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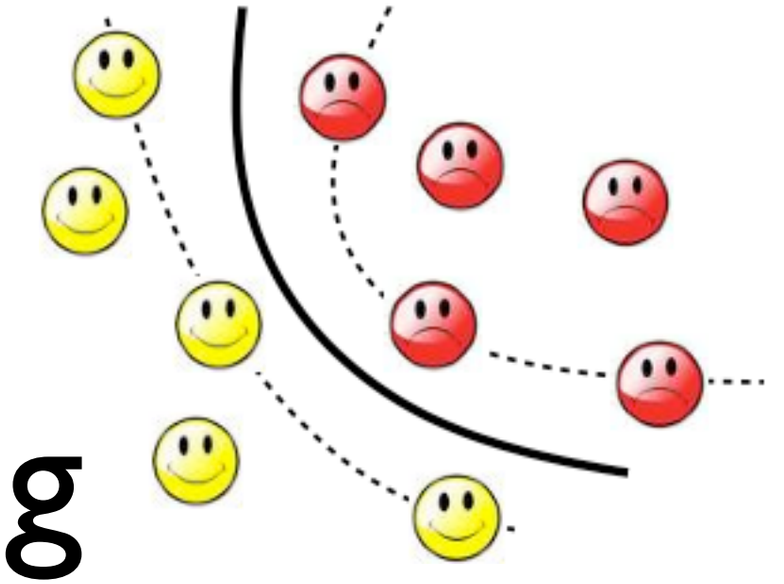

Machine Learning and Data Mining

(COMP 5318)

Logistic Regression and SVMs

Tongliang Liu

Announcements

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- This lecture is based on:
  - Murphy's book: Chapters 8, 14
  - Bishop's book: Chapters 4, 7
  - Ullman's book: Chapter 12

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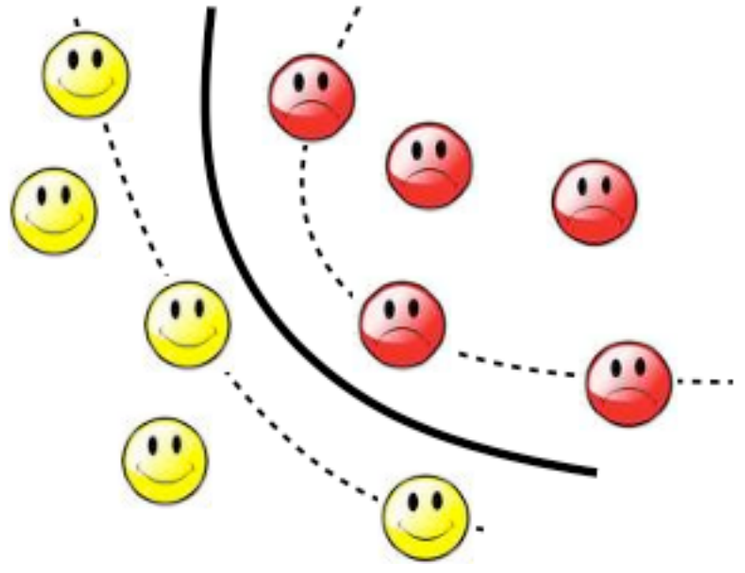

Quick Review

Supervised learning

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- Learn a mapping function *f* from $\mathbf{x}$ to y

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

  - If $y \in \{1, 2, \ldots, C\}$ the problem is called classification
  - If $y \in \mathbb{R}$ the problem is called regression

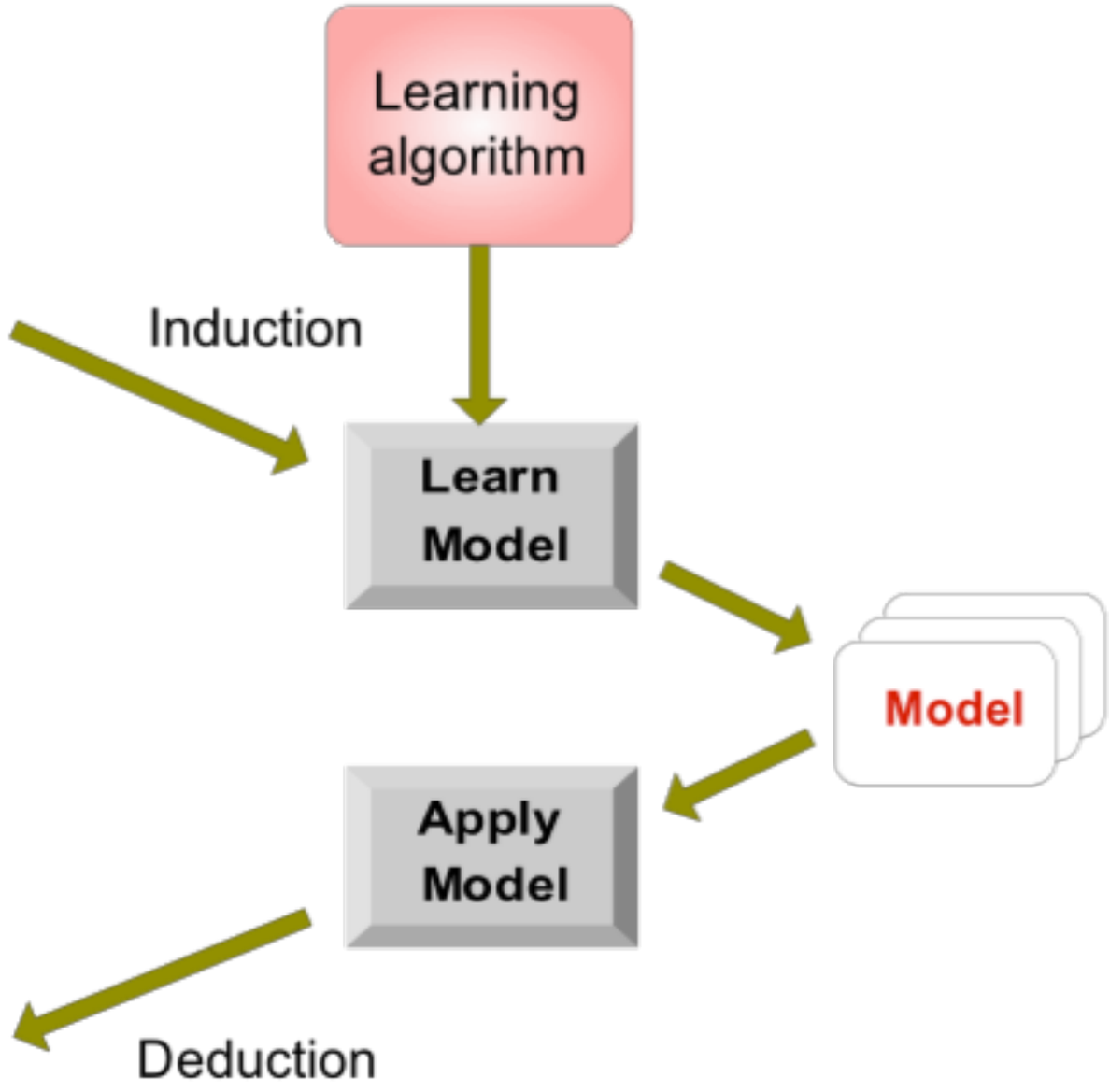
Illustrating Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

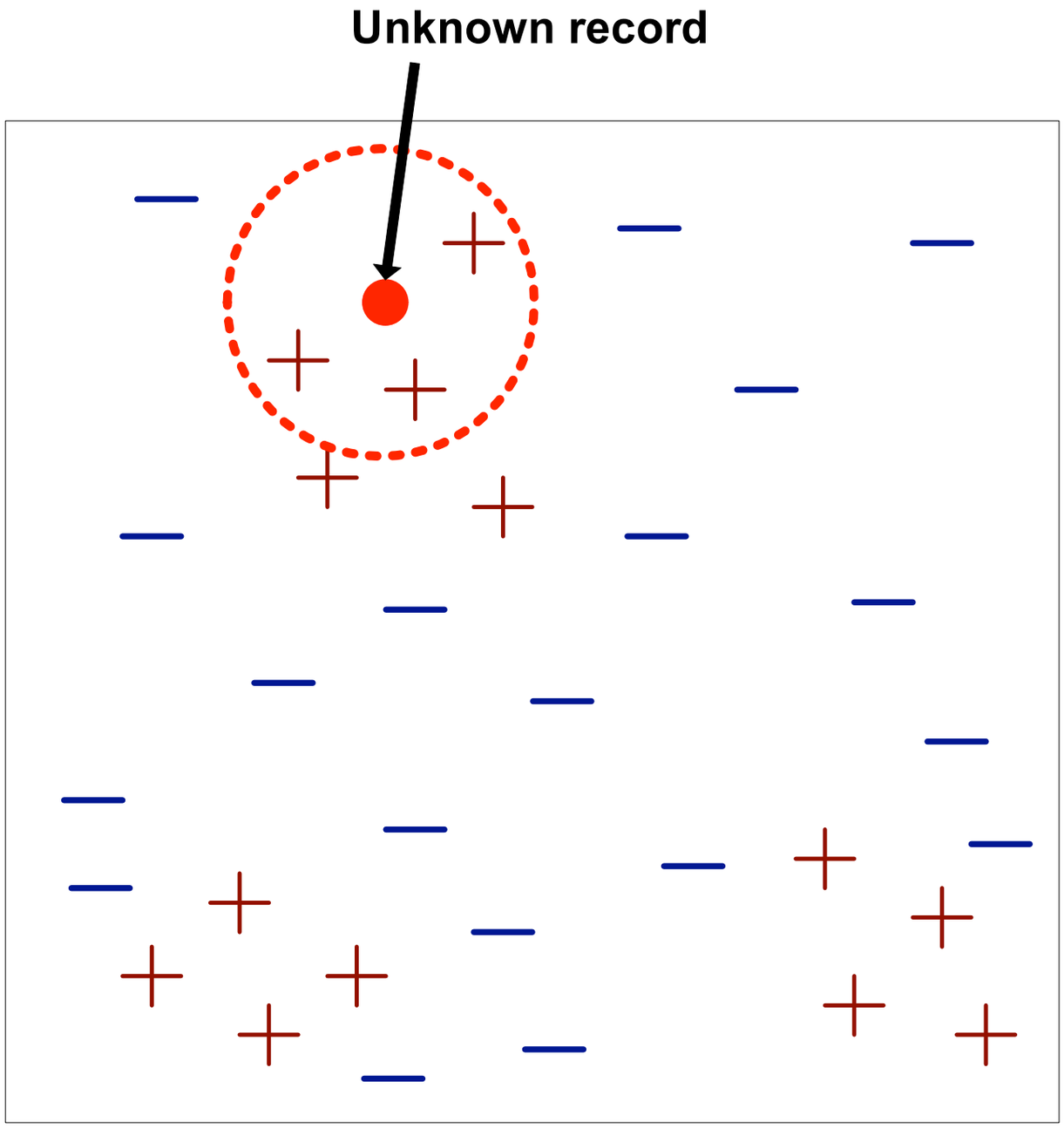
Training Set

Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Test Set



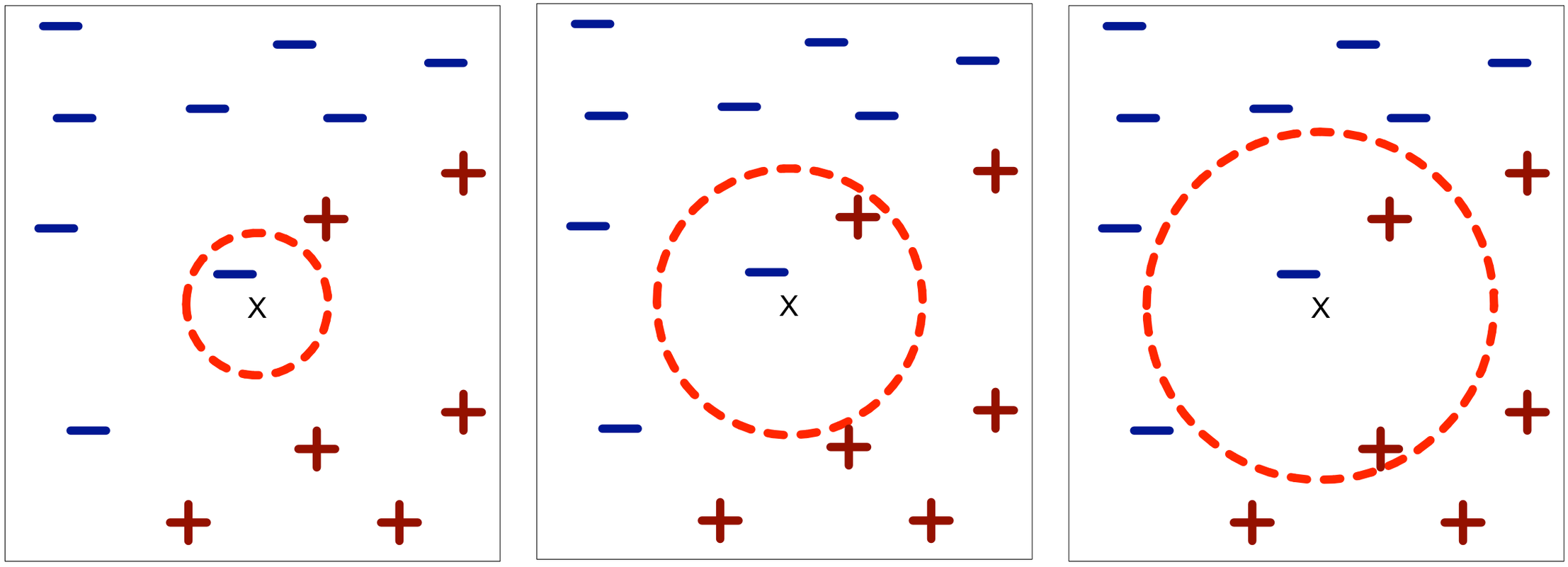
Nearest Neighbour Classifiers



- Requires three things
  - The set of stored records
  - Distance Metric to compute distance between records
  - The value of *k*, the number of nearest neighbours to retrieve

- To classify an unknown record:
  - Compute distance to other training records
  - Identify *k* nearest neighbours
  - Use class labels of nearest neighbours to determine the class label of unknown record (e.g., by taking majority vote)

Definition of Nearest Neighbour



(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

K-nearest neighbours of a record x are data points that have the k smallest distance to x

Bayesian Classifiers

- Approach:
  - compute the posterior probability $P(C \mid A_1, A_2, \ldots, A_n)$ for all values of C using the Bayes' theorem

$$P(C \mid A_1 A_2 \ldots A_n) = \frac{P(A_1 A_2 \ldots A_n \mid C) P(C)}{P(A_1 A_2 \ldots A_n)}$$

  - Choose value of C that maximises
    $P(C \mid A_1, A_2, \ldots, A_n)$
  - Equivalent to choosing value of C that maximises
    $P(A_1, A_2, \ldots, A_n \mid C)\, P(C)$
- How to estimate $P(A_1, A_2, \ldots, A_n \mid C)$?

Naïve Bayes Classifier

- Assume independence among attributes A_i when class is given:
  - $P(A_1, A_2, \ldots, A_n \mid C) = P(A_1 \mid C_j)\, P(A_2 \mid C_j) \ldots P(A_n \mid C_j)$

- Can estimate $P(A_i \mid C_j)$ for all A_i and C_j.

- New point is classified to C_j if $P(C_j) \prod P(A_i \mid C_j)$ is maximal.

How to Estimate Probabilities from Data?

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#	Refund	Status	Salary	Class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

- Class: $P(C) = N_c/N$
  - e.g., $P(No)$ = 7/10, $P(Yes)$ = 3/10
- For discrete attributes:

$$P(A_i \mid C_k) = |A_{ik}| / N_{c^k}$$

- where $|A_{ik}|$ is number of instances having attribute A_i and belongs to class C_k
- Examples:
  $P(Status=Married|No)$ = 4/7
  $P(Refund=Yes|Yes)$ = 0

Example of Naïve Bayes Classifier

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Name	Give Birth	Can Fly	Live in Water	Have Legs	Class
human	yes	no	no	yes	mammals
python	no	no	no	no	non-mammals
salmon	no	no	yes	no	non-mammals
whale	yes	no	yes	no	mammals
frog	no	no	sometimes	yes	non-mammals
komodo	no	no	no	yes	non-mammals
bat	yes	yes	no	yes	mammals
pigeon	no	yes	no	yes	non-mammals
cat	yes	no	no	yes	mammals
leopard shark	yes	no	yes	no	non-mammals
turtle	no	no	sometimes	yes	non-mammals
penguin	no	no	sometimes	yes	non-mammals
porcupine	yes	no	no	yes	mammals
eel	no	no	yes	no	non-mammals
salamander	no	no	sometimes	yes	non-mammals
gila monster	no	no	no	yes	non-mammals
platypus	no	no	no	yes	mammals
owl	no	yes	no	yes	non-mammals
dolphin	yes	no	yes	no	mammals
eagle	no	yes	no	yes	non-mammals

A: attributes

M: mammals

N: non-mammals

$$P(A \mid M) = \frac{6}{7} \times \frac{6}{7} \times \frac{2}{7} \times \frac{2}{7} = 0.06$$

$$P(A \mid N) = \frac{1}{13} \times \frac{10}{13} \times \frac{3}{13} \times \frac{4}{13} = 0.0042$$

$$P(A \mid M)P(M) = 0.06 \times \frac{7}{20} = 0.021$$

$$P(A \mid N)P(N) = 0.004 \times \frac{13}{20} = 0.0027$$

Give Birth	Can Fly	Live in Water	Have Legs	Class
yes	no	yes	no	?

$$P(A|M)P(M) > P(A|N)P(N)$$

=> Mammals

Metrics for Performance Evaluation

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- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a	b
	Class=No	c	d

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

Cost-Sensitive Measures

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$$\text{Precision (p)} = \frac{a}{a+c}$$

$$\text{Recall (r)} = \frac{a}{a+b}$$

$$\text{F - measure (F)} = \frac{2rp}{r+p} = \frac{2a}{2a+b+c}$$

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

- Precision is biased towards C(Yes | Yes) & C(Yes | No)
- Recall is biased towards C(Yes | Yes) & C(No | Yes)
- F-measure is biased towards all except C(No | No)

$$\text{Weighted Accuracy} = \frac{w_1 a + w_4 d}{w_1 a + w_2 b + w_3 c + w_4 d}$$

ROC Curve

- TP rate, TPR = TP/(TP+FN)
- FP rate, FPR = FP/(FP + TN)

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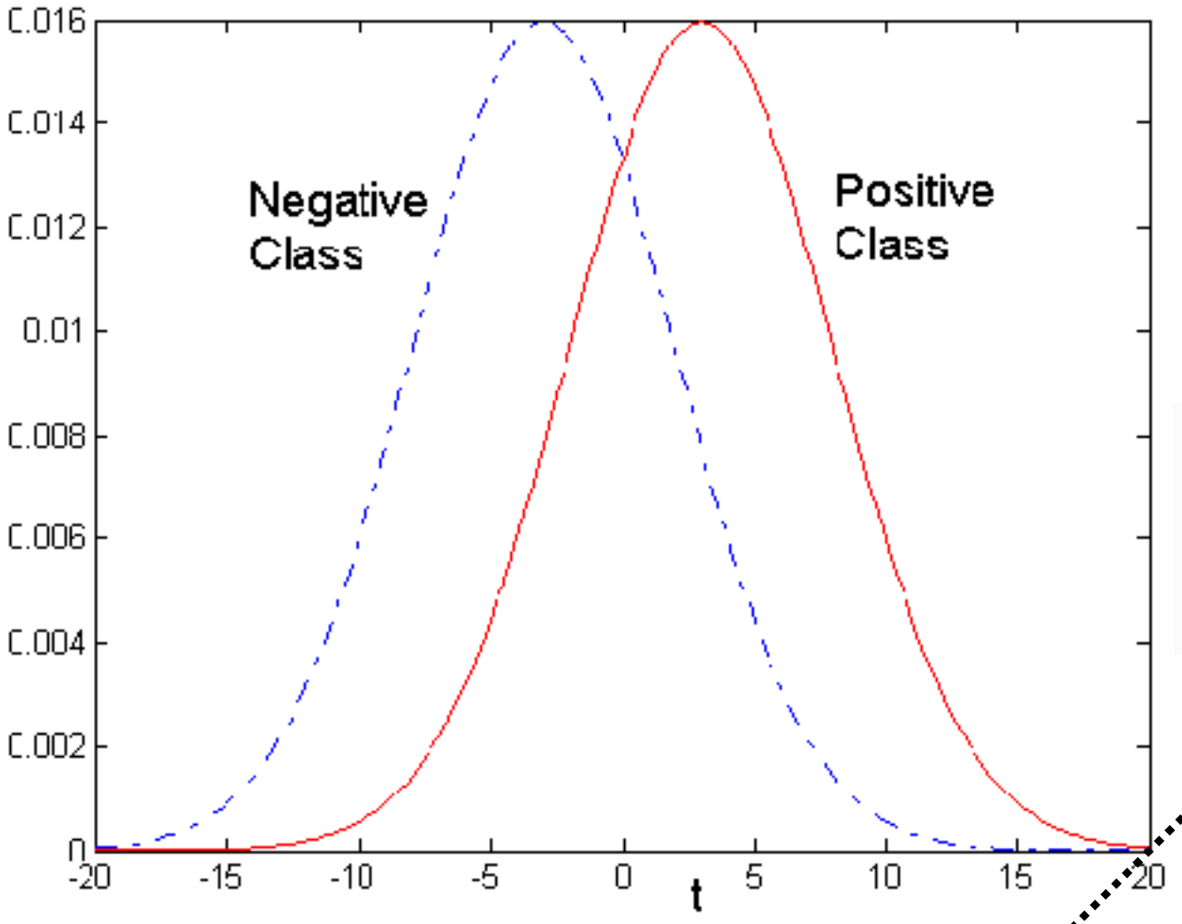
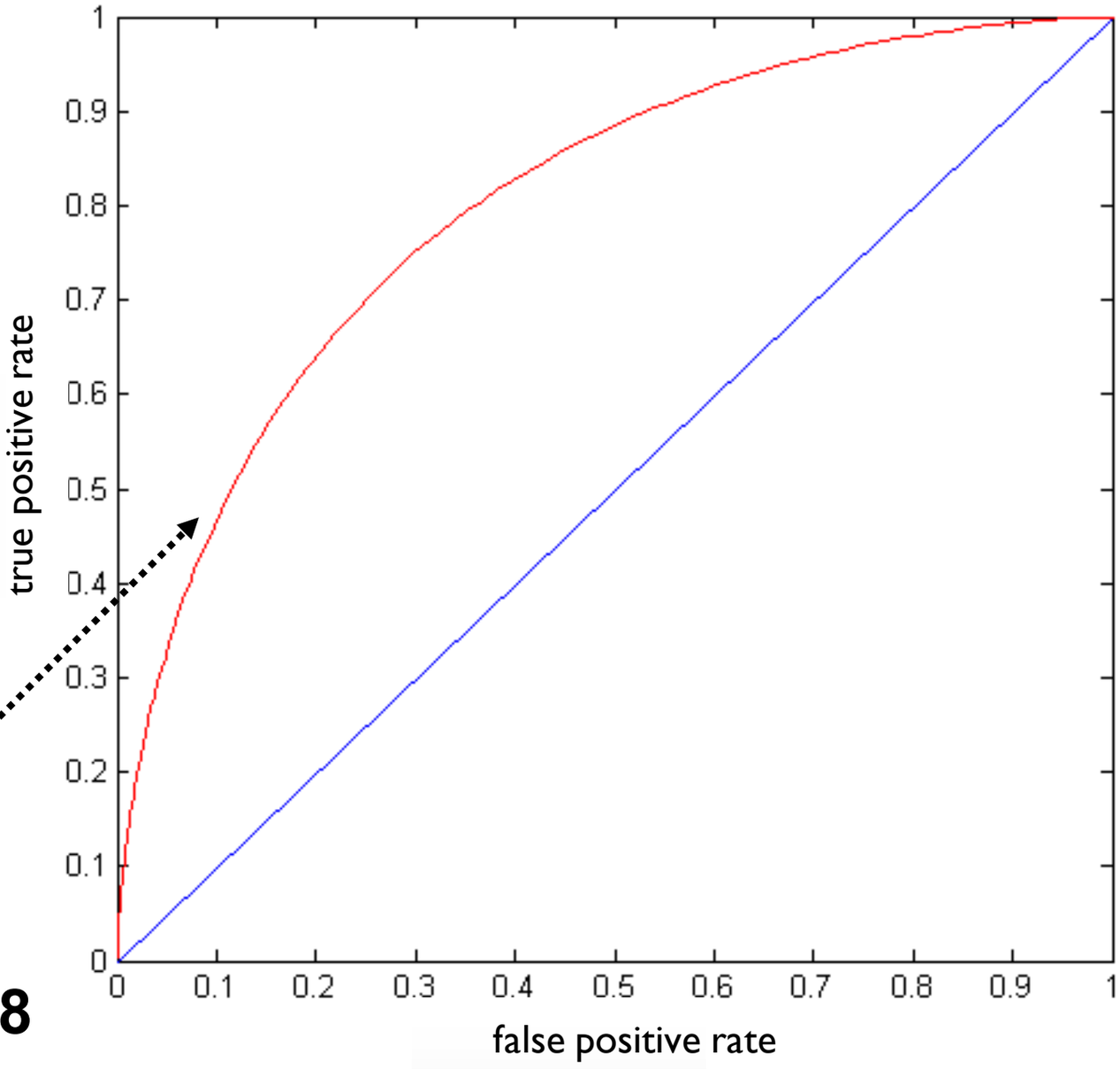
- 1-dimensional data set containing 2 classes (positive and negative)
- any points located at x > t is classified as positive





At threshold t:

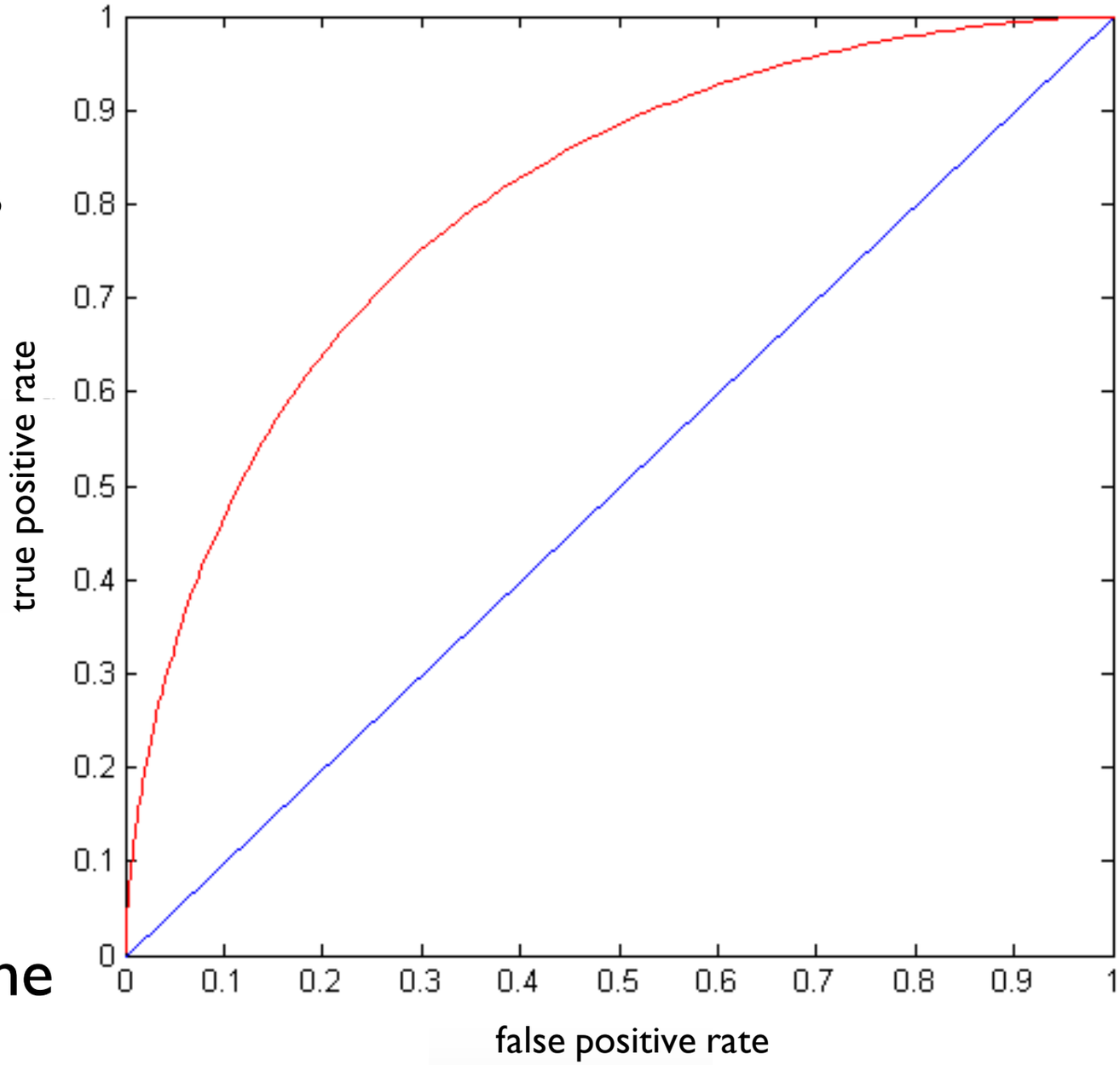
TP=0.5, FN=0.5, FP=0.12, FN=0.88

ROC Curve

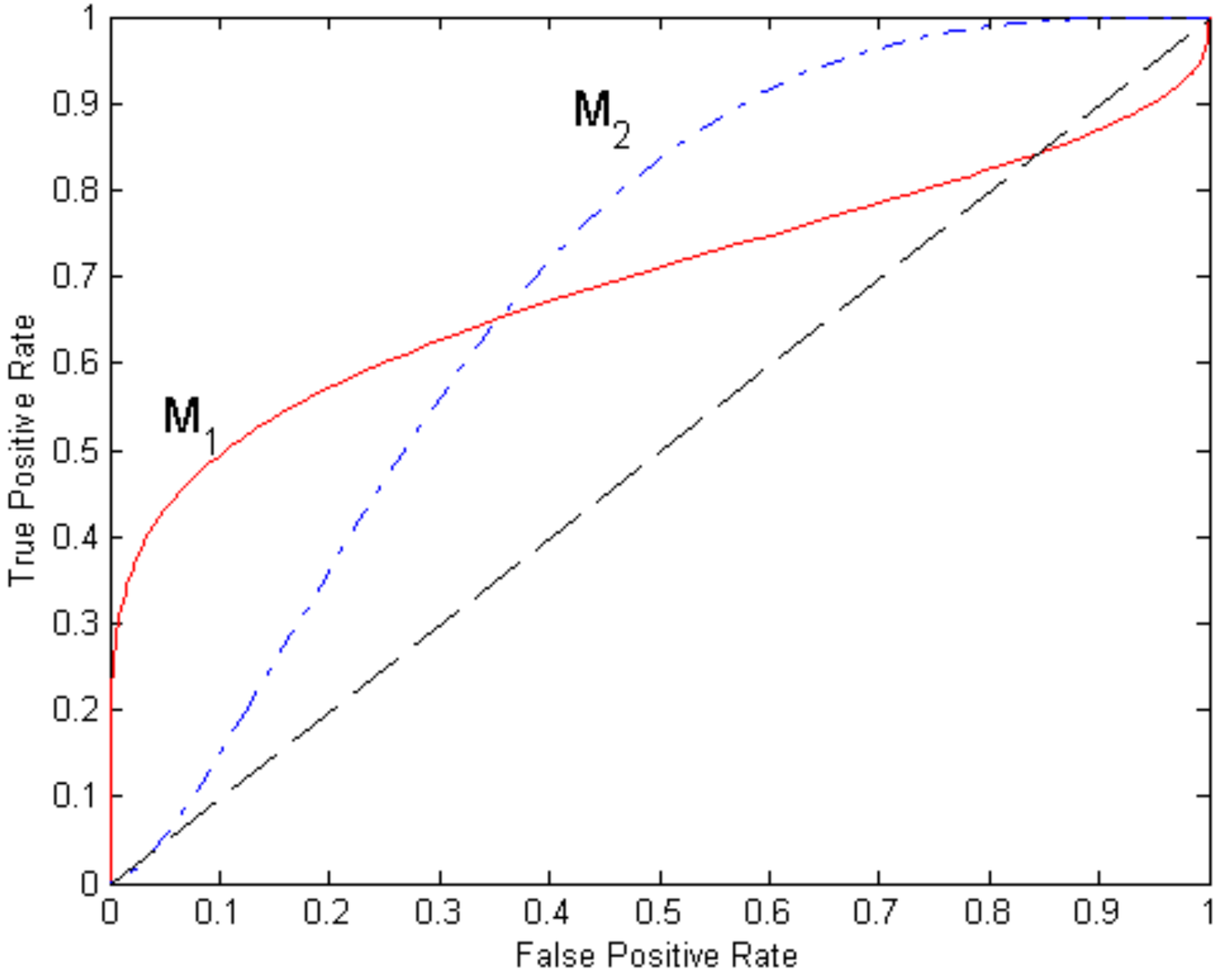
(TP,FP):

- (0,0): declare everything to be negative class
- (1,1): declare everything to be positive class
- (1,0): ideal

- Diagonal line:
  - Random guessing
  - Below diagonal line:
    - prediction is opposite of the true class



Using ROC for Model Comparison



- No model consistently outperform the other
- M_1 is better for small FPR
- M_2 is better for large FPR

- Area Under the ROC curve
  - Ideal:
    - Area = 1
  - Random guess:
    - Area = 0.5

How to construct a ROC curve

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Instance	$P(+\|A)$	True Class
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

- Use classifier that produces posterior probability for each test instance $P(+ \mid A)$
- Sort the instances according to $P(+ \mid A)$ in decreasing order
- Apply threshold at each unique value of $P(+ \mid A)$
- Count the number of TP, FP, TN, FN at each threshold
- TP rate, TPR = TP/(TP+FN)
- FP rate, FPR = FP/(FP + TN)

How to construct a ROC curve

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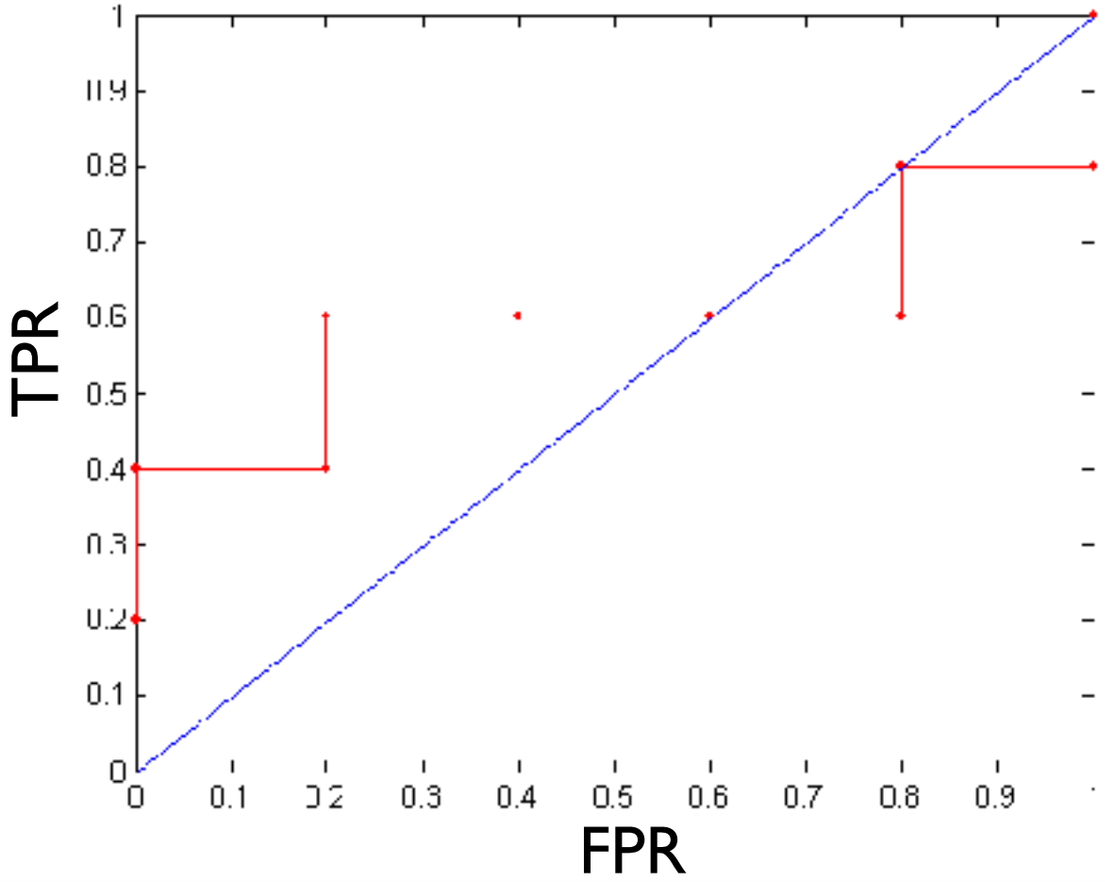
	Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=		0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
	TP	5	4	4	3	3	3	3	2	2	1	0
	FP	5	5	4	4	3	2	1	1	0	0	0
	TN	0	0	1	1	2	3	4	4	5	5	5
	FN	0	1	1	2	2	2	2	3	3	4	5
→	TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4	0.2	0
→	FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0	0	0

ROC Curve:



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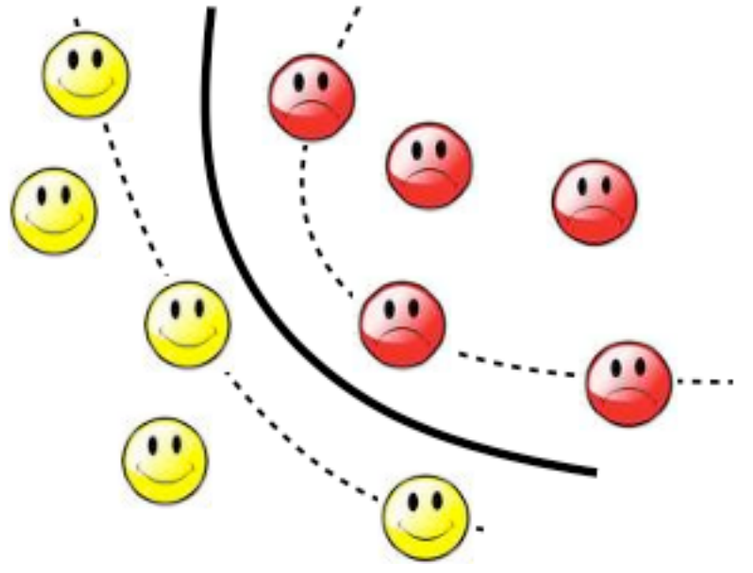
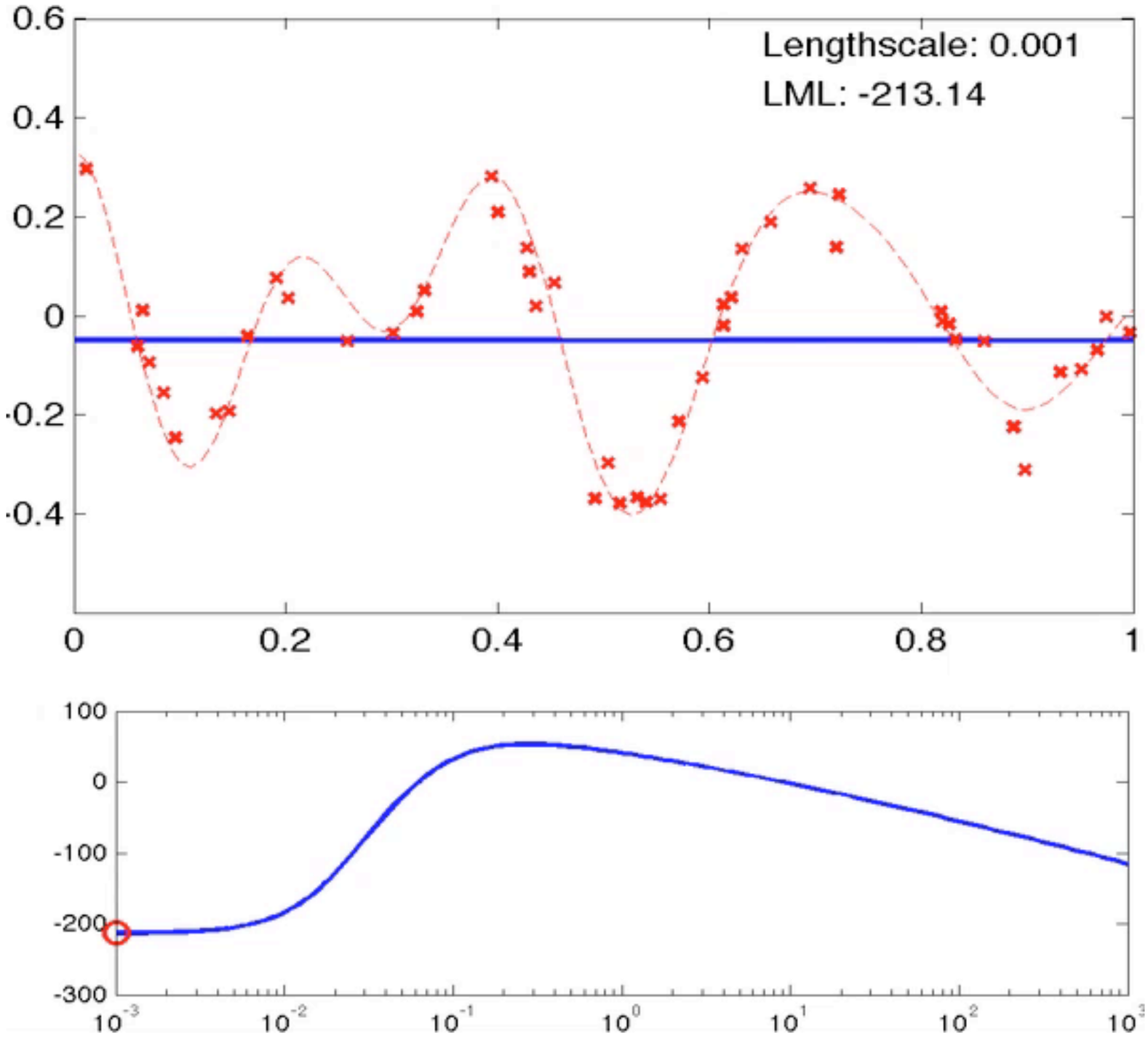


Classification II

Learning as optimisation



Loss functions

- Squared error, 0-1 Loss

$$L(y, \hat{y}) = (y - \hat{y})^2$$

$$L(y, \hat{y}) = I(y \neq \hat{y})$$

- Minimise risk, (expected risk, empirical risk)

$$R(\hat{f}) = E_{\mathbf{x},y} L(f(\mathbf{x}), \hat{f}(\mathbf{x}))$$

$$\hat{R}(\hat{f}) = \frac{1}{n} \sum_{i=1}^{n} L(y_i, \hat{f}(\mathbf{x}_i))$$

Loss for density estimation

- Suppose output is $\hat{p}(y|\mathbf{x})$, truth is $p(y|\mathbf{x})$
- Use KL (Kullback-Leibler) divergence

$$L(p(y|\mathbf{x}), \hat{p}(y|\mathbf{x})) = KL(p(y|\mathbf{x}), \hat{p}(y|\mathbf{x})) = \sum_y p(y|\mathbf{x}) \log \frac{p(y|\mathbf{x})}{\hat{p}(y|\mathbf{x})}$$

- Risk is expected negative log likelihood

$$R(\hat{p}) = -E_{\mathbf{x}} \sum_y p(y|\mathbf{x}) \log \hat{p}(y|\mathbf{x}) = -E_{\mathbf{x},y} \log \hat{p}(y|\mathbf{x})$$

Estimation vs Inference

- Learning as optimisation (frequentist): Given D, choose $\hat{f}$ to approximate f as closely as possible, so as to minimise (future) expected risk
- Usually compute parameter estimate $\hat{\theta}$
- Learning as inference (Bayesian): Given D, compute posterior over functions $p(f|D)$
- Or posterior over parameters

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)}$$

- Decision theory demonstrates that one of the best ways to minimise frequentist risk is to be Bayesian.

Generative vs Discriminative

- Generative approach:
  - Model $p(y, \mathbf{x}) = p(\mathbf{x}|y)p(y)$
  - Use Bayes' theorem $p(y|\mathbf{x}) = \dfrac{p(\mathbf{x}|y)p(y)}{p(\mathbf{x})}$

- Discriminative approach:
  - Model $p(y|\mathbf{x})$ directly

Naïve Bayes Classifier

Generative model:

$$p(\mathbf{x}, \mathcal{C}_k) = p(\mathcal{C}_k)p(\mathbf{x}_n|\mathcal{C}_k) = \pi\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \Sigma_k)$$

class posterior

class conditional density

class prior

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{\sum_{\mathcal{C}_j} p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)}$$

normalising constant

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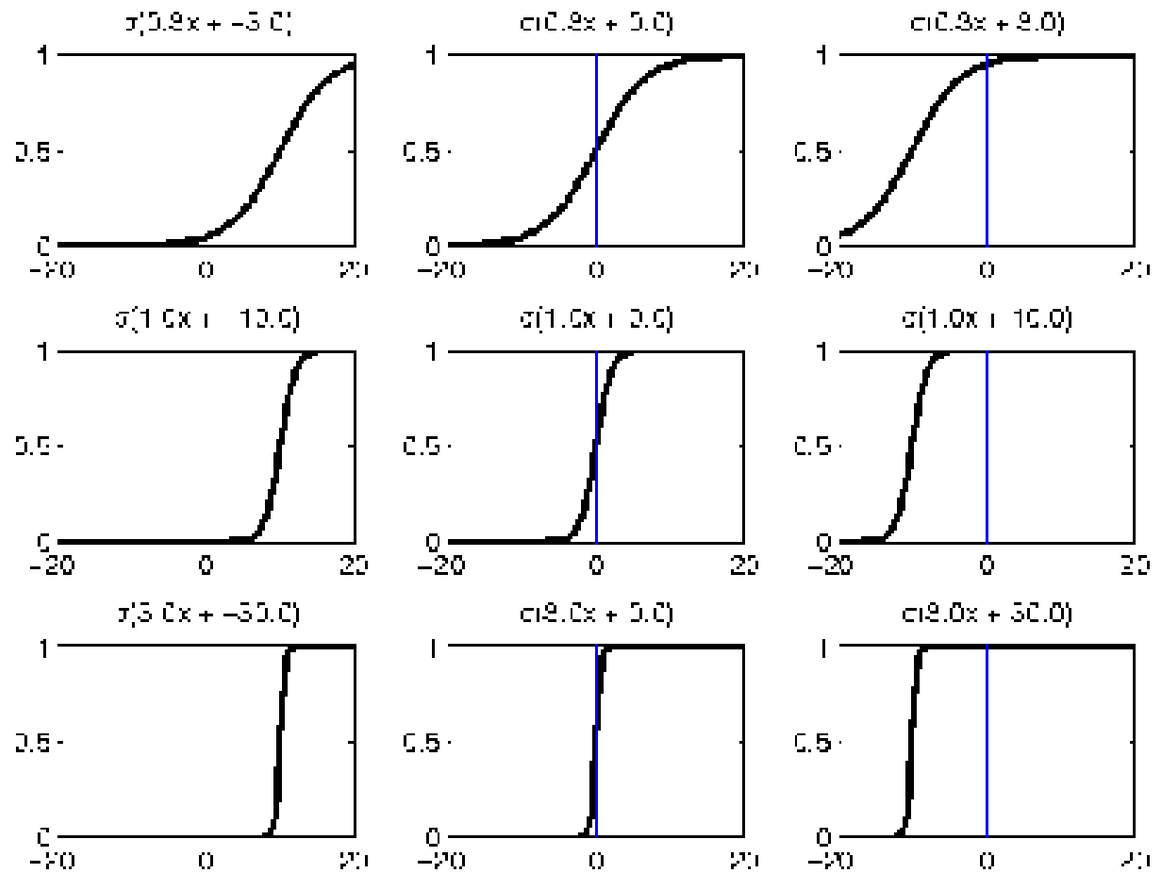
Logistic Regression

Logistic Regression

- Discriminative model for binary classification

$$
\begin{aligned}
p(y|\mathbf{x}, \mathbf{w}) &= \text{Ber}(y|\sigma(\eta)) = \sigma(\eta)^y (1-\sigma(\eta))^{1-y} \\
\eta &= \mathbf{w}^T \mathbf{x} \\
\sigma(\eta) &\stackrel{\text{def}}{=} \frac{1}{1+\exp(-\eta)} = \frac{e^\eta}{e^\eta + 1}
\end{aligned}
$$

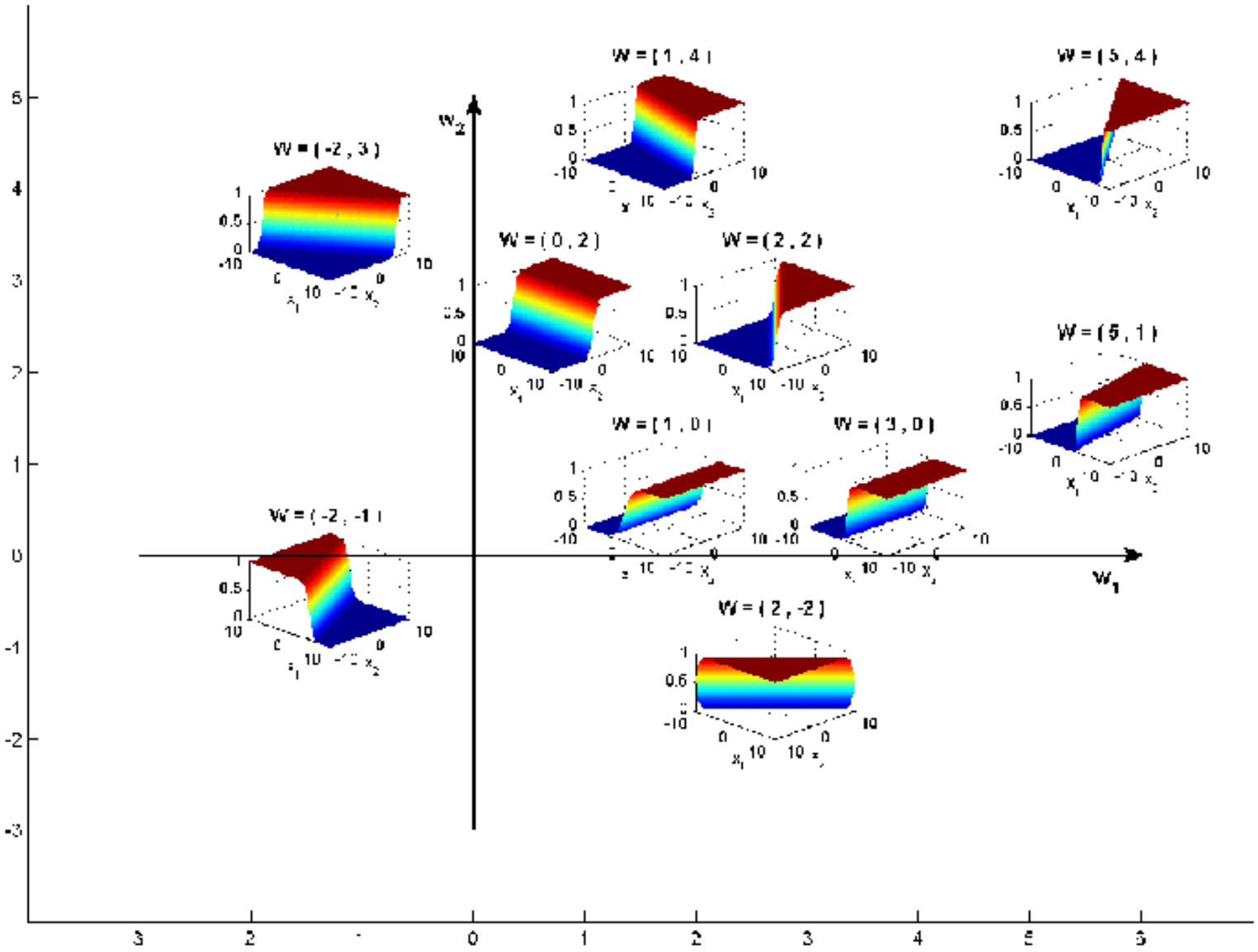


Sigmoid or Logistic function

Decision boundary

- Logistic Regression in 2D

$$p(y = 1|\mathbf{x}, \mathbf{w}) = \sigma(\mathbf{w}^T \mathbf{x})$$



Logistic Regression

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- Assumes a parametric form for directly estimating P(Y | X). For binary concepts, this is:

$$P(Y=0|X) = \frac{1}{1+\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$$

$$P(Y=1|X) = 1 - P(Y=0|X)$$

$$= \frac{\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}{1+\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$$

- Equivalent to a one-layer backpropagation neural net.
- Logistic regression is the source of the sigmoid function used in backpropagation.
- Objective function for training is somewhat different.

Logistic Regression as a Log-Linear Model

- Logistic regression is basically a linear model, which is demonstrated by taking logs.

$$\text{Assign label } Y = 0 \text{ iff } 1 < \frac{P(Y=0 \mid X)}{P(Y=1 \mid X)}$$

$$1 < \exp(w_0 + \sum_{i=1}^{n} w_i X_i)$$

$$0 < w_0 + \sum_{i=1}^{n} w_i X_i$$

$$\text{or equivalently} \quad w_0 > \sum_{i=1}^{n} -w_i X_i$$

- Also called a **maximum entropy model** (**MaxEnt**) because it can be shown that standard training for logistic regression gives the distribution with maximum entropy that is consistent with the training data.

Logistic Regression Training

- Weights are set during training to maximise the **conditional data likelihood** :

$$W \leftarrow \underset{W}{\operatorname{argmax}} \prod_{d \in D} P(Y^d \mid X^d, W)$$

where D is the set of training examples and Y^d and X^d denote, respectively, the values of Y and X for example d.

- Equivalently viewed as maximising the **conditional log likelihood** (CLL)

$$W \leftarrow \underset{W}{\operatorname{argmax}} \sum_{d \in D} \ln P(Y^d \mid X^d, W)$$

Logistic Regression Training

- Like neural-nets, can use standard gradient descent to find the parameters (weights) that optimise the CLL objective function.
- Many other more advanced training methods are possible to speed up convergence.
  - Conjugate gradient
  - Generalised Iterative Scaling (GIS)
  - Modified Iterative Scaling (MIS)
  - Limited-memory quasi-Newton (L-BFGS)
  - Stochastic gradient descent

Logistic Regression Training

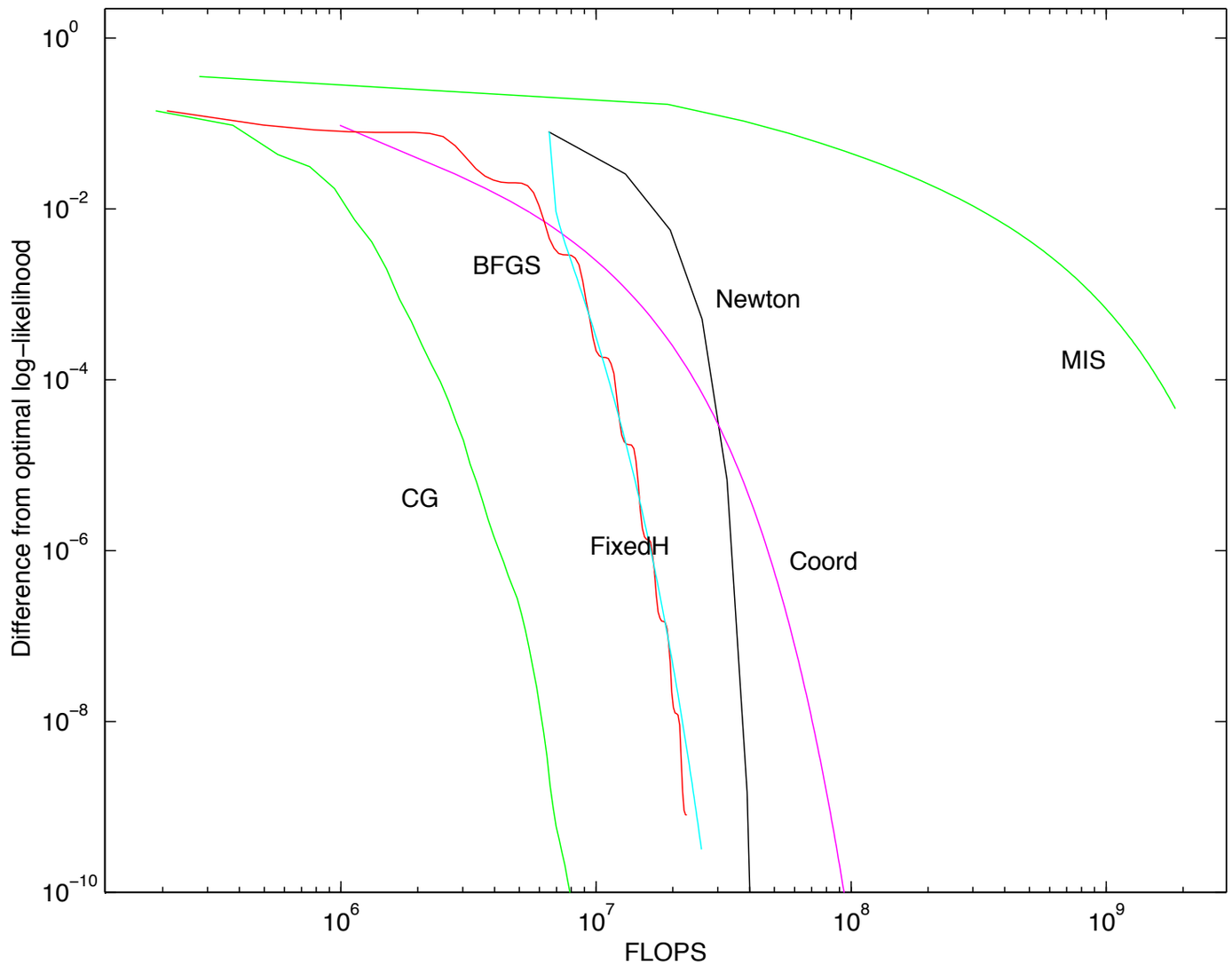

Figure 1: Cost vs. performance of six logistic regression algorithms. The dataset had 300 points in 100 dimensions. "CG" is conjugate gradient (section 4), "Coord" is coordinate-wise Newton, "FixedH" is Fixed-Hessian, and "MIS" is modified iterative scaling. CG also has the lowest actual time in Matlab.

See: "A comparison of numerical optimizers for logistic regression" by Thomas Minka, 2003.

Gradient Descent

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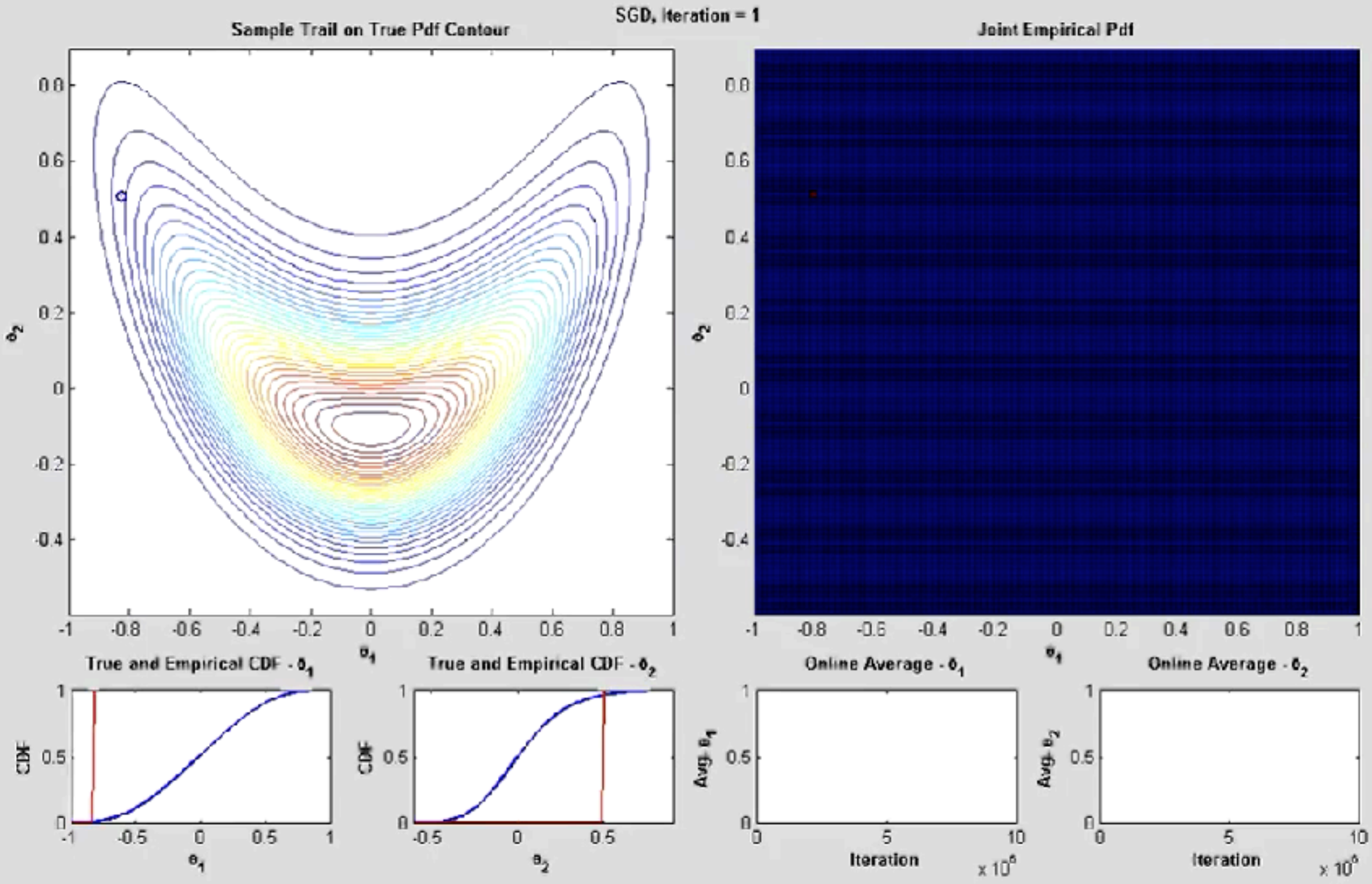

Preventing Overfitting in Logistic Regression

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- To prevent overfitting, one can use **regularisation** (a.k.a. smoothing) by penalising large weights by changing the training objective:

$$W \leftarrow \underset{W}{\operatorname{argmax}} \sum_{d \in D} \ln P(Y^d \mid X^d, W) - \frac{\lambda}{2} \|W\|^2$$

Where λ is a constant that determines the amount of smoothing

- This can be shown to be equivalent to assuming a Gaussian prior for *W* with zero mean and a variance related to $1/\lambda$.

Multinomial Logistic Regression

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- Logistic regression can be generalised to multi-class problems (where Y has a multinomial distribution).
- Effectively constructs a linear classifier for each category.

Relation Between NB and Logistic Regression

- Naïve Bayes with Gaussian distributions for features (GNB), can be shown to give the same functional form for the conditional distribution $P(Y \mid X)$.
  - But converse is not true, so Logistic Regression makes a weaker assumption.
- Logistic regression is a **discriminative** rather than generative model, since it models the conditional distribution $P(Y \mid X)$ and directly attempts to fit the training data for predicting Y from X. Does not specify a full joint distribution.

Relation Between NB and Logistic Regression (continued)

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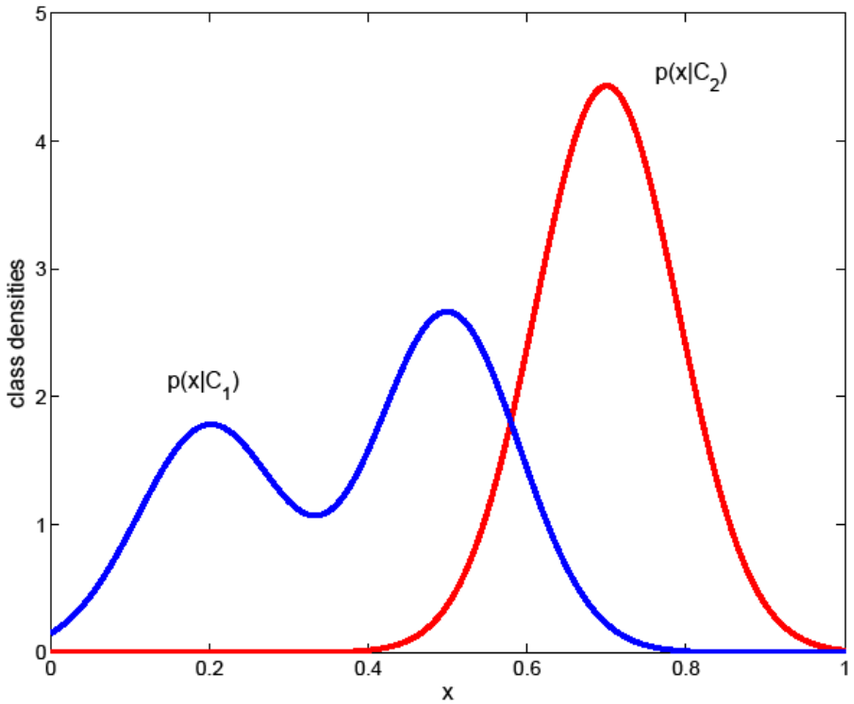
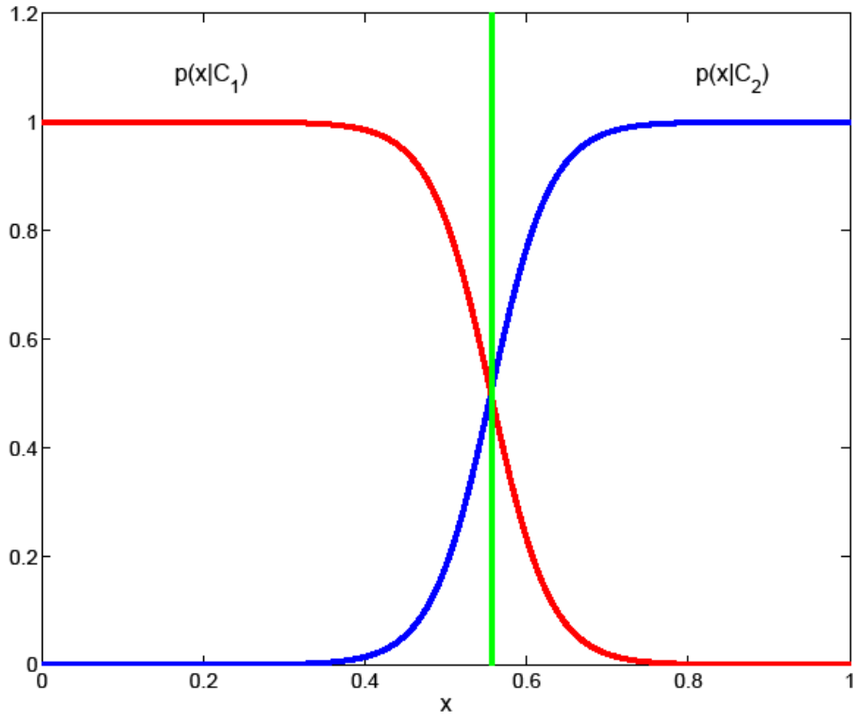
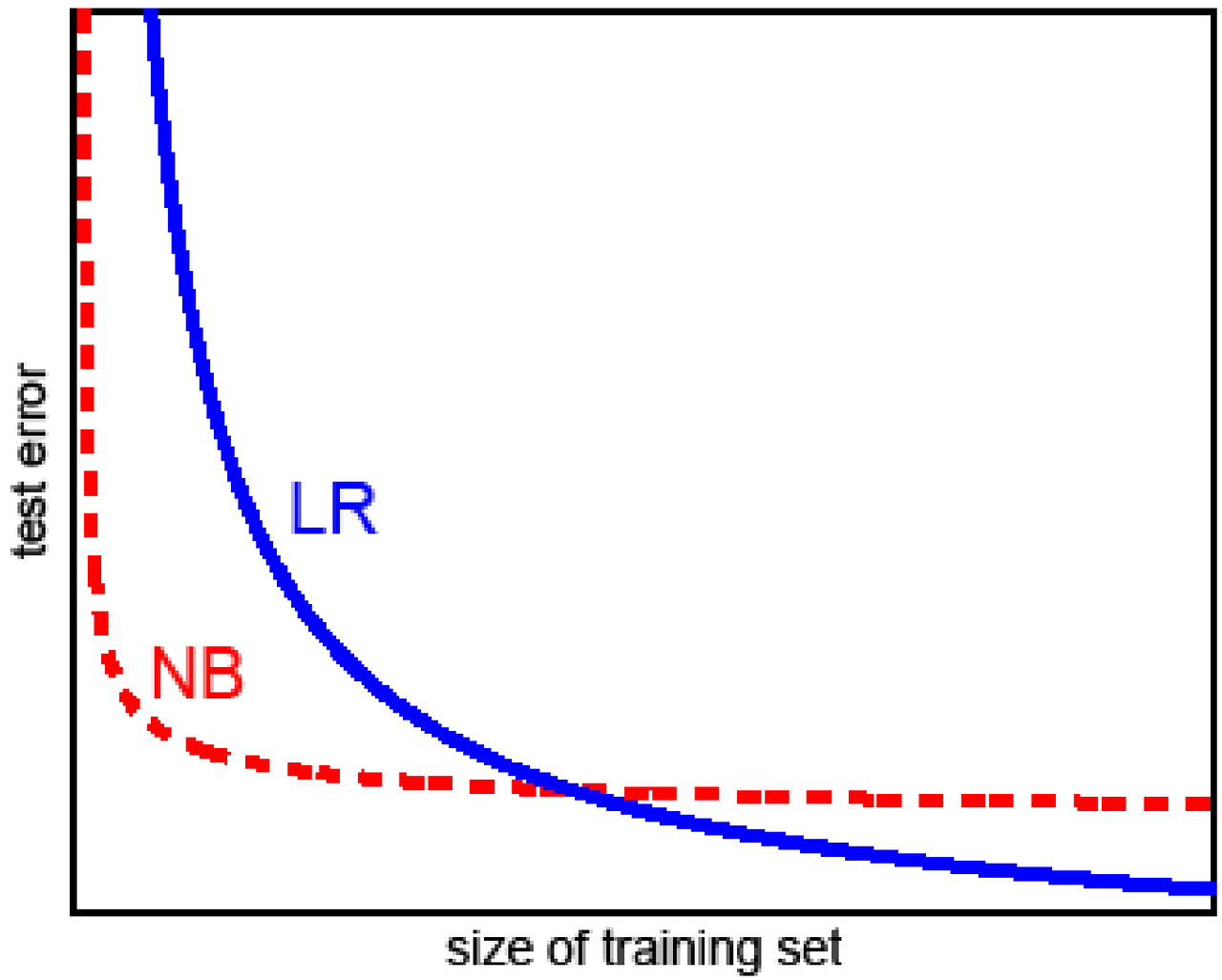
- When conditional independence is violated, logistic regression gives better generalisation if it is given sufficient training data.
- GNB converges to accurate parameter estimates faster ($O(\log n)$ examples for n features) compared to Logistic Regression ($O(n)$ examples).
- Experimentally, GNB is better when training data is scarce, logistic regression is better when it is plentiful.

Logistic Regression vs NB







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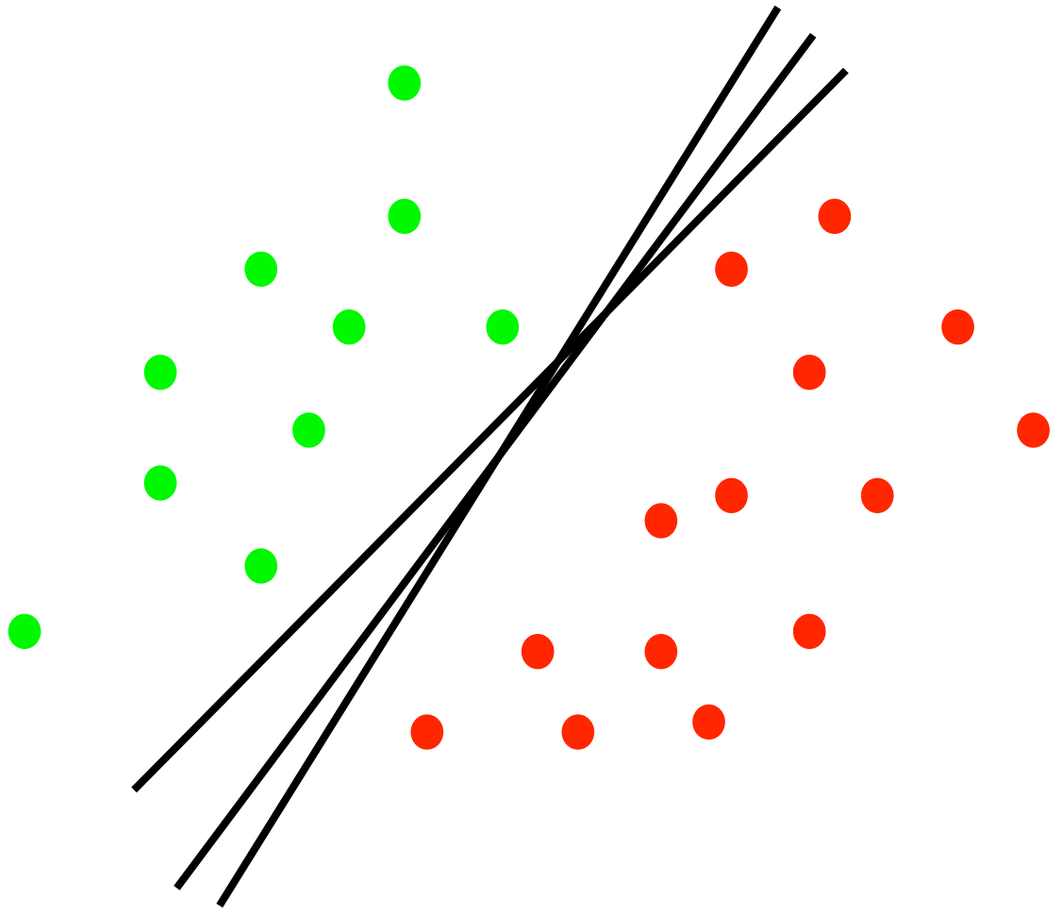
Support Vector Machines

Linear classifiers



Which line is better?

Maximum margin

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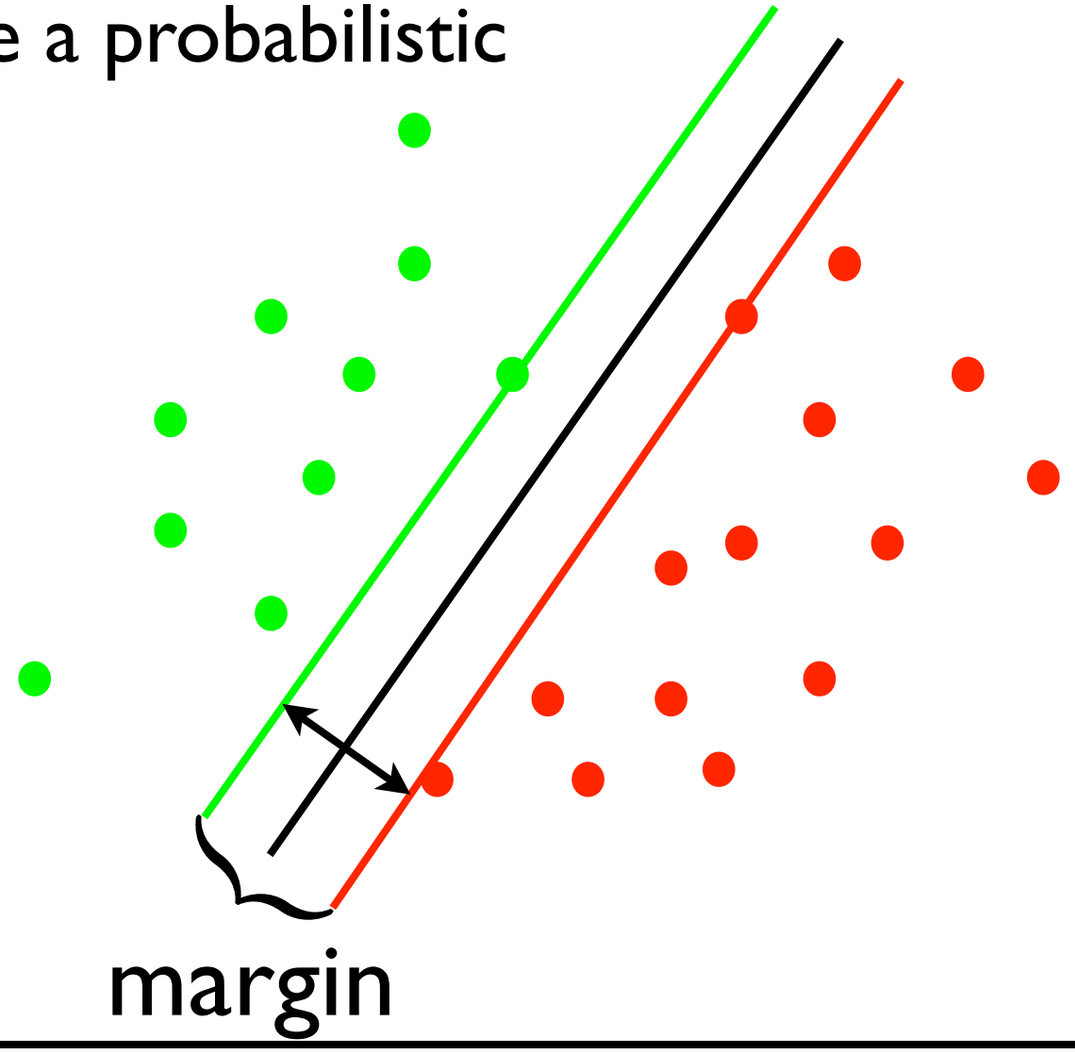
Things to note

- The boundary is defined by only a few points (support vectors)
- Difficult to define a probabilistic explanation



Linear Basis Function Models

Generally $$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$$

where $\phi_j(\mathbf{x})$ are known as *basis functions*.

Typically, $\phi_0(\mathbf{x}) = 1$, so that w_0 acts as a bias.

In the simplest case, we use linear basis functions :

$\phi_d(\mathbf{x}) = x_d$

Maximum margin classifiers (1)

Given a training set

Inputs $\mathbf{x}_1, \ldots, \mathbf{x}_N$

Targets

$t_1, \ldots, t_N$ where $t_n \in \{-1, 1\}$

Linear classifier

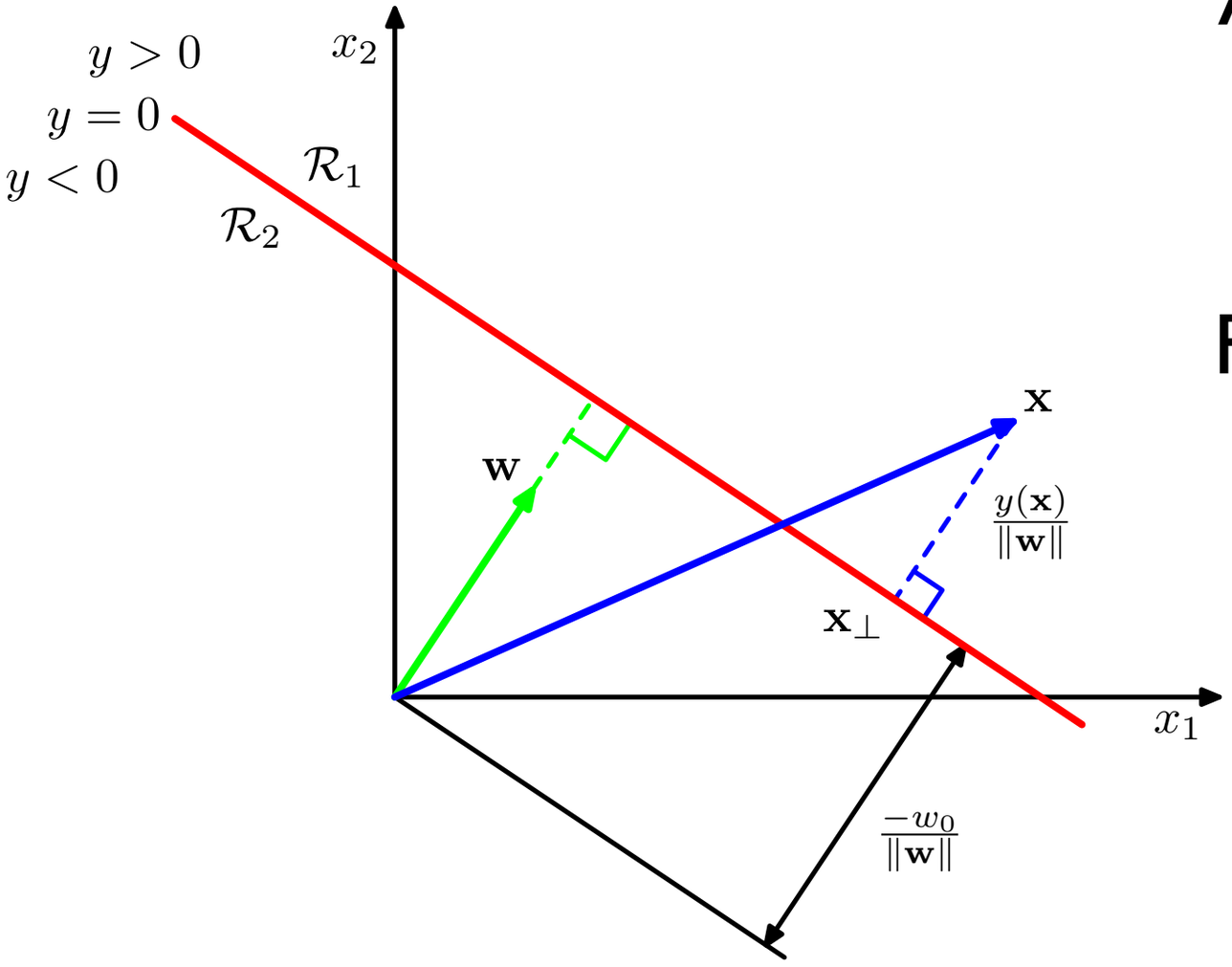
$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}) + b$$

Output sign of $y(\mathbf{x})$

so that $t_n y(\mathbf{x}_n) > 0$

for all points in the training set

Maximum margin classifiers(2)



Assuming $\phi(\mathbf{x}) = \mathbf{x}$

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0$$

For points in the boundary

$$y(\mathbf{x}) = 0 \quad \text{and}$$

$$\frac{\mathbf{w}^{\mathrm{T}}\mathbf{x}}{\|\mathbf{w}\|} = -\frac{w_0}{\|\mathbf{w}\|}$$

For arbitrary $\mathbf{x}$

$$\mathbf{x} = \mathbf{x}_\perp + r\frac{\mathbf{w}}{\|\mathbf{w}\|} \quad \text{and} \quad r = \frac{y(\mathbf{x})}{\|\mathbf{w}\|}$$

Maximum margin classifiers(3)

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For all points correctly classified $t_n y(\mathbf{x}_n) > 0$, $b = \omega_0$

and $$\frac{t_n y(\mathbf{x}_n)}{\|\mathbf{w}\|} = \frac{t_n(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n) + b)}{\|\mathbf{w}\|}$$

Maximum margin is found by

$$\arg\max_{\mathbf{w},b} \left\{ \frac{1}{\|\mathbf{w}\|} \min_n \left[t_n \left(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n) + b \right) \right] \right\}$$

However, this is too difficult to optimise !

Maximum margin classifiers(4)

Note that if $\mathbf{w} \to \kappa\mathbf{w}$ $b \to \kappa b$ $t_n y(\mathbf{x}_n)/\|\mathbf{w}\|$ is unchanged

Setting $t_n\left(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)+b\right)=1$ for the support vectors:

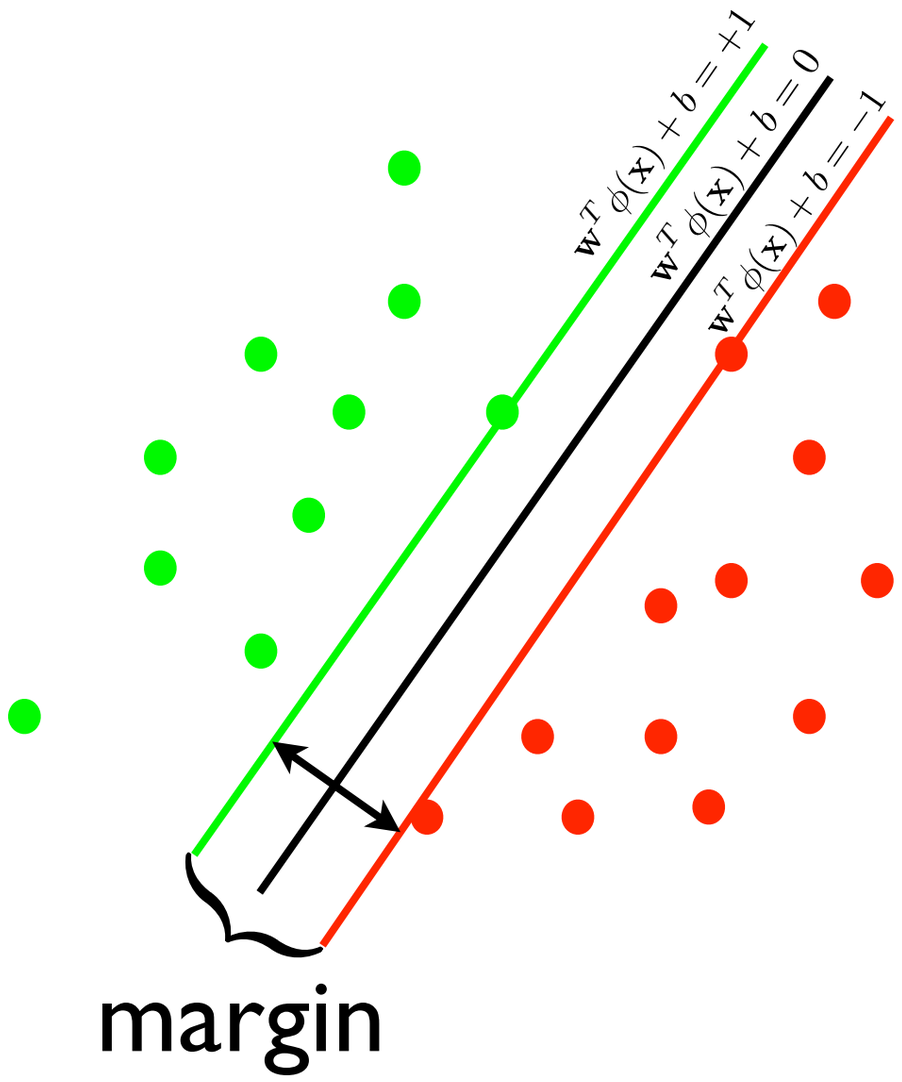
Quadratic programming

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

s.t.

$$t_n\left(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)+b\right)\geqslant 1,\ \ n=1,\ldots,N$$

Support Vector Machines



Quadratic programming

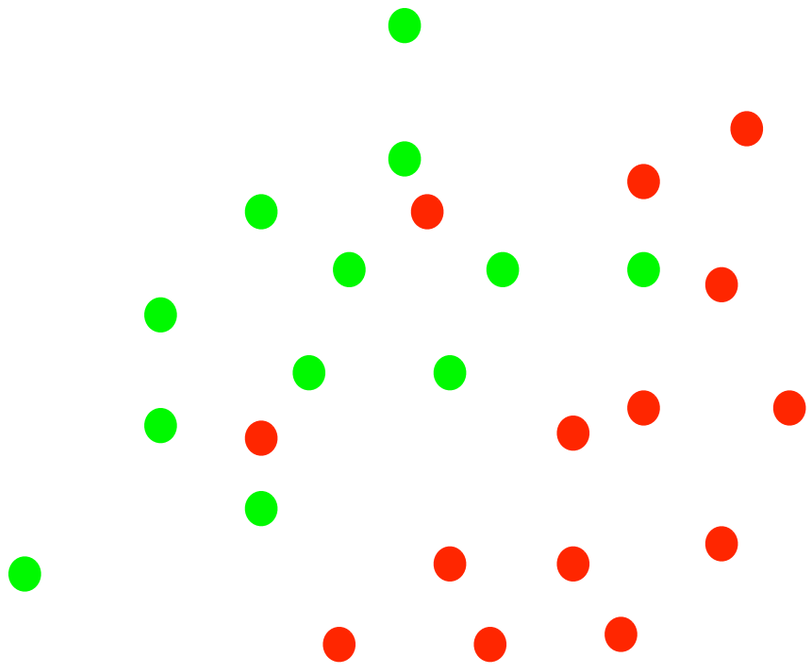
$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

s.t.

$$t_n\left(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)+b\right) \geqslant 1, \quad n=1,\ldots,N$$

- Solve efficiently by quadratic programming (QP)
- Hyperplane defined by support vectors

What happens if the data is not linearly separable?



Quadratic programming

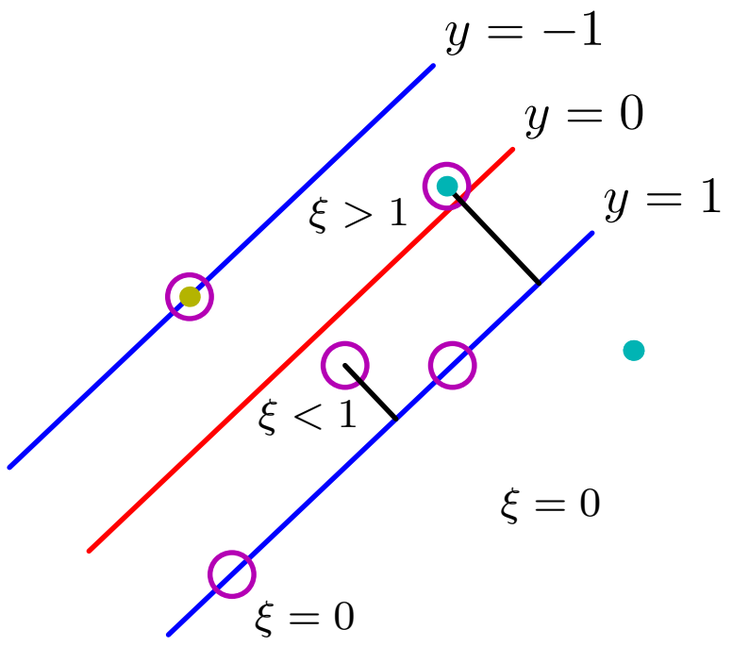
$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

s.t.

$$t_n\left(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)+b\right) \geqslant 1, \;\; n=1,\ldots,N$$

If margin ≥ 1, don't care
If margin < 1, pay linear penalty

Soft Margin Classification



Quadratic programming

$$\arg\min_{\mathbf{w},b} C\sum_{n=1}^{N}\xi_n + \frac{1}{2}\|\mathbf{w}\|^2$$

s.t.

$$t_n y(\mathbf{x}_n) \geqslant 1 - \xi_n \qquad n = 1, \ldots, N$$

$$\xi_n \geqslant 0$$

The Dual SVM formulation

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Quadratic programming

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

s.t.

$$t_n\left(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)+b\right) \geqslant 1, \;\; n=1,\ldots,N$$

Lagrangian function

$$L(\mathbf{w},b,\mathbf{a}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n\left\{t_n(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)+b)-1\right\}$$

setting the derivatives w.r.t. $\mathbf{w}$ and b equal to zero:

$$\begin{aligned}\mathbf{w} &= \sum_{n=1}^{N} a_n t_n \boldsymbol{\phi}(\mathbf{x}_n)\\ 0 &= \sum_{n=1}^{N} a_n t_n.\end{aligned}$$

$$\widetilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n,\mathbf{x}_m)$$

s.t.

$$\begin{aligned}a_n &\geqslant 0, \qquad n=1,\ldots,N,\\ \sum_{n=1}^{N} a_n t_n &= 0.\end{aligned}$$

Kernel trick

$$k(\mathbf{x},\mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}')$$

Kernel SVMs

- Solve the QP problem

$$\widetilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

with respect to $\mathbf{a}$ subject to the constraints

$$\begin{aligned} a_n &\geqslant 0, \qquad n = 1, \ldots, N, \\ \sum_{n=1}^{N} a_n t_n &= 0. \end{aligned}$$

- Support vectors satisfy

$$t_n \left(\sum_{m \in \mathcal{S}} a_m t_m k(\mathbf{x}_n, \mathbf{x}_m) + b \right) = 1$$

- For query points compute

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}, \mathbf{x}_n) + b.$$

Think about kernels not features

Polynomial kernel

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{z}) &= \left(1 + \mathbf{x}^{\mathrm{T}}\mathbf{z}\right)^2 = (1 + x_1 z_1 + x_2 z_2)^2 \\
&= 1 + 2x_1 z_1 + 2x_2 z_2 + x_1^2 z_1^2 + 2x_1 z_1 x_2 z_2 + x_2^2 z_2^2 \\
&= (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, \sqrt{2}x_1 x_2, x_2^2)(1, \sqrt{2}z_1, \sqrt{2}z_2, z_1^2, \sqrt{2}z_1 z_2, z_2^2)^{\mathrm{T}} \\
&= \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{z}).
\end{aligned}
$$

Gaussian kernel

$$k(\mathbf{x}, \mathbf{z}) = \exp(-\gamma\|\mathbf{x} - \mathbf{z}\|^2)$$

Infinite dimensional feature space!

What Functions are Kernels?

- For some functions $K(\mathbf{x}_i,\mathbf{x}_j)$ checking that $K(\mathbf{x}_i,\mathbf{x}_j)= \phi(\mathbf{x}_i)^{\mathrm{T}}\phi(\mathbf{x}_j)$ can be cumbersome.
- Mercer's theorem:

  Every semi-positive definite symmetric function is a kernel

- Semi-positive definite symmetric functions correspond to a semi-positive definite symmetric Gram matrix:

$K=$

$K(\mathbf{x}_1,\mathbf{x}_1)$	$K(\mathbf{x}_1,\mathbf{x}_2)$	$K(\mathbf{x}_1,\mathbf{x}_3)$	…	$K(\mathbf{x}_1,\mathbf{x}_n)$
$K(\mathbf{x}_2,\mathbf{x}_1)$	$K(\mathbf{x}_2,\mathbf{x}_2)$	$K(\mathbf{x}_2,\mathbf{x}_3)$		$K(\mathbf{x}_2,\mathbf{x}_n)$
…	…	…	…	…
$K(\mathbf{x}_n,\mathbf{x}_1)$	$K(\mathbf{x}_n,\mathbf{x}_2)$	$K(\mathbf{x}_n,\mathbf{x}_3)$	…	$K(\mathbf{x}_n,\mathbf{x}_n)$

Examples of Kernel Functions

- Linear: $K(\mathbf{x}_i,\mathbf{x}_j)= \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\phi}(\mathbf{x})$, where $\boldsymbol{\phi}(\mathbf{x})$ is $\mathbf{x}$ itself
- Polynomial of power p: $K(\mathbf{x}_i,\mathbf{x}_j)= (1+ \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j)^p$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\phi}(\mathbf{x})$, where $\boldsymbol{\phi}(\mathbf{x})$ has $\binom{d+p}{p}$ dimensions
- Gaussian (radial-basis function): $K(\mathbf{x}_i,\mathbf{x}_j) = e^{-\frac{\left\|\mathbf{x}_i-\mathbf{x}_j\right\|^2}{2\sigma^2}}$
  - Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\phi}(\mathbf{x})$, where $\boldsymbol{\phi}(\mathbf{x})$ is *infinite-dimensional*: every point is mapped to *a function* (a Gaussian); combination of functions for support vectors is the separator.
- Higher-dimensional space still has *intrinsic* dimensionality d (the mapping is not *onto*), but linear separators in it correspond to *non-linear* separators in original space.

Overfitting

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- Huge feature space with kernels, what about overfitting???
  - Maximising margin leads to sparse set of support vectors
  - Some interesting theory says that SVMs search for simple hypothesis with large margin
  - Often robust to overfitting

Summary

- SVM advantages
  - Efficient QP learning
  - Sparse
- SVM disadvantages
  - Not probabilistic
  - Do not directly handle multi-class problems
  - QP might struggle in very large datasets