Introduction to Statistical Machine Learning

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(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

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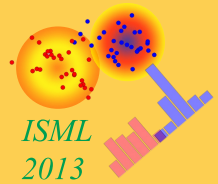

Outlines

Part XII

Sparse Kernel Machines

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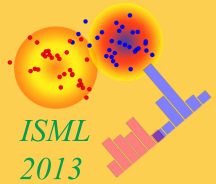

Sparse Kernel Machines - Motivation

- Nonlinear kernels extended our toolbox of methods considerably. Wherever an inner product was used in an algorithms, we can replace it with a kernel.
- Kernels act as a kind of 'similarity' measure and can be defined over graphs, sets, strings, and documents.
- But the kernel matrix is a square matrix with dimensions equal to the number of data points N. In order to calculate it, the kernel function must be evaluated for all pairs of training inputs.
- Sparse Kernel Machines implement learning algorithms which are based on sparse kernels. For prediction, these kernels are only evaluated at a subset of the training data.

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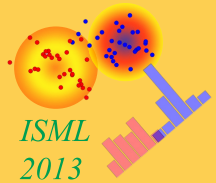

Maximum Margin Classifiers

- Return to the two-class classification with a linear model

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

  where $\phi(\mathbf{x})$ is some fixed feature space mapping, and b is the bias.
- Training data are N input vectors $\mathbf{x}_1, \ldots, \mathbf{x}_N$ with corresponding targets $t_1, \ldots, t_N$ where $t_n \in \{-1, +1\}$.
- The class of a new point is predicted as $\text{sign}\,(y(\mathbf{x}))$.
- Assume there exists a linear decision boundary. That means, there exist $\mathbf{w}$ and b such that

$$t_n \ \text{sign}\,(y(\mathbf{x}_n)) > 0 \qquad\qquad n = 1, \ldots, N.$$

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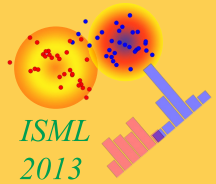
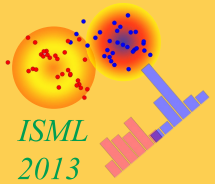


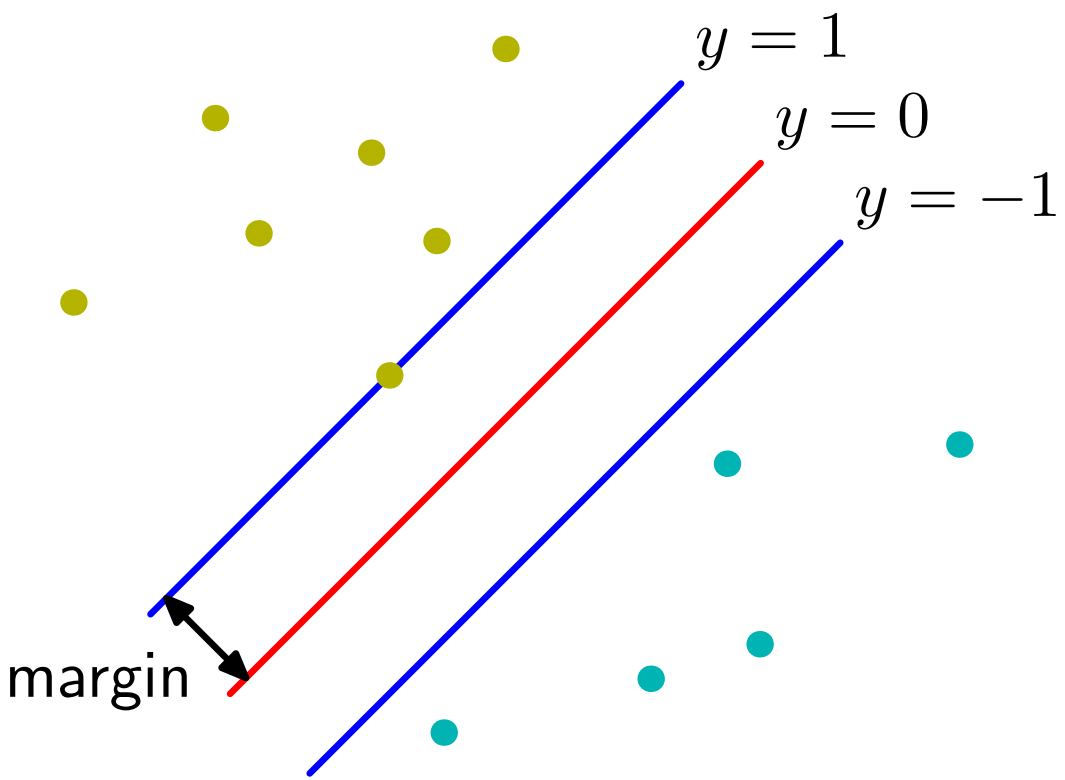
Maximum Margin Classifiers

- There may exist many solutions $\mathbf{w}$ and b for which the linear classifier perfectly separates the two classes.
- The perceptron algorithm can find a solution, but this depends on the initial choice of parameters.
- What is the decision boundary which results in the best generalisation (smallest generalisation error)?



Maximum Margin Classifiers

- The margin is the smallest distance between the decision boundary and any of the samples. (We will see later why $y = \pm 1$ on the margin.)



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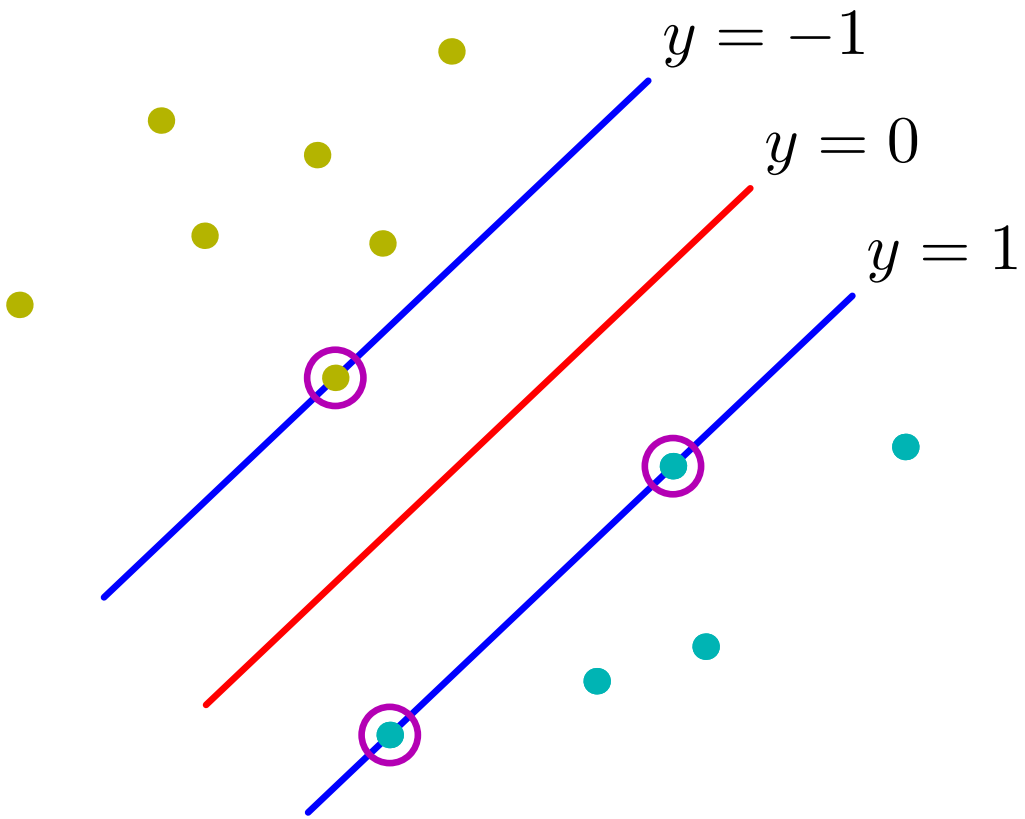
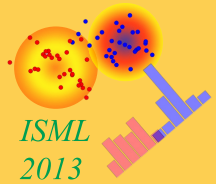
Maximum Margin Classifiers

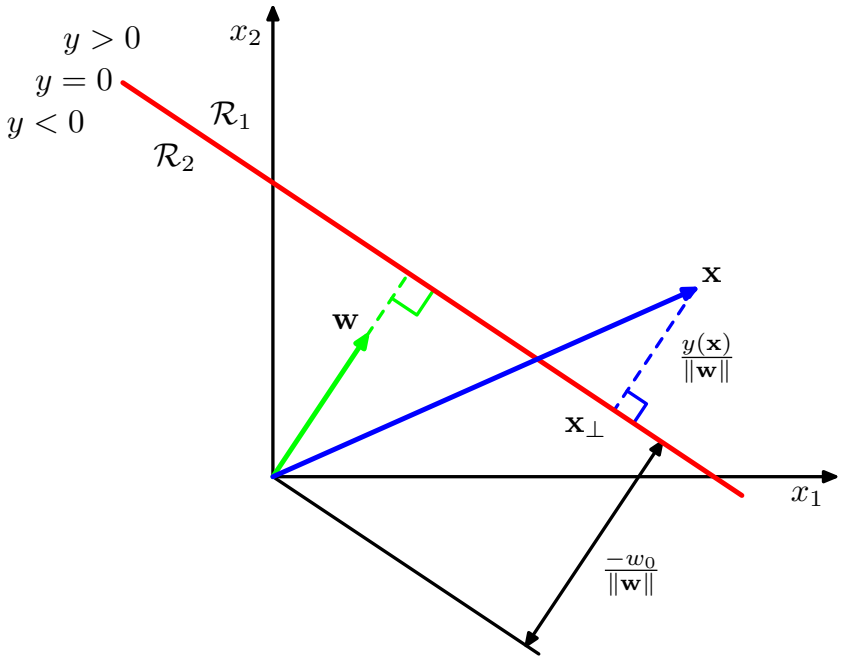
- Support Vector Machines choose the decision boundary which maximises the margin.





Reminder - Linear Classification

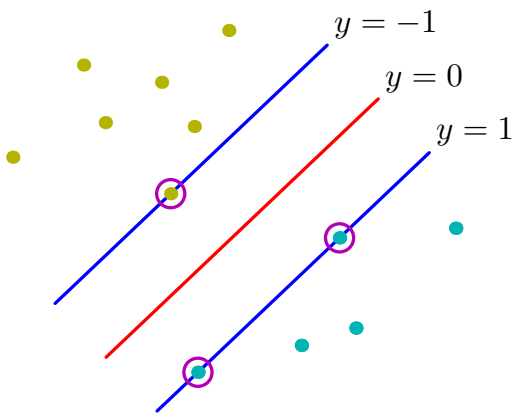
- $\mathbf{w}$ is orthogonal to the decision boundary ($0 = \mathbf{w}^T\mathbf{x_1} + w_0 = \mathbf{w}^T\mathbf{x_2} + w_0$ and $\mathbf{w}^T(\mathbf{x_1} - \mathbf{x_2}) = 0$.)
- Length of the projection of $\mathbf{x}$ onto $\mathbf{w}$ is $\frac{\mathbf{w}^T\mathbf{x}}{\|\mathbf{w}\|}$.
- If $\mathbf{x}$ sits on the decision boundary then $0 = y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$ and therefore the distance from the origin orthogonal to the decision boundary (and parallel to $\mathbf{w}$ is $\frac{\mathbf{w}^T\mathbf{x}}{\|\mathbf{w}\|} = -\frac{w_0}{\|\mathbf{w}\|}$.
- The distance of $\mathbf{x}$ from the decision boundary is therefore $\frac{\mathbf{w}^T\mathbf{x}}{\|\mathbf{w}\|} - (-\frac{w_0}{\|\mathbf{w}\|}) = \frac{y(\mathbf{x})}{\|\mathbf{w}\|}$.



Maximum Margin Classifiers

- Support Vector Machines choose the decision boundary which maximises the smallest distance to samples in both classes.
- We calculated the distance of a point $\mathbf{x}$ from the hyperplane $y(\mathbf{x}) = 0$ as $|y(\mathbf{x})|/\|\mathbf{w}\|$.
- Perfect classification means $t_n y(\mathbf{x}_n) > 0$ for all n.
- Thus, the distance of $\mathbf{x}_n$ from the decision boundary is

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



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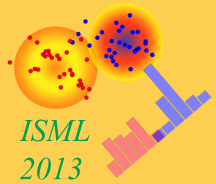

Maximum Margin Classifiers

- Support Vector Machines choose the decision boundary which maximises the smallest distance to samples in both classes.
- For the maximum margin solution, solve

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

- How can we solve this?

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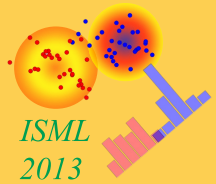

Maximum Margin Classifiers

- Maximum margin solution

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

- Observation: Rescaling $\mathbf{w}\to\kappa\mathbf{w}$ and $b\to\kappa b$ does not change the distance from the hypersurface.
- Scale in such a way that for the closest point

$$t_n\left(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n)+b\right)=1.$$

- The canonical representation for the decision hyperplane is therefore

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

- The constraints are active, if the equality holds, otherwise they are inactive.

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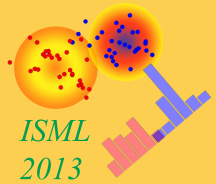


Maximum Margin Classifiers

- Maximum margin solution

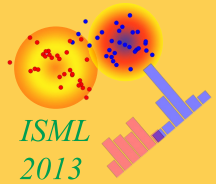
$$\arg\max_{\mathbf{w},b}\left\{\frac{1}{\|\mathbf{w}\|}\min_{n}\left[t_n\left(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n)+b\right)\right]\right\}$$

- Transformed once

$$\arg\max_{\mathbf{w},b}\left\{\frac{1}{\|\mathbf{w}\|}\right\} \quad \text{s.t. } t_n\left(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n)+b\right)\geq 1.$$

- Transformed again

$$\arg\min_{\mathbf{w},b}\left\{\frac{1}{2}\|\mathbf{w}\|^2\right\} \quad \text{s.t. } t_n\left(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n)+b\right)\geq 1.$$



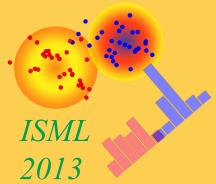
Maximum Margin Classifiers

- Quadratic Programming (QP) problem: minimise a quadratic function subject to linear constraints.

$$\arg\min_{\mathbf{w},b}\left\{\frac{1}{2}\|\mathbf{w}\|^2\right\} \quad \text{s.t. } t_n\left(\mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}_n)+b\right)\geq 1.$$

- Introduce Lagrange multipliers $\{a_n \geq 0\}$ to get the Lagrangian

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



Maximum Margin Classifiers

- Lagrangian

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

- Derivatives with respect to $\mathbf{w}$ and b are

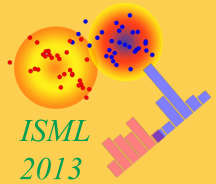
$$\mathbf{w} = \sum_{n=1}^{N} a_n \, t_n \, \boldsymbol{\phi}(\mathbf{x}_n) \qquad\qquad 0 = \sum_{n=1}^{N} a_n \, t_n$$

- Dual representation (again QP problem): Maximise

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

$$\sum_{n=1}^{N} a_n \, t_n = 0$$

$$a_n \geq 0 \qquad\qquad n = 1, \ldots, N.$$



Maximum Margin Classifiers

- Kernel function

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

  must imply a positive definite kernel (Gram matrix), otherwise the optimisation problem is not bounded from above.
- Solving the optimisation problem is of the order $O(N^3)$ in the number of data points N. The original optimisation problem is of order $O(M^3)$ where M was the number of basis functions.
- Again, kernel allows us to use large or infinite number of basis functions (feature maps), but disadvantegeous for $M < N$.

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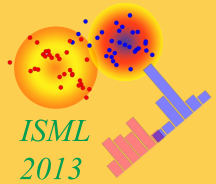


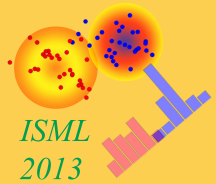
Maximum Margin Classifiers - Prediction

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

- The Karush-Kuhn-Tucker (KKT) conditions are

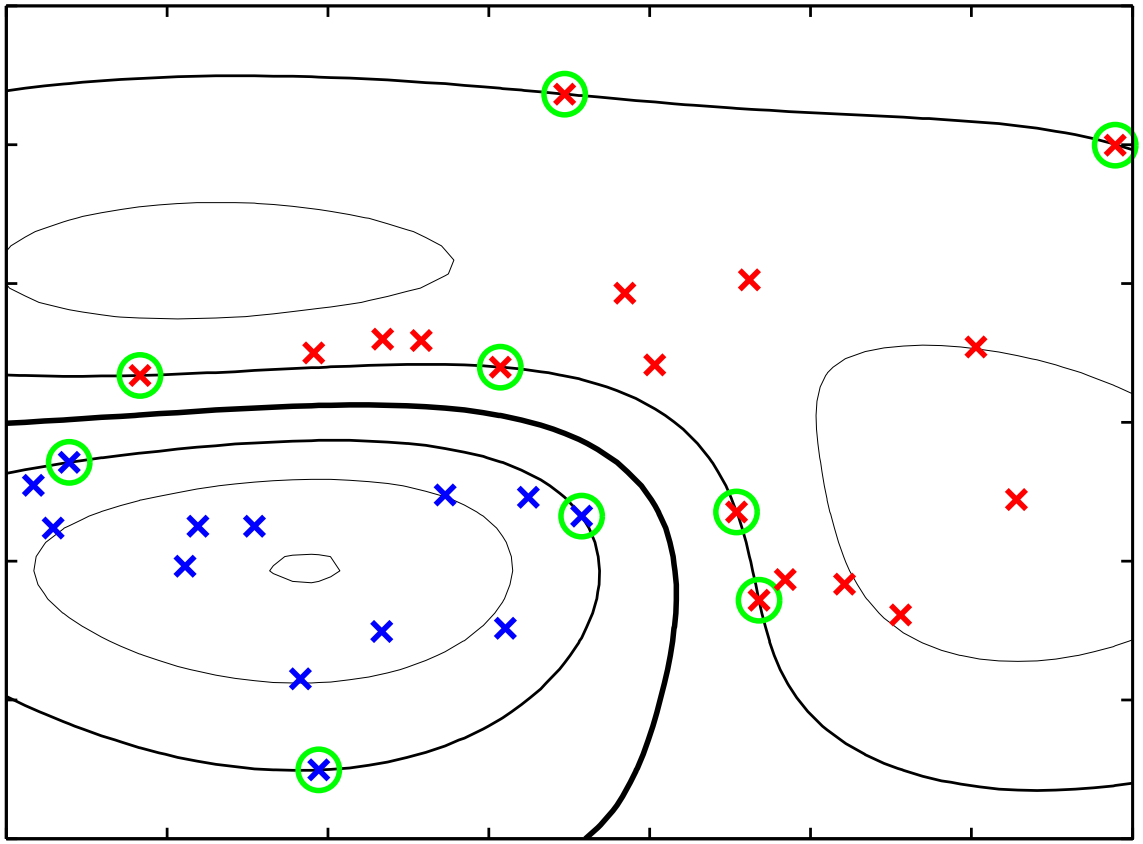
$$\begin{aligned} a_n &\geq 0 \\ t_n \, y(\mathbf{x}_n) - 1 &\geq 0 \\ a_n \left\{ t_n \, y(\mathbf{x}_n) - 1 \right\} &= 0. \end{aligned}$$

- Therefore, either $a_n = 0$ or $t_n \, y(\mathbf{x}_n) - 1 = 0$.
- If $a_n = 0$, no contribution to the prediction!
- After training, use only the set $\mathcal{S}$ of points for which $a_n > 0$ (and therefore $t_n \, y(\mathbf{x}_n) = 1$) holds.
- $\mathcal{S}$ contains only the support vectors.



Maximum Margin Classifiers - Support Vectors

- $\mathcal{S}$ contains only the support vectors.



Decision and margin boundaries for a two-class problem using Gaussian kernel functions.

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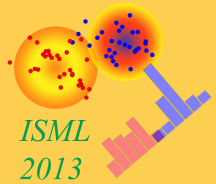

Maximum Margin Classifiers - Support Vectors

- Now for the bias b.
- Observe that for the support vectors, $t_n\, y(\mathbf{x}_n) = 1$.
- Therefore, we find

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

  and can use any support vector to calculate b.
- Numerically more stable: Multiply by t_n, observe $t_n^2 = 1$, and average over all support vectors.

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

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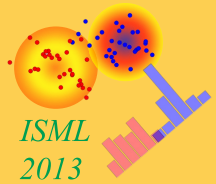

Maximum Margin Classifiers - Error

- Express the error for maximum margin classifiers with the help of a function

$$E_\infty(z) = \begin{cases} 0, & z \geq 0 \\ \infty, & z < 0 \end{cases}$$

enforcing the constraints as

$$\sum_{n=1}^{N} E_\infty(y(\mathbf{x}_n)t_n - 1)) + \lambda \|\mathbf{w}\|^2.$$

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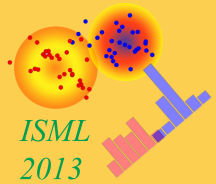

Overlapping Class distributions

- If the training data in the feature space are not linearly separable?
- Allow some data points to be on the 'wrong side' of the decision boundary.
- Increase a penalty with distance from the decision boundary.
- Assume, the penalty increases linearly with distance.
- Introduce slack variable $\xi_n \geq 0$ for each data point n .

$$\xi_n \begin{cases} = 0, & \text{data point is correctly classified and} \\ & \quad \text{on margin boundary or beyond} \\ < 1, & \text{data point is in correct margin} \\ = 1, & \text{data point is on the decision boundary} \\ > 1, & \text{data point is misclassified} \end{cases}$$

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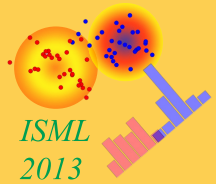
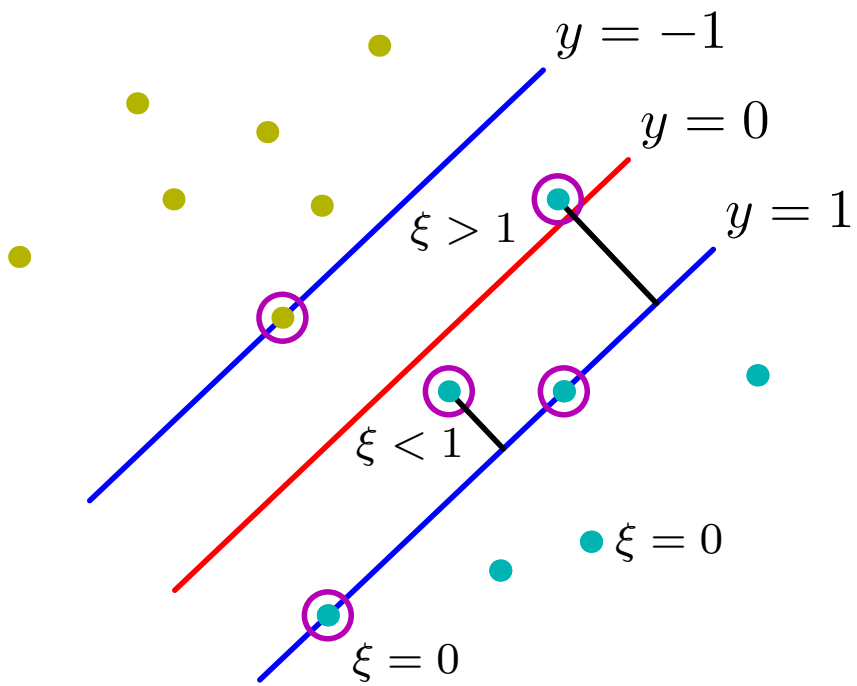


Overlapping Class distributions

- Introduce slack variable $\xi_n \geq 0$ for each data point n .

$$\xi_n = \begin{cases} 0, & \text{data point is correctly classified and} \\ & \text{on margin boundary or beyond} \\ |t_n - y(\mathbf{x})|, & \text{otherwise} \end{cases}$$



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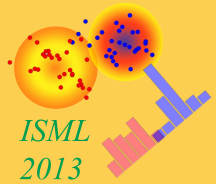


Overlapping Class distributions

- Constraints of the separable classification

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

change now to

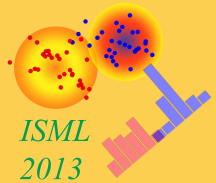
$$t_n\, y(\mathbf{x}_n) \geq 1 - \xi_n, \qquad n = 1, \ldots, N$$

- Minimise now

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

where C controls the trade-off between the slack variable penalty and the margin.

- Any misclassified point contributes $\xi_n >$, therefore $\sum_{n=1}^{N} \xi_n$ is an upper bound on the number of misclassified points.



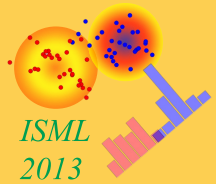
Overlapping Class distributions

- The Lagrangian with the Lagrange multipliers $\mathbf{a} = (a_1, \ldots, a_N)^T$ and $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_N)^T$ is now

$$L(\mathbf{w}, b, \boldsymbol{\xi}, \mathbf{a}, \boldsymbol{\mu}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{n=1}^{N}\xi_n - \sum_{n=1}^{N} a_n\{t_n\, y(\mathbf{x}_n) - 1 + \xi_n\} - \sum_{n=1}^{N}\mu_n\xi_n.$$

- The KKT conditions for $n = 1, \ldots, N$ are

$$\begin{aligned} a_n &\geq 0 \\ t_n\, y(\mathbf{x}_n) - 1 + \xi_n &\geq 0 \\ a_n(t_n\, y(\mathbf{x}_n) - 1 + \xi_n) &= 0 \\ \mu_n &\geq 0 \\ \xi_n &\geq 0 \\ \mu_n\xi_n &= 0. \end{aligned}$$



Overlapping Class distributions

- The dual Lagrangian after eliminating $\mathbf{w}$, b, $\boldsymbol{\xi}$, and $\boldsymbol{\mu}$ is then

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

$$\sum_{n=1}^{N} a_n \, t_n = 0$$

$$0 \leq a_n \leq C \qquad\qquad n = 1, \ldots, N.$$

- The only change from the separable case, is the box constraint via the parameter C.

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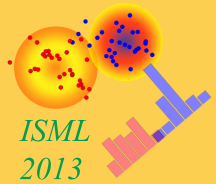

Overlapping Class distributions

- Equivalent formulation by Schölkopf et. al. (2000)

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

$$\sum_{n=1}^{N} a_n\, t_n = 0$$

$$0 \leq a_n \leq 1/N$$

$$\sum_{n=1}^{N} a_n \geq \nu \qquad\qquad n = 1, \ldots, N.$$

where ν is both

1. an upper bound on the fraction of margin errors, and,
2. a lower bound on the fraction of support vectors.

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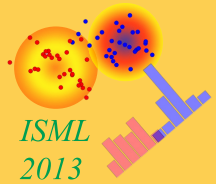
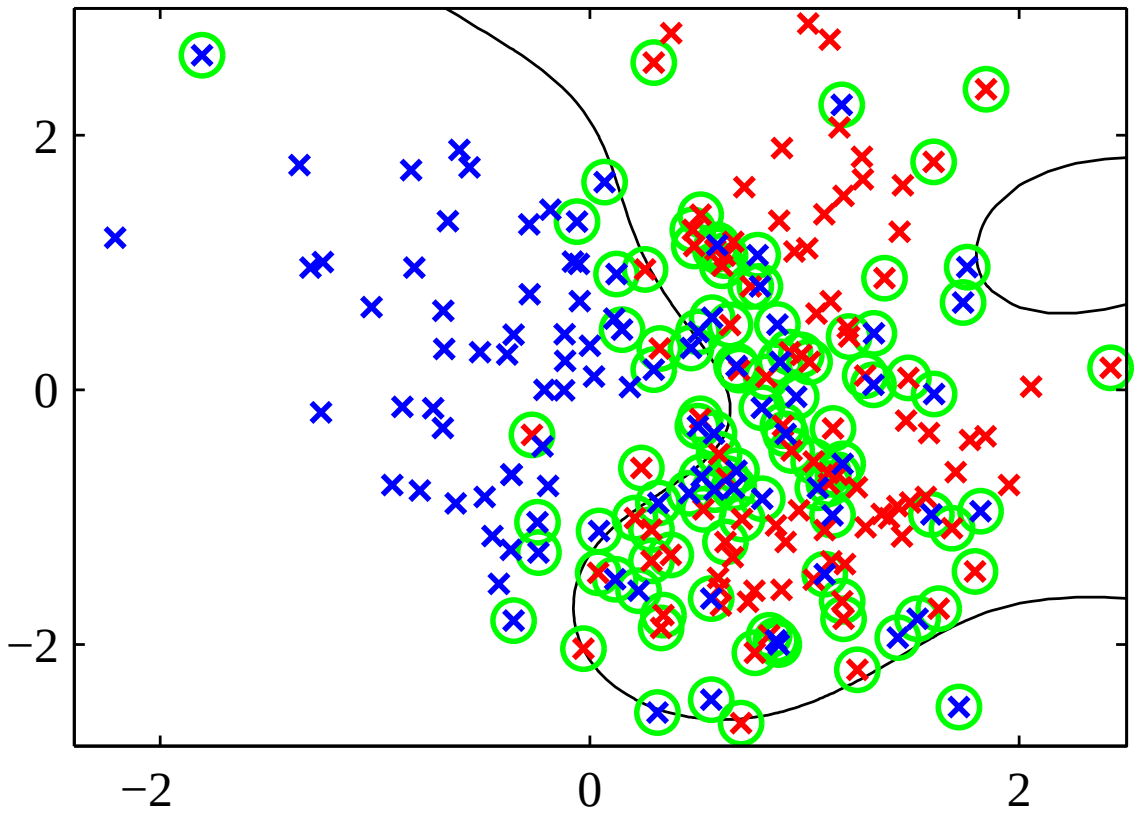


Overlapping Class distributions



The ν-SVM algorithm using Gaussian kernels $\exp(-\gamma\|\mathbf{x}-\mathbf{x}'\|^2)$ with $\gamma = 0.45$ applied to a nonseparable data set in two dimensions. Support vectors are indicated by circles.

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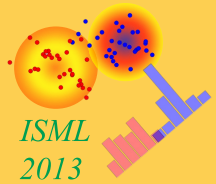

Support Vector Machines - Limitations

- Output are decisions, not posterior probabilities.
- Extension to classification with more than two classes is problematic.
- There is a complexity parameter C (or ν) which must be found (e.g. via cross-validation).
- Predictions are expressed as linear combinations of kernel functions that are centered on the training points.
- Kernel matrix is required to be positive definite.

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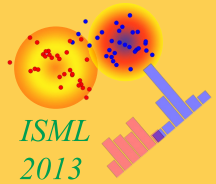

Relevance Vector Machines

- Assume a Bayesian model as in Bayesian Linear Regression with the probability of the target t given by

$$p(t \mid \mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t \mid y(\mathbf{x}), \beta^{-1}),$$

  and the linear model

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

  with fixed nonlinear basis functions $\boldsymbol{\phi}(\mathbf{x})$ (including a constant term to accomodate for the bias).
- But now the prior over $\mathbf{w}$ includes a different precision α_i for each of the components of $\mathbf{w}$

$$p(\mathbf{w} \mid \boldsymbol{\alpha}) = \prod_{i=1}^{M} \mathcal{N}(w_i \mid 0, \alpha_i^{-1}).$$

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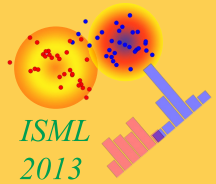

Relevance Vector Machines

- When using this prior for the weights $\mathbf{w}$

$$p(\mathbf{w} \mid \boldsymbol{\alpha}) = \prod_{i=1}^{M} \mathcal{N}(w_i \mid 0, \alpha_i^{-1})$$

  and maximising the evidence with respect to the hyperparameters α_i, a significant portion of the α_i will go to infinity.
- The corresponding w_i will therefore be concentrated at zero, and play no role for the prediction.

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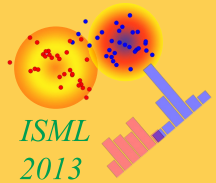

Relevance Vector Machines

- The Relevance Vector Machine iteratively calculates the α_i and β from the training data by optimising a nonconvex function.
- Disadvantages
  1. Nonconvex function means that the algorithm can get stuck in some local minimum.
  2. Training times can be longer than for SVM.
- Advantages
  1. As a Bayesian method, the parameters governing complexity and noise are determined from the input data. (Compare to SVM where we needed cross-validation).
  2. Number of relevance vectors is much smaller than the number of support vectors in a SVM.
  3. Therefore, prediction is much faster than with SVM.
  4. Extends well to multiclass learning.

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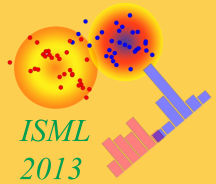
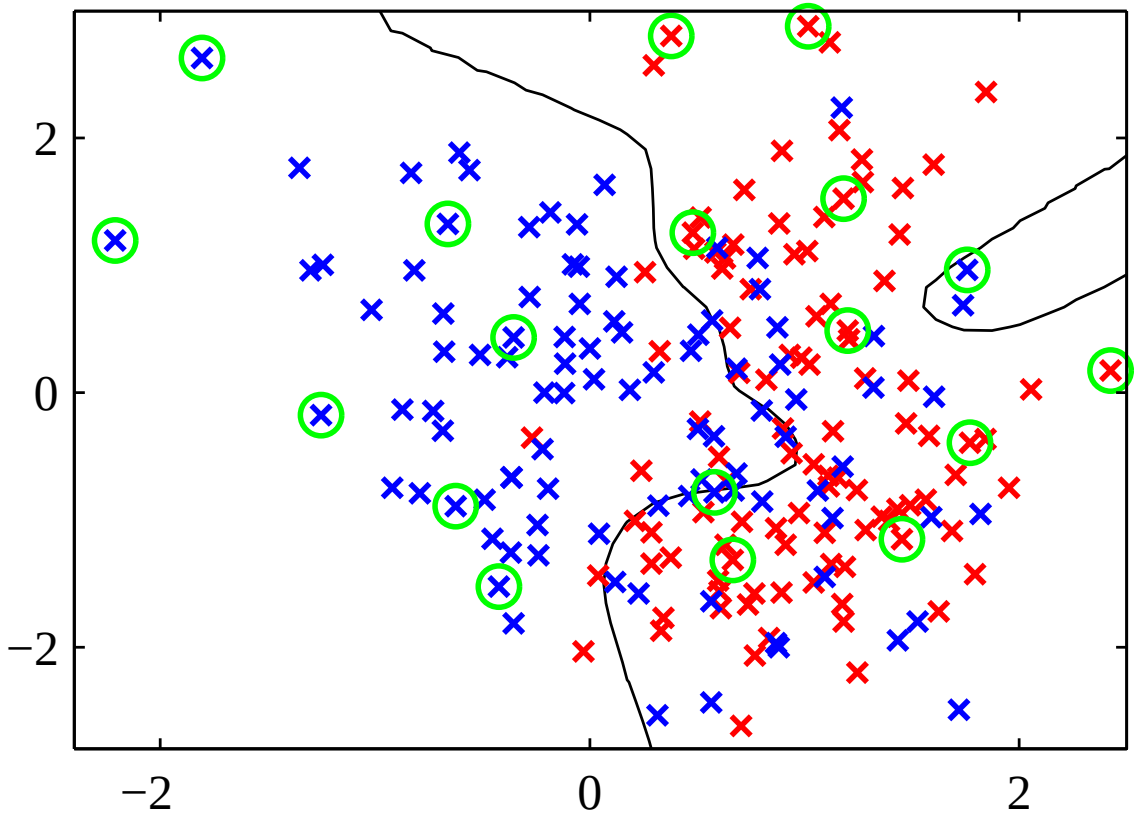


Relevance Vector Machines



Decision boundaries for a two-class problem found by a Relevance Vector Machine.

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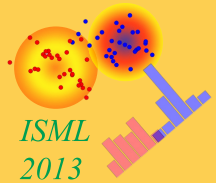
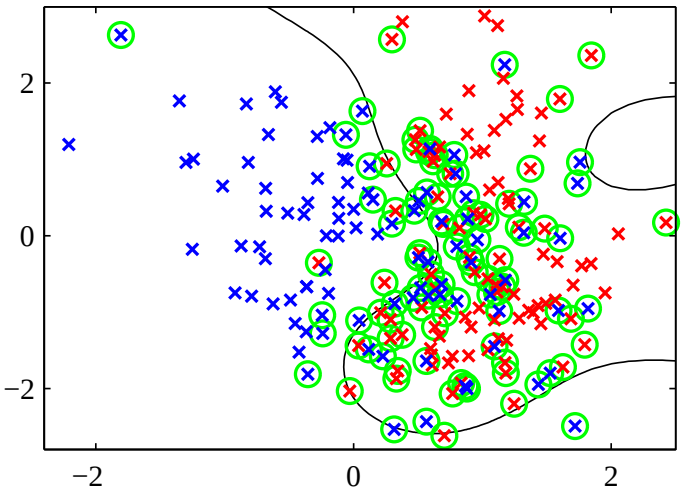
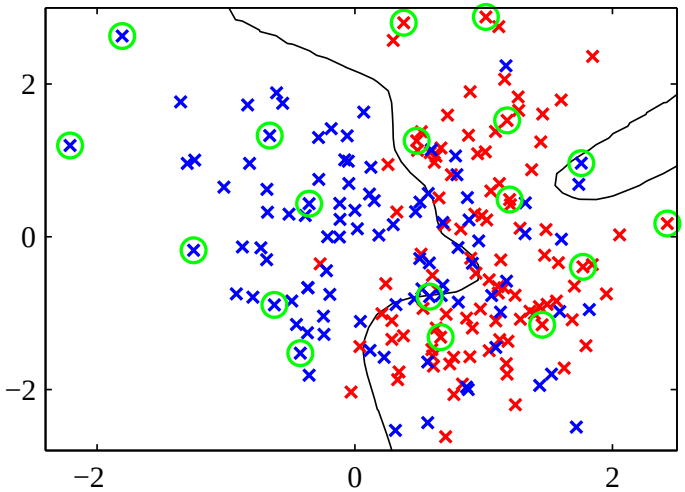


Relevance Vector Machines



Support Vector Machine



Relevance Vector Machine

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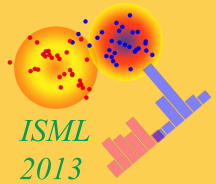
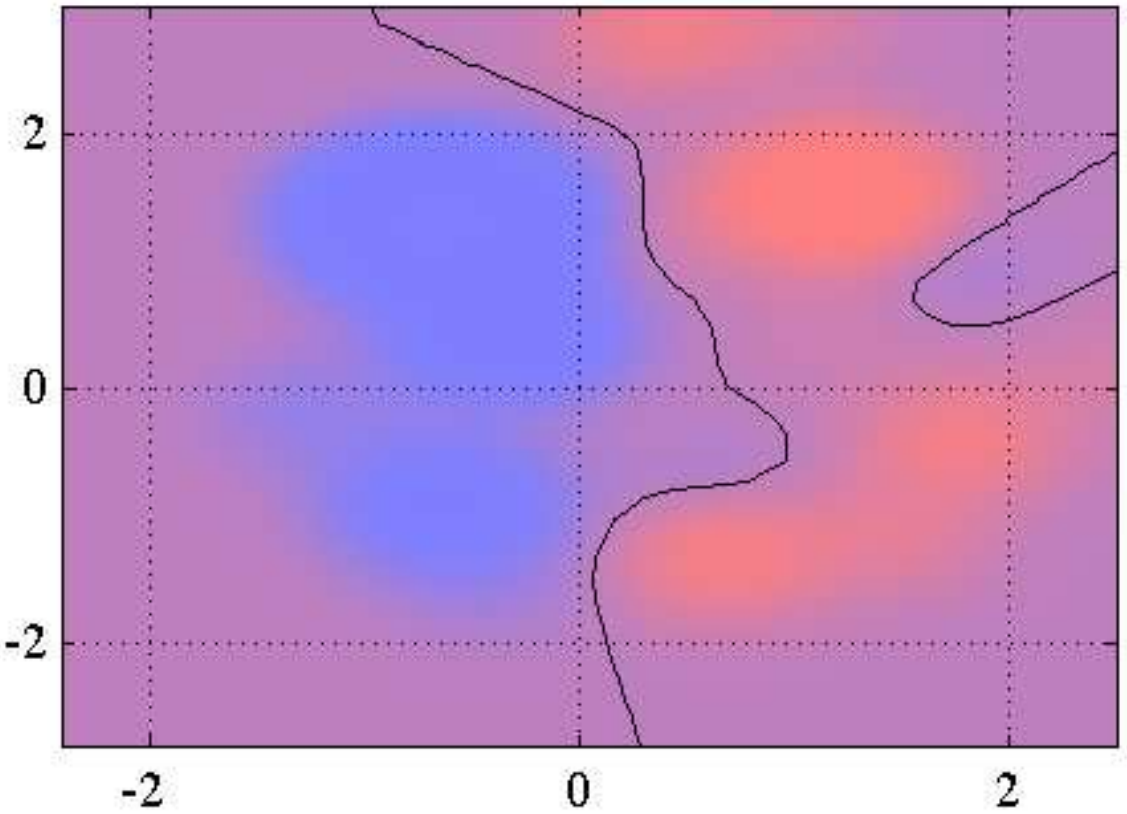


Relevance Vector Machines



Decision boundaries and posterior probability for a two-class problem found by a Relevance Vector Machine.

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