi-Newton methods over Newton's method is that the Hessian matrix (or, in the case of quasi-Newton methods, its approximation) B does not need to be inverted. The Hessian approximation B is chosen to satisfy

$$\nabla f(x^{k+1}) = \nabla f(x^k) + B(x^{k+1} - x^k),$$

which is called the **secant equation** (the Taylor series of the gradient itself).
In more than one dimension B is underdetermined. In one dimension, solving for B and applying the Newton's step with the updated value is equivalent to the secant method. The various quasi-Newton methods differ in their choice of the solution to the secant equation (in one dimension, all the variants are equivalent).

- Wikipedia page
- Newton-Raphson Visualization (1D)
- Newton-Raphson Visualization (2D)
- Newton's method
- Quasi-Newton method
- Using Gradient Descent for Optimization and Learning

Natural Gradient Descent

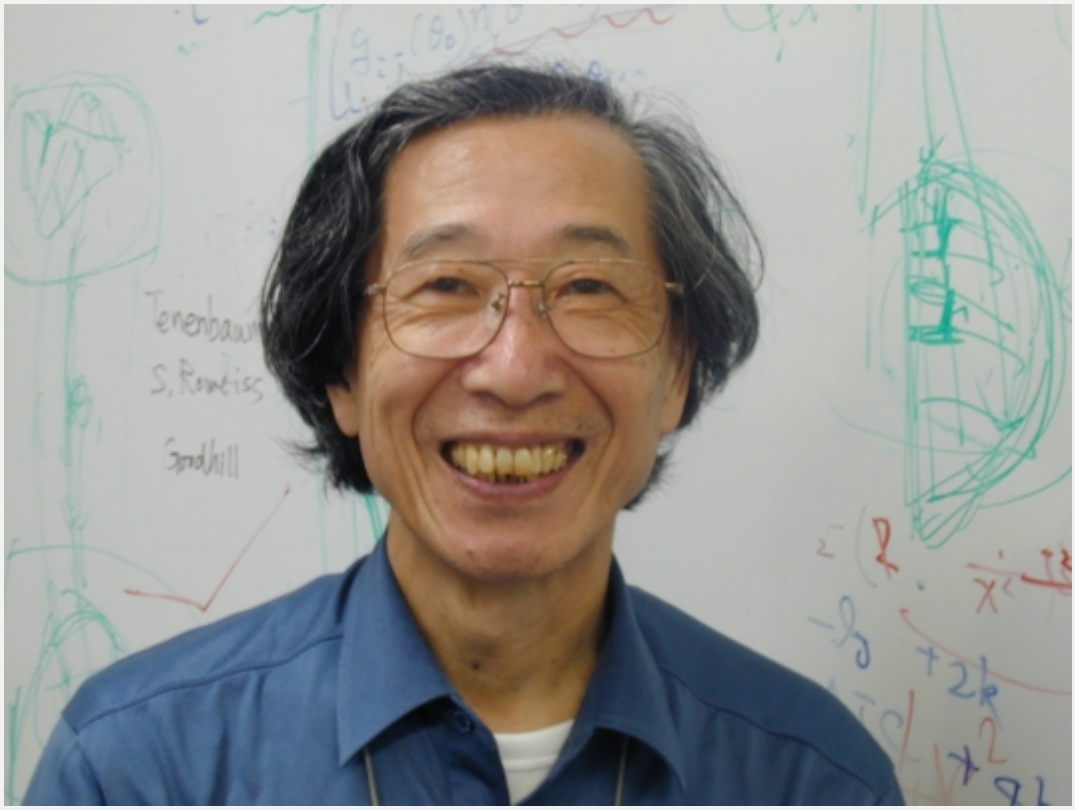
Natural gradient descent is to solve the optimization problem $\min_\theta L(\theta)$ by

$$\theta^{(t+1)} = \theta^{(t+1)} - \alpha_{(t)} F^{-1}(\theta^{(t)}) \nabla_\theta L(\theta^{(t)})$$

where $F^{-1}(\theta^{(t)})$ is the inverse of Remiann metric at the point $\theta^{(t)}$.
And **Fisher scoring** algorithm is a typical application of **Natural Gradient Descent** to statistics.
Natural gradient descent for manifolds corresponding to
exponential families can be implemented as a first-order method through **mirror descent**
(https://www.stat.wisc.edu/~raskutti/publication/MirrorDescent.pdf).

Originator of Information Geometry

Originator of Information Geometry



- http://www.yann-ollivier.org/rech/publs/natkal.pdf
- http://www.dianacai.com/blog/2018/02/16/natural-gradients-mirror-descent/
- https://www.zhihu.com/question/266846405
- http://bicmr.pku.edu.cn/~dongbin/Conferences/Mini-Course-IG/index.html
- http://ipvs.informatik.uni-stuttgart.de/mlr/wp-content/uploads/2015/01/mathematics_for_intelligent_systems_lecture12_notes_I.pdf
- http://www.luigimalago.it/tutorials/algebraicstatistics2015tutorial.pdf
- http://www.yann-ollivier.org/rech/publs/tango.pdf
- http://www.brain.riken.jp/asset/img/researchers/cv/s_amari.pdf

Expectation Maximization Algorithm

Expectation-Maximization algorithm, popularly known as the **EM algorithm** has become a standard piece in the statistician's repertoire.
It is used in incomplete-data problems or latent-variable problems such as Gaussian mixture model in maximum likelihood estimation.
The basic principle behind the **EM** is that instead of performing a complicated optimization,
one augments the observed data with latent data to perform a series of simple optimizations.

Let $\ell(\theta|Y_{obs}) \triangleq \log L(\theta|Y_{obs})$ denote the log-likelihood function of observed datum Y_{obs}。
We augment the observed data Y_{obs} with latent variables Z so that both the
complete-data log-likelihood $\ell(\theta|Y_{obs}, Z)$ and the conditional predictive distribution $f(z|Y_{obs}, \theta)$ are available.
Each iteration of the **EM** algorithm consists of an expectation step (E-step) and a maximization step (M-step)

Specifically, let $\theta^{(t)}$ be the current best guess at the MLE $\hat{\theta}$. The E-step
is to compute the **Q** function defined by

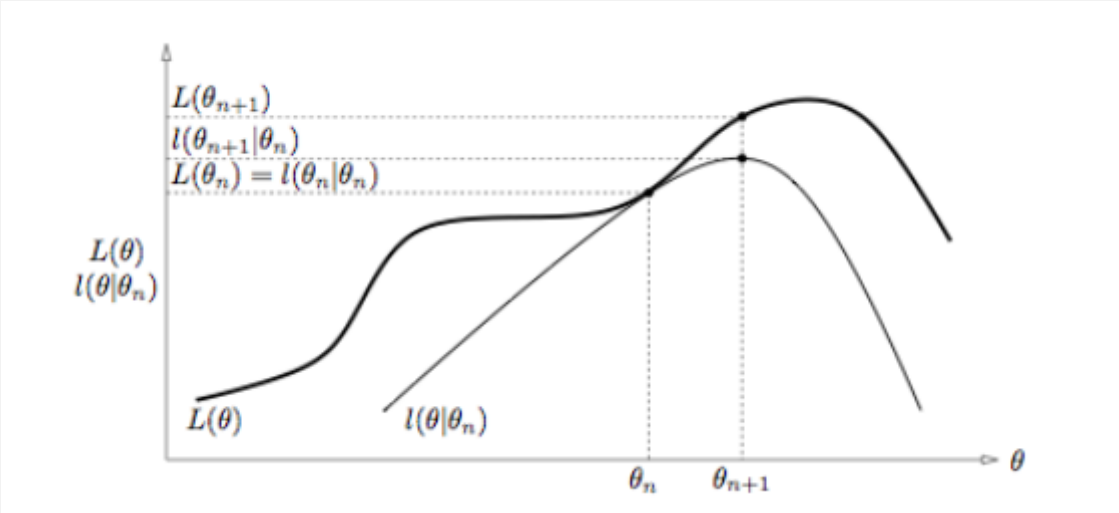
$$\begin{aligned} Q(\theta|\theta^{(t)}) &= \mathbb{E}(\ell(\theta|Y_{obs}, Z)|Y_{obs}, \theta^{(t)}) \\ &= \int_Z \ell(\theta|Y_{obs}, Z) \times f(z|Y_{obs}, \theta^{(t)}) \mathrm{d}z, \end{aligned}$$

and the M-step is to maximize **Q** with respect to θ to obtain

$$\theta^{(t+1)} = \arg\max_{\theta} Q(\theta|\theta^{(t)}).$$

- https://www.wikiwand.com/en/Expectation–maximization_algorithm
- http://cs229.stanford.edu/notes/cs229-notes8.pdf

Diagram of EM algorithm



Generalized EM Algorithm

Each iteration of the **generalized EM** algorithm consists of an expectation step (E-step) and a maximization step (M-step)
Specifically, let $\theta^{(t)}$ be the current best guess at the MLE $\hat{\theta}$. The E-step
is to compute the **Q** function defined by

$$\begin{aligned} Q(\theta|\theta^{(t)}) &= \mathbb{E}(\ell(\theta|Y_{obs}, Z)|Y_{obs}, \theta^{(t)}) \\ &= \int_Z \ell(\theta|Y_{obs}, Z) \times f(z|Y_{obs}, \theta^{(t)}) \mathrm{d}z, \end{aligned}$$

and the another step is to find θ that satisfies

$$\theta^{(t+1)} \in \{\theta|Q(\theta|\theta^{(t+1)} \geq Q(\theta|\theta^{(t)})\}.$$

It is not to maximize the conditional expectation.

See more on the book The EM Algorithm and Extensions, 2nd Edition by Geoffrey McLachlan , Thriyambakam Krishna.

Alternating Direction Method of Multipliers

Alternating direction method of multipliers is called **ADMM** shortly.
It is aimed to solve the following convex optimization problem:

$$\begin{aligned} \min F(x,y)\{ &= f(x)+g(y)\} && (\text{cost function}) \\ Ax+By &= b && (\text{constraint}) \end{aligned}$$

where $f(x)$ and $g(y)$ is convex; $A and B are matrices.

Define the augmented Lagrangian:

$$L_\mu(x,y)=f(x)+g(y)+\lambda^T(Ax+By-b)+\frac{\mu}{2}\|Ax+By-b\|_2^2.$$

It is iterative procedure:

$$\begin{aligned} &1.\ x^{k+1}=\arg\min_x L_\mu(x,y^k,\lambda^k); \\ &2.\ y^{k+1}=\arg\min_y L_\mu(x^{k+1},y,\lambda^k); \\ &3.\ \lambda^{k+1}=\lambda^k+\mu(Ax^{k+1}+By^{k+1}-b). \end{aligned}$$

Thanks to Professor He Bingsheng who taught me this.[10]

- https://www.ece.rice.edu/~tag7/Tom_Goldstein/Split_Bregman.html
- http://maths.nju.edu.cn/~hebma/
- http://stanford.edu/~boyd/admm.html
- http://shijun.wang/2016/01/19/admm-for-distributed-statistical-learning/
- https://www.wikiwand.com/en/Augmented_Lagrangian_method
- https://blog.csdn.net/shanglianlm/article/details/45919679

Stochastic Gradient Descent

Stochastic gradient descent takes advantages of stochastic or estimated gradient to replace the true gradient in gradient descent.
It is **stochastic gradient** but may not be **descent**.
The name **stochastic gradient methods** may be more appropriate to call the methods with stochastic gradient.
It can date back upto **stochastic approximation**.

It is aimed to solve the problem with finite sum optimization problem, i.e.

$$\arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} f(\theta|x_i)$$

where $n < \infty$ and $\{f(\theta|x_i)\}_{i=1}^{n}$ are in the same function family and $\{x_i\}_{i=1}^{n} \subset \mathbb{R}^d$ are constants while $\theta \in \mathbb{R}^p$ is the variable vector.

The difficulty is p, that the dimension of θ, is tremendous. In other words, the model is **overparameterized**. And the number n is far larger than p generally, i.e. $n \gg p \gg d$.
What is worse, the functions $\{f(\theta|x_i)\}_{i=1}^{n}$ are not convex in most case.

The stochastic gradient method is defined as

$$\theta^{k+1} = \theta^k - \alpha_k \frac{1}{m} \sum_{j=1}^{m} \nabla f(\theta^k|x'_j)$$

where x'_j is stochastically draw from $\{x_i\}_{i=1}^{n}$ and $m \ll n$.

It is the fact $m \ll n$ that makes it possible to compute the gradient of finite sum objective function and its side effect is that the objective function is not always descent.
There is fluctuations in the total objective function as gradient steps with respect to mini-batches are taken.

The fluctuations in the objective function as gradient steps with respect to mini-batches are taken

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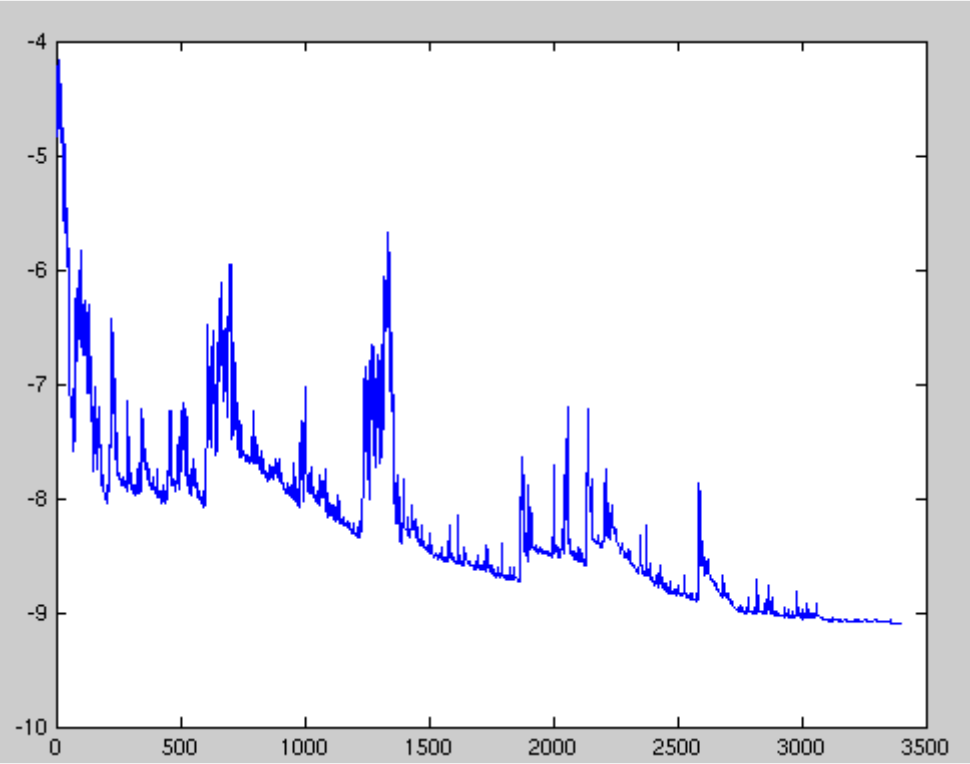
The fluctuations in the objective function as gradient steps with respect to mini-batches are taken



An heuristic proposal for avoiding the choice and for modifying the learning rate while the learning task runs is the **bold driver (BD) method**[11].
The learning rate increases *exponentially* if successive steps reduce the objective function f, and decreases rapidly if an "accident" is encountered (if objective function f increases), until a suitable value is found.
After starting with a small learning rate, its modifications are described by the following equation:

$$\alpha_{k+1} = \begin{cases} \rho\alpha_k, & f(\theta^{k+1}) < f(\theta^k); \\ \eta^n\alpha_k, & f(\theta^{k+1}) > f(\theta^k) \text{using } \alpha_k, \end{cases}$$

where ρ is close to 1 such as $\rho = 1.1$ in order to avoid frequent "accidents" because the objective function computation is wasted in these cases, η is chosen to provide a rapid reduction ($\eta = 0.5$), and n is the minimum integer such that the reduced rate η^n succeeds in diminishing the objective function.[12]

The fact that the sample size is far larger than the dimension of parameter, $n \gg p$, that makes it expensive to compute total objective function
$f(\theta) = \sum_{i=1}^{n} f(\theta|x_i)$.
Thus it is not clever to determine the learning rate α_k by line search. And most stochastic gradient methods are to find proper step length α_k to make it converge at least in convex optimization.
The variants of gradient descent such as momentum methods or mirror gradient methods have their stochastic counterparts.

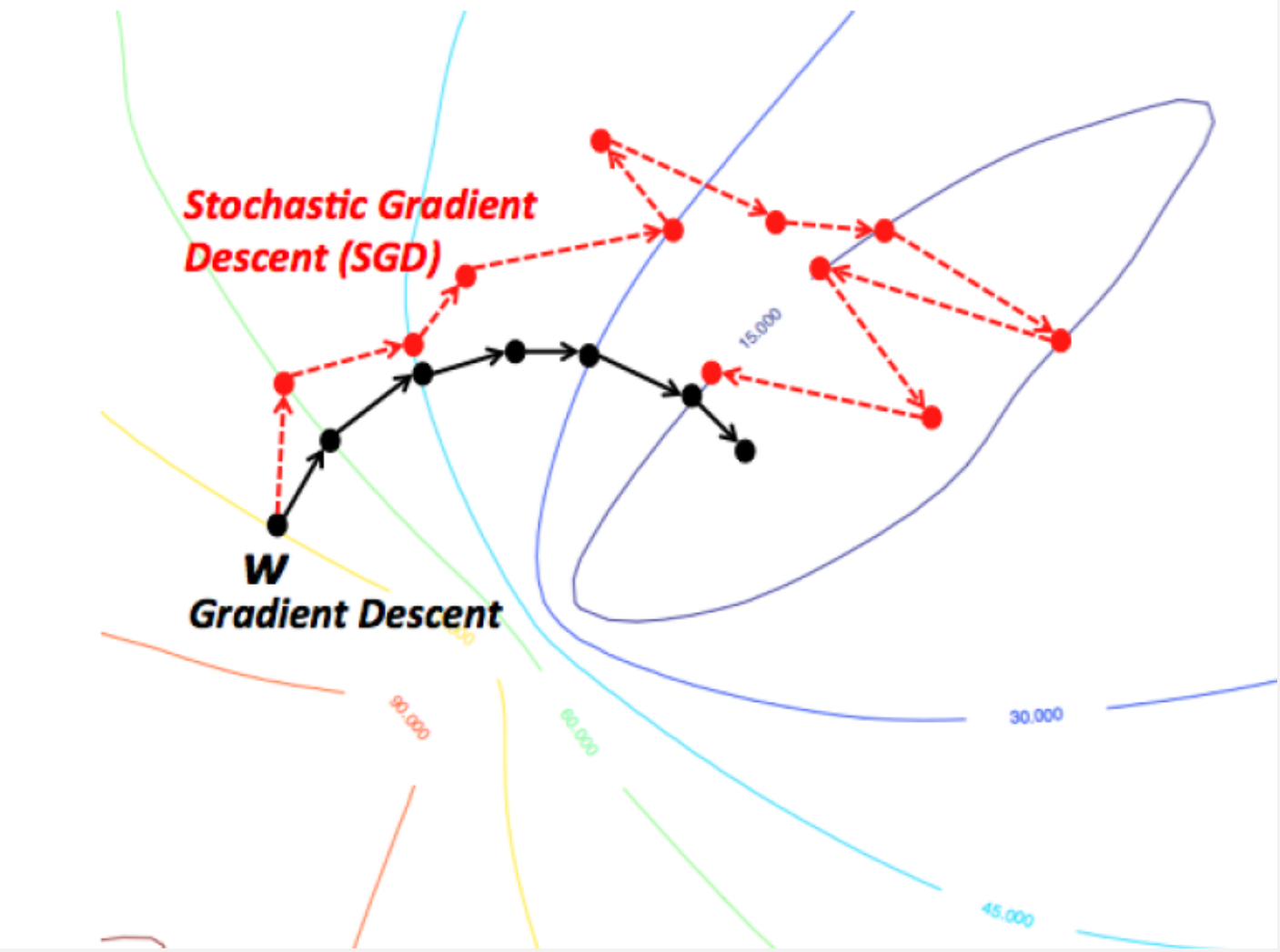
- It is simplest to set the step length a constant, such as $\alpha_k = 3 \times 10^{-3} \, \forall k$.
- There are decay schemes, i.e. the step length α_k diminishes such as $\alpha_k = \frac{\alpha}{k}$, where α is constant.
- And another strategy is to tune the step length adaptively such as *AdaGrad, ADAM*.

PS: the step length α_k is called **learning rate** in machine learning and stochastic gradient descent is also named as increment gradient methods in some case.

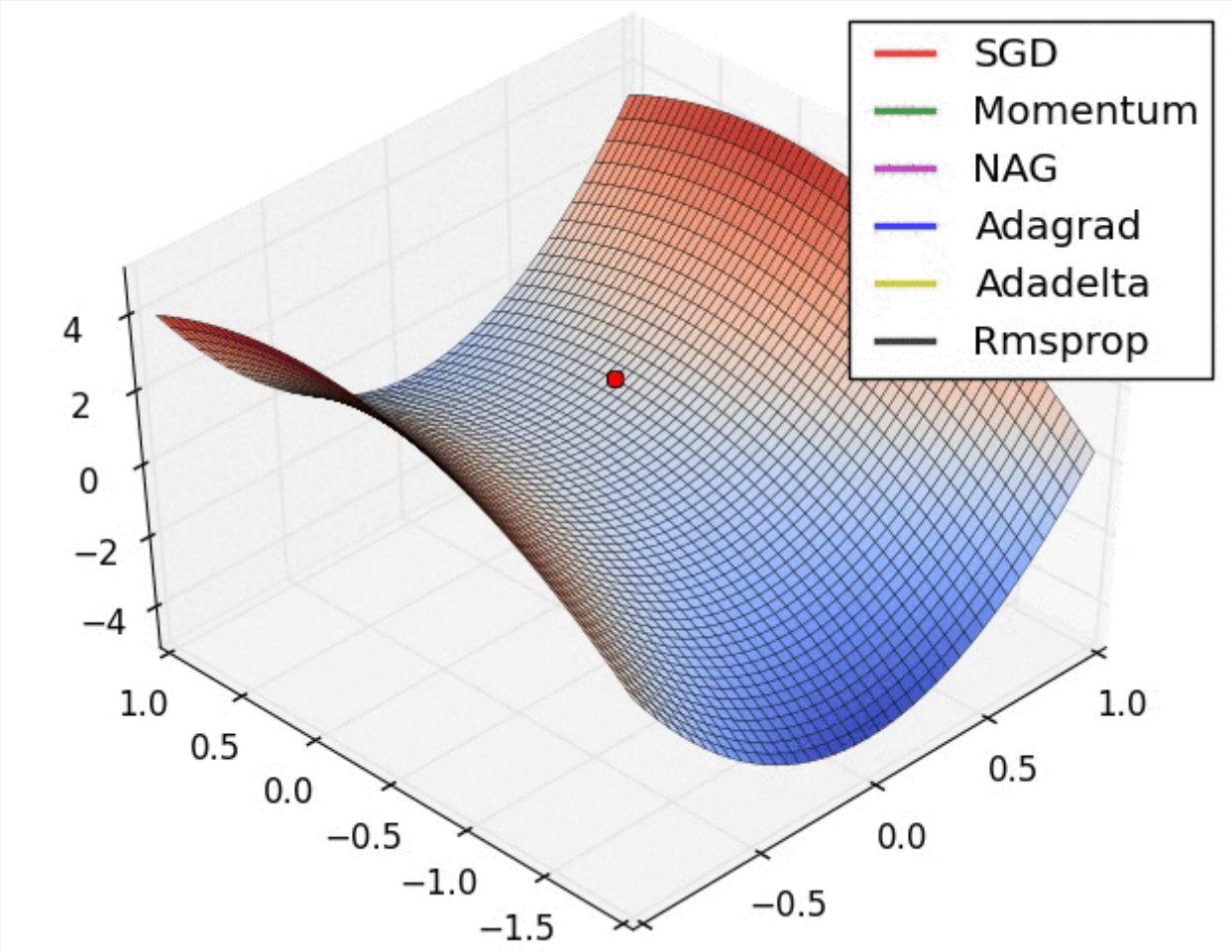
See the following links for more information on *stochastic gradient descent*.

- https://www.wikiwand.com/en/Stochastic_gradient_descent
- https://www.bonaccorso.eu/2017/10/03/a-brief-and-comprehensive-guide-to-stochastic-gradient-descent-algorithms/
- https://leon.bottou.org/projects/sgd
- https://leon.bottou.org/research/stochastic
- http://ruder.io/optimizing-gradient-descent/
- http://ruder.io/deep-learning-optimization-2017/
- https://zhuanlan.zhihu.com/p/22252270
- https://henripal.github.io/blog/stochasticdynamics
- https://henripal.github.io/blog/langevin

The Differences of Gradient Descent and Stochastic Gradient Descent



The Differences of Stochastic Gradient Descent and its Variants



Regression Analysis and Machine Learning

- http://shoefer.github.io/intuitivemi/
- http://karpathy.github.io/
- https://github.com/Hulalazz/100-Days-Of-ML-Code-1
- Machine Learning & Deep Learning Roadmap
- Regression in Wikipedia
- Machine Learning in Wikipedia
- Portal: Machine Learning

Regression Analysis

Regression is a method for studying the relationship between a response variable Y and a covariates X. The covariate is also called a **predictor** variable or a **feature**.

Regression is not function fitting. In function fitting, it is well-defined - $f(x_i)$ is fixed when x_i is fixed; in regression, it is not always so.

Linear regression is the "hello world" in statistical learning. It is the simplest model to fit the datum. We will induce it in the maximum likelihood estimation perspective.
See this link for more information https://www.wikiwand.com/en/Regression_analysis.

Ordinary Least Squares

Representation of Ordinary Least Squares

A linear regression model assumes that the regression function $E(Y|X)$ is
linear in the inputs $X_1, \cdots, X_p$. They are simple and often
provide an adequate and interpretable description of how the inputs affect the output.
Suppose that the datum $\{(x_i, y_i)\}_{i=1}^n$,

$$y_i = f(x_i) + \epsilon_i,$$

where the function f is linear, i.e. $f(x) = w^T x + b$.
Let $\epsilon = y - f(x)$.Then $\mathbb{E}(\epsilon|X) = \mathbb{E}(y - f(x)|x) = 0$
and the residual errors $\{\epsilon_i|\epsilon_i = y_i - f(x_i)\}_{i=1}^n$ are **i.i.d. in standard Gaussian distribution**.

By convention (**very important**!):

- x is assumed to be standardized (mean 0, unit variance);
- y is assumed to be centered.

For the linear regression, we could assume x is in Gaussian distribution.

Evaluation of Ordinary Least Squares

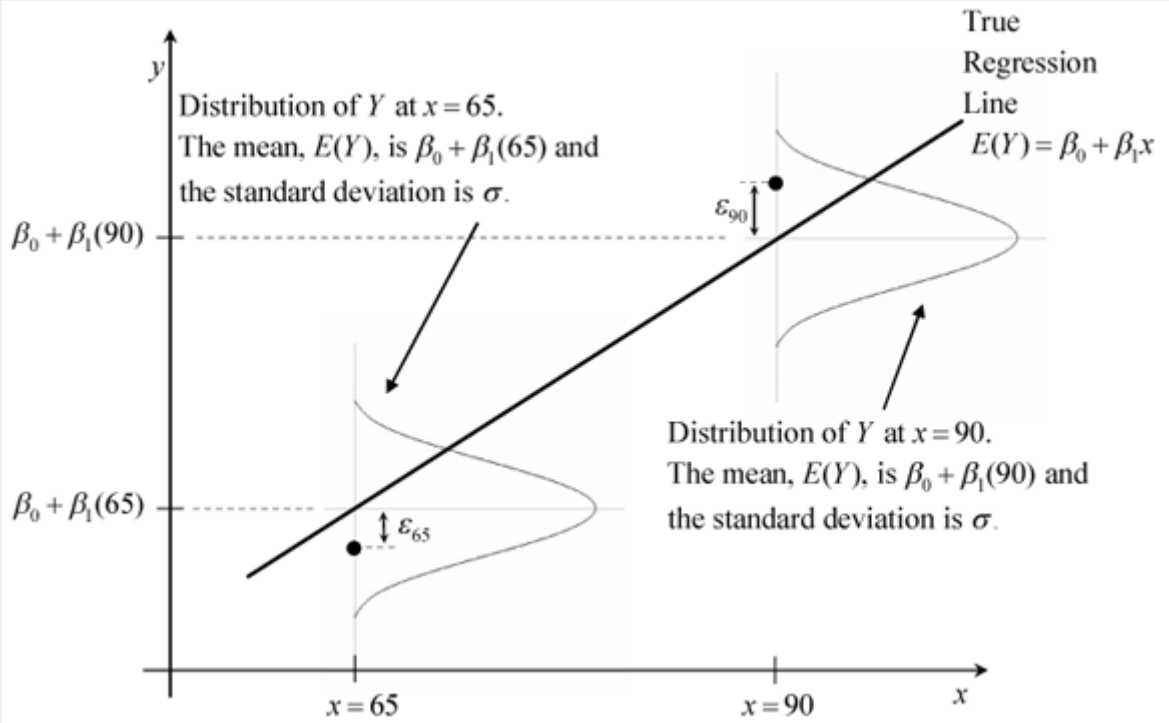
The likelihood of the errors are

$$L(\epsilon_1, \epsilon_2, \cdots, \epsilon_n) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-\epsilon_i^2}.$$

In MLE, we have shown that it is equivalent to

$$\arg\max \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-\epsilon_i^2} = \arg\min \sum_{i=1}^n \epsilon_i^2 = \arg\min \sum_{i=1}^n (y_i - f(x_i))^2.$$

Linear Regression and Likelihood Maximum Estimation



Optimization of Ordinary Least Squares

For linear regression, the function f is linear, i.e. $f(x) = w^T x$ where w is the parameters to tune. Thus $\epsilon_i = y_i - w^T x_i$ and $\sum_{i=1}^n (y_i - f(x_i))^2 = \sum_{i=1}^n (y_i - w^T x_i)^2$. It is also called *residual sum of squares* in statistics or *objective function* in optimization theory.
In a compact form,

$$\sum_{i=1}^{n} (y_i - w^T x_i)^2 = \|Y - Xw\|^2 , \tag{0}$$

where $Y = (y_1, y_2, \cdots, y_n)^T, X = (x_1, x_2, \cdots, x_n)$.
Let the gradient of objective function $\|Y - Xw\|^2$ be 0, i.e.

$$\nabla_w \|Y - Xw\|^2 = 2X^T(Y - Xw) = 0 , \tag{1}$$

then we gain that $w = (X^T X)^{-1} X^T Y$ if possible.

Note:

1. the residual error $\{\epsilon_i\}_{i=1}^n$ are i.i.d. in Gaussian distribution;
2. the inverse matrix $(X^T X)^{-1}$ may not exist in some extreme case.

See more on Wikipedia page.

Ridge Regression and LASSO

When the matrix X^TX is not inverse, ordinary least squares does not work.
And in ordinary least squares, the parameters w is estimated by MLE rather more general Bayesian estimator.

In the perspective of computation, we would like to consider the *regularization* technique;
In the perspective of Bayesian statistics, we would like to consider more proper *prior* distribution of the parameters.

Ridge Regression As Regularization

It is to optimize the following objective function with parameter norm penalty

$$PRSS_{\ell_2} = \sum_{i=1}^{n}(y_i - w^Tx_i)^2 + \lambda w^Tw = \|Y - Xw\|^2 + \lambda\|w\|^2 . \qquad \text{(Ridge)}$$

It is called penalized residual sum of squares.
Taking derivatives, we solve

$$\frac{\partial PRSS_{\ell_2}}{\partial w} = 2X^T(Y - Xw) + 2\lambda w = 0$$

and we gain that

$$w = (X^TX + \lambda I)^{-1}X^TY$$

where it is trackable if λ is large enough.

LASSO as Regularization

LASSO is the abbreviation of **Least Absolute Shrinkage and Selection Operator**.

1. It is to minimize the following objective function：

$$PRSS_{\ell_1} = \sum_{i=1}^{n}(y_i - w^Tx_i)^2 + \lambda\|w\|_1 = \|Y - Xw\|^2 + \lambda\|w\|_1 . \qquad \text{(LASSO)}$$

2. the optimization form:

$$\begin{aligned} &\arg\min_w \sum_{i=1}^{n}(y_i - w^Tx_i)^2 && \text{Objective function} \\ &\text{subject to } \|w\|_1 \le t && \text{constraint.} \end{aligned}$$

3. the selection form:

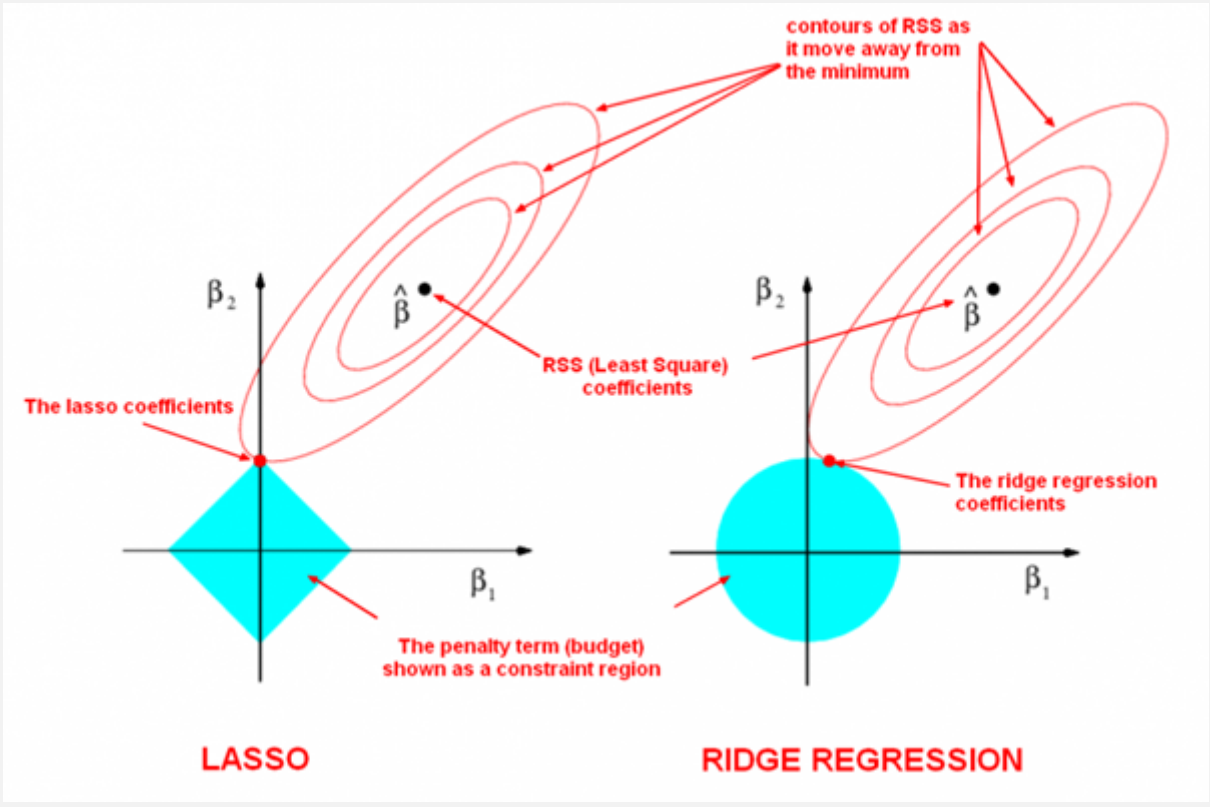
$$\begin{aligned} & \arg\min_{w} \|w\|_1 && \text{Objective function} \\ \text{subject to } & \sum_{i=1}^{n}(y_i - w^T x_i)^2 \le t && \text{constraint.} \end{aligned}$$

where $\|w\|_1 = \sum_{i=1}^{n} |w_i|$ if $w = (w_1, w_2, \cdots, w_n)^T$.

More solutions to this optimization problem:

- Q&A in zhihu.com;
- ADMM to LASSO;
- Regularization: Ridge Regression and the LASSO;
- Least angle regression;
- http://web.stanford.edu/~hastie/StatLearnSparsity/
- 历史的角度来看，Robert Tibshirani 的 Lasso 到底是不是革命性的创新？- 若羽的回答 - 知乎
- http://www.cnblogs.com/xingshansi/p/6890048.html

LASSO and Ridge Regression



The LASSO Page ,Wikipedia page and Q&A in zhihu.com

More References in Chinese blog

Bayesian Perspective

If we suppose the prior distribution of the parameters w is in Gaussian distribution, i.e. $f_W(w) \propto e^{-\lambda\|w\|^2}$, we will deduce the ridge regression.

If we suppose the prior distribution of the parameters w is in Laplacian distribution, i.e. $f_W(w) \propto e^{-\lambda \|w\|_1}$, we will deduce LASSO.

- Stat 305: Linear Models (and more)
- 机器学习算法实践-岭回归和LASSO - PytLab酱的文章 - 知乎

Elastic Net

When the sample size of training data n is far less than the number of features p, the objective function is:

$$PRSS_\alpha = \frac{1}{2n}\sum_{i=1}^{n}(y_i - w^T x_i)^2 + \lambda \sum_{j=1}^{p} P_\alpha(w_j), \qquad \text{(Elastic net)}$$

where $P_\alpha(w_j) = \alpha|w_j|_1 + \frac{1}{2}(1-\alpha)(w_j)^2$.

See more on http://web.stanford.edu/~hastie/TALKS/glmnet_webinar.pdf or http://www.princeton.edu/~yc5/ele538_math_data/lectures/model_selection.pdf.

We can deduce it by Bayesian estimation if we suppose the prior distribution of the parameters w is in mixture of Gaussian distribution and Laplacian distribution, i.e.

$$f_W(w) \propto e^{-\alpha\|w\|_1 - \frac{1}{2}(1-\alpha)\|w\|^2}.$$

See **Bayesian lasso regression** at http://faculty.chicagobooth.edu/workshops/econometrics/past/pdf/asp047v1.pdf.

Generalized Linear Model

In **ordinary least squares**, we assume that the errors $\{\epsilon_i\}_{i=1}^n$ are i.i.d. Gaussian, i.e. $\{\epsilon_i\} \overset{i.i.d}{\sim} N(0,1)$ for $i \in \{1, 2, \cdots, n\}$. It is not necessary to assume that they are in Gaussian distribution.
In statistics, the generalized linear model (GLM) is a flexible generalization of ordinary linear regression that allows for response variables that have error distribution models other than a normal distribution. The GLM generalizes linear regression by allowing the linear model to be related to the response variable via a link function and by allowing the magnitude of the variance of each measurement to be a function of its predicted value.

Intuition

Ordinary linear regression predicts the expected value of a given unknown quantity (the response variable, a random variable) as a linear combination of a set of observed values (predictors). This implies that a constant change in a predictor leads to a constant change in the response variable (i.e. a linear-response model).
This is appropriate when the response variable has a normal distribution (intuitively, when a response variable can vary essentially indefinitely in either direction with no fixed "zero value", or more generally for any quantity that only varies by a relatively small amount, e.g. human heights).

However, these assumptions are inappropriate for some types of response variables. For example, in cases where the response variable is expected to be always positive and varying over a wide range,
constant input changes lead to geometrically varying, rather than constantly varying, output changes. As an example, a prediction model might predict that 10 degree temperature decrease would lead to 1,000 fewer people visiting the beach is unlikely to generalize well over both small beaches
(e.g. those where the expected attendance was 50 at a particular temperature) and large beaches (e.g. those where the

expected attendance was 10,000 at a low temperature).
The problem with this kind of prediction model would imply a temperature drop of 10 degrees would lead to 1,000 fewer people visiting the beach, a beach whose expected attendance was 50 at a higher temperature would now be predicted to have the impossible attendance value of −950. Logically, a more realistic model would instead predict a constant rate of increased beach attendance (e.g. an increase in 10 degrees leads to a doubling in beach attendance, and a drop in 10 degrees leads to a halving in attendance).
Such a model is termed an exponential-response model (or log-linear model, since the logarithm of the response is predicted to vary linearly).

Model components

In a generalized linear model (GLM), each outcome Y of the dependent variables is assumed to be generated from a particular distribution in the **exponential family**, a large range of probability distributions that includes the normal, binomial, Poisson and gamma distributions, among others. The mean, μ, of the distribution depends on the independent variables, X, through:

$$\mathbb{E}(Y) = \mu = g^{-1}(X\beta)$$

where $\mathbb{E}(Y)$ is the expected value of Y; $X\beta$ is the linear predictor, a linear combination of unknown parameters β; g is the link function and g^{-1} is the inverse function of g.

The GLM consists of three elements:

Model components
1. A probability distribution from the exponential family.
2. A linear predictor $\eta = X\beta$.
3. A link function g such that $\mathbb{E}(Y) = \mu = g^{-1}(\eta)$.

- https://xg1990.com/blog/archives/304
- https://zhuanlan.zhihu.com/p/22876460
- https://www.wikiwand.com/en/Generalized_linear_model
- **Roadmap to generalized linear models in metacademy** at (https://metacademy.org/graphs/concepts/generalized_linear_models#lfocus=generalized_linear_models)
- Course in Princeton
- Exponential distribution familiy
- 14.1 - The General Linear Mixed Model

Logistic Regression

The logistic distribution:

$$y \triangleq P(Y = 1|X = x) = \frac{1}{1 + e^{-w^T x}} = \frac{e^{w^T x}}{1 + e^{w^T x}}$$

where w is the parameter vector. Thus, we can obtain:

$$\log \frac{P(Y=1|X=x)}{P(Y \neq 1|X=x)} = w^T x,$$

i.e.

$$\log \frac{y}{1-y} = w^T x$$

in theory.

- https://www.wikiwand.com/en/Logistic_regression
- http://www.omidrouhani.com/research/logisticregression/html/logisticregression.htm

Poisson Regression

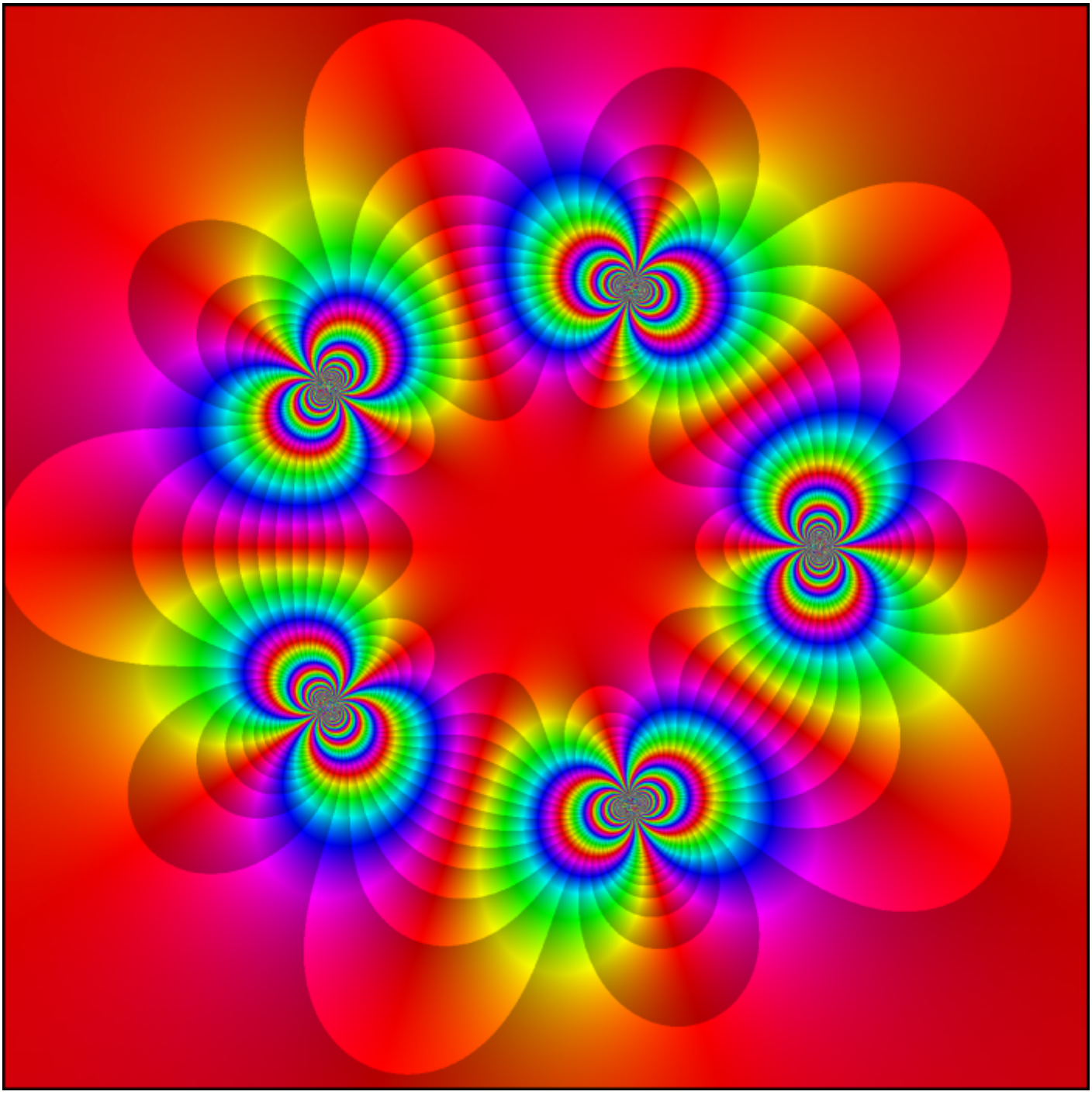
- http://www.cnblogs.com/kemaswill/p/3440780.html
- https://www.wikiwand.com/en/Poisson_regression

Projection pursuit regression

https://www.wikiwand.com/en/Projection_pursuit_regression

Nonparametric Regression

- https://www.wikiwand.com/en/Additive_model
- https://www.wikiwand.com/en/Generalized_additive_model
- http://iacs-courses.seas.harvard.edu/courses/am207/blog/lecture-20.html
- Nonparametric regression https://www.wikiwand.com/en/Nonparametric_regression
- Multilevel model https://www.wikiwand.com/en/Multilevel_model
- A Tutorial on Bayesian Nonparametric Models
- Hierarchical generalized linear model https://www.wikiwand.com/en/Hierarchical_generalized_linear_model
- http://doingbayesiandataanalysis.blogspot.com/2012/11/shrinkage-in-multi-level-hierarchical.html
- https://twiecki.github.io/blog/2014/03/17/bayesian-glms-3/
- http://www.stat.cmu.edu/~larry/=sml
- http://www.stat.cmu.edu/~larry/
- https://zhuanlan.zhihu.com/p/26830453



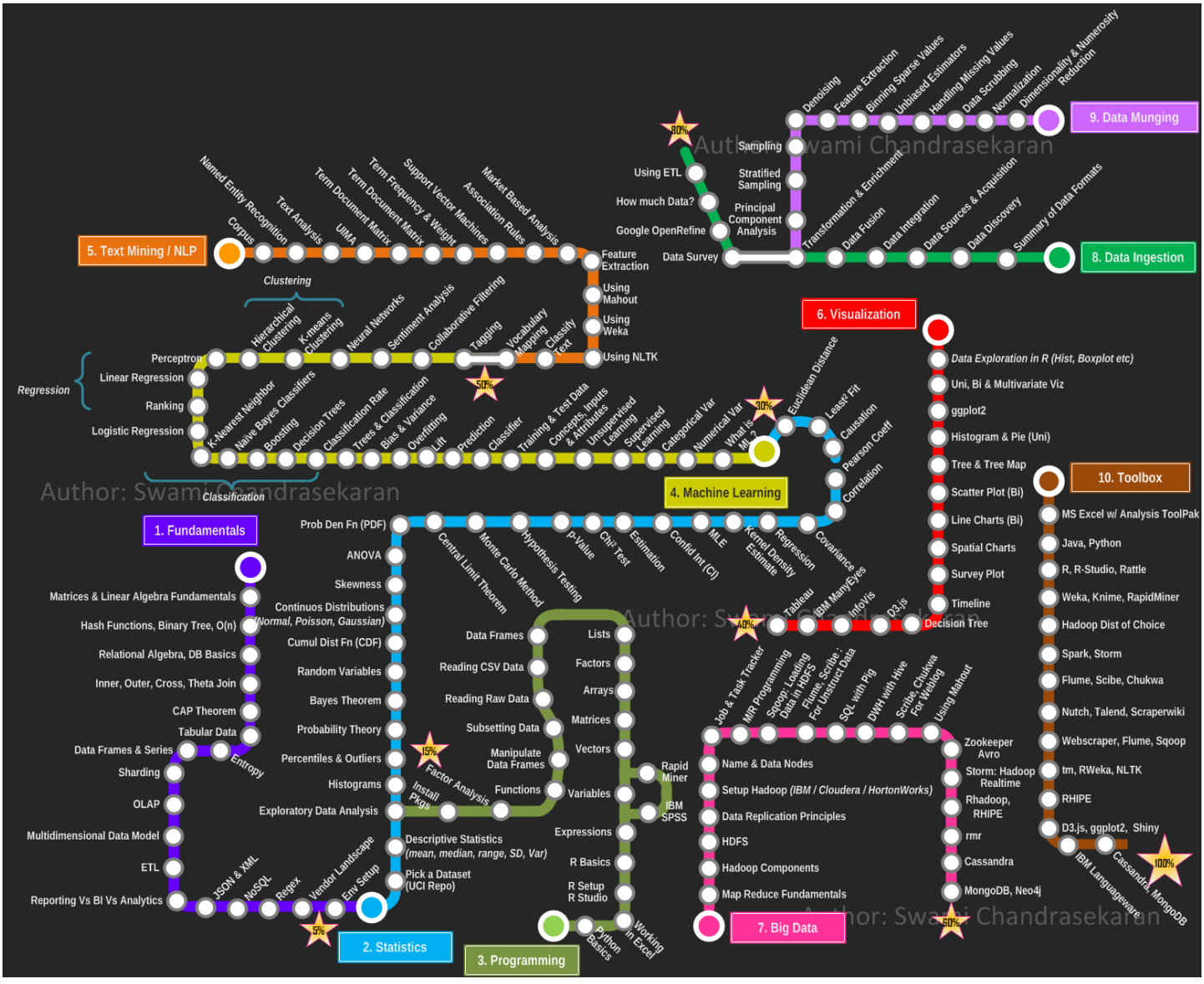
https://blogs.ams.org/visualinsight

Machine Learning

The goal of machine learning is to program computers to use example data or past experience to solve a given problem. Many successful applications of machine learning exist already, including systems that analyze past sales data to predict customer behavior, recognize faces or spoken speech, optimize robot behavior so that a task can be completed using minimum resources, and extract knowledge from bioinformatics data.
From ALPAYDIN, Ethem, 2004. Introduction to Machine Learning. Cambridge, MA: The MIT Press..

- http://www.machine-learning.martinsewell.com/
- https://arogozhnikov.github.io/2016/04/28/demonstrations-for-ml-courses.html

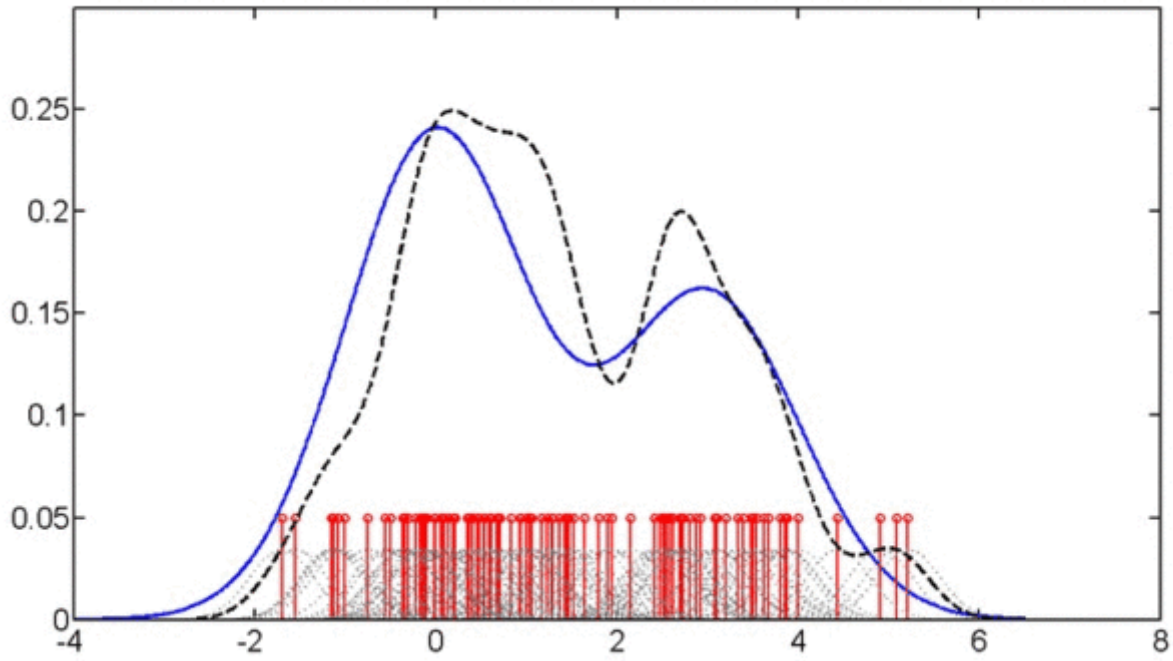
- https://www.analyticsvidhya.com/blog/2016/09/most-active-data-scientists-free-books-notebooks-tutorials-on-github/
- https://data-flair.training/blogs/machine-learning-tutorials-home/
- https://github.com/ty4z2008/Qix/blob/master/dl.md
- https://machinelearningmastery.com/category/machine-learning-resources/
- https://machinelearningmastery.com/machine-learning-checklist/
- https://ml-cheatsheet.readthedocs.io/en/latest/index.html
- https://sgfin.github.io/learning-resources/
- https://cedar.buffalo.edu/~srihari/CSE574/index.html
- http://interpretable.ml/
- https://christophm.github.io/interpretable-ml-book/
- https://csml.princeton.edu/readinggroup
- https://www.seas.harvard.edu/courses/cs281/
- https://developers.google.com/machine-learning/guides/rules-of-ml/



Road To Data Scientist

Density Estimation

Density estimation
https://www.cs.toronto.edu/~hinton/science.pdf



Classification

- https://en.wikipedia.org/wiki/Category:Classification_algorithms

Clustering

There are two different contexts in clustering, depending on how the entities to be clustered are organized.
In some cases one starts from an **internal representation** of each entity (typically an M-dimensional vector x_i assigned to entity i) and
derives mutual dissimilarities or mutual similarities from the internal representation.In
this case one can derive prototypes (or centroids) for each cluster, for example by averaging the characteristics of the contained entities (the vectors).
In other cases only an **external representation** of dissimilarities is available and the resulting model is an **undirected and weighted graph** of entities connected by edges. From https://www.intelligent-optimization.org/LIONbook/. [12:1]

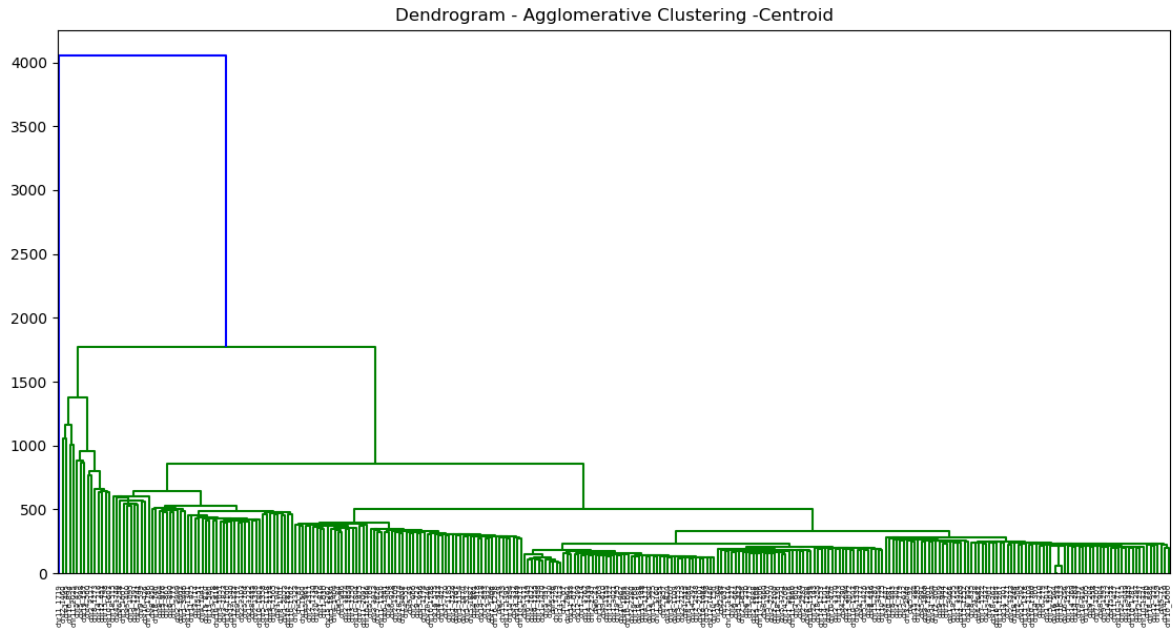
The external representation of dissimilarity will be discussed in **Graph Algorithm**.

K-means

K-means is also called **Lloyd's algorithm**.

Hierarchical clustering

- https://blog.csdn.net/qq_39388410/article/details/78240037
- http://iss.ices.utexas.edu/?p=projects/galois/benchmarks/agglomerative_clustering
- https://nlp.stanford.edu/IR-book/html/htmledition/hierarchical-agglomerative-clustering-1.html
- https://www.wikiwand.com/en/Hierarchical_clustering



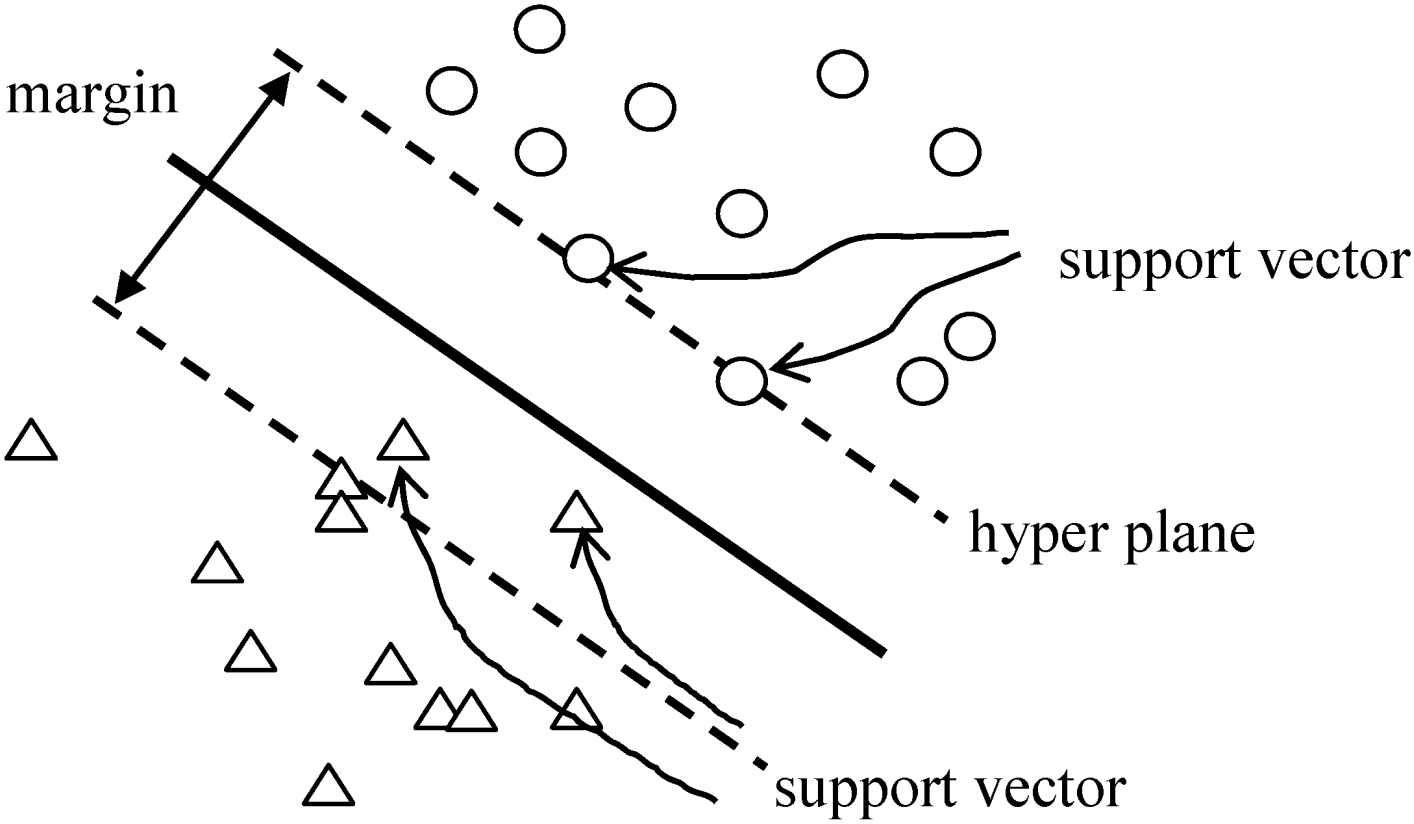
DBSCAN

- http://sklearn.apachecn.org/cn/0.19.0/modules/clustering.html
- https://www.wikiwand.com/en/Cluster_analysis
- https://www.toptal.com/machine-learning/clustering-algorithms

Support Vector Machine

http://www.svms.org/history.html
http://www.svms.org/
http://web.stanford.edu/~hastie/TALKS/svm.pdf

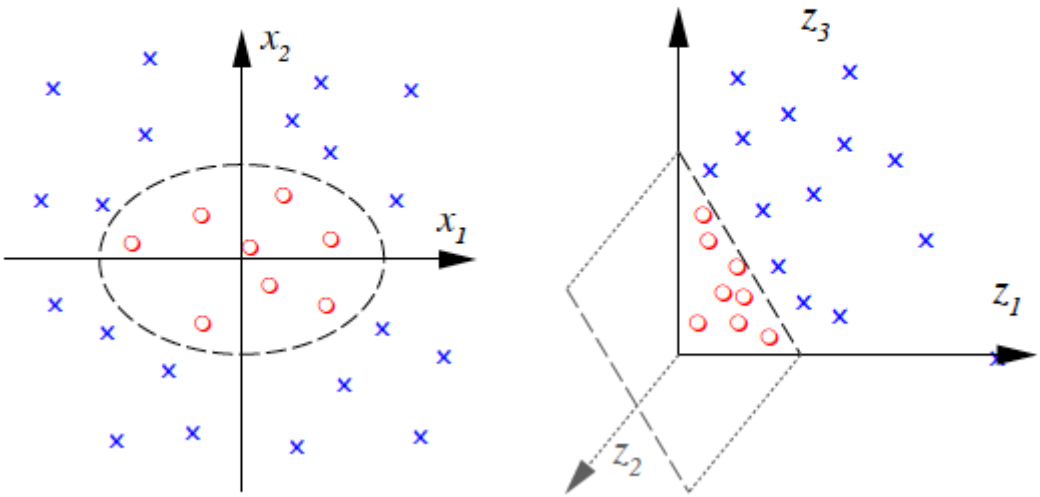
http://bytesizebio.net/2014/02/05/support-vector-machines-explained-well/



Kernel Methods

- Kernel method at Wikipedia;
- http://www.kernel-machines.org/
- http://onlineprediction.net/?n=Main.KernelMethods
- https://arxiv.org/pdf/math/0701907.pdf

$$\Phi : R^2 \to R^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{(2)}x_1x_2, x_2^2)$$



Principal Component Analysis and Singular Value Decomposition

Singular Value Decomposition

Singular value decomposition is an extension of eigenvector decomposition of a matrix.

For the square matrix $M_{n\times n}$, we can compute the eigenvalues and eigenvectors:

$$M_{n\times n}v = \lambda v$$

where the eigenvector $v \in \mathbb{R}^n$, the eigenvalue $\lambda \in \mathbb{R}$.
It is equivalent to solve the linear equation system $(M_{n\times n} - \lambda I_{n\times n})v = 0$ where $I_{n\times n}$ is the nth order identity matrix.
Especially, when $M_{n\times n}$ is symmetrical i.e. $M^T = M$, what are the properties of eigenvalue and eigenvector?

> ***Theorem***: *All eigenvalues of a symmetrical matrix are real.*
>
> ***Proof***: *Let A be a real symmetrical matrix and $Av = \lambda v$. We want to show the eigenvalue λ is real.*
> *Let $v^\star$ be conjugate transpose of v. $v^\star Av = \lambda v^\star v\,(1)$. If $Av = \lambda v$, thus $(Av)^\star = (\lambda v)^\star$, i.e. $v^\star A = \bar{\lambda} v^\star$.*
> *We can infer that $v^\star Av = \bar{\lambda} v^\star v\,(2)$.By comparing the equation (1) and (2), we can obtain that $\lambda = \bar{\lambda}$ where $\bar{\lambda}$ is the conjugate of λ.*

> ***Theorem***: *Every symmetrical matrix can be diagonalized.*

See more at http://mathworld.wolfram.com/MatrixDiagonalization.html.

When the matrix is rectangle i.e. the number of columns and the number of rows are not equal, what is the counterpart of eigenvalues and eigenvectors?
Another question is if every matrix $M_{m\times n} \in \mathbb{R}^{m\times n}$ can be written as the sum of rank-1 matrix and how?

$$M_{m\times n} = \sum_{i}^{r} p_i q_i = P_{m\times r} Q_{r\times n}$$

where $p_i \in \mathbb{R}^m$,$q_i \in \mathbb{R}^n$ and r is integer.
They are from the square matrices $M_{m\times n}^T M_{m\times n} = A_{n\times n}$ and $M_{m\times n} M_{m\times n}^T = B_{m\times m}$. It is obvious that the matrix A and B are symmetrical.

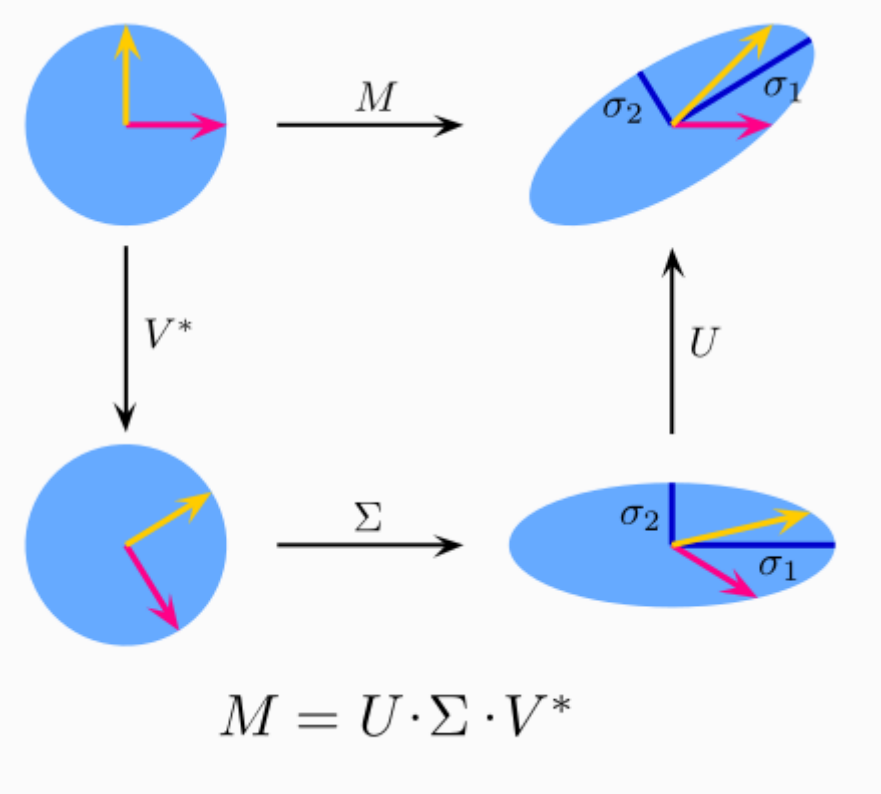
> ***Theorem***: *The matrix A and B has the same eigenvalues except zero.*
>
> ***Proof***: *We know that $A = M_{m\times n}^T M_{m\times n}$ and $B = M_{m\times n} M_{m\times n}^T$.*
> *Let $Av = \lambda v$ i.e. $M_{m\times n}^T M_{m\times n} v = \lambda v$, which can be rewritten as*
> *$M_{m\times n}^T (M_{m\times n} v) = \lambda v\ (1)$, where $v \in \mathbb{R}^n$.*
> *We multiply the matrix $M_{m\times n}$ in the left of both sides of equation (1), then we obtain*
> *$M_{m\times n} M_{m\times n}^T (M_{m\times n} v) = M_{m\times n}(\lambda v) = \lambda (M_{m\times n} v)$.*

> ***Theorem***: *The matrix A and B are non-negative definite, i.e. $\langle v, Av\rangle \geq 0, \forall v \in \mathbb{R}^n$ and $\langle u, Bu\rangle \geq 0, \forall u \in \mathbb{R}^m$.*
>
> ***Proof***: *It is $\langle v, Av\rangle = \left\langle v, M_{m\times n}^T M_{m\times n} v\right\rangle = (Mv)^T (Mv) = \|Mv\|_2^2 \geq 0$ as well as B.*

> ***Theorem***: *$M_{m\times n} = U_{m\times m} \Sigma_{m\times n} V_{n\times n}^T$, where*
>
> - *$U_{m\times m}$ is an $m \times m$ orthogonal matrix;*
> - *$\Sigma_{m\times n}$ is a diagonal $m \times n$ matrix with non-negative real numbers on the diagonal,*
> - *$V_{n\times n}^T$ is the transpose of an $n \times n$ orthogonal matrix.*

SVD

SVD

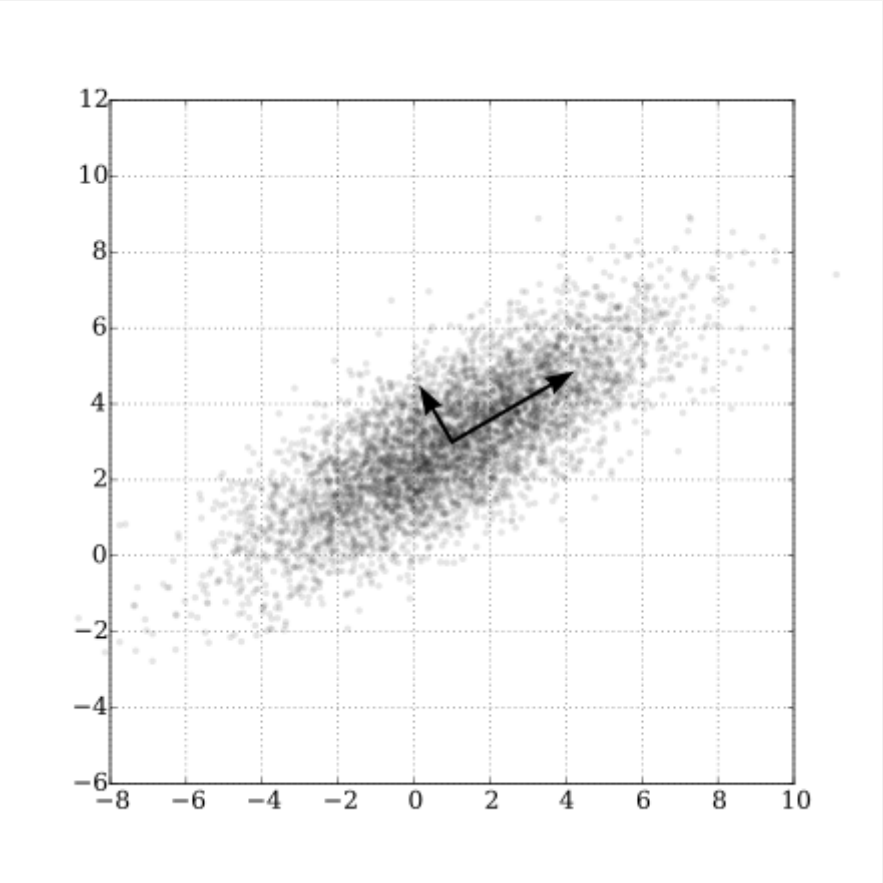


See more at http://mathworld.wolfram.com/SingularValueDecomposition.html.

- http://www-users.math.umn.edu/~lerman/math5467/svd.pdf
- http://www.nytimes.com/2008/11/23/magazine/23Netflix-t.html
- https://zhuanlan.zhihu.com/p/36546367
- http://www.cnblogs.com/LeftNotEasy/archive/2011/01/19/svd-and-applications.html
- Singular value decomposition
- http://www.cnblogs.com/endlesscoding/p/10033527.html
- http://www.flickering.cn/数学之美/2015/01/奇异值分解（we-recommend-a-singular-value-decomposition）/

Principal Component Analysis

Gaussian Scatter PCA



- Principal Component Analysis Explained Visually.
- https://www.zhihu.com/question/38319536
- Principal component analysis
- https://www.wikiwand.com/en/Principal_component_analysis
- https://onlinecourses.science.psu.edu/stat505/node/49/

Principal Component Regression

https://www.jianshu.com/p/d090721cf501

Graph Algorithms

Graph as Data Structure

Graph is mathematical abstract or generalization of the connection between entries.
A graph G consists of a finite set of vertices $V(G)$ and a set of edges $E(G)$ consisting of distinct, unordered pairs of vertices, where nodes stand for entities and edges stand for their connections.
It is the foundation of **network science**.
It is different from the common data where the feature is nothing except the connection.

> *Graphs provide a powerful way to represent and exploit these connections.*
> *Graphs can be used to model such diverse areas as computer vision, natural language*

processing, and recommender systems. [13]

The connections can be directed, weighted even probabilistic.

Definition: *Let G be a graph with $V(G) = 1, \ldots, n$ and $E(G) = e_1, \ldots, e_m$. Suppose each*
edge of G is assigned an orientation, which is arbitrary but fixed. The (vertex-edge) `incidence` *matrix of G, denoted by $Q(G)$, is the $n \times m$ matrix defined as follows. The rows and the columns of $Q(G)$ are indexed by $V(G)$ and $E(G)$, respectively. The (i, j)-entry of $Q(G)$ is 0 if vertex i and edge e_j are not incident, and otherwise it is 1 or -1 according as e_j originates or terminates at i, respectively. We often denote $Q(G)$ simply by Q. Whenever we mention $Q(G)$ it is assumed that the edges of G are oriented*

Definition: *Let G be a graph with $V(G) = 1, \ldots, n$ and $E(G) = e_1, \ldots, e_m$.The* `adjacency` *matrix of G, denoted by $A(G)$, is the $n \times n$ matrix defined as follows. The rows and*
the columns of $A(G)$ are indexed by $V(G)$. If $i \neq j$ then the (i, j)-entry of $A(G)$ is 0 for vertices i and j nonadjacent, and the (i, j)-entry is 1 for i and j adjacent. The (i, i)-entry of $A(G)$ is 0 for $i = 1, \ldots, n$. We often denote $A(G)$ simply by A. `Adjacency Matrix` *is also used to represent* `weighted graphs`*. If the (i, i)-entry of $A(G)$ is $w_{i,j}$, i.e. $A[i][j] = w_{i,j}$, then there is an edge from vertex i to vertex j with weight w.*
The `Adjacency Matrix` *of* `weighted graphs` *G is also called* `weight` *matrix of G, denoted by $W(G)$ or simply by W.*

See *Graph representations using set and hash* at https://www.geeksforgeeks.org/graph-representations-using-set-hash/.

Definition: *In graph theory, the degree (or valency) of a vertex of a graph is the number of edges incident to the vertex, with loops counted twice. From the Wikipedia page at https://www.wikiwand.com/en/Degree_(graph_theory).*
The degree of a vertex v is denoted $\deg(v)$ or $\deg v$. `Degree matrix` *D is a diagonal matrix such that $D_{i,i} = \sum_j w_{i,j}$ for the* `weighted graph` *with $W = (w_{i,j})$*
.

Definition: *Let G be a graph with $V(G) = 1, \ldots, n$ and $E(G) = e_1, \ldots, e_m$.The* `Laplacian` *matrix of G, denoted by $L(G)$, is the $n \times n$ matrix defined as follows.*

The rows and
the columns of $L(G)$ are indexed by $V(G)$. If $i \neq j$ then the (i,j)-entry of $L(G)$ is 0 for vertices i and j nonadjacent, and the (i,j)-entry is -1 for i and j adjacent. The (i,i)-entry of $L(G)$ is d_i, the degree of the vertex i, for $i = 1, \ldots, n$.
In other words, the (i,i)-entry of $L(G)$, $L(G)_{i,j}$, is defined by

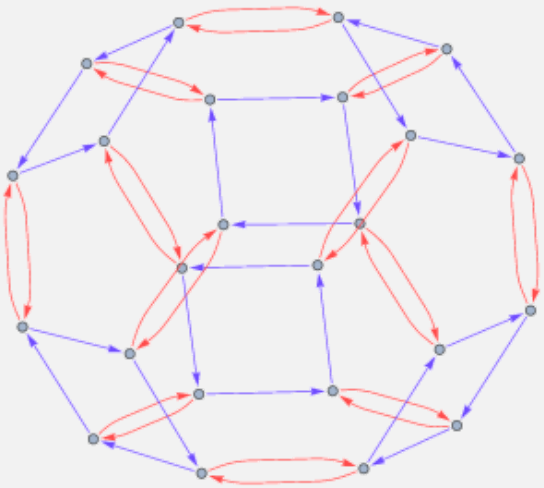
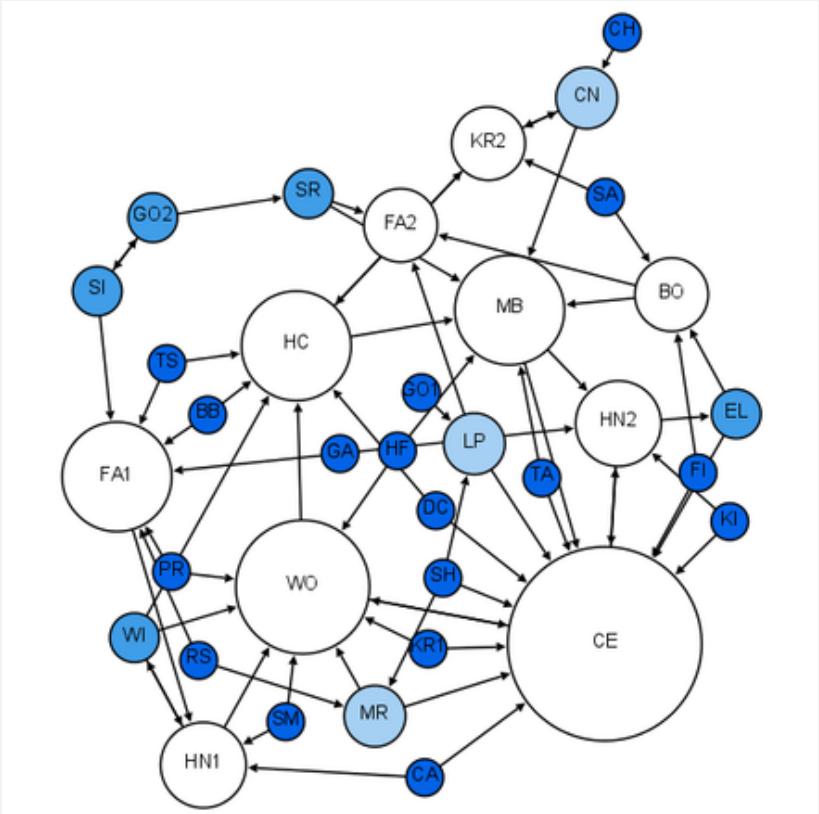
$$L(G)_{i,j} = \begin{cases} \deg(V_i) & \text{if } i = j, \\ -1 & \text{if } i \neq j \text{ and } V_i \text{ and } V_j \text{ is adjacent}, \\ 0 & \text{otherwise.} \end{cases}$$

Laplacian matrix of a graph G with `weighted matrix` *W is $L^W = D - W$, where D is the degree matrix of G.*
We often denote $L(G)$ simply by L.

***Definition**: A directed graph (or* `digraph` *) is a set of vertices and a collection of directed edges that each connects an ordered pair of vertices. We say that a directed edge points from the first vertex in the pair and points to the second vertex in the pair. We use the names 0 through V-1 for the vertices in a V-vertex graph. Via https://algs4.cs.princeton.edu/42digraph/.*

It seems that graph theory is the application of matrix theory at least partially.

Cayley graph of F2 in Wikimedia **Moreno Sociogram 1st Grade**

Cayley graph of F2 in Wikimedia	Moreno Sociogram 1st Grade
	

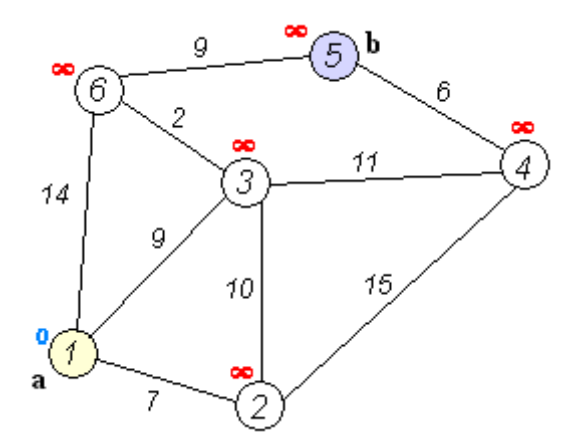
- http://mathworld.wolfram.com/Graph.html
- https://www.wikiwand.com/en/Graph_theory
- https://www.wikiwand.com/en/Gallery_of_named_graphs
- https://www.wikiwand.com/en/Laplacian_matrix
- http://www.ericweisstein.com/encyclopedias/books/GraphTheory.html
- https://www.wikiwand.com/en/Cayley_graph
- http://mathworld.wolfram.com/CayleyGraph.html
- https://www.wikiwand.com/en/Network_science
- https://www.wikiwand.com/en/Directed_graph
- https://www.wikiwand.com/en/Directed_acyclic_graph
- http://ww3.algorithmdesign.net/sample/ch07-weights.pdf
- https://www.geeksforgeeks.org/graph-data-structure-and-algorithms/
- https://www.geeksforgeeks.org/graph-types-and-applications/
- https://github.com/neo4j-contrib/neo4j-graph-algorithms
- https://algs4.cs.princeton.edu/40graphs/
- http://networkscience.cn/
- http://yaoyao.codes/algorithm/2018/06/11/laplacian-matrix
- The book **Graphs and Matrices** https://www.springer.com/us/book/9781848829800
- The book **Random Graph** https://www.math.cmu.edu/~af1p/BOOK.pdf.

A* Algorithm

In computer science, A* (pronounced "A star") is a computer algorithm that is widely used in pathfinding and graph traversal, which is the process of finding a path between multiple points, called "nodes". It enjoys widespread use due to its performance and accuracy. However, in practical travel-routing systems, it is generally outperformed by algorithms which can pre-process the graph to attain better performance, although other work has found A* to be superior to other approaches.
It is draw from Wikipedia page on A* algorithm.

First we learn the **Dijkstra's algorithm**.
Dijkstra's algorithm is an algorithm for finding the shortest paths between nodes in a graph, which may represent, for example, road networks. It was conceived by computer scientist Edsger W. Dijkstra in 1956 and published three years later.

Dijkstra algorithm



- https://www.wikiwand.com/en/Dijkstra's_algorithm
- https://www.geeksforgeeks.org/dijkstras-shortest-path-algorithm-greedy-algo-7/
- https://www.wikiwand.com/en/Shortest_path_problem

See the page at Wikipedia A* search algorithm

Graph Kernel

Like kernels in **kernel methods**, graph kernel is used as functions measuring the similarity of pairs of graphs.
They allow kernelized learning algorithms such as support vector machines to work directly on graphs, without having to do feature extraction to transform them to fixed-length, real-valued feature vectors.

- https://www.wikiwand.com/en/Graph_product
- https://www.wikiwand.com/en/Graph_kernel
- http://people.cs.uchicago.edu/~risi/papers/VishwanathanGraphKernelsJMLR.pdf
- https://www.cs.ucsb.edu/~xyan/tutorial/GraphKernels.pdf
- https://github.com/BorgwardtLab/graph-kernels

Spectral Clustering Algorithm

Spectral method is the kernel tricks applied to locality preserving projections as to reduce the dimension, which is as the data preprocessing for clustering.

In multivariate statistics and the clustering of data, spectral clustering techniques make use of the spectrum (eigenvalues) of the `similarity matrix` of the data to perform dimensionality reduction before clustering in fewer dimensions. The

similarity matrix is provided as an input and consists of a quantitative assessment of the relative similarity of each pair of points in the data set.

Similarity matrix is to measure the similarity between the input features $\{\mathbf{x}_i\}_{i=1}^n \subset \mathbb{R}^p$.
For example, we can use Gaussian kernel function

$$f(\mathbf{x_i}, \mathbf{x}_j) = exp(-\frac{\|\mathbf{x_i} - \mathbf{x}_j\|_2^2}{2\sigma^2})$$

to measure the *similarity* of inputs.

The element of *similarity matrix* S is $S_{i,j} = exp(-\frac{\|\mathbf{x_i}-\mathbf{x}_j\|_2^2}{2\sigma^2})$.
Thus S is symmetrical, i.e. $S_{i,j} = S_{j,i}$ for $i, j \in \{1, 2, \ldots, n\}$.
If the sample size $n \gg p$, the storage of **similarity matrix** is much larger than the original input $\{\mathbf{x}_i\}_{i=1}^n$, when we would only preserve the entries above some values.
The **Laplacian matrix** is defined by $L = D - S$ where $D = Diag\{D_1, D_2, \ldots, D_n\}$ and
$D_i = \sum_{j=1}^n S_{i,j} = \sum_{j=1}^n exp(-\frac{\|\mathbf{x_i}-\mathbf{x}_j\|_2^2}{2\sigma^2})$.

Then we can apply *principal component analysis* to the *Laplacian matrix* L to reduce the data dimension. After that we can perform $K - means$ or other clustering.

- https://zhuanlan.zhihu.com/p/34848710
- *On Spectral Clustering: Analysis and an algorithm* at http://papers.nips.cc/paper/2092-on-spectral-clustering-analysis-and-an-algorithm.pdf
- *A Tutorial on Spectral Clustering* at https://www.cs.cmu.edu/~aarti/Class/10701/readings/Luxburg06_TR.pdf.
- **谱聚类** https://www.cnblogs.com/pinard/p/6221564.html.
- *Spectral Clustering* http://www.datasciencelab.cn/clustering/spectral.
- https://en.wikipedia.org/wiki/Category:Graph_algorithms
- The course *Spectral Graph Theory, Fall 2015* athttp://www.cs.yale.edu/homes/spielman/561/.

Bootstrapping Methods

Bootstrapping methods are based on the bootstrap samples to compute new statistic.

- Bootstrapping_(statistics)
- Bootstrap Methods: Another Look at the Jackknife by B. Efron

Dimension Reduction

https://www.wikiwand.com/en/Nonlinear_dimensionality_reduction

Decision Tree

A decision tree is a set of questions organized in a hierarchical manner and represented graphically as a tree.

An Introduction to Recursive Partitioning: Rationale, Application and Characteristics of Classification and Regression Trees, Bagging and Random Forests

Ensemble methods

Zhou Zhihua's publication on ensemble methods

Bagging

Bagging, short for 'bootstrap aggregating', is a simple but highly effective ensemble method that creates diverse models on different random samples of the original data set.
Random forest is the application of bagging to decision tree algorithms.

- http://www.machine-learning.martinsewell.com/ensembles/bagging/
- https://www.cnblogs.com/earendil/p/8872001.html
- https://www.wikiwand.com/en/Bootstrap_aggregating

Boosting

- http://www.machine-learning.martinsewell.com/ensembles/boosting/
- Boosting at Wikipedia
- AdaBoost at Wikipedia, CSDN blog
- Gradient Boosting at Wikipedia
- https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3885826/
- https://explained.ai/gradient-boosting/index.html
- https://xgboost.ai/
- https://datascienceplus.com/extreme-gradient-boosting-with-r/
- https://data-flair.training/blogs/gradient-boosting-algorithm/
- http://blog.kaggle.com/2017/01/23/a-kaggle-master-explains-gradient-boosting/
- XGBoost: A Scalable Tree Boosting System
- xgboost的原理没你想像的那么难
- https://www.cnblogs.com/wxquare/p/5541414.html
- GBDT算法原理 - 飞奔的猫熊的文章 - 知乎

Stacking

Stacked generalization (or stacking) is a different way of combining multiple models, that introduces the concept of a meta learner. Although an attractive idea, it is less widely used than bagging and boosting. Unlike bagging and boosting, stacking may be (and normally is) used to combine models of different types. The procedure is as follows:

1. Split the training set into two disjoint sets.
2. Train several base learners on the first part.
3. Test the base learners on the second part.
4. Using the predictions from 3) as the inputs, and the correct responses as the outputs, train a higher level learner.

Note that steps 1) to 3) are the same as cross-validation, but instead of using a winner-takes-all approach, we combine the base learners, possibly nonlinearly.

- http://www.machine-learning.martinsewell.com/ensembles/stacking/
- https://www.jianshu.com/p/46ccf40222d6

- Deep forest
- https://cosx.org/2018/10/python-and-r-implementation-of-gcforest/
- https://blog.csdn.net/willduan1/article/details/73618677

- https://www.wikiwand.com/en/Ensemble_learning
- https://machinelearningmastery.com/gentle-introduction-gradient-boosting-algorithm-machine-learning/
- https://www.toptal.com/machine-learning/ensemble-methods-machine-learning

Deep Learning

Deep learning is the modern version of artificial neural networks full of tricks and techniques.
In mathematics, it is nonlinear nonconvex and composite of many functions. Its name -deep learning- is to distinguish from the classical machine learning "shallow" methods.
However, its complexity makes it yet engineering even art far from science. There is no first principle in deep learning but trial and error.
In theory, we do not clearly understand how to design more robust and efficient network architecture; in practice, we can apply it to diverse fields. It is considered as one approach to artificial intelligence

Deep learning is a typical hierarchy model.
The application of deep learning are partial listed in **Awesome deep learning**,MIT Deep Learning Book and Deep interests.

Father of Deep Learning

О.Г. Івахненко (1967 р.)

A history of deep learning

Three Giants' Survey in *(Nature 521 p 436)*

Father of Deep Learning

Critique of Paper by "Deep Learning Conspiracy" (Nature 521 p 436)

Deep Learning in Neural Networks: An Overview

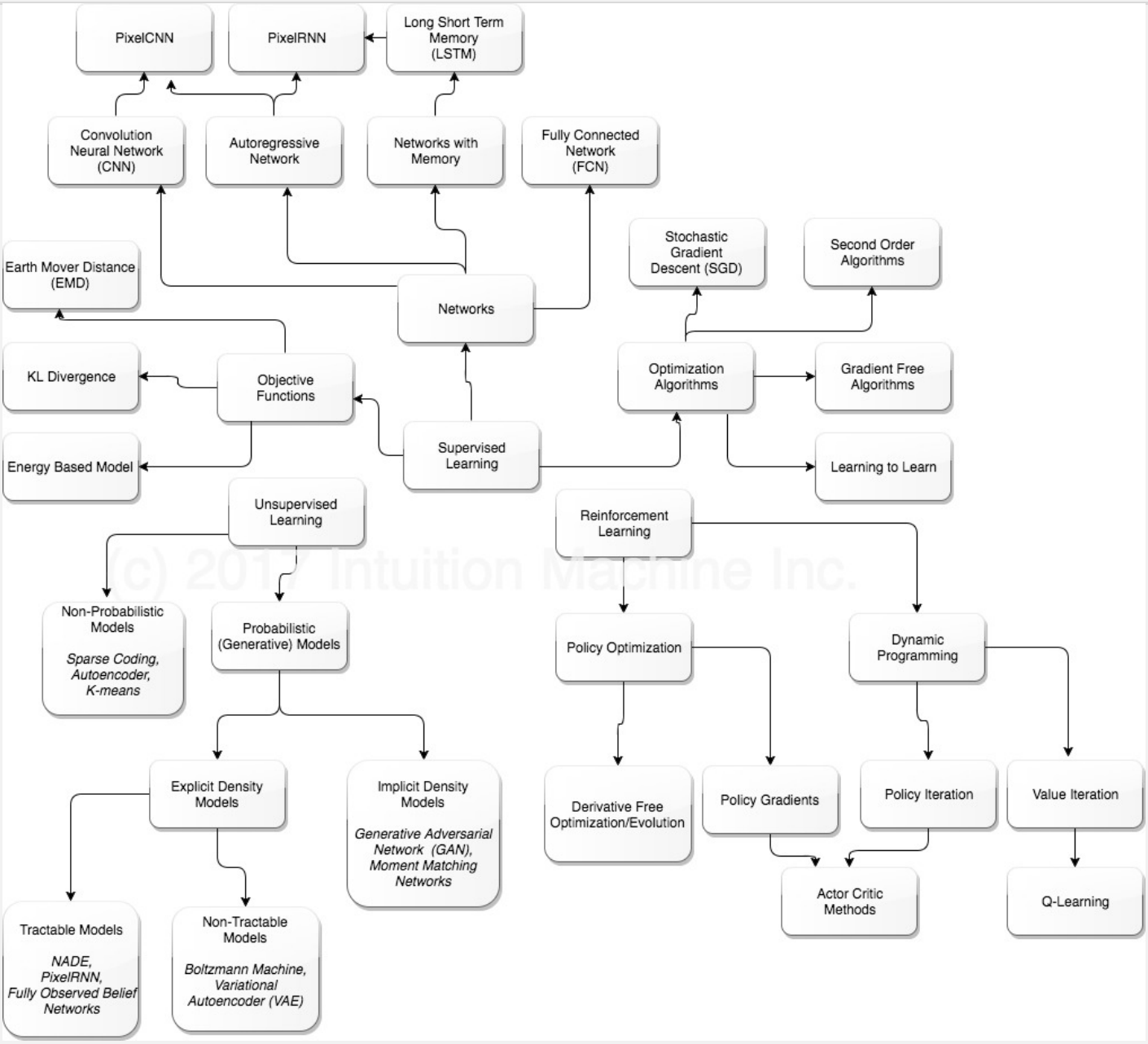
AI winter

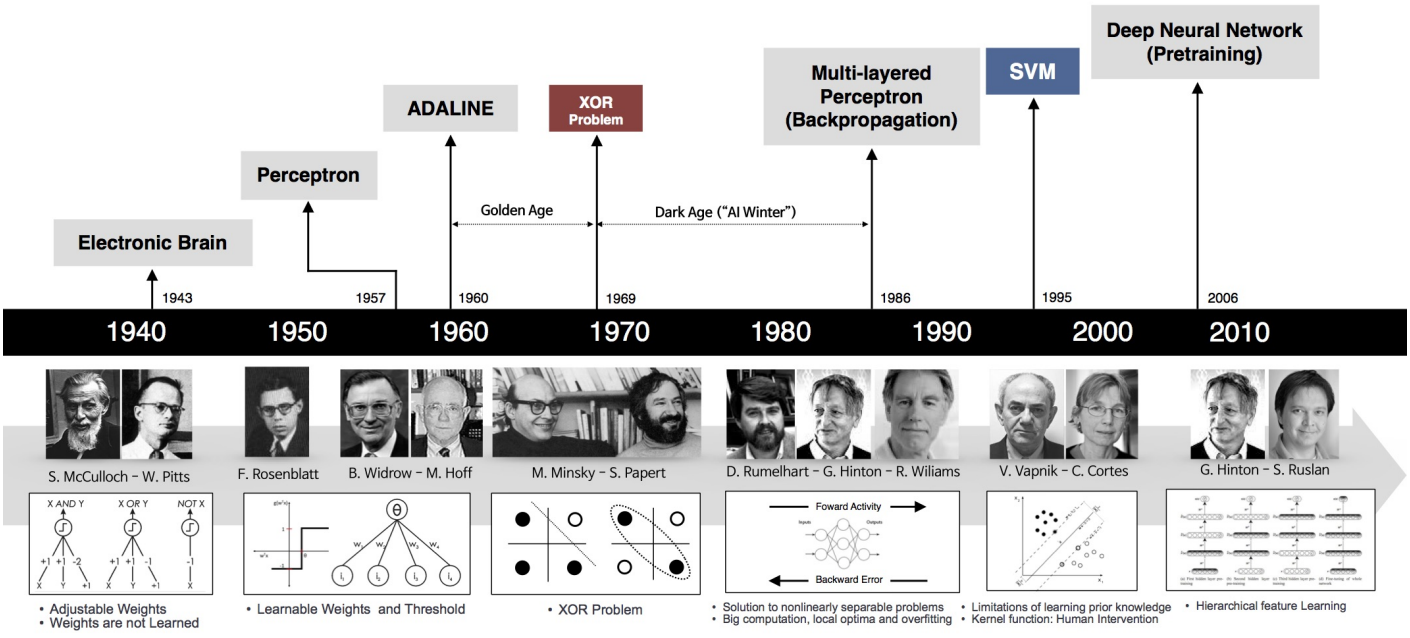
Deep learning in wiki and Deep Learning in Scholarpedia

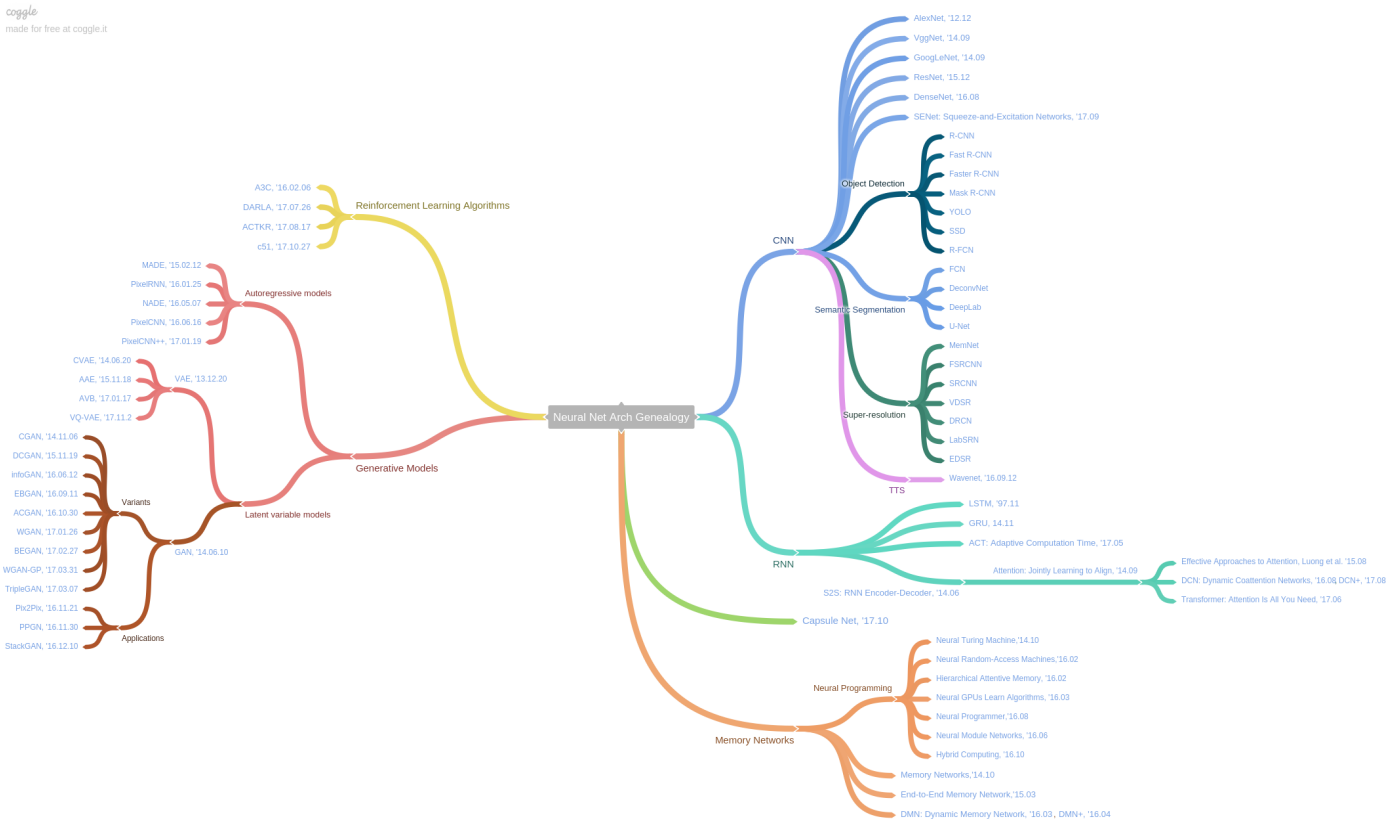
A Brief History of Deep Learning (Part One)

On the Origin of Deep Learning

Father of Deep Learning







Neural_Net_Arch_Genealogy

The **architecture** and **optimization** are the core content of deep learning models. We will focus on the first one.

Artificial Neural Network

Artificial neural networks are most easily visualized in terms of a **directed graph**. In the case of sigmoidal units, node s represents sigmoidal unit and directed edge $e = (u, v)$ indicates that one of sigmoidal unit v's inputs is the output of sigmoidal unit u.

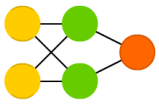
A mostly complete chart of

Neural Networks

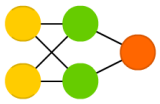
- Backfed Input Cell
- Input Cell
- Noisy Input Cell
- Hidden Cell
- Probablistic Hidden Cell
- Spiking Hidden Cell
- Output Cell
- Match Input Output Cell
- Recurrent Cell
- Memory Cell
- Different Memory Cell
- Kernel
- Convolution or Pool

Perceptron (P)

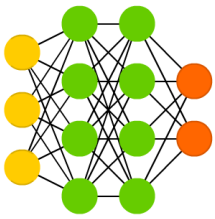
Feed Forward (FF)



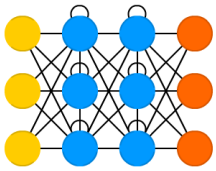
Radial Basis Network (RBF)



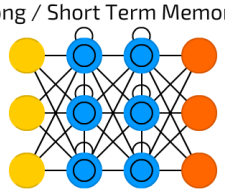
Deep Feed Forward (DFF)



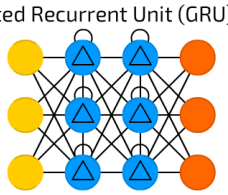
Recurrent Neural Network (RNN)



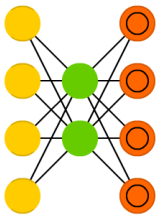
Long / Short Term Memory (LSTM)



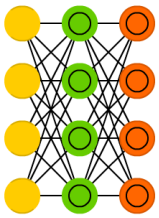
Gated Recurrent Unit (GRU)



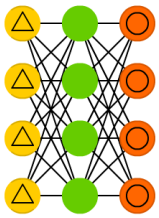
Auto Encoder (AE)



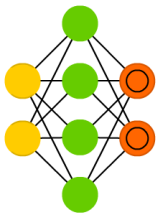
Variational AE (VAE)



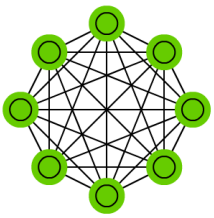
Denoising AE (DAE)



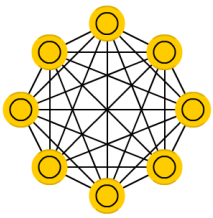
Sparse AE (SAE)



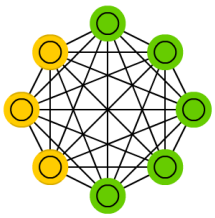
Markov Chain (MC)



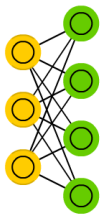
Hopfield Network (HN)



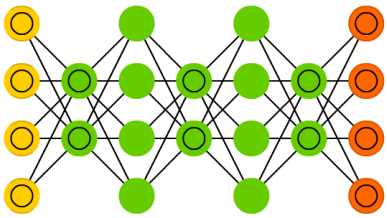
Boltzmann Machine (BM)



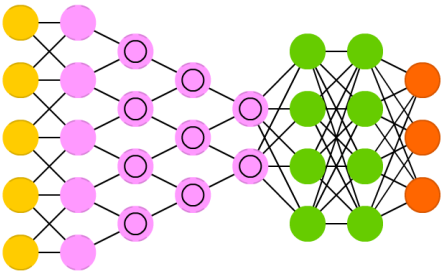
Restricted BM (RBM)



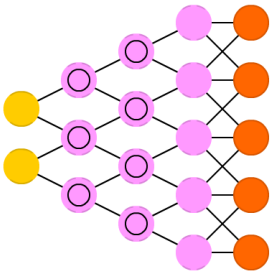
Deep Belief Network (DBN)



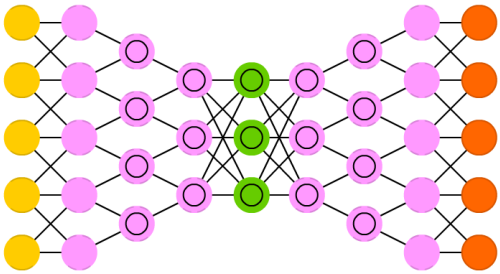
Deep Convolutional Network (DCN)



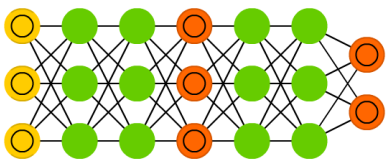
Deconvolutional Network (DN)



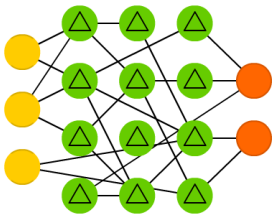
Deep Convolutional Inverse Graphics Network (DCIGN)



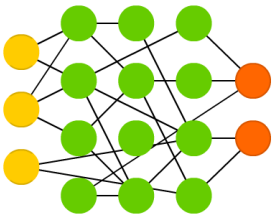
Generative Adversarial Network (GAN)



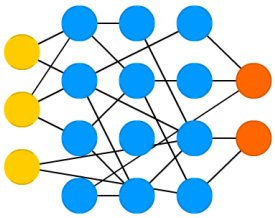
Liquid State Machine (LSM)



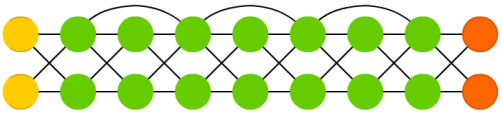
Extreme Learning Machine (ELM)



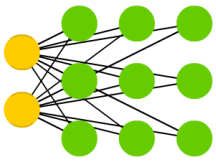
Echo State Network (ESN)



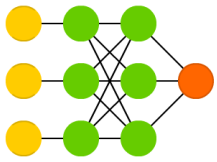
Deep Residual Network (DRN)



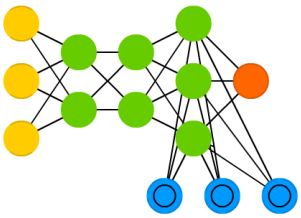
Kohonen Network (KN)



Support Vector Machine (SVM)



Neural Turing Machine (NTM)



- The Wikipedia page on ANN
- History of deep learning
- https://brilliant.org/wiki/artificial-neural-network/
- https://www.asimovinstitute.org/neural-network-zoo/

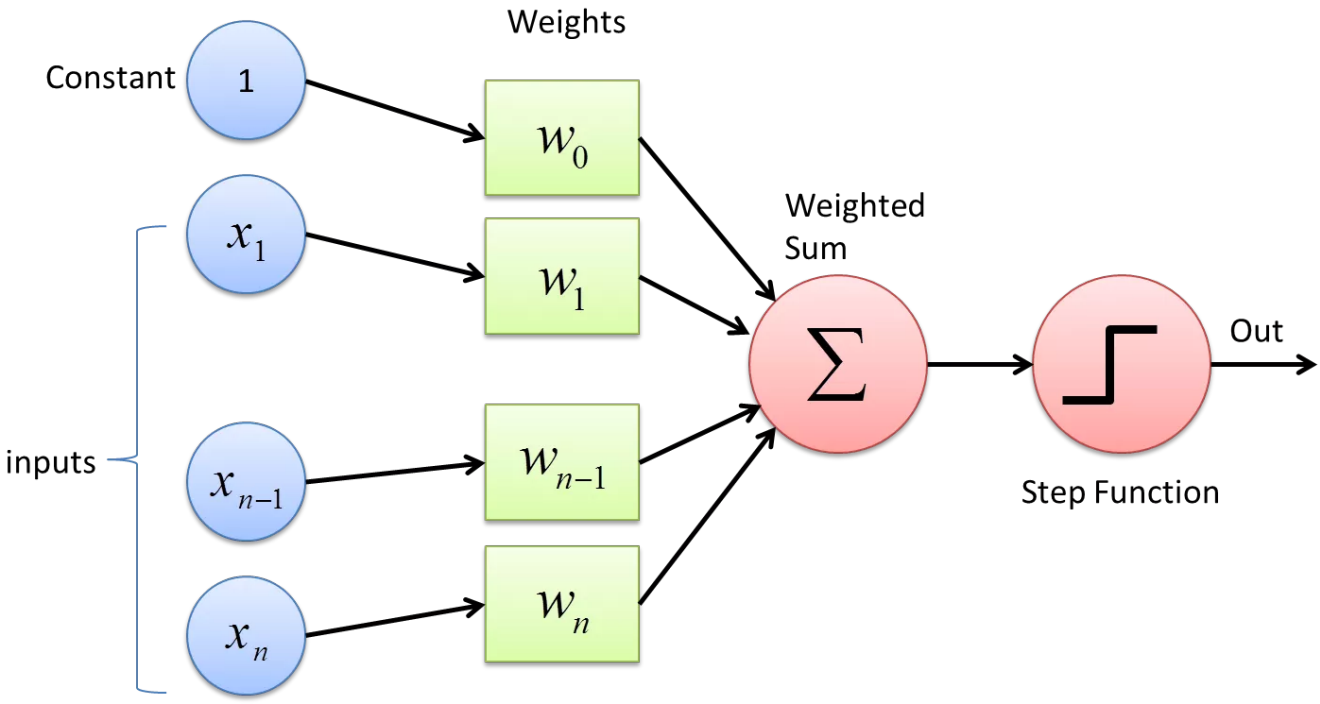
Perceptron

Perceptron can be seen as a generalized linear model.
In mathematics, it is a map

$$f : \mathbb{R}^n \to \mathbb{R}.$$

It can be decomposed into 2 steps:

1. Aggregate all the information: $z = \sum_{i=1}^{n} w_i x_i + b_0 = (x_1, x_2, \cdots, x_n, 1) \cdot (w_1, w_2, \cdots, w_n, b_0)^T$.
2. Transform the information to activate something: $y = \sigma(z)$, where σ is nonlinear such as step function.



Activation function

The nonlinear function σ is conventionally called activation function.
There are some activation functions in history.

- Sign function

$$f(x) = \begin{cases} 1, & \text{if } x > 0 \\ -1, & \text{if } x < 0 \end{cases}$$

- Step function

$$f(x) = \begin{cases} 1, & \text{if } x \geq 0 \\ 0, & \text{otherwise} \end{cases}$$

- Sigmoid function

$$\sigma(x) = \frac{1}{1 + e^{-x}}.$$

- Radical base function

$$\rho(x) = e^{-\beta(x - x_0)^2}.$$

- TanH function

$$tanh(x) = 2\sigma(2x) - 1 = \frac{2}{1 + e^{-2x}} - 1.$$

- ReLU function

$$ReLU(x) = (x)_+ = \max\{0, x\} = \begin{cases} x, & \text{if } x \geq 0 \\ 0, & \text{otherwise} \end{cases}.$$

- 神经网络激励函数的作用是什么？有没有形象的解释?
- Activation function in Wikipedia
- 激活函数https://blog.csdn.net/cyh_24/article/details/50593400
- 可视化超参数作用机制：一、动画化激活函数
- https://towardsdatascience.com/hyper-parameters-in-action-a524bf5bf1c
- https://www.cnblogs.com/makefile/p/activation-function.html
- http://www.cnblogs.com/neopenx/p/4453161.html

Learning algorithm

We draw it from the Wikipedia page.
Learning is to find optimal parameters of the model. Before that, we must feed data into the model.
The training data of n sample size is

$$D = \{(\mathbf{x}_i, d_i)\}_{i=1}^n$$

where

- $\mathbf{x}_i$ is the n-dimensional input vector;
- d_i is the desired output value of the perceptron for that input $\mathbf{x}_i$.

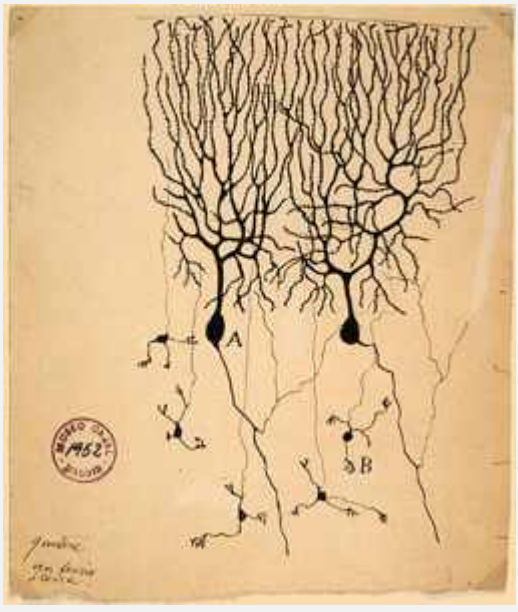
---

1. Initialize the weights and the threshold. Weights may be initialized to 0 or to a small random value. In the example below, we use 0.
2. For each example j in our training set D, perform the following steps over the input $\mathbf{x}_j$ and desired output d_j:
    - Calculate the actual output：

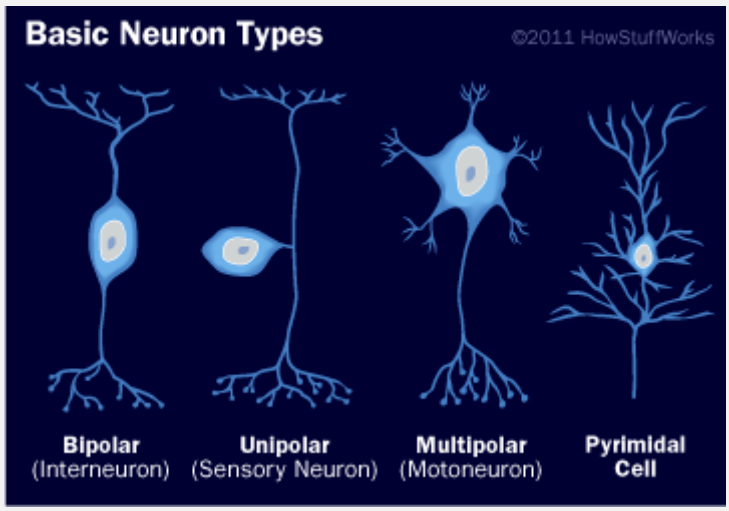
$$\begin{aligned} y_j(t) &= f[\mathbf{w}(t) \cdot \mathbf{x}_j] \\ &= f[w_0(t)x_{j,0} + w_1(t)x_{j,1} + w_2(t)x_{j,2} + \cdots + w_n(t)x_{j,n}] \end{aligned}$$

    - Update the weights:
      $w_i(t+1) = w_i(t) + r \cdot (d_j - y_j(t))x_{(j,i)}$,
      for all features $[0 \leq i \leq n]$, is the learning rate.
3. For offline learning, the second step may be repeated until the iteration error $\frac{1}{s}\sum_{j=1}^{s}|d_j - y_j(t)|$ is less than a user-specified error threshold γ, or a predetermined number of iterations have been completed, where *s* is again the size of the sample set.

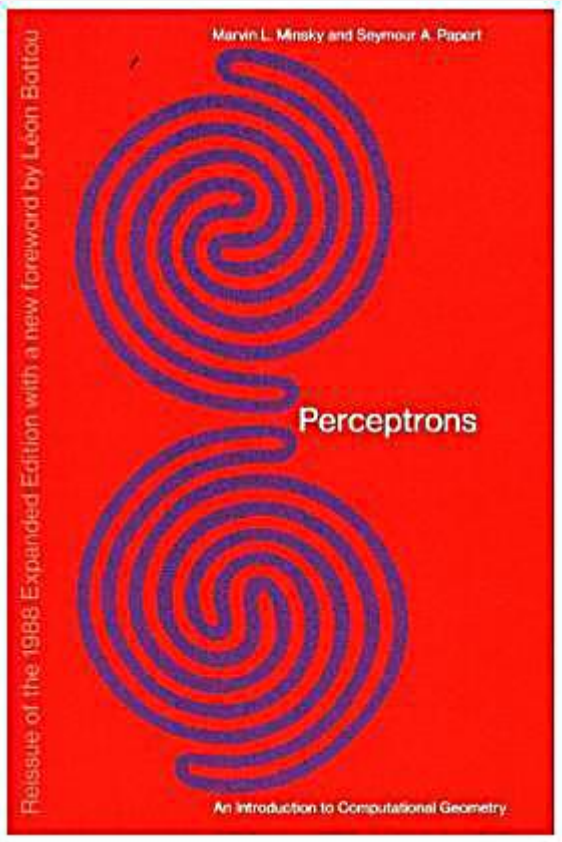
$Note$: the perceptron model is linear classifier, i.e. the training data set D is linearly separable such that the learning algorithm can converge.

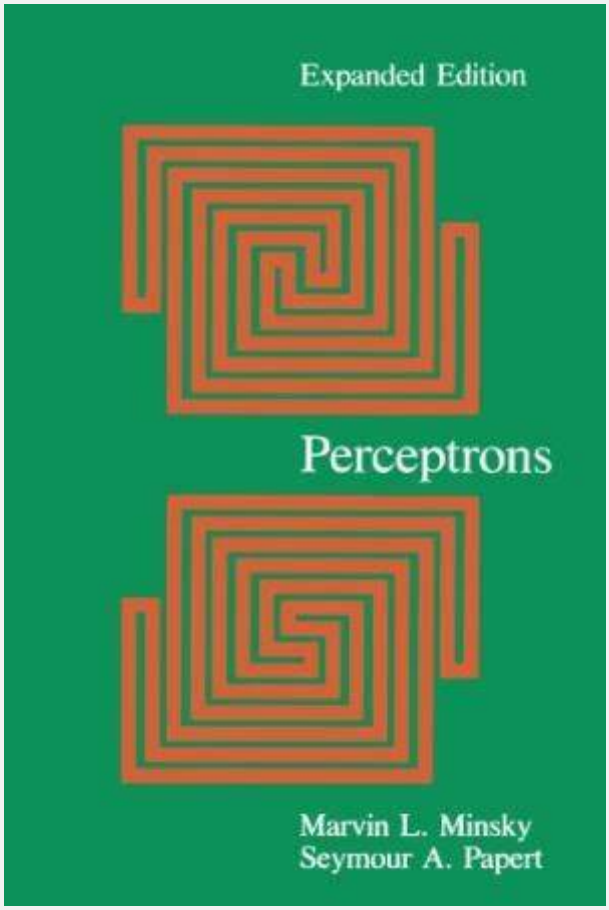


Perceptrons



人工神经网络真的像神经元一样工作吗？





More in Wikipedia page.

It is the first time to model cognition.

- Neural Networks, Types, and Functional Programming
- AI and Neuroscience: A virtuous circle
- Neuroscience-Inspired Artificial Intelligence
- 深度神经网络（DNN）是否模拟了人类大脑皮层结构？ - Harold Yue的回答 - 知乎
- Connectionist models of cognition https://stanford.edu/~jlmcc/papers/ThomasMcCIPCambEncy.pdf
- https://stats385.github.io/blogs

Feedforward Neural Network

Representation of Feedforward Neural Network

Given that the function of a single neuron is rather simple, it subdivides the input space into two regions by a hyperplane, the complexity must come from having more layers of neurons involved in a complex action (like recognizing your grandmother in all possible situations).The "squashing" functions introduce critical nonlinearities in the system, without their presence multiple layers would still create linear functions.
Organized layers are very visible in the human cerebral cortex, the part of our brain which plays a key role in memory, attention, perceptual awareness, thought, language, and consciousness.[12:2]

The **feedforward neural network** is also called multilayer perceptron. The best way to create complex functions from simple functions is by **composition**.

In mathematics, it can be considered as multi-layered non-linear composite function:

$$X \to \sigma \circ (W_1 X + b_1) = H_1 \to \sigma \circ (W_2 H_1 + b_2) = H_2 \to \cdots \sigma(WH + b) = y$$

where the notation $\circ$, $M_1, b_1, M_2, b_2, \cdots, W, b$ mean pointwise operation, the parameters in the affine mapping, respectively. Thus the data flow in the form of the chain:

$$\begin{aligned} f &= H_1 \circ H_2 \circ \cdots \circ \sigma && \text{Composite form} \\ X &\overset{\sigma}{\to} H_1 \overset{\sigma}{\to} H_2 \overset{\sigma}{\to} \cdots \overset{\sigma}{\to} y && \text{Hierarchy form} \\ \mathbb{R}^p &\to \mathbb{R}^{l_1} \to \mathbb{R}^{l_2} \to \cdots \to \mathbb{R} && \text{Dimension} \end{aligned}$$

where the circle notation $\circ$ means forward composite or as the input of afterward operation.
In hierarchy form, we omit the affine map.
It is can be written in the *recursive form*:

$$\begin{aligned} \mathbf{z}_i &= W_i H_{i-1} + b_i, \\ H_i &= \sigma \circ (\mathbf{z}_i), \forall i \{1, 2, \ldots, D\} \end{aligned} \tag{3}$$

where $H_0 = X \in \mathbb{R}^p$, b_i is a vector and W_i is matrix. And the number of recursive times D is called the depth of network.

1. In the first layer, we feed the input vector $X \in \mathbb{R}^p$ and connect it to each unit in the next layer $W_1 X + b_1 \in \mathbb{R}^{l_1}$ where $W_1 \in \mathbb{R}^{n \times l_1}$, $b_1 \in \mathbb{R}^{l_1}$. The output of the first layer is $H_1 = \sigma \circ (M_1 X + b)$, or in another word the output of jth unit in the first (hidden) layer is $h_j = \sigma(W_1 X + b_1)_j$ where $(W_1 X + b_1)_j$ is the jth element of l_1-dimensional vector $W_1 X + b_1$.
2. In the second layer, its input is the output of first layer,H_1, and apply linear map to it: $W_2 H_1 + b_2 \in \mathbb{R}^{l_2}$, where $W_2 \in \mathbb{R}^{l_1 \times l_2}$, $b_2 \in \mathbb{R}^{l_2}$. The output of the second layer is $H_2 = \sigma \circ (W_2 H_1 + b_2)$, or in another word the output of jth unit in the second (hidden) layer is $h_j = \sigma(W_2 H_1 + b_2)_j$ where $(W_2 H_1 + b_2)_j$ is the jth element of l_2-dimensional vector $W_2 H_1 + b_2$.
3. The map between the second layer and the third layer is similar to (1) and (2): the linear maps datum to different dimensional space and the nonlinear maps extract better representations.
4. In the last layer, suppose the input data is $H \in \mathbb{R}^l$. The output may be vector or scalar values and W may be a matrix or vector as well as y.

The ordinary feedforward neural networks take the *sigmoid* function $\sigma(x) = \frac{1}{1+e^{-x}}$ as the nonlinear activation function while the *RBF networks* take the Radial basis function as the activation function such as $\sigma(x) = e^{c\|x\|_2^2}$.

In theory, the universal approximation theorem show the power of feedforward neural network
if we take some proper activation functions such as sigmoid function.

- https://www.wikiwand.com/en/Universal_approximation_theorem
- http://mcneela.github.io/machine_learning/2017/03/21/Universal-Approximation-Theorem.html
- http://neuralnetworksanddeeplearning.com/chap4.html

Evaluation and Optimization in Multilayer Perceptron

The problem is how to find the optimal parameters $W_1, b_1, W_2, b_2, \cdots, W, b$?
The multilayer perceptron is as one example of supervised learning, which means that we feed datum $D = \{(\mathbf{x_i}, d_i)\}_{i=1}^n$ to it and evaluate it.

The general form of the evaluation is given by:

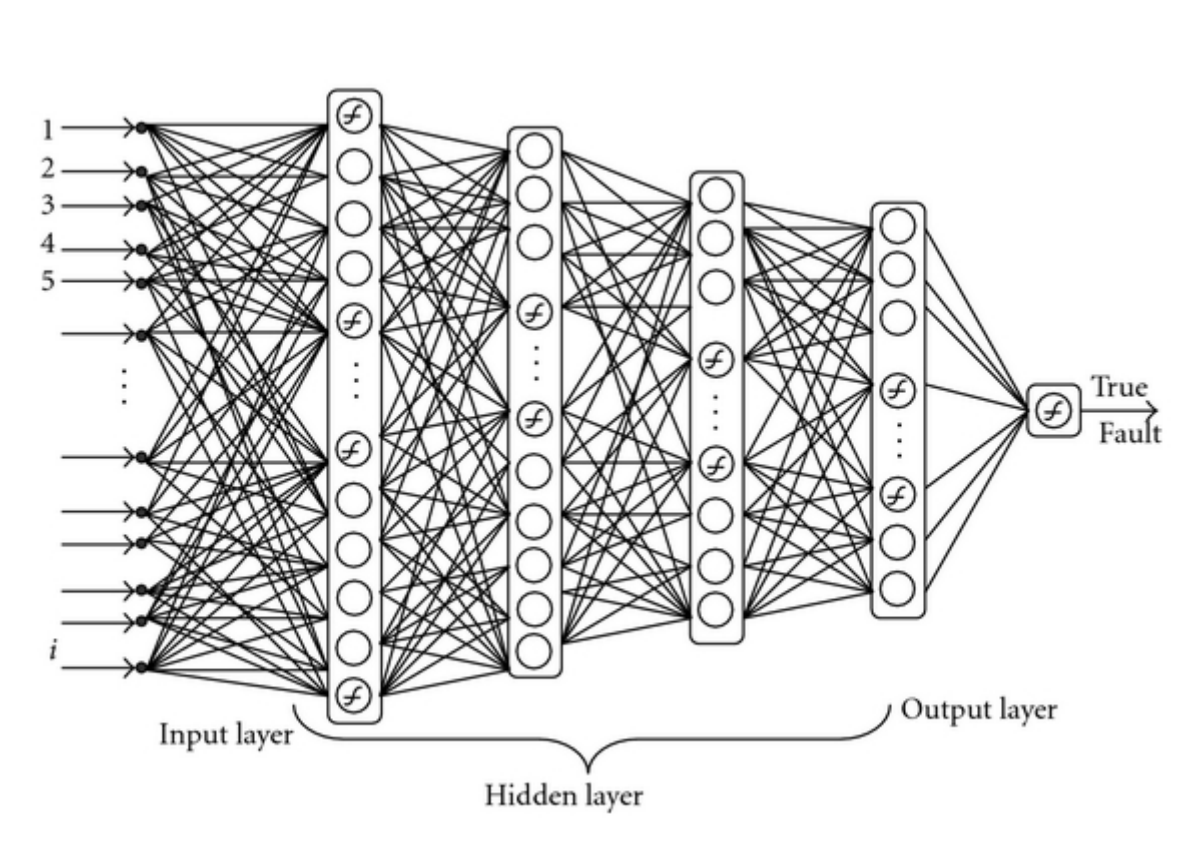
$$J(\theta) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{L}[f(\mathbf{x}_i|\theta), \mathbf{d}_i]$$

where $\mathbf{d}_i$ is the desired value of the input $\mathbf{x}_i$ and θ is the parameters of multilayer perceptron. The notation $f(\mathbf{x}_i|\theta)$ is the output given paramaters θ. The function $\mathbb{L}$ is **loss function** to measure the discrpency between the predicted value $f(\mathbf{x}_i|\theta)$ and the desired value $\mathbf{d}_i$.

In general, the number of parameters θ is less than the sample size n. And the objective function $J(\theta)$ is not convex.

We will solve it in the next section *Backpropagation, Optimization and Regularization*.

The diagram of MLP



Visualizing level surfaces of a neural network with raymarching

- https://devblogs.nvidia.com/deep-learning-nutshell-history-training/
- Deep Learning 101 Part 2
- https://www.wikiwand.com/en/Multilayer_perceptron

- https://www.wikiwand.com/en/Feedforward_neural_network
- https://www.wikiwand.com/en/Radial_basis_function_network

Evaluation for different tasks

Evaluation is to judge the models with different parameters in some sense via objective function.
In maximum likelihood estimation, it is likelihood or log-likelihood;
in parameter estimation, it is bias or mean square error;
in regression, it depends on the case.

In machine learning, evaluation is aimed to measure the discrepancy between the predicted values and trues value by **loss function**.
It is expected to be continuous smooth and differential but it is snot necessary.
The principle is the loss function make the optimization or learning tractable.
For classification, the loss function always is cross entropy;
for regression, the loss function can be any norm function such as the ℓ_2 norm;
in probability models, the loss function always is joint probability or logarithm of joint probability.

In classification, the last layer is to predict the degree of belief of the labels via softmax function,
i.e.

$$softmax(z) = (\frac{\exp(z_1)}{\sum_{i=1}^n \exp(z_i)}, \frac{\exp(z_2)}{\sum_{i=1}^n \exp(z_i)}, \cdots, \frac{\exp(z_n)}{\sum_{i=1}^n \exp(z_i)})$$

where n is the number of total classes. The labels are encoded as the one hot vector such as $\mathrm{d} = (1, 0, 0, \cdots, 0)$. The cross entropy is defined as:

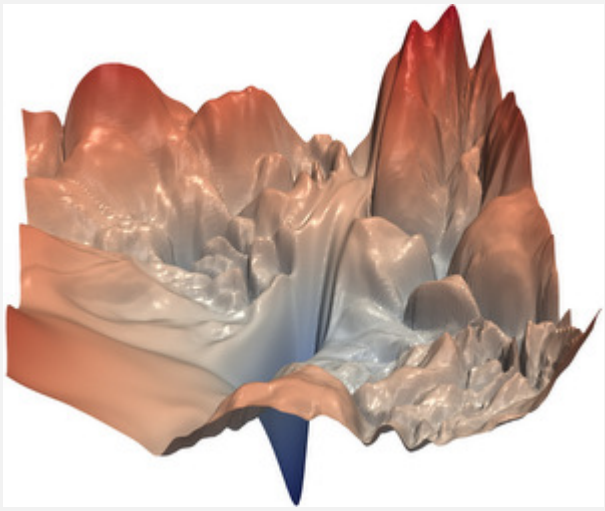
$$\mathbf{H}(d, p) = -\sum_{i=1}^n d_i \log(p_i) = \sum_{i=1}^n d_i \log(\frac{1}{p_i}),$$

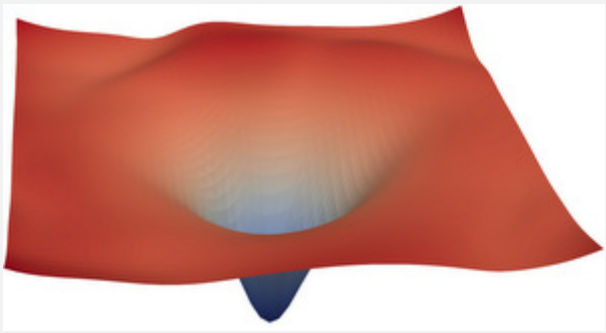
where d_i is the ith element of the one-hot vector d and $p_i = \frac{\exp(z_i)}{\sum_{j=1}^n \exp(z_j)}$ for all $i = 1, 2 \ldots, n$.

Suppose $\mathrm{d} = (1, 0, 0, \cdots, 0)$, the cross entropy is $\mathbf{H}(d, p) = -\log(p_1) = \log \sum_{i=1}^n \exp(z_i) - z_1$. The cost function is $\frac{1}{n} \sum_{i=1}^n \mathbf{H}(d^i, p^i)$ in the training data set $\{(\mathbf{x}_i, d^i)\}_{i=1}^n$ where $\mathbf{x}_i$ is the features of ith sample and d^i is the desired true target label encoded in **one-hot** vector meanwhile p^i is the predicted label of $\mathbf{x}_i$.
See the following links for more information on cross entropy and softmax.

VISUALIZING THE LOSS LANDSCAPE OF NEURAL NETS

VISUALIZING THE LOSS LANDSCAPE OF NEURAL NETS





- https://blog.csdn.net/u014380165/article/details/77284921;
- https://blog.csdn.net/u014380165/article/details/79632950;
- https://eli.thegreenplace.net/2016/the-softmax-function-and-its-derivative/;
- https://www.zhihu.com/question/65288314.

In regression, the loss function may simply be the squared ℓ_2 norm, i.e. $\mathbb{L}(d,p)=(d-p)^2$ where d is the desired target and p is the predicted result. And the cost function is *mean squared error*:

$$J(\theta)=\frac{1}{n}\sum_{i=1}^{n}[f(\mathbf{x}_i|\theta)-\mathrm{d}_i]^2.$$

In **robust statistics**, there are more loss functions such as *Huber loss*, *hinge loss*, *Tukey loss*.

- Huber loss function

$$Huber_{\delta}(x)=\begin{cases}\frac{|x|}{2}, & \text{if } |x|\le\delta\\ \delta(|x|-\frac{1}{2}\delta), & \text{otherwise}\end{cases}$$

- Hinge loss function

$$Hinge(x)=max\{0,1-tx\}$$

  where $t=+1$ or $t=-1$.

- Tukey loss function

$$Tukey_\delta(x) = \begin{cases} (1-[1-x^2/\delta^2]^3)\frac{\delta^2}{6}, & \text{if } |x| \le \delta \\ \frac{\delta^2}{6}, & \text{otherwise} \end{cases}$$

It is important to choose or design loss function or more generally objective function,
which can select variable as LASSO or confirm prior information as Bayesian estimation.
Except the *representation* or model, it is the objective function that affects the usefulness of learning algorithms.

For more on **loss function** see:

- https://blog.algorithmia.com/introduction-to-loss-functions/;
- https://www.learnopencv.com/understanding-activation-functions-in-deep-learning/;
- http://laid.delanover.com/activation-functions-in-deep-learning-sigmoid-relu-lrelu-prelu-rrelu-elu-softmax/;
- https://www.wikiwand.com/en/Robust_statistics
- https://www.wikiwand.com/en/Huber_loss
- https://github.com/Kulbear/deep-learning-nano-foundation/wiki/ReLU-and-Softmax-Activation-Functions;
- https://www.cs.umd.edu/~tomg/projects/landscapes/.

Backpropagation, Training and Regularization

Backpropagation

Automatic differentiation is the generic name for techniques that use the computational representation of a function to produce **analytic** values for the derivatives.
Automatic differentiation techniques are founded on the observation that any function, no matter how complicated, is evaluated by performing a sequence of simple elementary operations involving just one or two arguments at a time.
Backpropagation is one special case of automatic differentiation, i.e. *reverse-mode automatic differentiation*.

The backpropagation procedure to compute the gradient of an objective function with respect to the weights of a multilayer stack of modules is nothing more than a practical application of the **chain rule for derivatives**.
The key insight is that the derivative (or gradient) of the objective with respect to the input of a module can be computed by working backwards from the gradient with respect to the output of that module (or the input of the subsequent module).
The backpropagation equation can be applied repeatedly to
propagate gradients through all modules, starting from the output at the top (where the network produces its prediction) all the way to the bottom (where the external input is fed).
Once these gradients have been computed, it is straightforward to compute the gradients with respect to the weights of each module.[14]

Suppose that $f(x) = \sigma \circ (WH + b)$,where $H = \sigma \circ (W_4 H_3 + b_4)$, $H_3 = \sigma \circ (W_3 H_2 + b_3)$,$H_2 = \sigma \circ (W_2 H_1 + b_2)$, $H_1 = \sigma \circ (W_1 x + b_1)$,
we want to compute the gradient $L(x_0, d_0) = \|f(x_0) - d_0\|_2^2$ with respect to all weights W_1, W_2, W_3, W:

-

$$\frac{\partial L(x_0, d_0)}{\partial W_n^i} = \frac{\partial L(x_0, d_0)}{\partial f(x_0)} \frac{\partial f(x_0)}{\partial W_n^i} \forall i \in \{1, 2, \ldots, l_n\}, \forall\, n \in \{1, 2, 3, 4\}$$

and it is fundamental to compute the gradient with respect to the last layer as below.

- the gradient of loss function with respect to the prediction function:

$$\frac{\partial L(x_0, d_0)}{\partial f(x_0)} = 2[f(x_0) - d_0],$$

- the gradient of each unit in prediction function with respect to the weight in the last layer:

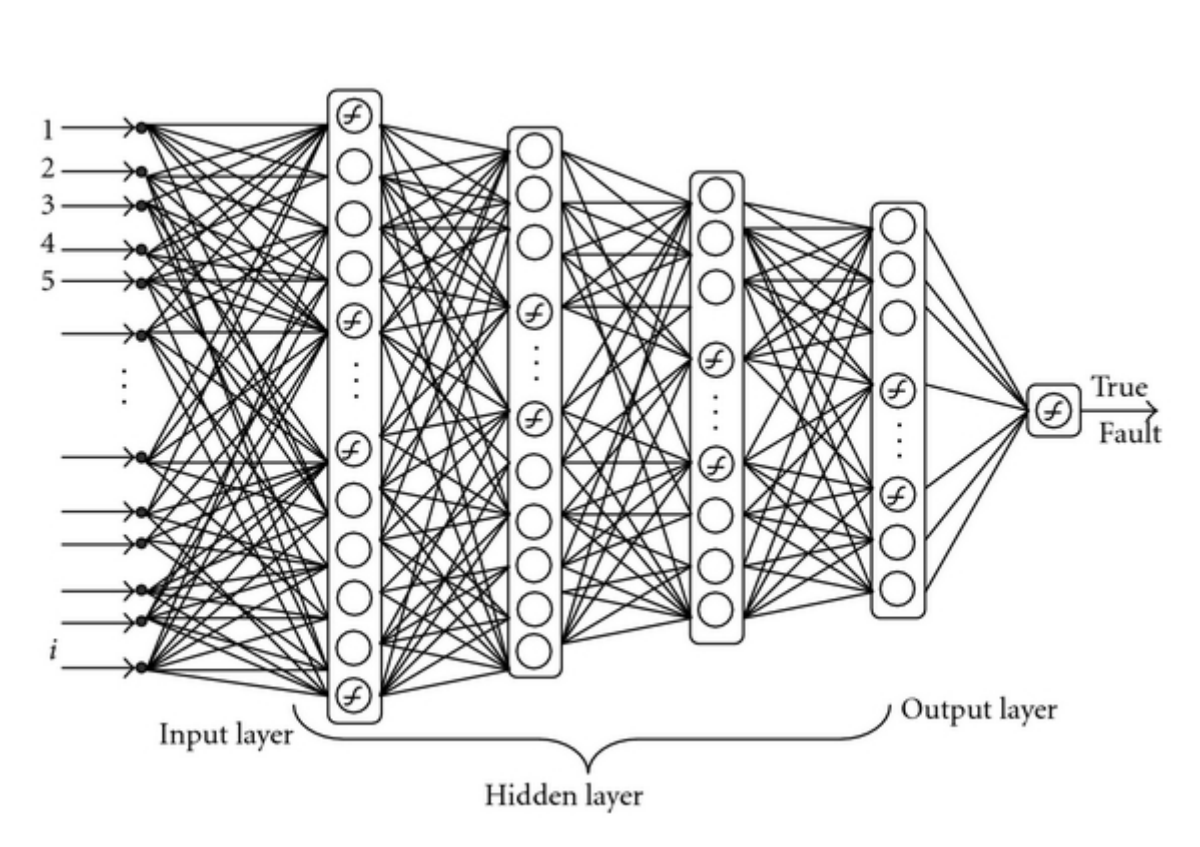
$$\frac{\partial f^j(x_0)}{\partial W^j} = \frac{\partial \sigma(W^j H + b^j)}{\partial W^j} = \sigma'(W^j H + b^j) H \ \forall j \in \{1, 2, \ldots, l\},$$

- the gradient of prediction function with respect to the last hidden state:

$$\frac{\partial f^j(x_0)}{\partial H} = \frac{\partial \sigma(W^j H + b^j)}{\partial H} = \sigma'(W^j H + b^j) W^j \ \forall j \in \{1, 2, \ldots, l\},$$

where $f^j(x_0)$, W^j, b^j and $\sigma'(z)$is the jth element of $f(x_0)$, the j-th row of matrix W, the jth element of vector b and $\frac{\mathrm{d}\sigma(z)}{\mathrm{d}z}$, respectively.

The Architecture of Feedforward Neural Networks



The Architecture of Feedforward Neural Networks

Each connection ,the black line, is attached with a weight parameter.

Recall the chain rule with more variables:

$$\frac{\partial f(m(x_0),n(x_0))}{\partial x_0}=\frac{\partial f(m(x_0),n(x_0))}{\partial m(x_0)}\frac{\partial m(x_0)}{\partial x_0}+\frac{\partial f(m(x_0),n(x_0))}{\partial n(x_0)}\frac{\partial n(x_0)}{\partial x_0}.$$

Similarly , we can compute following gradients:

$$\frac{\partial H^j}{\partial W_4^j}=\frac{\partial \sigma(W_4^jH_3+b_4^j)}{\partial W_4^j}=\sigma'(W_4^jH_3+b_4^j)H_3 \qquad \forall j\in\{1,2,\dots,l\};$$

$$\frac{\partial H^j}{\partial H_3}=\frac{\partial \sigma(W_4^jH_3+b_4^j)}{\partial H_3}=\sigma'(W_4^jH_3+b_4^j)W_4^j \qquad \forall j\in\{1,2,\dots,l_4\};$$

$$\frac{\partial H_3^j}{\partial W_3^j}=\frac{\partial \sigma(W_3^jH_2+b_3^j)}{\partial W_3^j}=\sigma'(W_3^jH_2+b_3^j)H_2 \qquad \forall j\in\{1,2,\dots,l_3\};$$

$$\frac{\partial H_3^j}{\partial H_2}=\frac{\partial \sigma(W_3^jH_2+b_3^j)}{\partial H_2}=\sigma'(W_3^jH_2+b_3^j)W_3^j \qquad \forall j\in\{1,2,\dots,l_3\};$$

$$\frac{\partial H_2^j}{\partial W_2^j}=\frac{\partial \sigma(W_2^jH_1+b_2^j)}{\partial W_2^j}=\sigma'(W_2^jH_1+b_2^j)H_1 \qquad \forall j\in\{1,2,\dots,l_2\};$$

$$\frac{\partial H_2^j}{\partial H_1}=\frac{\partial \sigma(W_2^jH_1+b_2^j)}{\partial H_1}=\sigma'(W_2^jH_1+b_2^j)W_2^j \qquad \forall j\in\{1,2,\dots,l_2\};$$

$$\frac{\partial H_1^j}{\partial W_1^j}=\frac{\partial \sigma(W_1^jx_0+b_1^j)}{\partial W_1^j}=\sigma'(W_1^jx_0+b_1^j)x_0 \qquad \forall j\in\{1,2,\dots,l_1\}.$$

The multilayer perceptron $f(x)$ can be written in a chain form:

$$X \overset{\sigma}{\to} H_1 \overset{\sigma}{\to} H_2 \overset{\sigma}{\to} H_3 \overset{\sigma}{\to} H_4 \overset{\sigma}{\to} H \overset{\sigma}{\to} f(x)$$
$$X \to W_1X \to W_2H_1 \to W_3H_2 \to W_4H_3 \to WH \to y$$
$$\mathbb{R}^p \to \mathbb{R}^{l_1} \to \mathbb{R}^{l_2} \to \mathbb{R}^{l_3} \to \mathbb{R}^{l} \to \mathbb{R}^{o}$$

while the backpropagation to compute the gradient is in the reverse order:

$$\frac{\partial y}{\partial W} \to \frac{\partial y}{\partial H} \to \frac{\partial H}{\partial W_4} \to \frac{\partial H}{\partial H_3} \to \frac{\partial H_3}{\partial W_3} \to \frac{\partial H_3}{\partial H_2} \to \frac{\partial H_2}{\partial W_2} \to \frac{\partial H_2}{\partial W_1} \to \frac{\partial H_1}{\partial W_1}.$$

In general, the gradient of any weight can be computed by *backpropagation* algorithm.
The first step is to compute the gradient of loss function with respect to the output $f(x_0) = y \in \mathbb{R}^o$, i.e.
$\frac{\partial L(x_0,d_0)}{\partial f(x_0)} = 2(f(x_0) - d_0) = 2(\sigma \circ (WH + b) - d_0)$
, of which the ith element is $2(y^i - d_0^i) = 2(\sigma(W^iH + b^i) - d_0^i)\, \forall i\{1, 2, \ldots, o\}$.
Thus

$$\frac{\partial L(x_0, d_0)}{\partial W^i} = \frac{\partial L(x_0, d_0)}{\partial y^i} \frac{\partial y^i}{\partial W^i} = 2(y^i - d_0^i)\sigma'(W^iH + b^i)H.$$

Thus we can compute all the gradients of W columns. Note that H has been computed through forwards propagation in that layer.

And $H = \sigma \circ (W_4H_3 + b_3)$, of which the ith element is $H^i = \sigma(W_4H_3 + b_4)^i = \sigma(W_4^iH_3 + b_4^i)$.

And we can compute the gradient of columns of W_4:

$$\begin{aligned}\frac{\partial L(x_0, y_0)}{\partial W_4^i} &= \sum_{j=1}^{o} \frac{\partial L(x_0, y_0)}{\partial f^j(x_0)} \frac{\partial f^j(x_0)}{\partial z} \frac{\partial z}{\partial W_4^i} = \sum_{j=1}^{o} \frac{\partial L(x_0, y_0)}{\partial y^j} \frac{\partial y^j}{\partial H^i} \frac{\partial H^i}{\partial W_4^i} \\ &= \sum_{j=1}^{o} \frac{\partial L}{\partial y^j} \frac{\partial\, y^j}{\partial (W^jH + b^j)} \frac{\partial (W^jH + b^j)}{\partial H^i} \frac{\partial (H^i)}{\partial W_4^i} \\ &= \sum_{j=1}^{l} \frac{\partial L}{\partial y^j}\, \sigma'(W^jH + b^j)\, W^{j,i}\, \sigma'(W_4^iH_3 + b_4^i)H_3,\end{aligned}$$

where $W^{j,i}$ is the ith element of jth column in matrix W.

$$\begin{aligned}\frac{\partial L(x_0, y_0)}{\partial W_3^i} &= \sum_{j=1}^{o} \frac{\partial L(x_0, y_0)}{\partial f^j(x_0)} [\frac{\partial f^j(x_0)}{\partial z}] \frac{\partial z}{\partial W_3^i} = \sum_{j=1}^{o} \frac{\partial L}{\partial y^j} [\frac{\partial y^j}{\partial H_3^i}] \frac{\partial H_3^i}{\partial W_3^i} \\ &= \sum_{j=1}^{o} \frac{\partial L}{\partial y^j} [\sum_{k=1} \frac{\partial y^j}{\partial H^k} \frac{\partial H^k}{\partial H_3^i}] \frac{\partial H_3^i}{\partial W_3^i}\end{aligned}$$

where all the partial derivatives or gradients have been computed or accessible. It is nothing except to add or multiply these values in the order when we compute the weights of hidden layer.

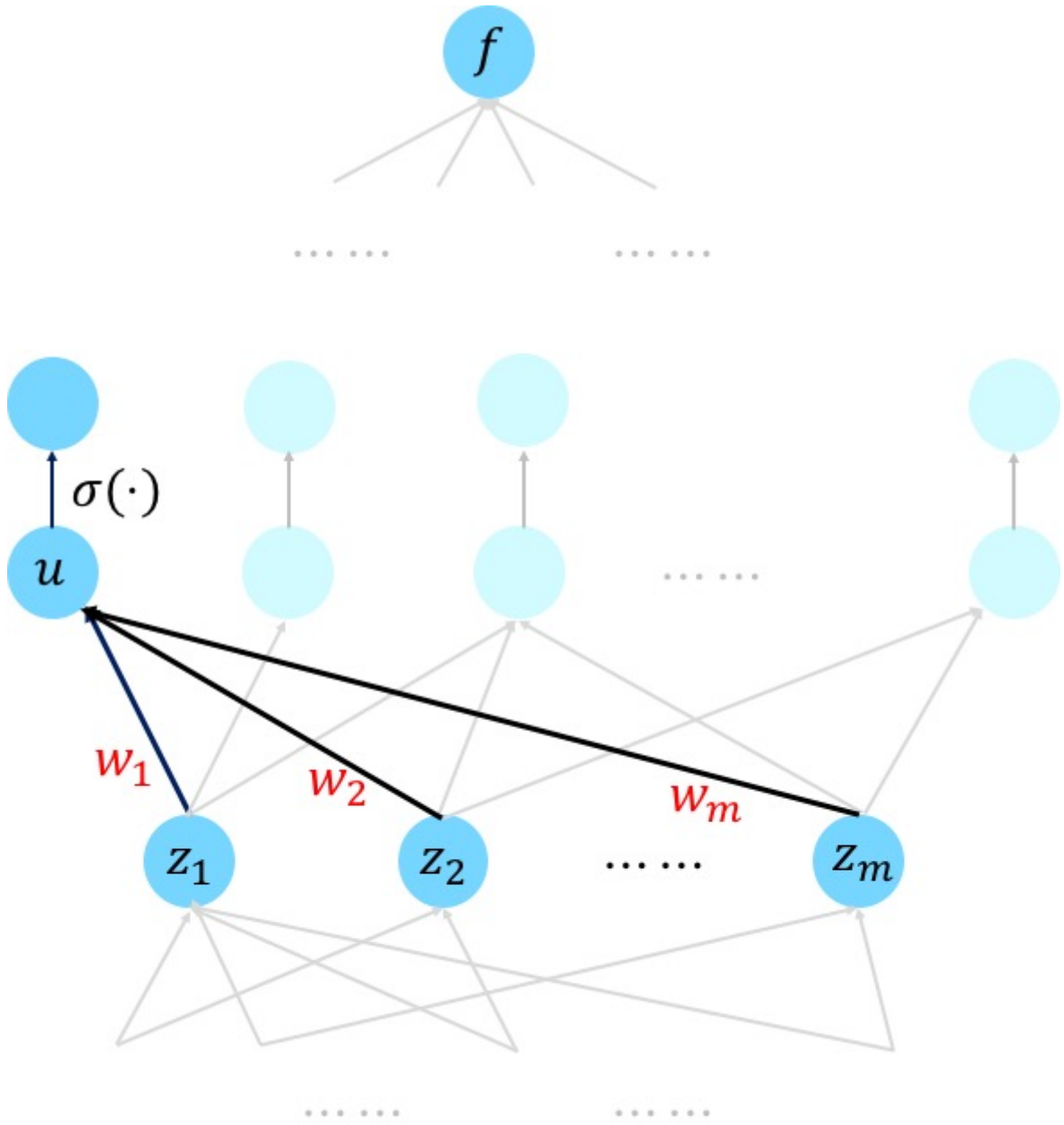
$$\frac{\partial L(x_0,y_0)}{\partial W_2^i} = \sum_{j=1}^{o} \frac{\partial L(x_0,y_0)}{\partial f^j(x_0)} [\frac{\partial f^j(x_0)}{\partial z}] \frac{\partial z}{\partial W_2^i} = \sum_{j=1}^{l} \frac{\partial L}{\partial y^j} [\frac{\partial y^j}{\partial H_2^i}] \frac{\partial H_2^i}{\partial W_2^i}$$
$$= \sum_{j=1}^{o} \frac{\partial L}{\partial y^j} \{\sum_{k=1} \frac{\partial y^j}{\partial H^k} [\sum_m \frac{\partial H^k}{\partial H_3^m} \frac{\partial H_3^m}{\partial H_2^i}]\} \frac{\partial H_2^i}{\partial W_2^i}$$

And the gradient of the first layer is computed by

$$\frac{\partial L(x_0,y_0)}{\partial W_1^i} = \sum_j \frac{\partial L(x_0,y_0)}{\partial y^j} \frac{\partial y^j}{\partial z} \frac{\partial z}{\partial W_1^i}$$
$$= \sum_j \frac{\partial L}{\partial y^j} [\sum_k \frac{\partial y^j}{\partial H^k} \sum_m \frac{\partial H^k}{\partial H_3^m} \sum_n \frac{\partial H_3^k}{\partial H_2^n} \sum_r \frac{\partial H_2^n}{\partial H_1^r}] \frac{\partial H_1^i}{\partial W_1^i}.$$

See more information on backpropagation in the following list

- Back-propagation, an introduction at offconvex.org;
- Backpropagation on Wikipedia;
- Automatic differentiation on Wikipedia;
- backpropagation on brilliant;
- An introduction to automatic differentiation at https://alexey.radul.name/ideas/2013/introduction-to-automatic-differentiation/;
- Reverse-mode automatic differentiation: a tutorial at https://rufflewind.com/2016-12-30/reverse-mode-automatic-differentiation.
- Who invented backpropagation ?;
- Autodiff Workshop
- 如何直观地解释 backpropagation 算法？ - 景略集智的回答 - 知乎
- The chapter 2 *How the backpropagation algorithm works* at the online book http://neuralnetworksanddeeplearning.com/chap2.html
- For more information on automatic differentiation see the book *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation, Second Edition* by Andreas Griewank and Andrea Walther_ at https://epubs.siam.org/doi/book/10.1137/1.9780898717761.



Training Methods

The training is to find the optimal parameters of the model based on the **training data set**. The training methods are usually based on the gradient of cost function as well as back-propagation algorithm in deep learning.
See **Stochastic Gradient Descent** in **Numerical Optimization** for details.
In this section, we will talk other optimization tricks such as **Normalization**.

Concepts	Interpretation
Overfitting and *Underfitting*	See Overfitting or Overfitting and Underfitting With Machine Learning Algorithms
Memorization and *Generalization*	Memorizing, given facts, is an obvious task in learning. This can be done by storing the input samples explicitly, or by identifying the concept behind the input data, and memorizing their general rules. The ability to identify the rules, to generalize, allows the system to make predictions on unknown data. Despite the strictly logical invalidity of this approach, the process of reasoning from specific samples to the general case can be observed in human learning. From https://www.teco.edu/~albrecht/neuro/html/node9.html.

Concepts	Interpretation
Normalization and *Standardization*	*Normalization* is to scale the data into the interval [0,1] while *Standardization* is to rescale the datum with zero mean 0 and unit variance 1. See Standardization vs. normalization.

Initialization

- Gradient Descent with Random Initialization: Fast Global Convergence for Nonconvex Phase Retrieva
- Gradient descent and variants
- off convex path
- graphcore.ai
- 可视化超参数作用机制：二、权重初始化
- 第 6 章 网络优化与正则化

Normalization

- Batch normalization 和 Instance normalization 的对比？ - Naiyan Wang的回答 - 知乎
- Weight Normalization 相比 batch Normalization 有什么优点呢？
- 深度学习中的Normalization模型
- Group Normalization
- https://blog.paperspace.com/busting-the-myths-about-batch-normalization/
- The original paper *Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift* at https://arxiv.org/pdf/1502.03167.pdf.

See **Improve the way neural networks learn** at http://neuralnetworksanddeeplearning.com/chap3.html.
See more on nonconvex optimization at http://sunju.org/research/nonconvex/.

Regularization

In mathematics, statistics, and computer science, particularly in the fields of machine learning and inverse problems, regularization is a process of introducing additional information in order to solve an ill-posed problem or to prevent overfitting. In general, regularization is a technique that applies to objective functions in ill-posed optimization problems. It changes the objective function or more generally the optimization procedure. However, it is not crystal clear that what is the relationship between the optimization techniques and generalization ability.
See the following links for more information on optimization and generalization.

- https://www.inference.vc/sharp-vs-flat-minima-are-still-a-mystery-to-me/
- https://arxiv.org/abs/1703.04933
- https://arxiv.org/abs/1810.05369
- https://blog.csdn.net/xzy_thu/article/details/80732220
- http://www.offconvex.org/2017/12/08/generalization1/
- http://www.offconvex.org/2018/02/17/generalization2/
- http://www.offconvex.org/2017/03/30/GANs2/

Parameter norm penalty

The ℓ_2 norm penalty is to add the squares of ℓ_2 norm of parameters to the objective function $J(\theta)$ to reduce the parameters(or weights) as shown in ridge regression with regular term coefficient λ, i.e.
$J(\theta) + \lambda\|\theta\|_2^2$.
Suppose $E(\theta) = J(\theta) + \lambda\|\theta\|_2^2$, the gradient descent take approximate (maybe inappropriate) form

$$\theta = \theta - \eta\frac{\partial E(\theta)}{\partial \theta} = \theta - \eta\frac{\partial J(\theta)}{\partial \theta} - 2\eta\lambda\theta$$

thus

$$\frac{\partial J(\theta)}{\partial \theta} = -2\lambda\theta \implies J(\theta) = e^{-2\lambda\theta}.$$

If we want to find the minima of $E(\theta)$, θ will decay to 0.
It extends to the following iterative formula:

$$\theta^{t+1} = (1-\lambda)\theta^t - \alpha_t\frac{\partial J(\theta^t)}{\partial \theta},$$

where λ determines how you trade off the original cost $J(\theta)$ with the large weights penalization.
The new term λ coming from the regularization causes the weight to decay in proportion to its size.

- https://stats.stackexchange.com/questions/70101/neural-networks-weight-change-momentum-and-weight-decay
- https://metacademy.org/graphs/concepts/weight_decay_neural_networks

The ℓ_1 norm penalty is also used in deep learning as in **LASSO**. It is to solve the following optimization problem:

$$\min_\theta J(\theta) + \lambda\|\theta\|_1,$$

where λ is a hyperparameter. Sparsity brings to the model as shown as in **LASSO**.

Early stop

Its essential is to make a balance in memorization and generalization.
Early stopping is to stop the procedure before finding the minima of cost in training data. It is one direct application of **cross validation**.

- https://www.wikiwand.com/en/Early_stopping
- https://www.wikiwand.com/en/Cross-validation_(statistics)

Dropout

It is to cripple the connections stochastically, which is often used in visual tasks. See the original paper Dropout: A Simple Way to Prevent Neural Networks from Overfitting.

- https://www.zhihu.com/question/24529483
- https://www.jiqizhixin.com/articles/2018-11-10-7

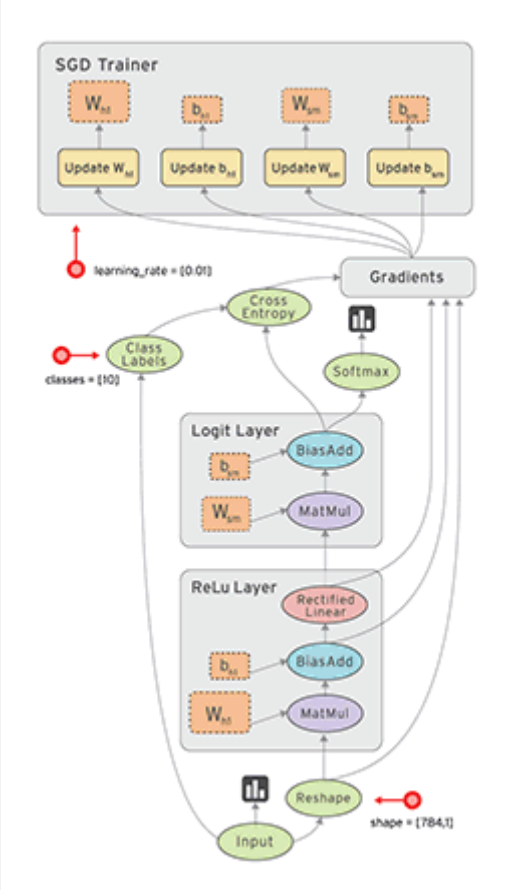
- https://www.jiqizhixin.com/articles/112501
- https://www.jiqizhixin.com/articles/2018-08-27-12
- https://yq.aliyun.com/articles/68901
- https://www.wikiwand.com/en/Regularization_(mathematics)
- CNN tricks
- https://www.jeremyjordan.me/deep-neural-networks-preventing-overfitting/
- https://www.doc.ic.ac.uk/~nd/surprise_96/journal/vol4/cs11/report.html#An engineering approach

Data Augmentation

Data augmentation is to augment the training datum specially in visual recognition.
Overfitting in supervised learning is data-dependent. In other words, the model may generalize better if the data set is more diverse.
It is to collect more datum in the statistical perspective.

- The Effectiveness of Data Augmentation in Image Classification using Deep Learning
- http://www.cnblogs.com/love6tao/p/5841648.html

Feed forward and Propagate backwards



Convolutional Neural Network

Convolutional neural network is originally aimed to solve visual tasks. In so-called Three Giants' Survey, the history of ConvNet and deep learning is curated.
Deep, Deep Trouble--Deep Learning's Impact on Image Processing, Mathematics, and Humanity tells us the mathematicians' impression on ConvNet in image processing.

Convolutional layer

Convolutional layer consists of padding, convolution, pooling.

Convolution Operation

Convolution operation is the basic element of convolution neural network.
We only talk the convolution operation in 2-dimensional space.

The image is represented as matrix or tensor in computer:

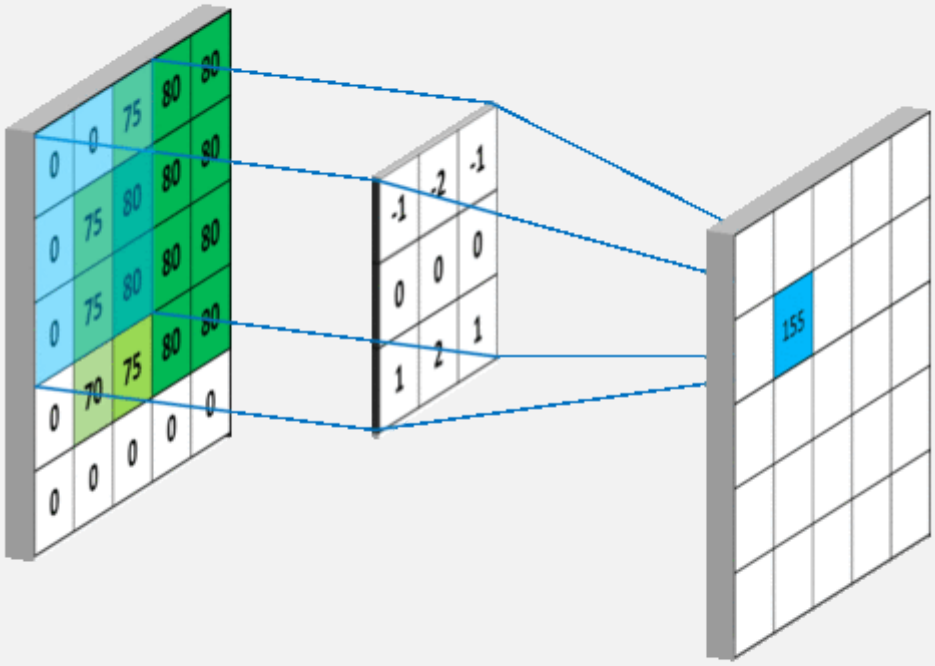
$$M = \begin{pmatrix} x_{11} & x_{12} & x_{13} & \cdots & x_{1n} \\ x_{21} & x_{22} & x_{23} & \cdots & x_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & x_{m3} & \cdots & x_{mn} \end{pmatrix}$$

where each entry $x_{ij} \in \{1, 2 \cdots, 256\}, i \in \{1, 2, \cdots, m\}, j \in \{1, 2, \cdots, n\}$.

- Transformation as matrix multiplication
  - The M under the transformation A is their product -MA- of which each column is the linear combination of columns of the matrix M. The spatial information or the relationship of the neighbors is lost.
- Spatial information extraction
  - Kernel in image processing takes the relationship of the neighboring entries into consideration. It transforms the neighboring entries into one real value. In 2-dimenional space, convolution corresponds to doubly block circulant matrix if the matrix is flatten. It is local pattern that we can learn.

The illustration of convolution operator

The illustration of convolution operator



(http://cs231n.github.io/assets/conv-demo/index.html)

As similar as the inner product of vector, the convolution operators can compute the similarity between the submatrix of images and the kernels (also called filters).

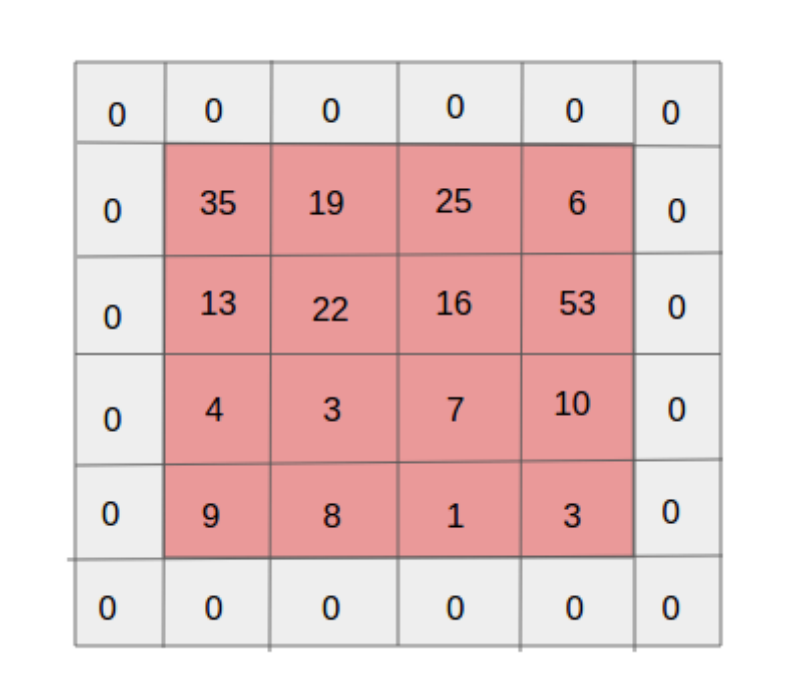
The convolution operators play the role as *parameter sharing* and *local connection*.
For more information on CNN, click the following links.

- CNN(卷积神经网络)是什么？有入门简介或文章吗？ - 机器之心的回答 - 知乎
- 能否对卷积神经网络工作原理做一个直观的解释？ - YJango的回答 - 知乎
- One by one convolution
- conv arithmetic
- Convolution deep learning

Padding

The standard convolution operation omit the information of the boundaries. Padding is to add some 0s outside the boundaries of the images.

Zero padding



https://zhuanlan.zhihu.com/p/36278093

Activation

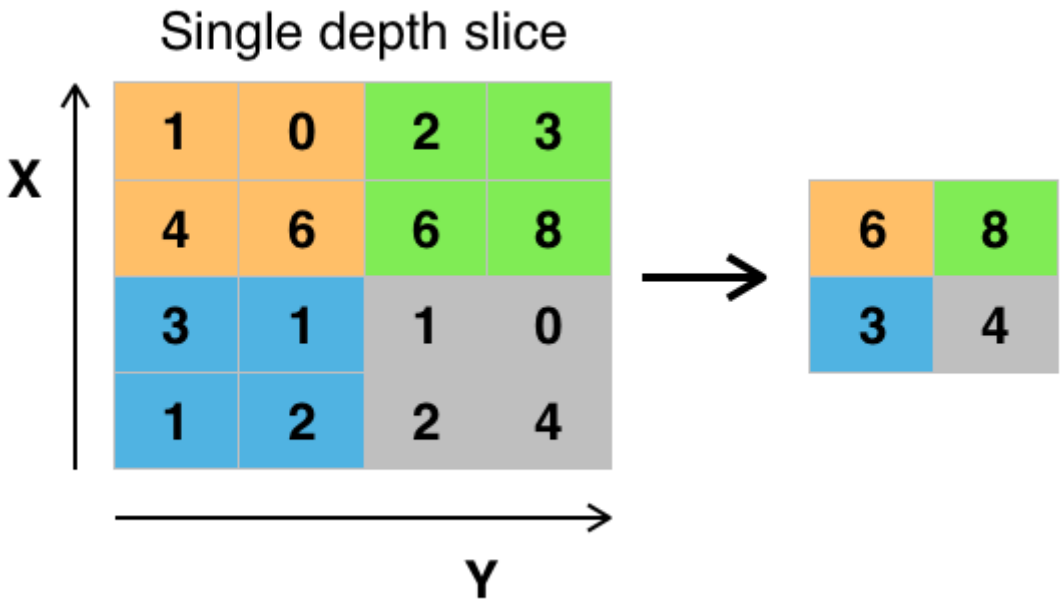
As in feedforward neural networks, an additional non-linear operation called **ReLU** has been used after every Convolution operation.

Pooling as Subsampling

Pooling as a special convolution is to make the model/network more robust.

Max Pooling

It is to use the maximum to represent the local information.



See https://www.superdatascience.com/convolutional-neural-networks-cnn-step-2-max-pooling/.

Sum Pooling

It is to use the sum to represent the local information.

Average Pooling

It is to use the average to represent the local information.

Random Pooling

It is to draw a sample from the receptive field to represent the local information.
https://www.cnblogs.com/tornadomeet/p/3432093.html

CNN

Convolution neural network (conv-net or CNN for short) is the assembly of convolution, padding, pooling and full connection , such as

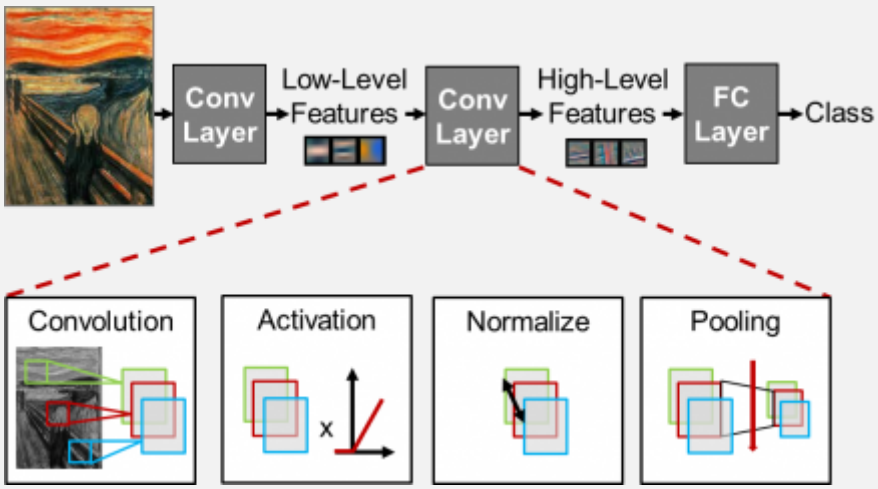
$$M \overset{Conv1}{\rightarrow} H_1 \overset{Conv2}{\rightarrow} H_2 \cdots \overset{Convl}{\rightarrow} H \overset{\sigma}{\rightarrow} y.$$

In the ith layer of convolutional neural network, it can be expressed as

$$\tilde{H}_i = C_i \otimes (P \oplus H_{i-1})$$
$$H_i = Pooling \cdot (\sigma \circ \tilde{H}_i)$$

where $\otimes, \oplus, \cdot$ represent convolution operation, padding and pooling, respectively.

Diagram of Convolutional neural network



- CS231n Convolutional Neural Network for Visual Recognition
- The *Wikipeida* page https://www.wikiwand.com/en/Convolutional_neural_network
- Awesome deep vision
- 解析深度学习——卷积神经网络原理与视觉实践
- Interpretable Convolutional Neural Networks
- An Intuitive Explanation of Convolutional Neural Networks
- Convolutional Neural Network Visualizations
- ConvNetJS
- https://www.vicarious.com/2017/10/20/toward-learning-a-compositional-visual-representation/

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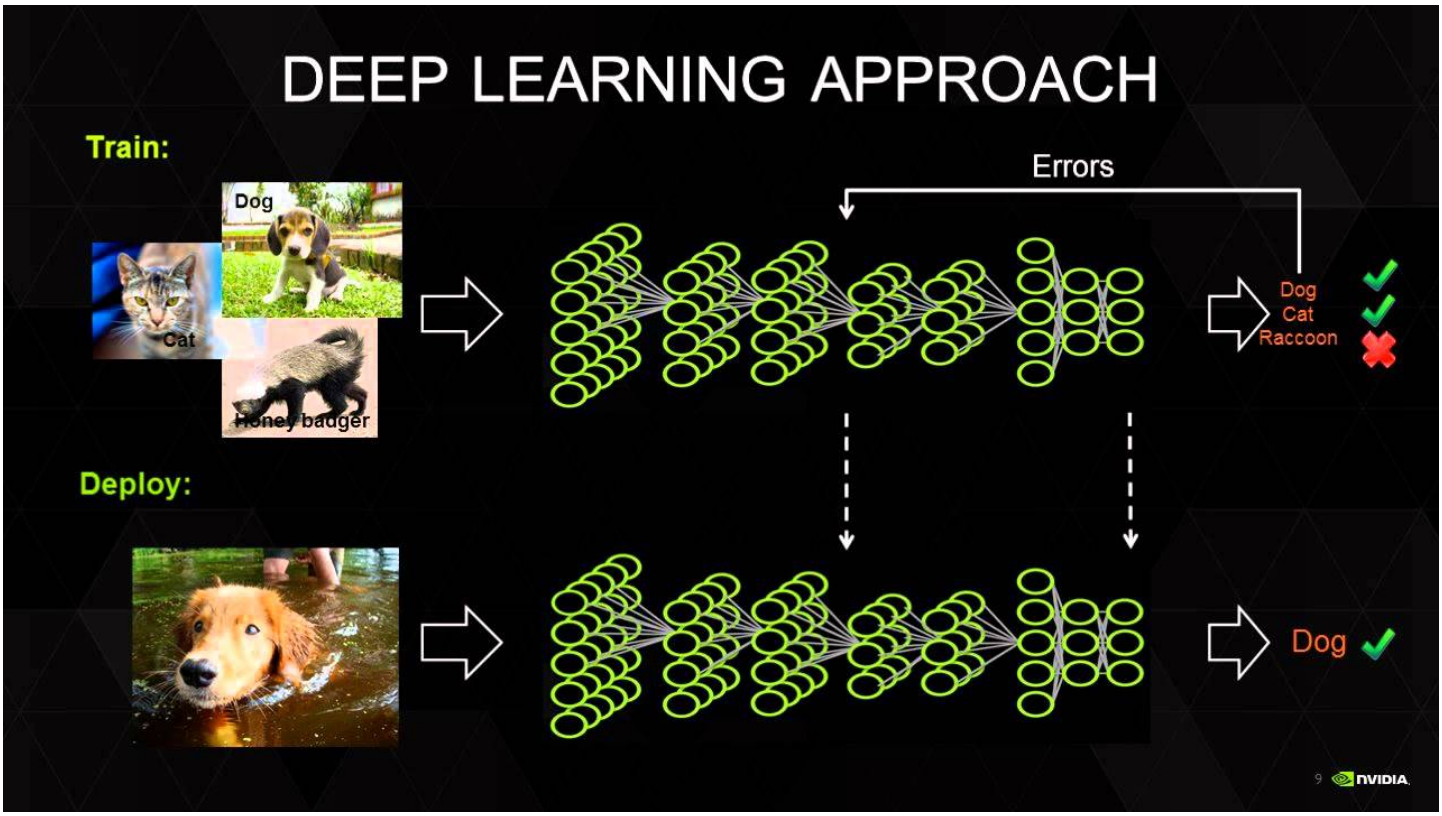
https://zhuanlan.zhihu.com/p/28749411



Visualization of CNN

- Deep Visualization
- Interpretable Representation Learning for Visual Intelligence
- https://www.zybuluo.com/lutingting/note/459569
- https://cs.nyu.edu/~fergus/papers/zeilerECCV2014.pdf
- https://zhuanlan.zhihu.com/p/24833574
- https://zhuanlan.zhihu.com/p/30403766
- https://blog.keras.io/how-convolutional-neural-networks-see-the-world.html
- http://people.csail.mit.edu/bzhou/ppt/presentation_ICML_workshop.pdf
- https://www.graphcore.ai/posts/what-does-machine-learning-look-like

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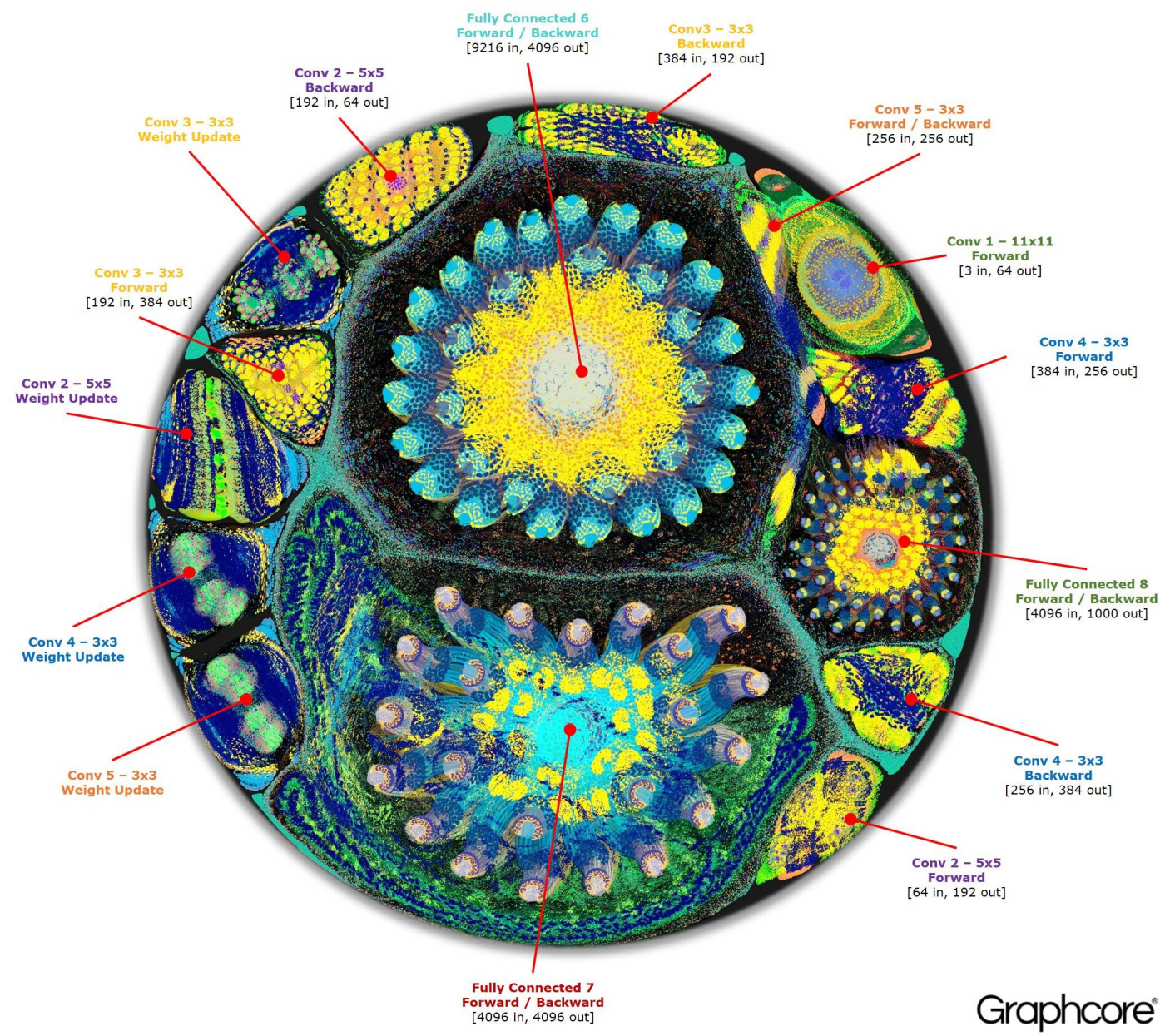


Recurrent Neural Networks and Long Short-Time Memory

Recurrent neural networks are aimed to handle sequence data such as time series.
Recall the recursive form of feedforward neural networks:

$$\begin{aligned}\mathbf{z}_i &= W_i H_{i-1} + b_i,\\ H_i &= \sigma \circ (\mathbf{z}_i),\end{aligned}$$

where $W_i \in \mathbb{R}^{l_i \times l_{i-1}}$, $H_i(\text{as well as } b_i) \in \mathbb{R}^{l_i} \forall i \in \{1, 2, \ldots, D\}$ and σ is activation function.
In convention, H_0 is defined as input $X \in \mathbb{R}^p$.
In short, the formula in the ith layer of feedforward neural network is given by

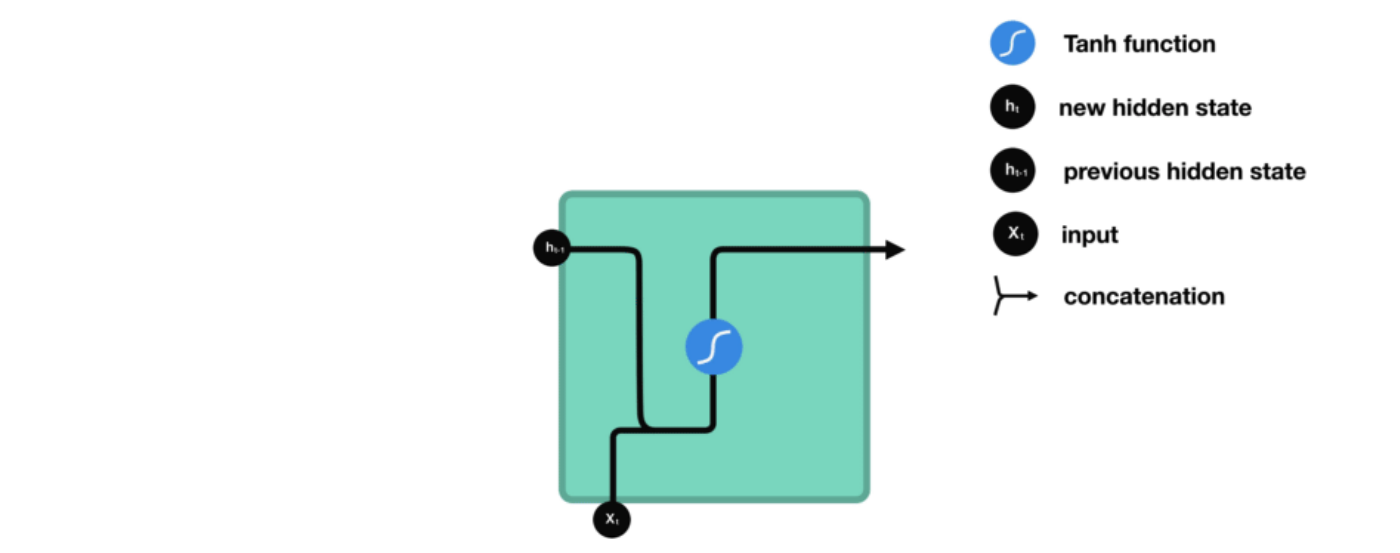
$$H_i = \sigma \circ (W_i H_{i-1} + b_i).$$

It may suit the **identically independently distributed** data set.
However, the sequence data is not **identically independently distributed** in most cases. For example, the outcome of current decision determines the next decision.
In mathematics it can be expressed as

$$H_t = \sigma \circ (X_t, H_{t-1}) = \sigma \circ (WH_{t-1} + UX_t + b),$$

where $X_t \in \mathbb{R}^p$ is the output $\forall t \in \{1, 2 \ldots, \tau\}$.

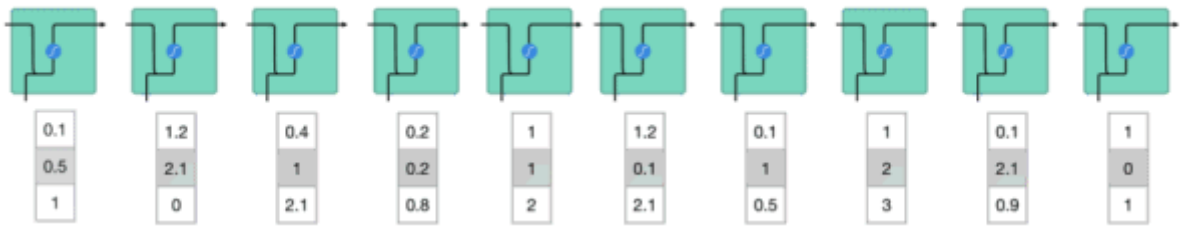
RNN Cell



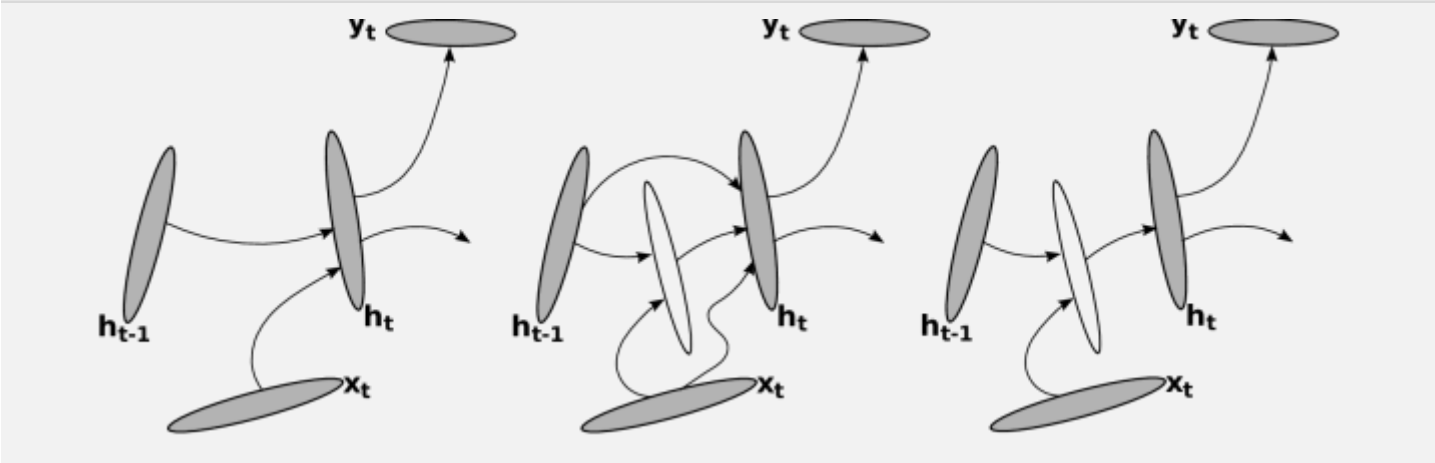
For each step from $t = 1$ to $t = \tau$, the complete update equations of RNN:

$$H_t = \sigma \circ (WH_{t-1} + UX_t + b)$$
$$O_t = \mathrm{softmax}(VH_t + c)$$

where the parameters are the bias vectors b and c along with the weight matrices
U, V and W, respectively for input-to-hidden, hidden-to-output and hidden-to-hidden connections.



Types of RNN



(https://www.altoros.com/blog/wp-content/uploads/2017/01/Deep-Learning-Using-TensorFlow-recurrent-neural-networks.png)

Bi-directional RNN

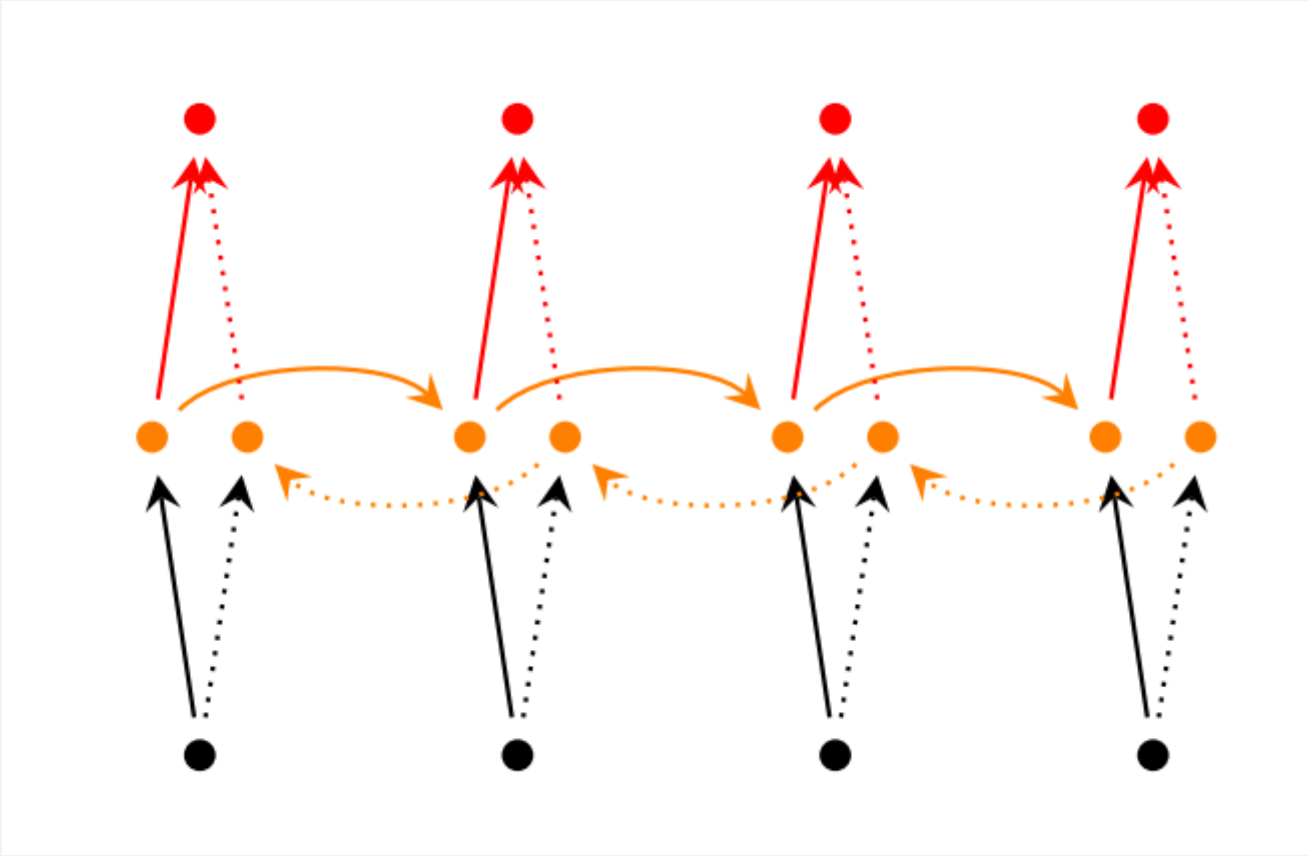
For each step from $t = 1$ to $t = \tau$, the complete update equations of RNN:

$$\begin{aligned}
\vec{H}_t &= \sigma \circ (W_1 \vec{H}_{t-1} + U_1 X_t + b_1) \\
\overleftarrow{H}_t &= \sigma \circ (W_2 \overleftarrow{H}_{t+1} + U_2 X_t + b_2) \\
O_t &= \mathrm{softmax}(V H_t + c)
\end{aligned}$$

where $H_t = [\vec{H}_t; \overleftarrow{H}_t]$.

Bi-directional RNN

Bi-directional RNN



The bold line(__) is computed earlier than the dotted line(...).

deepai.org

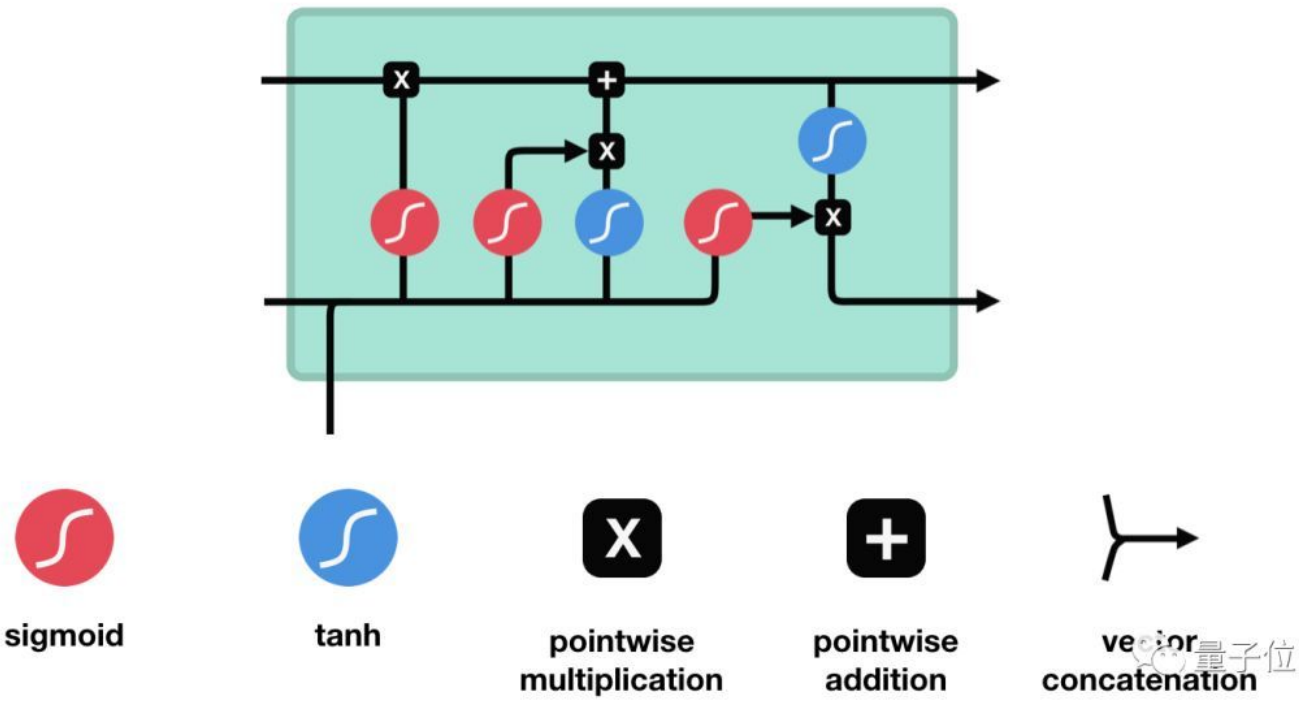
LSTM

There are several architectures of LSTM units. A common architecture is composed of a *memory cell, an input gate, an output gate and a forget gate*.
It is the first time to solve the **gradient vanishing problem** and
long-term dependencies in deep learning.

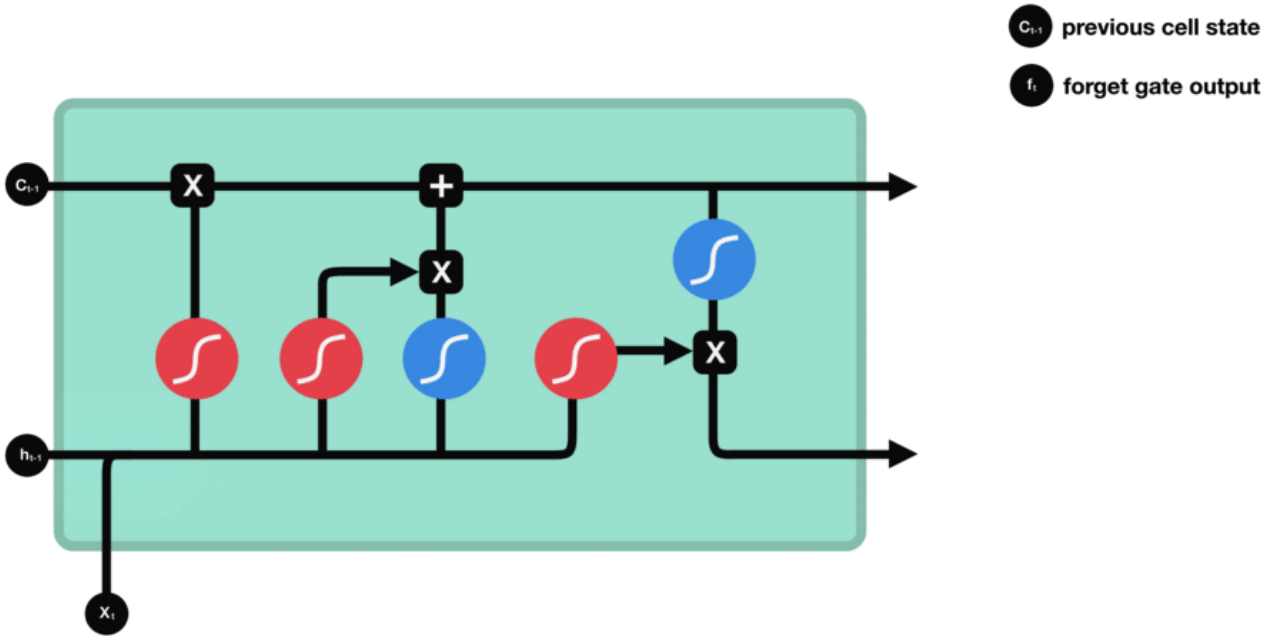
LSTM block

See *LSTM block* at(https://devblogs.nvidia.com/wp-content/uploads/2016/03/LSTM.png)

LSTM block

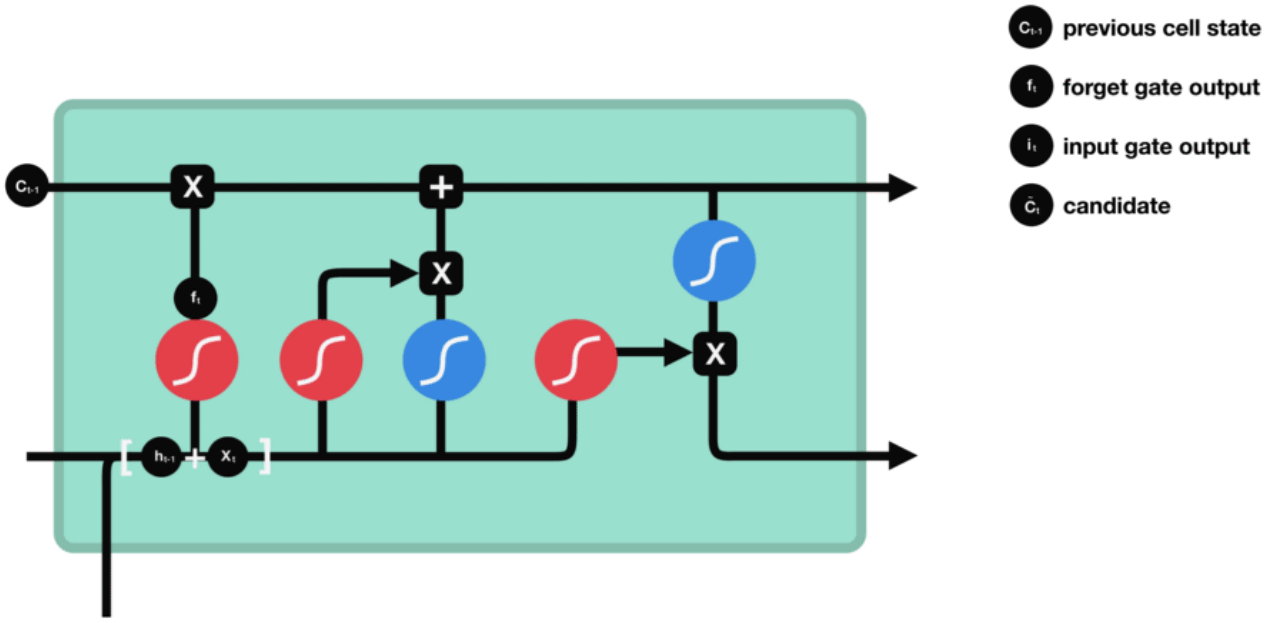


- forget gate
  $f_t = \sigma(W_f[h_{t-1}, x_t] + b_f)$

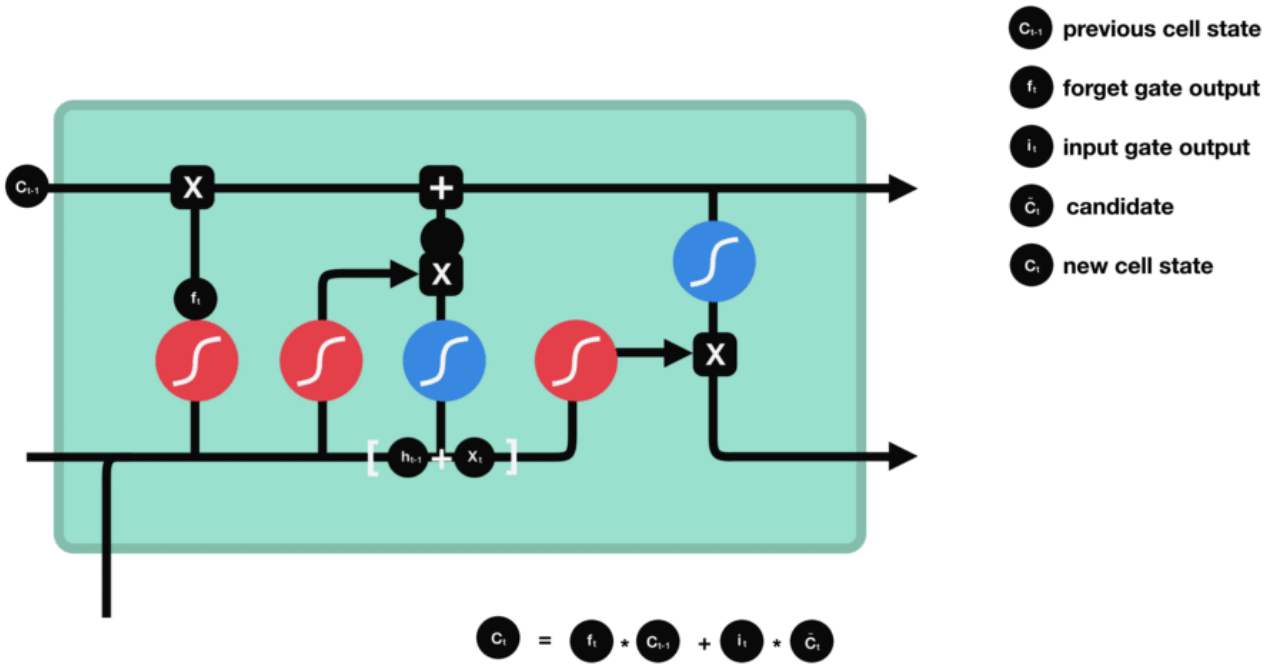


- input gate
  $i_t = \sigma(W_i[h_{t-1}, x_t] + b_i),$

$\tilde{C}_t = tanh(W_C[h_{t-1}, x_t] + b_C)$

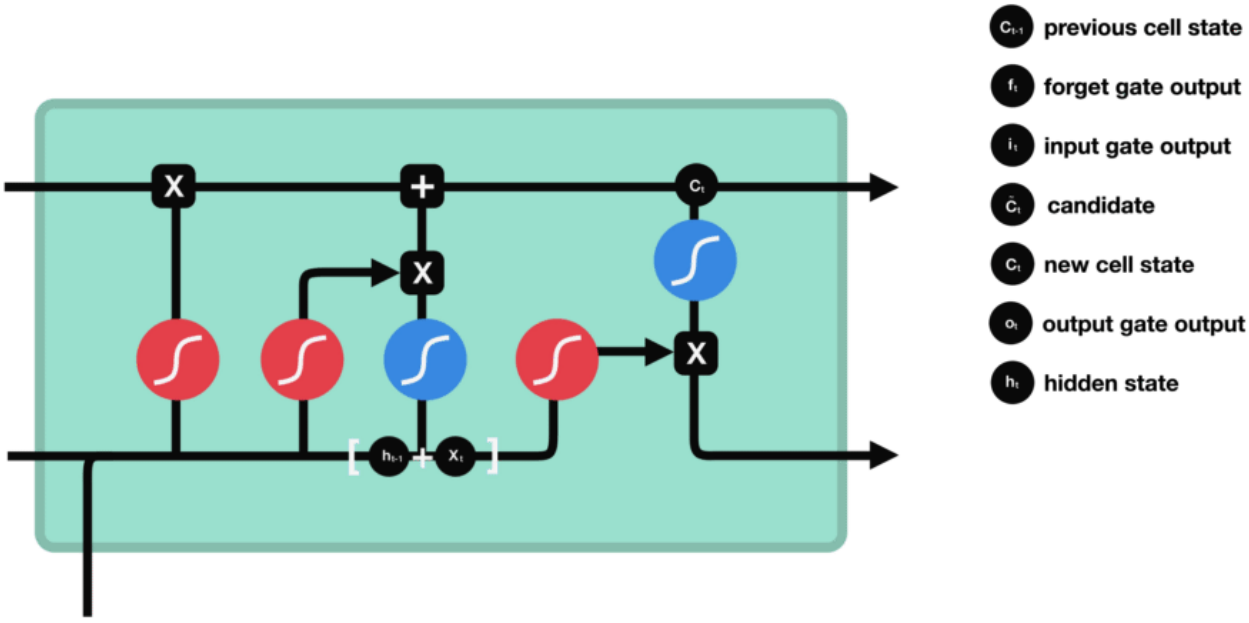


- memory cell
  $c_t = f_t \times c_{t-1} + i_t \times \tilde{C}_t$



- output gate
  $O_t = \sigma(W_O[h_{t-1}, x_t] + b_O)$ and

$$h_t = O_t \times tanh(c_t)$$



Inventor of LSTM

more on (http://people.idsia.ch/~juergen/)

- LSTM in Wikipeida
- Understanding LSTM Networks and its Chinese version https://www.jianshu.com/p/9dc9f41f0b29.
- LTSMvis
- Jürgen Schmidhuber's page on Recurrent Neural Networks
- https://www.analyticsvidhya.com/blog/2017/12/fundamentals-of-deep-learning-introduction-to-lstm/

Deep RNN

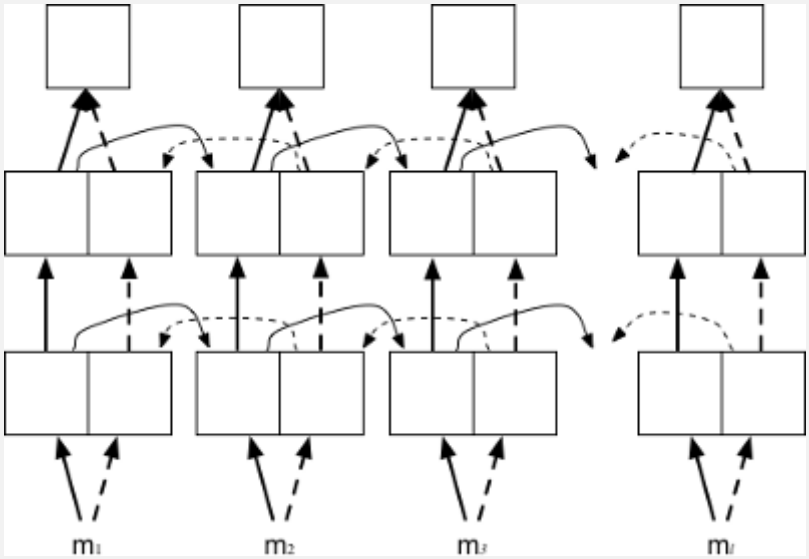
Deep RNN is composed of *RNN cell* as MLP is composed of perceptrons.
For each step from $t = 1$ to $t = \tau$, the complete update equations of deep d-RNN at the ith layer:

$$H_t^i = \sigma \circ (W_i H_{t-1} + U_i X_t + b)$$
$$O_t = \text{softmax}(V H_d + c)$$

where the parameters are the bias vectors b and c along with the weight matrices
U_i, V and W_i, respectively for input-to-hidden, hidden-to-output and hidden-to-hidden connections for $i \in \{1, 2, \cdots, d\}$.

Other RNN cells also can compose deep RNN via this stacking way such as deep Bi-RNN networks.

Deep Bi-RNN



- http://blog.songru.org/posts/notebook/Opinion_Mining_with_Deep_Recurrent_Neural_Networks_NOTE/
- http://opennmt.net/OpenNMT/training/models/
- https://machinelearningmastery.com/stacked-long-short-term-memory-networks/

- https://machinelearningmastery.com/recurrent-neural-network-algorithms-for-deep-learning/
- http://www.wildml.com/2015/09/recurrent-neural-networks-tutorial-part-1-introduction-to-rnns/
- http://www.wildml.com/2015/09/recurrent-neural-networks-tutorial-part-2-implementing-a-language-model-rnn-with-python-numpy-and-theano/
- https://zhuanlan.zhihu.com/p/27485750
- RNN in Wikipeida
- Awesome RNN
- RNN in metacademy
- https://zhuanlan.zhihu.com/p/49834993
- RNNs in Tensorflow, a Practical Guide and Undocumented Features

- The Unreasonable Effectiveness of Recurrent Neural Networks
- https://kvitajakub.github.io/2016/04/14/rnn-diagrams/
- http://www.zmonster.me/notes/visualization-analysis-for-rnn.html
- http://imgtec.eetrend.com/d6-imgtec/blog/2018-10/18051.html
- https://arxiv.org/pdf/1801.01078.pdf
- http://www.sohu.com/a/259957763_610300
- https://skymind.ai/wiki/lstm
- 循环神经网络(RNN, Recurrent Neural Networks)介绍

Attention Mechanism

An attention model is a method that takes n arguments $y_1, \dots, y_n$ and a context c. It return a vector z which is supposed to be the **summary** of the $y_i \in \mathbb{R}^d$, focusing on information linked to the context c. More formally, it returns a weighted arithmetic mean of the y_i, and the weights are chosen according the relevance of each y_i given the context c.
In mathematics, it can be expressed as:

$$\alpha_i = softmax(s(y_i, c))$$
$$z = \sum_{i=1}^{n} \alpha_i y_i$$

where $s(\cdot, \cdot)$ is the attention scoring function.
The attention scoring function $s(y_i, c)$ is diverse, such as:

- the additive model $s(y_i, c) = v^T tanh \circ (Wy_i + Uc)$, where $v \in \mathbb{R}^d$, $W \in \mathbb{R}^{d \times d}$, $U \in \mathbb{R}^d$ are parameters to learn;
- the inner product model $s(y_i, c) = \langle y_i, c \rangle$, i.e. the inner product of y_i, c;
- the scaled inner product model $s(y_i, c) = \frac{\langle y_i, c \rangle}{d}$,where d is the dimension of input y_i;
- the bilinear model $s(y_i, c) = y_i^T W c$, where $W \in \mathbb{R}^{d \times d}$ is parameter matrix to learn.

It is always as one component of some complex network as normalization.

- 第 8 章 注意力机制与外部记忆
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- https://distill.pub/2016/augmented-rnns/
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- Attention and Memory in Deep Learning and NLP
- http://www.deeplearningpatterns.com/doku.php?id=attention
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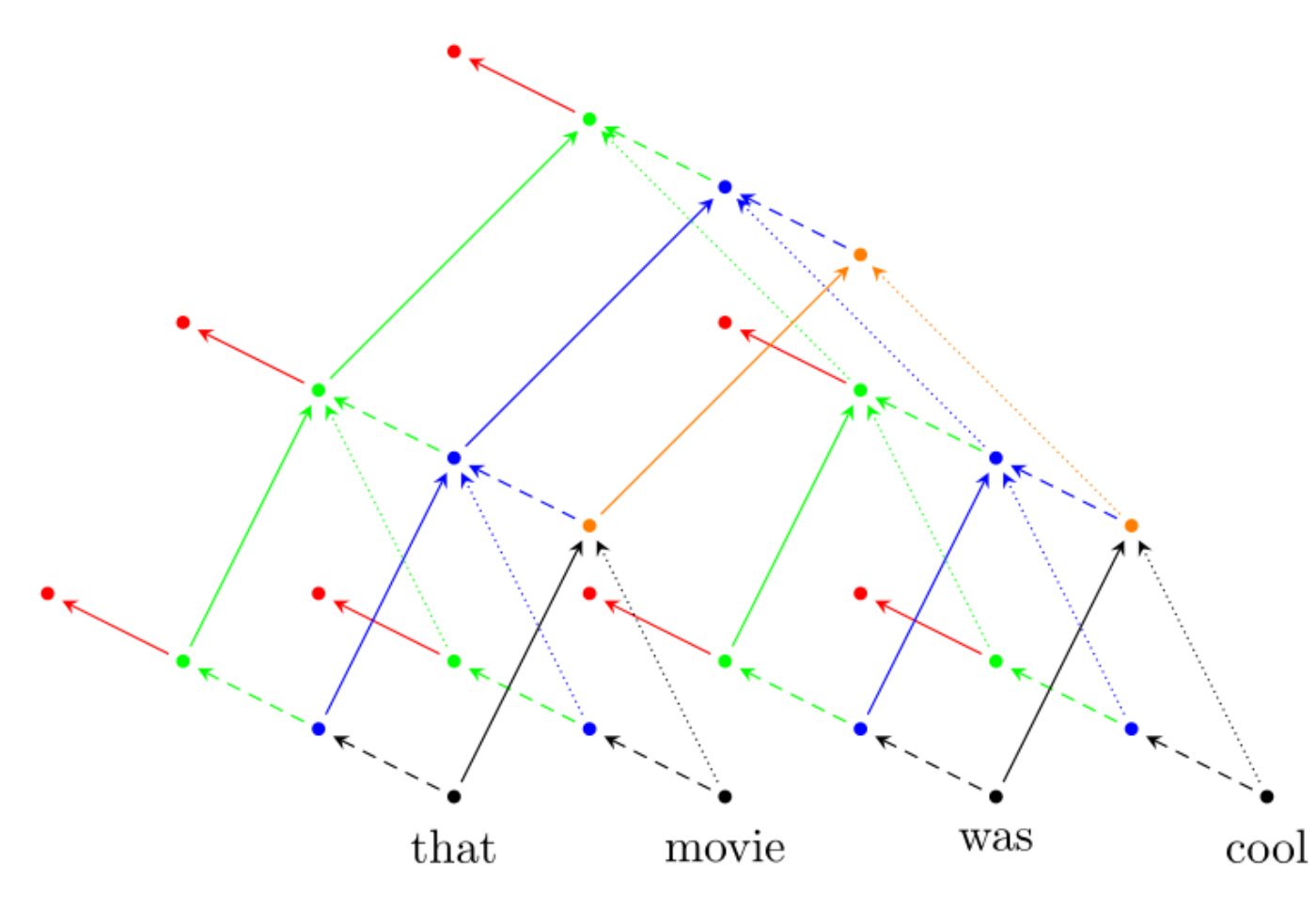
Recursive Neural Network

- https://www.wikiwand.com/en/Recursive_neural_network

- https://cs224d.stanford.edu/lectures/CS224d-Lecture10.pdf

Diagram of Recursive Neural Network



Graph Convolution Network

Graph can be represented as `adjacency matrix` as shown in *Graph Algorithm*. However, the adjacency matrix only describe the connections between the nodes. The feature of the nodes does not appear. The node itself really matters. A naive approach is to concatenate the `feature matrix` $X \in \mathbb{R}^{N\times E}$ and `adjacency matrix` $A \in \mathbb{R}^{N\times N}$, i.e. $X_{in} = [X, A] \in \mathbb{R}^{N\times(N+E)}$. And what is the output?

How can deep learning apply to them?

> *For these models, the goal is then to learn a function of signals/features on a graph* $G = (V, E)$ *which takes as input:*

- *A feature description* x_i *for every node* i*; summarized in a* $N \times D$ *feature matrix* X *(*N*: number of nodes,* D*: number of input features)*
- *A representative description of the graph structure in matrix form; typically in the form of an adjacency matrix* A *(or some function thereof)*

> *and produces a node-level output Z (an $N \times F$ feature matrix, where F is the number of output features per node). Graph-level outputs can be modeled by introducing some form of pooling operation (see, e.g. Duvenaud et al., NIPS 2015).*

Every neural network layer can then be written as a non-linear function

$$H_{i+1} = \sigma \circ (H_i, A)$$

with $H_0 = X_{in}$ and $H_d = Z$ (or Z for graph-level outputs), d being the number of layers. The specific models then differ only in how σ is chosen and parameterized.

For example, we can consider a simple form of a layer-wise propagation rule

$$H_{i+1} = \sigma \circ (H_i, A) = \sigma \circ (AH_iW_i)$$

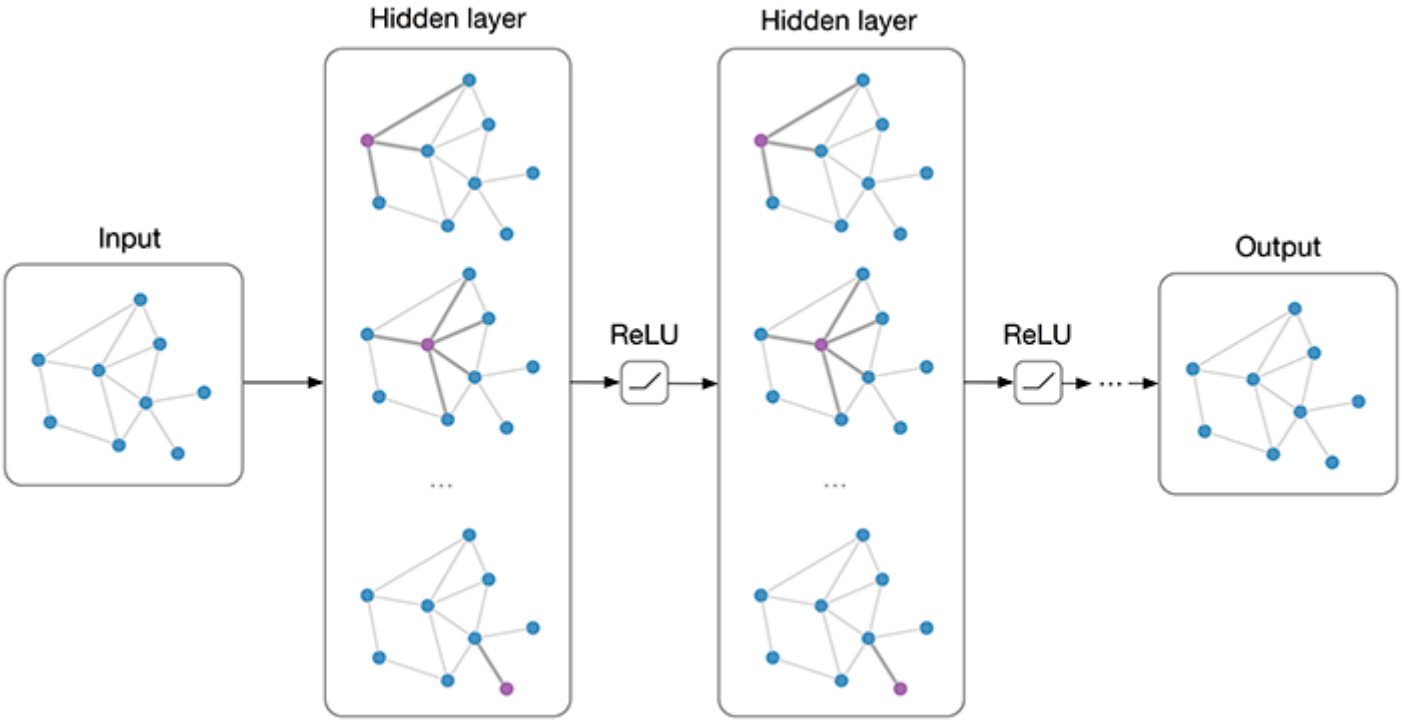
where W_i is a weight matrix for the i-th neural network layer and $\sigma(\cdot)$ is is a non-linear activation function such as *ReLU*.

- But first, let us address two limitations of this simple model: multiplication with A means that, for every node, we sum up all the feature vectors of all neighboring nodes but not the node itself (unless there are self-loops in the graph). We can "fix" this by enforcing self-loops in the graph: we simply add the identity matrix I to A.
- The second major limitation is that A is typically not normalized and therefore the multiplication with A will completely change the scale of the feature vectors (we can understand that by looking at the eigenvalues of A).Normalizing A such that all rows sum to one, i.e. $D^{-1}A$, where D is the diagonal node degree matrix, gets rid of this problem.

In fact, the propagation rule introduced in Kipf & Welling (ICLR 2017) is given by:

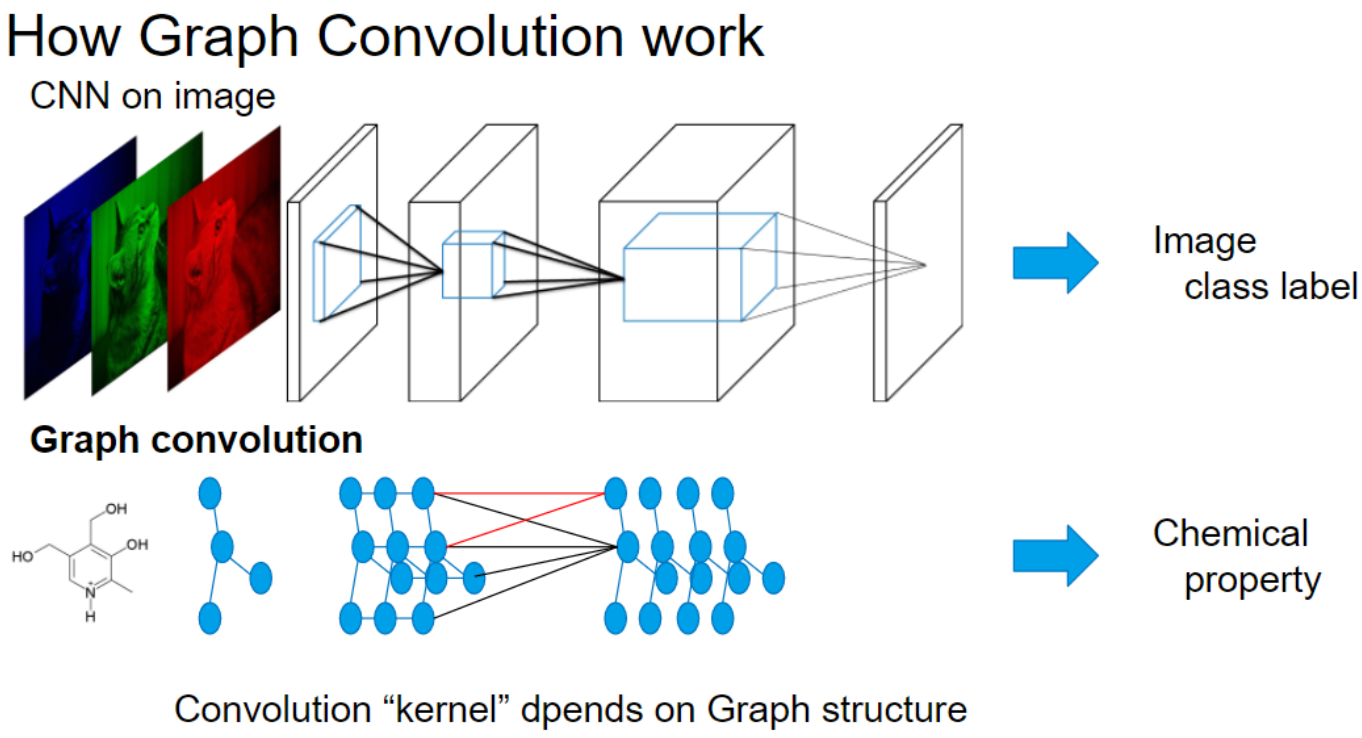
$$H_{i+1} = \sigma \circ (H_i, A) = \sigma \circ (\hat{D}^{-\frac{1}{2}}\hat{A}\hat{D}^{-\frac{1}{2}}H_iW_i),$$

with $\hat{A} = A + I$, where I is the identity matrix and $\hat{D}$ is the diagonal node degree matrix of $\hat{A}$.



GCN

See more details at Multi-layer Graph Convolutional Network (GCN) with first-order filters.



CNN VS. GCNN

- http://deeploria.gforge.inria.fr/thomasTalk.pdf
- https://arxiv.org/abs/1812.04202
- https://skymind.ai/wiki/graph-analysis
- Graph-based Neural Networks
- Geometric Deep Learning

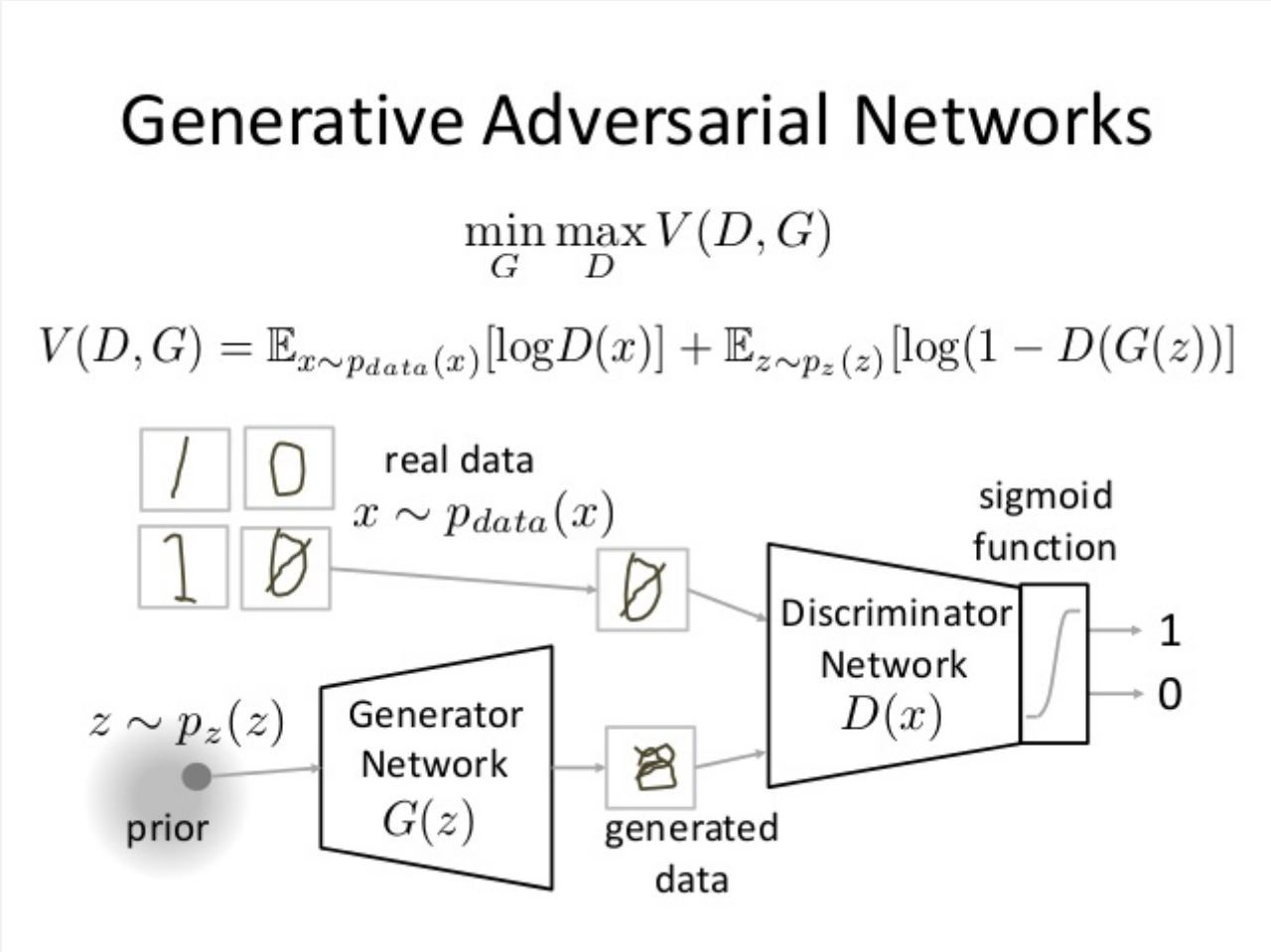
- Deep Chem
- GRAM: Graph-based Attention Model for Healthcare Representation Learning
- https://zhuanlan.zhihu.com/p/49258190
- https://www.experoinc.com/post/node-classification-by-graph-convolutional-network
- http://sungsoo.github.io/2018/02/01/geometric-deep-learning.html
- https://sites.google.com/site/deepgeometry/slides-1
- https://rusty1s.github.io/pytorch_geometric/build/html/notes/introduction.html
- .mp4 illustration
- Deep Graph Library (DGL)

Graph convolution network is potential to *reasoning* as the blend of probabilistic graph model and *deep learning*.

Generative Adversarial Network

It origins from http://papers.nips.cc/paper/5423-generative-adversarial-nets.pdf.

- https://skymind.ai/wiki/generative-adversarial-network-gan
- 千奇百怪的GAN变体，都在这里了（持续更新嘤） - 量子学园的文章 - 知乎
- 生成模型中的左右互搏术：生成对抗网络GAN——深度学习第二十章（四） - 川陀学者的文章 - 知乎 https://zhuanlan.zhihu.com/p/37846221)
- Really awesome GANs
- GAN zoo
- https://gandissect.csail.mit.edu/
- https://poloclub.github.io/ganlab/
- https://github.com/nndl/Generative-Adversarial-Network-Tutorial



Network Compression

- Distiller
- Deep Compression and EIE
- Network Speed and Compression
- https://arxiv.org/pdf/1712.01887.pdf
- https://hanlab.mit.edu/projects/tsm/
- Papers Reading List of *Embeded Neural Network*
- SigDL -- Deep Learning for IoT Device and Edge Computing Embedded Targets
- https://arxiv.org/abs/1804.03294

Bayesian Deep Learning

- https://alexgkendall.com/computer_vision/phd_thesis/
- http://bayesiandeeplearning.org/
- http://twiecki.github.io/blog/2016/06/01/bayesian-deep-learning/

Theories of Deep Learning

- Short Course of Deep Learning 2016 Autumn, PKU
- 深度学习名校课程大全 - 史博的文章 - 知乎
- Theories of Deep Learning (STATS 385)
- Topics Course on Deep Learning for Spring 2016 by Joan Bruna, UC Berkeley, Statistics Department
- Mathematical aspects of Deep Learning
- MATH 6380p. Advanced Topics in Deep Learning Fall 2018
- CoMS E6998 003: Advanced Topics in Deep Learning
- Deep Learning Theory: Approximation, Optimization, Generalization
- Theory of Deep Learning, ICML'2018
- Neural Networks, Manifolds, and Topology
- Theory of Deep Learning, project in researchgate
- THE THEORY OF DEEP LEARNING - PART I
- Magic paper
- Principled Approaches to Deep Learning
- The Science of Deep Learning
- The thermodynamics of learning
- A Convergence Theory for Deep Learning via Over-Parameterization
- MATHEMATICS OF DEEP LEARNING, NYU, Spring 2018
- Advancing AI through cognitive science
- https://zhuanlan.zhihu.com/p/45695998
- https://www.zhihu.com/question/265917569
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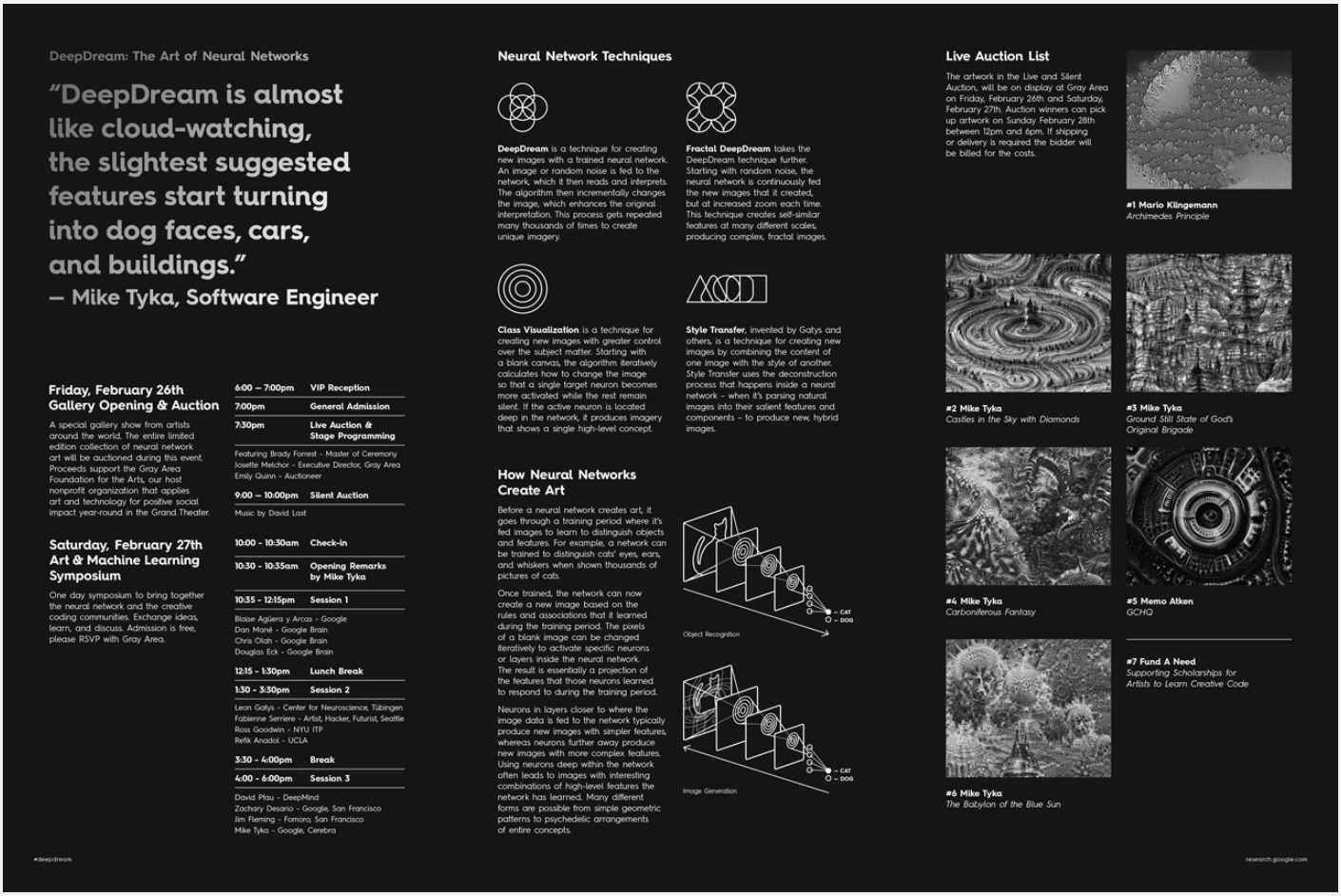
Deep Dream

Deep Dream



- A guide to deep learning
- 500 Q&A on Deep Learning
- Deep learning Courses
- Deep Learning note
- Deep learning from the bottom up
- Deep Learning Papers Reading Roadmap
- Some websites on deep learning:
    - [http://colah.github.io/]
    - [https://distill.pub/]
    - [http://www.wildml.com/]
    - [https://www.fast.ai/]
- Deep learning 101
- Design pattern of deep learning
- A Quick Introduction to Neural Networks
- A Primer on Deep Learning
- Deep learning and neural network
- An Intuitive Explanation of Convolutional Neural Networks
- Recurrent Neural Network

- THE ULTIMATE GUIDE TO RECURRENT NEURAL NETWORKS (RNN)
- LSTM at skymind.ai
- Deep Learning Resources
- Deep Learning meeting
- Online courses
- Some personal experience in deep learning
- **11-485/785** Introduction to Deep Learning
- **Deep Learning: Do-It-Yourself!**
- **Deep Learning course: lecture slides and lab notebooks**
- EE-559 – DEEP LEARNING (SPRING 2018)
- The Functions of Deep Learning
- https://stanford.edu/~shervine/teaching/cs-229/cheatsheet-deep-learning
- https://www.deeplearningwizard.com/
- https://www.stateoftheart.ai/
- 神经网络与深度学习
- https://mchromiak.github.io/articles/2017/Sep/01/Primer-NN/#.XBXb42h3hPY

Probabilistic Programming and Topological Data Analysis

Probabilistic Graphical Model

A graphical model or probabilistic graphical model (PGM) or structured probabilistic model is a probabilistic model for which a graph expresses the conditional dependence structure between random variables. They are commonly used in probability theory, statistics—particularly Bayesian statistics—and machine learning.
It is a marriage of graph theory and probability theory.

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- https://www.cs.cmu.edu/~aarti/Class/10701/lecs.html
- http://www.cs.cmu.edu/~epxing/Class/10708/lecture.html

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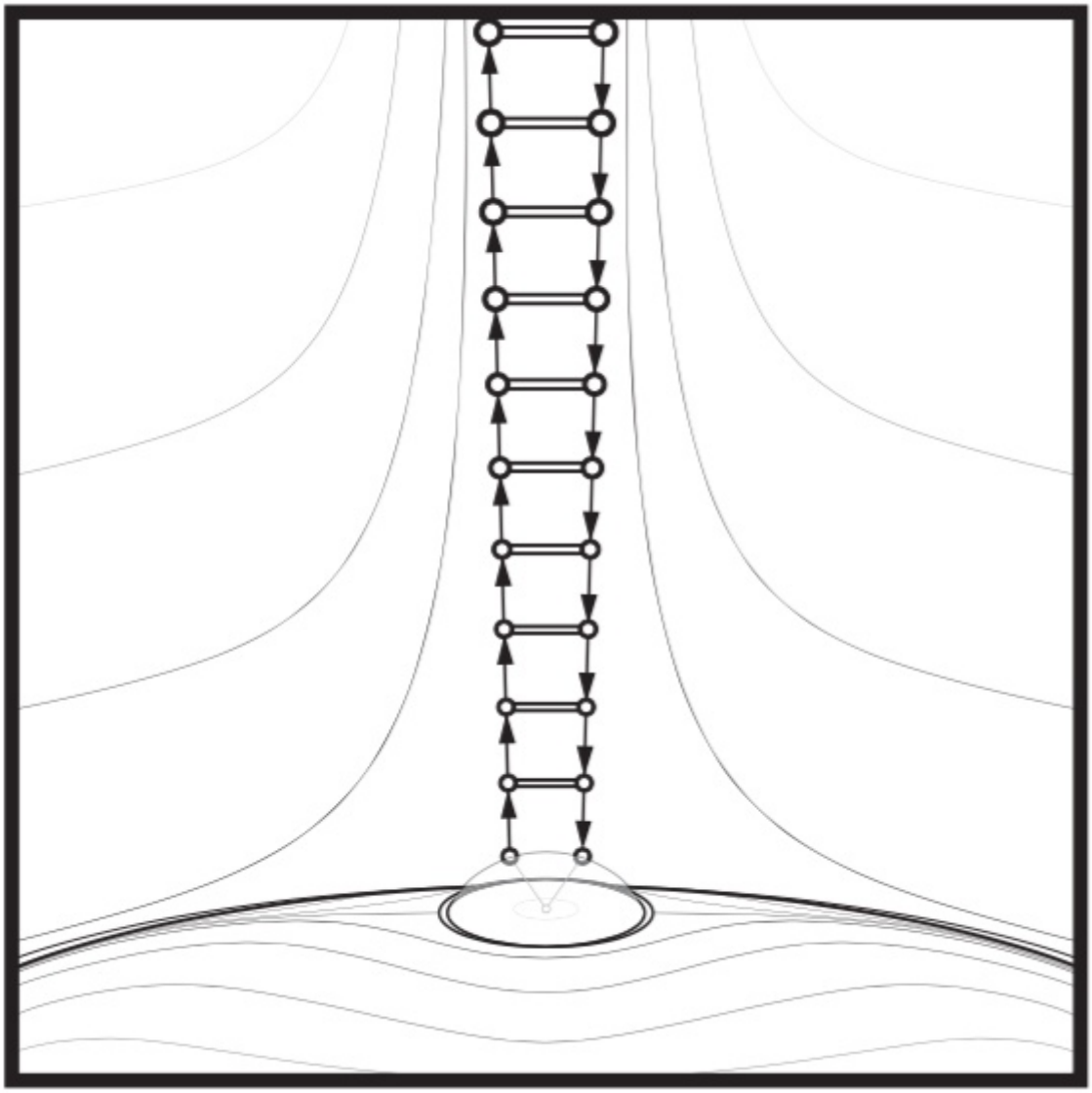
Graph Nets library and TDA

Graph Nets library and TDA



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- http://pyro.ai/examples/
- http://dustintran.com/blog/a-quick-update-edward-and-some-motivations
- https://www.wikiwand.com/en/Topological_data_analysis
- https://www.wikiwand.com/en/Random_graph
- TDA overview
- Studying the Shape of Data Using Topology

- Topological Data Analysis
- Why TDA works?
- http://outlace.com/TDApart1.html
- https://www.springer.com/cn/book/9783642150135

AutoML

- https://arxiv.org/abs/1810.13306
- https://github.com/hibayesian/awesome-automl-papers
- https://github.com/pierre-chaville/automlk
- https://www.simonwenkel.com/2018/08/29/introduction-to-autokeras.html

Computational Intelligence

Computational intelligence is rooted in the artificial neural network and evolutionary algorithms.

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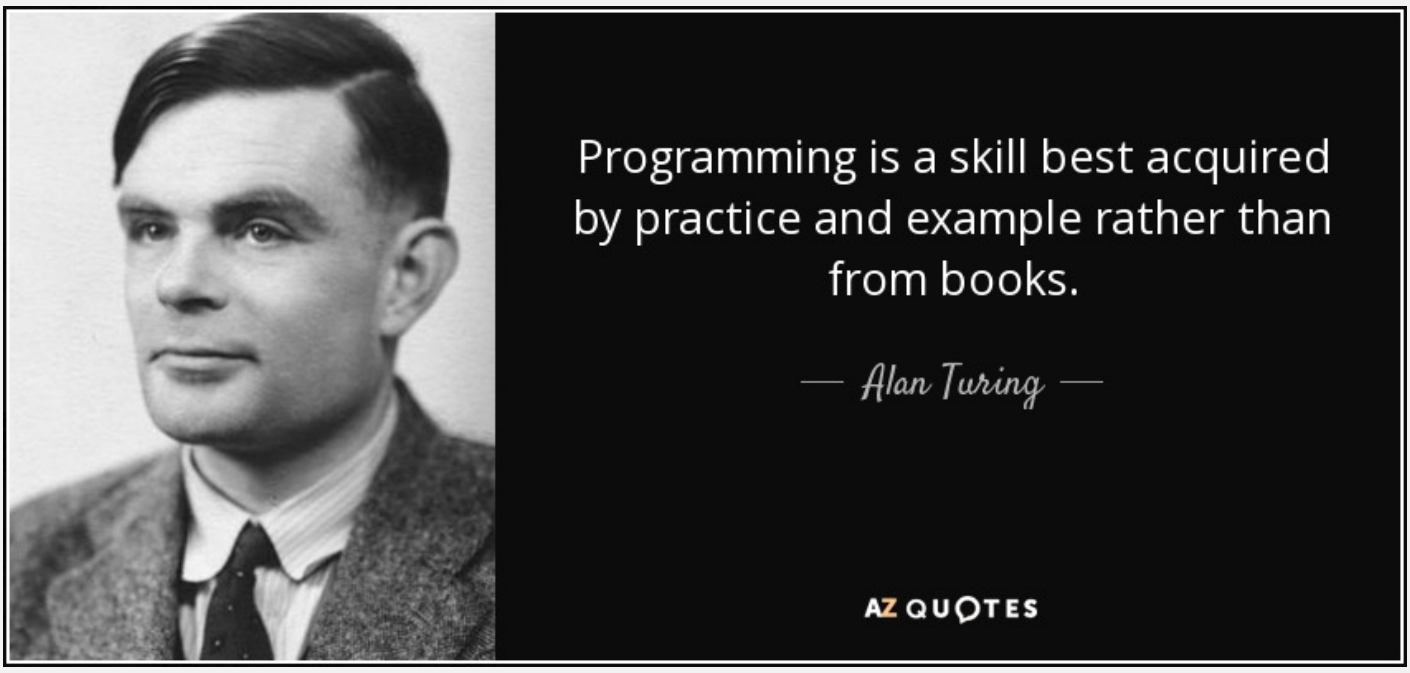
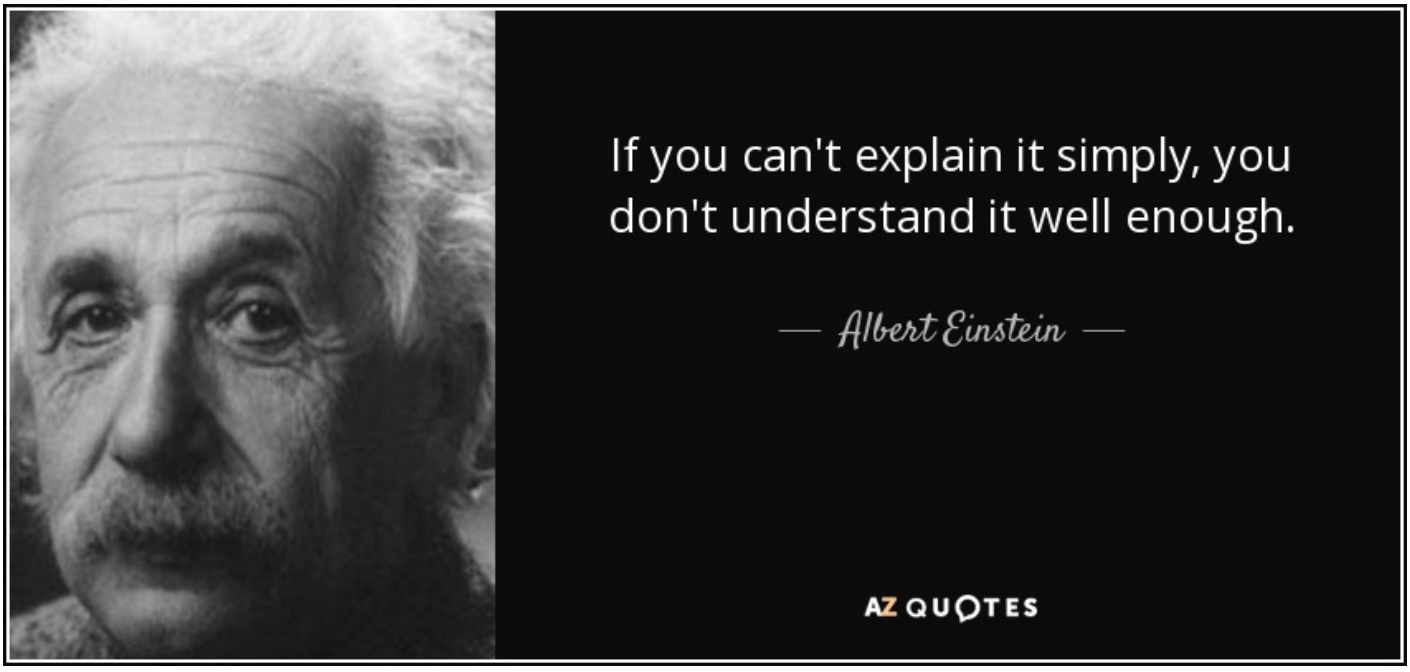
1. https://readyforai.com/
2. http://cleveralgorithms.com/
3. https://course.elementsofai.com/
4. https://intelligence.org/blog/
5. https://github.com/Siyeong-Lee/CIO
6. https://github.com/owainlewis/awesome-artificial-intelligence
7. https://github.com/JordanMicahBennett/Supermathematics-and-Artificial-General-Intelligence
8. https://github.com/gopala-kr/AI-Learning-Roadmap
9. http://emergentcomputation.com/Pseudo.html
10. https://wiki.opencog.org/w/Special:WhatLinksHere/The_Open_Cognition_Project
11. 人工智能(AI)资料大全 - 猿助猿的文章 - 知乎

路漫漫其修远兮，吾将上下而求索。





*Stay hungry, stay young, stay foolish, stay curious, and above all, stay humble because just when you think got all the answers, is the moment when some bitter twist of fate in the universe will **remind you that you very much don't**. --Tom Hiddleston*

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6. https://en.wikipedia.org/wiki/Thomas_Bayes ↩
7. All of Statistics ↩ ↩
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14. http://www.cs.toronto.edu/~hinton/absps/NatureDeepReview.pdf ↩