Universität Augsburg University

Deep Learning

Maths Refresher

Tuesday 29th November 2019

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Lecture Outline

- Linear Algebra
- Probability
- Differential Calculus
- Gradient Descent

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Why Linear Algebra?

- It is a key foundation to the field of machine learning
  - Present from notations used to describe the operation of algorithms to the implementation of algorithms in code
- Also needed to understanding the calculus and statistics used in machine learning
- Enables a deeper intuition in algorithms
  - Implement algorithms from scratch
  - Devise new algorithms

Linear Algebra (Refresher)

- **Scalar**
  - A one-dimensional vector, i.e. 1 x 1
- **Vector**
  - A single-dimensional array of numbers
  - i.e. 1 x m
- **Matrix**
  - A two-dimensional array of numbers
  - An $m \times n$ matrix has m rows and n columns
- **Tensor**
  - A multidimensional array of numbers

Scalar:

$$a$$

Vector:

$$\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix}$$

Matrix:

n columns, j →

m rows, i ↓

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \ddots & \ddots & \vdots \\ a_{m1} & \dots & \dots & a_{mn} \end{bmatrix}$$

- **Norm of a vector**
  - The norm is a measure of magnitude
    - The l^p norm is given by:

$$l^p = (|x_1|^p + |x_2|^p + \cdots + |x_n|^p)^{1/P}$$

  - Machine learning generally uses the l^1 and l^2 norms
    - The least squares cost function is the l^2 norm of an error vector
    - Norm of a parameter vector can be used in regularization

- **Norm of a vector**
  - l^1 norm example

$$v = \begin{bmatrix} 1 \\ -4 \\ 5 \end{bmatrix}, \|v\|_1 = |1| + |-4| + |5| = 10$$

  - l^2 norm example

$$v = \begin{bmatrix} 1 \\ -4 \\ 5 \end{bmatrix}, \|v\|_2 = \sqrt{|1|^2 + |-4|^2 + |5|^2} = \sqrt{42}$$

- **Dot product**
  - The dot product of two vectors, $v_1 \in \mathbb{R}^{n\times 1}$ and $v_2 \in \mathbb{R}^{n\times 1}$, is the sum of the product of the corresponding elements:

$$v_1 \cdot v_2 = v_1^T v_2 = v_2^T v_1 = v_{1_1} v_{2_1} + v_{1_2} v_{2_2} + \cdots + v_{1_n} v_{2_n} = \sum_{k=1}^{n} v_{1_k} v_{2_k}$$

- **Dot product**
  - Example:

$$v_1 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}, v_2 = \begin{bmatrix} 3 \\ 5 \\ -1 \end{bmatrix}$$

$$v_1 \cdot v_2 = \ v_1^T v_2 = = 1 \times 3 + 2 \times 5 - 3 \times 1 = 10$$

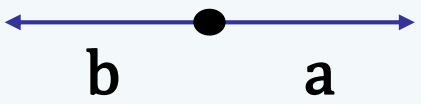
- **Why is the dot product important?**
  - The dot product encodes information about the angle between two vectors

$$\boldsymbol{v}_1 \cdot \boldsymbol{v}_1 = \|\boldsymbol{v}_1\| \|\boldsymbol{v}_1\| \cos\theta$$

$$\theta = arccos\left(\frac{\boldsymbol{v}_1 \cdot \boldsymbol{v}_1}{\|\boldsymbol{v}_1\| \|\boldsymbol{v}_1\|}\right)$$

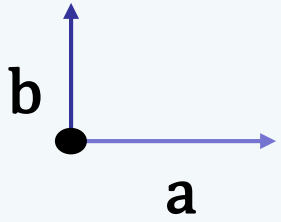
- **Why is the dot product important?**

$\cos \pi = -1$



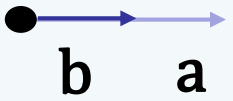
Dot product is negative

$\cos \frac{\pi}{2} = 0$



Dot product is zero

$\cos 0 = 1$



Dot product is positive

– The dot product measures how similar two vectors are

- **Matrix multiplication**
  - For $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{p \times q}$ to be multipliable n must equal p and the resulting matrix is C $\in \mathbb{R}^{m \times q}$

$$C_{i,j} = \sum_{k=1}^{n} a_{i,k}\, b_{k,j}$$

$$\forall\, i \in \{1,2,\ldots,m\}$$

$$\forall\, j\, \{1,2,\ldots,q\}$$

- **Matrix multiplication**
  - Example:

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}, B = \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix}, C = A \times B$$

$$C_{11} = \begin{bmatrix} 1 & 2 \end{bmatrix} \begin{bmatrix} 5 \\ 7 \end{bmatrix}, 1 \times 5 + 2 \times 7 = 19 \, , C_{12} = \begin{bmatrix} 1 & 2 \end{bmatrix} \begin{bmatrix} 6 \\ 8 \end{bmatrix}, 1 \times 6 + 2 \times 8 = 22$$

$$C_{21} = \begin{bmatrix} 3 & 4 \end{bmatrix} \begin{bmatrix} 5 \\ 7 \end{bmatrix}, 3 \times 5 + 4 \times 7 = 43 \, , C_{22} = \begin{bmatrix} 3 & 4 \end{bmatrix} \begin{bmatrix} 6 \\ 8 \end{bmatrix}, 3 \times 6 + 4 \times 8 = 50$$

$$C = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} = \begin{bmatrix} 19 & 22 \\ 43 & 50 \end{bmatrix}$$

- **Matrix transpose**
  - The transpose of a matrix $A \in \mathbb{R}^{m \times n}$ is generally represented as $A^T \in \mathbb{R}^{n \times m}$
  - This is performed by transposing the column vectors as row vectors

$$a'_{ji} = a_{i,j}, \forall\, i \in \{1,2,\dots,m\}, \forall\, j\, \{1,2,\dots,n\}$$

where $a'_{ji} \in A^T$ and $a_{i,j} \in A$

  - Transpose is important as it relates in inner products
    - The dot product of two column vectors a and b can be computed as the single entry of the matrix product: $[a \cdot b] = a^T b$

- **Matrix transpose**
  - Examples:

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \text{ then } A^T = \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & 4 & 3 \\ 8 & 2 & 6 \\ 7 & 8 & 3 \\ 4 & 9 & 6 \\ 7 & 8 & 1 \end{bmatrix} \text{ then } A^T = \begin{bmatrix} 1 & 8 & 7 & 4 & 7 \\ 4 & 2 & 8 & 9 & 8 \\ 3 & 6 & 3 & 6 & 1 \end{bmatrix}$$

- **Determinant of a matrix**
  - The determinant of a square matrix $A \in \mathbb{R}^{n \times n}$ is a number denoted by $|A|$ or $\det(A)$ and is given by:

$$\boldsymbol{det}(\boldsymbol{A}) = \pm \prod a_{1j_i}\, a_{2j_2}, \ldots, a_{nj_n}$$

  - where the column indices $j_1, j_2, .., j_n$ are taken from the set $\{1, 2, \ldots\ n\}$, with no repetitions allowed. The plus (minus) sign is taken if the permutation $(j_1, j_2, .., j_n)$ is even (odd)

- **Determinant of a matrix**
  - Examples:

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{21}a_{12}$$

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$$

$$= a_{11}(a_{22}a_{33} - a_{32}a_{23}) - a_{21}(a_{12}a_{33} - a_{32}a_{13}) + a_{31}(a_{12}a_{23} - a_{22}a_{13})$$

- **Inverse of a matrix**
  - For a square matrix $A \in \mathbb{R}^{n \times n}$, the inverse is denoted as A^{-1} and produces the identity when multiplied by A

$$AA^{-1} = A^{-1}A$$

$$A^{-1} = \frac{(cofactor\ matrix\ of\ A)^T}{\det(A)}$$

  - Cofactor for $a_{\mathrm{i,j}} = (-1)^{i+j} d_{ij}$
    - Where d_{ij} is the determinate of the matrix formed by deleting row i and column j from A

- **Inverse of a matrix**
  - Examples

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}^{-1} = \frac{1}{a_{11} \times a_{22} - a_{21} \times a_{12}} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}$$

$$\begin{bmatrix} 4 & 7 \\ 2 & 6 \end{bmatrix}^{-1} = \frac{1}{4 \times 6 - 2 \times 7} \begin{bmatrix} 6 & -7 \\ -2 & 4 \end{bmatrix} = \frac{1}{10} \begin{bmatrix} 6 & -7 \\ -2 & 4 \end{bmatrix} = \begin{bmatrix} 0.6 & -0.7 \\ -0.2 & 0.4 \end{bmatrix}$$

$$\begin{bmatrix} 3 & 4 \\ 6 & 8 \end{bmatrix}^{-1} = \frac{1}{3 \times 8 - 6 \times 4} \begin{bmatrix} 8 & -4 \\ -6 & 3 \end{bmatrix} \rightarrow \text{inverse does not exist}$$

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- **Why probability?**
  - Machine learning must always deal with uncertain quantities
  - Laws of probability govern how a machine learning algorithm should reason
    - We design machine learning algorithms to approximate expressions derived from probability theory
  - Analyse the behaviour of a proposed approach

- **Definitions**
  - **Experiment:** any process of observation
  - **Random experiment:** An experiment in which the outcomes cannot be precisely predicted
  - **Sample space:** set of all possible outcomes
  - **Probability measure P:** an assignment of a number between 0 and 1 to a particular event in the sample space

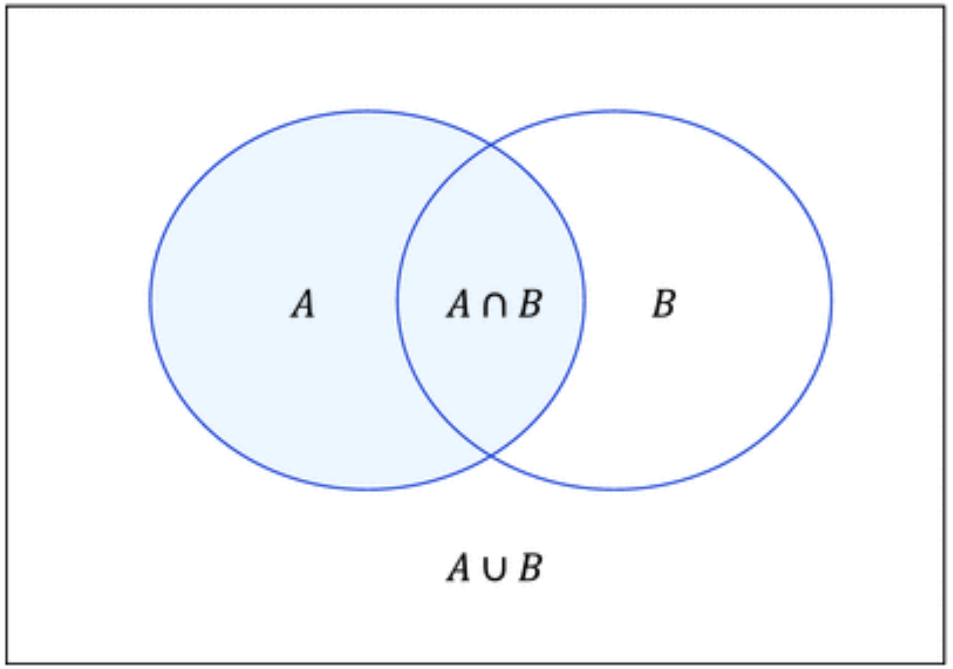
$P(A)$: the probability that an event A will occur

$$0 \leq P(A) \leq 1$$

- **Rules of Probability**
  - **Intersection of events**
    - The probability that Events A *and* B occur, denoted $P(A \cap B)$
  - **Mutually exclusive events**
    - Cannot occur at the same time i.e. $P(A \cap B) = 0$
  - **Union of events**
    - The probability that events A *or* B occur, denoted $P(A \cup B)$
  - **Conditional probability**
    - The probability that Event A occurs, given that Event B has occurred
    - Denoted $P(A|B)$

- **Rules of probability**
  - **Rule of multiplication**
    - $P(A \cap B) = P(A)\,P(B|A)$

      $= P(B)P(A|B)$
    - Note, $P(A \cap B)$ is denoted as $P(AB)$
  - **Rule of addition**
    - $P(A \cup B) = P(A) + P(B) - P(A \cap B)$



- **Rules of probability**
  - **Chain rule of probability**
    - Extension of the rule of multiplication

$$P(A_1A_2A_3 \dots A_n) = P(A_1)P(A_2|A_1)P(A_3|A_1A_2)P(A_n|A_1A_2A_3 \dots A_{n-1})$$
$$= P(A_1)\prod_{i-2}^{n} P(A_i|A_1A_2A_3 \dots A_{n-1})$$

  - **Mutually exclusive events $\mathbf{P(AB) = 0}$**

$$P(A_1 \cup A_2 \cup A_3 \cup \cdots \cup A_n) = P(A_1) + P(A_2) + P(A_3) + \cdots + P(A_n)$$
$$= \sum_{i=1}^{n} P(A_n)$$

- **Rules of probability**
  - **Independence of events**

$$P(AB) = P(A)P(B)$$

  - **Bayes' rule**
    - From multiplication rule

$$P(AB) = P(A)P(B|A) = P(B)P(A|B)$$

    - Therefore

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

- **Random experiment**
  - An experiment or a process for which the outcome cannot be predicted with absolute certainty
    - However, we have knowledge of the *sample space*, the set of all possible outcomes
- **Random variable**
  - Individual outcomes of a random experiment
    - A function that maps the outcomes of random experiment (the samples space) to a subset of real numers (i.e. $\mathbb{R}$).
      - E.g. A random variable can be used to describe the process of rolling a fair die and the possible outcomes $\{1, 2, 3, 4, 5, 6\}$

- **Probability Mass Function (PMF)**
  - Let X be a random variable with domain D
  - The probability mass function is then defined as the probability that X is equal to some value x

$$\sum_{x \in D} P(X = x) = 1$$

  - To be a PMF, P must satisfy
    - P must be the sets of all possible states of X
    - $0 \leq P(X) \leq 1$
    - $\sum_{x \in D} P(X) = 1$

- **Expectation**
  - The average value that some function takes when x is drawn from P

$$\mathbb{E}_{x\sim P}[f(x)] = \mu = \sum_x P(x)f(x)$$

- **Variance**
  - Variation in different sample values of x when drawn from its probability distribution

$$Var[f(x)] = \sigma^2 = \mathbb{E}[f(x) - \mathbb{E}[f(x)]^2]$$

- **Covariance**
  - Measure joint variability between two random variables

$$Cov\big(f(x), g(y)\big) = \mathbb{E}[(f(x) - \mathbb{E}[f(x)])(g(x) - \mathbb{E}[g(x)])]$$

- **Random processes**
  - A collection of random variables defined over a common PMF
    - Consider a random process η with N observed values

- **Mean**

$$\mu_{\eta} = \frac{1}{N}\sum_{n=0}^{N-1}\eta(n)$$

- **Mean-Square**
  - The 'power' of the process

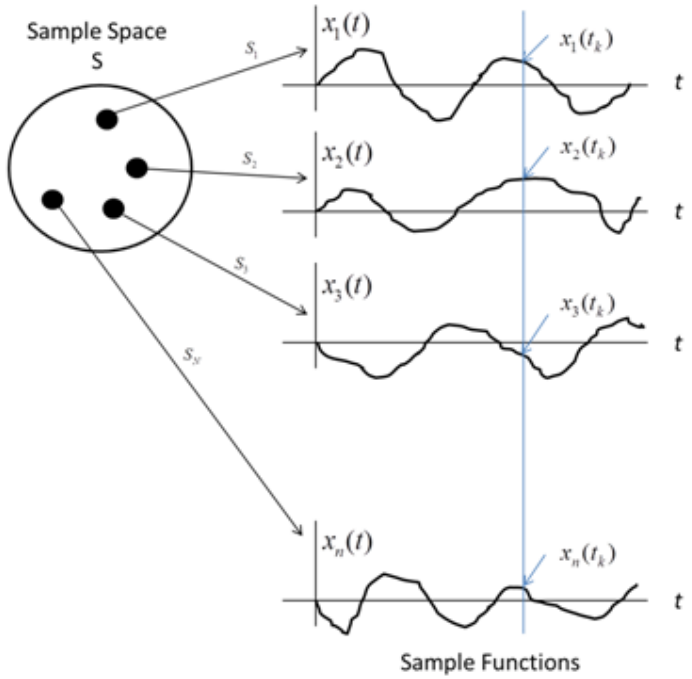
$$MS_{\eta} = \frac{1}{N}\sum_{n=0}^{N-1}(\eta(n))^2$$

- **Variance**

$$\sigma_{\eta}^2 = \frac{1}{N}\sum_{n=0}^{N-1}\left(\eta(n) - \mu_{\eta}\right)^2$$

Image Source:
https://www.vocal.com

- **Random signal**
  - When the values of a random process η form a time series
    - Also known as a stochastic process
  - Denoted $\eta(t)$
- Key properties
  - μ_η represents the DC component
    - DC component is the amplitude signal fluctuates around
      - Assumed to be zero for random noise
  - MS_η represents the average power
    - If μ_η is zero $\sigma_\eta^2 = MS_\eta$



- **Information Theory**
  - Quantifying how much information is present in a signal
    - Likely events should have low information content
      - Likely events are uninformative
    - Less likely events should have higher information content
      - Unlikely events are more informative
  - Self-Information: $$I(x) = -logP(x)$$
  - Entropy: $$H(x) = E_{x\sim P}[I(x)] = -E_{x\sim P}[logP(x)]$$
    - Distribution of expected information

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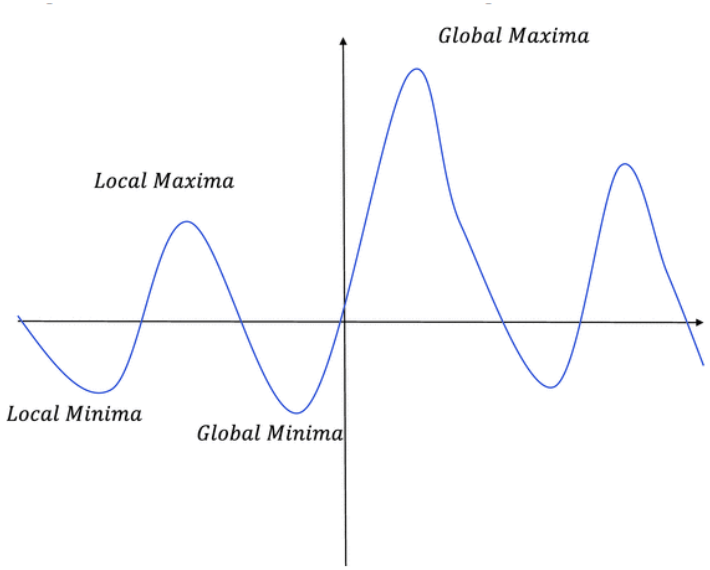
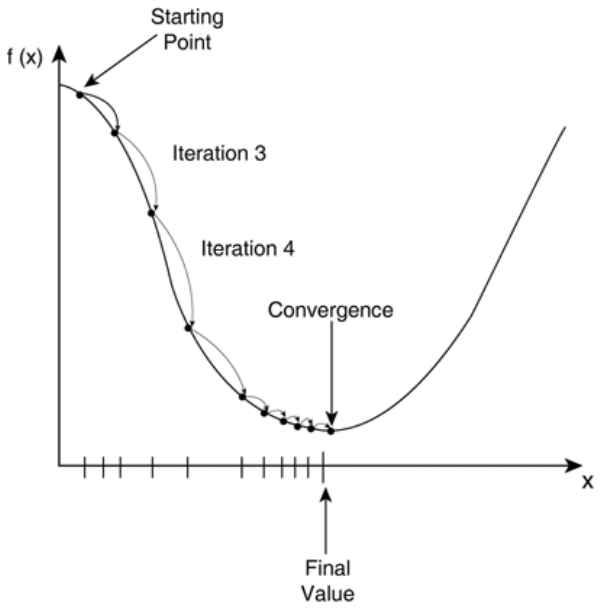
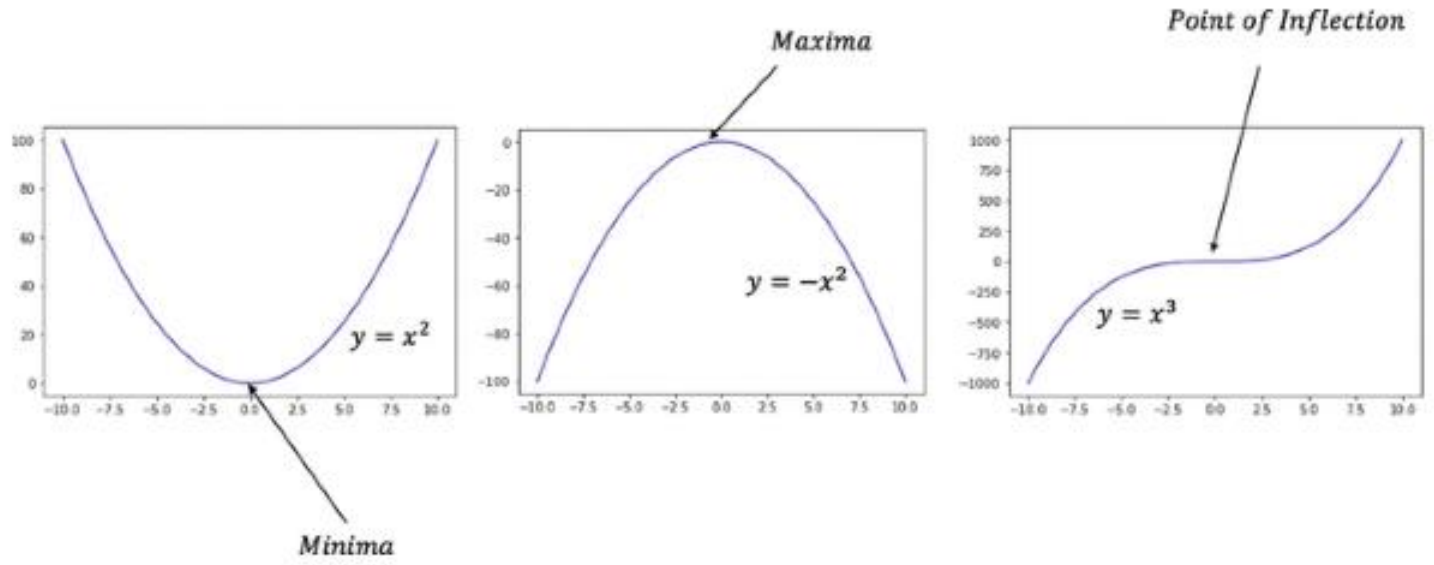
- **A good understanding of calculus is essential for machine learning**
  - Machine learning models are (normally) a function of several variables
  - In building a model we generally need to compute a cost function, we derive the models that best explain the training data by optimising this cost function
  - Optimisation refers to the task of minimising (or maximising) a function $f(\boldsymbol{x})$

- **Maxima and Minima of Functions**
  - Building machine-learning models relies on iteratively minimising a cost function



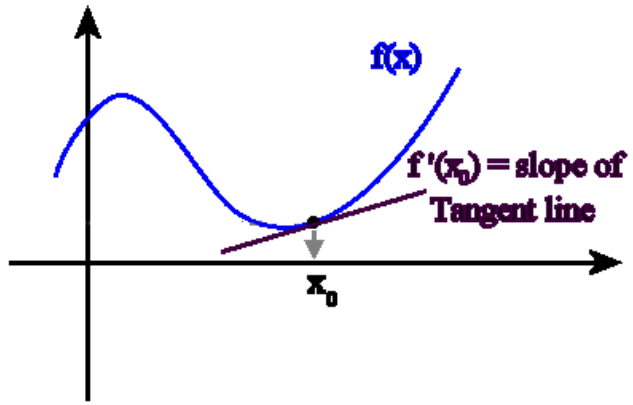


- **Rules for locating maxima/minima**
  - 1st order derivative is zero
  - Maxima: 2nd order derivative is *less* than zero
  - Minima: 2nd order derivative is *greater* than zero
  - Point of inflection: 2nd order derivative equals zero



- **Derivative of a function $f(t)$**
  - Rate of change of a quantity represented by a function with respect to another quantity on which the function is dependent on.

$$\frac{df}{dt} = \lim_{h \to 0} \frac{f(t+h) - f(t)}{h}$$



- **Derivative of a function $f(t)$**

$f(x)$	$f'(x)$	$f(x)$	$f'(x)$
x^n	nx^{n-1}	e^x	e^x
$\ln(x)$	$1/x$	$\sin(x)$	$\cos(x)$
$\cos(x)$	$-\sin(x)$	$\tan(x)$	$\sec^2(x)$
$\cot(x)$	$-\mathrm{cosec}^2(x)$	$\sec(x)$	$\sec(x)\tan(x)$
$\mathrm{cosec}(x)$	$-\mathrm{cosec}(x)\cot(x)$	$\tan^{-1}(x)$	$1/(1+x^2)$
$\sin^{-1}(x)$	$1/\sqrt{1-x^2}$ for $\lvert x\rvert < 1$	$\cos^{-1}(x)$	$-1/\sqrt{1-x^2}$ for $\lvert x\rvert < 1$
$\sinh(x)$	$\cosh(x)$	$\cosh(x)$	$\sinh(x)$
$\tanh(x)$	$\mathrm{sech}^2(x)$	$\coth(x)$	$-\mathrm{cosech}^2(x)$
$\mathrm{sech}(x)$	$-\mathrm{sech}(x)\tanh(x)$	$\mathrm{cosech}(x)$	$-\mathrm{cosech}(x)\coth(x)$
$\sinh^{-1}(x)$	$1/\sqrt{x^2+1}$	$\cosh^{-1}(x)$	$1/\sqrt{x^2-1}$ for $x > 1$
$\tanh^{-1}(x)$	$1/(1-x^2)$ for $\lvert x\rvert < 1$	$\coth^{-1}(x)$	$-1/(x^2-1)$ for $\lvert x\rvert > 1$

- **Product Rule**
  - If $f(x)$ and $g(x)$ are differentiable on x then:

$$(f \cdot g)'(x) = f(x)g'(x) + g(x)f'(x)$$

- **Chain Rule**
  - If $f(x)$ and $g(x)$ are differentiable on x

$$(f \circ g)'(x) = f'\big(g(x)\big)g'(x)$$

  - If $y = g(u)$ and $u = g(x)$ the derivative of y is

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}$$

- **Partial derivatives $z = f(x, y)$**

$$\frac{\partial z}{\partial x} = \lim_{h \to 0} \frac{f(x+h, y) - f(x, y)}{h}$$

$$\frac{\partial z}{\partial y} = \lim_{h \to 0} \frac{f(y+h, x) - f(x, y)}{h}$$

  - Successive Partial Derivatives

$$\frac{\partial}{\partial y}\left(\frac{\partial z}{\partial x}\right) = \frac{\partial^2 z}{\partial y \partial x}$$

$$\frac{\partial}{\partial x}\left(\frac{\partial z}{\partial y}\right) = \frac{\partial^2 z}{\partial x \partial y}$$

    - Note that if the second derivatives are continuous, $\frac{\partial^2 z}{\partial y \partial x} = \frac{\partial^2 z}{\partial x \partial y}$

- **Gradient of a function**
  - Vector of first order partial derivatives

$$f(\boldsymbol{x}), \text{where } \boldsymbol{x} = [x_1, x_2, \dots, x_n]^T \epsilon \mathbb{R}^{n \times 1}$$

Then,

$$\nabla f(\boldsymbol{x}) = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n}\right]^T$$

  - The gradient is important in machine-learning algorithms when we try to maximize or minimize cost functions with respect to the model parameters,

- **Hessian Matrix of a function**
  - Matrix of second order partial derivatives
    - Useful in optimisation problems
      - Especially when cost function is non linear

For a function: $f(x, y, z)$:

$$Hf(x, y, z) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial x \partial z} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} & \frac{\partial^2 f}{\partial y \partial z} \\ \frac{\partial^2 f}{\partial z \partial x} & \frac{\partial^2 f}{\partial z \partial y} & \frac{\partial^2 f}{\partial z^2} \end{bmatrix}$$

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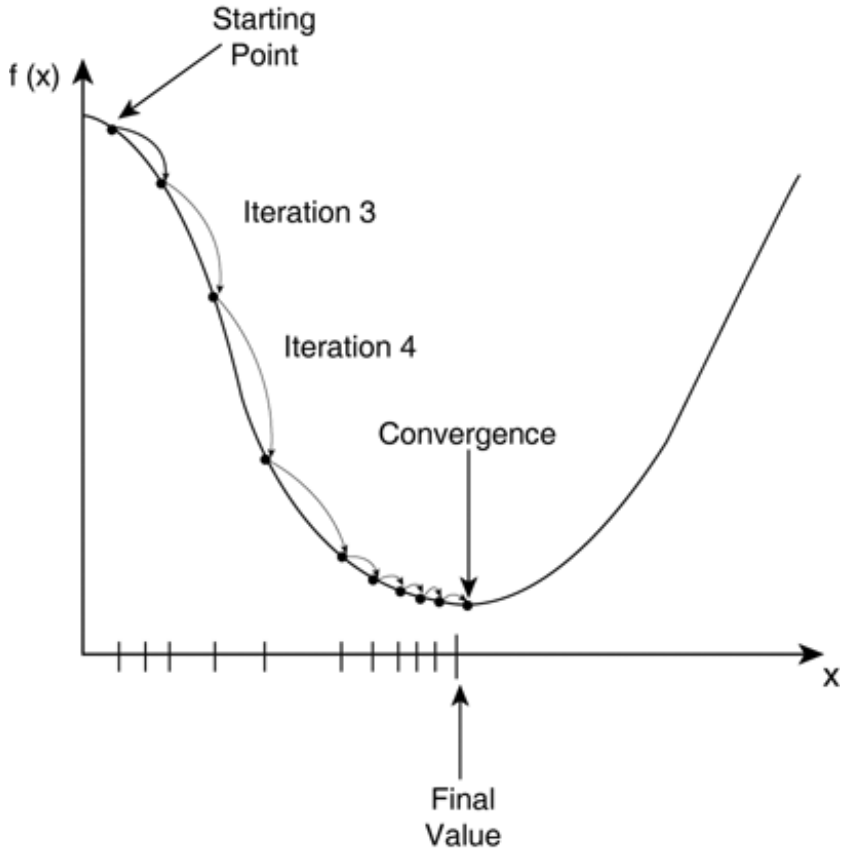
- **Gradient Descent Algorithms**
  - Arguably the most widely used optimisation technique
  - Iterative solution
    - Uses the negative gradient of the cost function to determine the direction they parameters need updating

$$\theta^{(t+1)} = \theta^{(t)} - \eta \nabla C(\theta^{(t)})$$

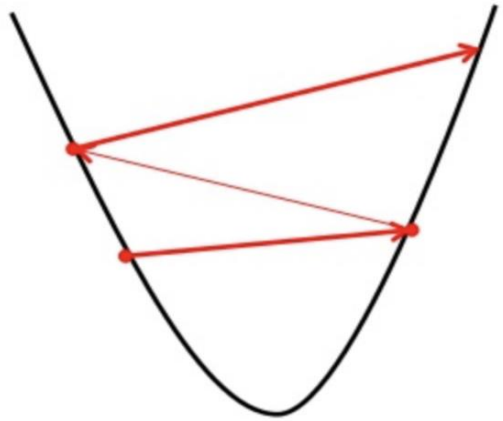


- **Gradient Descent Algorithms**

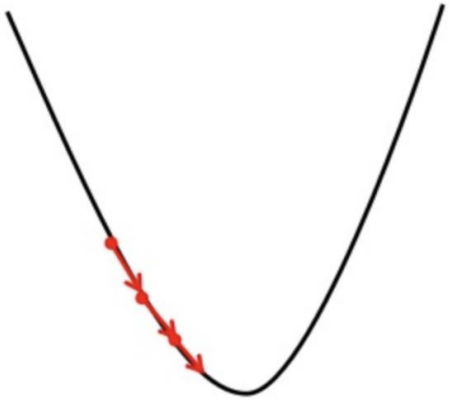
$$\theta^{(t+1)} = \theta^{(t)} - \eta \nabla C(\theta^{(t)})$$

  - η is the learning rate
  - A constant that defines the size of the gradient descent step
  - Size is important:
    - To large and the update function might oscillate over the minima
    - To small and convergence is slow

Big learning rate



Small learning rate



Source: https://towardsdatascience.com/

- **Multivariate Gradient Descent Algorithms**
  - Lets consider a cost function $C(\theta)$ where $\theta \in \mathbb{R}^{n\times 1}$
  - At every iteration we want to update θ to $\theta + \Delta\theta$ such that $C(\theta + \Delta\theta)$ is less than $C(\theta)$
  - Achieved by assuming linearity and using a *Taylor series expansion* we get:

$$C(\theta + \Delta\theta) = C(\theta) + \Delta\theta^T \nabla C(\theta)$$

  - Need to choose $\Delta\theta$ such that $C(\theta + \Delta\theta)$ is less than $C(\theta)$

- **Multivariate Gradient Descent Algorithms**
  - Need to choose $\Delta\theta$ such that $C(\theta + \Delta\theta)$ is less than $C(\theta)$

$$C(\theta + \Delta\theta) = C(\theta) + \Delta\theta^T \nabla C(\theta)$$

  - To get the minimum value of the dot product $\Delta\theta^T \nabla C(\theta)$, the direction of $\Delta\theta$ should be the opposite of $\nabla C(\theta)$

$$\Delta\theta \propto -\nabla C(\theta)$$

Hence

$$\Delta\theta = -\eta \nabla C(\theta)$$

$$\theta + \Delta\theta = \theta - \eta \nabla C(\theta)$$

$$\theta^{(t+1)} = \theta^{(t)} - \eta \nabla C(\theta^{(t)})$$