Supervised Learning – Classification

COMP9417 Machine Learning and Data Mining

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Acknowledgements

Material derived from slides for the book
"Elements of Statistical Learning (2nd Ed.)" by T. Hastie,
R. Tibshirani & J. Friedman. Springer (2009)
http://statweb.stanford.edu/~tibs/ElemStatLearn/

Material derived from slides for the book
"Machine Learning: A Probabilistic Perspective" by P. Murphy
MIT Press (2012)
http://www.cs.ubc.ca/~murphyk/MLbook

Material derived from slides for the book
"Machine Learning" by P. Flach
Cambridge University Press (2012)
http://cs.bris.ac.uk/~flach/mlbook

Material derived from slides for the book
"Bayesian Reasoning and Machine Learning" by D. Barber
Cambridge University Press (2012)
http://www.cs.ucl.ac.uk/staff/d.barber/brml

Material derived from slides for the book
"Machine Learning" by T. Mitchell
McGraw-Hill (1997)
http://www-2.cs.cmu.edu/~tom/mlbook.html

Material derived from slides for the course
"Machine Learning" by A. Srinivasan
BITS Pilani, Goa, India (2016)

Aims

This lecture will introduce you to machine learning approaches to the problem of *classification*. Following it you should be able to reproduce theoretical results, outline algorithmic techniques and describe practical applications for the topics:

- describe distance measures and how they are used in classification
- outline the basic k-nearest neighbour classification method
- define MAP and ML inference using Bayes theorem
- define the Bayes optimal classification rule in terms of MAP inference
- outline the Naive Bayes classification algorithm
- describe typical applications of Naive Bayes for text classification
- outline the Perceptron classification algorithm
- outline the logistic regression classification algorithm

Note: slides with titles marked * are for background only.

Introduction

Classification (sometimes called *concept learning*) methods dominate machine learning . . .

. . . however, they often don't have convenient mathematical properties like regression, so are more complicated to analyse. The idea is to learn a *classifier*, which is usually a function mapping from an input data point to one of a set of discrete outputs, i.e., the *classes*.

We will mostly focus on their advantages and disadvantages as learning methods first, and point to unifying ideas and approaches where applicable. In this lecture we focus on classification methods that are essentially *linear models* . . .

and in later lectures we will see other, more expressive, classifier learning methods.

Nearest neighbour classification

- Related to the simplest form of learning: rote learning or memorization
  - Training instances are searched for instance that **most closely resembles** new or *query* instance
  - The *instances* themselves represent the knowledge
  - Called: *instance-based*, *memory-based* learning or *case-based* learning; often a form of *local* learning
- The *similarity* or *distance* function defines "learning", i.e., how to go beyond simple memorization
- Intuitive idea — instances "close by", i.e., neighbours or *exemplars*, should be classified similarly
- Instance-based learning is *lazy* learning
- Methods: *nearest-neighbour*, *k-nearest-neighbour*, *lowess*, ...
- Ideas also important for *unsupervised* methods, e.g., clustering (later lectures)

Minkowski distance

Minkowski distance If $\mathcal{X} = \mathbb{R}^d$, the *Minkowski distance* of order $p > 0$ is defined as

$$\text{Dis}_p(\mathbf{x}, \mathbf{y}) = \left(\sum_{j=1}^{d} |x_j - y_j|^p \right)^{1/p} = ||\mathbf{x} - \mathbf{y}||_p$$

where $||\mathbf{z}||_p = \left(\sum_{j=1}^{d} |z_j|^p \right)^{1/p}$ is the p-*norm* (sometimes denoted L_p norm) of the vector $\mathbf{z}$.

Minkowski distance

- The 2-norm refers to the familiar *Euclidean distance*

$$\text{Dis}_2(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{j=1}^{d}(x_j - y_j)^2} = \sqrt{(\mathbf{x} - \mathbf{y})^{\mathrm{T}}(\mathbf{x} - \mathbf{y})}$$

  which measures distance 'as the crow flies'.

- The 1-*norm* denotes *Manhattan distance*, also called *cityblock distance*:

$$\text{Dis}_1(\mathbf{x}, \mathbf{y}) = \sum_{j=1}^{d} |x_j - y_j|$$

  This is the distance if we can only travel along coordinate axes.

Minkowski distance

- If we now let p grow larger, the distance will be more and more dominated by the largest coordinate-wise distance, from which we can infer that $\text{Dis}_\infty(\mathbf{x}, \mathbf{y}) = \max_j |x_j - y_j|$; this is also called *Chebyshev distance*.
- You will sometimes see references to the 0-*norm* (or L_0 norm) which counts the number of non-zero elements in a vector. The corresponding distance then counts the number of positions in which vectors $\mathbf{x}$ and $\mathbf{y}$ differ. This is not strictly a Minkowski distance; however, we can define it as

$$\text{Dis}_0(\mathbf{x}, \mathbf{y}) = \sum_{j=1}^{d} (x_j - y_j)^0 = \sum_{j=1}^{d} I[x_j = y_j]$$

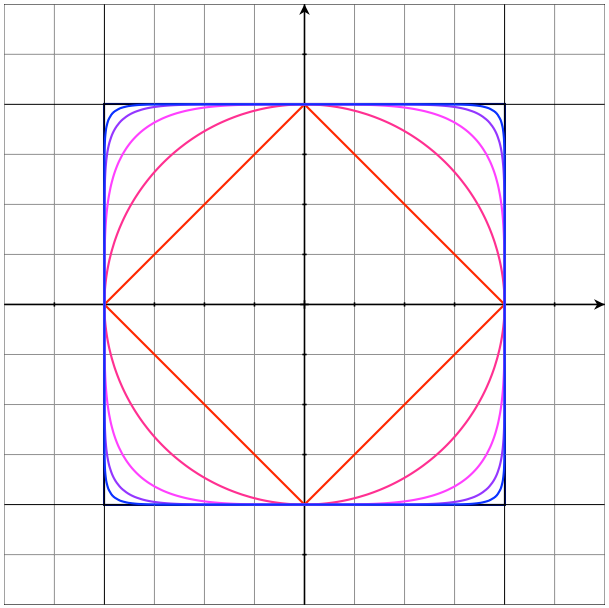
under the understanding that $x^0 = 0$ for $x = 0$ and 1 otherwise.

Minkowski distance

Sometimes the data $\mathcal{X}$ is not naturally in $\mathbb{R}^d$, but if we can turn it into Boolean features, or character sequesnces, we can still apply distance measures. For example:

- If $\mathbf{x}$ and $\mathbf{y}$ are binary strings, this is also called the *Hamming distance*. Alternatively, we can see the Hamming distance as the number of bits that need to be flipped to change $\mathbf{x}$ into $\mathbf{y}$.
- For non-binary strings of unequal length this can be generalised to the notion of *edit distance* or *Levenshtein distance*.

Circles and ellipses



Lines connecting points at order-p Minkowski distance 1 from the origin for (from inside) $p = 0.8$; $p = 1$ (Manhattan distance, the rotated square in red); $p = 1.5$; $p = 2$ (Euclidean distance, the violet circle); $p = 4$; $p = 8$; and $p = \infty$ (Chebyshev distance, the blue rectangle). Notice that for points on the coordinate axes all distances agree. For the other points, our reach increases with p; however, if we require a rotation-invariant distance metric then Euclidean distance is our only choice.

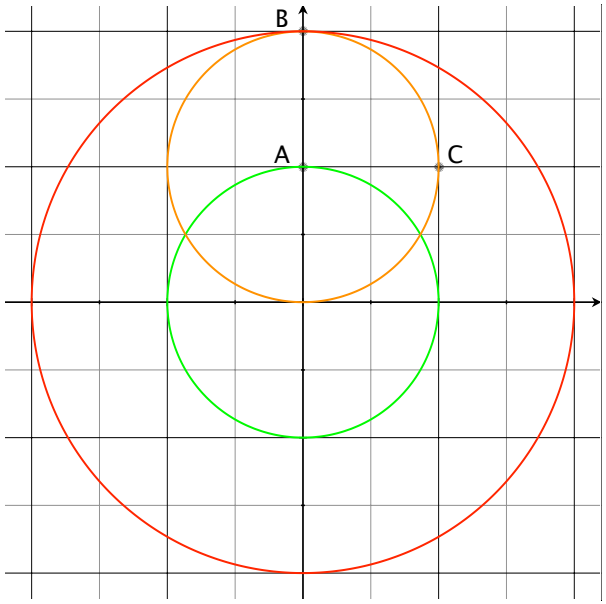
Distance metric

Distance metric Given an instance space $\mathcal{X}$, a *distance metric* is a function $\mathrm{Dis} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ such that for any $x, y, z \in \mathcal{X}$:

- distances between a point and itself are zero: $\mathrm{Dis}(x, x) = 0$;
- all other distances are larger than zero: if $x \neq y$ then $\mathrm{Dis}(x, y) > 0$;
- distances are symmetric: $\mathrm{Dis}(y, x) = \mathrm{Dis}(x, y)$;
- detours can not shorten the distance: $\mathrm{Dis}(x, z) \leq \mathrm{Dis}(x, y) + \mathrm{Dis}(y, z)$.

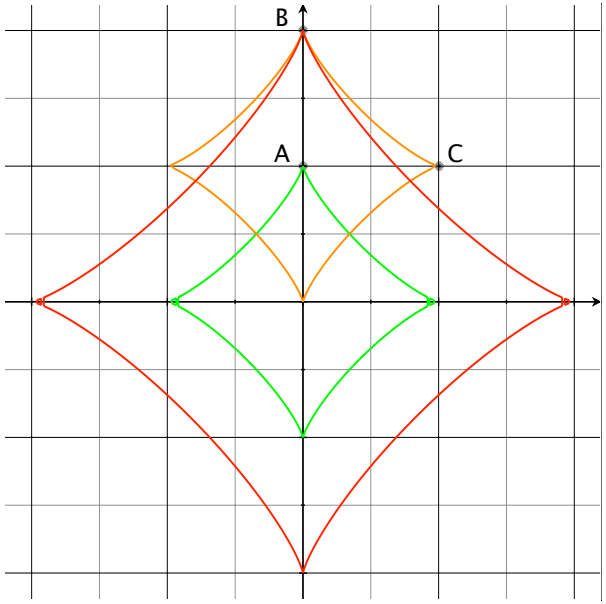
If the second condition is weakened to a non-strict inequality – i.e., $\mathrm{Dis}(x, y)$ may be zero even if $x \neq y$ – the function Dis is called a *pseudo-metric*.

The triangle inequality – Minkowski distance for $p = 2$



The green circle connects points the same Euclidean distance (i.e., Minkowski distance of order $p = 2$) away from the origin as A. The orange circle shows that B and C are equidistant from A. The red circle demonstrates that C is closer to the origin than B, which conforms to the triangle inequality.

The triangle inequality – Minkowski distance for $p \leq 1$



With Manhattan distance ($p = 1$), B and C are equally close to the origin and also equidistant from A. With $p < 1$ (here, $p = 0.8$) C is further away from the origin than B; since both are again equidistant from A, it follows that travelling from the origin to C via A is quicker than going there directly, which violates the triangle inequality.

Mahalanobis distance *

Often, the shape of the ellipse is estimated from data as the inverse of the covariance matrix: $\mathbf{M} = \mathbf{\Sigma}^{-1}$. This leads to the definition of the *Mahalanobis distance*

$$\text{Dis}_M(\mathbf{x}, \mathbf{y}|\mathbf{\Sigma}) = \sqrt{(\mathbf{x} - \mathbf{y})^{\mathrm{T}} \mathbf{\Sigma}^{-1} (\mathbf{x} - \mathbf{y})}$$

Using the covariance matrix in this way has the effect of decorrelating and normalising the features.

Clearly, Euclidean distance is a special case of Mahalanobis distance with the identity matrix $\mathbf{I}$ as covariance matrix: $\text{Dis}_2(\mathbf{x}, \mathbf{y}) = \text{Dis}_M(\mathbf{x}, \mathbf{y}|\mathbf{I})$.

Means and distances

The arithmetic mean minimises squared Euclidean distance *The arithmetic mean $\boldsymbol{\mu}$ of a set of data points D in a Euclidean space is the unique point that minimises the sum of squared Euclidean distances to those data points.*

Proof. We will show that $\arg\min_{\mathbf{y}} \sum_{\mathbf{x}\in D} ||\mathbf{x}-\mathbf{y}||^2 = \boldsymbol{\mu}$, where $||\cdot||$ denotes the 2-norm. We find this minimum by taking the gradient (the vector of partial derivatives with respect to y_i) of the sum and setting it to the zero vector:

$$\nabla_{\mathbf{y}} \sum_{\mathbf{x}\in D} ||\mathbf{x}-\mathbf{y}||^2 = -2 \sum_{\mathbf{x}\in D} (\mathbf{x}-\mathbf{y}) = -2 \sum_{\mathbf{x}\in D} \mathbf{x} + 2|D|\mathbf{y} = \mathbf{0}$$

from which we derive $\mathbf{y} = \frac{1}{|D|} \sum_{\mathbf{x}\in D} \mathbf{x} = \boldsymbol{\mu}$.

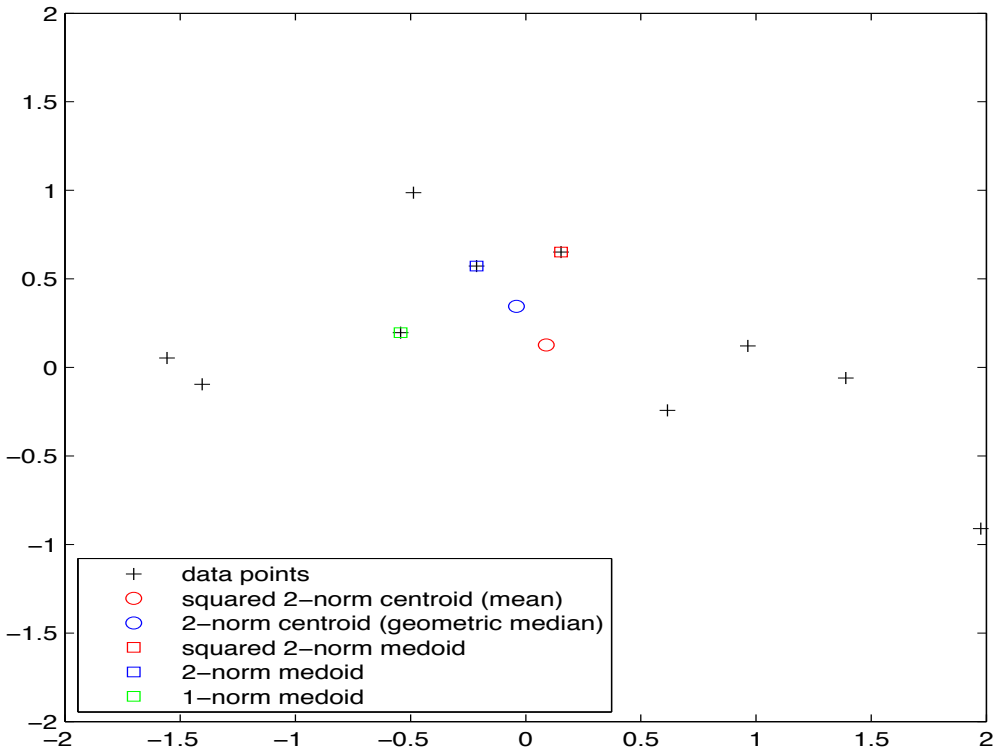
Means and distances

- Notice that minimising the sum of squared Euclidean distances of a given set of points is the same as minimising the *average* squared Euclidean distance.
- You may wonder what happens if we drop the square here: wouldn't it be more natural to take the point that minimises total Euclidean distance as exemplar?
- This point is known as the *geometric median*, as for univariate data it corresponds to the median or 'middle value' of a set of numbers. However, for multivariate data there is no closed-form expression for the geometric median, which needs to be calculated by successive approximation.

Means and distances

- In certain situations it makes sense to restrict an exemplar to be one of the given data points. In that case, we speak of a *medoid*, to distinguish it from a *centroid* which is an exemplar that doesn't have to occur in the data.
- Finding a medoid requires us to calculate, for each data point, the total distance to all other data points, in order to choose the point that minimises it. Regardless of the distance metric used, this is an $O(n^2)$ operation for n points.
- So for medoids there is no computational reason to prefer one distance metric over another.
- There may be more than one medoid.

Centroids and medoids

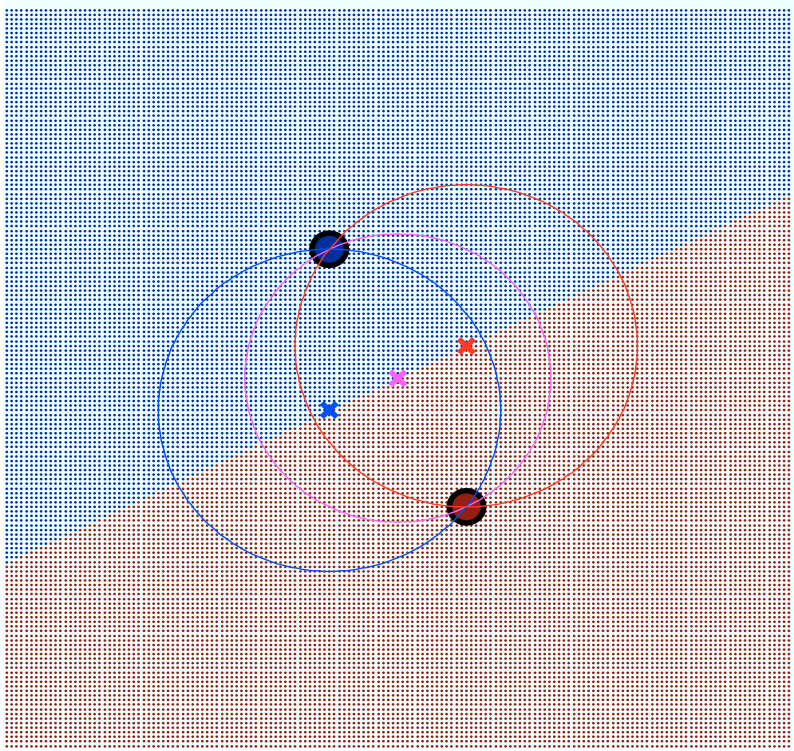


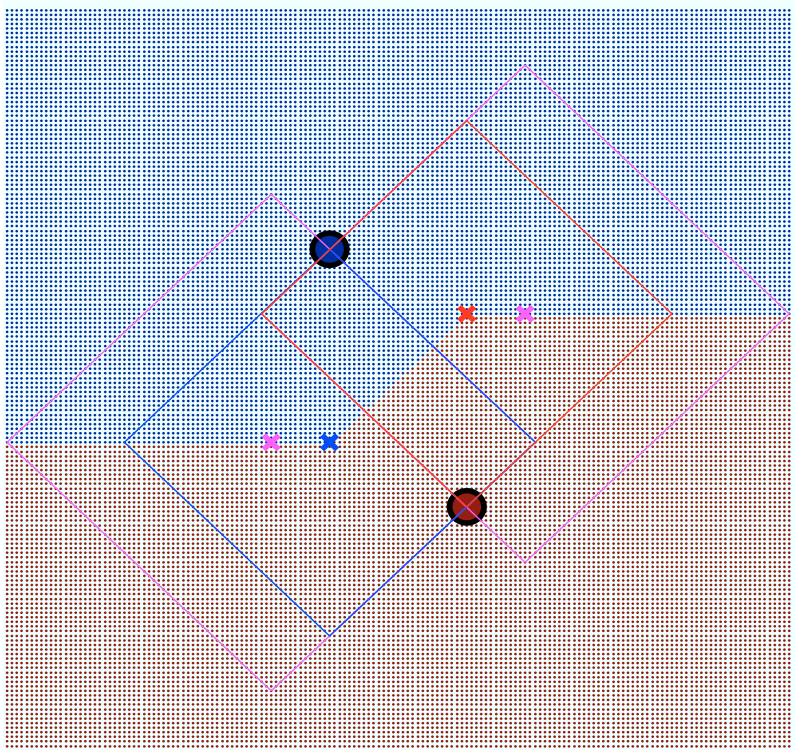
A small data set of 10 points, with circles indicating centroids and squares indicating medoids (the latter must be data points), for different distance metrics. Notice how the outlier on the bottom-right 'pulls' the mean away from the geometric median; as a result the corresponding medoid changes as well.

The basic linear classifier is distance-based

- The basic linear classifier constructs the decision boundary as the perpendicular bisector of the line segment connecting the two exemplars (one for each class).
- An alternative, distance-based way to classify instances without direct reference to a decision boundary is by the following decision rule: if $\mathbf{x}$ is nearest to $\boldsymbol{\mu}^{\oplus}$ then classify it as positive, otherwise as negative; or equivalently, classify an instance to the class of the *nearest* exemplar.
- If we use Euclidean distance as our closeness measure, simple geometry tells us we get exactly the same decision boundary.
- So the basic linear classifier can be interpreted from a distance-based perspective as constructing exemplars that minimise squared Euclidean distance within each class, and then applying a nearest-exemplar decision rule.

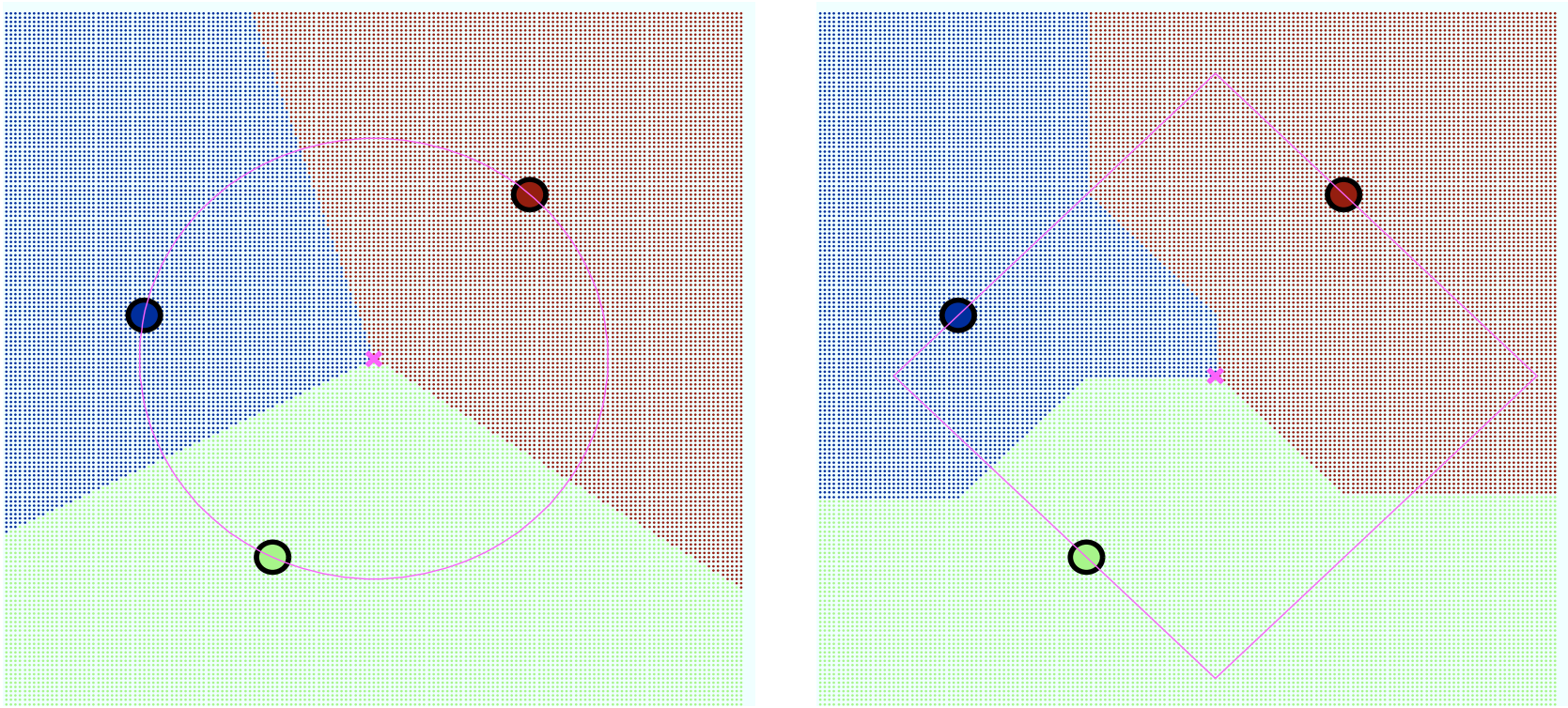
Two-exemplar decision boundaries





(left) For two exemplars the nearest-exemplar decision rule with Euclidean distance results in a linear decision boundary coinciding with the perpendicular bisector of the line connecting the two exemplars. (right) Using Manhattan distance the circles are replaced by diamonds.

Three-exemplar decision boundaries



(left) Decision regions defined by the 2-norm nearest-exemplar decision rule for three exemplars. (right) With Manhattan distance the decision regions become non-convex.

Distance-based models

To summarise, the main ingredients of distance-based models are

- distance metrics, which can be Euclidean, Manhattan, Minkowski or Mahalanobis, among many others;
- exemplars: centroids that find a centre of mass according to a chosen distance metric, or medoids that find the most centrally located data point; and
- distance-based decision rules, which take a vote among the k nearest exemplars.

Nearest Neighbour

Stores all training examples $\langle x_i, f(x_i) \rangle$.

Nearest neighbour:

- Given query instance x_q, first locate nearest training example x_n, then estimate $\hat{f}(x_q) \leftarrow f(x_n)$

k-Nearest neighbour:

- Given x_q, take vote among its k nearest neighbours (if discrete-valued target function)
- take mean of f values of k nearest neighbours (if real-valued)

$$\hat{f}(x_q) \leftarrow \frac{\sum_{i=1}^{k} f(x_i)}{k}$$

k-Nearest Neighbour Algorithm

Training algorithm:

- For each training example $\langle x_i, f(x_i) \rangle$, add the example to the list *training_examples*.

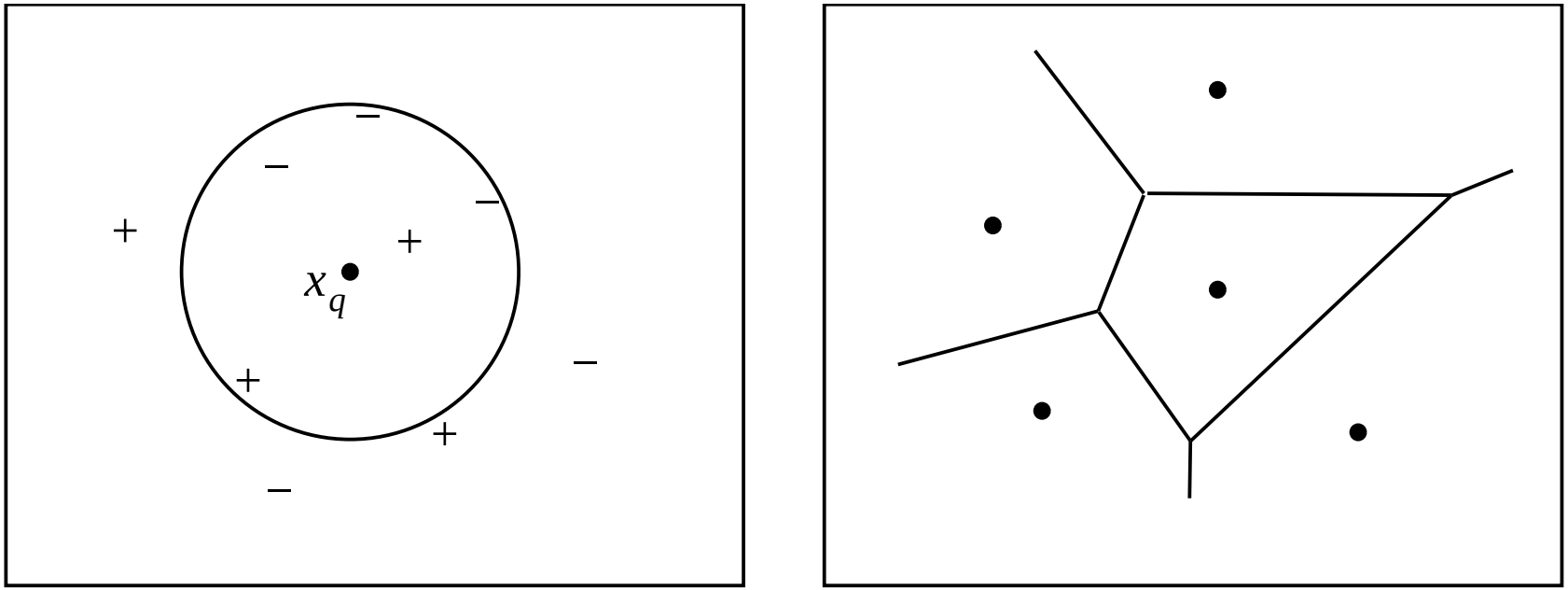
Classification algorithm:

- Given a query instance x_q to be classified,
  - Let $x_1 \ldots x_k$ be the k instances from *training_examples* that are *nearest* to x_q by the distance function
  - Return

$$\hat{f}(x_q) \leftarrow \arg\max_{v \in V} \sum_{i=1}^{k} \delta(v, f(x_i))$$

where $\delta(a, b) = 1$ if $a = b$ and 0 otherwise.

"Hypothesis Space" for Nearest Neighbour



2 classes, $+$ and $-$ and query point x_q. On left, note effect of varying k. On right, $1-$NN induces a Voronoi tessellation of the instance space. Formed by the perpendicular bisectors of lines between points.

Distance function again

The distance function defines what is learned.
Instance x is described by a feature vector (list of attribute-value pairs)

$$\langle a_1(x), a_2(x), \ldots a_m(x) \rangle$$

where $a_r(x)$ denotes the value of the rth attribute of x.
Most commonly used distance function is *Euclidean* distance ...

- distance between two instances x_i and x_j is defined to be

$$d(x_i, x_j) = \sqrt{\sum_{r=1}^{m} (a_r(x_i) - a_r(x_j))^2}$$

Distance function again

Many other distance functions could be used ...

- e.g., *Manhattan* or *city-block* distance (sum of absolute values of differences between attributes)

$$d(x_i, x_j) = \sum_{r=1}^{m} |a_r(x_i) - a_r(x_j)|$$

Vector-based formalization – use *norm* L_1, L_2, ...
The idea of distance functions will appear again in *kernel methods*.

Normalization and other issues

- Different attributes measured on different scales
- Need to be *normalized* (why ?)

$$a_r = \frac{v_r - \min v_r}{\max v_r - -\min v_r}$$

  where v_r is the actual value of attribute r
- Nominal attributes: distance either 0 or 1
- Common policy for missing values: assumed to be maximally distant (given normalized attributes)

When To Consider Nearest Neighbour

- Instances map to points in $\Re^n$
- Less than 20 attributes per instance
  - or number of attributes can be reduced ...
- Lots of training data
- No requirement for "explanatory" model to be learned

When To Consider Nearest Neighbour

Advantages:

- Statisticians have used k-NN since early 1950s
- Can be very accurate
  - at most twice the "Bayes error" for 1-NN (Cover & Hart, 1967)
- Training is very fast
- Can learn complex target functions
- Don't lose information by generalization - keep all instances

When To Consider Nearest Neighbour

Disadvantages:

- Slow at query time: basic algorithm scans entire training data to derive a prediction
- "Curse of dimensionality"
- Assumes all attributes are equally important, so easily fooled by irrelevant attributes
  - Remedy: attribute selection or weights
- Problem of noisy instances:
  - Remedy: remove from data set
  - not easy – how to know which are noisy ?

When To Consider Nearest Neighbour

What is the inductive bias of k-NN ?

- an assumption that the classification of query instance x_q will be most similar to the classification of other instances that are nearby according to the distance function

k-NN uses terminology from statistical pattern recognition (see below)

- *Regression* approximating a real-valued target function
- *Residual* the error $\hat{f}(x) - f(x)$ in approximating the target function
- *Kernel function* function of distance used to determine weight of each training example, i.e., kernel function is the function K s.t. $w_i = K(d(x_i, x_q))$

Nearest-neighbour classifier

- kNN uses the training data as exemplars, so training is $O(n)$ (but prediction is also $O(n)$!)
- 1NN perfectly separates training data, so low bias but high variance
- By increasing the number of neighbours k we increase bias and decrease variance (what happens when $k = n$?)
- Easily adapted to real-valued targets, and even to structured objects (nearest-neighbour retrieval). Can also output probabilities when $k > 1$
- Warning: in high-dimensional spaces everything is far away from everything and so pairwise distances are uninformative (curse of dimensionality)

Distance-Weighted kNN

- Might want to weight nearer neighbours more heavily ...
- Use distance function to construct a weight w_i
- Replace the final line of the classification algorithm by:

$$\hat{f}(x_q) \leftarrow \arg\max_{v \in V} \sum_{i=1}^{k} w_i \delta(v, f(x_i))$$

where

$$w_i \equiv \frac{1}{d(x_q, x_i)^2}$$

and $d(x_q, x_i)$ is distance between x_q and x_i

Distance-Weighted kNN

For real-valued target functions replace the final line of the algorithm by:

$$\hat{f}(x_q) \leftarrow \frac{\sum_{i=1}^{k} w_i f(x_i)}{\sum_{i=1}^{k} w_i}$$

(denominator normalizes contribution of individual weights).
Now we can consider using *all* the training examples instead of just k

$\rightarrow$ using all examples (i.e., when $k = n$) with the rule above is called Shepard's method

Evaluation

Lazy learners do not construct an explicit model, so how do we evaluate the output of the learning process ?

- 1-NN – training set error is always zero !
  - each training example is always closest to itself
- k-NN – overfitting may be hard to detect

Leave-one-out cross-validation (LOOCV) – leave out each example and predict it given the rest:

$$(x_1, y_1), (x_2, y_2), \ldots, (x_{i-1}, y_{i-1}), (x_{i+1}, y_{i+1}), \ldots, (x_n, y_n)$$

Error is mean over all predicted examples. Fast – no models to be built !

Curse of Dimensionality

Bellman (1960) coined this term in the context of dynamic programming

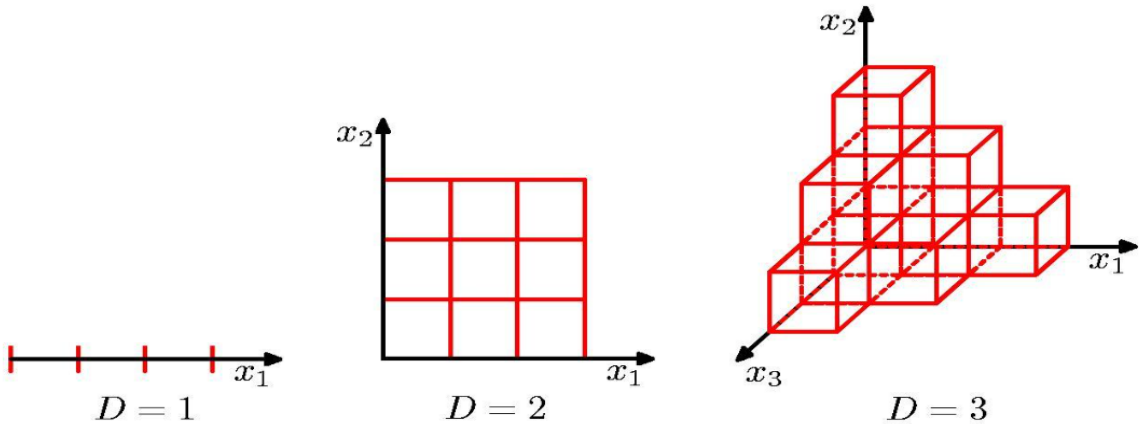
Imagine instances described by 20 attributes, but only 2 are relevant to target function — "similar" examples will appear "distant".

Curse of dimensionality: nearest neighbour is easily mislead when high-dimensional X – problem of irrelevant attributes

One approach:

- Stretch jth axis by weight z_j, where $z_1, \ldots, z_n$ chosen to minimize prediction error
- Use cross-validation to automatically choose weights $z_1, \ldots, z_n$
- Note setting z_j to zero eliminates this dimension altogether

Curse of Dimensionality



- number of "cells" in the instance space grows exponentially in the number of features
- with exponentially many cells we would need exponentially many data points to ensure that each cell is sufficiently populated to make nearest-neighbour predictions reliably

Curse of Dimensionality

Some ideas to address this for instance-based (nearest-neighbour) learning

- Euclidean distance with weights on attributes

$$\sqrt{\sum w_r(a_r(x_q) - a_r(x))^2}$$

- updating of weights based on nearest neighbour classification error
  - class correct/incorrect: weight increased/decreased
  - can be useful if not all features used in classification

See Moore and Lee (1994) "*Efficient Algorithms for Minimizing Cross Validation Error*"

Instance-based (nearest-neighbour) learning

Recap – Practical problems of 1-NN scheme:

- Slow (but fast $k-d$ tree-based approaches exist)
  - Remedy: removing irrelevant data
- Noise (but k-NN copes quite well with noise)
  - Remedy: removing noisy instances
- All attributes deemed equally important
  - Remedy: attribute weighting (or simply selection)
- Doesn't perform explicit generalization
  - Remedy: rule-based or tree-based NN approaches

Refinements of instance-based (nearest-neighbour) classifiers *

- Edited NN classifiers *discard* some of the training instances before making predictions
- Saves memory and speeds up classification
- IB2: *incremental* NN learner: only incorporates misclassified instances into the classifier
  - Problem: noisy data gets incorporated
- IB3: store *classification performance* information with each instance & only use in prediction if above a threshold

Dealing with noise *

Use larger values of k (why ?) How to find the "right" k ?

- One way: cross-validation-based k-NN classifier (but slow)
- Different approach: discarding instances that don't perform well by keeping success records of how well an instance does at prediction (IB3)
  - Computes confidence interval for an instance's success rate and for default accuracy of its class
  - If lower limit of first interval is above upper limit of second one, instance is accepted (IB3: 5%-level)
  - If upper limit of first interval is below lower limit of second one, instance is rejected (IB3: 12.5%-level)

Uncertainty

As far as the laws of mathematics refer to reality, they are not certain; as far as they are certain, they do not refer to reality.

–Albert Einstein

Two Roles for Bayesian Methods

Provides practical learning algorithms:

- Naive Bayes classifier learning
- Bayesian network learning, etc.
- Combines prior knowledge (prior probabilities) with observed data
- How to get prior probabilities ?

Provides useful conceptual framework:

- Provides a "gold standard" for evaluating other learning algorithms
- Some additional insight into Occam's razor

Bayes Theorem

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

where

- $P(h)$ = prior probability of hypothesis h
- $P(D)$ = prior probability of training data D
- $P(h|D)$ = probability of h given D
- $P(D|h)$ = probability of D given h

Choosing Hypotheses

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

Generally want the most probable hypothesis given the training data
Maximum a posteriori hypothesis h_{MAP}:

$$\begin{aligned} h_{MAP} &= \arg\max_{h \in H} P(h|D) \\ &= \arg\max_{h \in H} \frac{P(D|h)P(h)}{P(D)} \\ &= \arg\max_{h \in H} P(D|h)P(h) \end{aligned}$$

Choosing Hypotheses

If assume $P(h_i) = P(h_j)$ then can further simplify, and choose the *Maximum likelihood* (ML) hypothesis

$$h_{ML} = \arg\max_{h_i \in H} P(D|h_i)$$

Applying Bayes Theorem

Does patient have cancer or not?

A patient takes a lab test and the result comes back positive. The test returns a correct positive result in only 98% of the cases in which the disease is actually present, and a correct negative result in only 97% of the cases in which the disease is not present. Furthermore, $.008$ of the entire population have this cancer.

$$P(cancer) = \qquad P(\neg cancer) =$$
$$P(\oplus \mid cancer) = \qquad P(\ominus \mid cancer) =$$
$$P(\oplus \mid \neg cancer) = \qquad P(\ominus \mid \neg cancer) =$$

Applying Bayes Theorem

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$$P(cancer) = .008 \qquad P(\neg cancer) = .992$$
$$P(\oplus \mid cancer) = .98 \qquad P(\ominus \mid cancer) = .02$$
$$P(\oplus \mid \neg cancer) = .03 \qquad P(\ominus \mid \neg cancer) = .97$$

Applying Bayes Theorem

Does patient have cancer or not?

We can find the maximum a posteriori (MAP) hypothesis

$$\begin{aligned} P(\oplus \mid cancer)P(cancer) &= 0.98 \times 0.008 = 0.00784 \\ P(\oplus \mid \neg cancer)P(\neg cancer) &= 0.03 \times 0.992 = 0.02976 \end{aligned}$$

Thus $h_{MAP} = \ldots$.

Applying Bayes Theorem

Does patient have cancer or not?

We can find the maximum a posteriori (MAP) hypothesis

$$\begin{aligned} P(\oplus \mid cancer)P(cancer) &= 0.98 \times 0.008 = 0.00784 \\ P(\oplus \mid \neg cancer)P(\neg cancer) &= 0.03 \times 0.992 = 0.02976 \end{aligned}$$

Thus $h_{MAP} = \neg cancer$.

Also note: posterior probability of hypothesis $cancer$ higher than prior.

Applying Bayes Theorem

How to get the posterior probability of a hypothesis h ?
Divide by $P(\oplus)$, probability of data, to normalize result for h:

$$P(h|D) = \frac{P(D|h)P(h)}{\sum_{h_i \in H} P(D|h_i)P(h_i)}$$

Denominator ensures we obtain posterior probabilities that sum to 1.
Sum for all possible numerator values, since hypotheses are mutually exclusive (e.g., patient either has cancer or does not).
Marginal likelihood (marginalizing out over hypothesis space) — prior probability of the data.

Basic Formulas for Probabilities

Product Rule: probability $P(A \wedge B)$ of conjunction of two events A and B:

$$P(A \wedge B) = P(A|B)P(B) = P(B|A)P(A)$$

Sum Rule: probability of disjunction of two events A and B:

$$P(A \vee B) = P(A) + P(B) - P(A \wedge B)$$

Theorem of total probability: if events $A_1, \ldots, A_n$ are mutually exclusive with $\sum_{i=1}^{n} P(A_i) = 1$, then:

$$P(B) = \sum_{i=1}^{n} P(B|A_i)P(A_i)$$

Basic Formulas for Probabilities

Also worth remembering:

- *Conditional Probability*: probability of A given B:

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

- Rearrange sum rule to get:

$$P(A \wedge B) = P(A) + P(B) - P(A \vee B)$$

Exercise: Derive Bayes Theorem.

Brute Force MAP Hypothesis Learner

Idea: view learning as finding the *most probable* hypothesis

- For each hypothesis h in H, calculate the posterior probability

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

- Output the hypothesis h_{MAP} with the highest posterior probability

$$h_{MAP} = \arg\max_{h \in H} P(h|D)$$

Relation to Concept Learning (i.e., classification)

Canonical concept learning task:

- instance space X, hypothesis space H, training examples D
- consider a learning algorithm that outputs most specific hypothesis from the *version space* $VS_{H,D}$ (i.e., set of all consistent or "zero-error" classification rules)

What would Bayes rule produce as the MAP hypothesis?

Does this algorithm output a MAP hypothesis??

Relation to Concept Learning

Brute Force MAP Framework for Concept Learning:

Assume fixed set of instances $\langle x_1, \ldots, x_m \rangle$

Assume D is the set of classifications $D = \langle c(x_1), \ldots, c(x_m) \rangle$

Choose $P(h)$ to be *uniform* distribution:

- $P(h) = \frac{1}{|H|}$ for all h in H

Choose $P(D|h)$:

- $P(D|h) = 1$ if h consistent with D
- $P(D|h) = 0$ otherwise

Relation to Concept Learning

Then:

$$P(h|D) = \begin{cases} \frac{1}{|VS_{H,D}|} & \text{if } h \text{ is consistent with } D \\ 0 & \text{otherwise} \end{cases}$$

Relation to Concept Learning

Note that since likelihood is zero if h is inconsistent then the posterior is also zero. But how did we obtain the posterior for consistent h ?

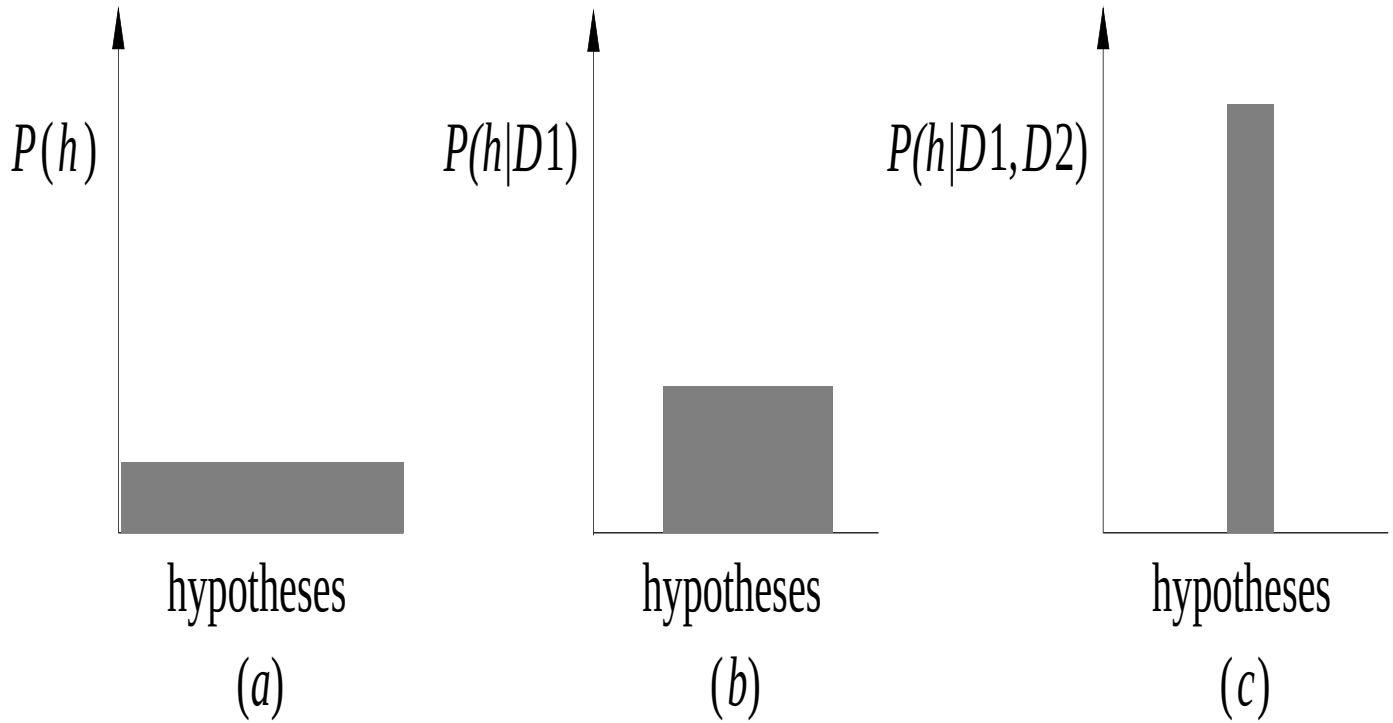
$$\begin{aligned} P(h|D) &= \frac{1 \cdot \frac{1}{|H|}}{P(D)} \\ &= \frac{1 \cdot \frac{1}{|H|}}{\frac{|VS_{H,D}|}{|H|}} \\ &= \frac{1}{|VS_{H,D}|} \end{aligned}$$

Relation to Concept Learning

How did we obtain $P(D)$? From theorem of total probability:

$$
\begin{aligned}
P(D) &= \sum_{h_i \in H} P(D|H_i)P(h_i) \\
&= \sum_{h_i \in VS_{H,D}} 1 \cdot \frac{1}{|H|} + \sum_{h_i \notin VS_{H,D}} 0 \cdot \frac{1}{|H|} \\
&= \sum_{h_i \in VS_{H,D}} 1 \cdot \frac{1}{|H|} \\
&= \frac{|VS_{H,D}|}{|H|}
\end{aligned}
$$

Evolution of Posterior Probabilities



Relation to Concept Learning

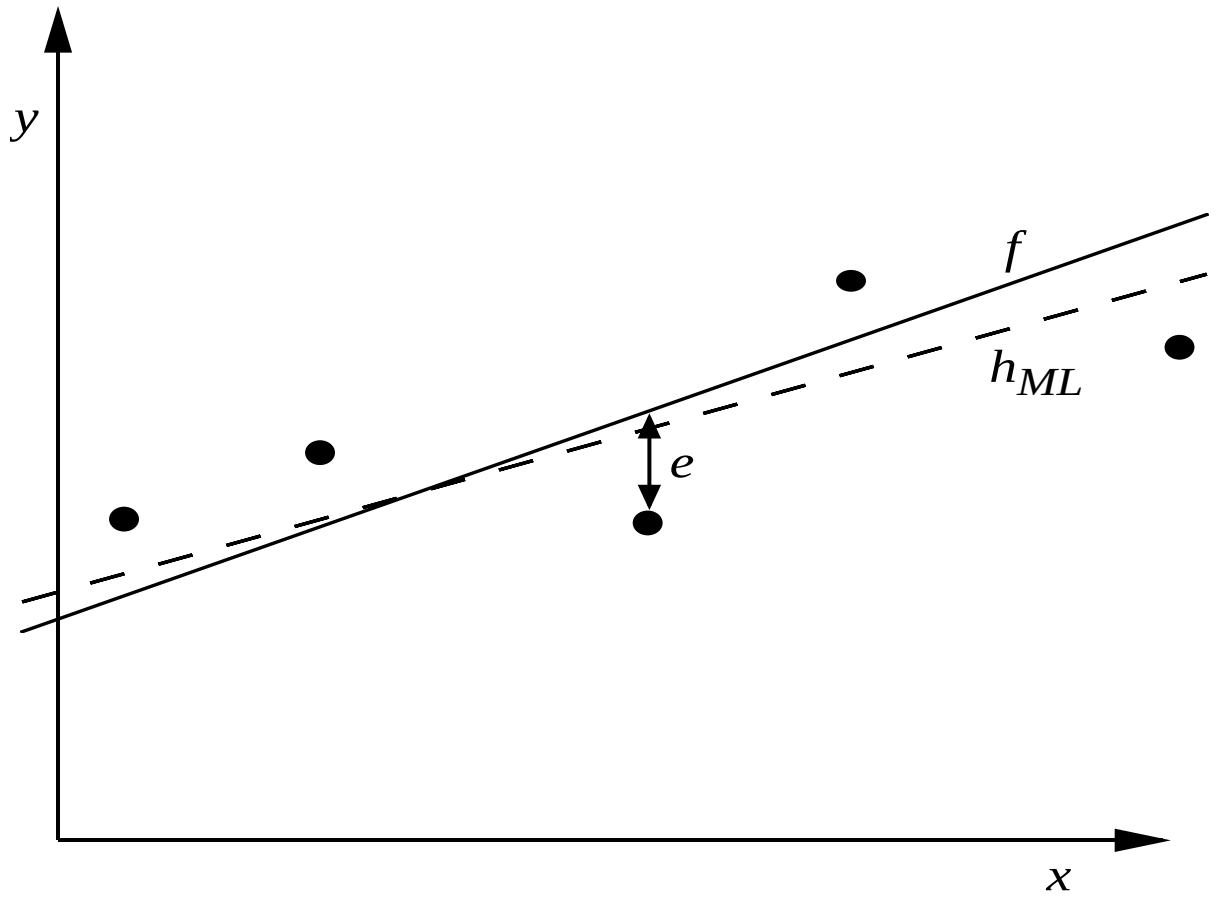
Every hypothesis consistent with D is a MAP hypothesis, if we assume

- uniform probability over H
- target function $c \in H$
- deterministic, noise-free data
- etc. (see above)

So, this learning algorithm *will* output a MAP hypothesis, even though it does not explicitly use *probabilities* in learning.

Learning A Real Valued Function

E.g., learning a linear target function f from noisy examples:



Learning A Real Valued Function

Consider any real-valued target function f
Training examples $\langle x_i, d_i \rangle$, where d_i is noisy training value

- $d_i = f(x_i) + e_i$
- e_i is random variable (noise) drawn independently for each x_i according to some Gaussian (normal) distribution with mean=0

Then the **maximum likelihood** hypothesis h_{ML} is the one that **minimizes the sum of squared errors**:

$$h_{ML} = \arg\min_{h \in H} \sum_{i=1}^{m} (d_i - h(x_i))^2$$

Learning A Real Valued Function

How did we obtain this ?

$$
\begin{aligned}
h_{ML} &= \arg\max_{h \in H} p(D|h) \\
&= \arg\max_{h \in H} \prod_{i=1}^{m} p(d_i|h) \\
&= \arg\max_{h \in H} \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{d_i - h(x_i)}{\sigma}\right)^2}
\end{aligned}
$$

Recall that we treat each probability $p(D|h)$ **as if** $h = f$, i.e., **we assume** $\mu = f(x_i) = h(x_i)$, which is the key idea behind maximum likelihood !

Learning A Real Valued Function

Maximize natural log to give simpler expression:

$$
\begin{aligned}
h_{ML} &= \arg\max_{h \in H} \sum_{i=1}^{m} \ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2}\left(\frac{d_i - h(x_i)}{\sigma}\right)^2 \\
&= \arg\max_{h \in H} \sum_{i=1}^{m} -\frac{1}{2}\left(\frac{d_i - h(x_i)}{\sigma}\right)^2 \\
&= \arg\max_{h \in H} \sum_{i=1}^{m} -\left(d_i - h(x_i)\right)^2
\end{aligned}
$$

Equivalently, we can minimize the positive version of the expression:

$$
h_{ML} = \arg\min_{h \in H} \sum_{i=1}^{m} \left(d_i - h(x_i)\right)^2
$$

Discriminative and generative probabilistic models

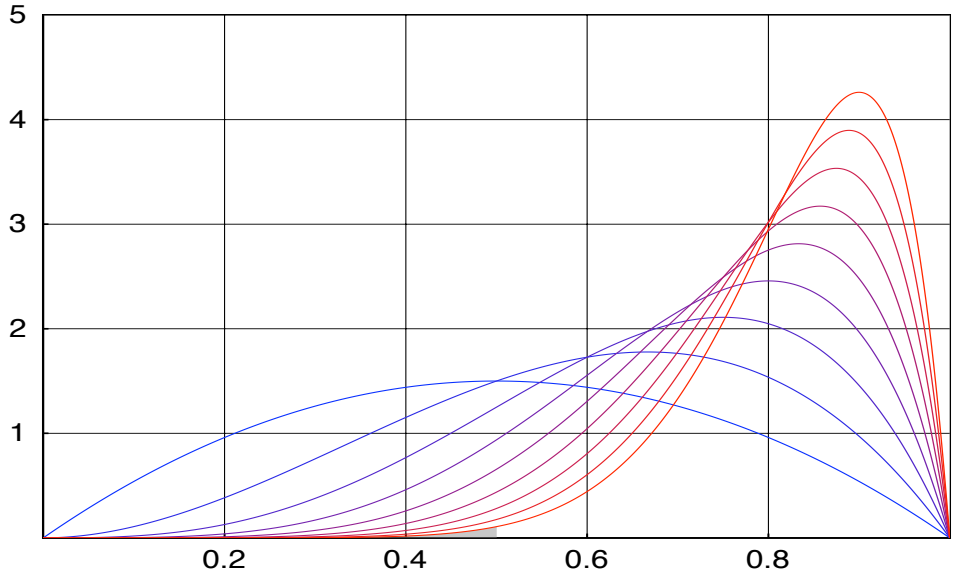
- *Discriminative models* model the posterior probability distribution $P(Y|X)$, where Y is the target variable and X are the features. That is, given X they return a probability distribution over Y.
- *Generative models* model the joint distribution $P(Y, X)$ of the target Y and the feature vector X. Once we have access to this joint distribution we can derive any conditional or marginal distribution involving the same variables. In particular, since $P(X) = \sum_y P(Y = y, X)$ it follows that the posterior distribution can be obtained as $P(Y|X) = \frac{P(Y,X)}{\sum_y P(Y=y,X)}$.
- Alternatively, generative models can be described by the likelihood function $P(X|Y)$, since $P(Y, X) = P(X|Y)P(Y)$ and the target or prior distribution (usually abbreviated to 'prior') can be easily estimated or postulated.
- Such models are called 'generative' because we can sample from the joint distribution to obtain new data points together with their labels. Alternatively, we can use $P(Y)$ to sample a class and $P(X|Y)$ to sample an instance for that class.

Assessing uncertainty in estimates

Suppose we want to estimate the probability θ that an arbitrary e-mail is spam, so that we can use the appropriate prior distribution.

- The natural thing to do is to inspect n e-mails, determine the number of spam e-mails d, and set $\hat{\theta} = d/n$; we don't really need any complicated statistics to tell us that.
- However, while this is the most likely estimate of θ – the maximum a posteriori (MAP) estimate – this doesn't mean that other values of θ are completely ruled out.
- We model this by a probability distribution over θ (a Beta distribution in this case) which is updated each time new information comes in. This is further illustrated in the figure for a distribution that is more and more skewed towards spam.
- For each curve, its bias towards spam is given by the area under the curve and to the right of $\theta = 1/2$.

Assessing uncertainty in estimates



Each time we inspect an e-mail, we are reducing our uncertainty regarding the prior spam probability θ. After we inspect two e-mails and observe one spam, the possible θ values are characterised by a symmetric distribution around $1/2$. If we inspect a third, fourth, ..., tenth e-mail and each time (except the first one) it is spam, then this distribution narrows and shifts a little bit to the right each time. The distribution for n e-mails reaches its maximum at $\hat{\theta}_{\text{MAP}} = \frac{n-1}{n}$ (e.g., $\hat{\theta}_{\text{MAP}} = 0.8$ for $n = 5$).

The Bayesian perspective

Explicitly modelling the posterior distribution over the parameter θ has a number of advantages that are usually associated with the 'Bayesian' perspective:

- We can precisely characterise the uncertainty that remains about our estimate by quantifying the spread of the posterior distribution.
- We can obtain a generative model for the parameter by sampling from the posterior distribution, which contains much more information than a summary statistic such as the MAP estimate can convey – so, rather than using a single e-mail with $\theta = \theta_{\mathrm{MAP}}$, our generative model can contain a number of e-mails with θ sampled from the posterior distribution.

The Bayesian perspective

- We can quantify the probability of statements such as 'e-mails are biased towards ham' (the tiny shaded area in the figure demonstrates that after observing one ham and nine spam e-mails this probability is very small, about 0.6%).
- We can use one of these distributions to encode our prior beliefs: e.g., if we believe that the proportions of spam and ham are typically 50–50, we can take the distribution for $n = 2$ (the lowest, symmetric one in the figure on the previous slide) as our prior.

The key point is that probabilities do not have to be interpreted as estimates of relative frequencies, but can carry the more general meaning of (possibly subjective) degrees of belief.

Consequently, we can attach a probability distribution to almost anything: not just features and targets, but also model parameters and even models.

Minimum Description Length Principle

Once again, the MAP hypothesis

$$h_{MAP} = \arg\max_{h \in H} P(D|h)P(h)$$

Which is equivalent to

$$h_{MAP} = \arg\max_{h \in H} \log_2 P(D|h) + \log_2 P(h)$$

Or

$$h_{MAP} = \arg\min_{h \in H} -\log_2 P(D|h) - \log_2 P(h)$$

Minimum Description Length Principle

Interestingly, this is an expression about a quantity of *bits*.

$$h_{MAP} = \arg\min_{h \in H} -\log_2 P(D|h) - \log_2 P(h) \quad (1)$$

From information theory:

> *The optimal (shortest expected coding length) code for an event with probability p is $-\log_2 p$ bits.*

Minimum Description Length Principle

So interpret (1):

- $-\log_2 P(h)$ is length of h under optimal code
- $-\log_2 P(D|h)$ is length of D given h under optimal code

Note well: assumes *optimal* encodings, when the priors and likelihoods are known. In practice, this is difficult, and makes a difference.

Minimum Description Length Principle

Occam's razor: prefer the shortest hypothesis

MDL: prefer the hypothesis h that minimizes

$$h_{MDL} = \arg\min_{h \in H} L_{C_1}(h) + L_{C_2}(D|h)$$

where $L_C(x)$ is the description length of x under optimal encoding C

Minimum Description Length Principle

Without loss of generality, classifier is here assumed to be a decision tree

Example: H = decision trees, D = training data labels

- $L_{C_1}(h)$ is # bits to describe tree h
- $L_{C_2}(D|h)$ is # bits to describe D given h
  - Note $L_{C_2}(D|h) = 0$ if examples classified perfectly by h. Need only describe exceptions
- Hence h_{MDL} trades off tree size for training errors
  - i.e., prefer the hypothesis that minimizes

$$length(h) + length(misclassifications)$$

Most Probable Classification of New Instances

So far we've sought the most probable *hypothesis* given the data D (i.e., h_{MAP})

Given new instance x, what is its most probable *classification*?

- $h_{MAP}(x)$ is not the most probable classification!

Most Probable Classification of New Instances

Consider:

- Three possible hypotheses:

$$P(h_1|D) = .4,\ P(h_2|D) = .3,\ P(h_3|D) = .3$$

- Given new instance x,

$$h_1(x) = +,\ h_2(x) = -,\ h_3(x) = -$$

- What's most probable classification of x?

Bayes Optimal Classifier

Bayes optimal classification:

$$\arg\max_{v_j \in V} \sum_{h_i \in H} P(v_j|h_i)P(h_i|D)$$

Example:

$$\begin{aligned} P(h_1|D) &= .4, \quad P(-|h_1) = 0, \quad P(+|h_1) = 1 \\ P(h_2|D) &= .3, \quad P(-|h_2) = 1, \quad P(+|h_2) = 0 \\ P(h_3|D) &= .3, \quad P(-|h_3) = 1, \quad P(+|h_3) = 0 \end{aligned}$$

Bayes Optimal Classifier

therefore

$$\sum_{h_i \in H} P(+|h_i)P(h_i|D) = .4$$

$$\sum_{h_i \in H} P(-|h_i)P(h_i|D) = .6$$

and

$$\arg\max_{v_j \in V} \sum_{h_i \in H} P(v_j|h_i)P(h_i|D) = -$$

No other classification method using the same hypothesis space and same prior knowledge can outperform this method on average

Bayes Error

What is the best performance attainable by a (two-class) classifier ?

Define the probability of error for classifying some instance x by

$$\begin{aligned} P(\text{error}|x) &= P(\text{class}_1|x) \quad \text{if we predict class}_2 \\ &= P(\text{class}_2|x) \quad \text{if we predict class}_1 \end{aligned}$$

This gives

$$\Sigma_x \quad P(\text{error}) = P(\text{error}|x)\ P(x)$$

So we can justify the use of the decision rule

$$\begin{aligned} \text{if} \quad P(\text{class}_1|x) > P(\text{class}_2|x) \quad &\text{then} \quad \text{predict class}_1 \\ &\text{else} \quad \text{predict class}_2 \end{aligned}$$

On average, this decision rule minimises probability of classification error.

Naive Bayes Classifier

Along with decision trees, neural networks, nearest neighbour, one of the most practical learning methods.

When to use

- Moderate or large training set available
- Attributes that describe instances are conditionally independent given classification

Successful applications:

- Classifying text documents
- Gaussian Naive Bayes for real-valued data

Naive Bayes Classifier

Assume target function $f : X \to V$, where each instance x described by attributes $\langle a_1, a_2 \ldots a_n \rangle$.
Most probable value of $f(x)$ is:

$$
\begin{aligned}
v_{MAP} &= \arg\max_{v_j \in V} P(v_j | a_1, a_2 \ldots a_n) \\
v_{MAP} &= \arg\max_{v_j \in V} \frac{P(a_1, a_2 \ldots a_n | v_j) P(v_j)}{P(a_1, a_2 \ldots a_n)} \\
&= \arg\max_{v_j \in V} P(a_1, a_2 \ldots a_n | v_j) P(v_j)
\end{aligned}
$$

Naive Bayes Classifier

Naive Bayes assumption:

$$P(a_1, a_2 \ldots a_n | v_j) = \prod_i P(a_i | v_j)$$

- Attributes are statistically independent (given the class value)
  - which means knowledge about the value of a particular attribute tells us nothing about the value of another attribute (if the class is known)

which gives

Naive Bayes classifier: $v_{NB} = \arg\max_{v_j \in V} P(v_j) \prod_i P(a_i | v_j)$

Naive Bayes Algorithm

Naive_Bayes_Learn($examples$)

For each target value v_j

$\hat{P}(v_j) \leftarrow$ estimate $P(v_j)$

For each attribute value a_i of each attribute a

$\hat{P}(a_i|v_j) \leftarrow$ estimate $P(a_i|v_j)$

Classify_New_Instance(x)

$$v_{NB} = \arg\max_{v_j \in V} \hat{P}(v_j) \prod_{a_i \in x} \hat{P}(a_i|v_j)$$

Naive Bayes Example

Consider *PlayTennis* again ...

Outlook			Temperature			Humidity			Windy		
	Yes	No		Yes	No		Yes	No		Yes	No
Sunny	2	3	Hot	2	2	High	3	4	False	6	2
Overcast	4	0	Mild	4	2	Normal	6	1	True	3	3
Rainy	3	2	Cool	3	1						
Sunny	2/9	3/5	Hot	2/9	2/5	High	3/9	4/5	False	6/9	2/5
Overcast	4/9	0/5	Mild	4/9	2/5	Normal	6/9	1/5	True	3/9	3/5
Rainy	3/9	2/5	Cool	3/9	1/5						
Play											
Yes	No										
9	5										
9/14	5/14										

Naive Bayes Example

Say we have the new instance:

$$\langle Outlk = sun, Temp = cool, Humid = high, Wind = true \rangle$$

We want to compute:

$$v_{NB} = \underset{v_j \in \{\text{“yes”}, \text{“no”}\}}{\arg\max} P(v_j) \prod_i P(a_i | v_j)$$

Naive Bayes Example

So we first calculate the likelihood of the two classes, "yes" and "no"

$$\text{for "yes"} = P(y) \times P(sun|y) \times P(cool|y) \times P(high|y) \times P(true|y)$$
$$0.0053 = \frac{9}{14} \times \frac{2}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{3}{9}$$

$$\text{for "no"} = P(n) \times P(sun|n) \times P(cool|n) \times P(high|n) \times P(true|n)$$
$$0.0206 = \frac{5}{14} \times \frac{3}{5} \times \frac{1}{5} \times \frac{4}{5} \times \frac{3}{5}$$

Naive Bayes Example

Then convert to a probability by normalisation

$$
\begin{aligned}
P(\text{“yes”}) &= \frac{0.0053}{(0.0053 + 0.0206)} \\
&= 0.205 \\
P(\text{“no”}) &= \frac{0.0206}{(0.0053 + 0.0206)} \\
&= 0.795
\end{aligned}
$$

The Naive Bayes classification is “no”.

Naive Bayes: Subtleties

Conditional independence assumption is often violated

$$P(a_1, a_2 \ldots a_n | v_j) = \prod_i P(a_i | v_j)$$

- ...but it works surprisingly well anyway. Note don't need estimated posteriors $\hat{P}(v_j|x)$ to be correct; need only that

$$\arg\max_{v_j \in V} \hat{P}(v_j) \prod_i \hat{P}(a_i|v_j) = \arg\max_{v_j \in V} P(v_j) P(a_1 \ldots, a_n | v_j)$$

i.e. maximum probability is assigned to correct class

- see [Domingos & Pazzani, 1996] for analysis
- Naive Bayes posteriors often unrealistically close to 1 or 0
- adding too many redundant attributes will cause problems (e.g. identical attributes)

Naive Bayes: "zero-frequency" problem

What if none of the training instances with target value v_j have attribute value a_i? Then

$$\hat{P}(a_i|v_j) = 0, \text{ and...}$$

$$\hat{P}(v_j)\prod_i \hat{P}(a_i|v_j) = 0$$

Pseudo-counts add 1 to each count (a version of the *Laplace Estimator*)

Naive Bayes: "zero-frequency" problem

- In some cases adding a constant different from 1 might be more appropriate
- Example: attribute *outlook* for class *yes*

Sunny	*Overcast*	*Rainy*
$\frac{2+\frac{\mu}{2}}{9+\mu}$	$\frac{4+\frac{\mu}{3}}{9+\mu}$	$\frac{3+\frac{\mu}{3}}{9+\mu}$

- Weights don't need to be equal (if they sum to 1) – a form of *prior*

Sunny	*Overcast*	*Rainy*
$\frac{2+\mu p_1}{9+\mu}$	$\frac{4+\mu p_2}{9+\mu}$	$\frac{3+\mu p_3}{9+\mu}$

Naive Bayes: "zero-frequency" problem

This generalisation is a Bayesian estimate for $\hat{P}(a_i|v_j)$

$$\hat{P}(a_i|v_j) \leftarrow \frac{n_c + mp}{n + m}$$

where

- n is number of training examples for which $v = v_j$,
- n_c number of examples for which $v = v_j$ and $a = a_i$
- p is prior estimate for $\hat{P}(a_i|v_j)$
- m is weight given to prior (i.e. number of "virtual" examples)

This is called the m-estimate of probability.

Naive Bayes: missing values

- Training: instance is not included in frequency count for attribute value-class combination
- Classification: attribute will be omitted from calculation

Naive Bayes: numeric attributes

- Usual assumption: attributes have a *normal* or *Gaussian* probability distribution (given the class)
- The *probability density function* for the normal distribution is defined by two parameters:

  The sample mean μ:

$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$$

  The standard deviation σ:

$$\sigma = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \mu)^2$$

Naive Bayes: numeric attributes

Then we have the density function $f(x)$:

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

Example: continuous attribute *temperature* with mean $= 73$ and standard deviation $= 6.2$. Density value

$$f(\text{temperature} = 66 | \text{“yes”}) = \frac{1}{\sqrt{2\pi}6.2} \; e^{-\frac{(66-73)^2}{2\times 6.2^2}} = 0.0340$$

Missing values during training are not included in calculation of mean and standard deviation.

Naive Bayes: numeric attributes

Note: the normal distribution is based on the simple exponential function

$$f(x) = e^{-|x|^m}$$

As the power m in the exponent increases, the function approaches a step function.
Where $m = 2$

$$f(x) = e^{-|x|^2}$$

and this is the basis of the normal distribution – the various constants are the result of scaling so that the integral (the area under the curve from $-\infty$ to $+\infty$) is equal to 1.
from "Statistical Computing" by Michael J. Crawley (2002) Wiley.

Categorical random variables

Categorical variables or features (also called discrete or nominal) are ubiquitous in machine learning.

- Perhaps the most common form of the Bernoulli distribution models whether or not a word occurs in a document. That is, for the i-th word in our vocabulary we have a random variable X_i governed by a Bernoulli distribution. The joint distribution over the *bit vector* $X = (X_1, \ldots, X_k)$ is called a *multivariate Bernoulli distribution*.
- Variables with more than two outcomes are also common: for example, every word position in an e-mail corresponds to a categorical variable with k outcomes, where k is the size of the vocabulary. The multinomial distribution manifests itself as a *count vector*: a histogram of the number of occurrences of all vocabulary words in a document. This establishes an alternative way of modelling text documents that allows the number of occurrences of a word to influence the classification of a document.

Categorical random variables

Both these document models are in common use. Despite their differences, they both assume independence between word occurrences, generally referred to as the *naive Bayes assumption*.

- In the multinomial document model, this follows from the very use of the multinomial distribution, which assumes that words at different word positions are drawn independently from the same categorical distribution.
- In the multivariate Bernoulli model we assume that the bits in a bit vector are statistically independent, which allows us to compute the joint probability of a particular bit vector $(x_1, \ldots, x_k)$ as the product of the probabilities of each component $P(X_i = x_i)$.
- In practice, such word independence assumptions are often not true: if we know that an e-mail contains the word 'Viagra', we can be quite sure that it will also contain the word 'pill'. Violated independence assumptions reduce the quality of probability estimates but may still allow good classification performance.

Example application: Learning to Classify Text

In machine learning, the classic example of applications of Naive Bayes is learning to classify text documents.

Here is a simplified version in the multinomial document model.

Learning to Classify Text

Why?

- Learn which news articles are of interest
- Learn to classify web pages by topic

Naive Bayes is among most effective algorithms

What attributes shall we use to represent text documents??

Learning to Classify Text

Target concept $Interesting? : Document \rightarrow \{+, -\}$

1. Represent each document by vector of words
   - one attribute per word position in document
2. Learning: Use training examples to estimate
   - $P(+)$
   - $P(-)$
   - $P(doc|+)$
   - $P(doc|-)$

Learning to Classify Text

Naive Bayes conditional independence assumption

$$P(doc|v_j) = \prod_{i=1}^{length(doc)} P(a_i = w_k|v_j)$$

where $P(a_i = w_k|v_j)$ is probability that word in position i is w_k, given v_j

one more assumption: $P(a_i = w_k|v_j) = P(a_m = w_k|v_j), \forall i, m$

"bag of words"

Learning to Classify Text

LEARN_NAIVE_BAYES_TEXT($Examples, V$)

// collect all words and other tokens that occur in $Examples$

$Vocabulary \leftarrow$ all distinct words and other tokens in $Examples$

// calculate the required $P(v_j)$ *and* $P(w_k|v_j)$ *probability terms*

for each target value v_j in V do

- $docs_j \leftarrow$ subset of $Examples$ for which the target value is v_j
- $P(v_j) \leftarrow \frac{|docs_j|}{|Examples|}$
- $Text_j \leftarrow$ a single document created by concatenating all members of $docs_j$
- $n \leftarrow$ total number of words in $Text_j$ (counting duplicate words multiple times)
- for each word w_k in $Vocabulary$
  - $n_k \leftarrow$ number of times word w_k occurs in $Text_j$
  - $P(w_k|v_j) \leftarrow \frac{n_k+1}{n+|Vocabulary|}$

Learning to Classify Text

CLASSIFY_NAIVE_BAYES_TEXT(Doc)

- $positions \leftarrow$ all word positions in Doc that contain tokens found in $Vocabulary$
- Return v_{NB}, where

$$v_{NB} = \arg\max_{v_j \in V} P(v_j) \prod_{i \in positions} P(a_i|v_j)$$

Application: 20 Newsgroups

Given: 1000 training documents from each group
Learning task: classify each new document by newsgroup it came from

comp.graphics	misc.forsale
comp.os.ms-windows.misc	rec.autos
comp.sys.ibm.pc.hardware	rec.motorcycles
comp.sys.mac.hardware	rec.sport.baseball
comp.windows.x	rec.sport.hockey
alt.atheism	sci.space
soc.religion.christian	sci.crypt
talk.religion.misc	sci.electronics
talk.politics.mideast	sci.med
talk.politics.misc	
talk.politics.guns	

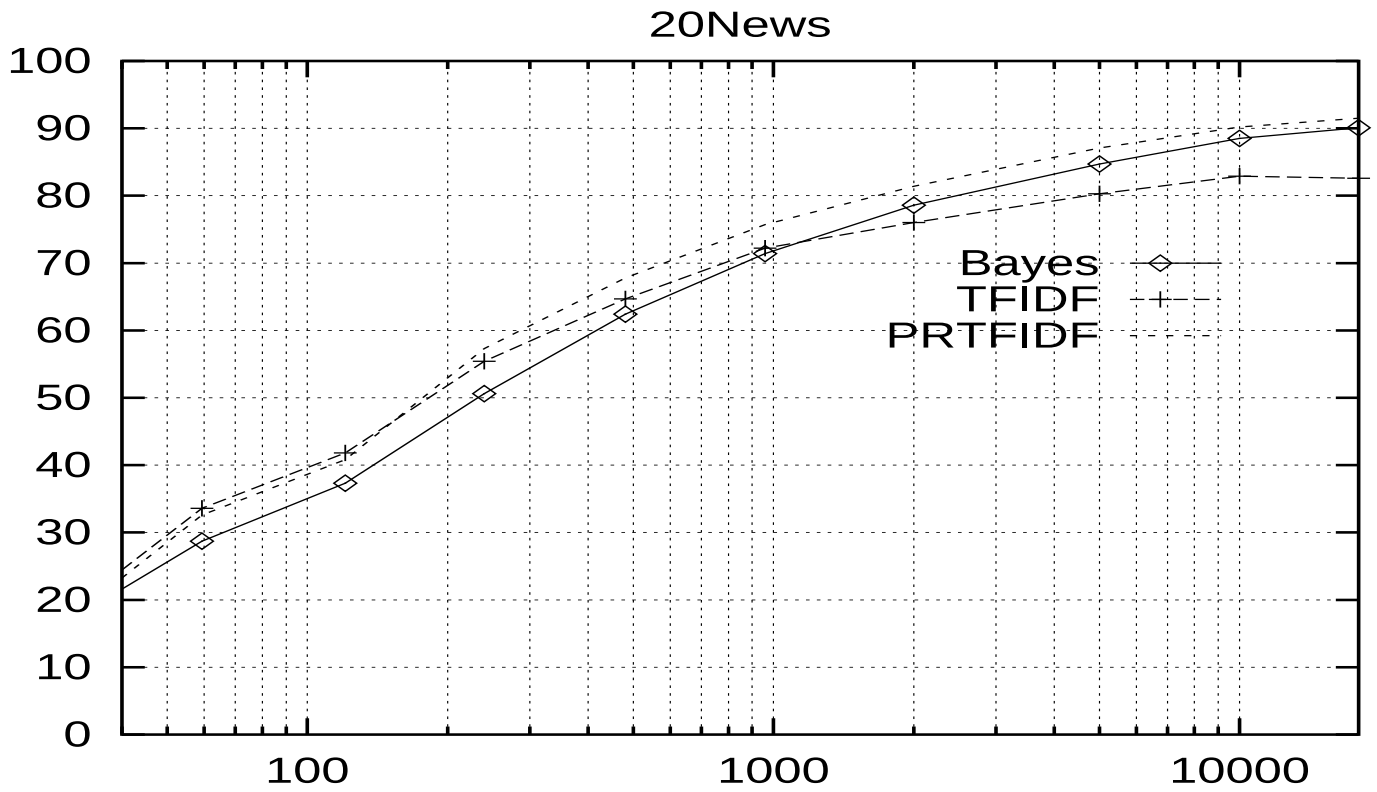
Naive Bayes: 89% classification accuracy

Article from rec.sport.hockey

```
Path: cantaloupe.srv.cs.cmu.edu!das-news.harvard.edu!ogicse!uwm.edu
From: xxx@yyy.zzz.edu (John Doe)
Subject: Re: This year's biggest and worst (opinion)...
Date: 5 Apr 93 09:53:39 GMT

I can only comment on the Kings, but the most obvious candidate
for pleasant surprise is Alex Zhitnik. He came highly touted as
a defensive defenseman, but he's clearly much more than that.
Great skater and hard shot (though wish he were more accurate).
In fact, he pretty much allowed the Kings to trade away that
huge defensive liability Paul Coffey. Kelly Hrudey is only the
biggest disappointment if you thought he was any good to begin
with. But, at best, he's only a mediocre goaltender. A better
choice would be Tomas Sandstrom, though not through any fault
of his own, but because some thugs in Toronto decided ...
```

Learning Curve for 20 Newsgroups



Accuracy vs. Training set size (1/3 withheld for test)

Probabilistic decision rules

We have chosen one of the possible distributions to model our data X as coming from either class.

- The more different $P(X|Y = \text{spam})$ and $P(X|Y = \text{ham})$ are, the more useful the features X are for classification.
- Thus, for a specific e-mail x we calculate both $P(X = x|Y = \text{spam})$ and $P(X = x|Y = \text{ham})$, and apply one of several possible decision rules:

maximum likelihood (ML) – predict $\arg\max_y P(X = x|Y = y)$;

maximum a posteriori (MAP) – predict

$$\arg\max_y P(X = x|Y = y)P(Y = y);$$

The relation between the first two decision rules is that ML classification is equivalent to MAP classification with a uniform class distribution.

Probabilistic decision rules

We again use the example of Naive Bayes for text classification to illustrate, using both the multinomial and multivariate Bernoulli models.

Prediction using a naive Bayes model

Suppose our vocabulary contains three words a, b and c, and we use a multivariate Bernoulli model for our e-mails, with parameters

$$\boldsymbol{\theta}^{\oplus} = (0.5, 0.67, 0.33) \qquad \boldsymbol{\theta}^{\ominus} = (0.67, 0.33, 0.33)$$

This means, for example, that the presence of b is twice as likely in spam ($+$), compared with ham.
The e-mail to be classified contains words a and b but not c, and hence is described by the bit vector $\mathbf{x} = (1, 1, 0)$. We obtain likelihoods

$$P(\mathbf{x}|\oplus) = 0.5 \cdot 0.67 \cdot (1 - 0.33) = 0.222$$
$$P(\mathbf{x}|\ominus) = 0.67 \cdot 0.33 \cdot (1 - 0.33) = 0.148$$

The ML classification of $\mathbf{x}$ is thus spam.

Prediction using a naive Bayes model

In the case of two classes it is often convenient to work with likelihood ratios and odds.

- The likelihood ratio can be calculated as

$$\frac{P(\mathbf{x}|\oplus)}{P(\mathbf{x}|\ominus)} = \frac{0.5}{0.67}\frac{0.67}{0.33}\frac{1-0.33}{1-0.33} = 3/2 > 1$$

- This means that the MAP classification of $\mathbf{x}$ is also spam if the prior odds are more than $2/3$, but ham if they are less than that.
- For example, with 33% spam and 67% ham the prior odds are $\frac{P(\oplus)}{P(\ominus)} = \frac{0.33}{0.67} = 1/2$, resulting in a posterior odds of

$$\frac{P(\oplus|\mathbf{x})}{P(\ominus|\mathbf{x})} = \frac{P(\mathbf{x}|\oplus)}{P(\mathbf{x}|\ominus)}\frac{P(\oplus)}{P(\ominus)} = 3/2 \cdot 1/2 = 3/4 < 1$$

In this case the likelihood ratio for $\mathbf{x}$ is not strong enough to push the decision away from the prior.

Prediction using a naive Bayes model

Alternatively, we can employ a multinomial model. The parameters of a multinomial establish a distribution over the words in the vocabulary, say

$$\boldsymbol{\theta}^{\oplus} = (0.3, 0.5, 0.2) \qquad \boldsymbol{\theta}^{\ominus} = (0.6, 0.2, 0.2)$$

The e-mail to be classified contains three occurrences of word a, one single occurrence of word b and no occurrences of word c, and hence is described by the count vector $\mathbf{x} = (3, 1, 0)$. The total number of vocabulary word occurrences is $n = 4$. We obtain likelihoods

$$P(\mathbf{x}|\oplus) = 4! \frac{0.3^3}{3!} \frac{0.5^1}{1!} \frac{0.2^0}{0!} = 0.054$$

$$P(\mathbf{x}|\ominus) = 4! \frac{0.6^3}{3!} \frac{0.2^1}{1!} \frac{0.2^0}{0!} = 0.1728$$

The likelihood ratio is $\left(\frac{0.3}{0.6}\right)^3 \left(\frac{0.5}{0.2}\right)^1 \left(\frac{0.2}{0.2}\right)^0 = 5/16$. The ML classification of $\mathbf{x}$ is thus ham, the opposite of the multivariate Bernoulli model. This is mainly because of the three occurrences of word a, which provide strong evidence for ham.

Training data for naive Bayes

A small e-mail data set described by count vectors.

E-mail	$\#a$	$\#b$	$\#c$	Class
e_1	0	3	0	$+$
e_2	0	3	3	$+$
e_3	3	0	0	$+$
e_4	2	3	0	$+$
e_5	4	3	0	$-$
e_6	4	0	3	$-$
e_7	3	0	0	$-$
e_8	0	0	0	$-$

Training data for naive Bayes

The same data set described by bit vectors.

E-mail	$a?$	$b?$	$c?$	Class
e_1	0	1	0	$+$
e_2	0	1	1	$+$
e_3	1	0	0	$+$
e_4	1	1	0	$+$
e_5	1	1	0	$-$
e_6	1	0	1	$-$
e_7	1	0	0	$-$
e_8	0	0	0	$-$

Training a naive Bayes model

Consider the following e-mails consisting of five words a, b, c, d, e:

e_1: $b\ d\ e\ b\ b\ d\ e$
e_2: $b\ c\ e\ b\ b\ d\ d\ e\ c\ c$
e_3: $a\ d\ a\ d\ e\ a\ e\ e$
e_4: $b\ a\ d\ b\ e\ d\ a\ b$

e_5: $a\ b\ a\ b\ a\ b\ a\ e\ d$
e_6: $a\ c\ a\ c\ a\ c\ a\ e\ d$
e_7: $e\ a\ e\ d\ a\ e\ a$
e_8: $d\ e\ d\ e\ d$

We are told that the e-mails on the left are spam and those on the right are ham, and so we use them as a small training set to train our Bayesian classifier.

- First, we decide that d and e are so-called *stop words* that are too common to convey class information.
- The remaining words, a, b and c, constitute our vocabulary.

Training a naive Bayes model

For the multinomial model, we represent each e-mail as a count vector, as before.

- In order to estimate the parameters of the multinomial, we sum up the count vectors for each class, which gives $(5, 9, 3)$ for spam and $(11, 3, 3)$ for ham.
- To smooth these probability estimates we add one pseudo-count for each vocabulary word, which brings the total number of occurrences of vocabulary words to 20 for each class.
- The estimated parameter vectors are thus
  $\hat{\boldsymbol{\theta}}^{\oplus} = (6/20, 10/20, 4/20) = (0.3, 0.5, 0.2)$ for spam and
  $\hat{\boldsymbol{\theta}}^{\ominus} = (12/20, 4/20, 4/20) = (0.6, 0.2, 0.2)$ for ham.

Training a naive Bayes model

In the multivariate Bernoulli model e-mails are represented by bit vectors, as before.

- Adding the bit vectors for each class results in $(2, 3, 1)$ for spam and $(3, 1, 1)$ for ham.
- Each count is to be divided by the number of documents in a class, in order to get an estimate of the probability of a document containing a particular vocabulary word.
- Probability smoothing now means adding two pseudo-documents, one containing each word and one containing none of them.
- This results in the estimated parameter vectors $\hat{\boldsymbol{\theta}}^{\oplus} = (3/6, 4/6, 2/6) = (0.5, 0.67, 0.33)$ for spam and $\hat{\boldsymbol{\theta}}^{\ominus} = (4/6, 2/6, 2/6) = (0.67, 0.33, 0.33)$ for ham.

Linear discriminants

Many forms of linear discriminant from statistics and machine learning, e.g.,

- Fisher's Linear Discriminant Analysis
  - the basic linear classifier in lecture 1 is a version of this
- Logistic Regression
  - a probabilistic linear classifier
- Perceptron
  - a linear threshold classifier
  - an early version of an artificial "neuron"
  - still a useful method, and source of ideas

Logistic regression

In the case of a two-class problem, model the probability of one class $P(Y = 1)$ vs. the alternative $(1 - P(Y = 1))$:

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

or

$$\ln \frac{P(Y = 1|\mathbf{x})}{1 - P(Y = 1|\mathbf{x})} = \mathbf{w}^T\mathbf{x}$$

The quantity on the l.h.s. is called the *logit* and all we are doing is a linear model for the logit.

Note: to fit this is actually more complex than linear regression, so we omit the details.

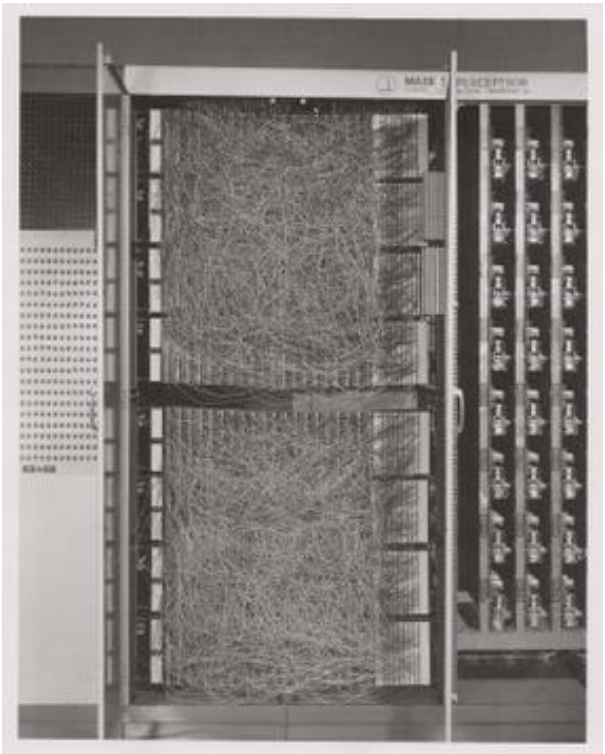
Generalises to multiple class versions (Y can have more than two values).

Perceptron

A linear classifier that can achieve perfect separation on linearly separable data is the *perceptron*, originally proposed as a simple *neural network* by F. Rosenblatt in the late 1950s.

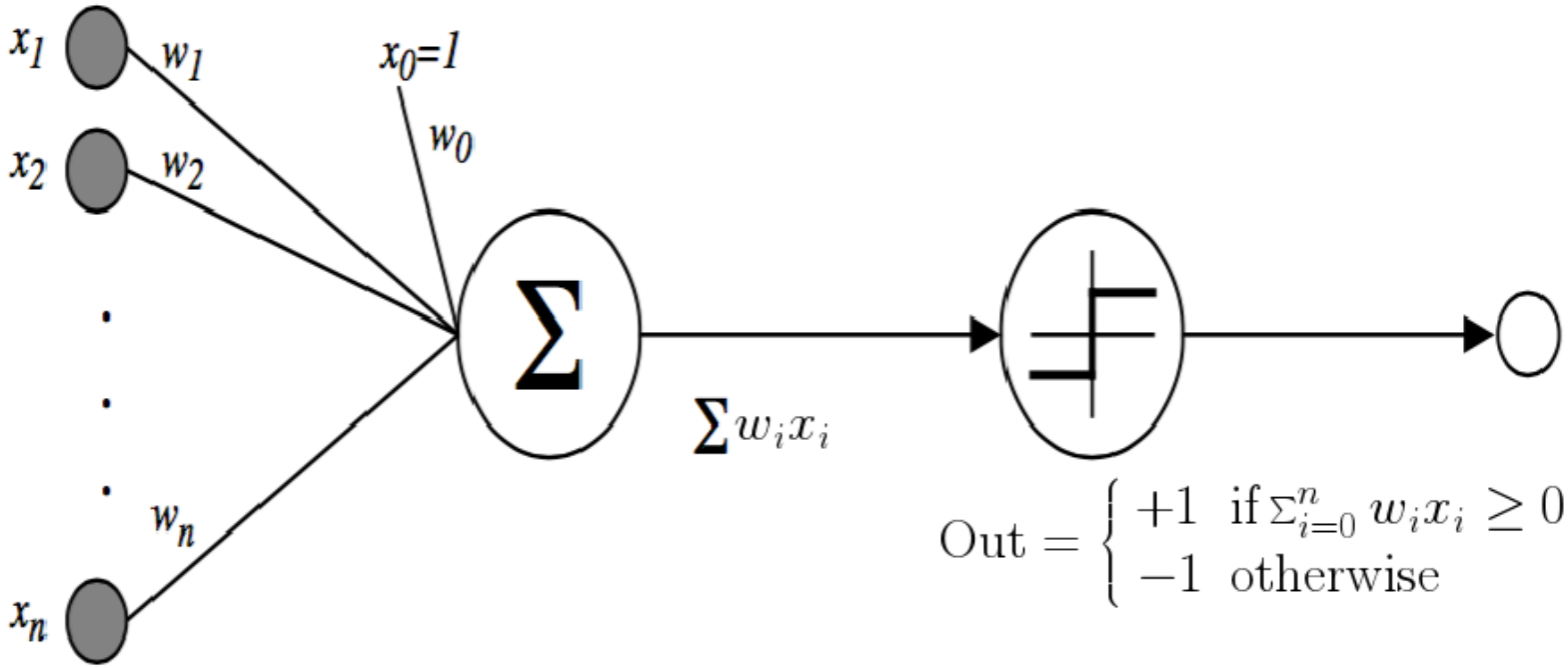
Perceptron

Originally implemented in software (based on the McCulloch-Pitts neuron from the 1940s), then in hardware as a 20x20 visual sensor array with potentiometers for adaptive weights.



Source `http://en.wikipedia.org/w/index.php?curid=47541432`

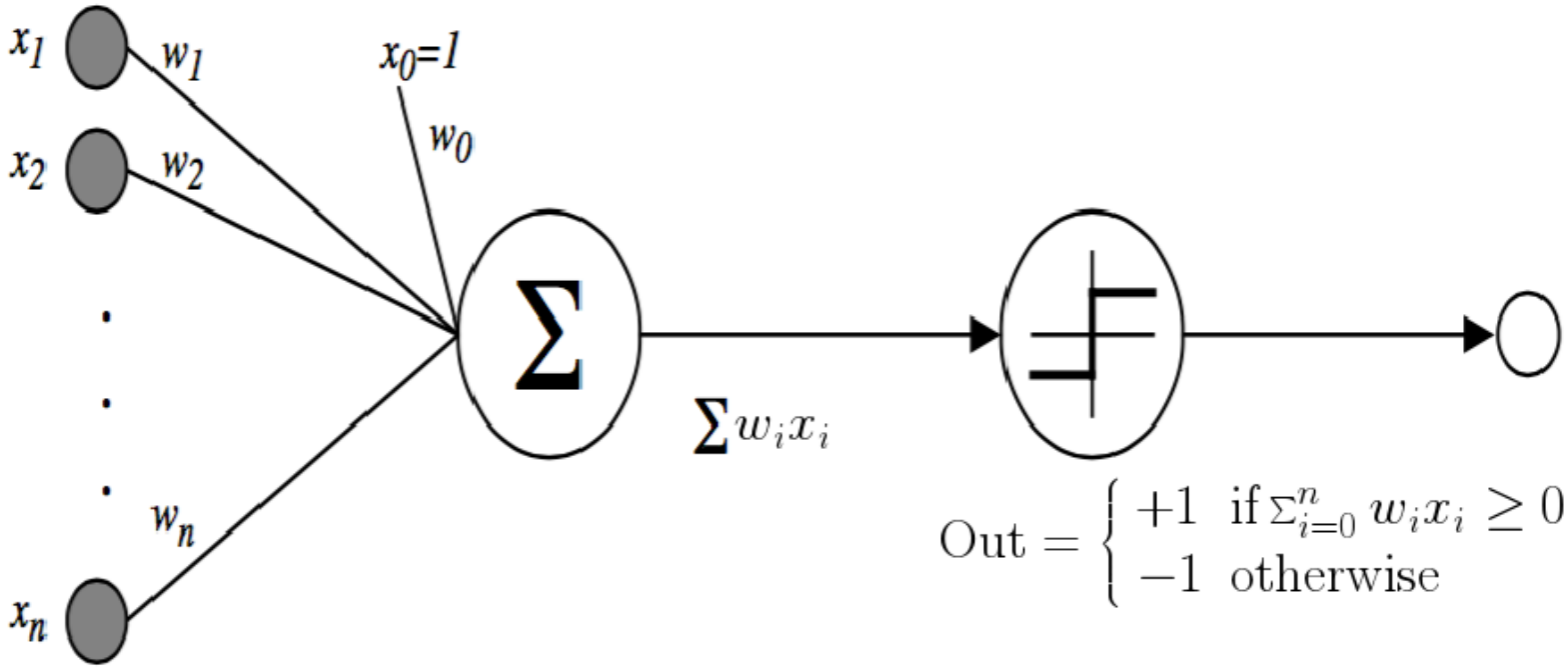
Perceptron



Output o is thresholded sum of products of inputs and their weights:

$$o(x_1, \ldots, x_n) = \begin{cases} +1 & \text{if } w_0 + w_1 x_1 + \cdots + w_n x_n > 0 \\ -1 & \text{otherwise.} \end{cases}$$

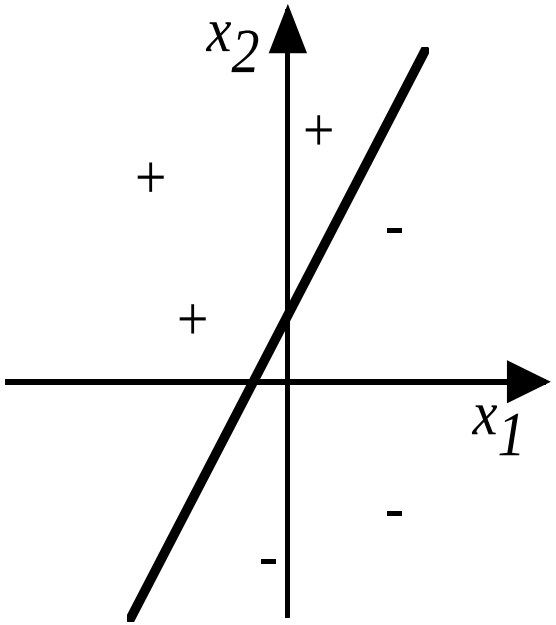
Perceptron



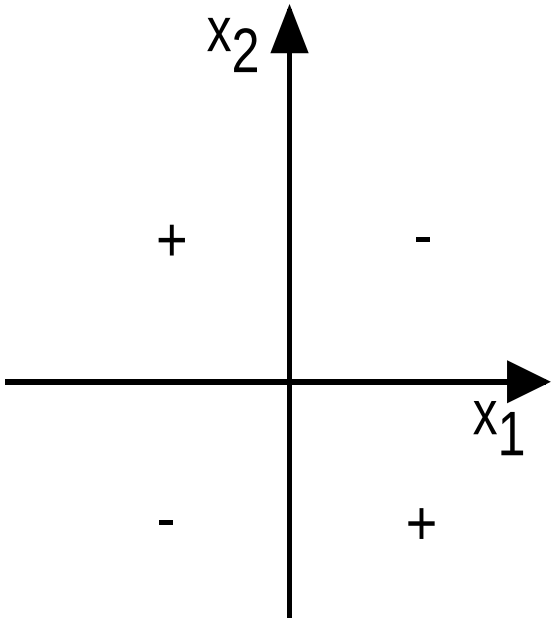
Or in vector notation:

$$o(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{w} \cdot \mathbf{x} > 0 \\ -1 & \text{otherwise.} \end{cases}$$

Decision Surface of a Perceptron



(a)



(b)

Represents some useful functions

- What weights represent $o(x_1, x_2) = AND(x_1, x_2)$?
- What weights represent $o(x_1, x_2) = XOR(x_1, x_2)$?

Decision Surface of a Perceptron

So some functions not representable

- e.g., not linearly separable
  - a labelled data set is linearly separable if there is a linear decision boundary that separates the classes
- for non-linearly separable data we'll need something else
  - e.g., networks of these ...
  - the start of "deep" networks ...

Perceptron learning

Key idea:

Learning is "finding a good set of weights"

Perceptron learning is simply an iterative weight-update scheme:

$$w_i \leftarrow w_i + \Delta w_i$$

where the weight update Δw_i depends only on *misclassified* examples and is modulated by a "smoothing" parameter η typically referred to as the "learning rate".

Can prove that perceptron learning will converge:

- if training data is linearly separable
- and η sufficiently small

Perceptron learning

The perceptron iterates over the training set, updating the weight vector every time it encounters an incorrectly classified example.

- For example, let $\mathbf{x}_i$ be a misclassified positive example, then we have $y_i = +1$ and $\mathbf{w} \cdot \mathbf{x}_i < t$. We therefore want to find $\mathbf{w}'$ such that $\mathbf{w}' \cdot \mathbf{x}_i > \mathbf{w} \cdot \mathbf{x}_i$, which moves the decision boundary towards and hopefully past x_i.
- This can be achieved by calculating the new weight vector as $\mathbf{w}' = \mathbf{w} + \eta \mathbf{x}_i$, where $0 < \eta \leq 1$ is the *learning rate* (again, assume set to 1). We then have $\mathbf{w}' \cdot \mathbf{x}_i = \mathbf{w} \cdot \mathbf{x}_i + \eta \mathbf{x}_i \cdot \mathbf{x}_i > \mathbf{w} \cdot \mathbf{x}_i$ as required.
- Similarly, if $\mathbf{x}_j$ is a misclassified negative example, then we have $y_j = -1$ and $\mathbf{w} \cdot \mathbf{x}_j > t$. In this case we calculate the new weight vector as $\mathbf{w}' = \mathbf{w} - \eta \mathbf{x}_j$, and thus $\mathbf{w}' \cdot \mathbf{x}_j = \mathbf{w} \cdot \mathbf{x}_j - \eta \mathbf{x}_j \cdot \mathbf{x}_j < \mathbf{w} \cdot \mathbf{x}_j$.

Perceptron learning

- The two cases can be combined in a single update rule:

$$\mathbf{w}' = \mathbf{w} + \eta y_i \mathbf{x}_i$$

- Here y_i acts to change the sign of the update, corresponding to whether a positive or negative example was misclassified
- This is the basis of the *perceptron training algorithm* for linear classification
- The algorithm just iterates over the training examples applying the weight update rule until all the examples are correctly classified
- If there is a linear model that separates the positive from the negative examples, i.e., the data is linearly separable, it can be shown that the perceptron training algorithm will converge in a finite number of steps.

Perceptron training algorithm

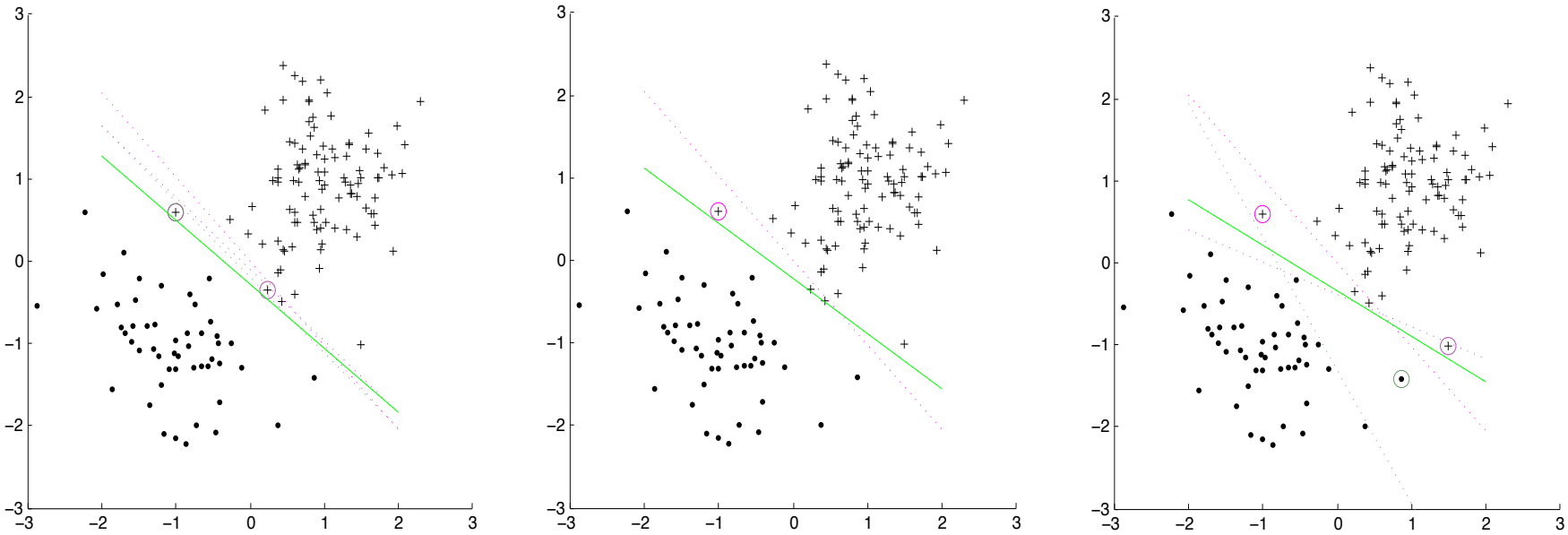
Algorithm Perceptron(D, η) // perceptron training for linear classification

Input: labelled training data D in homogeneous coordinates; learning rate η.

Output: weight vector $\mathbf{w}$ defining classifier $\hat{y} = \text{sign}(\mathbf{w} \cdot \mathbf{x})$.

$\mathbf{w} \leftarrow \mathbf{0}$ // Other initialisations of the weight vector are possible
converged$\leftarrow$false
while *converged* $=$ false **do**
    converged$\leftarrow$true
    for $i = 1$ to $|D|$ **do**
        if $y_i \mathbf{w} \cdot \mathbf{x}_i \leq 0$ **then** // i.e., $\hat{y}_i \neq y_i$
            $\mathbf{w} \leftarrow \mathbf{w} + \eta y_i \mathbf{x}_i$
            converged$\leftarrow$false // We changed $\mathbf{w}$ so haven't converged yet
        end
    end
end

Perceptron training – varying learning rate



(left) A perceptron trained with a small learning rate ($\eta = 0.2$). The circled examples are the ones that trigger the weight update. (middle) Increasing the learning rate to $\eta = 0.5$ leads in this case to a rapid convergence. (right) Increasing the learning rate further to $\eta = 1$ may lead to too aggressive weight updating, which harms convergence.
The starting point in all three cases was the basic linear classifier.

Summary

- Two major frameworks for classification by linear models
  Distance-based. The key ideas are geometric.
  Probabilistic. The key ideas are Bayesian.
- We also discussed Logistic Regression and the Perceptron, a simple form of threshold model.
- These classifiers are also, in some sense, linear models
- So we have established the basis for learning classifiers
- Later we will see how to extend by building on these ideas