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**
- Soft-Margin SVM
- Kernels - Kernel SVM
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The margin

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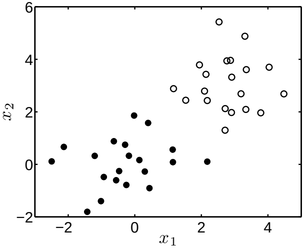
  - Minimise the loss.
  - Maximise the likelihood.
  - Maximise the posterior (MAP).

The margin

- 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.

Some data

- We'll 'think' in 2-dimensions.



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

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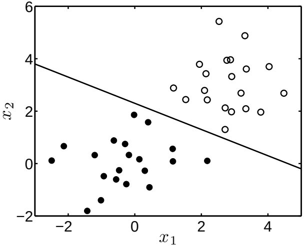

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- A linear *decision boundary* can be represented as a straight line:

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

2-dim

$w^T x = w_1 x_1 + w_2 x_2$

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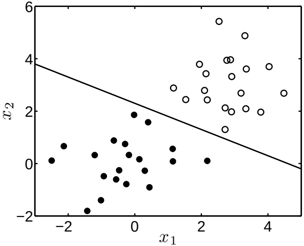

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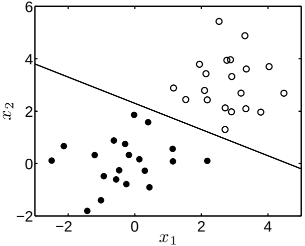

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$$\mathbf{w}^\mathsf{T}\mathbf{x} + b = 0$$

- Our task is to find $\mathbf{w}$ and b
- Once we have these, classification is easy:

$$\begin{cases} \mathbf{w}^\mathsf{T}\mathbf{x}_{\text{new}} + b > 0 & : \quad t_{\text{new}} = 1 \\ \mathbf{w}^\mathsf{T}\mathbf{x}_{\text{new}} + b < 0 & : \quad t_{\text{new}} = -1 \end{cases}$$

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

The margin

- How do we choose $\mathbf{w}$ and b?
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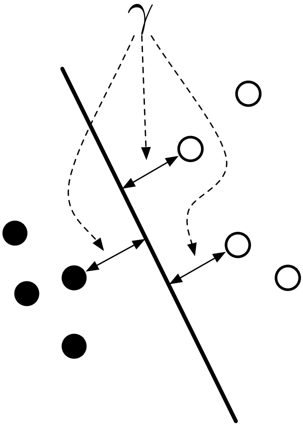
- Need a quantity to optimise!
- Use the margin, γ
- Maximise it!



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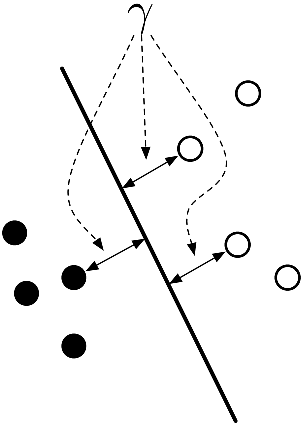
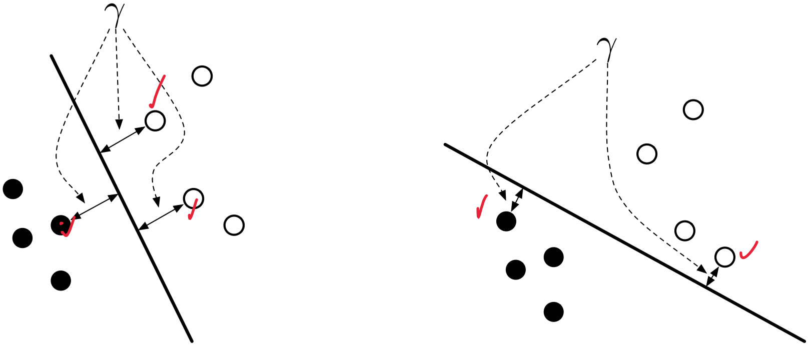


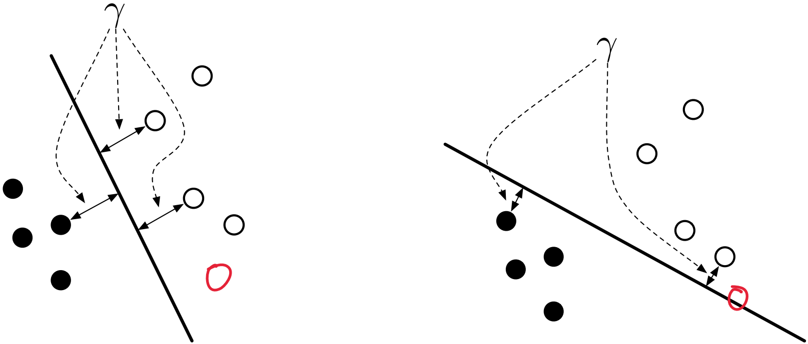
Perpendicular distance from the decision boundary to the closest points on each side.

Why maximise the margin?



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

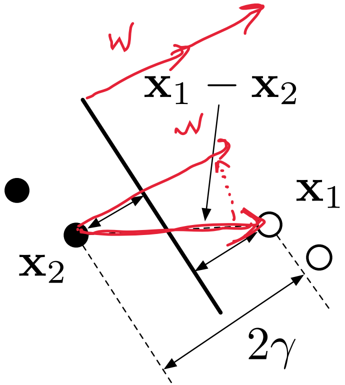
Why maximise the margin?



- 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

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

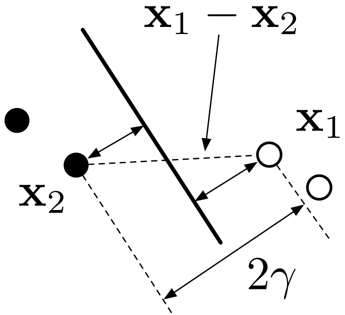


Computing the margin

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

Fix the scale such that:

$$\begin{aligned} \mathbf{w}^T\mathbf{x}_1 + b &= 1 \quad > 0 \\ \mathbf{w}^T\mathbf{x}_2 + b &= -1 \quad < 0 \end{aligned}$$



Computing the margin

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

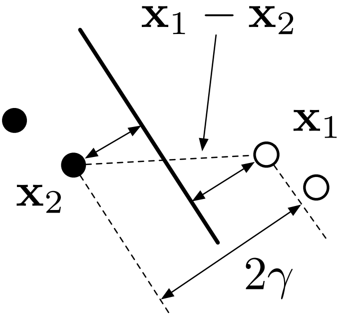
Fix the scale such that:

$$\begin{aligned} \mathbf{w}^T\mathbf{x}_1 + b &= 1 \\ \mathbf{w}^T\mathbf{x}_2 + b &= -1 \end{aligned}$$

Therefore:

$$\begin{aligned} \underbrace{(\mathbf{w}^T\mathbf{x}_1 + \cancel{b})}_{+1} - \underbrace{(\mathbf{w}^T\mathbf{x}_2 + \cancel{b})}_{-1} &= 2 \\ \mathbf{w}^T(\mathbf{x}_1 - \mathbf{x}_2) &= 2 \end{aligned}$$

$$\boxed{\gamma = \frac{1}{||\mathbf{w}||}}$$



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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 $t_n = 1$: $\mathbf{w}^\mathsf{T}\mathbf{x}_n + b \geq 1$
  - For $\mathbf{x}_n$ with $t_n = -1$: $\mathbf{w}^\mathsf{T}\mathbf{x}_n + b \leq -1$

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- Which can be expressed more neatly as:

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

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

Maximising the margin

- We have the following optimisation problem:

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

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

Maximising the margin

$$\frac{\partial (w^T w)}{\partial w} = \cancel{2}w \; ?$$

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

- Can put the constraints into the minimisation using Lagrange multipliers:

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

$$\text{Subject to: } \alpha_n \geq 0$$

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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\begin{aligned}
\frac{\partial}{\partial \mathbf{w}} &= \mathbf{w} - \sum_n \alpha_n t_n \mathbf{x}_n = 0 \\
\frac{\partial}{\partial b} &= -\sum_n \alpha_n t_n = 0
\end{aligned}
$$

- From which we can infer that:

$$
\begin{aligned}
\mathbf{w} &= \sum_n \alpha_n t_n \mathbf{x}_n \\
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- From which we can infer that:

$$\begin{aligned}\mathbf{w} &= \sum_n \alpha_n t_n \mathbf{x}_n \\ \sum_n \alpha_n t_n &= 0\end{aligned}$$

- Substitute these back into our optimisation problem:

$$\frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w} - \sum_n \alpha_n(t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) - 1) \quad \Longrightarrow \cdots + b\underbrace{\sum \alpha_n t_n}_{0}$$

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

$$= \sum_n \alpha_n - \frac{1}{2}\sum_{n,m}\alpha_n\alpha_m t_n t_m \mathbf{x}_n^\mathsf{T}\mathbf{x}_m$$

$$
\begin{aligned}
& \frac{1}{2}\mathbf{w}^{\mathsf{T}}\mathbf{w} - \sum_{n} \alpha_n (t_n(\mathbf{w}^{\mathsf{T}}\mathbf{x}_n + b) - 1) \\
& \vdots \qquad\qquad\qquad \vdots \qquad\qquad\qquad \vdots \\
= \; & \sum_{n} \alpha_n - \frac{1}{2} \sum_{n,m} \alpha_n \alpha_m t_n t_m \mathbf{x}_n^{\mathsf{T}} \mathbf{x}_m
\end{aligned}
$$

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

$$
\begin{aligned}
\alpha_n &\geq 0 \\
\sum_{n} \alpha_n t_n &= 0
\end{aligned}
$$

$$\frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w} - \sum_n \alpha_n(t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) - 1)$$

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- Subject to:

$$\begin{cases} \alpha_n \geq 0 \\ \sum_n \alpha_n t_n = 0 \end{cases}$$

$w^T x_1 + b = +1$

$\Rightarrow \boxed{b = 1 - w^T x_1}$

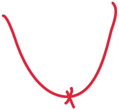
- Decision function was $\mathrm{sign}(\mathbf{w}^\mathsf{T}\mathbf{x}_{\text{new}} + b)$ and is now:

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

So?

$$\underset{\boldsymbol{\alpha}}{\operatorname{argmax}} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n,m=1}^{N} \alpha_n \alpha_m t_n t_m \mathbf{x}_n^{\mathsf{T}} \mathbf{x}_m$$

$$\text{subject to} \quad \sum_{n=1}^{N} \alpha_n t_n = 0, \quad \alpha_n \geq 0$$



- 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, `CVXOPT` in Python ...

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$$\underset{\boldsymbol{\alpha}}{\text{argmax}} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n,m=1}^{N} \alpha_n \alpha_m t_n t_m \mathbf{x}_n^{\mathsf{T}} \mathbf{x}_m$$

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- This is a standard optimisation problem (quadratic programming)
- Has a single, global solution. This is very useful!
- Many algorithms around to solve it.
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- Once we have α_n:

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

Primal and Dual

Primal

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

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

Dual

$$\underset{\boldsymbol{\alpha}}{\operatorname{argmax}} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n,m=1}^{N} \alpha_n \alpha_m t_n t_m \mathbf{x}_n^{\mathsf{T}} \mathbf{x}_m$$

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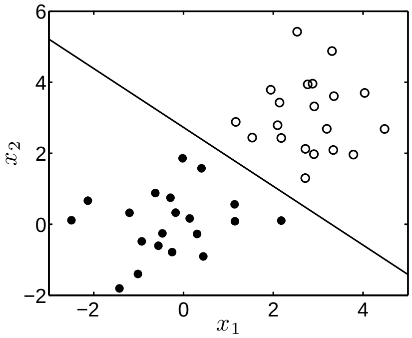
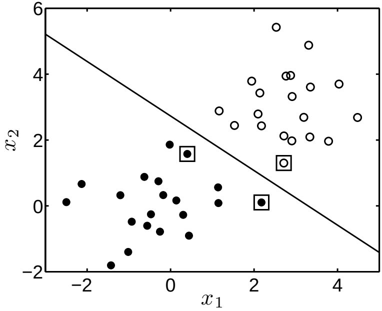
Optimal boundary



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

Support Vectors

- At the optimum, only 3 non-zero α values (squares).



α_n

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

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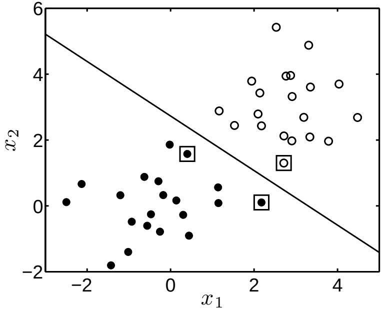

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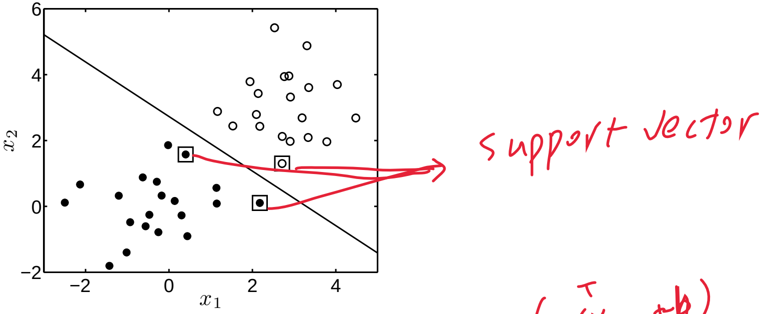

- $t_{\text{new}} = \text{sign}\left(\sum_n \alpha_n t_n \mathbf{x}_n^{\mathsf{T}} \mathbf{x}_{\text{new}} + b\right)$ = sign($w^T x_{new} + b$)
- Predictions only depend on these data-points!
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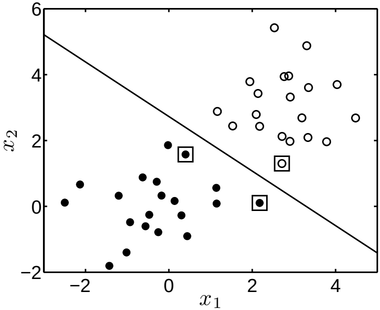
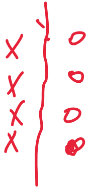
Support Vectors

- At the optimum, only 3 non-zero α values (squares).

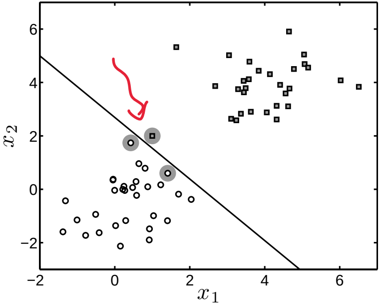




- $t_{\text{new}} = \text{sign}\left(\sum_n \alpha_n t_n \mathbf{x}_n^{\mathsf{T}} \mathbf{x}_{\text{new}} + b\right)$
- Predictions only depend on these data-points!
- We knew that – margin is only a function of closest points.
- These are called Support Vectors
- Normally a small proportion of the data:
  - Solution is *sparse*.

Is sparseness good?

- Not always:



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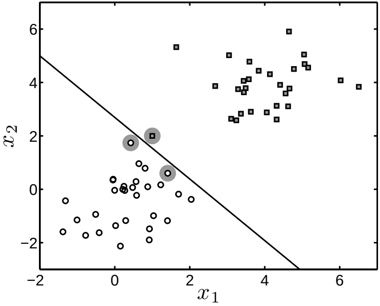

- Why does this happen?

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

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

Topics ...

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

Soft margin

- We can relax the constraints:

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

$$\boxed{t_n(w^T x_n + b) \geqslant 1}$$

Soft margin

- We can relax the constraints:

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

- Our optimisation becomes:

$$\operatorname*{argmin}_{\mathbf{w}} \overbrace{\frac{1}{2}\mathbf{w}^\mathsf{T}\mathbf{w}}^{\text{margin}} + C \overbrace{\sum_{n=1}^{N}}^{\text{softness constraints}} \xi_n$$

$$\text{subject to} \;\; \underbrace{t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) \geq 1 - \xi_n}_{\text{contraints}}$$

Soft margin

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- And when we add Lagrange etc:

$$\begin{aligned} \underset{\boldsymbol{\alpha}}{\operatorname{argmax}} \; & \sum_{n=1}^{N}\alpha_n - \frac{1}{2}\sum_{n,m=1}^{N}\alpha_n\alpha_m t_n t_m \mathbf{x}_n^\mathsf{T}\mathbf{x}_m \\ \text{subject to} \;\; & \sum_{n=1}^{N}\alpha_n t_n = 0, \;\; 0 \leq \alpha_n \leq C \end{aligned}$$

Soft margin

- We can relax the constraints:

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

- Our optimisation becomes:

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$$\text{subject to}\ \ t_n(\mathbf{w}^\mathsf{T}\mathbf{x}_n + b) \geq 1 - \xi_n$$

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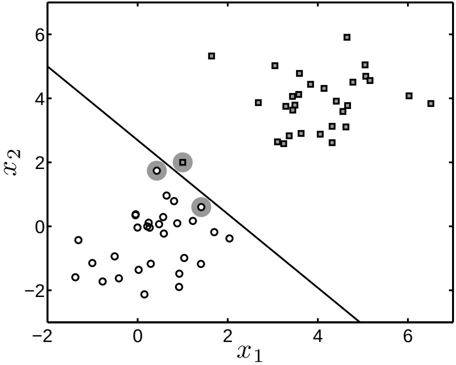
$$\operatorname*{argmax}_{\boldsymbol{\alpha}} \sum_{n=1}^{N}\alpha_n - \frac{1}{2}\sum_{n,m=1}^{N}\alpha_n\alpha_m t_n t_m \mathbf{x}_n^\mathsf{T}\mathbf{x}_m$$

$$\text{subject to}\ \ \sum_{n=1}^{N}\alpha_n t_n = 0,\ \ 0 \leq \alpha_n \leq C$$

- The **only** change is an upper-bound on α_n!

Soft margins

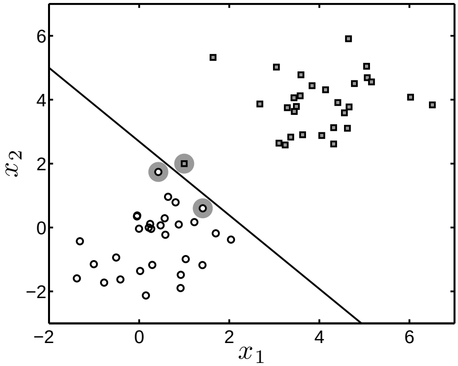
- Here's our problematic data again:



- α_n for the 'bad' square is 3.5.

Soft margins

- Here's our problematic data again:

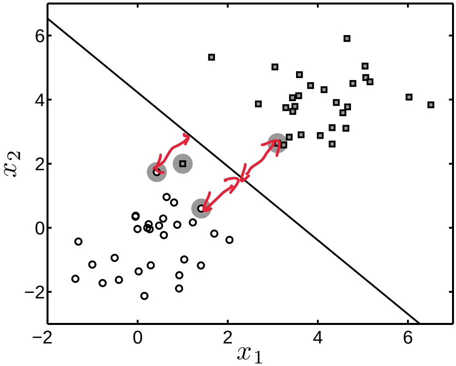


- α_n for the 'bad' square is 3.5.
- So, if we set $C < 3.5$, we should see this point having less influence and the boundary moving to somewhere more sensible...

Soft margins

- Try $C = 1$

$0 \leq \alpha_n \leq C = 1$



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

Soft margins

- The choice of C is very important.
- Too high and we *over-fit* to noise. $\to$ C is too large
- Too low and we *underfit* $\to$ C is too small
  - ...and lose any sparsity.

Soft margins

- The choice of C is very important.
- 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:

$$\mathbf{w} = [w_1, w_2]^\mathsf{T}, \quad b$$

$w^T x + b = 0$

- In general: D+1.

SVMs – some observations

- In our example, we started with 3 parameters:

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- We now have N: $\alpha_1, \ldots, \alpha_N$

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- In general: D+1.
- 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 ...

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

Inner products

- Here's the optimisation problem:

$$\underset{\boldsymbol{\alpha}}{\operatorname{argmax}} \sum_n \alpha_n - \frac{1}{2} \sum_{n,m} \alpha_n \alpha_m t_n t_m \mathbf{x}_n^\mathsf{T} \mathbf{x}_m$$

- Here's the decision function:

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

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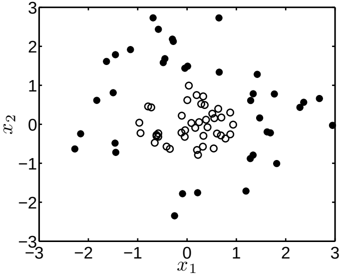
- Data ($\mathbf{x}_n, \mathbf{x}_m, \mathbf{x}_{\text{new}}$, etc) only appears as inner (dot) products:

$$\mathbf{x}_n^\mathsf{T} \mathbf{x}_m, \ \mathbf{x}_n^\mathsf{T} \mathbf{x}_{\text{new}}, \text{etc}$$

Projections

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



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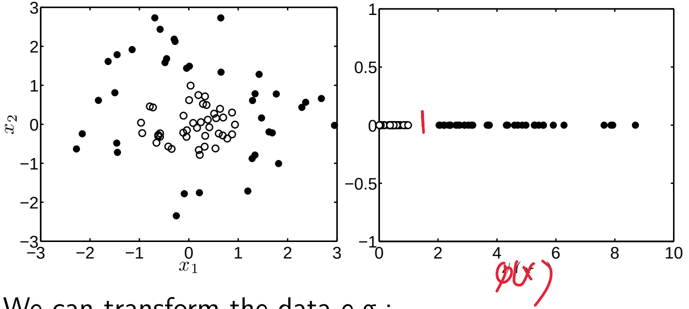

- We can transform the data e.g.:

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

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

Projections

- Our optimisation is now:

$$\underset{\boldsymbol{\alpha}}{\operatorname{argmax}} \sum_n \alpha_n - \frac{1}{2} \sum_{n,m} \alpha_n \alpha_m t_n t_m \phi(\mathbf{x}_n)^\mathsf{T} \phi(\mathbf{x}_m)$$

- And predictions:

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$$\phi(\mathbf{x}_n)^\mathsf{T} \phi(\mathbf{x}_m) = (x_{n1}^2 + x_{n2}^2)(x_{m1}^2 + x_{m2}^2) = k(\mathbf{x}_n, \mathbf{x}_m)$$

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

Projections

- We needn't directly think of projections at all. def. of $\phi(x_n)$
- Can just think of functions $k(\mathbf{x}_n, \mathbf{x}_m)$ that *are dot products in some space*.

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- Polynomial:
$$k(\mathbf{x}_n, \mathbf{x}_m) = (1 + \mathbf{x}_n^\mathsf{T}\mathbf{x}_m)^\beta$$
- These all correspond to $\phi(\mathbf{x}_n)^\mathsf{T}\phi(\mathbf{x}_m)$ 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, $\mathbf{w}$ is defined as:

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

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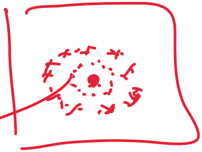
- We **only know** $\phi(\mathbf{x}_n)^\mathsf{T}\phi(\mathbf{x}_m) = k(\mathbf{x}_n, \mathbf{x}_m)$
- So, we can't compute $\mathbf{w}$ or the boundary!
- But we can evaluate the predictions on a grid of $\mathbf{x}_{\text{new}}$ and use Python/Matlab to draw a contour:

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



Aside: kernelising other algorithms

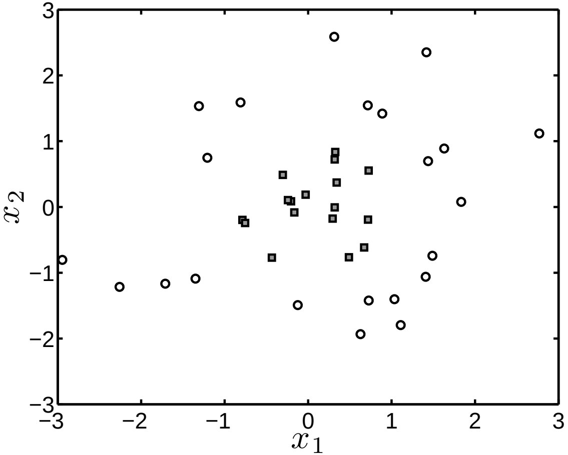
- **Many** algorithms can be kernelised.
  - Any that can be written with data only appearing as inner products.
- Simple algorithms can be used to solve very complex problems!
- Class exercise:
  - KNN requires the distance between $\mathbf{x}_{\text{new}}$ and each $\mathbf{x}_n$:

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

  - Can we kernelise it?

$$= \underbrace{x_{new}^T x_{new}}_{k(\cdot,\cdot)} - 2 \underbrace{x_n^T x_{new}}_{k(\cdot,\cdot)} + \underbrace{x_n^T x_n}_{k(\cdot,\cdot)}$$

Example – nonlinear data

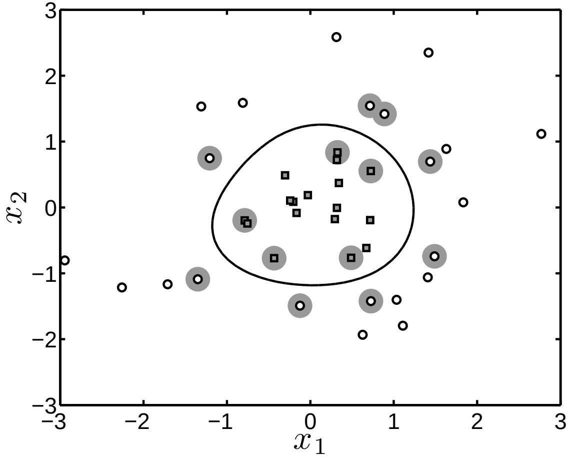


- We'll use a Gaussian kernel:

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

- And vary β ($C = 10$).

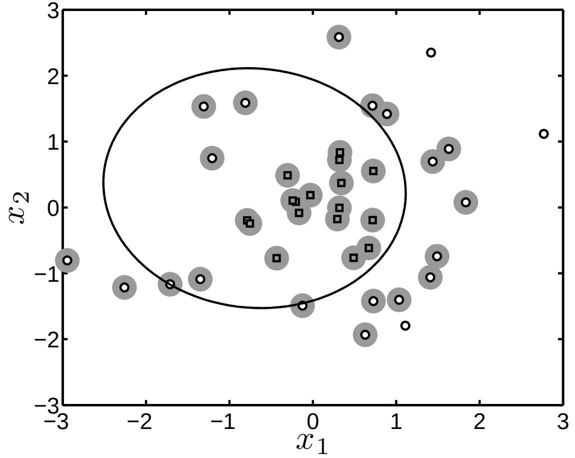
Examples



- $\beta = 1$.

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

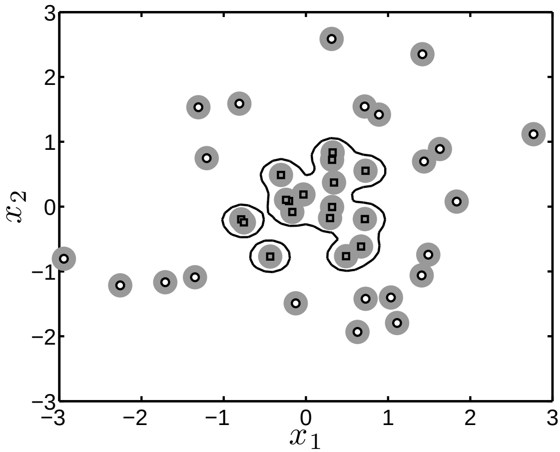
Examples



- $\beta = 0.01$.

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

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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The Gaussian kernel

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- $\beta = 0.01$ was too simple:
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- $\beta = 50$ was too complex:
  - *Memorises* the data.
- $\beta = 1$ was about right.
- Neither $\beta = 50$ or $\beta = 0.01$ will *generalise* well.
- Both are also non-sparse (lots of support vectors).

Choosing kernel function, parameters and C

- Kernel function and parameter choice is data dependent.
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  - C too high – overfitting.
  - C too low – underfitting.
- Cross-validation!
- 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.
- Loosened the SVM constraints to allow points on the wrong side of boundary.
- 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.
- 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 3 classification algorithms, more will come later ...
- How do we choose?
  - Which algorithm?
  - Which parameters?
- Need performance indicators.

Performance evaluation

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

0/1 loss

- 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:

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

δ (cond) = 1 if cond is True
0 otherwise.

- ($\delta(a)$ is 1 if a is true and 0 otherwise)

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

0/1 loss

Disadvantage: Doesn't take into account class imbalance:

0/1 loss

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- We're building a classifier to detect a rare disease.
- Assume only 1% of population is diseased.

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- Diseased: $t = 1$
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0/1 loss

Disadvantage: Doesn't take into account class imbalance:

- We're building a classifier to detect a rare disease.
- Assume only 1% of population is diseased.
- Diseased: $t = 1$ 1%
- Healthy: $t = 0$ 99% $\implies$ 0/1 loss = 0.01
- What if we always predict healthy? $(t = 0)$

0/1 loss

Disadvantage: Doesn't take into account class imbalance:

- We're building a classifier to detect a rare disease.
- 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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- We'll stick with our disease example.
- Need to define 4 quantities. The numbers of:

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True

- **True negatives (TN)** – the number of objects with $\boxed{t_n^* = 0}$ that are classified as $t_n = 0$ (healthy people diagnosed as healthy).

Sensitivity and specificity

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- Need to define 4 quantities. The numbers of:
- 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).

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

Sensitivity

$\{t_n^* = 1, t_n = 1\}$

$$S_e = \frac{TP}{\underbrace{TP + FN}_{\{t_n^* = 1\}}}$$

$\{t_n^* = 1, t_n = 1\}$ $\{t_n^* = 1, t_n = 0\}$

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

Specificity

$\{t_n^* = 0, t_n = 0\}$

$\{t_n^* = 0, t_n = 0\}$

$$S_p = \frac{TN}{\underbrace{TN + FP}_{\{t_n^* = 0\}}} = 1$$

$\{t_n^* = 0, t_n = 1\}$

- 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

other threshold(s).

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

$$t_{\text{new}} = \text{sign}\left(\sum_{n=1}^{N} t_n \alpha_n k(\mathbf{x}_n, \mathbf{x}_{\text{new}}) + b\right) \begin{cases} > 0 \to + \\ < 0 \to - \end{cases}$$

- Implies a threshold of zero (sign function)

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- e.g. SVM:

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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.

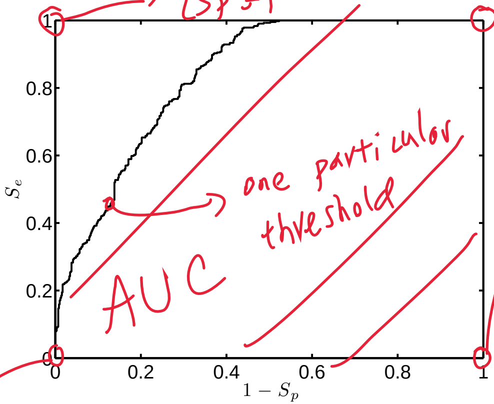
ROC curve

Se = 1
Sp = 1

Se = 1
Sp = 0

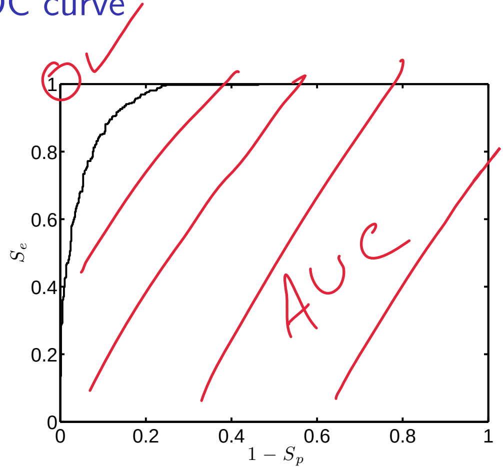
Se = 0
Sp = 0

Se = 0
Sp = 1



- 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 ($S_e = 1, S_p = 1$).

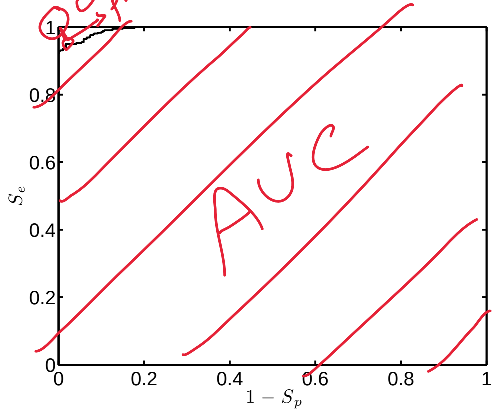
ROC curve



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

ROC curve

prefer se



- 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.

  - $\beta = 50$: AUC=0.8348
  - $\beta = 0.01$: AUC= 0.9551
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    - $\beta = 50$: AUC=0.8348
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- 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	True class 0
Predicted class	1	TP	FP
	0	FN	TN

/TN+FP

- 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 (≈ 50000 dimensions (words)!)
    - Details in book Chapter.
- ≈ 7000 independent test documents.
- Summarise results in 20×20 confusion matrix:

		True class										
		...	10	11	12	13	14	15	16	17	18	19	20
Predicted class	1	...	4	2	0	2	10	4	7	1	12	7	47
	2	...	0	0	4	18	7	8	2	0	1	1	3
	3	...	0	0	1	0	1	0	1	0	0	0	0
	4	...	1	0	1	28	3	0	0	0	0	0	0
							⋮						
	16	...	3	2	2	5	17	4	376	3	7	2	**68**
	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**

True class

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  - 17: talk.politics.guns
  - 19: talk.politics.misc

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  - 16: talk.religion.misc
  - 20: soc.religion.christian

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- Maybe we need more data in these classes?

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

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- Linear classifier – (possibly) nonlinear data transformation.
- Introduced two different performance measures:
  - 0/1 loss
  - ROC/AUC
- Introduced confusion matrices – a way of assessing the performance of a multi-class classifier.