Lecture 1. StatML Welcome and Maths Review

COMP90051 Statistical Machine Learning

Lecturer: Jean Honorio

This lecture

- About COMP90051
- Review: Probability theory
- Review: Linear algebra
- Review: Sequences and limits

Subject objectives

- Develop an appreciation for the role of statistical ML, advanced foundations and applications
- Gain an understanding of a representative selection of ML techniques – *how ML works*
- Be able to design, implement and evaluate ML systems
- Become a discerning ML consumer

Subject content

- The subject will cover topics from

  Foundations of statistical learning, linear models, non-linear bases, regularised linear regression, generalisation theory, kernel methods, deep neural nets, experts, multi-armed bandits, Bayesian learning, probabilistic graphical models

- Classical / in-person teaching
  - Theory in lectures (2x per week), subject assessment;
  - Hands-on experience in weekly workshop (starts week 2), subject assessment;
  - *Strongly recommend you keep up (viz. quizzes)*

Subject staff / Contact

Lecturers: [Jean Honorio](#) [Week 1 to Week 5]
Zahra Dasht Bozorgi [Week 6 to first lecture of Week 10]
Ben Rubinstein [Second lecture of Week 10 to Week 12]

Tutors: Shijie Liu (Head Tutor),
Qianjun Ding, Jinhao Li, Paul Ou, Xunye Tian, Jedwin Villanueva
See Canvas for latest list and contact details.

Ed discussion *Will open after this first lecture*

Contacting staff *Combined staff email*
comp90051-2024s2-staff@lists.unimelb.edu.au

Advanced ML: Expected Background

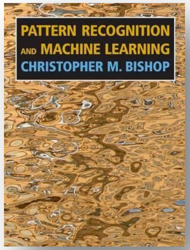
- **ML**: COMP90049, COMP20008, MAST90105
- **Algorithms & complexity**: big-O, termination; basic data structures & algorithms
- **Solid coding**, ideally experience in Python
- **Mathematics and statistics**

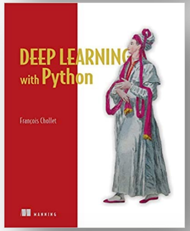
Maths / stats requirements

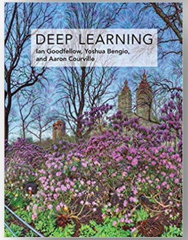
- Probability theory: probability calculus; discrete/continuous distributions; multivariate; exponential families; Bayes rule
- Sequences: sequences, limits, supremum
- Linear algebra: vector inner products & norms; orthonormal bases; matrix operations, inverses, eigenvectors/values
- Calculus & optimisation: partial derivatives; gradient descent; convexity; Lagrange multipliers

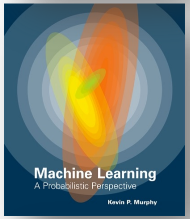
Textbooks

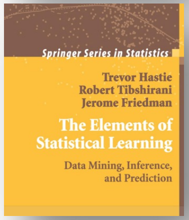
- We don't have only one reference. We prefer to pick good bits from several. We may also supplement with other readings as we go.
- All are available free online or through the library digitally. See the Canvas subject overview for links. Therefore, no need to buy**.**
- Primarily we refer to (good all rounder): ***Bishop (2007) Pattern Recognition and Machine Learning***
- ***Practical Deep Nets: Chollet (2017) Deep learning with Python***
- ***More deep learning detail: Goodfellow, Bengio, Courville (2016) Deep learning***
- For more on PGMs/Bayesian inference: Murphy (2012) *Machine Learning: A Probabilistic Perspective*
- For reference on frequentist ideas, SVMs, lasso, etc.:
  Hastie, Tibshirani, Friedman (2001) *The Elements of Statistical Learning: Data Mining, Inference and Prediction*
- For reference on learning theory (though goes deeper/broader than we need)
  Shalev-Shwartz and Ben-David *"Understanding Machine Learning: From Theory to Algorithms"*











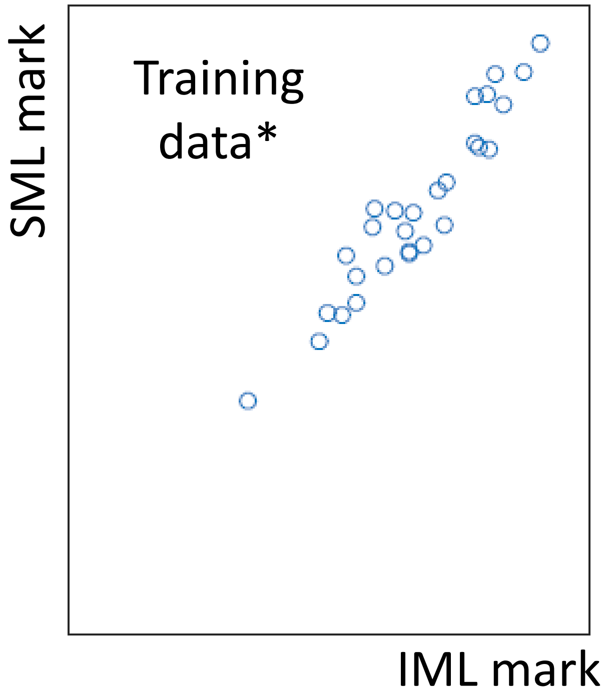
Assessment

- Assessment components
  - Timing may differ from handbook due to non-teaching week
  - Two assignments – w5-8 (12.5% each, individual)
    - ~1.5 weeks to complete
    - One written assignment, one programming assignment
  - A group project – w8-12 (25%, group size 3)
    - ~4 weeks to complete
  - Quizzes 30min fortnightly (10% - best 5 of 6)
    - Q1 to **open August 4 at 11.59pm** and **close August 5 at 11.59pm**
  - Final Exam (40%): 2hr open book **on-campus exam** (40%)

- 50% hurdles applied to **exam**

Probability theory

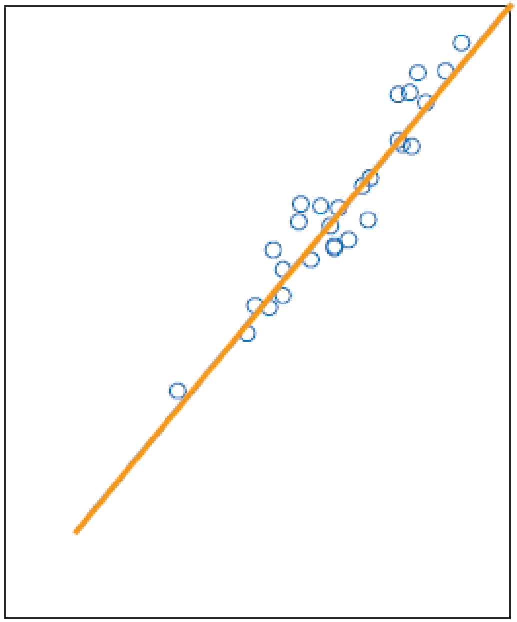
Data is noisy (almost always)



- Example:
  - given mark for Intro ML (IML)
  - predict mark for Stat Machine Learning (SML)

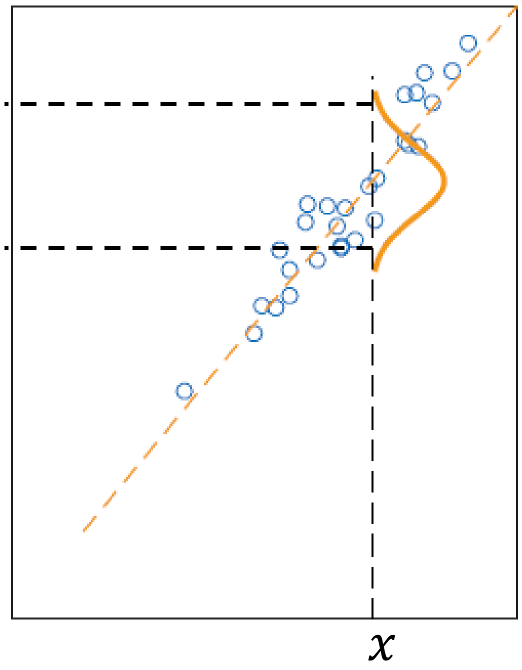
* synthetic data :)

Types of models



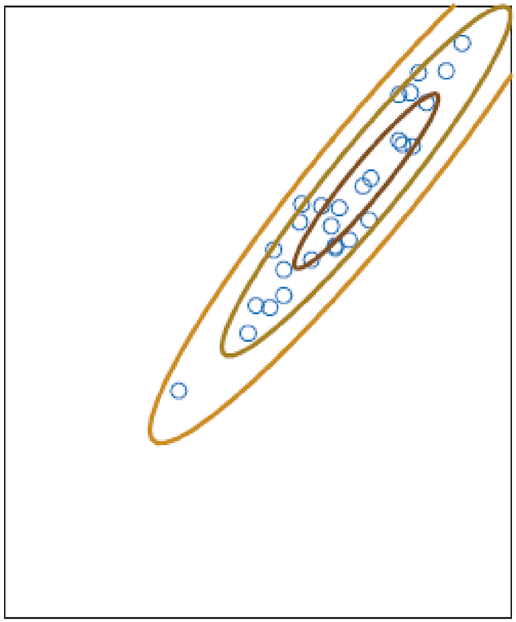
$\hat{y} = f(x)$

IntroML mark was 95, SML mark is predicted to be 95



$P(y|x)$

IntroML mark was 95, SML mark is likely to be in (92, 97)



$P(x, y)$

probability of having $(IML = x, SML = y)$

Basics of probability theory

- A probability space:
  - Set Ω of possible outcomes
  - Set *F* of events (subsets of outcomes)
  - Probability measure P: *F* → **R**
- Example: a die roll
  - {1, 2, 3, 4, 5, 6}
  - { φ, {1}, …, {6}, {1,2}, …, {5,6}, …, {1,2,3,4,5,6} }
  - P(φ)=0, P({1})=1/6, P({1,2})=1/3, …

Axioms of probability

F contains all of: Ω; all complements $\Omega \backslash f$, $f \in F$; the union of any countable set of events in F.

1. $P(f) \geq 0$ for every event $f \in F$.
2. $P\left(\bigcup_f f\right) = \sum_f P(f)$ for all countable sets of pairwise disjoint events.
3. $P(\Omega) = 1$

Random variables (**r.v.'s**)

- A random variable *X* is a numeric function of outcome $X(\omega) \in \boldsymbol{R}$
- $P(X \in A)$ denotes the probability of the outcome being such that *X* falls in the range *A*

- Example: *X* winnings on $5 bet on even die roll
  * *X* maps 1,3,5 to -5
    X maps 2,4,6 to 5
  * P(*X*=5) = P(*X*=-5) = ½

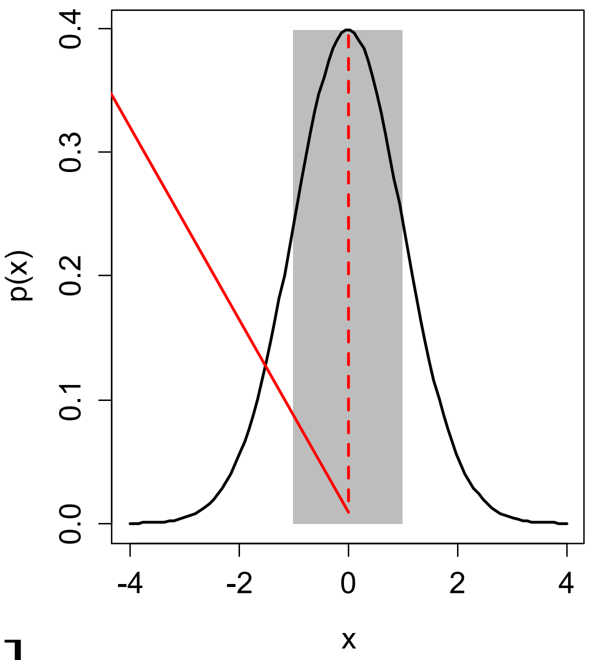
Discrete vs. continuous distributions

- Discrete distributions
  - Govern r.v. taking discrete values
  - Described by probability mass function p(x) which is P(X=x)
  - $P(X \leq x) = \sum_{a=-\infty}^{x} p(a)$
  - **Examples**: Bernoulli, Binomial, Multinomial, Poisson

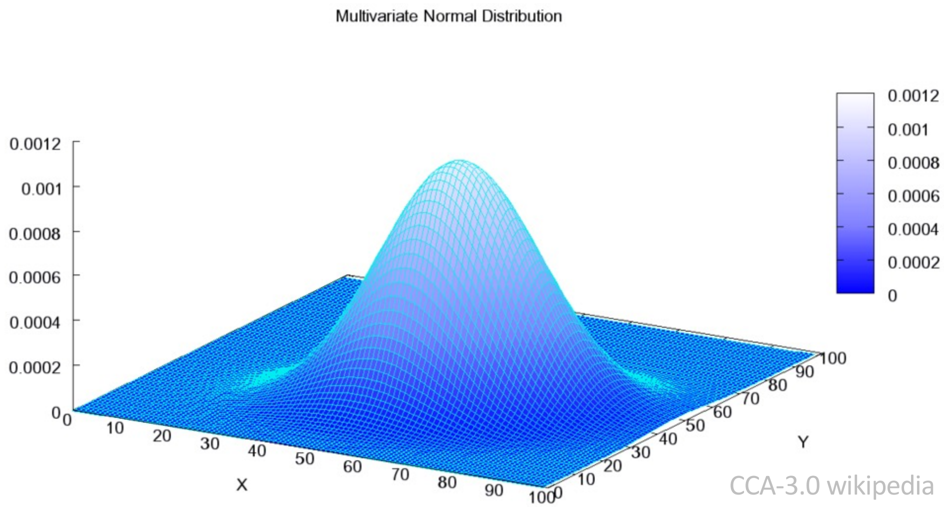
- Continuous distributions
  - Govern real-valued r.v.
  - Cannot talk about PMF but rather probability density function p(x)
  - $P(X \leq x) = \int_{-\infty}^{x} p(a) da$
  - **Examples**: Uniform, Normal, Laplace, Gamma, Beta, Dirichlet

Expectation

- Expectation $E[X]$ is the r.v. X's "average" value
  - Discrete: $E[X] = \sum_x x\, P(X = x)$
  - Continuous: $E[X] = \int_x \; x\, p(x)\, dx$
- Properties
  - Linear: $E[aX + b] = aE[X] + b$
    $E[X + Y] = E[X] + E[Y]$
  - Monotone: $X \geq Y \;\Rightarrow\; E[X] \geq E[Y]$
- Variance: $Var(X) = E[(X - E[X])^2]$



Multivariate distributions



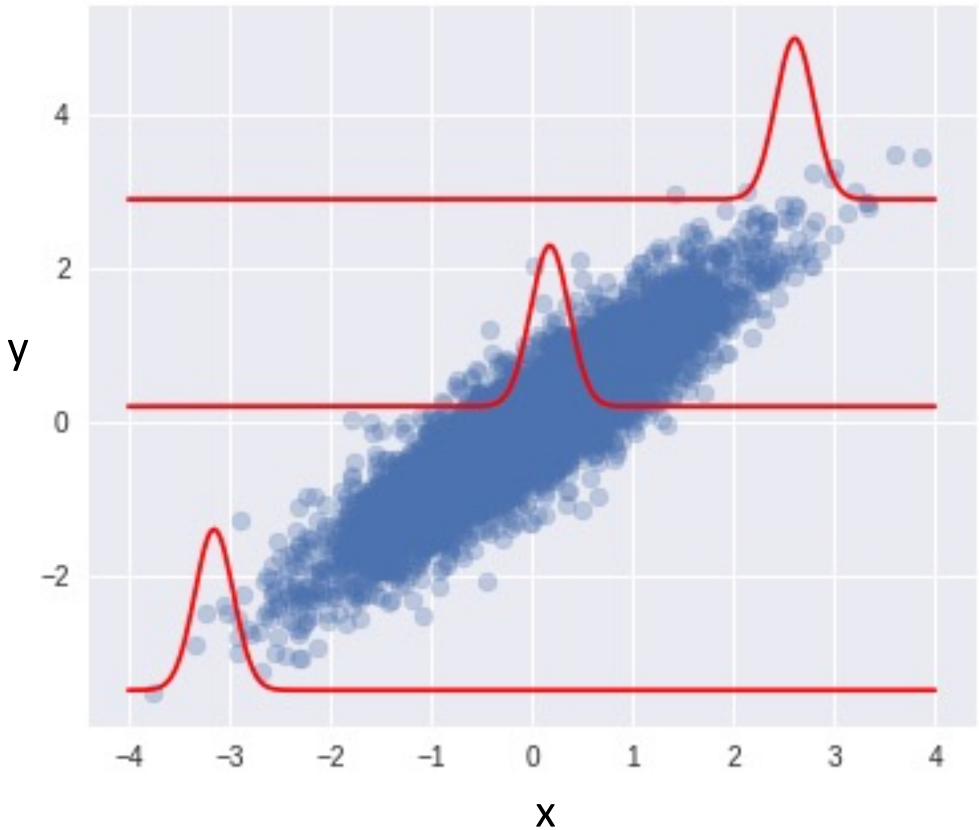
- Specify joint distribution over multiple variables
- Probabilities are computed as in univariate case, we now just have repeated summations or repeated integrals
- Discrete: $P((X, Y) \in A) = \sum_{(x,y) \in A} p(x, y)$
- Continuous: $P((X, Y) \in A) = \int_A \; p(x, y) dx dy$

Independence and conditioning

- X, Y are independent if
  - $P(X \in A, Y \in B) = P(X \in A)P(Y \in B)$
  - Similarly for densities: $p_{X,Y}(x, y) = p_X(x)p_Y(y)$
  - **Intuitively**: knowing value of Y reveals nothing about X
  - **Algebraically**: the joint on X,Y factorises!

- Conditional probability
  - $P(A|B) = \frac{P(A \cap B)}{P(B)}$
  - Similarly for densities $p(y|x) = \frac{p(x,y)}{p(x)}$
  - **Intuitively**: probability event A will occur given we know event B has occurred
  - **The Product Rule:** $P(A \cap B)$ **=** $P(A|B)\ P(B)$
  - X,Y independent equiv to $P(Y = y|X = x) = P(Y = y)$

Independence and conditioning



- Not independent: knowing the value of *y* gives you insight into the value that *x* will take

https://math.stackexchange.com/questions/3063616/variance-of-conditional-multivariate-gaussian

Inverting conditioning: Bayes' Theorem

Bayes

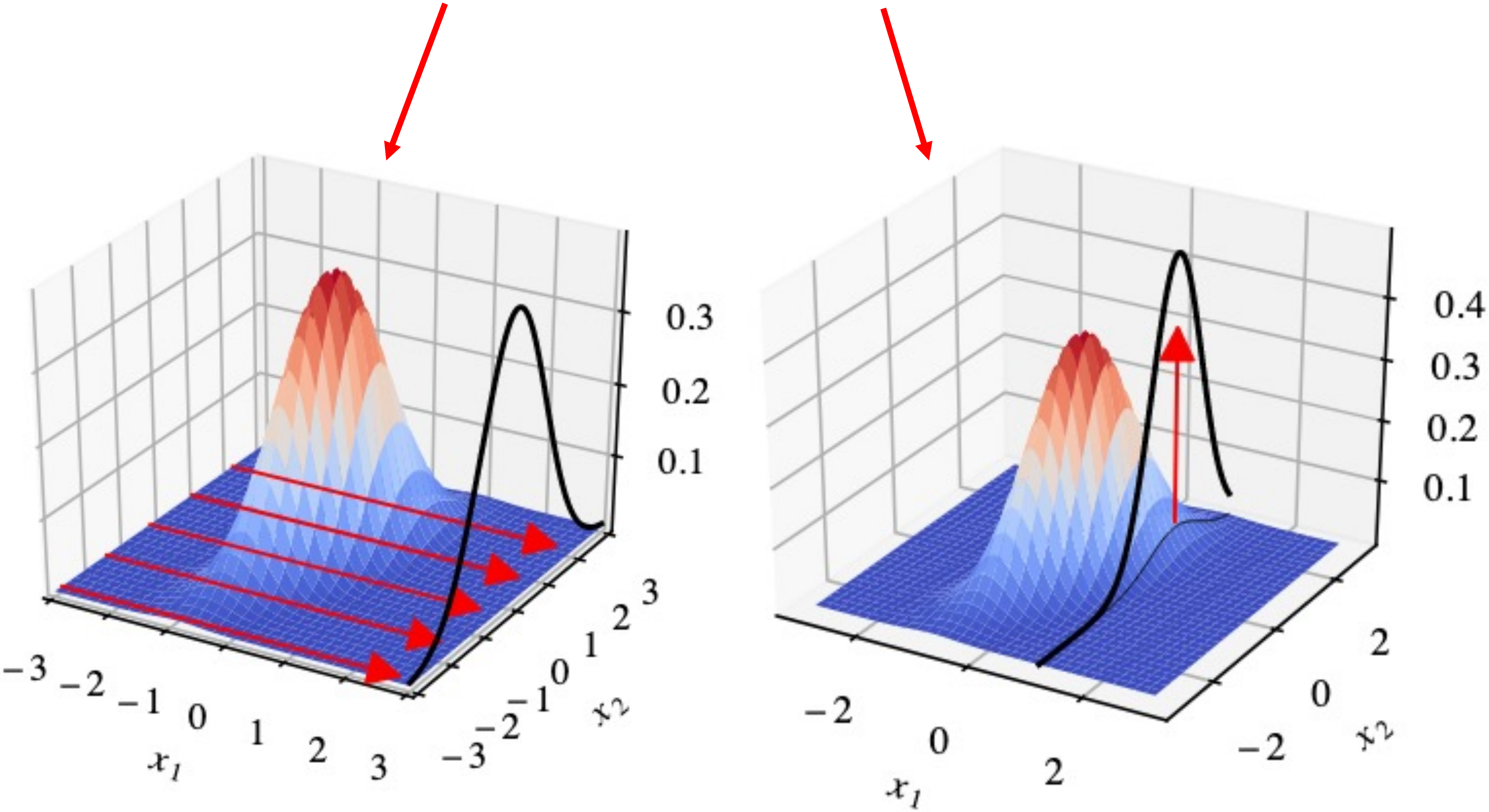
- In terms of events *A*, *B*
  - $P(A \cap B) = P(A|B)P(B) = P(B|A)P(A)$
  - $P(A|B) = \frac{P(B|A)\,P(A)}{P(B)}$
- Simple rule that lets us swap conditioning order

Inverting conditioning: Bayes' Theorem

Bayes

- In terms of events *A*, *B*
  - $P(A \cap B) = P(A|B)P(B) = P(B|A)P(A)$
  - $P(A|B) = \dfrac{P(B|A)\,P(A)}{P(B)}$
- Simple rule that lets us swap conditioning order
- Probabilistic and Bayesian inference make heavy use
  - Marginals: probabilities of individual variables
  - The Sum Rule of marginalisation: summing away all but r.v.'s of interest. $P(A) = \sum_b P(A, B = b)$

Marginalisation vs conditioning



https://motion.cs.illinois.edu/RoboticSystems/Probability.html

Mini Summary

- Probability spaces, axioms of probability
- Discrete vs continuous; Univariate vs multivariate
- Expectation, Variance
- Independence and conditioning
- Bayes rule and marginalisation

Next: Linear algebra primer/review

Vectors

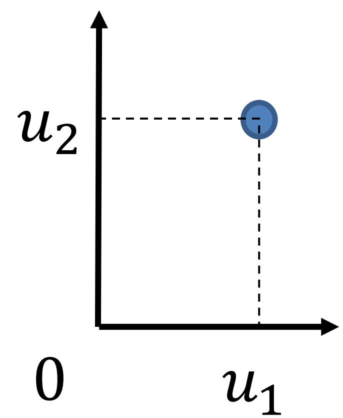
Link between geometric and algebraic interpretation of ML methods

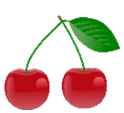
What are vectors?

Suppose $\boldsymbol{u} = [u_1, u_2]'$. What does $\boldsymbol{u}$ really represent?

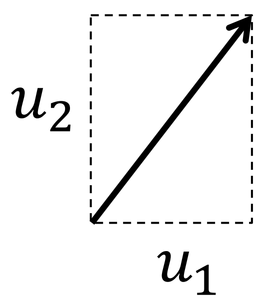
Ordered set of numbers $\{u_1, u_2\}$

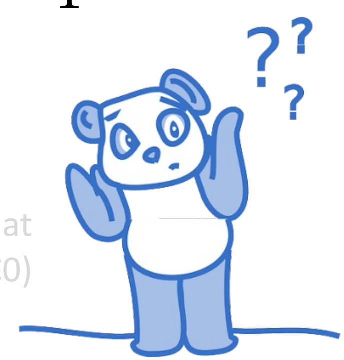
Cartesian coordinates of a point





A direction





art: OpenClipartVectors at pixabay.com (CC0)

Dot product: Algebraic definition

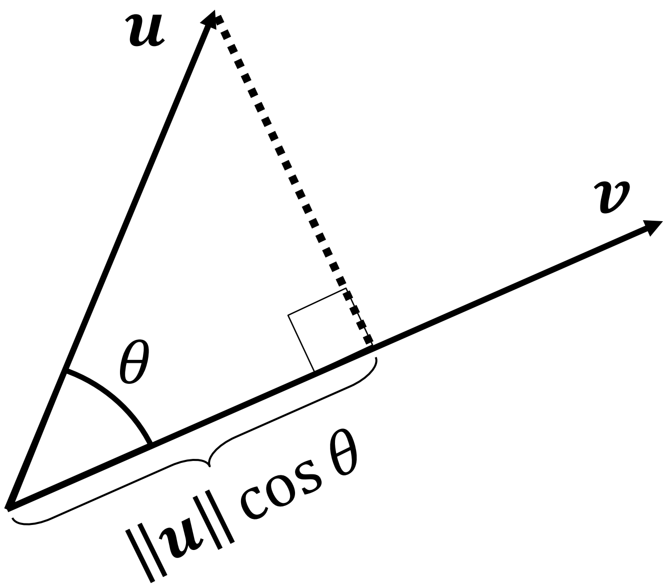
- Given two m-dimensional vectors $\boldsymbol{u}$ and $\boldsymbol{v}$, their dot product is $\boldsymbol{u} \cdot \boldsymbol{v} \equiv \boldsymbol{u}'\boldsymbol{v} \equiv \sum_{i=1}^{m} u_i v_i$
  - E.g., weighted sum of terms is a dot product $\boldsymbol{x}'\boldsymbol{w}$

- If k is a scalar, $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ are vectors then

$$(k\boldsymbol{a})'\boldsymbol{b} = k(\boldsymbol{a}'\boldsymbol{b}) = \boldsymbol{a}'(k\boldsymbol{b})$$
$$\boldsymbol{a}'(\boldsymbol{b} + \boldsymbol{c}) = \boldsymbol{a}'\boldsymbol{b} + \boldsymbol{a}'\boldsymbol{c}$$

Dot product: Geometric definition

- Given two m-dimensional Euclidean vectors $\boldsymbol{u}$ and $\boldsymbol{v}$, their dot product is $\boldsymbol{u} \cdot \boldsymbol{v} \equiv \boldsymbol{u}'\boldsymbol{v} \equiv \|\boldsymbol{u}\|\|\boldsymbol{v}\| \cos\theta$
  - $\|\boldsymbol{u}\|, \|\boldsymbol{v}\|$ are L_2 *norms* for $\boldsymbol{u}, \boldsymbol{v}$ also written as $\|\boldsymbol{u}\|_{\boldsymbol{2}}$
  - θ is the angle between the vectors



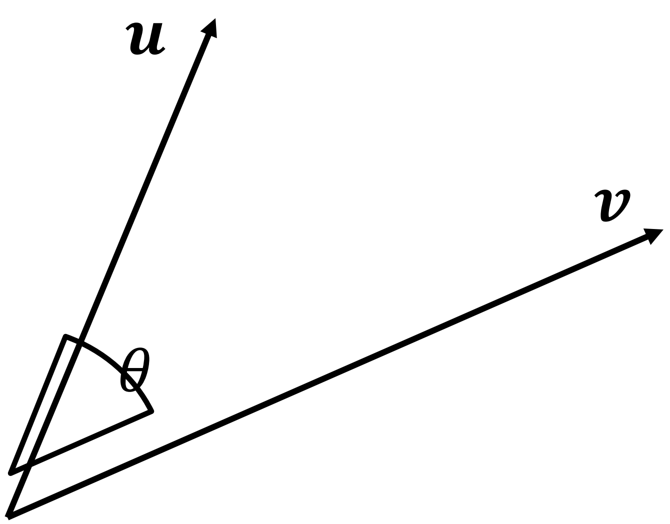
The *scalar projection* of $\boldsymbol{u}$ onto $\boldsymbol{v}$ is given by

$$u_{\boldsymbol{v}} = \|\boldsymbol{u}\| \cos\theta$$

Thus dot product is
$\boldsymbol{u}'\boldsymbol{v} = u_{\boldsymbol{v}}\|\boldsymbol{v}\| = v_{\boldsymbol{u}}\|\boldsymbol{u}\|$

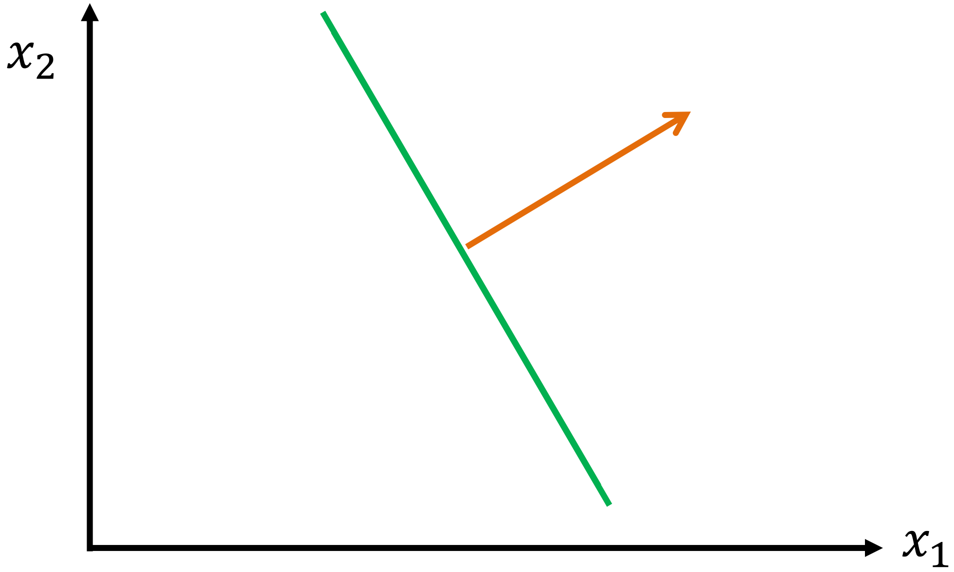
Geometric properties of the dot product

- If the two vectors are orthogonal then $\boldsymbol{u}'\boldsymbol{v} = 0$
- If the two vectors are parallel then $\boldsymbol{u}'\boldsymbol{v} = \|\boldsymbol{u}\|\|\boldsymbol{v}\|$, if they are anti-parallel then $\boldsymbol{u}'\boldsymbol{v} = -\|\boldsymbol{u}\|\|\boldsymbol{v}\|$
- $\boldsymbol{u}'\boldsymbol{u} = \|\boldsymbol{u}\|^2$, so $\|\boldsymbol{u}\| = \sqrt{\boldsymbol{u}'\boldsymbol{u}} = \sqrt{u_1^2 + \cdots + u_m^2}$ defines the Euclidean vector length



Hyperplanes and normal vectors

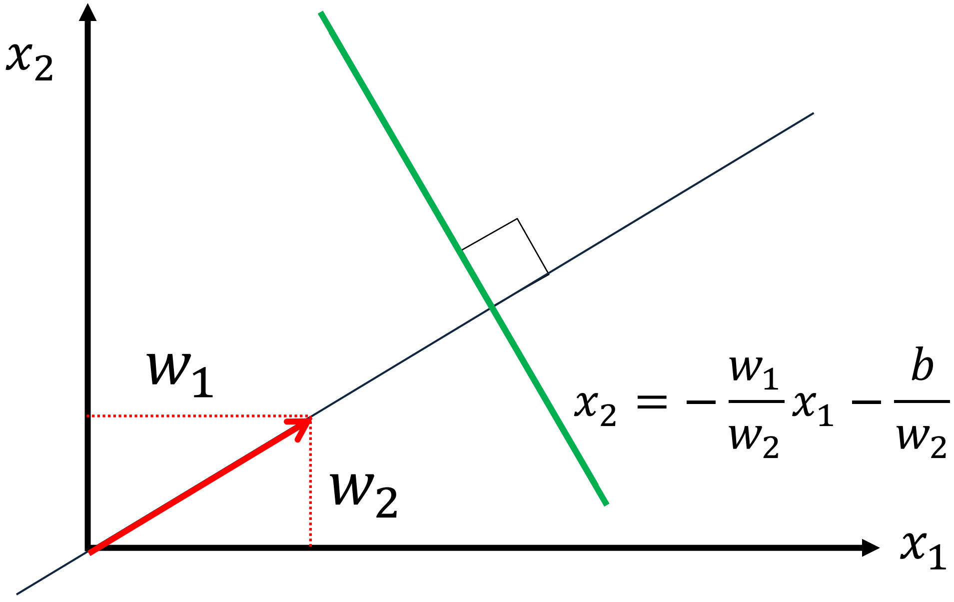
- A *hyperplane* defined by parameters $\boldsymbol{w}$ and b is a set of points $\boldsymbol{x}$ that satisfy $\boldsymbol{x}'\boldsymbol{w} + b = 0$
- In 2D, a hyperplane is a line: a line is a set of points that satisfy $w_1 x_1 + w_2 x_2 + b = 0$



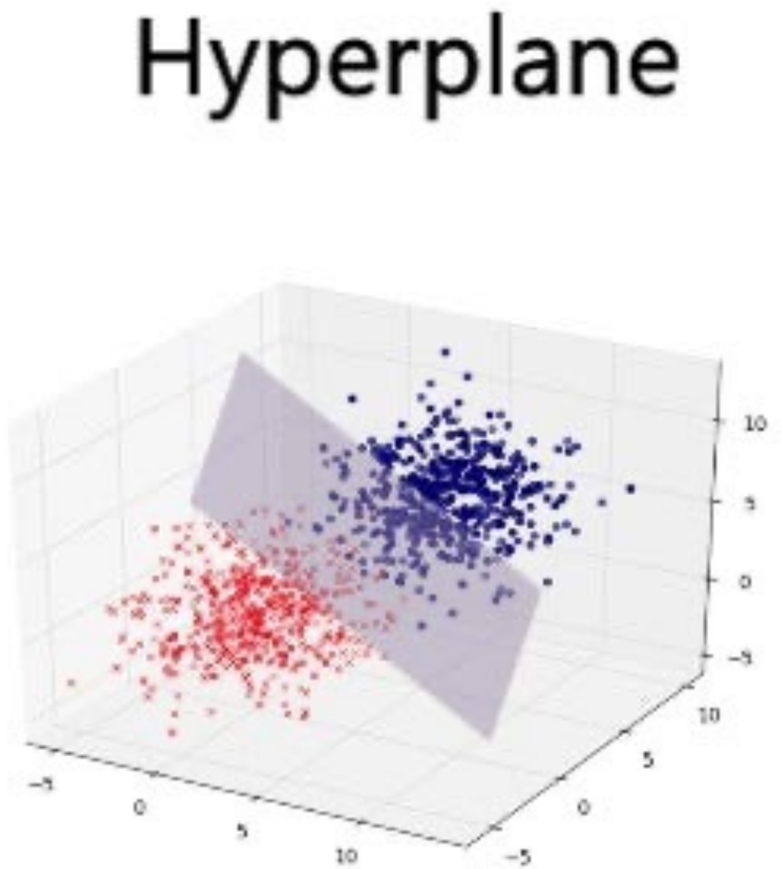
A *normal vector* for a hyperplane is a vector perpendicular to that hyperplane

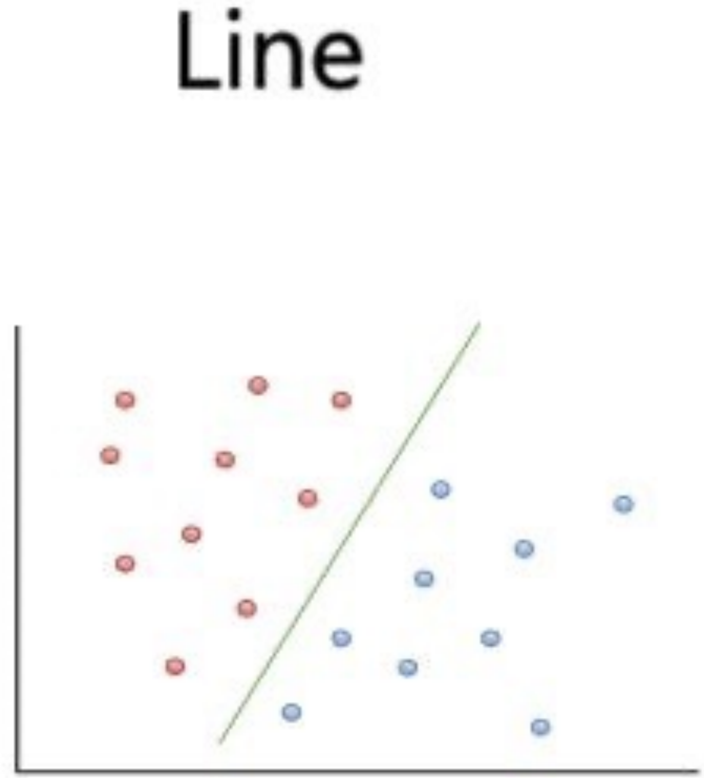
Hyperplanes and normal vectors

- Consider a line defined by w_1, w_2 and b
- Vector $\boldsymbol{w} = [w_1, w_2]'$ is a normal vector



Hyperplane vs line





L_1 and L_2 norms

- Throughout the subject we will often encounter norms that are functions $\mathbb{R}^n \to \mathbb{R}$ of a particular form
  * Intuitively, norms measure lengths of vectors in some sense
  * Often component of objectives or stopping criteria in optimisation-for-ML
- More specifically, we will often use the L_2 norm (*aka* Euclidean distance)

$$\|\boldsymbol{a}\| = \|\boldsymbol{a}\|_2 \equiv \sqrt{a_1^2 + \cdots + a_n^2}$$

- And also the L_1 norm (*aka* absolute norm or Manhattan distance)

$$\|\boldsymbol{a}\|_1 \equiv |a_1| + \cdots + |a_n|$$

Vector Spaces and Bases

Useful in interpreting matrices and some algorithms like PCA

Linear combinations, Independence

- A linear combination of vectors $v_1, \ldots, v_k \in V$ some vector space, is a new vector $\sum_{i=1}^{k} a_i v_i$ for some scalars $a_1, \ldots, a_k$
- A set of vectors $\{v_1, \ldots, v_k\} \subseteq V$ is called linearly dependent if one element v_j can be written as a linear combination of the other elements
- A set that isn't linearly dependent is linearly independent
- For formal definition of vector spaces: https://en.wikipedia.org/wiki/Vector_space#Definition

Spans, Bases

- The span of vectors $v_1, \ldots, v_k \in V$ is the set of all obtainable linear combinations (ranging over all scalar coefficients) of the vectors

- A set of vectors $B = \{v_1, \ldots, v_k\} \subseteq V$ is called a basis for a vector subspace $V' \subseteq V$ if
  1. The set B is linearly independent; and
  2. Every $\mathrm{v} \in V'$ is a linear combination of the set B.

- An orthonormal basis is a basis in which:
  1. Each pair of basis vectors are orthogonal (zero dot prod); and
  2. Each vector has norm equal to 1.

Matrices

Some useful facts for ML

Basic matrices

- A rectangular array, often denoted by upper-case, with two indices first for row, second for column
- Square matrix has equal dimensions (numbers of rows and columns)
- Matrix transpose **A**' or $\mathbf{A}^T$ of *m* by *n* matrix **A** is an *n* by *m* matrix with entries $A'_{ij}=A_{ji}$
- A square matrix **A** with **A**=**A**' is called symmetric
- The (square) identity matrix **I** has 1 on the diagonal, 0 off-diagonal
- Matrix inverse $\mathbf{A}^{-1}$ of square matrix **A** (if it exists) satisfies $\mathbf{A}^{-1}\mathbf{A}=\mathbf{I}$
- See more: https://en.wikipedia.org/wiki/Matrix_(mathematics)
  - Including matrix-matrix and matrix-vector products

Matrix eigenspectrum

- Scalar, vector pair (λ, v) are called an eigenvalue-eigenvector pair of a square matrix **A** if $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$
  - Intuition: matrix **A** doesn't rotate **v** it just stretches it
  - Intuition: the eigenvalue represents stretching factor
- In general eigenvalues may be zero, negative or even complex (imaginary) – we'll only encounter reals

Spectra of common matrices

- Eigenvalues of symmetric matrices are always real (no imaginary component)
- A matrix with linear dependent columns has some zero eigenvalues (called rank deficient) → no matrix inverse exists

Positive (semi)definite matrices

- A symmetric square matrix **A** is called positive semidefinite if for all vectors **v** we have $\mathbf{v}'\mathbf{A}\mathbf{v} \geq 0$.
  - Then **A** has non-negative eigenvalues
  - For example, any $\mathbf{A} = \mathbf{X}'\mathbf{X}$ since: $\mathbf{v}'\mathbf{X}'\mathbf{X}\mathbf{v} = \|\mathbf{X}\mathbf{v}\|^2 \geq 0$
- Further if $\mathbf{v}'\mathbf{A}\mathbf{v} > 0$ holds as a strict inequality then **A** is called positive definite
  - Then **A** has (strictly) positive eigenvalues

Mini Summary

- Vectors: Vector spaces, dot products, independence, hyperplanes
- Matrices: Eigenvalues, positive semidefinite matrices

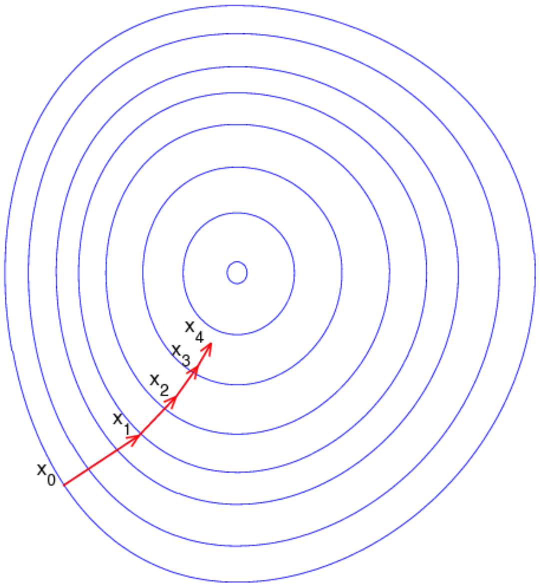
Next: Sequences and limits review/primer

Sequences and Limits

Sequences arise whenever we have iterations (e.g. training loops, growing data sample size). Limits tell us about where sequences tend towards.

Infinite Sequences

- Written like $x_1, x_2, \ldots$ or $\{x_i\}_{i \in \mathbb{N}}$
- Formally: a function from the positive (from 1) or non-negative (from 0) integers
- Index set: subscript set e.g. $\mathbb{N}$
- Sequences allow us to reason about test error when training data grows indefinitely, or training error (or a stopping criterion) when training runs arbitrarily long



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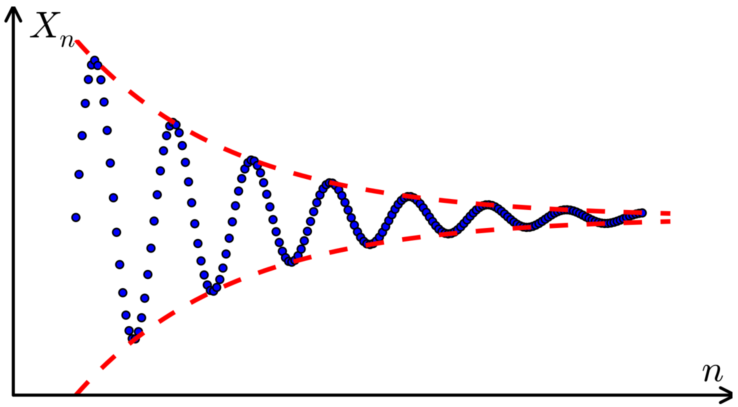
Limits and Convergence

- A sequence $\{x_i\}_{i\in\mathbb{N}}$ converges if its elements become and remain arbitrarily close to a fixed limit point L.
- Formally: $x_i \rightarrow L$ if, for all $\varepsilon > 0$, there exists $N \in \mathbb{N}$ such that for all $n \geq N$ we have $\|x_n - L\| < \varepsilon$

Notes:

- Epsilon ε represents distance of sequence to limit point
- Distance can be arbitrarily small
- Definition says we eventually get that close (at some finite N) and we stay *at least* that close for ever more



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Supremum

Generalising the maximum: When a sequence never quite peaks.

When does the Maximum Exist?

- Can you always take a max of a set?
- Finite sets: what's the max of {1, 7, 3, 2, 9}?
- Closed, bounded intervals: what's the max of [0,1]?
- Open, bounded intervals: what's the max of [0,1)?
- Open, unbounded intervals: what's the max of [0,∞)?

What about "Least Upper Bound"?

- Can you always take a least-upper-bound of a set? (much more often!)
- Finite sets: what's the max of {1, 7, 3, 2, 9}?

  max=9 LUB=9

- Closed, bounded intervals: what's the max of [0,1]?

  max=1 LUB=1

- Open, bounded intervals: what's the max of [0,1)?

  max=N/A LUB=1

- Open, unbounded intervals: what's the max of $[0,\infty)$?

  max=N/A LUB=∞

The Supremum

- Consider any subset S of the reals
- Upper bound $u \in \mathbb{R}^+$ of set S has: $u \geq x$ for all $x \in S$
- If u is no bigger than any other upper bound of S then it's called a least upper bound or supremum of S, written as $\sup(S)$ and pronounced "soup":
  * $z \geq u$ for all upper bounds $z \in \mathbb{R}^+$ of S

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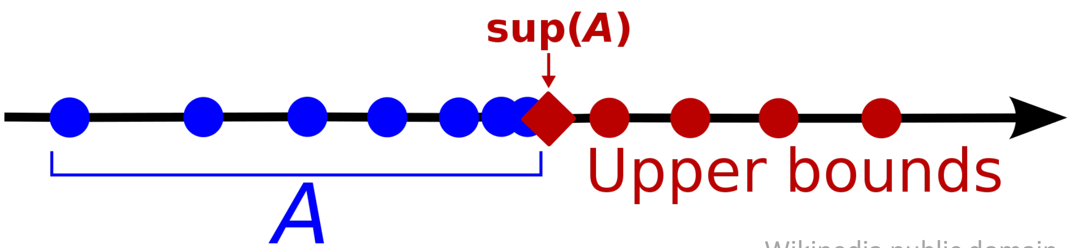
- When we don't know, or can't guarantee, that a set or sequence has a max, it is better to use its sup



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Infimum

- The greatest lower bound or infimum is generalisation of the minimum
- Written inf(S) pronounced “inf”
- Useful if we’re minimising training error but don’t know if the minimum is ever attained.

Mini Summary

- Sequences
- Limits of sequences
- Supremum is the new maximum

Next time: L02 Statistical schools

Jupyter notebooks setup and launch (at home)

Homework 0 (no credit) will be released soon