12.02.2019

Statistical Methods in AI (CSE/ECE 471)

Lecture-10: Support Vector Machines

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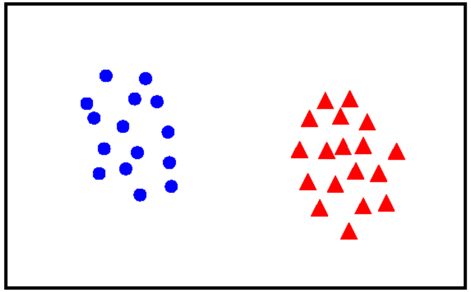
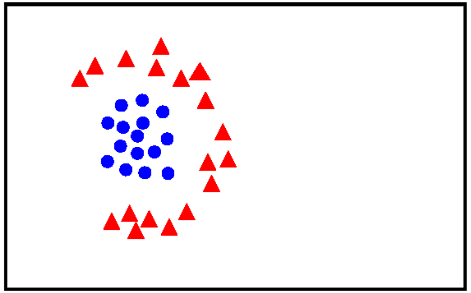
Binary Classification

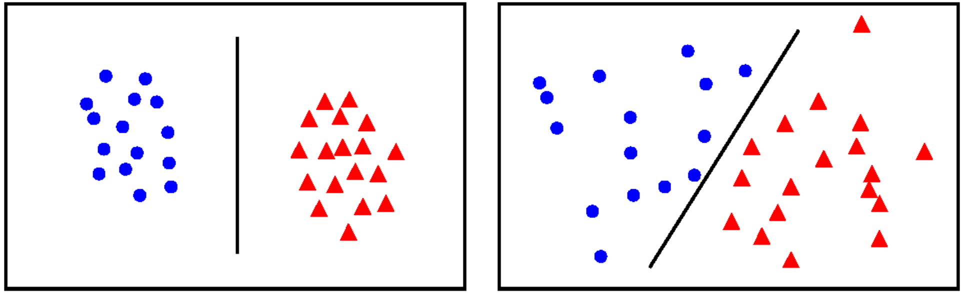
Given training data $(\mathbf{x}_i, y_i)$ for $i = 1 \ldots N$, with $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{-1, 1\}$



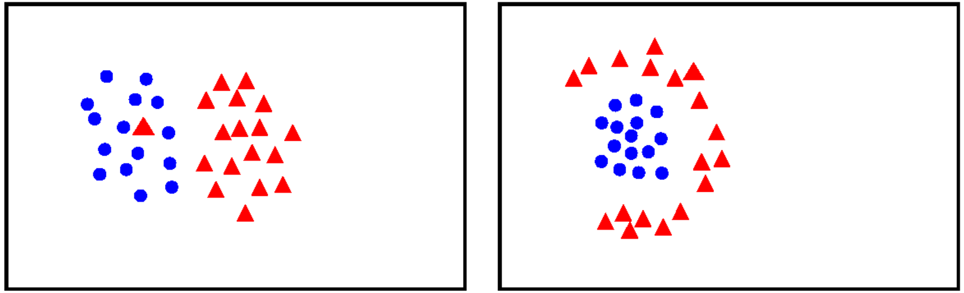


Linear separability

linearly
separable



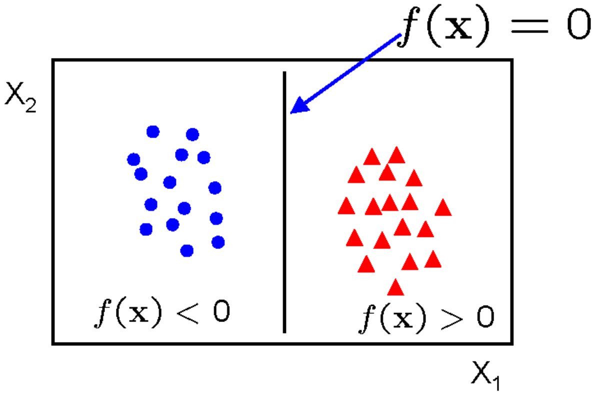
not
linearly
separable



Linear classifiers

A linear classifier has the form

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

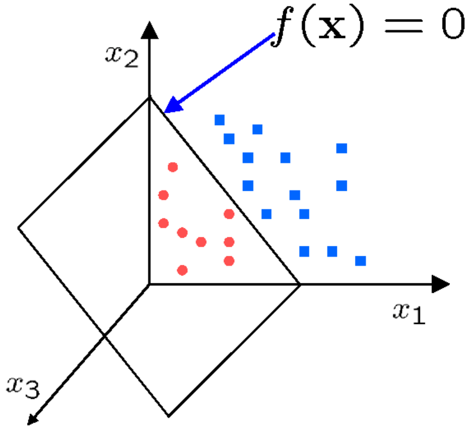


- in 2D the discriminant is a line
- $\mathbf{w}$ is the normal to the line, and b the bias
- $\mathbf{w}$ is known as the weight vector

Linear classifiers

A linear classifier has the form

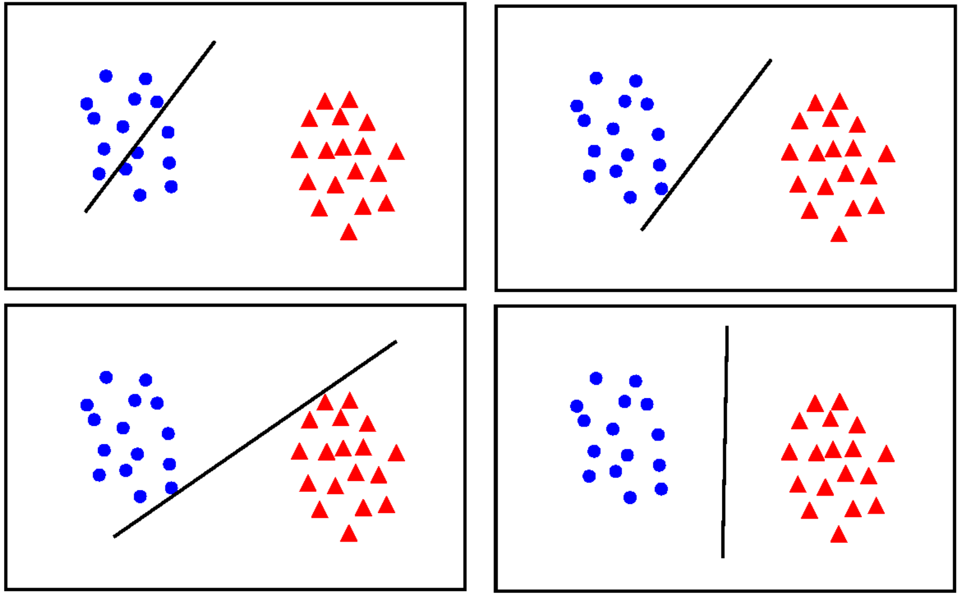
$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$



- in 3D the discriminant is a plane, and in nD it is a hyperplane

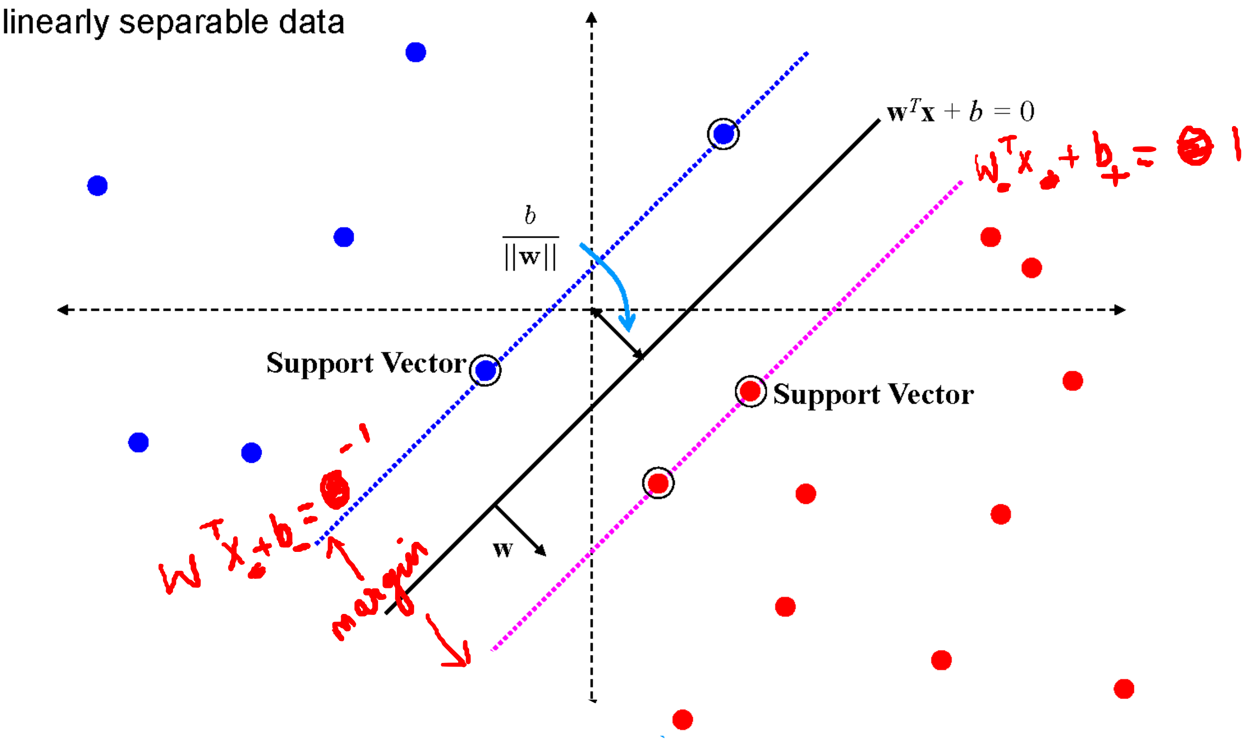
The Perceptron Classifier

What is the best w?



- maximum margin solution: most stable under perturbations of the inputs

Support Vector Machine



What is the advantage of support vectors ?

SVM – sketch derivation

- Since $\mathbf{w}^\top \mathbf{x} + b = 0$ and $c(\mathbf{w}^\top \mathbf{x} + b) = 0$ define the same plane, we have the freedom to choose the normalization of $\mathbf{w}$

SVM – sketch derivation

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- Choose normalization such that $\mathbf{w}^\top \mathbf{x}_+ + b = +1$ and $\mathbf{w}^\top \mathbf{x}_- + b = -1$ for the positive and negative support vectors respectively

SVM – sketch derivation

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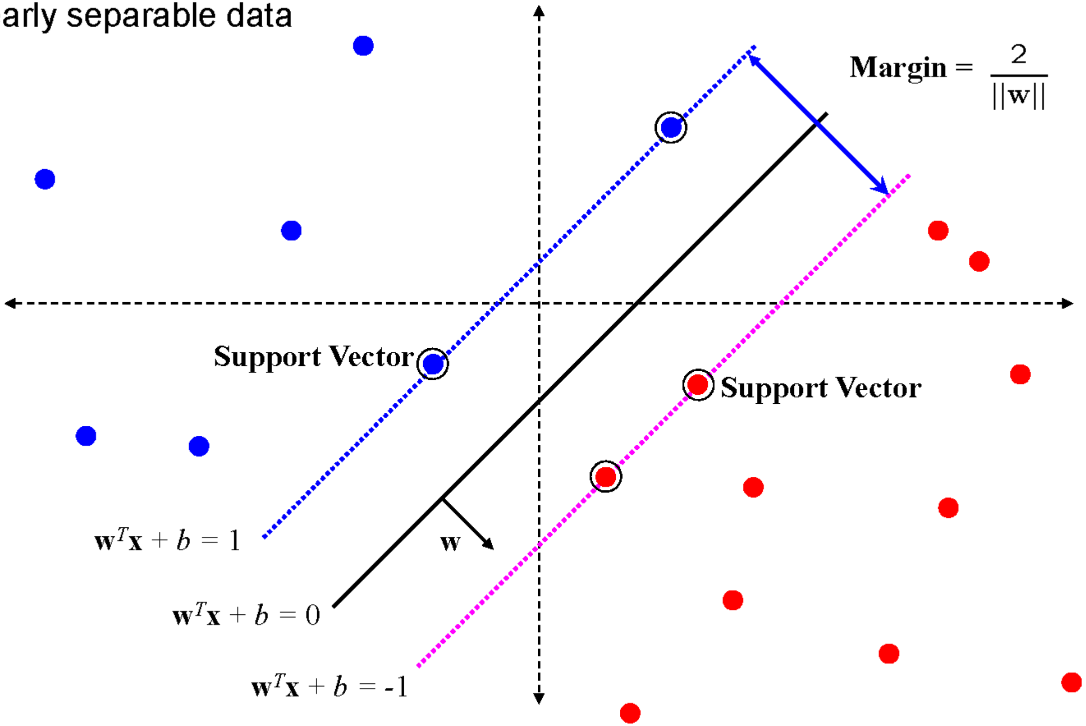
- Choose normalization such that $\mathbf{w}^\top \mathbf{x}_+ + b = +1$ and $\mathbf{w}^\top \mathbf{x}_- + b = -1$ for the positive and negative support vectors respectively

- Then the margin is given by

$$= \frac{2}{||\mathbf{w}||}$$

Support Vector Machine

linearly separable data



Margin = $\frac{2}{||\mathbf{w}||}$
Support Vector
Support Vector
$\mathbf{w}^T\mathbf{x} + b = 1$
$\mathbf{w}$
$\mathbf{w}^T\mathbf{x} + b = 0$
$\mathbf{w}^T\mathbf{x} + b = -1$

SVM – Optimization

- Learning the SVM can be formulated as an optimization:

$$arg \max_{\mathbf{w}} \frac{2}{||\mathbf{w}||} \text{ subject to } \mathbf{w}^\top \mathbf{x}_i + b \begin{array}{ll} \geq 1 & \text{if } y_i = +1 \\ \leq -1 & \text{if } y_i = -1 \end{array} \text{ for } i = 1 \ldots N$$

SVM – Optimization

- Learning the SVM can be formulated as an optimization:

$$\max_{\mathbf{w}} \frac{2}{||\mathbf{w}||} \text{ subject to } \mathbf{w}^\top \mathbf{x}_i + b \begin{array}{ll} \geq 1 & \text{if } y_i = +1 \\ \leq -1 & \text{if } y_i = -1 \end{array} \text{ for } i = 1 \ldots N$$

- Or equivalently

$$\min_{\mathbf{w}} ||\mathbf{w}||^2 \text{ subject to } y_i \left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 \text{ for } i = 1 \ldots N$$

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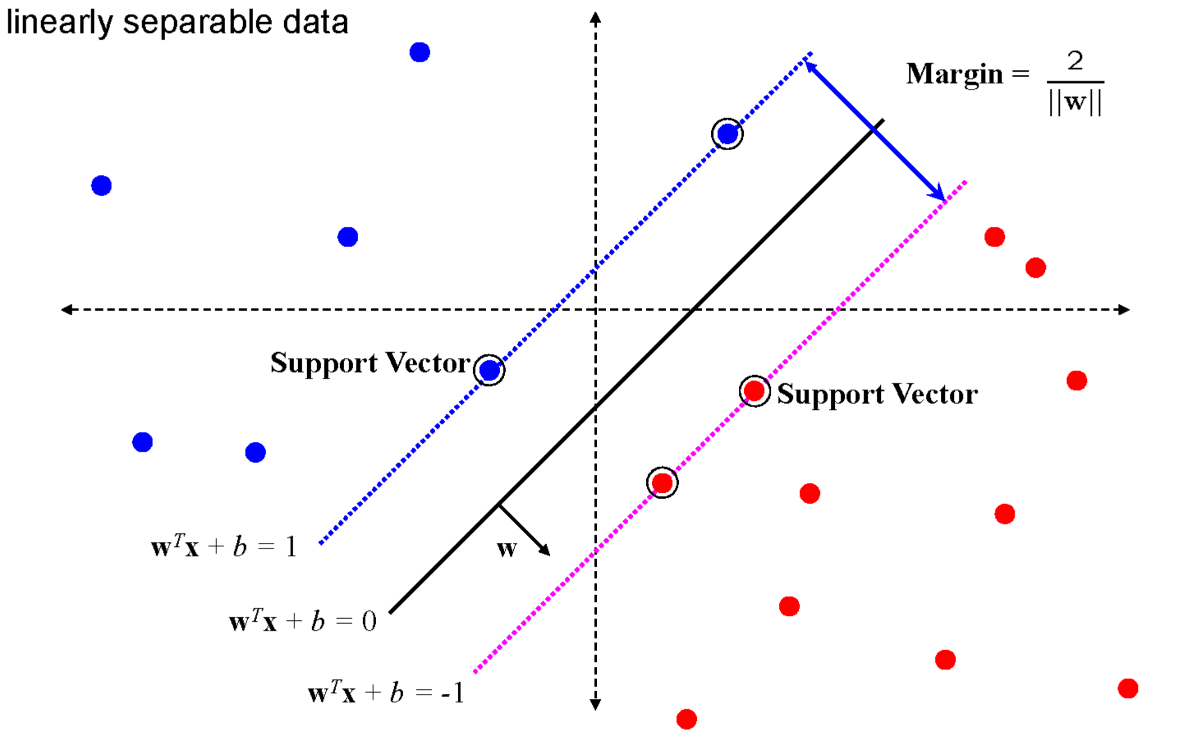
- This is a quadratic optimization problem subject to linear constraints and there is a unique minimum

Quadratic programming in python: https://scaron.info/blog/quadratic-programming-in-python.html

How to find support vectors ?

Support Vector Machine


linearly separable data
Margin = $\frac{2}{||\mathbf{w}||}$
Support Vector
Support Vector
$\mathbf{w}$
$\mathbf{w}^T\mathbf{x} + b = 1$
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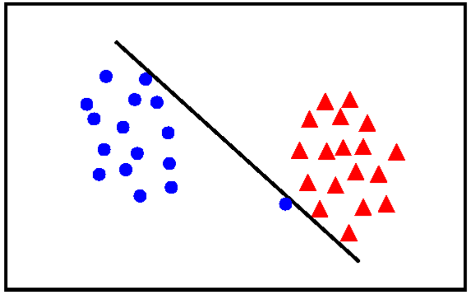
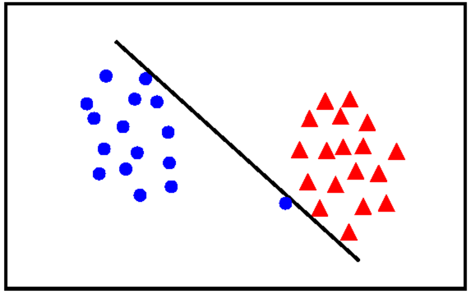
Linear separability again: What is the best w?

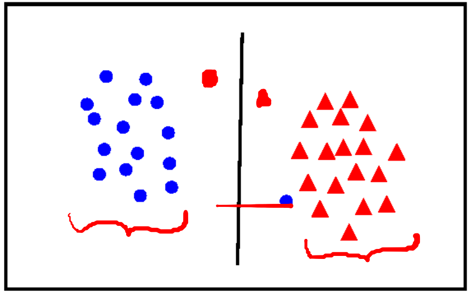


- the points can be linearly separated but there is a very narrow margin

Linear separability again: What is the best w?

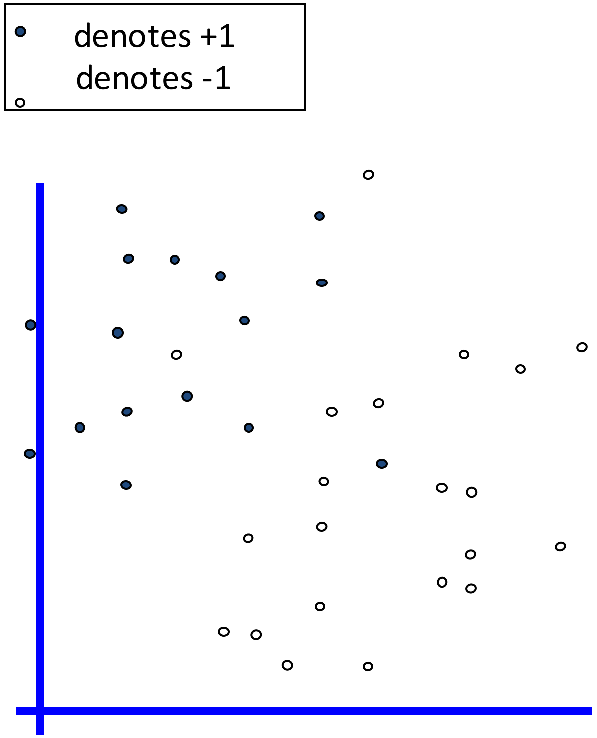


- the points can be linearly separated but there is a very narrow margin



- but possibly the large margin solution is better, even though one constraint is violated

In general there is a trade off between the margin and the number of mistakes on the training data



Idea 1:

Find minimum ***w.w***, while minimizing number of training set errors.

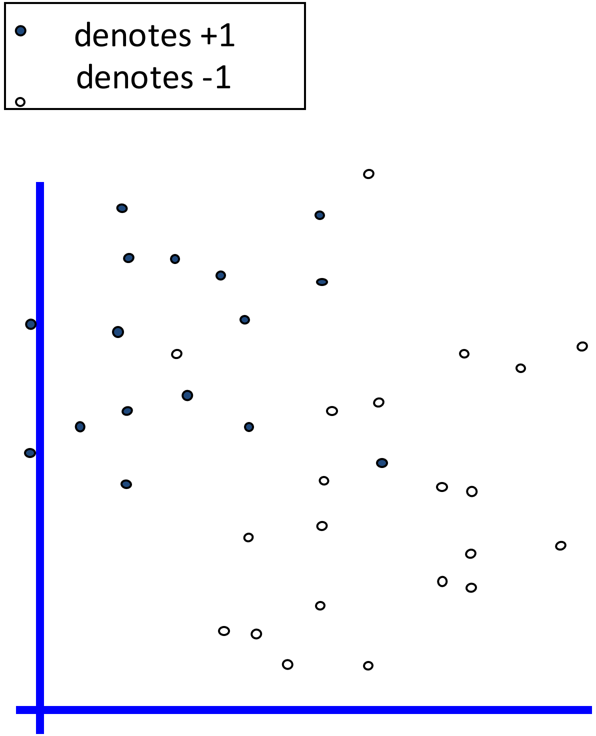
Problemette: Two things to minimize makes for an ill-defined optimization

Idea 1.1:

Minimize

w.w *+ C (#train errors)*

Tradeoff parameter



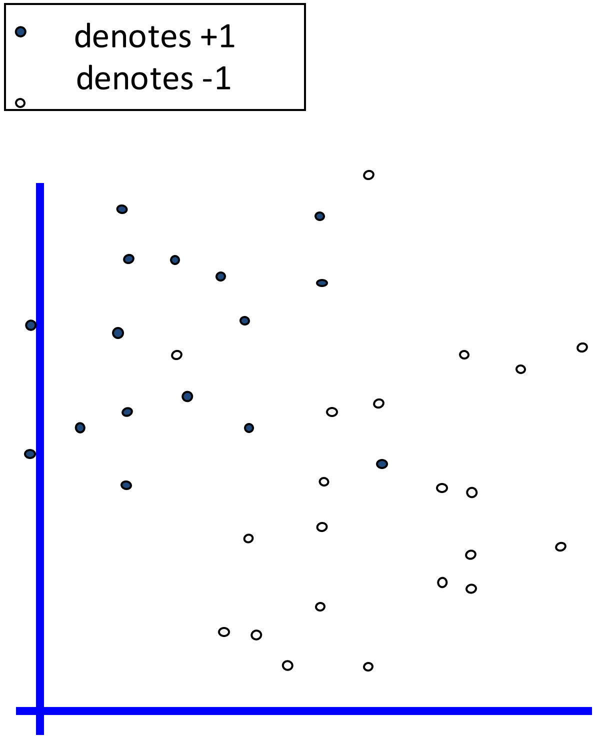
Idea 1.1:

Minimize

$$\mathbf{w.w} + C\ (\#train\ errors)$$

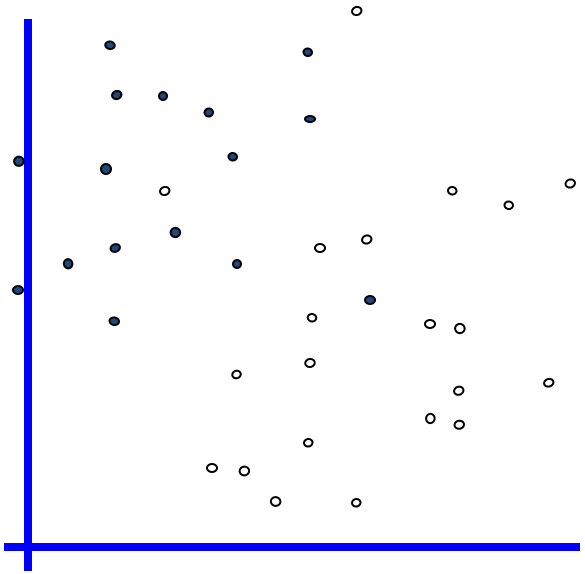
Tradeoff parameter

This is problematic. Why ?



Uh-oh!

● denotes +1
○ denotes -1



This is going to be a problem!
What should we do?

Idea 1.1:

Minimize

w.w *+ C (#train errors)*

Tradeoff parameter

This is problematic. Why ?

Can't be expressed as a Quadratic Programming problem.

Solving it may be too slow.

(Also, doesn't distinguish between disastrous errors and near misses)

Uh-oh!

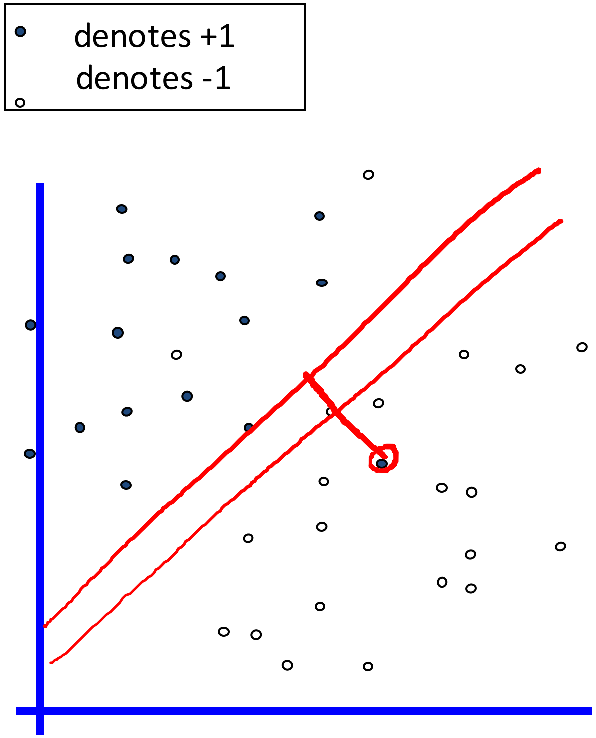
This is going to be a problem!

What should we do?

Idea 2.0:

Minimize

w.w *+ C (distance of error points to their correct place)*



Support Vector Machine (SVM) for Noisy Data

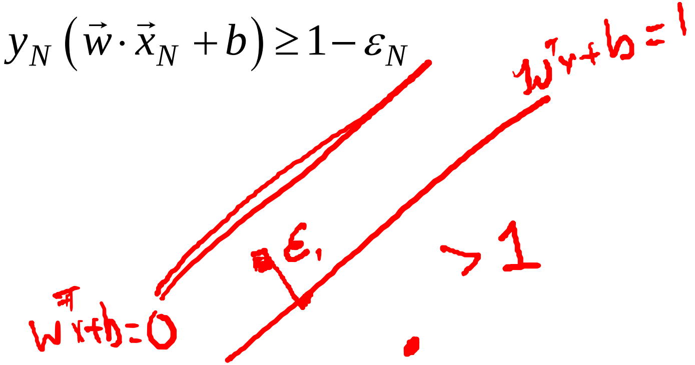
$$\{\vec{w}^*, b^*\} = \min_{\vec{w},b} \sum_{i=1}^{d} w_i^2 + c\sum_{j=1}^{N}\varepsilon_j$$

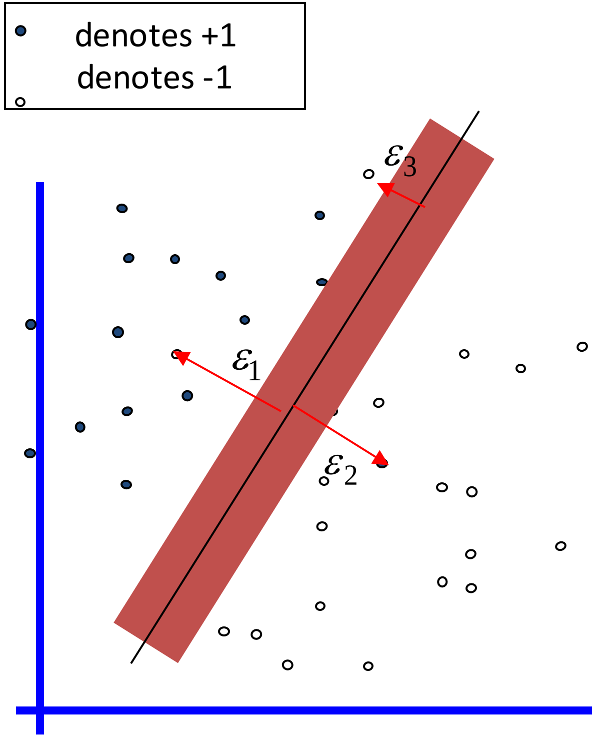
$$y_1\left(\vec{w}\cdot\vec{x}_1+b\right)\ge 1-\varepsilon_1 \quad \checkmark \quad \varepsilon_1$$

$$y_2\left(\vec{w}\cdot\vec{x}_2+b\right)\ge 1-\varepsilon_2 \quad \checkmark \quad \varepsilon_2$$

...

$$y_N\left(\vec{w}\cdot\vec{x}_N+b\right)\ge 1-\varepsilon_N$$





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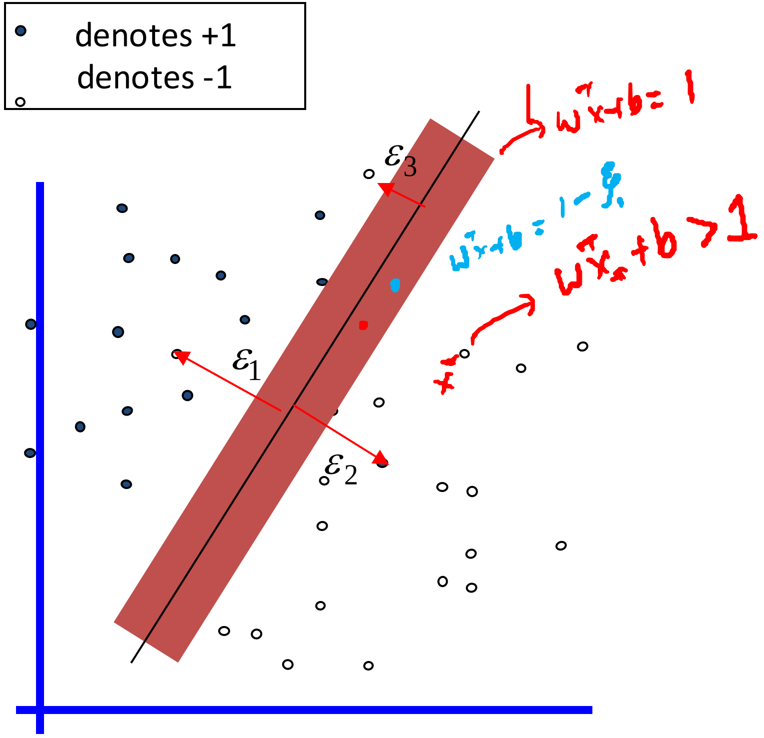
$$y_1\left(\vec{w}\cdot\vec{x}_1 + b\right) \geq 1 - \varepsilon_1$$

$$y_2\left(\vec{w}\cdot\vec{x}_2 + b\right) \geq 1 - \varepsilon_2$$

$$\ldots$$

$$y_N\left(\vec{w}\cdot\vec{x}_N + b\right) \geq 1 - \varepsilon_N$$


● denotes +1

○ denotes -1

- Any problem with the above formulation ?

Support Vector Machine (SVM) for Noisy Data

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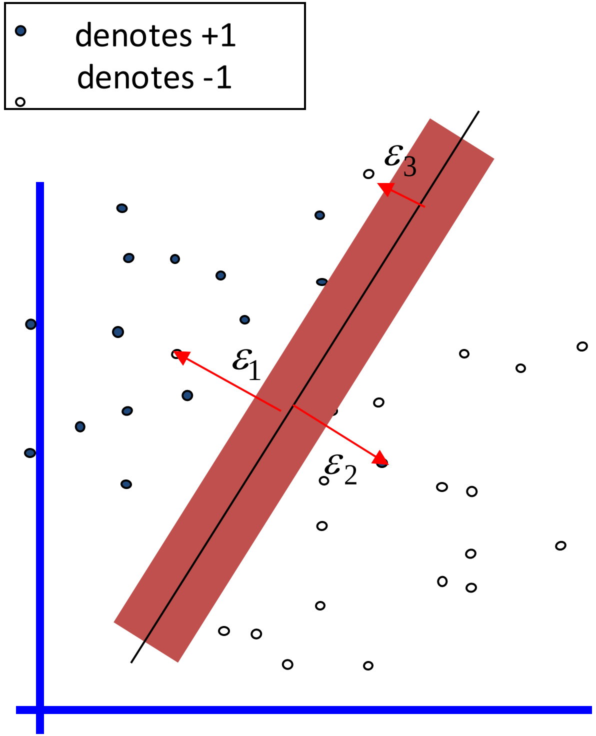
$$y_1\left(\vec{w}\cdot\vec{x}_1 + b\right) \geq 1 - \varepsilon_1, \varepsilon_1 \geq 0$$

$$y_2\left(\vec{w}\cdot\vec{x}_2 + b\right) \geq 1 - \varepsilon_2, \varepsilon_2 \geq 0$$

$$\ldots$$

$$y_N\left(\vec{w}\cdot\vec{x}_N + b\right) \geq 1 - \varepsilon_N, \varepsilon_N \geq 0$$

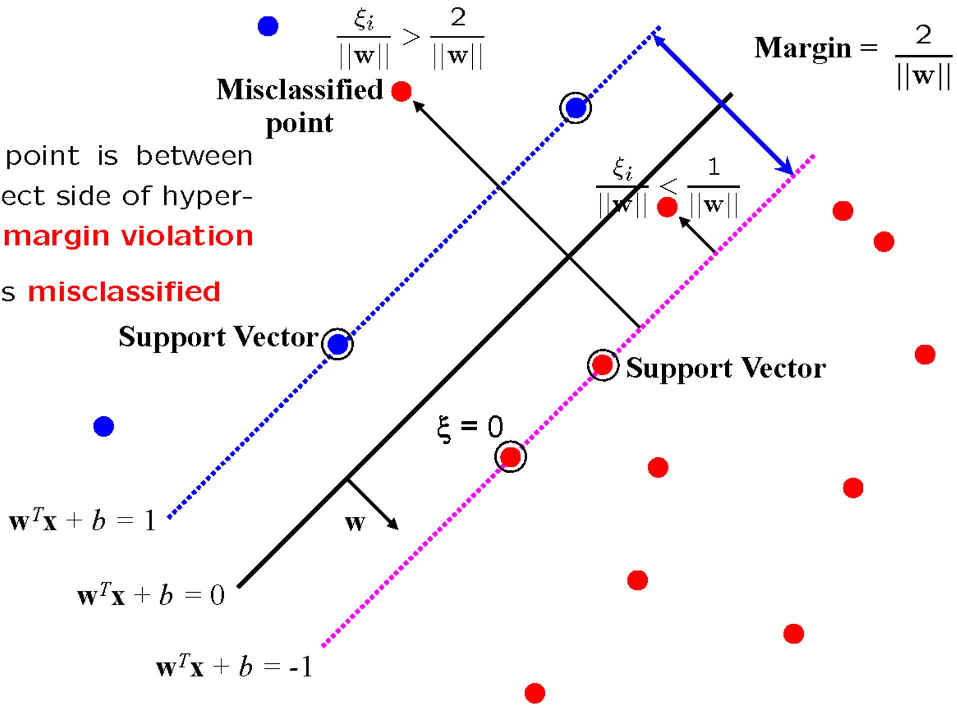
- Balance the trade off between margin and classification errors



Introduce “slack” variables

$$\xi_i \geq 0$$

- for $0 < \xi \leq 1$ point is between margin and correct side of hyper-plane. This is a **margin violation**
- for $\xi > 1$ point is **misclassified**



$\frac{\xi_i}{||\mathbf{w}||} > \frac{2}{||\mathbf{w}||}$
Misclassified point
Margin = $\frac{2}{||\mathbf{w}||}$
$\frac{\xi_i}{||\mathbf{w}||} < \frac{1}{||\mathbf{w}||}$
Support Vector
Support Vector
$\xi = 0$
$\mathbf{w}$
$\mathbf{w}^T\mathbf{x} + b = 1$
$\mathbf{w}^T\mathbf{x} + b = 0$
$\mathbf{w}^T\mathbf{x} + b = -1$

“Soft” margin solution

The optimization problem becomes

$$\min_{\mathbf{w}\in\mathbb{R}^d, \xi_i \in \mathbb{R}^+} ||\mathbf{w}||^2 + C\sum_i^N \xi_i$$

subject to

$$y_i\left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1 \ldots N$$

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subject to

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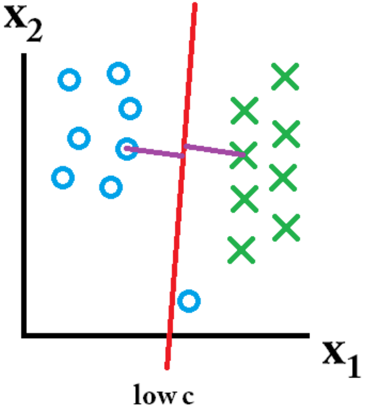
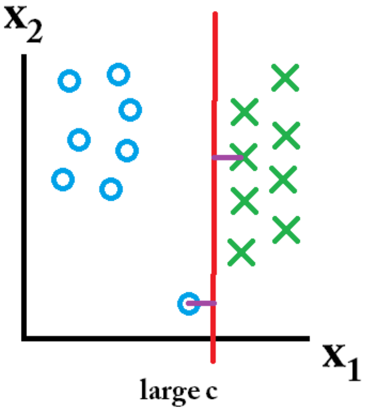
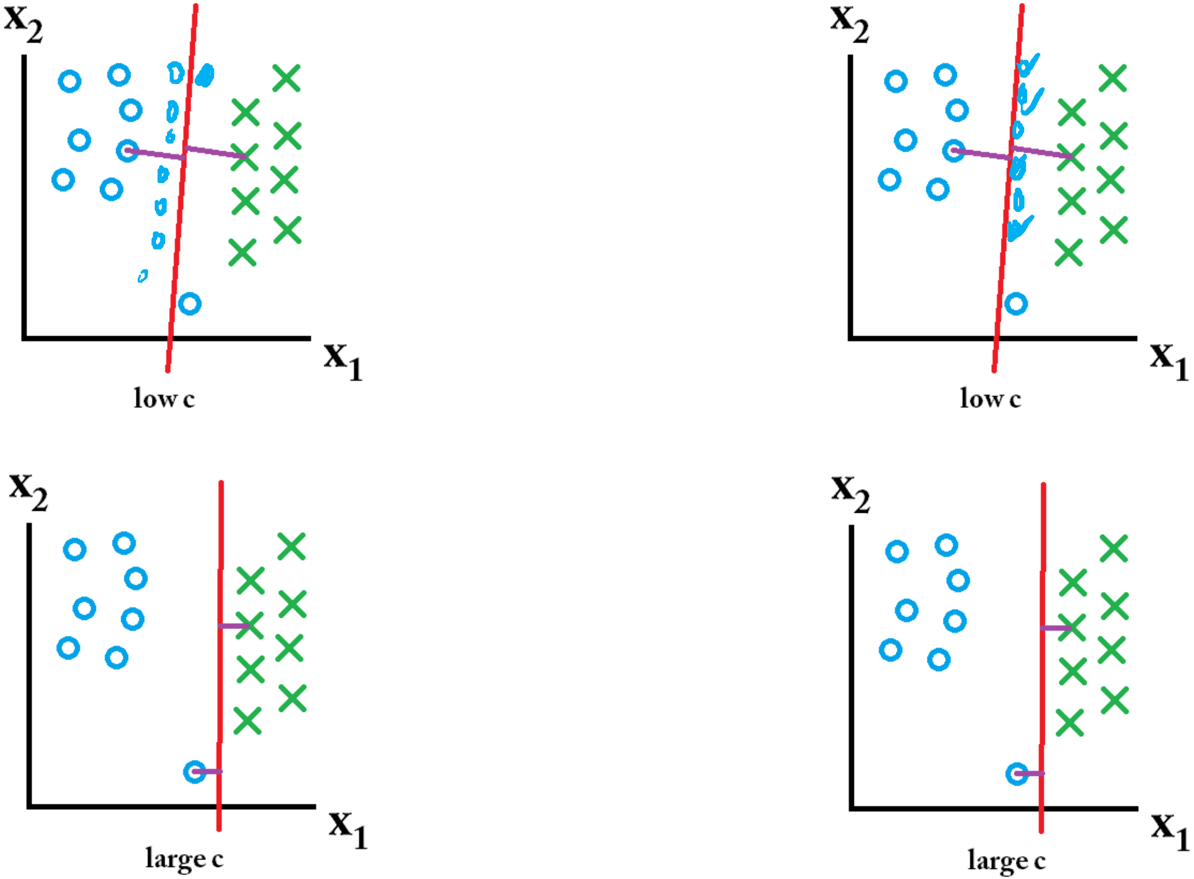
- Every constraint can be satisfied if ξ_i is sufficiently large
- C is a regularization parameter:
  - small C allows constraints to be easily ignored → large margin
  - large C makes constraints hard to ignore → narrow margin
  - $C = \infty$ enforces all constraints: hard margin
- This is still a quadratic optimization problem and there is a unique minimum. Note, there is only one parameter, C.

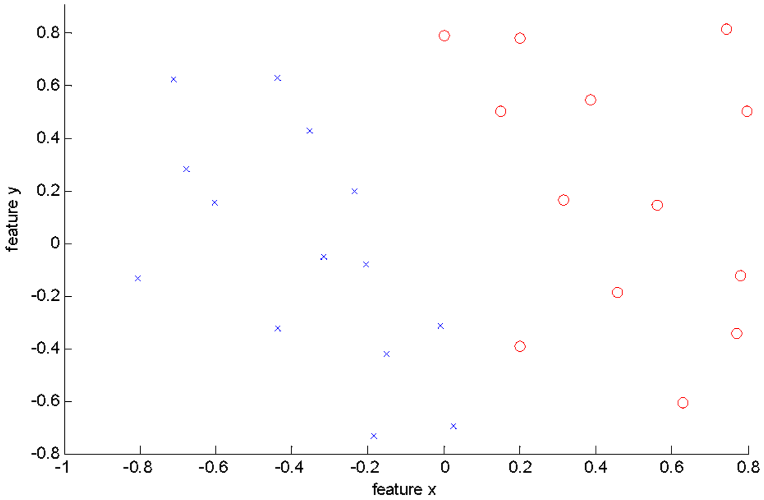
C = 0 ???





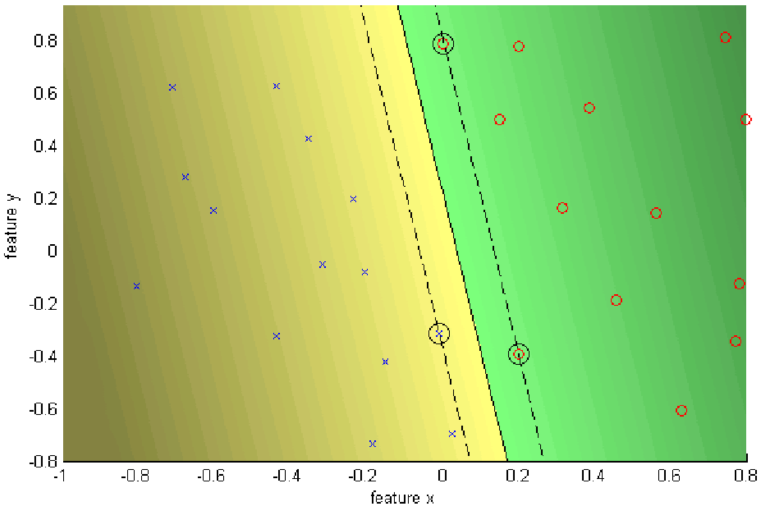
NOTE: Best margin = That which generalizes to ‘unseen’ data

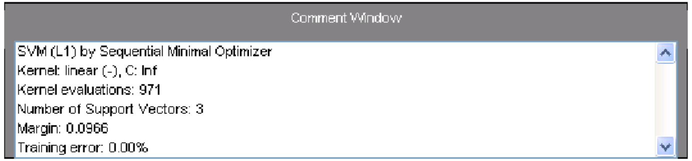




- data is linearly separable
- but only with a narrow margin

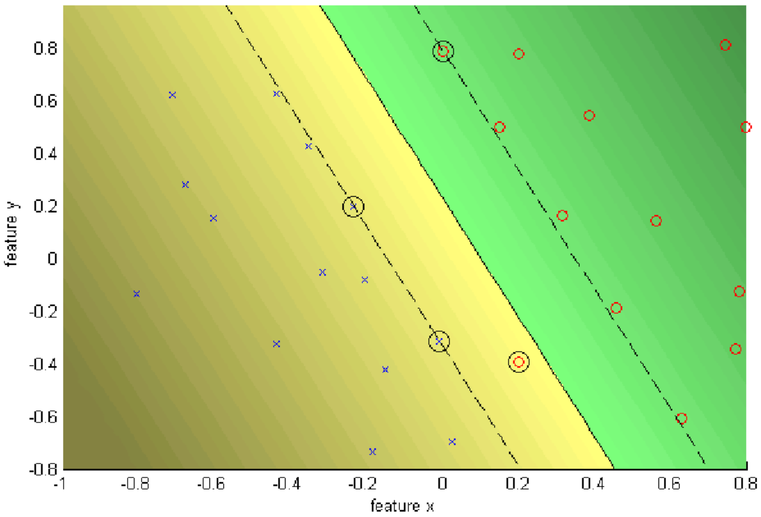
C = Infinity   hard margin

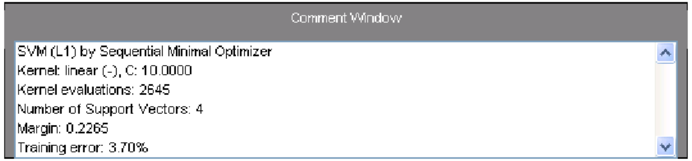




```
SVM (L1) by Sequential Minimal Optimizer
Kernel: linear (-), C: Inf
Kernel evaluations: 971
Number of Support Vectors: 3
Margin: 0.0966
Training error: 0.00%
```

C = 10 soft margin





```
SVM (L1) by Sequential Minimal Optimizer
Kernel: linear (-), C: 10.0000
Kernel evaluations: 2645
Number of Support Vectors: 4
Margin: 0.2265
Training error: 3.70%
```

Optimization

Learning an SVM has been formulated as a constrained optimization problem over $\mathbf{w}$ and ξ

$$\min_{\mathbf{w}\in\mathbb{R}^d,\xi_i\in\mathbb{R}^+} ||\mathbf{w}||^2 + C\sum_i^N \xi_i \text{ subject to } y_i\left(\mathbf{w}^\top\mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1 \ldots N$$

The constraint $y_i\left(\mathbf{w}^\top\mathbf{x}_i + b\right) \geq 1 - \xi_i$, can be written more concisely as

$$y_i f(\mathbf{x}_i) \geq 1 - \xi_i$$

which, together with $\xi_i \geq 0$, is equivalent to

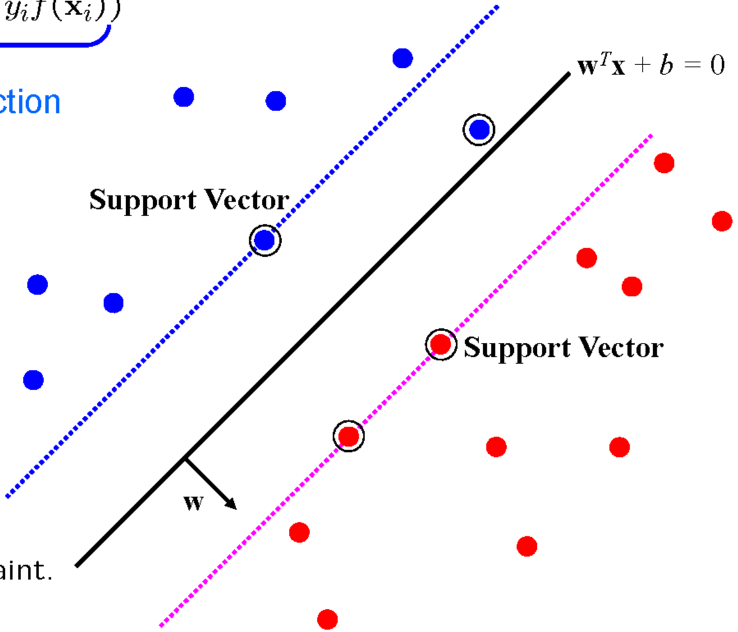
$$\xi_i = \max\left(0, 1 - y_i f(\mathbf{x}_i)\right)$$

Hence the learning problem is equivalent to the unconstrained optimization problem over $\mathbf{w}$

$$\min_{\mathbf{w}\in\mathbb{R}^d} \underbrace{||\mathbf{w}||^2}_{\text{regularization}} + C\sum_i^N \underbrace{\max\left(0, 1 - y_i f(\mathbf{x}_i)\right)}_{\text{loss function}}$$

Loss function

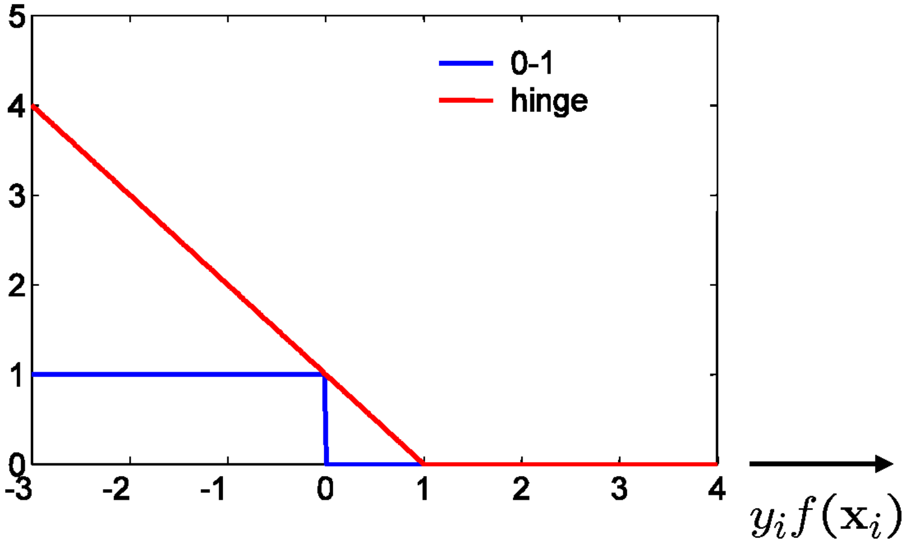
$$\min_{\mathbf{w}\in\mathbb{R}^d} ||\mathbf{w}||^2 + C\sum_i^N \underbrace{\max\left(0, 1 - y_i f(\mathbf{x}_i)\right)}_{\text{loss function}}$$



Points are in three categories:

1. $y_i f(x_i) > 1$
   Point is outside margin.
   No contribution to loss
2. $y_i f(x_i) = 1$
   Point is on margin.
   No contribution to loss.
   As in hard margin case.
3. $y_i f(x_i) < 1$
   Point violates margin constraint.
   Contributes to loss

Loss functions



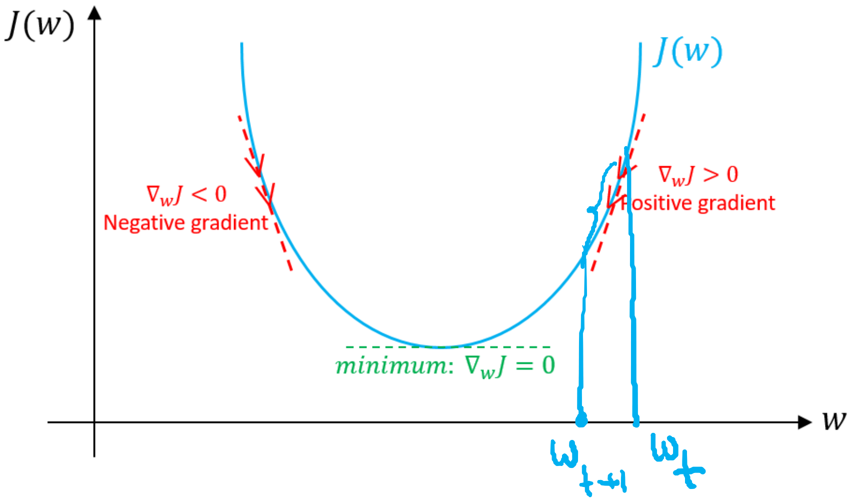
- SVM uses “hinge” loss $\max(0, 1 - y_i f(\mathbf{x}_i))$
- an approximation to the 0-1 loss

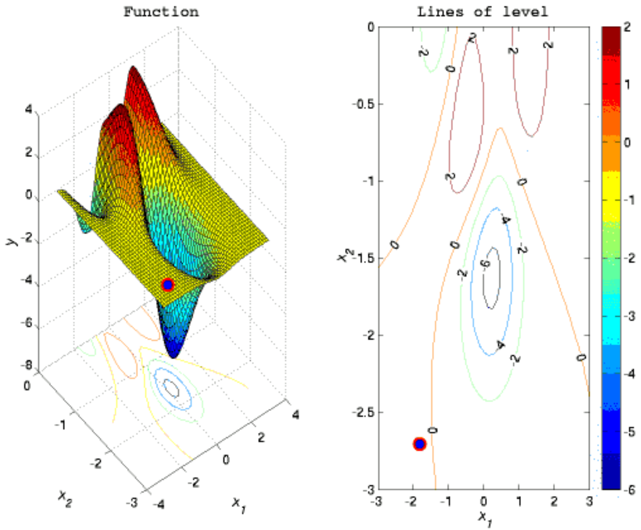
Gradient (or steepest) descent algorithm for SVM

To minimize a cost function $\mathcal{C}(\mathbf{w})$ use the iterative update

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \nabla_{\mathbf{w}} \mathcal{C}(\mathbf{w}_t)$$

where η is the learning rate.





Gradient (or steepest) descent algorithm for SVM

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where η is the learning rate.

First, rewrite the optimization problem as an average

$$\begin{aligned}\min_{\mathbf{w}} \mathcal{C}(\mathbf{w}) &= \frac{\lambda}{2}||\mathbf{w}||^2 + \frac{1}{N}\sum_i^N \max\left(0, 1 - y_i f(\mathbf{x}_i)\right) \\ &= \frac{1}{N}\sum_i^N \left(\frac{\lambda}{2}||\mathbf{w}||^2 + \max\left(0, 1 - y_i f(\mathbf{x}_i)\right)\right)\end{aligned}$$

(with $\lambda = 2/(NC)$ up to an overall scale of the problem) and $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$

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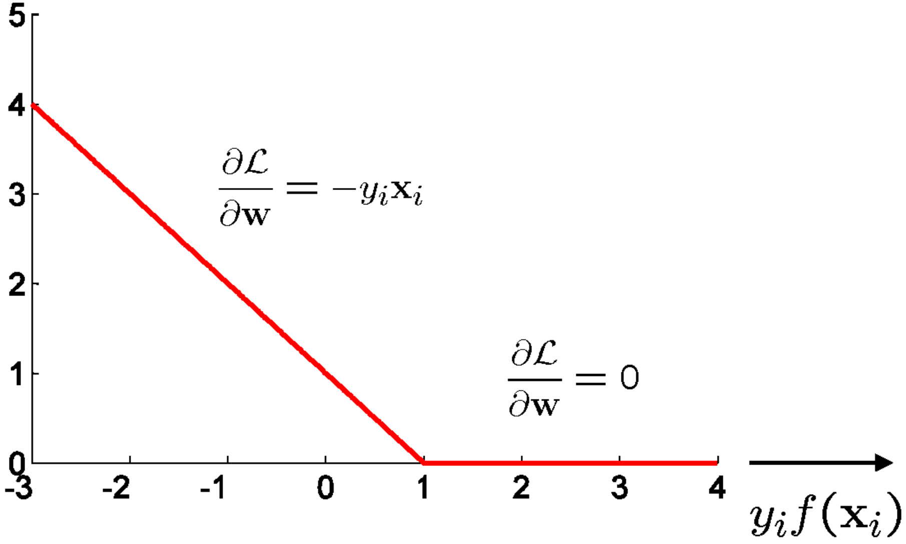
(with $\lambda = 2/(NC)$ up to an overall scale of the problem) and $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$

Because the hinge loss is not differentiable, a sub-gradient is computed

Sub-gradient for hinge loss

$$\mathcal{L}(\mathbf{x}_i, y_i; \mathbf{w}) = \max(0, 1 - y_i f(\mathbf{x}_i)) \qquad f(\mathbf{x}_i) = \mathbf{w}^\top \mathbf{x}_i + b$$



Sub-gradient descent algorithm for SVM

$$\mathcal{C}(\mathbf{w}) = \frac{1}{N}\sum_{i}^{N}\left(\frac{\lambda}{2}||\mathbf{w}||^2 + \mathcal{L}(\mathbf{x}_i, y_i; \mathbf{w})\right)$$

The iterative update is

$$\begin{aligned}\mathbf{w}_{t+1} &\leftarrow \mathbf{w}_t - \eta\nabla_{\mathbf{w}_t}\mathcal{C}(\mathbf{w}_t)\\ &\leftarrow \mathbf{w}_t - \eta\frac{1}{N}\sum_{i}^{N}(\lambda\mathbf{w}_t + \nabla_{\mathbf{w}}\mathcal{L}(\mathbf{x}_i, y_i; \mathbf{w}_t))\end{aligned}$$

where η is the learning rate.

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where η is the learning rate.

Then each iteration t involves cycling through the training data with the updates:

$$\begin{aligned} \mathbf{w}_{t+1} &\leftarrow \mathbf{w}_t - \eta(\lambda \mathbf{w}_t - y_i \mathbf{x}_i) && \text{if } y_i f(\mathbf{x}_i) < 1 \\ &\leftarrow \mathbf{w}_t - \eta \lambda \mathbf{w}_t && \text{otherwise} \end{aligned}$$

In the Pegasos algorithm the learning rate is set at $\eta_t = \frac{1}{\lambda t}$

SVM – review

- We have seen that for an SVM learning a linear classifier

$$f(x) = \mathbf{w}^\top \mathbf{x} + b$$

is formulated as solving an optimization problem over $\mathbf{w}$:

$$\min_{\mathbf{w} \in \mathbb{R}^d} ||\mathbf{w}||^2 + C \sum_i^N \max\left(0, 1 - y_i f(\mathbf{x}_i)\right)$$

- This quadratic optimization problem is known as the primal problem.

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- This quadratic optimization problem is known as the primal problem.

- Instead, the SVM can be formulated to learn a linear classifier

$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

by solving an optimization problem over α_i.

- This is know as the dual problem, and we will look at the advantages of this formulation.

Sketch derivation of dual form

The Representer Theorem states that the solution $\mathbf{w}$ can always be written as a linear combination of the training data:

$$\mathbf{w} = \sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j$$

Now, substitute for $\mathbf{w}$ in $f(x) = \mathbf{w}^\top \mathbf{x} + b$

$$f(x) = \left(\sum_{j=1}^{N} \alpha_j y_j \mathbf{x}_j \right)^\top \mathbf{x} + b = \sum_{j=1}^{N} \alpha_j y_j \left(\mathbf{x}_j{}^\top \mathbf{x} \right) + b$$

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and for $\mathbf{w}$ in the cost function $\min_{\mathbf{w}} ||\mathbf{w}||^2$ subject to $y_i \left(\mathbf{w}^\top \mathbf{x}_i + b \right) \geq 1, \forall i$

$$||\mathbf{w}||^2 = \left\{ \sum_j \alpha_j y_j \mathbf{x}_j \right\}^\top \left\{ \sum_k \alpha_k y_k \mathbf{x}_k \right\} = \sum_{jk} \alpha_j \alpha_k y_j y_k (\mathbf{x}_j{}^\top \mathbf{x}_k)$$

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and for $\mathbf{w}$ in the cost function $\min_{\mathbf{w}} ||\mathbf{w}||^2$ subject to $y_i \left(\mathbf{w}^\top \mathbf{x}_i + b \right) \geq 1, \forall i$

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Hence, an equivalent optimization problem is over α_j

$$\min_{\alpha_j} \sum_{jk} \alpha_j \alpha_k y_j y_k (\mathbf{x}_j{}^\top \mathbf{x}_k) \quad \text{subject to } y_i \left(\sum_{j=1}^{N} \alpha_j y_j (\mathbf{x}_j{}^\top \mathbf{x}_i) + b \right) \geq 1, \forall i$$

Primal and dual formulations

N is number of training points, and d is dimension of feature vector $\mathbf{x}$.

Primal problem: for $\mathbf{w} \in \mathbb{R}^d$

$$\min_{\mathbf{w} \in \mathbb{R}^d} ||\mathbf{w}||^2 + C \sum_i^N \max\left(0, 1 - y_i f(\mathbf{x}_i)\right)$$

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Dual problem: for $\boldsymbol{\alpha} \in \mathbb{R}^N$ (stated without proof):

$$\max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k (\mathbf{x}_j{}^\top \mathbf{x}_k) \text{ subject to } 0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and} \sum_i \alpha_i y_i = 0$$

- Need to learn d parameters for primal, and N for dual

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- Need to learn d parameters for primal, and N for dual
- If $N << d$ then more efficient to solve for α than $\mathbf{w}$
- Dual form only involves $(\mathbf{x}_j{}^\top \mathbf{x}_k)$. We will return to why this is an advantage when we look at kernels.

Primal and dual formulations

Primal version of classifier:

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

Dual version of classifier:

$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

This is a problem !

Primal and dual formulations

Primal version of classifier:

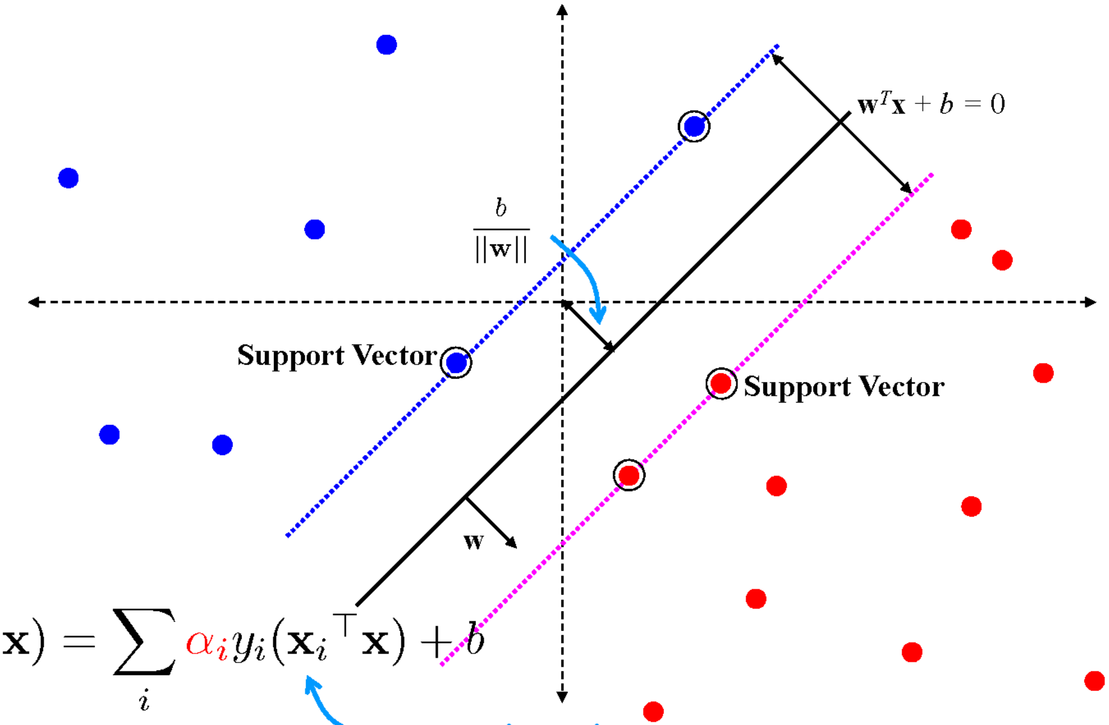
$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

Dual version of classifier:

$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

At first sight the dual form appears to have the disadvantage of a K-NN classifier – it requires the training data points $\mathbf{x}_i$. However, many of the α_i's are zero. The ones that are non-zero define the support vectors $\mathbf{x}_i$.

Support Vector Machine



$$f(\mathbf{x}) = \sum_i {\color{red}\alpha_i} y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

support vectors

Dual Classifier

Classifier:

$$f(\mathbf{x}) \;=\; \sum_{i}^{N} \alpha_i y_i \, \mathbf{x}_i{}^{\top} \mathbf{x} + b$$

$$N$$

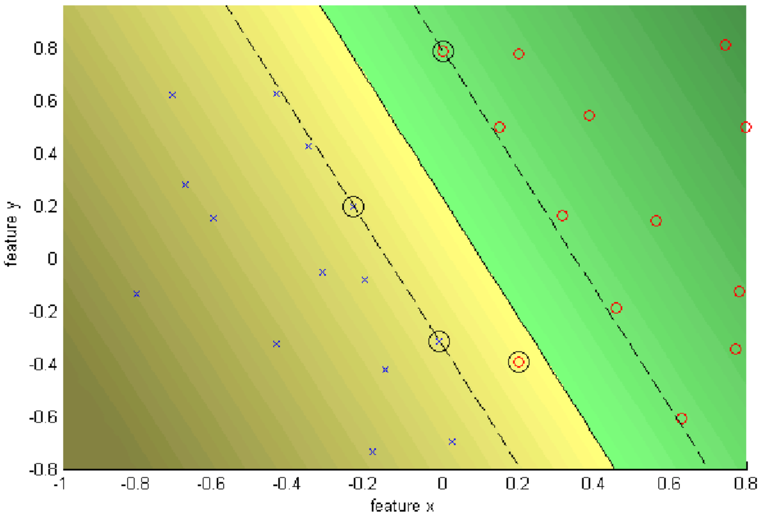
Learning:

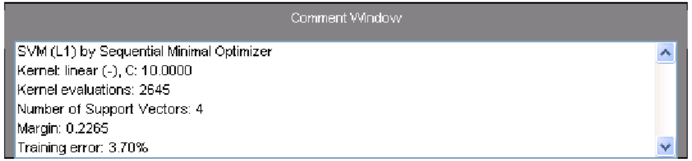
$$\max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k \mathbf{x}_j{}^{\top} \mathbf{x}_k$$

subject to

$$0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and} \sum_i \alpha_i y_i = 0$$

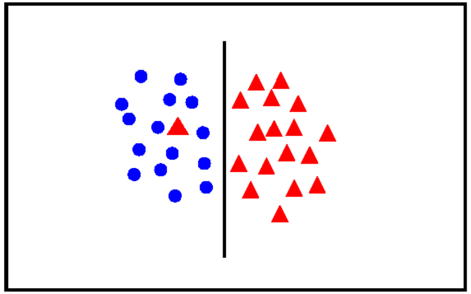
C = 10   soft margin





```
SVM (L1) by Sequential Minimal Optimizer
Kernel: linear (-), C: 10.0000
Kernel evaluations: 2645
Number of Support Vectors: 4
Margin: 0.2265
Training error: 3.70%
```

Handling data that is not linearly separable



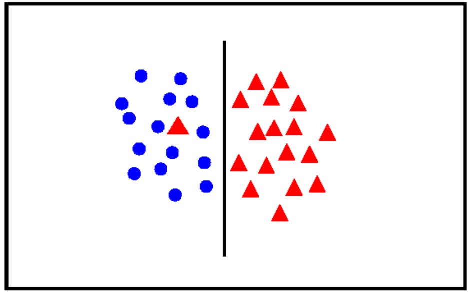
- introduce slack variables

$$\min_{\mathbf{w}\in\mathbb{R}^d, \xi_i \in \mathbb{R}^+} ||\mathbf{w}||^2 + C\sum_i^N \xi_i$$

subject to

$$y_i\left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1 \ldots N$$

Handling data that is not linearly separable



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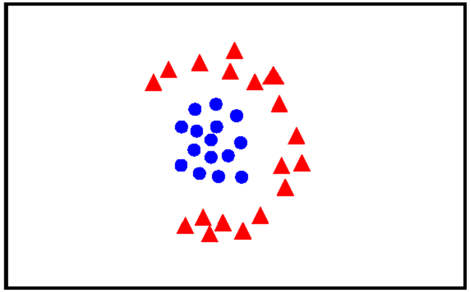
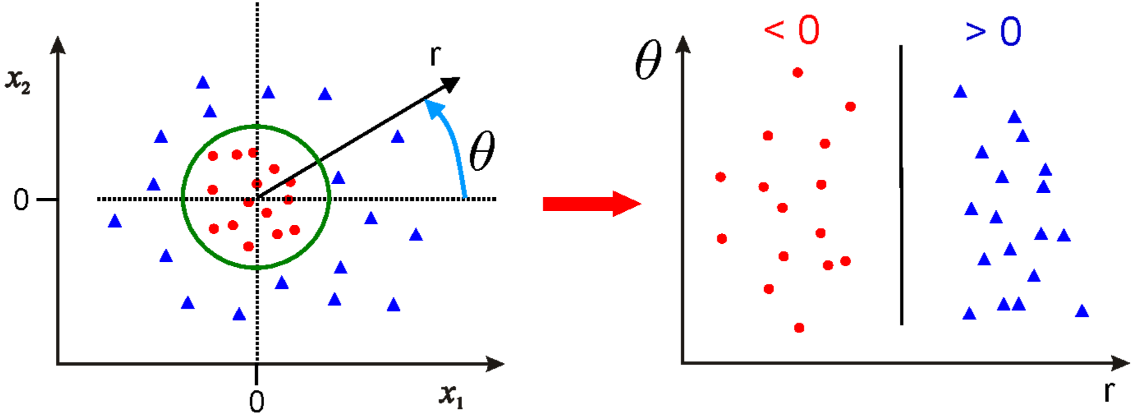


- linear classifier not appropriate

??

Solution 1: use polar coordinates

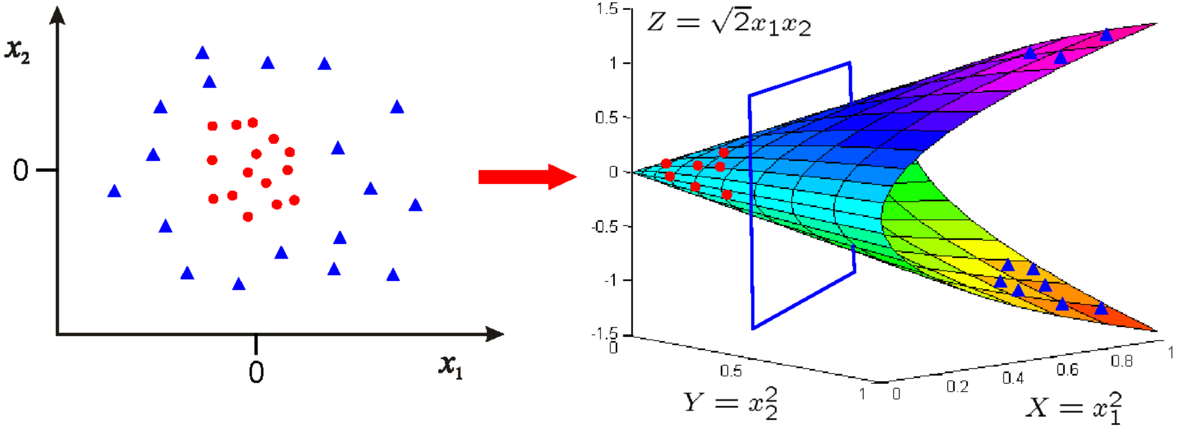


- Data is linearly separable in polar coordinates
- Acts non-linearly in original space

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \to \begin{pmatrix} r \\ \theta \end{pmatrix} \qquad \mathbb{R}^2 \to \mathbb{R}^2$$

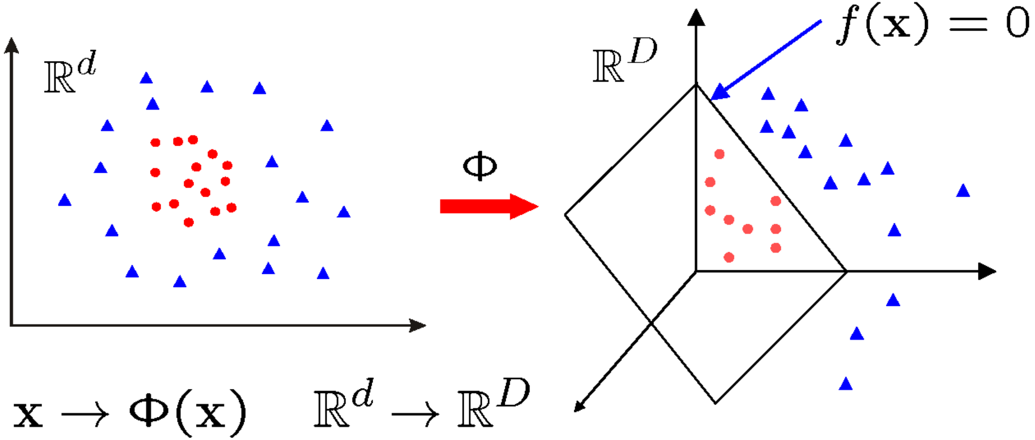
Solution 2: map data to higher dimension

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix} \qquad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$



- Data is linearly separable in 3D
- This means that the problem can still be solved by a linear classifier

SVM classifiers in a transformed feature space



$$\Phi : \mathbf{x} \rightarrow \Phi(\mathbf{x}) \quad \mathbb{R}^d \rightarrow \mathbb{R}^D$$

Learn classifier linear in $\mathbf{w}$ for $\mathbb{R}^D$:

$$f(\mathbf{x}) = \mathbf{w}^\top \Phi(\mathbf{x}) + b$$

$\Phi(\mathbf{x})$ is a feature map

Primal Classifier in transformed feature space

Classifier, with $\mathbf{w} \in \mathbb{R}^D$:

$$f(\mathbf{x}) = \mathbf{w}^\top \Phi(\mathbf{x}) + b$$

Primal Classifier in transformed feature space

Classifier, with $\mathbf{w} \in \mathbb{R}^D$:

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Learning, for $\mathbf{w} \in \mathbb{R}^D$

$$\min_{\mathbf{w} \in \mathbb{R}^D} ||\mathbf{w}||^2 + C \sum_i^N \max\left(0, 1 - y_i f(\mathbf{x}_i)\right)$$

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$$\min_{\mathbf{w} \in \mathbb{R}^D} ||\mathbf{w}||^2 + C \sum_i^N \max\left(0, 1 - y_i f(\mathbf{x}_i)\right)$$

- Simply map $\mathbf{x}$ to $\Phi(\mathbf{x})$ where data is separable
- Solve for $\mathbf{w}$ in high dimensional space $\mathbb{R}^D$

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Learning, for $\mathbf{w} \in \mathbb{R}^D$

$$\min_{\mathbf{w} \in \mathbb{R}^D} ||\mathbf{w}||^2 + C \sum_i^N \max\left(0, 1 - y_i f(\mathbf{x}_i)\right)$$

- Simply map $\mathbf{x}$ to $\Phi(\mathbf{x})$ where data is separable
- Solve for $\mathbf{w}$ in high dimensional space $\mathbb{R}^D$
- If $D >> d$ then there are many more parameters to learn for $\mathbf{w}$. Can this be avoided?

Dual Classifier

Classifier:

$$f(\mathbf{x}) \;=\; \sum_{i}^{N} \alpha_i y_i \, \mathbf{x}_i{}^\top \mathbf{x} + b$$

$$N$$

Learning:

$$\max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k \mathbf{x}_j{}^\top \mathbf{x}_k$$

subject to

$$0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and } \sum_i \alpha_i y_i = 0$$

Dual Classifier in transformed feature space

Classifier:

$$
\begin{aligned}
f(\mathbf{x}) &= \sum_{i}^{N} \alpha_i y_i \, \mathbf{x}_i{}^\top \mathbf{x} + b \\
\rightarrow f(\mathbf{x}) &= \sum_{i}^{N} \alpha_i y_i \, \mathbf{\Phi}(\mathbf{x}_i)^\top \mathbf{\Phi}(\mathbf{x}) + b
\end{aligned}
$$

Learning:

$$
\max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k \mathbf{x}_j{}^\top \mathbf{x}_k
$$

$$
\rightarrow \quad \max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k \mathbf{\Phi}(\mathbf{x}_j)^\top \mathbf{\Phi}(\mathbf{x}_k)
$$

subject to

$$
0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and } \sum_i \alpha_i y_i = 0
$$

Dual Classifier in transformed feature space

- Note, that $\Phi(\mathbf{x})$ only occurs in pairs $\Phi(\mathbf{x}_j)^\top \Phi(\mathbf{x}_i)$
- Once the scalar products are computed, only the N dimensional vector $\boldsymbol{\alpha}$ needs to be learnt; it is not necessary to learn in the D dimensional space, as it is for the primal
- Write $k(\mathbf{x}_j, \mathbf{x}_i) = \Phi(\mathbf{x}_j)^\top \Phi(\mathbf{x}_i)$. This is known as a Kernel

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Classifier:

$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i \, k(\mathbf{x}_i, \mathbf{x}) + b$$

Dual Classifier in transformed feature space

- Note, that $\Phi(\mathbf{x})$ only occurs in pairs $\Phi(\mathbf{x}_j)^\top \Phi(\mathbf{x}_i)$
- Once the scalar products are computed, only the N dimensional vector $\boldsymbol{\alpha}$ needs to be learnt; it is not necessary to learn in the D dimensional space, as it is for the primal
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Classifier:

$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i \, k(\mathbf{x}_i, \mathbf{x}) + b$$

Learning:

$$\max_{\alpha_i \geq 0} \sum_i \alpha_i - \frac{1}{2} \sum_{jk} \alpha_j \alpha_k y_j y_k \, k(\mathbf{x}_j, \mathbf{x}_k)$$

subject to

$$0 \leq \alpha_i \leq C \text{ for } \forall i, \text{ and} \sum_i \alpha_i y_i = 0$$

Special transformations

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \to \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix} \qquad \mathbb{R}^2 \to \mathbb{R}^3$$

$$\begin{aligned} \Phi(\mathbf{x})^\top \Phi(\mathbf{z}) &= \left(x_1^2, x_2^2, \sqrt{2}x_1x_2\right) \begin{pmatrix} z_1^2 \\ z_2^2 \\ \sqrt{2}z_1z_2 \end{pmatrix} \\ &= x_1^2z_1^2 + x_2^2z_2^2 + 2x_1x_2z_1z_2 \\ &= (x_1z_1 + x_2z_2)^2 \\ &= (\mathbf{x}^\top\mathbf{z})^2 \end{aligned}$$

Special transformations

$$\Phi : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1 x_2 \end{pmatrix} \qquad \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

$$\begin{aligned} \Phi(\mathbf{x})^\top \Phi(\mathbf{z}) &= \left(x_1^2, x_2^2, \sqrt{2}x_1 x_2\right) \begin{pmatrix} z_1^2 \\ z_2^2 \\ \sqrt{2}z_1 z_2 \end{pmatrix} \\ &= x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1 x_2 z_1 z_2 \\ &= (x_1 z_1 + x_2 z_2)^2 \\ &= (\mathbf{x}^\top \mathbf{z})^2 \end{aligned}$$

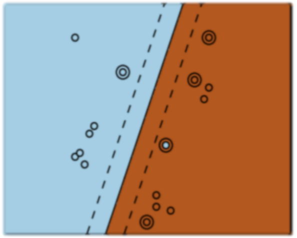
Kernel Trick

- Classifier can be learnt and applied without explicitly computing $\Phi(\mathbf{x})$
- All that is required is the kernel $k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z})^2$
- Complexity of learning depends on N not on D

Example kernels

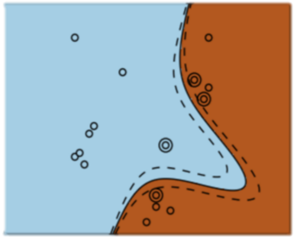
- Linear kernels $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{x}'$
- Polynomial kernels $k(\mathbf{x}, \mathbf{x}') = \left(1 + \mathbf{x}^\top \mathbf{x}'\right)^d$ for any $d > 0$
  - Contains all polynomials terms up to degree d
- Gaussian kernels $k(\mathbf{x}, \mathbf{x}') = \exp\left(-||\mathbf{x} - \mathbf{x}'||^2 / 2\sigma^2\right)$ for $\sigma > 0$
  - Infinite dimensional feature space

Linear Kernel



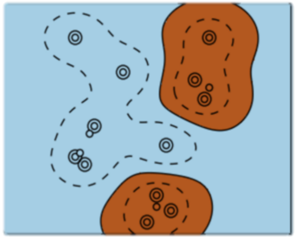
C hyperparameter

Polynomial Kernel



C plus gamma, degree and coefficient hyperparameters

RBF Kernel



C plus gamma hyperparameter

SVM classifier with Gaussian kernel

N = size of training data

$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}) + b$$

weight (may be zero)

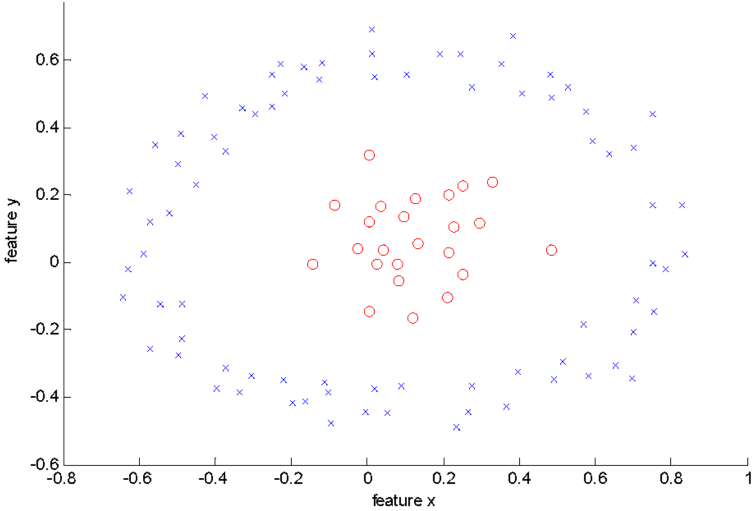
support vector

Gaussian kernel $k(\mathbf{x}, \mathbf{x}') = \exp\left(-||\mathbf{x} - \mathbf{x}'||^2/2\sigma^2\right)$

Radial Basis Function (RBF) SVM

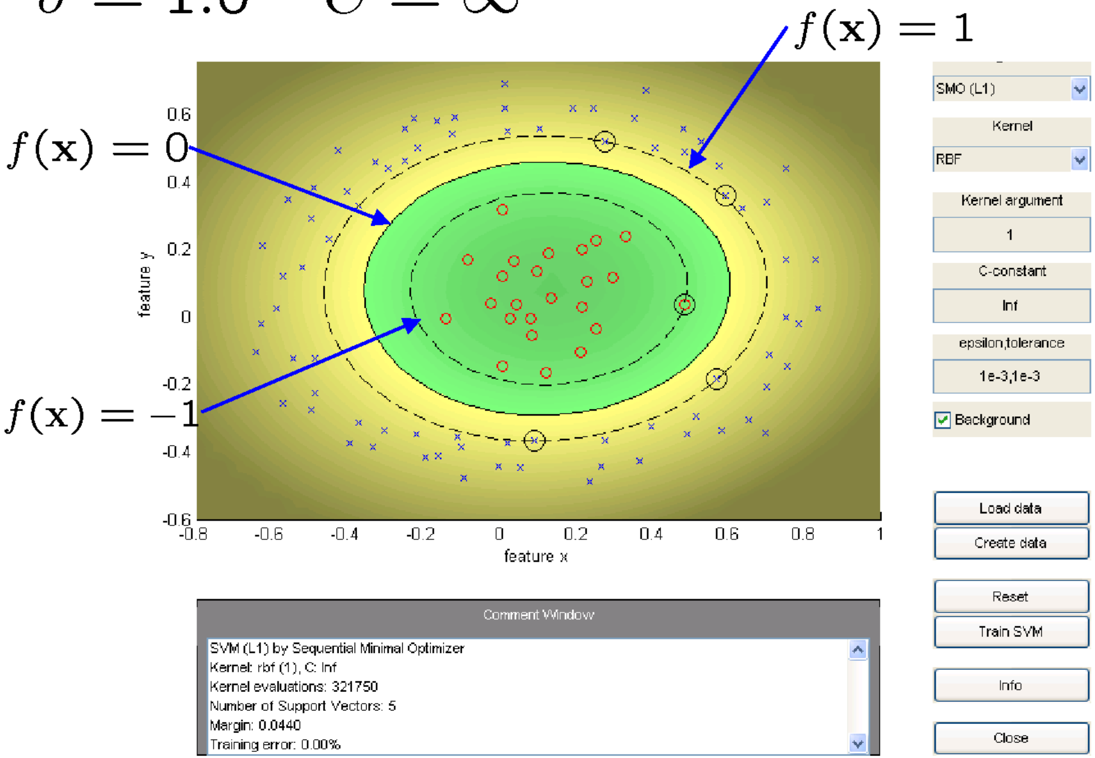
$$f(\mathbf{x}) = \sum_i^N \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2/2\sigma^2\right) + b$$

RBF Kernel SVM Example



- data is not linearly separable in original feature space

$$\sigma = 1.0 \quad C = \infty$$



$f(\mathbf{x}) = 1$

$f(\mathbf{x}) = 0$

$f(\mathbf{x}) = -1$

SMO (L1)

Kernel: RBF

Kernel argument: 1

C-constant: Inf

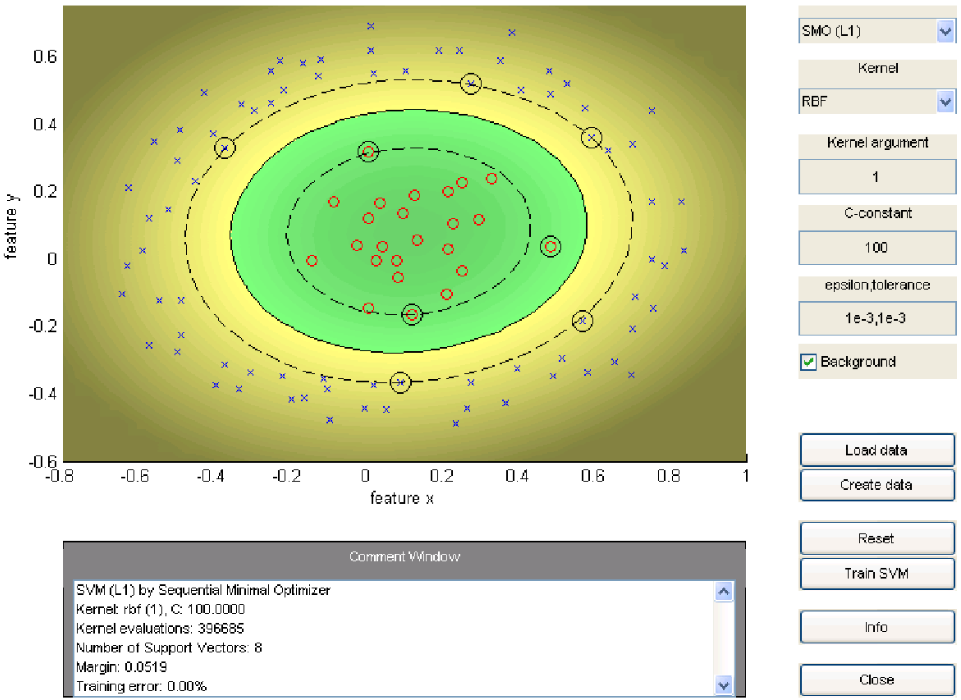
epsilon,tolerance: 1e-3,1e-3

☑ Background

```
SVM (L1) by Sequential Minimal Optimizer
Kernel: rbf (1), C: Inf
Kernel evaluations: 321750
Number of Support Vectors: 5
Margin: 0.0440
Training error: 0.00%
```

$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2 / 2\sigma^2\right) + b$$

$$\sigma = 1.0 \quad C = 100$$



SMO (L1)

Kernel: RBF

Kernel argument: 1

C-constant: 100

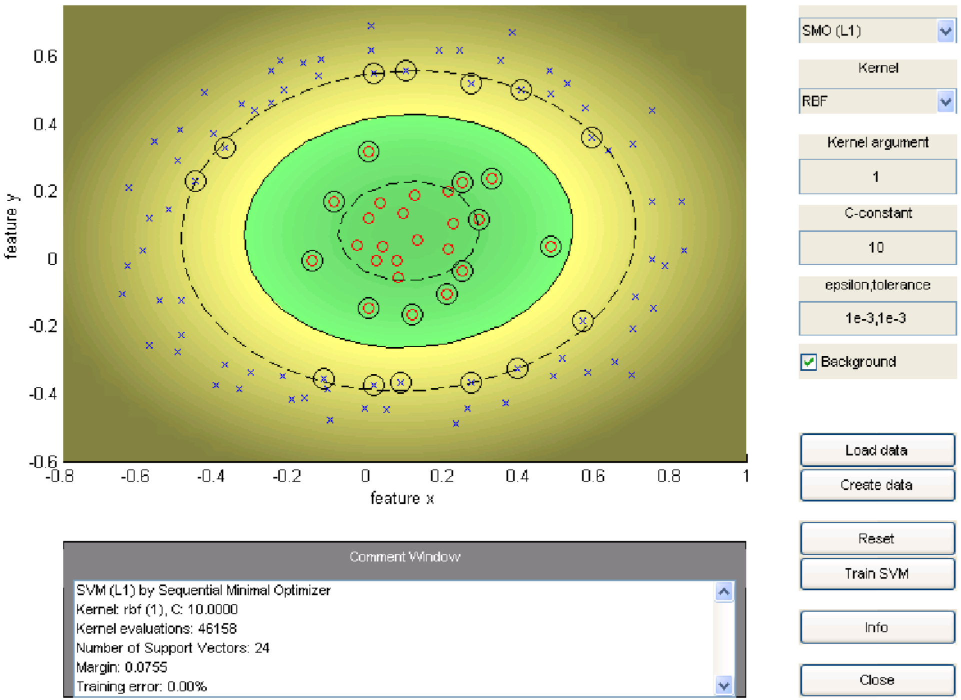
epsilon,tolerance: 1e-3,1e-3

☑ Background

```
SVM (L1) by Sequential Minimal Optimizer
Kernel: rbf (1), C: 100.0000
Kernel evaluations: 396685
Number of Support Vectors: 8
Margin: 0.0519
Training error: 0.00%
```

Decrease C, gives wider (soft) margin

$$\sigma = 1.0 \quad C = 10$$



SMO (L1)

Kernel: RBF

Kernel argument: 1

C-constant: 10

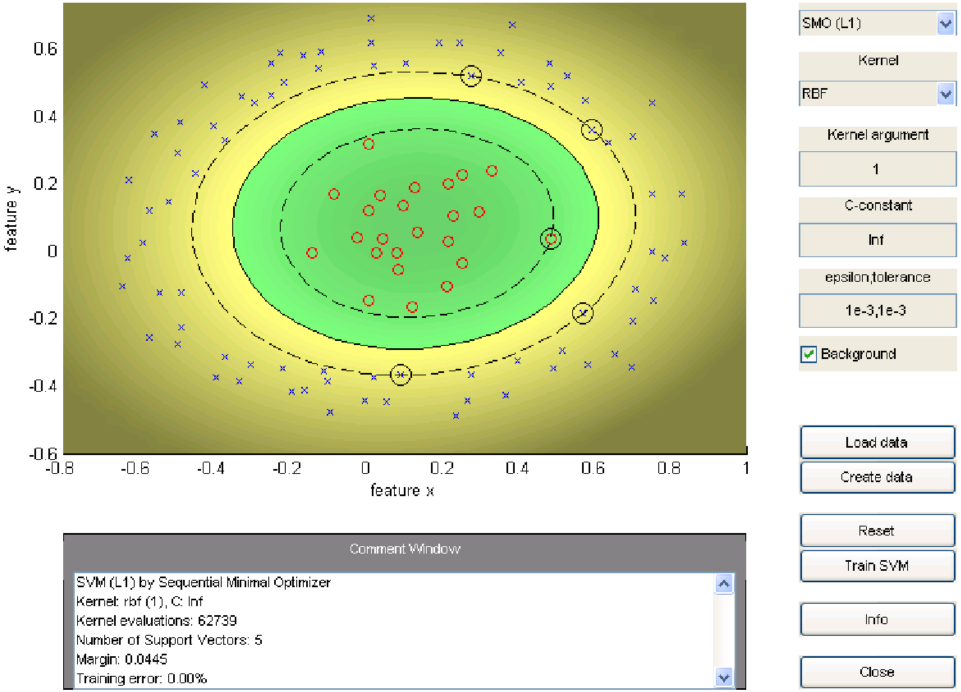
epsilon,tolerance: 1e-3,1e-3

☑ Background

```
SVM (L1) by Sequential Minimal Optimizer
Kernel: rbf (1), C: 10.0000
Kernel evaluations: 46158
Number of Support Vectors: 24
Margin: 0.0755
Training error: 0.00%
```

$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2 / 2\sigma^2\right) + b$$

$$\sigma = 1.0 \quad C = \infty$$



SMO (L1)

Kernel: RBF

Kernel argument: 1

C-constant: Inf

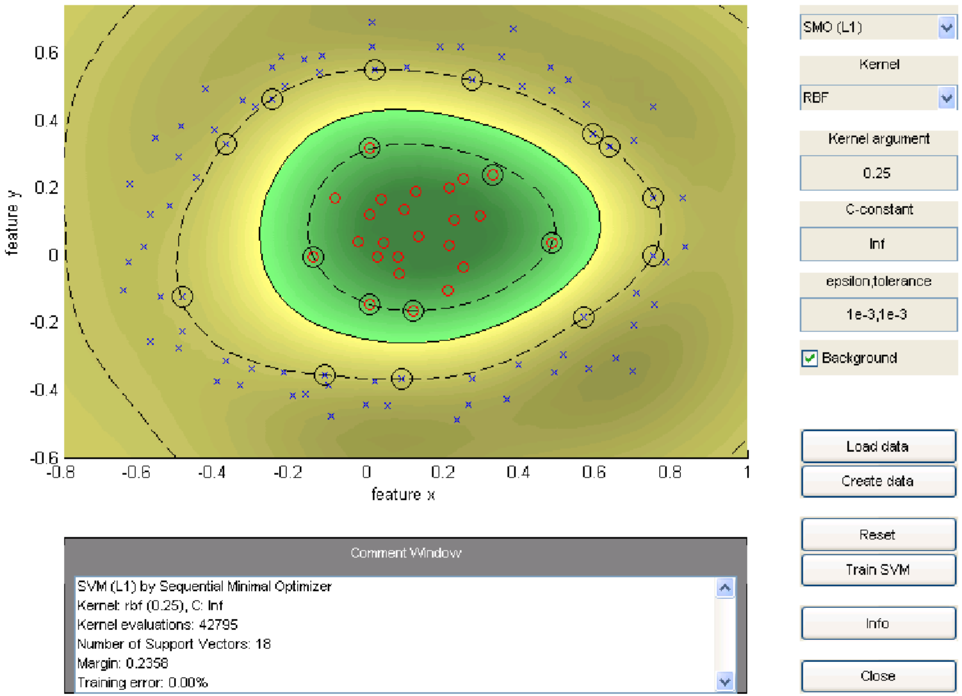
epsilon,tolerance: 1e-3,1e-3

☑ Background

```
SVM (L1) by Sequential Minimal Optimizer
Kernel: rbf (1), C: Inf
Kernel evaluations: 62739
Number of Support Vectors: 5
Margin: 0.0445
Training error: 0.00%
```

$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2 / 2\sigma^2\right) + b$$

$\sigma = 0.25 \quad C = \infty$



SMO (L1)

Kernel

RBF

Kernel argument

0.25

C-constant

Inf

epsilon,tolerance

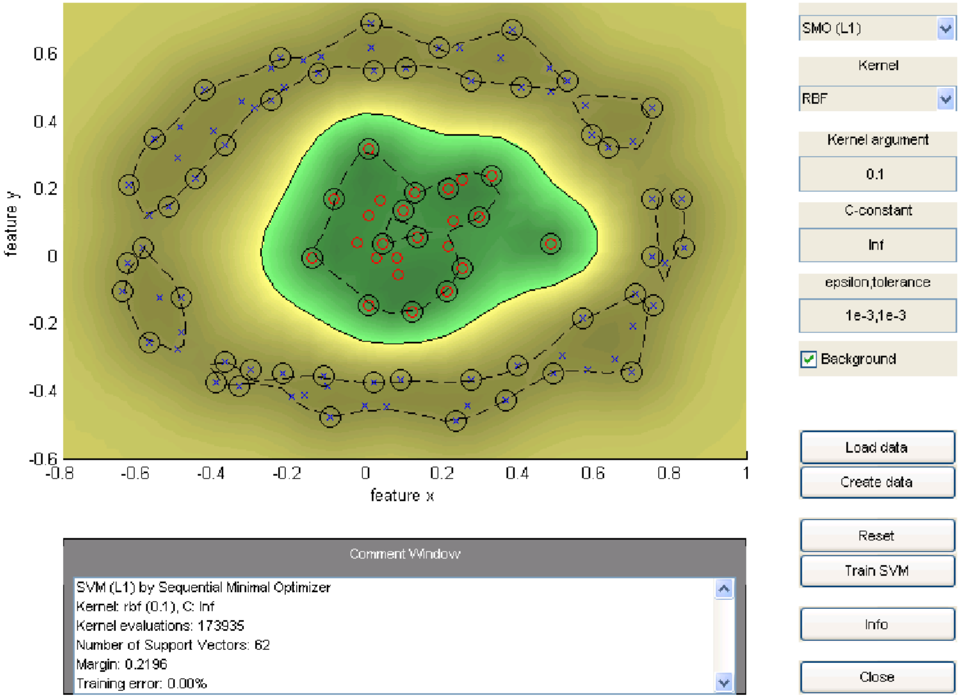
1e-3,1e-3

☑ Background

```
SVM (L1) by Sequential Minimal Optimizer
Kernel: rbf (0.25), C: Inf
Kernel evaluations: 42795
Number of Support Vectors: 18
Margin: 0.2358
Training error: 0.00%
```

Decrease sigma, moves towards nearest neighbour classifier

$$\sigma = 0.1 \quad C = \infty$$



SMO (L1)

Kernel: RBF

Kernel argument: 0.1

C-constant: Inf

epsilon,tolerance: 1e-3,1e-3

☑ Background

```
SVM (L1) by Sequential Minimal Optimizer
Kernel: rbf (0.1), C: Inf
Kernel evaluations: 173935
Number of Support Vectors: 62
Margin: 0.2196
Training error: 0.00%
```

$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_i y_i \exp\left(-||\mathbf{x} - \mathbf{x}_i||^2 / 2\sigma^2\right) + b$$

Kernel Trick - Summary

- Classifiers can be learnt for high dimensional features spaces, without actually having to map the points into the high dimensional space

- Data may be linearly separable in the high dimensional space, but not linearly separable in the original feature space

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- Classifiers can be learnt for high dimensional features spaces, without actually having to map the points into the high dimensional space

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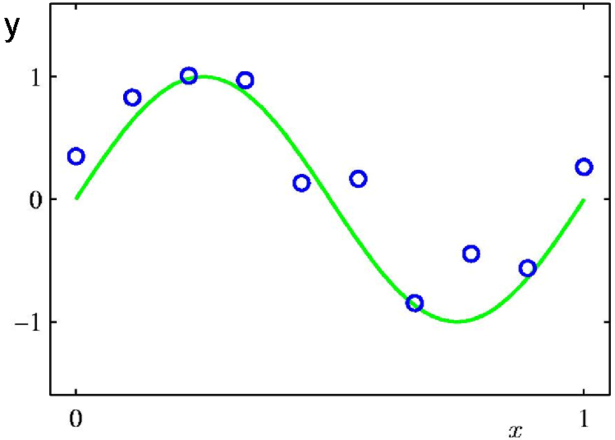
- Kernels apply also to objects that are not vectors, e.g.

$$k(h, h') = \sum_k \min(h_k, h'_k) \text{ for histograms with bins } h_k, h'_k$$

Regression



- Suppose we are given a training set of N observations

$$((\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)) \text{ with } \mathbf{x}_i \in \mathbb{R}^d, y_i \in \mathbb{R}$$

- The regression problem is to estimate $f(\mathbf{x})$ from this data such that

$$y_i = f(\mathbf{x}_i)$$

Learning by optimization

- As in the case of classification, learning a regressor can be formulated as an optimization:

Minimize with respect to $f \in \mathcal{F}$

$$\sum_{i=1}^{N} \underbrace{l\left(f(\mathbf{x}_i), y_i\right)}_{\text{loss function}}$$

Choice of regression function – non-linear basis functions

- Function for regression $y(\mathbf{x}, \mathbf{w})$ is a non-linear function of $\mathbf{x}$, but linear in $\mathbf{w}$:

$$f(\mathbf{x}, \mathbf{w}) = w_0 + w_1\phi_1(\mathbf{x}) + w_2\phi_2(\mathbf{x}) + \ldots + w_M\phi_M(\mathbf{x}) = \mathbf{w}^\top\Phi(\mathbf{x})$$

- For example, for $x \in \mathbb{R}$, polynomial regression with $\phi_j(x) = x^j$:

$$f(x, \mathbf{w}) = w_0 + w_1\phi_1(\mathbf{x}) + w_2\phi_2(\mathbf{x}) + \ldots + w_M\phi_M(\mathbf{x}) = \sum_{j=0}^{M} w_j x^j$$

e.g. for $M = 3$,

$$f(x, \mathbf{w}) = (w_0, w_1, w_2, w_3)\begin{pmatrix} 1 \\ x \\ x^2 \\ x^3 \end{pmatrix} = \mathbf{w}^\top\Phi(x)$$

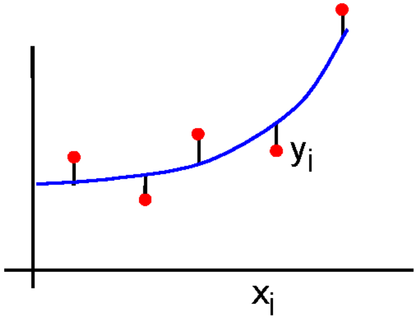
$$\Phi : x \rightarrow \Phi(x) \quad \mathbb{R}^1 \rightarrow \mathbb{R}^4$$

Least squares regression”

- Cost function – squared loss:

target value

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N} \underbrace{\{f(x_i, \mathbf{w}) - y_i\}^2}_{\text{loss function}}$$



- Regression function for x (1D):

$$f(\mathbf{x}, \mathbf{w}) = w_0 + w_1\phi_1(\mathbf{x}) + w_2\phi_2(\mathbf{x}) + \ldots + w_M\phi_M(\mathbf{x}) = \mathbf{w}^\top \Phi(\mathbf{x})$$

Solving for the weights w

Notation: write the target and regressed values as N-vectors

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ . \\ . \\ y_N \end{pmatrix} \qquad \mathbf{f} = \begin{pmatrix} \Phi(x_1)^\top \mathbf{w} \\ \Phi(x_2)^\top \mathbf{w} \\ . \\ . \\ \Phi(x_N)^\top \mathbf{w} \end{pmatrix} = \boldsymbol{\Phi}\mathbf{w} = \begin{bmatrix} 1 & \phi_1(x_1) & \dots & \phi_M(x_1) \\ 1 & \phi_1(x_2) & \dots & \phi_M(x_2) \\ . & & & . \\ . & & & . \\ 1 & \phi_1(x_N) & \dots & \phi_M(x_N) \end{bmatrix} \begin{pmatrix} w_0 \\ w_1 \\ . \\ . \\ w_M \end{pmatrix}$$

$\boldsymbol{\Phi}$ is an $N \times M$ design matrix

e.g. for polynomial regression with basis functions up to x^2

$$\boldsymbol{\Phi}\mathbf{w} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ . & & . \\ . & & . \\ 1 & x_N & x_N^2 \end{bmatrix} \begin{pmatrix} w_0 \\ w_1 \\ w_2 \end{pmatrix}$$

$$\begin{aligned}\widetilde{E}(\mathbf{w}) &= \frac{1}{2}\sum_{i=1}^{N}\{f(x_i,\mathbf{w})-y_i\}^2+\frac{\lambda}{2}\|\mathbf{w}\|^2\\ &= \frac{1}{2}\sum_{i=1}^{N}\left(y_i-\mathbf{w}^\top\boldsymbol{\Phi}(x_i)\right)^2+\frac{\lambda}{2}\|\mathbf{w}\|^2\\ &= \frac{1}{2}(\mathbf{y}-\boldsymbol{\Phi}\mathbf{w})^2+\frac{\lambda}{2}\|\mathbf{w}\|^2\end{aligned}$$

$$\begin{aligned}
\widetilde{E}(\mathbf{w}) &= \frac{1}{2}\sum_{i=1}^{N}\{f(x_i,\mathbf{w}) - y_i\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2 \\
&= \frac{1}{2}\sum_{i=1}^{N}\left(y_i - \mathbf{w}^\top \mathbf{\Phi}(x_i)\right)^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2 \\
&= \frac{1}{2}(\mathbf{y} - \Phi\mathbf{w})^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2
\end{aligned}$$

Now, compute where derivative w.r.t. $\mathbf{w}$ is zero for minimum

$$\frac{\widetilde{E}(\mathbf{w})}{d\mathbf{w}} = -\mathbf{\Phi}^\top(\mathbf{y} - \Phi\mathbf{w}) + \lambda\mathbf{w} = \mathbf{0}$$

Hence

$$\left(\mathbf{\Phi}^\top\mathbf{\Phi} + \lambda\mathtt{I}\right)\mathbf{w} = \mathbf{\Phi}^\top\mathbf{y}$$

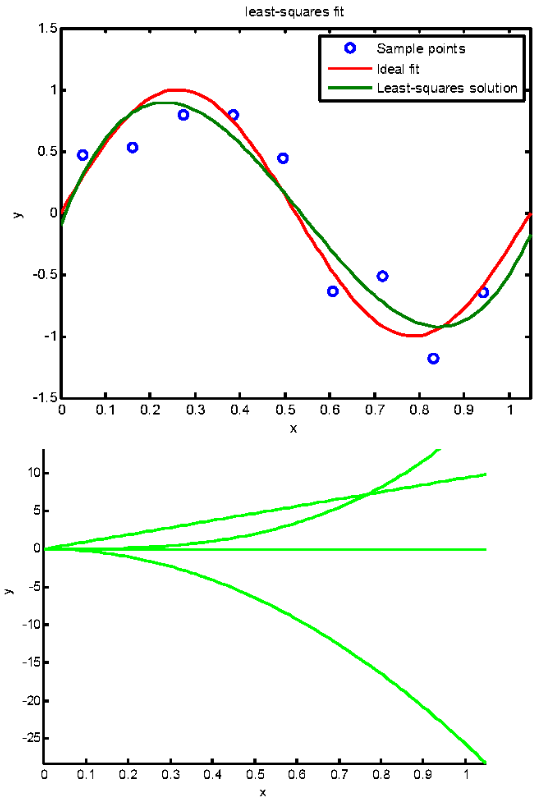
$$\mathbf{w} = \left(\mathbf{\Phi}^\top\mathbf{\Phi} + \lambda\mathtt{I}\right)^{-1}\mathbf{\Phi}^\top\mathbf{y}$$

$$\mathbf{w} = \left(\mathbf{\Phi}^\top \mathbf{\Phi} + \lambda \mathtt{I}\right)^{-1} \mathbf{\Phi}^\top \mathbf{y}$$

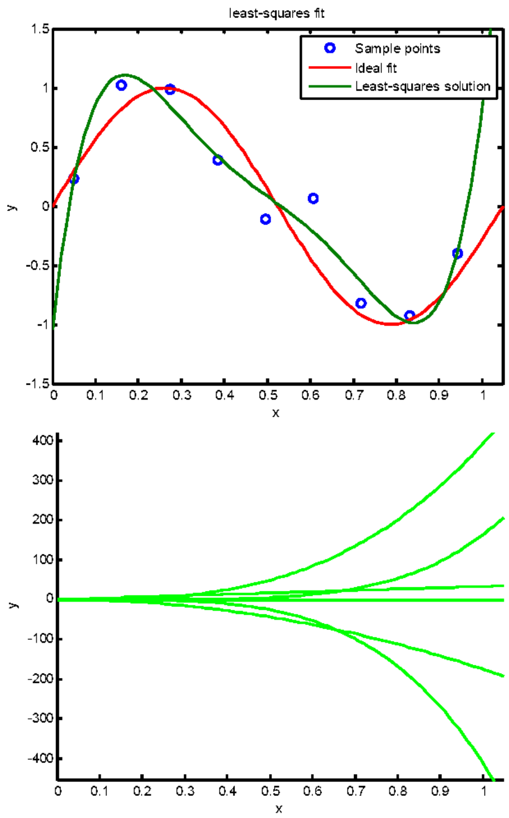
$$\begin{aligned} f(x, \mathbf{w}) &= \mathbf{w}^\top \Phi(x) = \Phi(x)^\top \mathbf{w} \\ &= \Phi(x)^\top \left(\mathbf{\Phi}^\top \mathbf{\Phi} + \lambda \mathtt{I}\right)^{-1} \mathbf{\Phi}^\top \mathbf{y} \\ &= \mathbf{b}(x)^\top \mathbf{y} \end{aligned}$$

Output is a linear blend, $\mathbf{b}(x)$, of the training values $\{y_i\}$

M = 3


least-squares fit
Sample points
Ideal fit
Least-squares solution
1.5
1
0.5
0
-0.5
-1
-1.5
y
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x
10
5
0
-5
-10
-15
-20
-25
y
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x

M = 5


least-squares fit
Sample points
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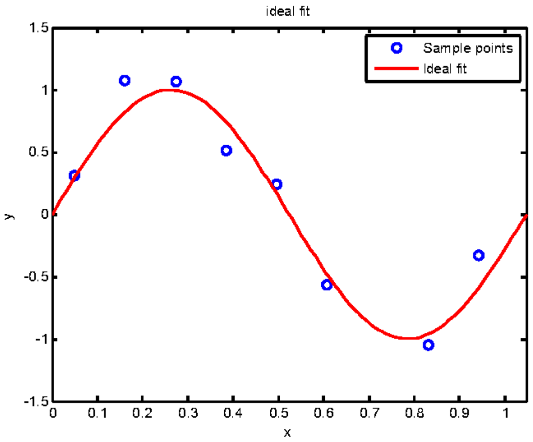
1.5
1
0.5
0
-0.5
-1
-1.5
y
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x
400
300
200
100
0
-100
-200
-300
-400
y
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x

Example 2: Gaussian basis functions

- The red curve is the true function (which is not a polynomial)
- The data points are samples from the curve with added noise in y.

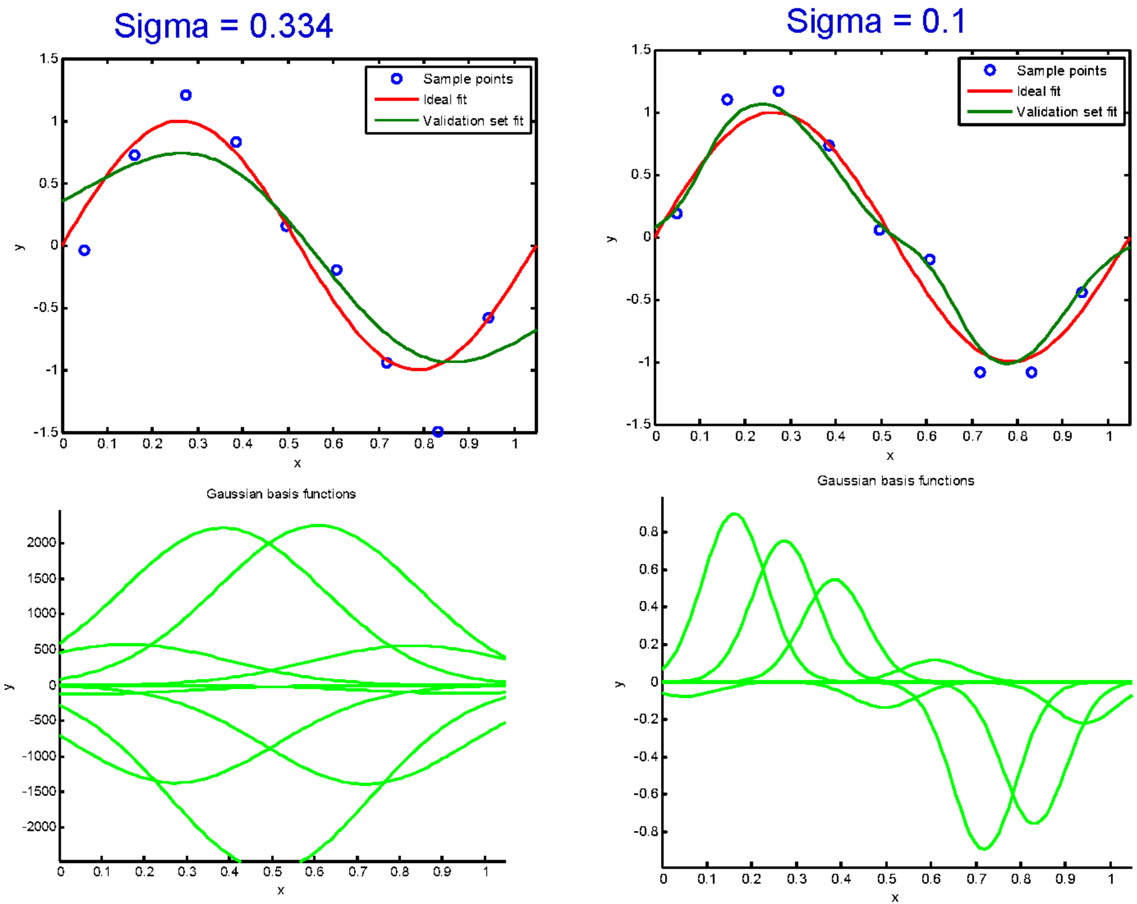
- Basis functions are centred on the training data (N points)



$$f(x, \mathbf{w}) = \sum_{i=1}^{N} w_i e^{-(x-x_i)^2/\sigma^2} = \mathbf{w}^\top \Phi(x) \qquad \Phi : x \to \Phi(x) \quad \mathbb{R} \to \mathbb{R}^N$$

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} \{f(x_i, \mathbf{w}) - y_i\}^2$$

w is a N-vector



Sigma = 0.334

Sigma = 0.1

Kernel Trick – other uses

- Kernel PCA
- Kernel K-NN
- ….

Multiclass SVM (Intuition)

- Recall: Binary SVM
  - Maximize margin
  - Equivalently,

    Minimize norm of weights such that the closest points to the hyperplane have a score §1

- Multiclass SVM
  - Each label has a different weight vector (like one-vs-all)
  - Maximize multiclass margin
  - Equivalently,

    Minimize total norm of the weights such that the true label is scored at least 1 more than the second best one

Multiclass SVM in the separable case

Recall hard binary SVM

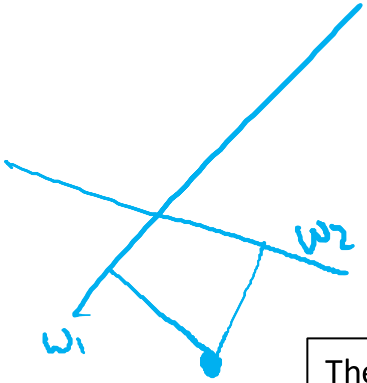
$$\begin{aligned} \min_{\mathbf{w}} \quad & \frac{1}{2}\mathbf{w}^T\mathbf{w} \\ \text{s.t.} \forall i, \quad & y_i \mathbf{w}^T \mathbf{x}_i \geq 1 \end{aligned}$$

Size of the weights.
Effectively, regularizer

$$\begin{aligned} \min_{\mathbf{w}_1, \mathbf{w}_2, \cdots, \mathbf{w}_K} \quad & \overline{\frac{1}{2}\sum_k \mathbf{w}_k^T \mathbf{w}_k} \\ \text{s.t.} \quad & \underline{\mathbf{w}_{\mathbf{y}_i}^T \mathbf{x} - \mathbf{w}_k^T \mathbf{x} \geq 1} \qquad \forall (\mathbf{x}_i, \mathbf{y}_i) \in D, \\ & \qquad\qquad\qquad\qquad\quad k \in \{1, 2, \cdots, K\}, k \neq \mathbf{y}_i, \end{aligned}$$

The score for the true label is higher
than the score for ***any*** other label by 1

Multiclass SVM: General case



Size of the weights. Effectively, regularizer

Total slack. Effectively, don't allow too many examples to violate the margin constraint

$$
\begin{aligned}
\min_{\mathbf{w}_1,\mathbf{w}_2,\cdots,\mathbf{w}_K,\xi} \quad & \frac{1}{2}\sum_k \mathbf{w}_k^T\mathbf{w}_k + C\sum_{(\mathbf{x}_i,\mathbf{y}_i)\in D}\xi_i \\
\text{s.t.} \quad & \mathbf{w}_{\mathbf{y}_i}^T\mathbf{x} - \mathbf{w}_k^T\mathbf{x} \geq 1-\xi_i, \qquad \forall(\mathbf{x}_i,\mathbf{y}_i)\in D, \\
& \qquad\qquad k\in\{1,2,\cdots,K\}, k\neq \mathbf{y}_i, \\
& \xi_i \geq 0, \qquad \forall i.
\end{aligned}
$$

The score for the true label is higher than the score for ***any*** other label by $1-\xi_i$

Slack variables. Not all examples need to satisfy the margin constraint.

Slack variables can only be positive

Multiclass SVM: Summary

- Training:
  - Optimize the SVM objective

- Prediction:
  - Winner takes all

    $\text{argmax}_i\ \mathbf{w}_i^T\mathbf{x}$

Advantages and Disadvantages of SVM

- Advantages
  - prediction accuracy is generally high
  - robust, works when training examples contain errors
  - fast evaluation of the learned target function
- Criticism
  - long training time
  - difficult to understand the learned function (weights)
  - not easy to incorporate domain knowledge

References

- Idiot’s Guide to SVM: http://web.mit.edu/6.034/wwwbob/svm-notes-long-08.pdf
- https://www.svm-tutorial.com/2015/06/svm-understanding-math-part-3/
- [PRML] Bishop, Ch 6-7
- Examples with scikit-learn
  - https://jakevdp.github.io/PythonDataScienceHandbook/05.07-support-vector-machines.html
  - https://stackabuse.com/implementing-svm-and-kernel-svm-with-pythons-scikit-learn/