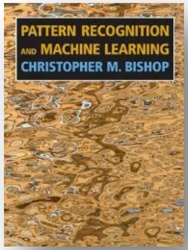
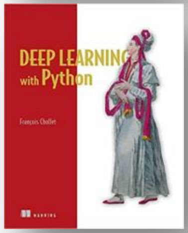
This lecture

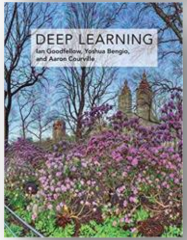
- Review: Probability theory
- Review: Linear algebra
- Review: Sequences and limits

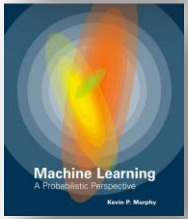
Textbooks

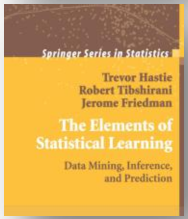
- We don’t have only one reference. We prefer to pick good bits from several. We may also supplement with other readings as we go.
- All are available free online or through the library digitally. See the Canvas lecture outline for links. Therefore, no need to buy**.**
- Primarily we refer to (good all 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*











Assessment

- Assessment components
  - Two projects – one group (w4-7), one individual (w9-11)
    - Each (25%)
    - Each has ~3 weeks to complete
  - Regular Quiz, ~fortnightly (5 x 2% = 10%)
  - Final Exam (40%)

- 50% hurdles applied to both **exam**, and **combined projects** ~~+ quiz~~

*updated 1/3 to reflect handbook; namely hurdle only applied to projects, not the quiz results. Note there are **two** separate hurdles.*

Machine Learning Basics

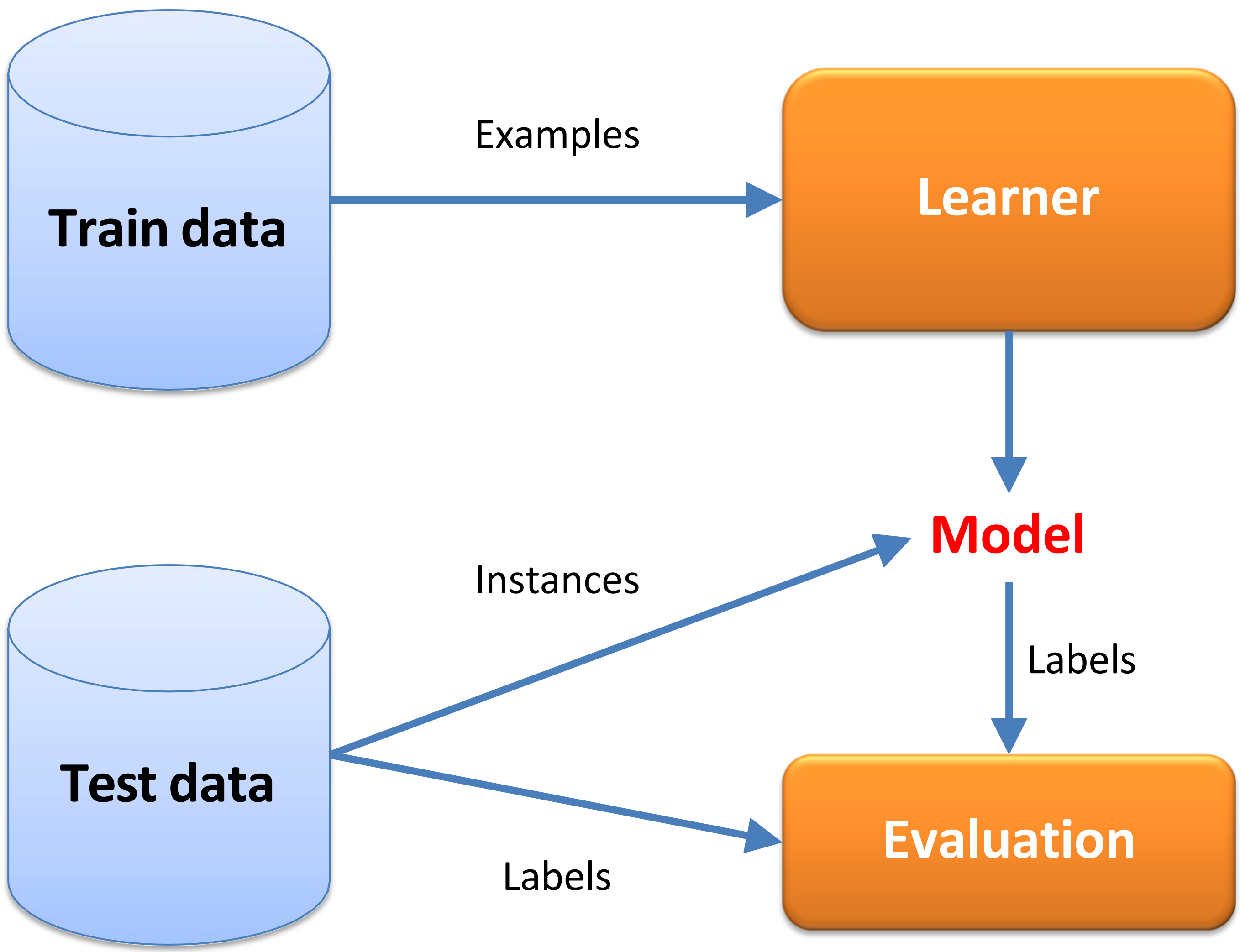
Terminology

- Input to a machine learning system can consist of
  - Instance: measurements about individual entities/objects
    a loan application
  - Attribute (aka Feature, explanatory var.): component of the instances
    the applicant's salary, number of dependents, etc.
  - Label (aka Response, dependent var.): an outcome that is categorical, numeric, etc.
    forfeit vs. paid off
  - Examples: instance coupled with label
    <(100k, 3), "forfeit">
  - Models: discovered relationship between attributes and/or label

Supervised vs unsupervised learning

	Data	Model used for
Supervised learning	Labelled	Predict labels on new instances
Unsupervised learning	Unlabelled	Cluster related instances; Project to fewer dimensions; Understand attribute relationships

Architecture of a supervised learner

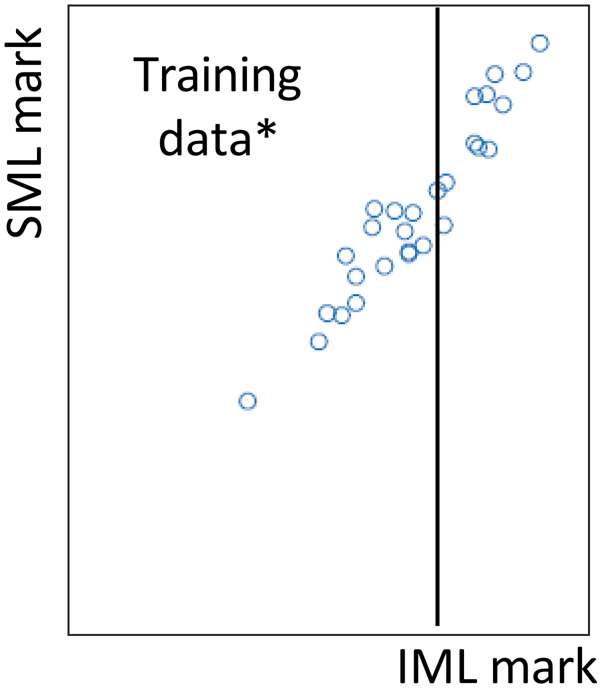


Evaluation (supervised learners)

- How you measure quality depends on your problem!
- Typical process
  - Pick an evaluation metric comparing label vs prediction
  - Procure an independent, labelled test set
  - “Average” the evaluation metric over the test set
- Example evaluation metrics
  - Accuracy, Contingency table, Precision-Recall, ROC curves
- When data poor, cross-validate

Probability theory

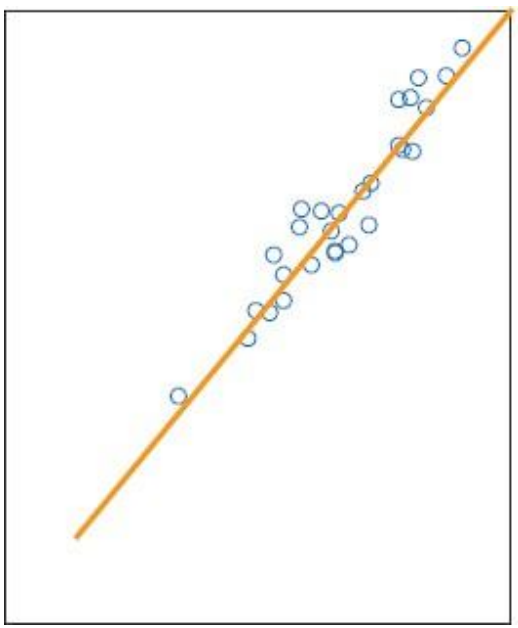
Data is noisy (almost always)



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

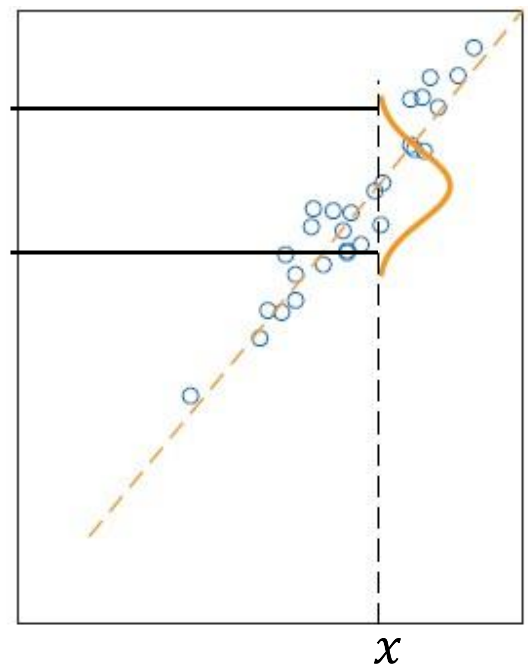
* synthetic data :)

Types of models



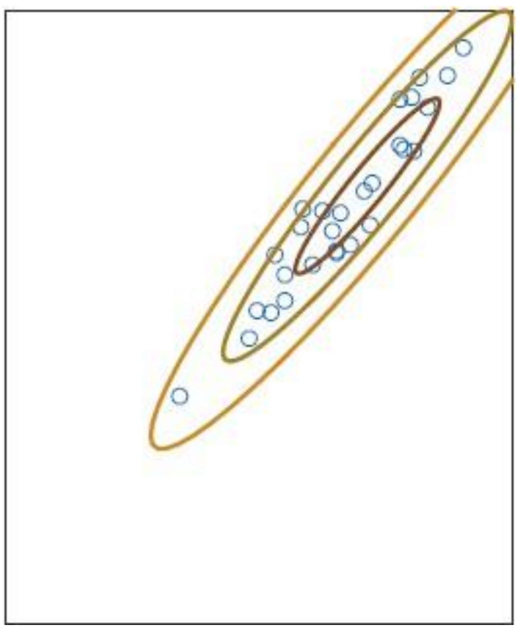
$$\hat{y} = f(x)$$

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*

1. F contains all of: Ω; all complements $\Omega \backslash f$, $f \in F$; the union of any countable set of events in F.
2. $P(f) \geq 0$ for every event $f \in F$.
3. $P\left(\bigcup_f f\right) = \sum_f P(f)$ for all countable sets of pairwise disjoint events.
4. $P(\Omega) = 1$

* We won't delve further into advanced probability theory, which starts with measure theory – a beautiful subject and the only way to "fully" formulate probability.

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*

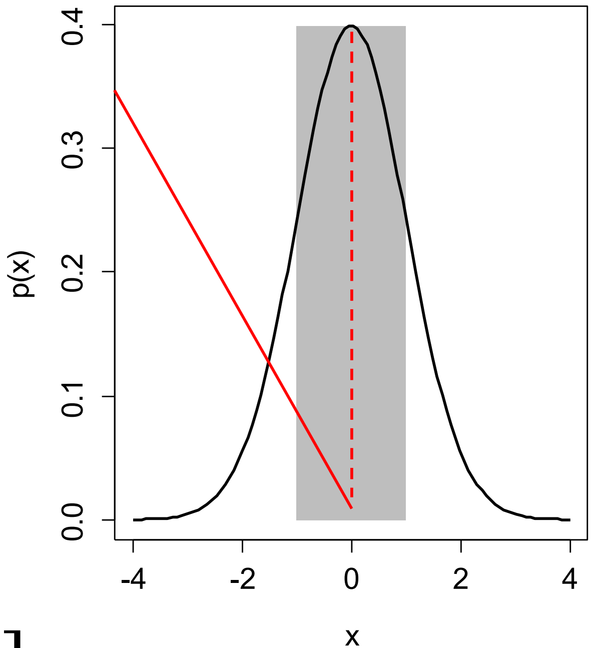
- Example: *X* winnings on \$5 bet on even die roll
  - *X* maps 1,3,5 to -5
    X maps 2,4,6 to 5
  - P(*X*=5) = P(*X*=-5) = ½

Discrete vs. continuous distributions

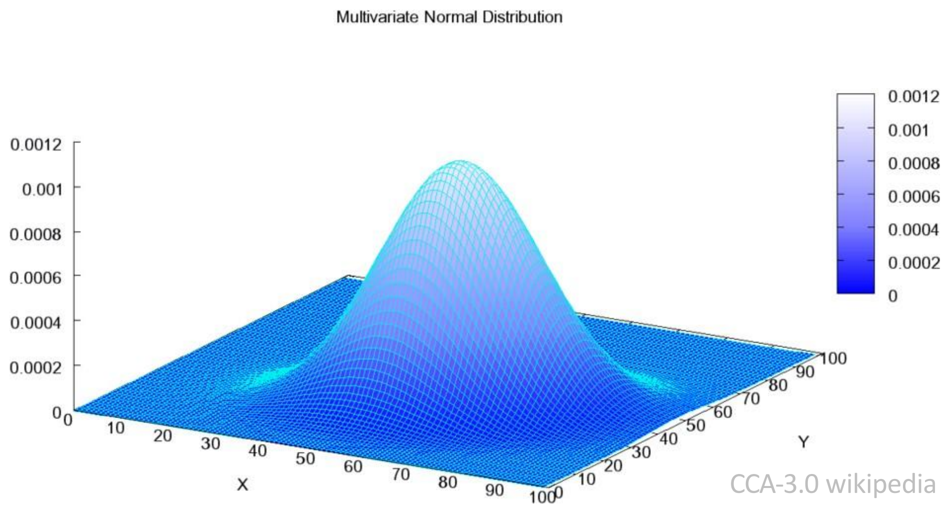
- Discrete distributions
  - Govern r.v. taking discrete values
  - Described by probability mass function p(x) which is P(X=x)
  - $P(X \leq x) = \sum_{a=-\infty}^{x} p(a)$
  - **Examples**: Bernoulli, Binomial, Multinomial, Poisson
- Continuous distributions
  - Govern real-valued r.v.
  - Cannot talk 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: $p_{X,\mathrm{F}}(x, y) = p_X(x) p_{\mathrm{F}}(y)$
  - **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
  - X,Y independent equiv to $P(Y = y|X = x) = P(Y = y)$

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
- Probabilistic and Bayesian inference make heavy use
  - Marginals: probabilities of individual variables
  - Marginalisation: summing away all but r.v.'s of interest

    $P(A) = \sum_b P(A, B = b)$

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

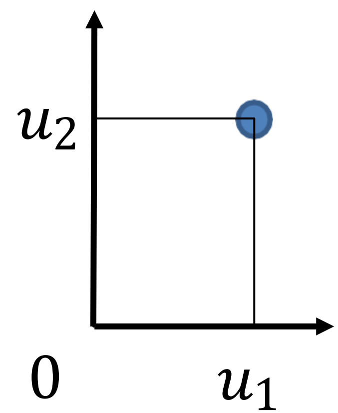
Link between geometric and algebraic interpretation of ML methods

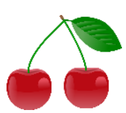
What are vectors?

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

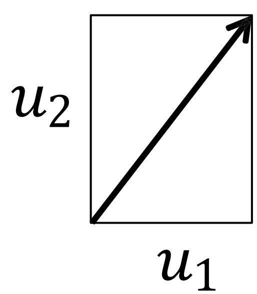
Ordered set of numbers $\{u_1, u_2\}$

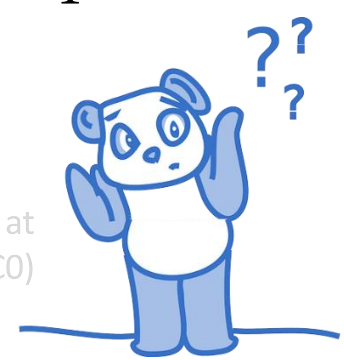
Cartesian coordinates of a point





A direction





art: OpenClipartVectors at pixabay.com (CC0)

Dot product: Algebraic definition

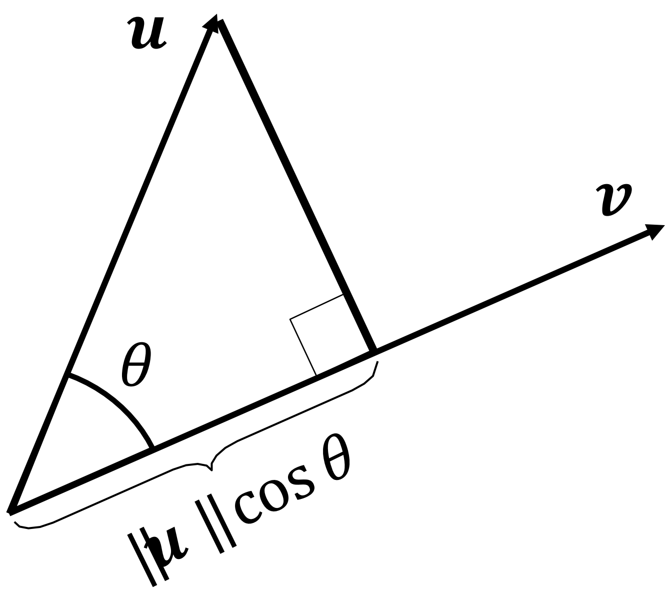
- Given two m-dimensional vectors $\boldsymbol{u}$ and $\boldsymbol{v}$, their dot product is $\boldsymbol{u} \cdot \boldsymbol{v} \equiv \boldsymbol{u}'\boldsymbol{v} \equiv \sum_{i31}^{m} u_i v_i$
  - E.g., weighted sum of terms is a dot product $\boldsymbol{x}'\boldsymbol{w}$
- If k is a scalar, $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ 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

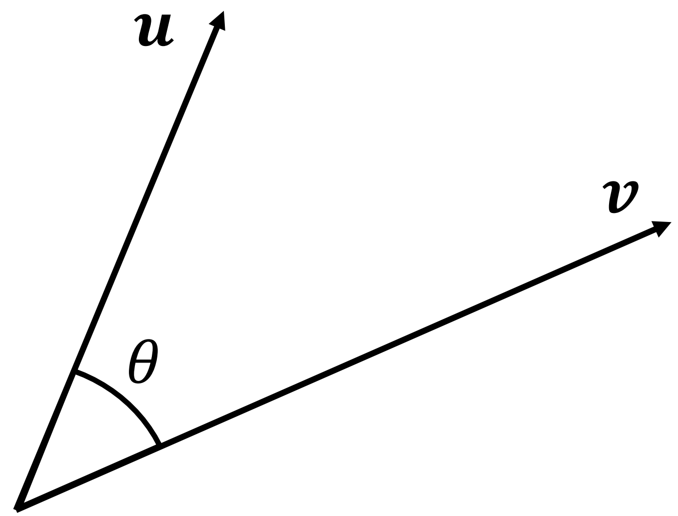
$$u_{\boldsymbol{v}} = \|\boldsymbol{u}\| \cos\theta$$

Thus dot product is

$$\boldsymbol{u}'\boldsymbol{v} = u_{\boldsymbol{v}}\|\boldsymbol{v}\| = v_{\boldsymbol{u}}\|\boldsymbol{u}\|$$

Geometric properties of the dot product

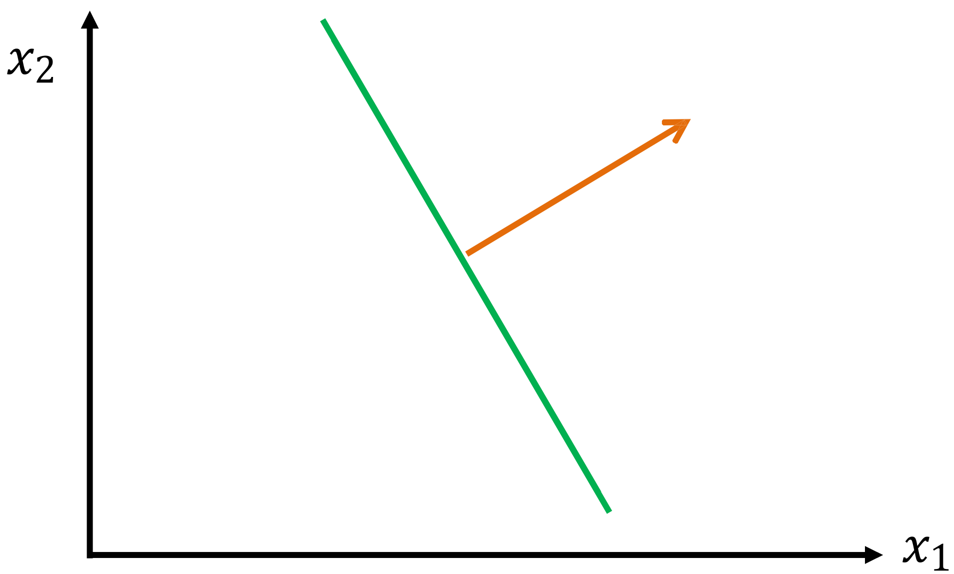
- If the two vectors are orthogonal then $\boldsymbol{u}'\boldsymbol{v} = 0$
- If the two vectors are parallel then $\boldsymbol{u}'\boldsymbol{v} = \|\boldsymbol{u}\|\|\boldsymbol{v}\|$, if they are anti-parallel then $\boldsymbol{u}'\boldsymbol{v} = -\|\boldsymbol{u}\|\|\boldsymbol{v}\|$
- $\boldsymbol{u}'\boldsymbol{u}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

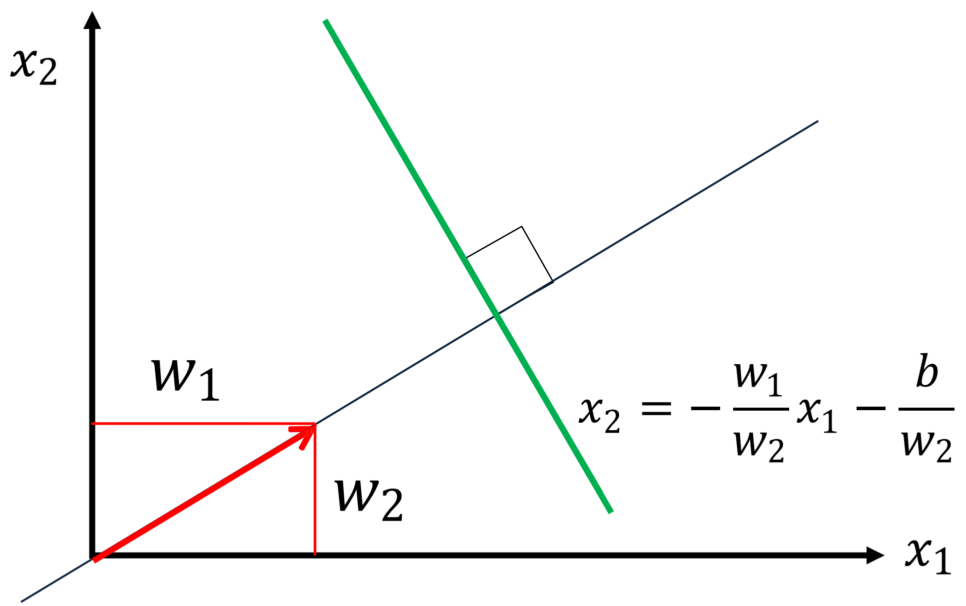
- Consider a hyperplane defined by parameters $\boldsymbol{w}$ and b. Note that $\boldsymbol{w}$ is itself a vector

- Lemma: Vector $\boldsymbol{w}$ is normal to the hyperplane

- Proof sketch:
  - Choose any two points $\boldsymbol{u}$ and $\boldsymbol{v}$ on the hyperplane. Note that vector $(\boldsymbol{u}-\boldsymbol{v})$ lies on the hyperplane
  - Consider dot product $(\boldsymbol{u}-\boldsymbol{v})'\boldsymbol{w} = \boldsymbol{u}'\boldsymbol{w} - \boldsymbol{v}'\boldsymbol{w}$
    $$= (\boldsymbol{u}'\boldsymbol{w} + b) - (\boldsymbol{v}'\boldsymbol{w} + b) = 0$$
  - Thus $(\boldsymbol{u}-\boldsymbol{v})$ lies on the hyperplane, but is perpendicular to $\boldsymbol{w}$, and so $\boldsymbol{w}$ is a vector normal

Example in 2D

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



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

- For formal definition of vector spaces:
  https://en.wikipedia.org/wiki/Vector_space#Definition
- A linear combination of vectors $v_1, \dots, v_k \in V$ some vector space, is a new vector $\sum_{i=1}^{k} a_i v_i$ for some scalars $a_1, \dots, a_k$
- A set of vectors $\{v_1, \dots, v_k\} \subseteq V$ 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

Spans, Bases

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

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

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

Matrices

Some useful facts for ML

Basic matrices

- See more: https://en.wikipedia.org/wiki/Matrix_(mathematics)
  - Including matrix-matrix and matrix-vector products
- 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 $\mathbf{A}'$ or $\mathbf{A}^T$ of m by n matrix $\mathbf{A}$ is an n by m matrix with entries $A'_{ij}=A_{ji}$
- A square matrix $\mathbf{A}$ with $\mathbf{A}=\mathbf{A}'$ is called symmetric
- The (square) identity matrix $\mathbf{I}$ has 1 on the diagonal, 0 off-diagonal
- Matrix inverse $\mathbf{A}^{-1}$ of square matrix $\mathbf{A}$ (if it exists) satisfies $\mathbf{A}^{-1}\mathbf{A}=\mathbf{I}$

Matrix eigenspectrum

- Scalar, vector pair (λ, v) are called an eigenvalue-eigenvector pair of a square matrix **A** if $\mathbf{Av} = \lambda\mathbf{v}$
  - 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

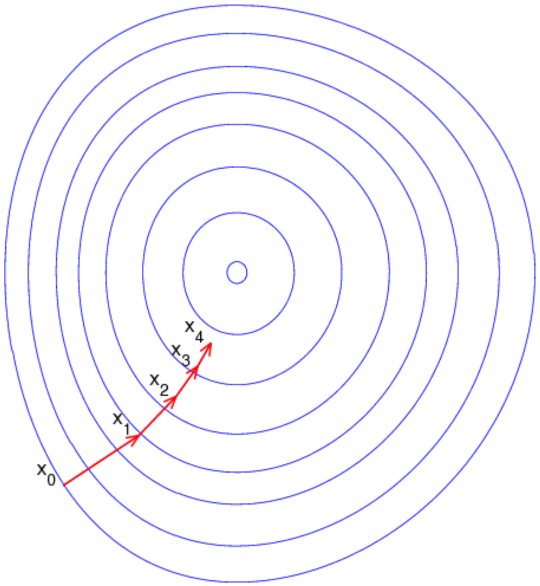
Next: Sequences and limits review/primer

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 $\{x_i\}_{i \in \mathbb{N}}$
- Index set: subscript set e.g. $\mathbb{N}$



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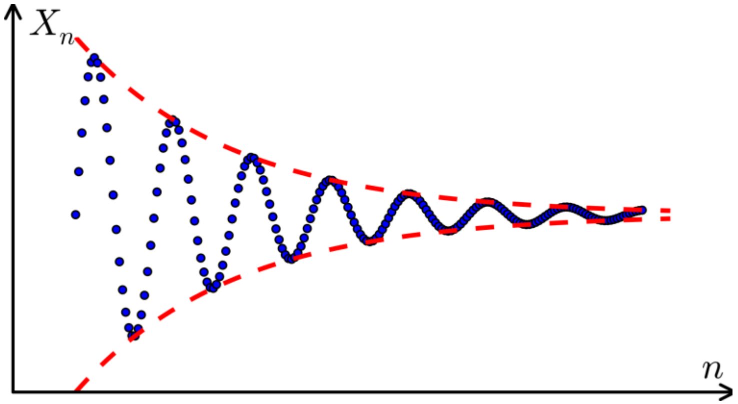
- Sequences allow us to reason about test error when training data grows indefinitely, or training error (or a stopping criterion) when training runs arbitrarily long

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: $x_i \to L$ 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 $[0,\infty)$?

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 $u \in \mathbb{R}^8$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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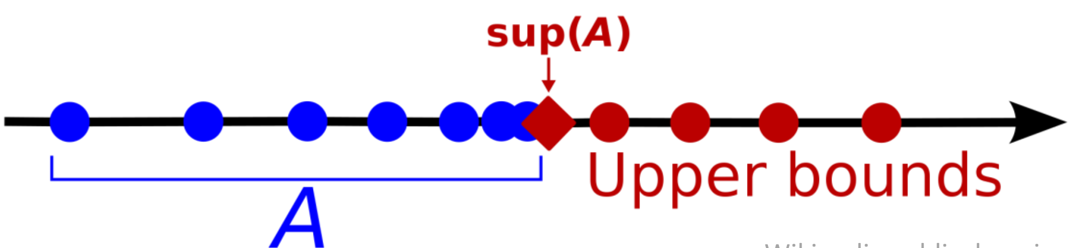
- When we don't know, or can't guarantee, that a set or sequence has a max, it is better to use its sup



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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.