Support Vector Machines and Kernel methods

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Reference

The content and the slides are adapted from

S. Rogers and M. Girolami, A First Course in Machine Learning (FCML), 2nd edition, Chapman & Hall/CRC 2016, ISBN: 9781498738484

Classification syllabus

- 4 classification algorithms.
- Of which:
 - 2 are probabilistic.
 - Bayes classifier.
 - Logistic regression.
 - 2 non-probabilistic.
 - K-nearest neighbours.
 - Support Vector Machines (SVM).
- There are many others!

Topics ...

- Linear SVM
- ► Soft-Margin SVM
- Kernels Kernel SVM
- Classifier Performance

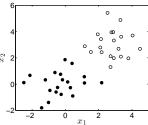
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- Linear SVM
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- ▶ We have seen several algorithms where we find the parameters that optimise something:
 - Minimise the loss.
 - Maximise the likelihood.
 - Maximise the posterior (MAP).

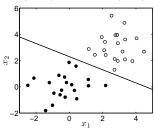
- ▶ We have seen several algorithms where we find the parameters that optimise something:
 - Minimise the loss.
 - Maximise the likelihood.
 - Maximise the posterior (MAP).
- ► The Support Vector Machine (SVM) is no different:
- ▶ It finds the *decision boundary* that maximises the margin.

► We'll 'think' in 2-dimensions.



SVM is a binary classifier. N data points, each with attributes $\mathbf{x} = [x_1, x_2]^\mathsf{T}$ and target $t = \pm 1$

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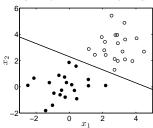


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► A linear *decision boundary* can be represented as a straight line:

$$\mathbf{w}^\mathsf{T}\mathbf{x} + b = 0$$

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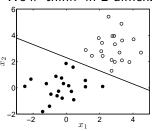
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- Our task is to find w and b
- Once we have these, classification is easy:

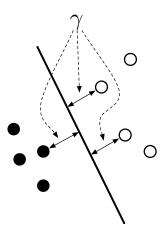
$$\mathbf{w}^{\mathsf{T}}\mathbf{x}_{\mathsf{new}} + b > 0$$
 : $t_{\mathsf{new}} = 1$
 $\mathbf{w}^{\mathsf{T}}\mathbf{x}_{\mathsf{new}} + b < 0$: $t_{\mathsf{new}} = -1$

ightharpoonup i.e. $t_{\text{new}} = \text{sign}(\mathbf{w}^{\mathsf{T}}\mathbf{x}_{\text{new}} + b)$

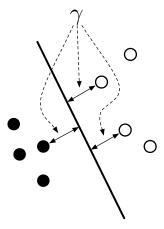


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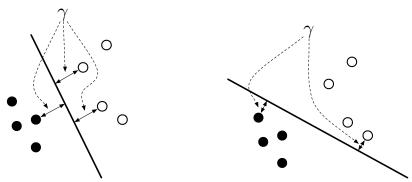


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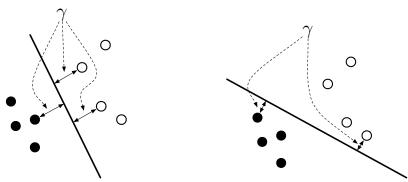
Perpendicular distance from the decision boundary to the closest points on each side.

Why maximise the margin?



Maximum margin decision boundary (left) seems to better reflect the data characteristics than other boundary (right).

Why maximise the margin?

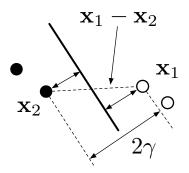


- Maximum margin decision boundary (left) seems to better reflect the data characteristics than other boundary (right).
- Note how margin is much smaller on right and closest points have changed.
- There is going to be one 'best' boundary (w.r.t margin)
- Statistical theory justifying the choice.



Computing the margin

$$2\gamma = \frac{1}{||\mathbf{w}||} \mathbf{w}^\mathsf{T} (\mathbf{x}_1 - \mathbf{x}_2)$$



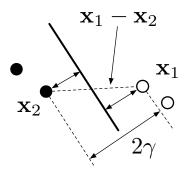
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Fix the scale such that:

$$\mathbf{w}^{\mathsf{T}}\mathbf{x}_1 + b = 1$$

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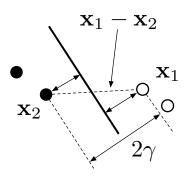
$$\mathbf{w}^{\mathsf{T}}\mathbf{x}_1 + b = 1$$

 $\mathbf{w}^{\mathsf{T}}\mathbf{x}_2 + b = -1$

Therefore:

$$(\mathbf{w}^{\mathsf{T}}\mathbf{x}_1 + b) - (\mathbf{w}^{\mathsf{T}}\mathbf{x}_2 + b) = 2$$

 $\mathbf{w}^{\mathsf{T}}(\mathbf{x}_1 - \mathbf{x}_2) = 2$
 $\gamma = \frac{1}{||\mathbf{x}_1||}$



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- ▶ Equivalent to minimising $\frac{1}{2}||\mathbf{w}||^2 = \frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w}$
- ► There are some constraints:
 - For \mathbf{x}_n with $t_n = 1$: $\mathbf{w}^\mathsf{T} \mathbf{x}_n + b \ge 1$
 - ▶ For \mathbf{x}_n with $t_n = -1$: $\mathbf{w}^\mathsf{T} \mathbf{x}_n + b \le -1$

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- Which can be expressed more neatly as:

$$t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n+b)\geq 1$$

▶ (This is why we use $t_n = \pm 1$ and not $t_n = \{0, 1\}$.)

▶ We have the following optimisation problem:

$$\underset{\mathbf{w}}{\operatorname{argmin}} \ \frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w}$$
 Subject to: $t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) \geq 1$

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Can put the constraints into the minimisation using Lagrange multipliers:

$$\underset{\mathbf{w}}{\operatorname{argmin}} \ \frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w} - \sum_{n=1}^N \alpha_n (t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) - 1)$$
 Subject to: $\alpha_n \geq 0$

What now?

- ► Let's think about what happens at the solution (we'll see why...)
- ▶ We know that $\frac{\partial}{\partial \mathbf{w}} = 0$ and $\frac{\partial}{\partial b} = 0$.

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$$\frac{\partial}{\partial b} = -\sum_{n} \alpha_{n} t_{n} = 0$$

From which we can infer that:

$$\mathbf{w} = \sum_{n} \alpha_{n} t_{n} \mathbf{x}_{n}$$
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▶ Substitute these back into our optimisation problem:



$$\frac{1}{2}\mathbf{w}^{\mathsf{T}}\mathbf{w} - \sum_{n} \alpha_{n} (t_{n}(\mathbf{w}^{\mathsf{T}}\mathbf{x}_{n} + b) - 1)$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$= \sum_{n} \alpha_{n} - \frac{1}{2} \sum_{n,m} \alpha_{n} \alpha_{m} t_{n} t_{m} \mathbf{x}_{n}^{\mathsf{T}} \mathbf{x}_{m}$$

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- ► Instead of minimising the previous expression, we can maximise this one (for reasons we won't go into).
- Subject to:

$$\sum_{n} \alpha_{n} t_{n} = 0$$

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▶ Decision function was sign($\mathbf{w}^{\mathsf{T}}\mathbf{x}_{\mathsf{new}} + b$) and is now:

$$t_{\text{new}} = \operatorname{sign}\left(\sum_{n=1}^{N} \alpha_n t_n \mathbf{x}_n^{\mathsf{T}} \mathbf{x}_{\text{new}} + b\right)$$



So?

$$\begin{split} \operatorname*{argmax} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n.m=1}^{N} \alpha_n \alpha_m t_n t_m \mathbf{x}_n^\mathsf{T} \mathbf{x}_m \\ \mathrm{subject \ to} \quad \sum_{n=1}^{N} \alpha_n t_n = 0, \quad \alpha_n \geq 0 \end{split}$$

- This is a standard optimisation problem (quadratic programming)
- Has a single, global solution. This is very useful!
- Many algorithms around to solve it.
- e.g. quadprog in Matlab...

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- Many algorithms around to solve it.
- e.g. quadprog in Matlab...
- ▶ Once we have α_n :

$$t_{\text{new}} = \operatorname{sign}\left(\sum_{n=1}^{N} \alpha_n t_n \mathbf{x}_n^{\mathsf{T}} \mathbf{x}_{\text{new}} + b\right)$$

Primal and Dual

Primal

$$\underset{\mathbf{w}}{\operatorname{argmin}} \ \frac{1}{2} \mathbf{w}^\mathsf{T} \mathbf{w}$$

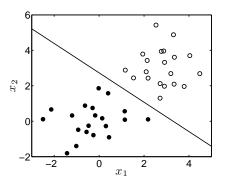
Subject to: $t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) \ge 1$

Dual

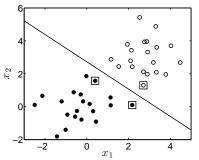
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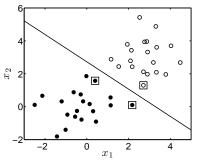
Optimal boundary



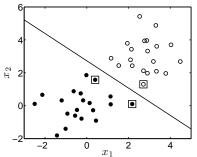
- ▶ Optimisation gives us $\alpha_1, \ldots, \alpha_N$
- Compute $\mathbf{w} = \sum_{n} \alpha_n t_n \mathbf{x}_n$
- ► Compute $b = t_n \mathbf{w}^\mathsf{T} \mathbf{x}_n$ (for one of the closest points)
 - ▶ Recall that we defined $\mathbf{w}^\mathsf{T}\mathbf{x}_n + b = \pm 1 = t_n$ for closest points.
- Plot $\mathbf{w}^\mathsf{T} \mathbf{x} + b = 0$



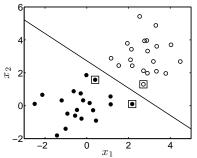
- $t_{\text{new}} = \text{sign} \left(\sum_{n} \alpha_{n} t_{n} \mathbf{x}_{n}^{\mathsf{T}} \mathbf{x}_{\text{new}} + b \right)$
- Predictions only depend on these data-points!



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- ► These are called Support Vectors

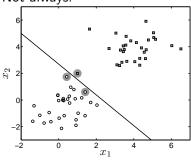


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- Predictions only depend on these data-points!
- ▶ We knew that margin is only a function of closest points.
- ► These are called Support Vectors
- ▶ Normally a small proportion of the data:
 - Solution is sparse.



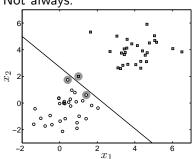
Is sparseness good?

► Not always:



Is sparseness good?

Not always:



▶ Why does this happen?

$$t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n+b)\geq 1$$

- All points must be on correct side of boundary.
- ► This is a hard margin

Topics ...

- Linear SVM
- ► Soft-Margin SVM
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We can relax the constraints:

$$t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) \ge 1 - \xi_n, \ \xi_n \ge 0$$

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$$\underset{\mathbf{w}}{\operatorname{argmin}} \frac{1}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w} + C \sum_{n=1}^{N} \xi_{n}$$
 subject to $t_{n}(\mathbf{w}^{\mathsf{T}} \mathbf{x}_{n} + b) \geq 1 - \xi_{n}$

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And when we add Lagrange etc:

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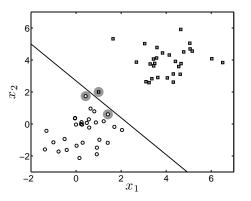
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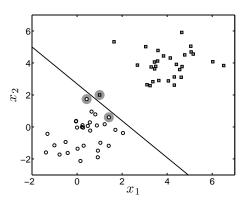
▶ The **only** change is an upper-bound on $\alpha_n!$

► Here's our problematic data again:



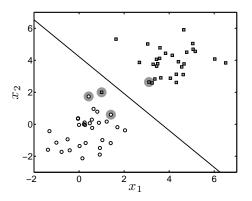
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► Here's our problematic data again:



- \triangleright α_n for the 'bad' square is 3.5.
- ▶ So, if we set C < 3.5, we should see this point having less influence and the boundary moving to somewhere more sensible...

► Try *C* = 1



- ▶ We have an extra support vector.
- ► And a better decision boundary.

- ▶ The choice of *C* is very important.
- ► Too high and we *over-fit* to noise.
- Too low and we underfit
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- ► Too high and we *over-fit* to noise.
- ► Too low and we underfit
 - ...and lose any sparsity.
- ► Choose it using cross-validation.

SVMs – some observations

▶ In our example, we started with 3 parameters:

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▶ In general: D+1.

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- ▶ In general: D+1.
- \blacktriangleright We now have $N: \alpha_1, \ldots, \alpha_N$
- Sounds harder?
- Depends on data dimensionality:
 - Typical Microarray dataset:
 - ► $D \sim 3000$, $N \sim 30$.
 - ▶ In some cases $N \ll D$

Topics ...

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- ► Soft-Margin SVM
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Inner products

Here's the optimisation problem:

$$\underset{\alpha}{\operatorname{argmax}} \sum_{n} \alpha_{n} - \frac{1}{2} \sum_{n,m} \alpha_{n} \alpha_{m} t_{n} t_{m} \mathbf{x}_{n}^{\mathsf{T}} \mathbf{x}_{m}$$

Here's the decision function:

$$t_{\text{new}} = \text{sign}\left(\sum_{n} \alpha_{n} t_{n} \mathbf{x}_{n}^{\mathsf{T}} \mathbf{x}_{\text{new}} + b\right)$$

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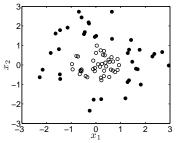
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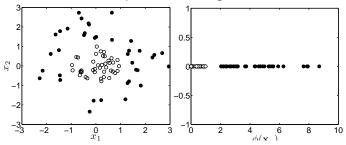
▶ Data $(\mathbf{x}_n, \mathbf{x}_m, \mathbf{x}_{\text{new}}, \text{ etc})$ only appears as inner (dot) products:

$$\mathbf{x}_{n}^{\mathsf{T}}\mathbf{x}_{m}, \ \mathbf{x}_{n}^{\mathsf{T}}\mathbf{x}_{\mathsf{new}}, \mathsf{etc}$$

- Our SVM can find linear decision boundaries.
- ▶ What if the data requires something nonlinear?



- Our SVM can find linear decision boundaries.
- What if the data requires something nonlinear?



We can transform the data e.g.:

$$\phi(\mathbf{x}_n) = x_{n1}^2 + x_{n2}^2$$

- ▶ So that it can be separated with a straight line.
- And use $\phi(\mathbf{x}_n)$ instead of \mathbf{x}_n in our optimisation.



Our optimisation is now:

$$\underset{\alpha}{\operatorname{argmax}} \sum_{n} \alpha_{n} - \frac{1}{2} \sum_{n,m} \alpha_{n} \alpha_{m} t_{n} t_{m} \phi(\mathbf{x}_{n})^{\mathsf{T}} \phi(\mathbf{x}_{m})$$

And predictions:

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We can think of the dot product in the projected space as a function of the original data.

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- ► These all correspond to $\phi(\mathbf{x}_n)^T \phi(\mathbf{x}_m)$ for some transformation $\phi(\mathbf{x}_n)$.
- ▶ Don't know what the projections $\phi(\mathbf{x}_n)$ are don't need to know!

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- ...but we're finding linear boundaries in some other space.
- ► The optimisation is just as simple, regardless of the kernel choice.
 - Still a quadratic program.
 - Still a single, global optimum.
- We can find very complex decision boundaries with a linear algorithm!

A technical point

- Our decision boundary was defined as $\mathbf{w}^\mathsf{T}\mathbf{x} + b = 0$.
- Now, w is defined as:

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n t_n \phi(\mathbf{x}_n)$$

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- ► So, we can't compute **w** or the boundary!
- But we can evaluate the predictions on a grid of x_{new} and use Matlab to draw a contour:

$$\sum_{n=1}^{N} \alpha_n t_n k(\mathbf{x}_n, \mathbf{x}_{\text{new}}) + b$$

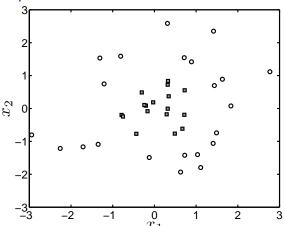
Aside: kernelising other algorithms

- Many algorithms can be kernelised.
 - Any that can be written with data only appearing as inner products.
- Simple algorithms can be used to solve very complex problems!
- Class exercise:
 - NNN requires the distance between \mathbf{x}_{new} and each \mathbf{x}_n :

$$(\mathbf{x}_{\mathsf{new}} - \mathbf{x}_n)^\mathsf{T} (\mathbf{x}_{\mathsf{new}} - \mathbf{x}_n)$$

Can we kernelise it?

Example – nonlinear data



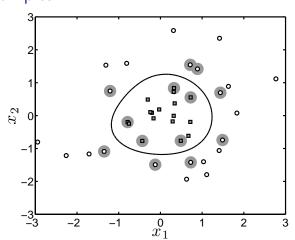
► We'll use a Gaussian kernel:

$$k(\mathbf{x}_n, \mathbf{x}_m) = \exp\left\{-\beta(\mathbf{x}_n - \mathbf{x}_m)^{\mathsf{T}}(\mathbf{x}_n - \mathbf{x}_m)\right\}$$

And vary β (C = 10).



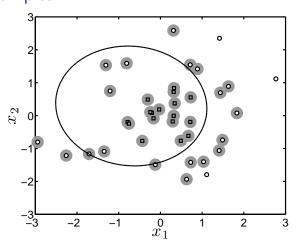
Examples



$$\beta = 1.$$

$$k(\mathbf{x}_n, \mathbf{x}_m) = \exp\left\{-\beta(\mathbf{x}_n - \mathbf{x}_m)^{\mathsf{T}}(\mathbf{x}_n - \mathbf{x}_m)\right\}$$

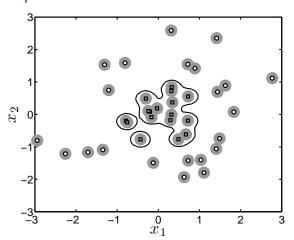
Examples



$$\beta = 0.01.$$

$$k(\mathbf{x}_n, \mathbf{x}_m) = \exp\left\{-\beta(\mathbf{x}_n - \mathbf{x}_m)^{\mathsf{T}}(\mathbf{x}_n - \mathbf{x}_m)\right\}$$

Examples



▶
$$\beta = 50$$
.

$$k(\mathbf{x}_n, \mathbf{x}_m) = \exp\left\{-\beta(\mathbf{x}_n - \mathbf{x}_m)^{\mathsf{T}}(\mathbf{x}_n - \mathbf{x}_m)\right\}$$

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 - Not flexible enough to surround just the square class.
- $ightharpoonup \beta = 50$ was too complex:
 - Memorises the data.
- \triangleright $\beta = 1$ was about right.
- Neither $\beta = 50$ or $\beta = 0.01$ will generalise well.
- Both are also non-sparse (lots of support vectors).

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- Easy to overfit.

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 - ► *C* too high overfitting.
 - C too low underfitting.
- Cross-validation!
- ightharpoonup Search over β and C
 - ► SVM scales with N^3 (naive implementation)
 - For large N, cross-validation over many C and β values is infeasible.

Summary - SVMs

- Described a classifier that is optimised by maximising the margin.
- Did some re-arranging to turn it into a quadratic programming problem.
- Saw that data only appear as inner products.
- Introduced the idea of kernels.
- Can fit a linear boundary in some other space without explicitly projecting.
- Loosened the SVM constraints to allow points on the wrong side of boundary.
- Other algorithms can be kernelised...we'll see a clustering one in the future.

Topics ...

- Linear SVM
- ► Soft-Margin SVM
- Kernels Kernel SVM
- Classifier Performance

Performance evaluation

- ▶ We've seen 4 classification algorithms.
- ► How do we choose?
 - ▶ Which algorithm?
 - Which parameters?
- Need performance indicators.

Performance evaluation

- We've seen 4 classification algorithms.
- ► How do we choose?
 - ▶ Which algorithm?
 - Which parameters?
- Need performance indicators.
- ▶ We'll cover:
 - ▶ 0/1 loss.
 - ► ROC analysis (sensitivity and specificity)
 - Confusion matrices

- ightharpoonup 0/1 loss: proportion of times classifier is wrong.
- Consider a set of predictions t_1, \ldots, t_N and a set of true labels t_1^*, \ldots, t_N^* .
- Mean loss is defined as:

$$\frac{1}{N}\sum_{n=1}^{N}\delta(t_n\neq t_n^*)$$

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- \blacktriangleright ($\delta(a)$ is 1 if a is true and 0 otherwise)
- Advantages:
 - Can do binary or multiclass classification.
 - Simple to compute.
 - Single value.

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- ► Assume only 1% of population is diseased.

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- ► Assume only 1% of population is diseased.
- ▶ Diseased: t = 1
- ▶ Healthy: t = 0
- ▶ What if we always predict healthy? (t = 0)
- Accuracy 99%
- But classifier is rubbish!

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- ▶ False positives (FP) the number of objects with $t_n^* = 0$ that are classified as $t_n = 1$ (healthy people diagnosed as diseased).

Sensitivity and specificity

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- ▶ True positives (TP) the number of objects with $t_n^* = 1$ that are classified as $t_n = 1$ (diseased people diagnosed as diseased).
- ▶ True negatives (TN) the number of objects with $t_n^* = 0$ that are classified as $t_n = 0$ (healthy people diagnosed as healthy).
- False positives (FP) the number of objects with $t_n^* = 0$ that are classified as $t_n = 1$ (healthy people diagnosed as diseased).
- ▶ False negatives (FN) the number of objects with $t_n^* = 1$ that are classified as $t_n = 0$ (diseased people diagnosed as healthy).

Sensitivity

$$S_{\rm e} = \frac{TP}{TP + FN}$$

- ▶ The proportion of diseased people that we classify as diseased.
- ► The higher the better.
- ▶ In our example, $S_e = 0$.

Specificity

$$S_p = \frac{TN}{TN + FP}$$

- ▶ The proportion of healthy people that we classify as healthy.
- ► The higher the better.
- ▶ In our example, $S_p = 1$.

Optimising sensitivity and specificity

- ▶ We would like both to be as high as possible.
- ▶ Often increasing one will decrease the other.

Optimising sensitivity and specificity

- ▶ We would like both to be as high as possible.
- ▶ Often increasing one will decrease the other.
- Balance will depend on application:
- e.g. diagnosis:
 - ► We can probably tolerate a decrease in specificity (healthy people diagnosed as diseased)....
 - ...if it gives us an increase in sensitivity (getting diseased people right).

ROC analysis

- ▶ Many classification algorithms involve setting a threshold.
- e.g. SVM:

$$t_{\text{new}} = \operatorname{sign}\left(\sum_{n=1}^{N} t_n \alpha_n k(\mathbf{x}_n, \mathbf{x}_{\text{new}}) + b\right)$$

► Implies a threshold of zero (sign function)

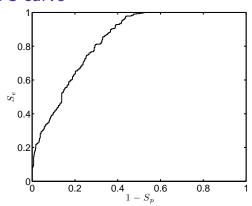
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- ► Implies a threshold of zero (sign function)
- However, we could use any threshold we like....
- The Receiver Operating Characteristic (ROC) curve shows how S_e and $1 S_p$ vary as the threshold changes.

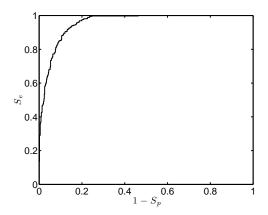
ROC curve



- ▶ SVM for nonlinear data with $\beta = 50$.
- Each point is a threshold value.
 - ▶ Bottom left everything classified as 0 (-1 in SVM)
 - ► Top right everything classified as 1.
- ▶ Goal: get the curve to the top left corner perfect classification ($S_e = 1, S_p = 1$).

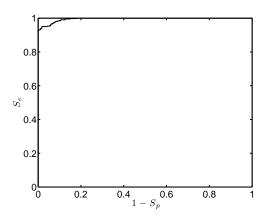


ROC curve



- ▶ SVM for nonlinear data with $\beta = 0.01$.
- ▶ Better than $\beta = 50$
 - Closer to top left corner.

ROC curve



- ▶ SVM for nonlinear data with $\beta = 1$.
- ► Better still.

AUC

- We can quantify performance by computing the Area Under the ROC Curve (AUC)
- The higher this value, the better.
 - β = 50: AUC=0.8348
 - β = 0.01: AUC= 0.9551
 - $\beta = 1$: AUC=0.9936

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 - β = 50: AUC=0.8348
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 - $\beta = 1$: AUC=0.9936
- ▶ AUC is generally a safer measure than 0/1 loss.

Confusion matrices

The quantities we used to compute S_e and S_p can be neatly summarised in a table:

		True class				
		1	0			
Predicted class	1	TP	FP			
Predicted class	0	FN	TN			

- This is known as a confusion matrix
- It is particularly useful for multi-class classification.
- ► Tells us where the mistakes are being made.
- Note that normalising columns gives us S_e and S_p

Confusion matrices – example

- 20 newsgroups data.
- Thousands of documents from 20 classes (newsgroups)
- ▶ Use a Naive Bayes classifier (\approx 50000 dimensions (words)!)
 - Details in book Chapter.
- $ightharpoonup \approx 7000$ independent test documents.
- ▶ Summarise results in 20×20 confusion matrix:

	True class												
			10	11	12	13	14	15	16	18	18	19	20
	1		4	2	0	2	10	4	7	1	12	7	47
	2		0	0	4	18	7	8	2	0	1	1	3
SS	3		0	0	1	0	1	0	1	0	0	0	0
class	4		1	0	1	28	3	0	0	0	0	0	0
Predicted							:						
je.	16		3	2	2	5	17	4	376	3	7	2	68
ш	17		1	0	9	0	3	1	3	325	3	95	19
	18		2	1	0	2	6	2	1	2	325	4	5
	19		8	4	8	0	10	21	1	16	19	185	7
	20		0	0	1	0	1	1	2	4	0	1	92

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▶ Algorithm is getting 'confused' between classes 20 and 16, and 19 and 17.

▶ 17: talk.politics.guns

▶ 19: talk.politics.misc

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► Maybe these should be just one class?

▶ Maybe we need more data in these classes?

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20: soc.religion.christian

Maybe these should be just one class?

▶ Maybe we need more data in these classes?

Confusion matrix helps us direct our efforts to improving the classifier.



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