Lecture 3: SVM dual, kernels and regression

C19 Machine Learning

Hilary 2015

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- Primal and dual forms
- Linear separability revisted
- Feature maps
- Kernels for SVMs
- Regression
 - Ridge regression
 - Basis functions

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 ${\bf w}$:

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

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

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

Proof: see example sheet.

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

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

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

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

Hence, an equivalent optimization problem is over α_i

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

and a few more steps are required to complete the derivation.

Primal and dual formulations

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

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

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

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

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

- ullet Need to learn d parameters for primal, and N for dual
- If N << d then more efficient to solve for α than 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:

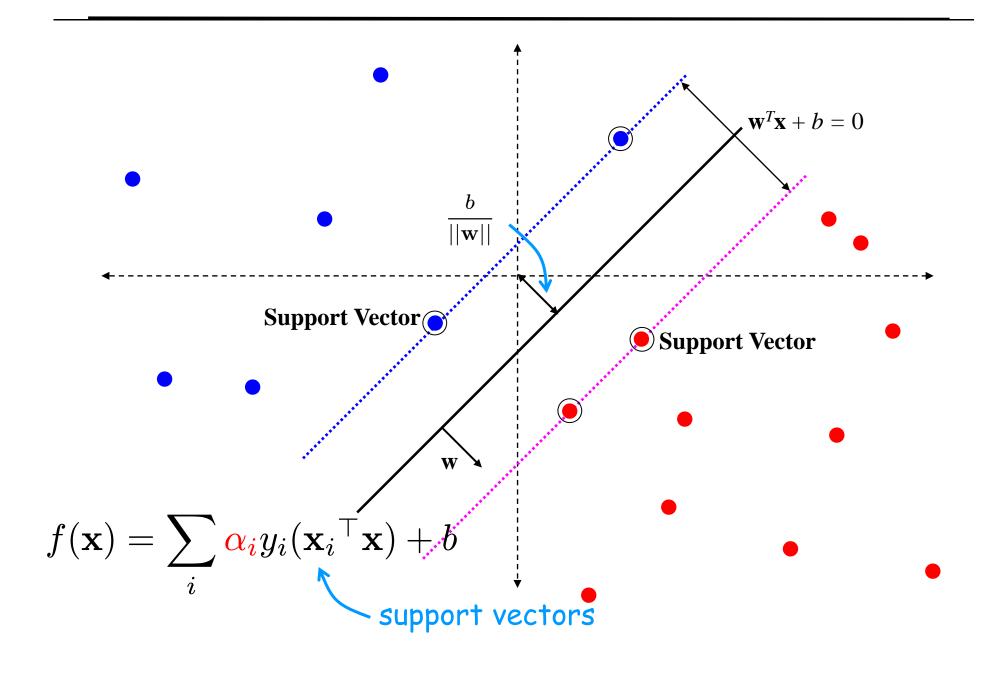
$$f(\mathbf{x}) = \mathbf{w}^{\top} \mathbf{x} + b$$

Dual version of classifier:

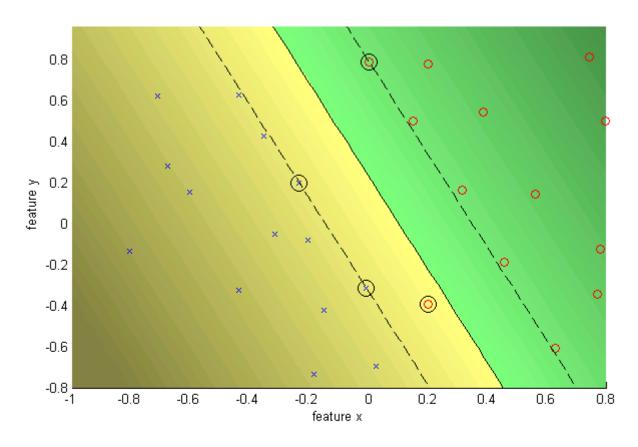
$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_{i} y_{i}(\mathbf{x}_{i}^{\top} \mathbf{x}) + b$$

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

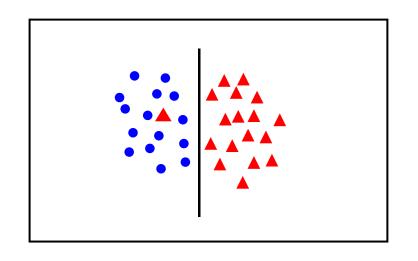


C = 10 soft margin





Handling data that is not linearly separable

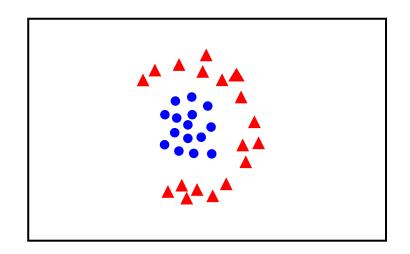


• introduce slack variables

$$\min_{\mathbf{w} \in \mathbb{R}^d, \xi_i \in \mathbb{R}^+} ||\mathbf{w}||^2 + C \sum_{i=1}^N \xi_i$$

subject to

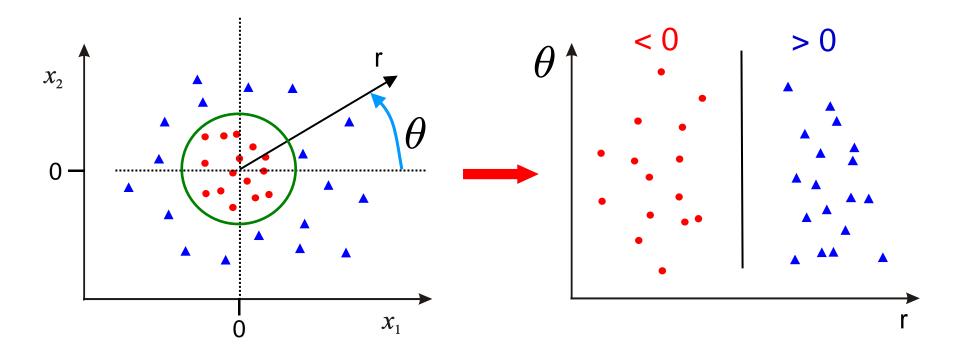
$$y_i\left(\mathbf{w}^{\top}\mathbf{x}_i + b\right) \geq 1 - \xi_i \text{ for } i = 1 \dots N$$



• linear classifier not appropriate

??

Solution 1: use polar coordinates

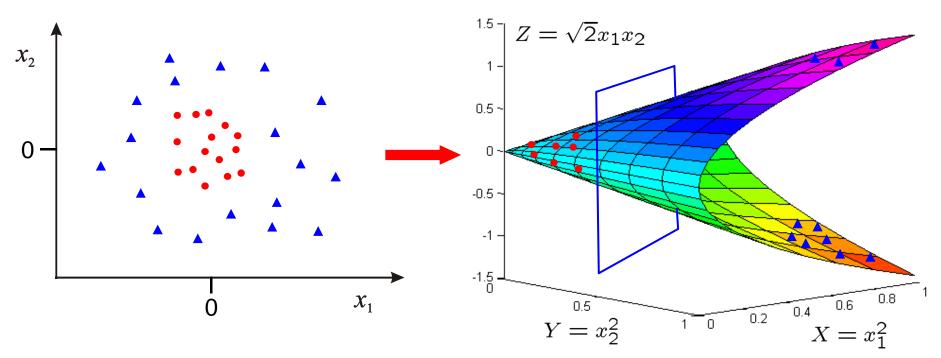


- Data is linearly separable in polar coordinates
- Acts non-linearly in original space

$$\Phi: \left(\begin{array}{c} x_1 \\ x_2 \end{array}\right) \to \left(\begin{array}{c} r \\ \theta \end{array}\right) \quad \mathbb{R}^2 \to \mathbb{R}^2$$

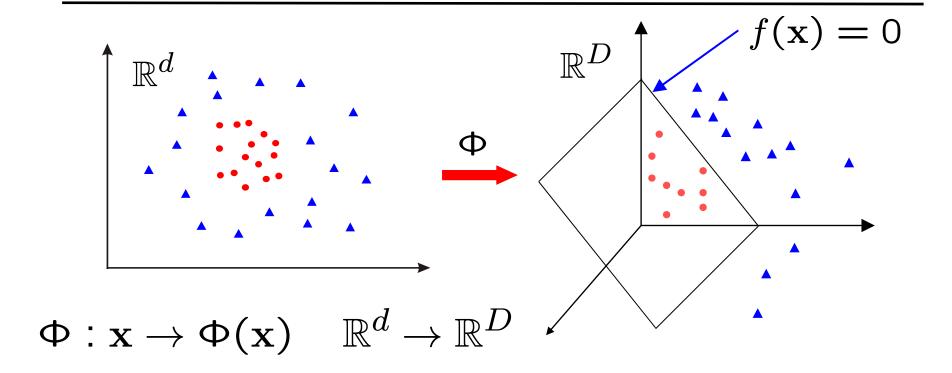
Solution 2: map data to higher dimension

$$\Phi: \left(\begin{array}{c} x_1 \\ x_2 \end{array}\right) \to \left(\begin{array}{c} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{array}\right) \quad \mathbb{R}^2 \to \mathbb{R}^3$$



- 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



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

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

 $\Phi(x)$ is a feature map

Primal Classifier in transformed feature space

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

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

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

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

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

Dual Classifier in transformed feature space

Classifier:

$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_{i} y_{i} \mathbf{x}_{i}^{\top} \mathbf{x} + b$$

$$\to f(\mathbf{x}) = \sum_{i}^{N} \alpha_{i} y_{i} \Phi(\mathbf{x}_{i})^{\top} \Phi(\mathbf{x}) + b$$

Learning:

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

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

subject to

$$0 \le \alpha_i \le C$$
 for $\forall i$, and $\sum_i \alpha_i y_i = 0$

Dual Classifier in transformed feature space

- Note, that $\Phi(\mathbf{x})$ only occurs in pairs $\Phi(\mathbf{x}_j)^{\top}\Phi(\mathbf{x}_i)$
- ullet Once the scalar products are computed, only the N dimensional vector $oldsymbol{lpha}$ 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

Classifier:

$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_{i} y_{i} \, k(\mathbf{x}_{i}, \mathbf{x}) + b$$

Learning:

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

subject to

$$0 \le \alpha_i \le C$$
 for $\forall i$, and $\sum_i \alpha_i y_i = 0$

Special transformations

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

$$\Phi(\mathbf{x})^{\top} \Phi(\mathbf{z}) = \begin{pmatrix} x_1^2, x_2^2, \sqrt{2}x_1x_2 \end{pmatrix} \begin{pmatrix} z_1^2 \\ z_2^2 \\ \sqrt{2}z_1z_2 \end{pmatrix}$$

$$= x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1x_2 z_1 z_2$$

$$= (x_1 z_1 + x_2 z_2)^2$$

$$= (\mathbf{x}^{\top} \mathbf{z})^2$$

Kernel Trick

- Classifier can be learnt and applied without explicitly computing $\Phi(x)$
- All that is required is the kernel $k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^{\top} \mathbf{z})^2$
- Complexity of learning depends on N (typically it is $O(N^3)$) 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

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)

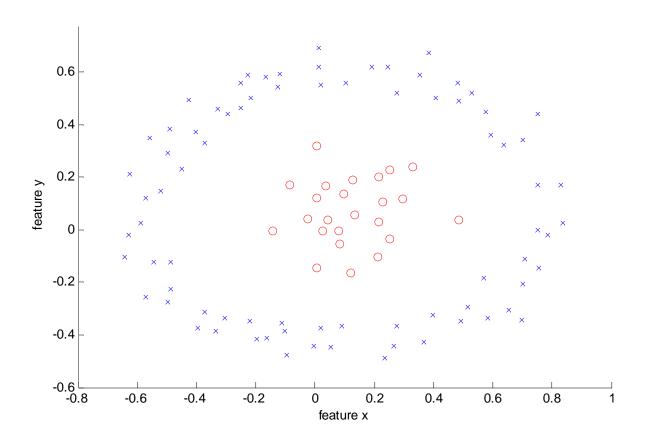
support vector

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

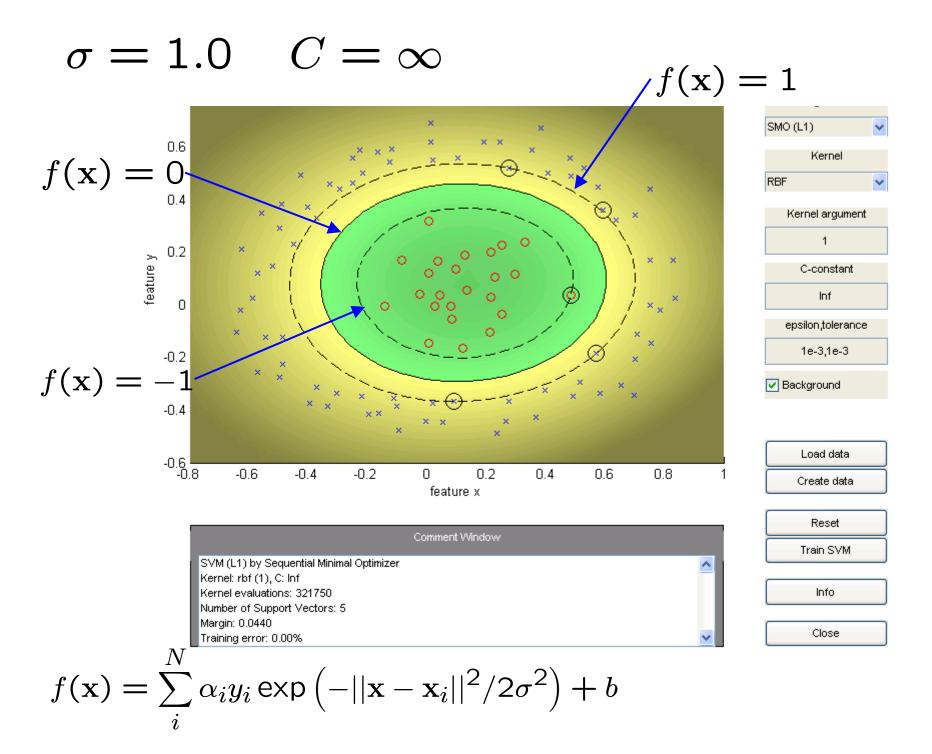
Radial Basis Function (RBF) SVM

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

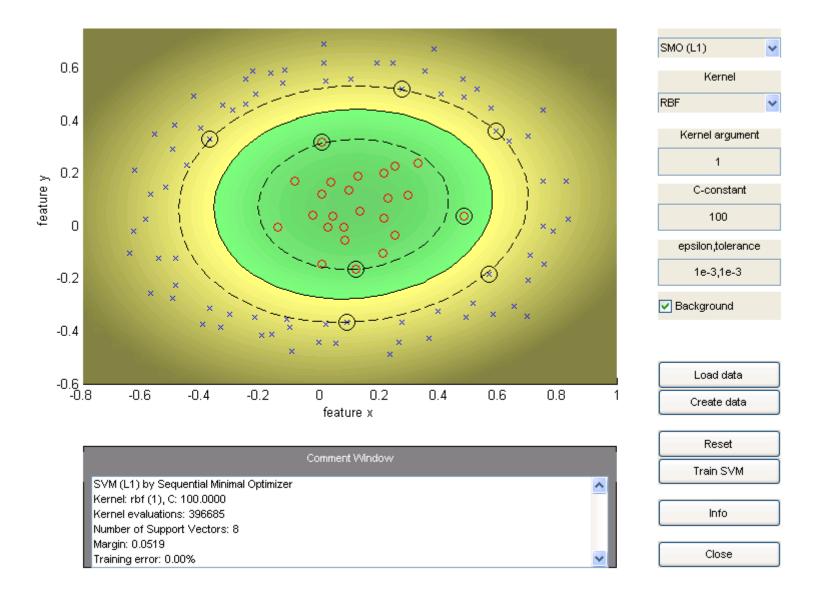
RBF Kernel SVM Example



• data is not linearly separable in original feature space

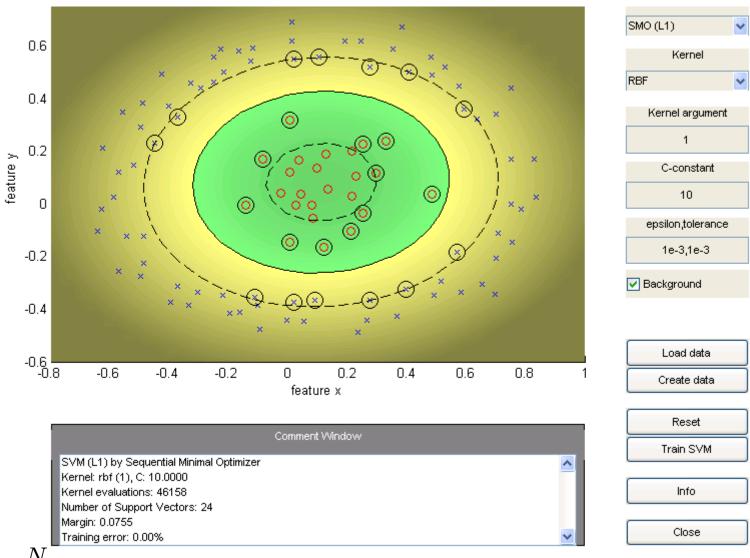


$\sigma = 1.0$ C = 100



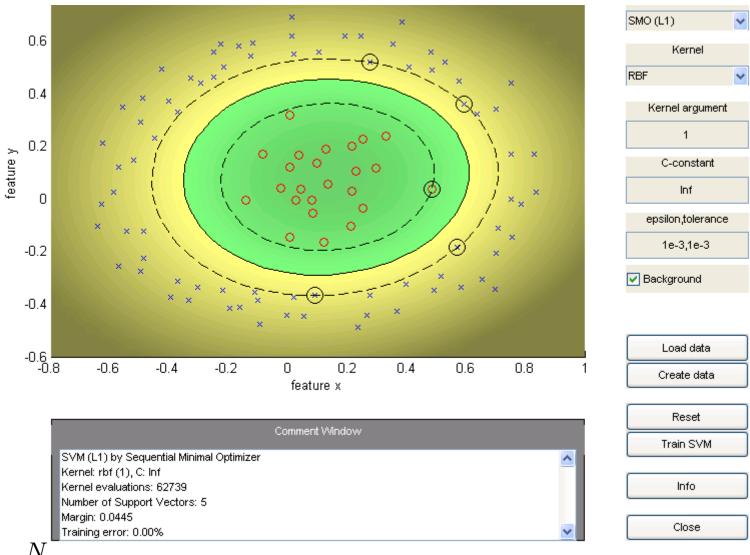
Decrease C, gives wider (soft) margin

$\sigma = 1.0$ C = 10



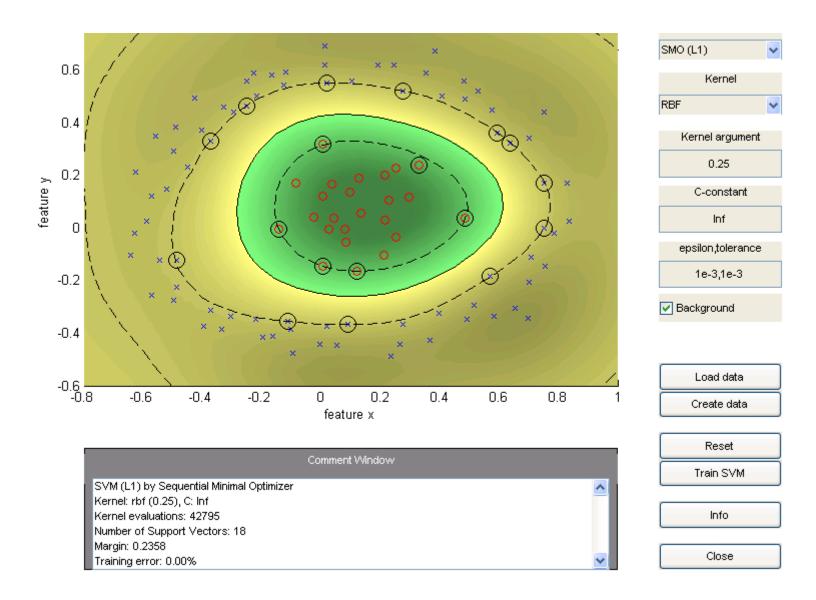
 $f(\mathbf{x}) = \sum_{i}^{N} \alpha_{i} y_{i} \exp\left(-||\mathbf{x} - \mathbf{x}_{i}||^{2}/2\sigma^{2}\right) + b$

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



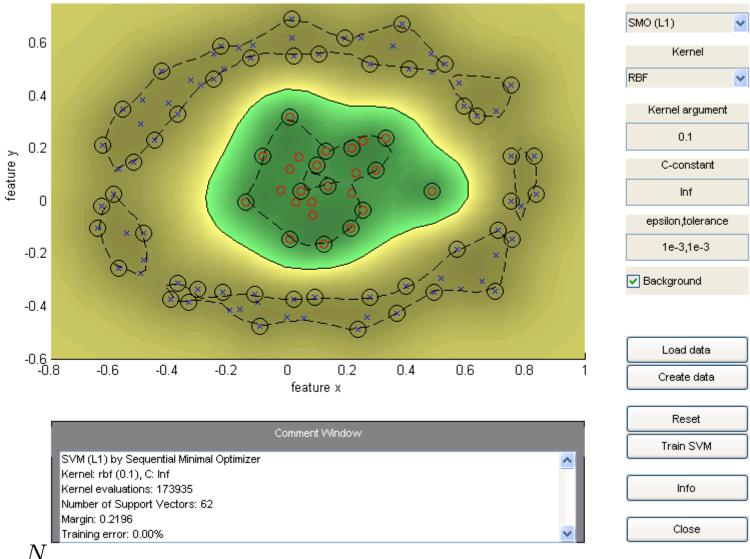
$$f(\mathbf{x}) = \sum_{i}^{N} \alpha_{i} y_{i} \exp\left(-||\mathbf{x} - \mathbf{x}_{i}||^{2}/2\sigma^{2}\right) + b$$

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



Decrease sigma, moves towards nearest neighbour classifier

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



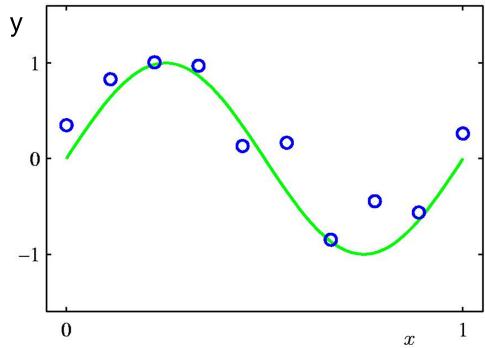
 $f(\mathbf{x}) = \sum_{i}^{N} \alpha_{i} y_{i} \exp\left(-||\mathbf{x} - \mathbf{x}_{i}||^{2}/2\sigma^{2}\right) + b$

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
- Kernels can be used for an SVM because of the scalar product in the dual form, but can also be used elsewhere they are not tied to the SVM formalism
- Kernels apply also to objects that are not vectors, e.g.

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

Regression



ullet Suppose we are given a training set of N observations

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

ullet 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 $f \in \mathcal{F}$

$$\sum_{i=1}^{N} l\left(f(\mathbf{x}_i), y_i\right) + \lambda R\left(f\right)$$
loss function regularization

- There is a choice of both loss functions and regularization
 - e.g. squared loss, SVM "hinge-like" loss
 - squared regularizer, lasso regularizer

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 $\phi_j(x) = x^j$:

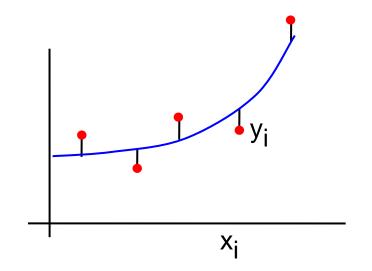
$$f(x, \mathbf{w}) = w_0 + w_1 \phi_1(\mathbf{x}) + w_2 \phi_2(\mathbf{x}) + \dots + w_M \phi_M(\mathbf{x}) = \sum_{j=0}^M w_j x^j$$

e.g. for
$$M = 3$$
,
$$f(x, \mathbf{w}) = (w_0, w_1, w_2, w_3) \begin{pmatrix} 1 \\ x \\ x^2 \\ x^3 \end{pmatrix} = \mathbf{w}^{\top} \Phi(x)$$
$$\Phi : x \to \Phi(x) \quad \mathbb{R}^1 \to \mathbb{R}^4$$

Least squares "ridge regression"

Cost function – squared loss:

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} \left\{ f(x_i, \mathbf{w}) - y_i \right\}^2 + \frac{\lambda}{2} ||\mathbf{w}||^2$$
 loss function regularization



Regression function for x (1D):

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

• NB squared loss arises in Maximum Likelihood estimation for an error model

$$y_i = ilde{y}_i + n_i \qquad n_i \sim \mathcal{N}(0, \sigma^2)$$
 measured value true value

Solving for the weights w

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

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

 Φ is an $N \times M$ design matrix

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

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

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

Now, compute where derivative w.r.t. w is zero for minimum

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

Hence

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

M basis functions, N data points

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

$$[] = [] () () () () assume N > M$$

$$M \times 1 () M \times M () M \times N () N \times 1$$

- This shows that there is a unique solution.
- If $\lambda = 0$ (no regularization), then

$$\mathbf{w} = (\mathbf{\Phi}^{\top} \mathbf{\Phi})^{-1} \mathbf{\Phi}^{\top} \mathbf{y} = \mathbf{\Phi}^{+} \mathbf{y}$$

where Φ^+ is the pseudo-inverse of Φ (pinv in Matlab)

- Adding the term λI improves the conditioning of the inverse, since if Φ is not full rank, then $(\Phi^{\top}\Phi + \lambda I)$ will be (for sufficiently large λ)
- ullet As $\lambda o \infty$, $\mathbf{w} o rac{1}{\lambda} \mathbf{\Phi}^ op \mathbf{y} o \mathbf{0}$
- Often the regularization is applied only to the inhomogeneous part of \mathbf{w} , i.e. to $\tilde{\mathbf{w}}$, where $\mathbf{w}=(w_0,\tilde{\mathbf{w}})$

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

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

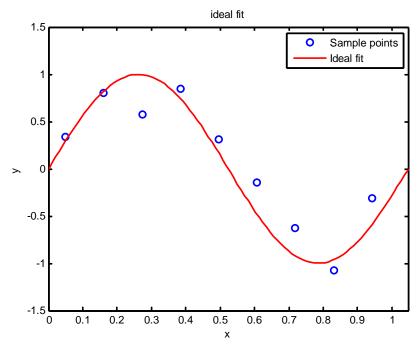
$$= \mathbf{\Phi}(x)^{\top} (\mathbf{\Phi}^{\top} \mathbf{\Phi} + \lambda \mathbf{I})^{-1} \mathbf{\Phi}^{\top} \mathbf{y}$$

$$= \mathbf{b}(x)^{\top} \mathbf{y}$$

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

Example 1: polynomial 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.
- There is a choice in both the degree, M, of the basis functions used, and in the strength of the regularization

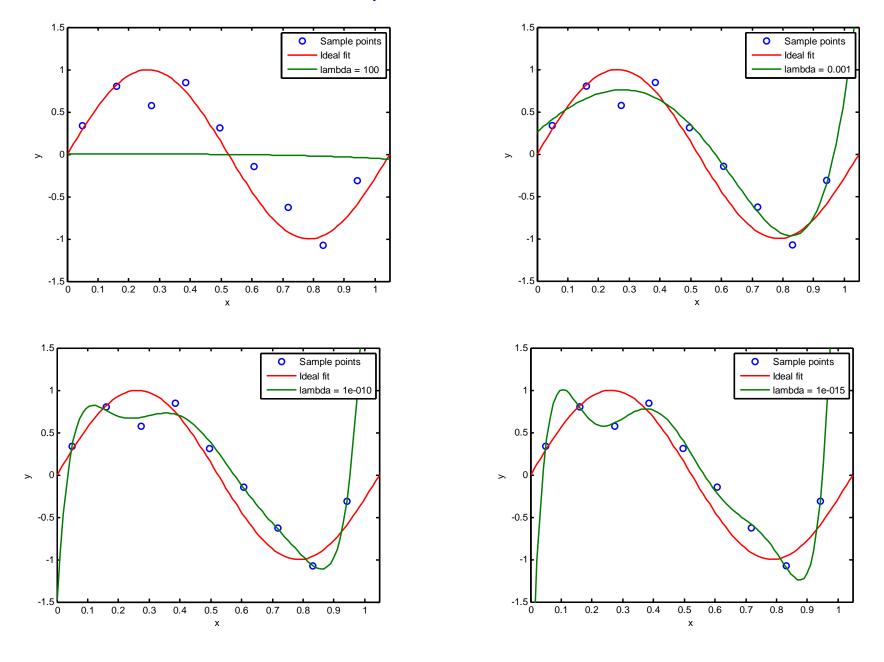


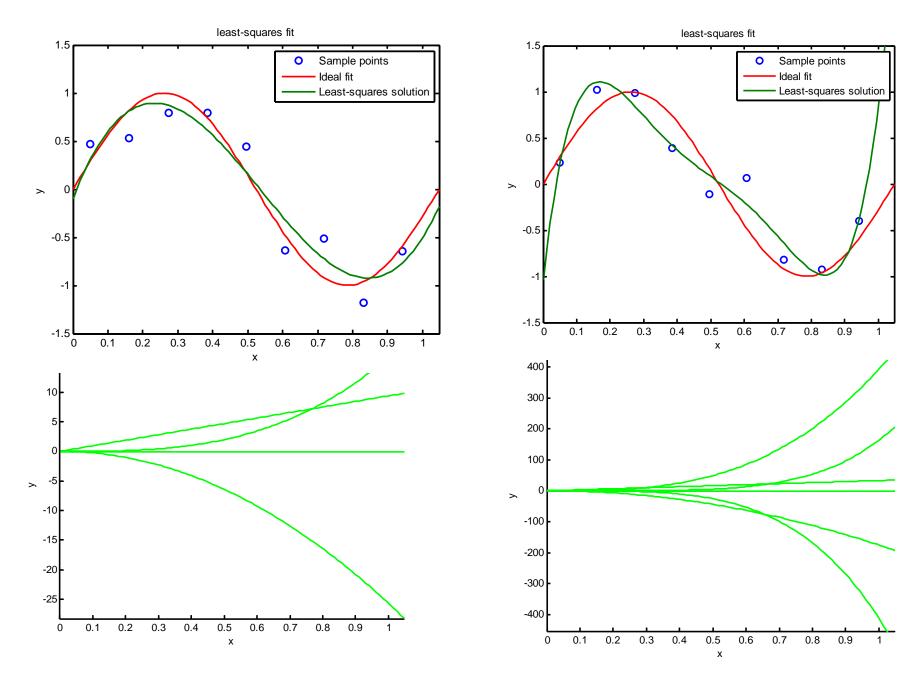
dimensional vector

$$f(x, \mathbf{w}) = \sum_{j=0}^{M} w_j x^j = \mathbf{w}^{\top} \Phi(x) \qquad \Phi : x \to \Phi(x) \quad \mathbb{R} \to \mathbb{R}^{M+1}$$

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} \left\{ f(x_i, \mathbf{w}) - y_i \right\}^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2 \qquad \text{w is a M+1}$$
dimensional vector

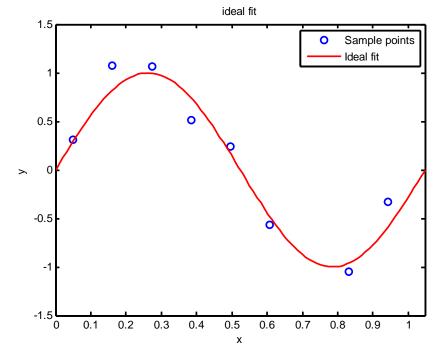
N = 9 samples, M = 7





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)
- There is a choice in both the scale, sigma, of the basis functions used, and in the strength of the regularization



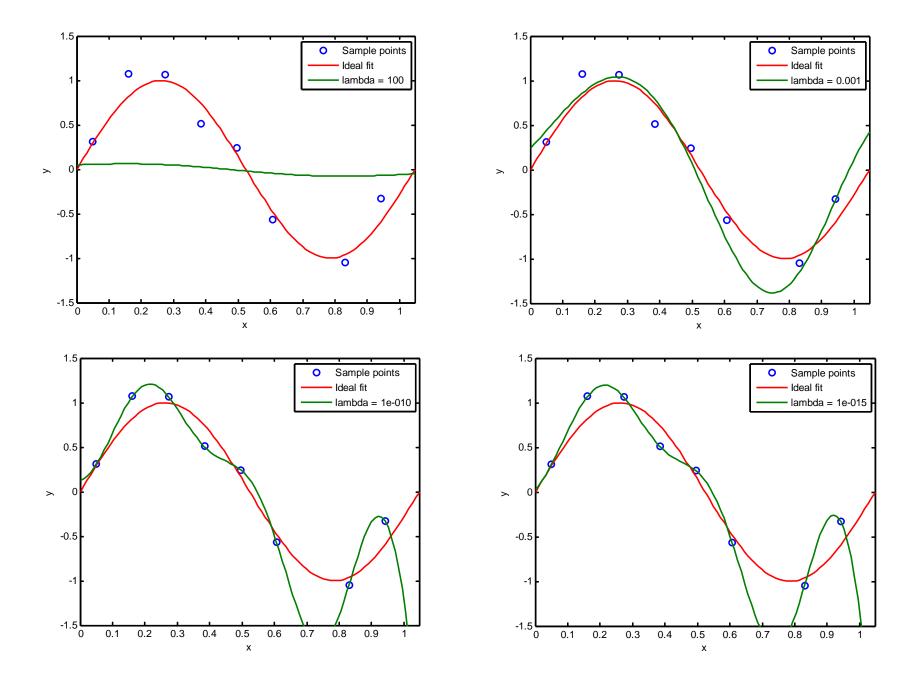
$$f(x, \mathbf{w}) = \sum_{i=1}^{N} w_i e^{-(x-x_i)^2/\sigma^2} = \mathbf{w}^{\top} \Phi(x) \qquad \Phi : x \to \Phi(x) \quad \mathbb{R} \to \mathbb{R}^N$$

$$\Phi: x \to \Phi(x) \quad \mathbb{R} \to \mathbb{R}^N$$

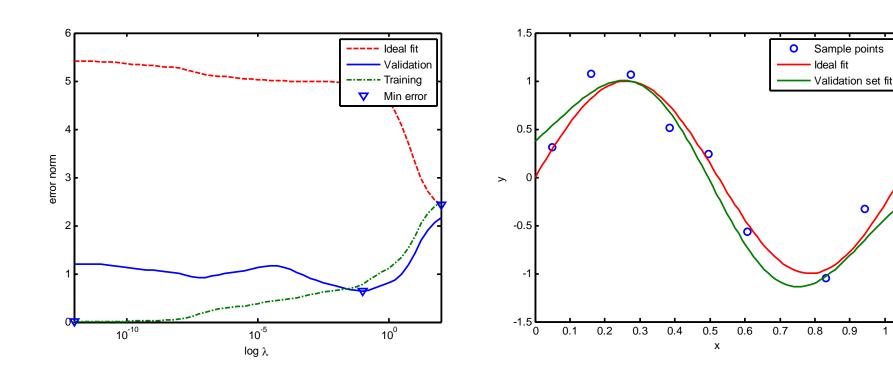
$$\widetilde{E}(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} \{f(x_i, \mathbf{w}) - y_i\}^2 + \frac{\lambda}{2} ||\mathbf{w}||^2$$

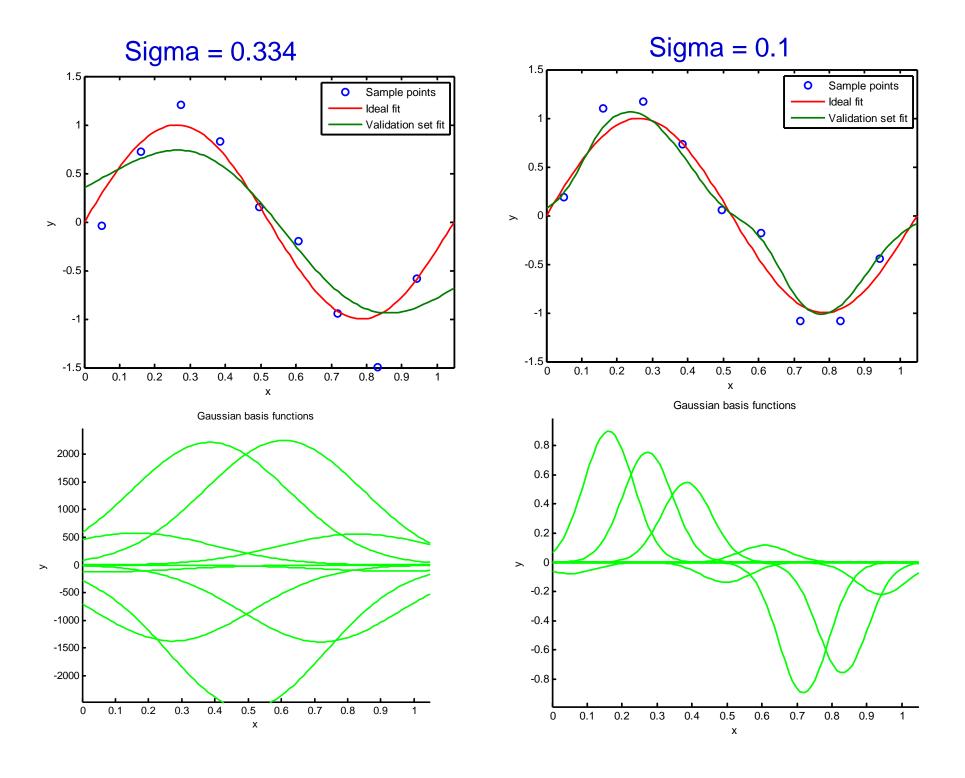
w is a N-vector

N = 9 samples, sigma = 0.334



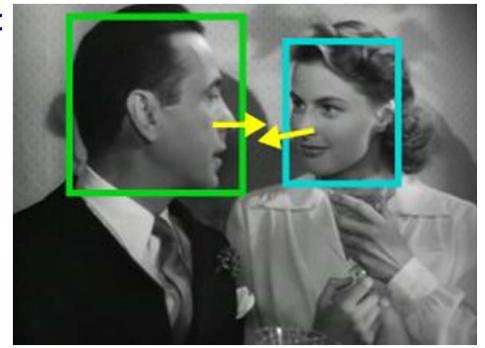
Choosing lambda using a validation set





Application: regressing face pose

- Estimate two face pose angles:
 - yaw (around the Y axis)
 - pitch (around the X axis)
- Compute a HOG feature vector for each face region
- Learn a regressor from the HOG vector to the two pose angles



Summary and dual problem

So far we have considered the primal problem where

$$f(\mathbf{x}, \mathbf{w}) = \sum_{i=1}^{M} w_i \phi_i(\mathbf{x}) = \mathbf{w}^{\top} \Phi(\mathbf{x})$$

and we wanted a solution for $\mathbf{w} \in \mathbb{R}^M$

As in the case of SVMs, we can also consider the dual problem where

$$\mathbf{w} = \sum_{i=1}^{N} a_i \Phi(x_i)$$
 and $f(\mathbf{x}, \mathbf{a}) = \sum_{i=1}^{N} a_i \Phi(x_i)^{\top} \Phi(x)$

and obtain a solution for $\mathbf{a} \in \mathbb{R}^N$.

Again

- there is a closed form solution for a,
- the solution involves the $N \times N$ Gram matrix $k(x_i, x_j) = \Phi(x_i)^\top \Phi(x_j)$,
- so we can use the kernel trick again to replace scalar products

Background reading and more

- Bishop, chapters 6 & 7 for kernels and SVMs
- Hastie et al, chapter 12
- Bishop, chapter 3 for regression
- More on web page:

http://www.robots.ox.ac.uk/~az/lectures/ml