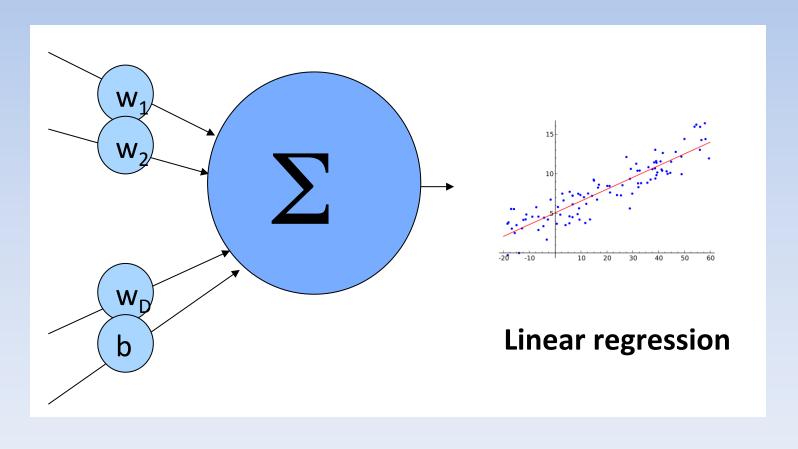
# UCB - CS189 Introduction to Machine Learning Fall 2015

Lecture 8: Kernel machines

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ChaLearn

# Come to my office hours... Wed 2:30-4:30 Soda 329

#### Last time



# Come to my office hours... Wed 2:30-4:30 Soda 329

#### **Today**

#### Kernel machines

**PARAMETRIC (Perceptons)** 

$$f(x) = w \cdot \Phi(x)$$

$$\mathbf{w} = \sum_{k} \underline{\alpha}_{k} \Phi(\mathbf{x}^{k})$$

(Large margin) Perceptron

$$\Delta \mathbf{w} \sim \mathbf{y}_k \Phi(\mathbf{x}^k)$$
 if  $\mathbf{y}_k f(\mathbf{x}^k) < 1$   
  $\sim \mathbf{1}(1-\mathbf{z}_k) \mathbf{y}_k \Phi(\mathbf{x}^k)$   $\mathbf{z}_k = \mathbf{y}_k f(\mathbf{x}^k)$   
(Rosenblatt 1958)

Logistic regression

$$\Delta \mathbf{w} \sim S(-\mathbf{z}_k) \mathbf{y}_k \Phi(\mathbf{x}^k)$$
(Cox 1958)

LMS regression or classification  $\Delta \mathbf{w} \sim (\mathbf{y}_k - \mathbf{f}(\mathbf{x}^k)) \Phi(\mathbf{x}^k) \sim (1 - \mathbf{z}_k) \mathbf{y}_k \Phi(\mathbf{x}^k)$ 

(Widrow-Hoff, 1960)

NON PARAMETRIC (Kernel machines)

$$f(\mathbf{x}) = \sum_{k} \underline{\alpha}_{\underline{k}} k(\underline{\mathbf{x}}^{\underline{k}}, \mathbf{x})$$

$$k(\mathbf{x}^k, \mathbf{x}) = \Phi(\mathbf{x}^k).\Phi(\mathbf{x})$$

Potential Function algorithm

$$\Delta \alpha_k \sim y_k$$
 if  $y_k f(\mathbf{x}^k) < 1$   
  $\sim \mathbf{1}(1-z_k) y_k$   
(Aizerman et al 1964)

Dual logistic regression

$$\Delta \alpha_k \sim S(-z_k) y_k$$

**Dual LMS** 

$$\Delta \alpha_k \simeq (\underline{y}_k - f(\underline{x}^k)) \simeq (1 - \underline{z}_k) \underline{y}_k$$

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# Linear regression

#### Problem setting:

- $\circ$  N training input/output pairs  $\{(\mathbf{x}^k, \mathbf{y}^k)\}$ ; y is continuous.
- Linear model  $f(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x}$  ( $\mathbf{w}_0$  corresponds to  $\mathbf{x}_0 \equiv 1$ ,  $\dim(\mathbf{x}) = d$ )
- O Solve a system of N equations  $y^k = w_0 + w_1 x_0 + ...$  of (d +1) unknown.

#### Matrix notation:

- $\circ$  X  $\mathbf{w}^{\mathsf{T}} = \mathbf{y}$
- o  $X = [x_i^k]$  of dim(N,d);  $y = [y_i^k]$  of dim(N,1);  $w = [w_i]$  of dim(1,d).

#### Solution:

- <u>Case 1</u>: N > d, over-determined, no exact solution.  $\mathbf{w}^T = X^+ \mathbf{y}$  is the best solution in the least-square sense. RSS= $\Sigma_k(f(\mathbf{x})-\mathbf{y}^k)^2$ .
- Case 2: N < d, under-determined,  $\mathbf{w}^T = X^+ \mathbf{y}$  is the solution of min  $\|\mathbf{w}\|$ .

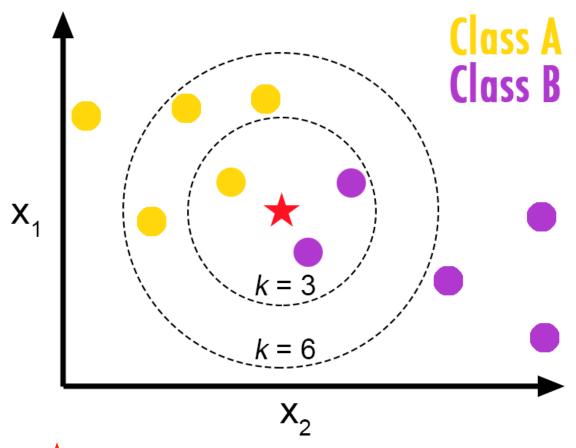
#### Pseudo-inverse:

- $O X^{+} = \lim_{\lambda \to 0^{+}} (X^{T}X + \lambda I)^{-1} X^{T} = \lim_{\lambda \to 0^{+}} X^{T} (X X^{T} + \lambda I)^{-1}$
- o Inverse the smallest matrix and adjust  $\lambda>0$  by cross-validation (see SVD trick).

#### Kernel trick:

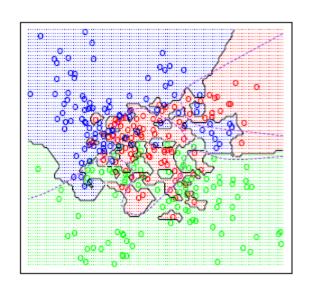
- o in case 2, N<<d, replace X  $X^T$  by a (N, N) kernel matrix  $K = k(\mathbf{x}^k, \mathbf{x}^h)$
- $\circ$  **α** = (K+ λI)<sup>-1</sup> **y**, gives you a non linear regression function  $f(\mathbf{x}) = \Sigma_k \alpha_k k(\mathbf{x}, \mathbf{x}_k)$ .

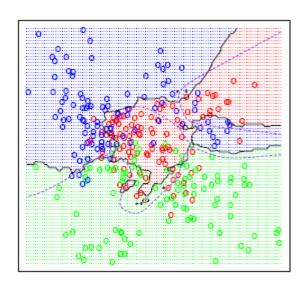
#### Ancestor of kernel methods: KNN



Assign to the class label of the majority of the k closest examples.

# Optimum k in k-nearest neighbors



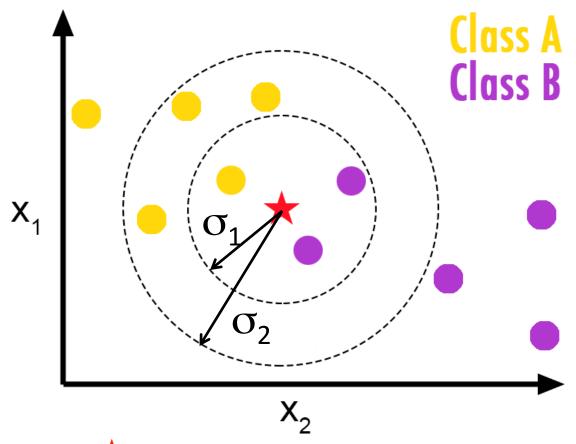


k=1 k=15

#### Fit vs. robustness tradeoff in kNN:

- kNN does not have any parameters (non parametric method).
- The "complexity" (of the decision function) decreases with k.
- k is a hyper-parameter adjustable by cross-validation.
- kNN can also be used for regression.

#### Parzen windows



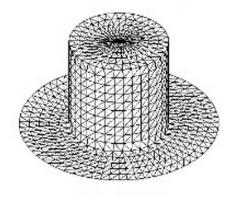
Assign to  $\bigstar$  the class label of the majority of the examples enclosed in a sphere of radius  $\mathbf{O}_{\mathbf{r}}$ .

#### Parzen windows is a kernel method

• Assign to  $\mathbf{x}$  the class label of the majority of the examples enclosed in a sphere of radius  $\sigma$ .

• 
$$f(\mathbf{x}) = \sum_{k=1:N} y_k k(\mathbf{x}, \mathbf{x}_k)$$

• Top hat kernel:  $k(\mathbf{x}, \mathbf{x}_k) = \mathbf{1}(\|\mathbf{x} - \mathbf{x}_k\|^2 < \sigma^2)$ 



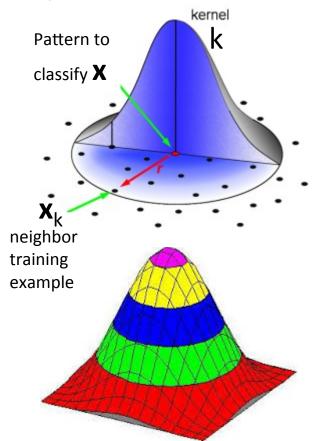
#### Parzen windows is a kernel method

• Assign to  $\mathbf{x}$  the class label of the majority of the examples enclosed in a sphere of radius  $\sigma$ .

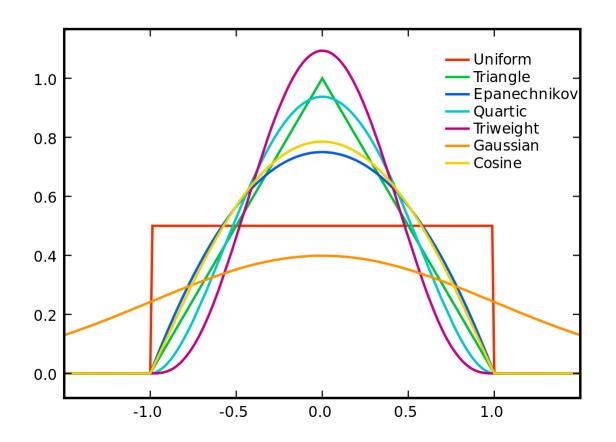
• 
$$f(\mathbf{x}) = \sum_{k=1:N} y_k k(\mathbf{x}, \mathbf{x}_k)$$

• Top hat kernel:  $k(\mathbf{x}, \mathbf{x}_k) = \mathbf{1}(\|\mathbf{x} - \mathbf{x}_k\|^2 < \sigma^2)$ 

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



#### Some radial kernels



Source: <a href="https://en.wikipedia.org/wiki/Kernel\_(statistics">https://en.wikipedia.org/wiki/Kernel\_(statistics)</a>

See also: <a href="http://crsouza.com/2010/03/kernel-functions-for-machine-learning-applications">http://crsouza.com/2010/03/kernel-functions-for-machine-learning-applications</a>
<a href="http://crsouza.com/2010/03/kernel-functions-for-machine-learning-applications">http://crsouza.com/2010/03/kernel-functions-for-machine-learning-applications</a>
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#### Non radial kernels

$$f(\mathbf{x}) = \sum_{k=1:N} y_k k(\mathbf{x}, \mathbf{x}_k)$$

• Linear kernel:

$$k(\mathbf{x}, \mathbf{x}_k) = \mathbf{x}.\mathbf{x}_k$$
  
The Parzen windows  $f(\mathbf{x})$  for the linear kernel is just Hebb's rule!

• Polynomial kernel:  $k(\mathbf{x}, \mathbf{x}_{k}) = (1 + \mathbf{x}.\mathbf{x}_{k})^{q}$ 

#### What makes k(x, x') a "good" kernel?

- Symmetric  $k(\mathbf{x}, \mathbf{x'}) = k(\mathbf{x'}, \mathbf{x})$
- Kernel matrix  $K = [k(\mathbf{x}_k, \mathbf{x}_h)]_{k=1:N, h=1:N}$  invertible, possibly after "regularization"  $(K+\lambda I)$ ,  $\lambda > 0$ . Satisfied if all eigenvalues  $\geq 0$  (PSD matrix).
- True in particular if:
  - k(x, x') is a PSD kernel i.e.
     satisfies Mercer's condition.

```
\sum_{i=1}^n \sum_{j=1}^n K(x_i,x_j)c_ic_j \geq 0 for all finite sequences of points x_1,...,x_n of [a,b] and all choices of real numbers c_1,...,c_n
```

There exists an eigen decomposition  $k(\mathbf{x}, \mathbf{x'}) = \sum_{i=1:\infty} \lambda_i \psi_i(\mathbf{x}) \psi_i(\mathbf{x'})$ 

- K is a Gram matrix (outer product  $K = XX^T$  or  $K = \Phi\Phi^T$ )
- K is a covariance matrix.
- The sigmoid kernel tanh(x.x') is NOT PSD.

#### Remember the "kernel trick"

• 
$$f(\mathbf{x}) = \sum_{k} \alpha_{k} k(\mathbf{x}^{k}, \mathbf{x})$$

NON PARAMETRIC

• 
$$k(\mathbf{x}^k, \mathbf{x}) = \Phi(\mathbf{x}^k) \bullet \Phi(\mathbf{x})$$



# **Dual forms**

•  $f(x) = w \cdot \Phi(x)$ 

**PARAMETRIC** 

• 
$$\mathbf{w} = \sum_{k} \alpha_{k} \Phi(\mathbf{x}^{k})$$

# Reproducing kernels

- A Hilbert space H is a space of functions {f(x)}.
- A "reproducing kernel" Hilbert space (RKHS) is endowed with a dot product:

$$\langle f, g \rangle_H = \int f(\mathbf{x}) g(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}$$

H has a (unique) positive definite "reproducing kernel":

$$k(s, t) = \langle k(., s), k(., t) \rangle_{H}$$

Reproducing kernel property:

$$f(x) = \langle k(., x), f \rangle_{H}$$

#### Representer theorem

Kimeldorf, George S.; Wahba, Grace (1970) Schölkopf, Bernhard; Herbrich, Ralf; Smola, Alex J. (2001)

- $f(\mathbf{x})$  is a function in RKHS H, w.  $\langle f, g \rangle_H = \int f(\mathbf{x}) g(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}$ , and kernel k:  $f(\mathbf{x}) = \langle k(., \mathbf{x}), f \rangle_H$ .
- Given a risk functional R[f] and a regularizer  $\Omega[f]$  and training examples  $\{\mathbf{x}^k, \mathbf{y}^k\}$  on which we evaluate R[f] +  $\lambda\Omega[f]$ ,  $\lambda>0$ .
- $f^*(\mathbf{x}) = \operatorname{argmin}_f R_{train}[f] + \lambda \Omega[f]$  admits a representation

$$f^*(\mathbf{x}) = \sum_k \alpha_k k(\mathbf{x}, \mathbf{x}^k)$$

• This means that we only have to solve for  $\alpha_k$  and that the solution lies in the span of  $k(., \mathbf{x}^k)$  that can be thought of as special kind of features. The kernel determines the type of function used and the type of regularization (smoothness).

#### Mercer kernels and kernel trick

$$k(\mathbf{x}, \mathbf{x'}) = \sum_{i=1:\infty} \lambda_i \, \psi_i(\mathbf{x}) \, \psi_i(\mathbf{x'})$$

Use 
$$\phi_i(\mathbf{x}) = \sqrt{\lambda_i} \psi_i(\mathbf{x})$$

$$f(\mathbf{x}) = \sum_{k} \alpha_{k} k(\mathbf{x}^{k}, \mathbf{x}) = \sum_{k} \alpha_{k} \sum_{i} \phi_{i}(\mathbf{x}^{k}) \phi_{i}(\mathbf{x})$$

$$= \sum_{i} \left( \sum_{k} \alpha_{k} \phi_{i}(\mathbf{x}^{k}) \right) \phi_{i}(\mathbf{x})$$

$$= \sum_{i} w_{i} \phi_{i}(\mathbf{x})$$

See for details: https://en.wikipedia.org/wiki/Representer\_theorem

### Kernel algebra

Cristianini and Shaw-Taylor, 2001

**Proposition 3.22 (Closure properties)** Let  $\kappa_1$  and  $\kappa_2$  be kernels over  $X \times X$ ,  $X \subseteq \mathbb{R}^n$ ,  $a \in \mathbb{R}^+$ ,  $f(\cdot)$  a real-valued function on X,  $\phi: X \longrightarrow \mathbb{R}^N$  with  $\kappa_3$  a kernel over  $\mathbb{R}^N \times \mathbb{R}^N$ , and  $\mathbf{B}$  a symmetric positive semi-definite  $n \times n$  matrix. Then the following functions are kernels:

(i) 
$$\kappa(\mathbf{x}, \mathbf{z}) = \kappa_1(\mathbf{x}, \mathbf{z}) + \kappa_2(\mathbf{x}, \mathbf{z}),$$

(ii) 
$$\kappa(\mathbf{x}, \mathbf{z}) = a\kappa_1(\mathbf{x}, \mathbf{z}),$$

(iii) 
$$\kappa(\mathbf{x}, \mathbf{z}) = \kappa_1(\mathbf{x}, \mathbf{z}) \kappa_2(\mathbf{x}, \mathbf{z}),$$

(iv) 
$$\kappa(\mathbf{x}, \mathbf{z}) = f(\mathbf{x})f(\mathbf{z}),$$

(v) 
$$\kappa(\mathbf{x}, \mathbf{z}) = \kappa_3(\phi(\mathbf{x}), \phi(\mathbf{z})),$$

(vi) 
$$\kappa(\mathbf{x}, \mathbf{z}) = \mathbf{x}' \mathbf{B} \mathbf{z}$$
.

**Proposition 3.24** Let  $\kappa_1(\mathbf{x}, \mathbf{z})$  be a kernel over  $X \times X$ , where  $\mathbf{x}, \mathbf{z} \in X$ , and p(x) is a polynomial with positive coefficients. Then the following functions are also kernels:

(i) 
$$\kappa(\mathbf{x}, \mathbf{z}) = p(\kappa_1(\mathbf{x}, \mathbf{z})),$$

(ii) 
$$\kappa(\mathbf{x}, \mathbf{z}) = \exp(\kappa_1(\mathbf{x}, \mathbf{z})),$$

(iii) 
$$\kappa(\mathbf{x}, \mathbf{z}) = \exp(-\|\mathbf{x} - \mathbf{z}\|^2 / (2\sigma^2)).$$

#### Favorite kernel

$$k(\mathbf{x}, \mathbf{x}') = (\mathbf{a} + \mathbf{x} \cdot \mathbf{x}')^{b} \exp(-\mathbf{d} \|\mathbf{x} - \mathbf{x}_{k}\|^{c})$$

Of 4 hyper-parameters a, b, c, d.

Simplify: take a = 1 and c = 2.

Then:  $b = 0 \rightarrow Gaussian kernel$ 

 $d = 0 \rightarrow Polynomial kernel$ 

Adjust the hyper-parameters by cross-validation.

#### Kernel machines

#### **PARAMETRIC (Perceptons)**

$$f(x) = w \bullet \Phi(x)$$

$$\mathbf{w} = \sum_{k} \alpha_{k} \, \Phi(\mathbf{x}^{k})$$

(Large margin) Perceptron

$$\Delta \mathbf{w} \sim y_k \Phi(\mathbf{x}^k)$$
 if  $y_k f(\mathbf{x}^k) < 1$   
  $\sim \mathbf{1}(1-z_k) y_k \Phi(\mathbf{x}^k)$   $z_k = y_k f(\mathbf{x}^k)$ 

(Rosenblatt 1958)

Logistic regression

$$\Delta \mathbf{w} \sim S(-z_k) y_k \Phi(\mathbf{x}^k)$$

(Cox 1958)

LMS regression or classification  $\Delta w \sim (v - f(\mathbf{x}^k)) \Phi(\mathbf{x}^k) \sim (1 - 7) v \Phi(\mathbf{x}^k)$ 

$$\Delta \mathbf{w} \sim (\mathbf{y}_k - \mathbf{f}(\mathbf{x}^k)) \Phi(\mathbf{x}^k) \sim (1 - \mathbf{z}_k) \mathbf{y}_k \Phi(\mathbf{x}^k)$$

(Widrow-Hoff, 1960)

#### **NON PARAMETRIC (Kernel machines)**

$$f(\mathbf{x}) = \sum_{k} \alpha_{k} k(\mathbf{x}^{k}, \mathbf{x})$$

$$k(\mathbf{x}^k, \mathbf{x}) = \Phi(\mathbf{x}^k).\Phi(\mathbf{x})$$

Potential Function algorithm

$$\Delta\alpha_k \sim y_k$$
 if  $y_k f(\mathbf{x}^k) < 1$   
  $\sim \mathbf{1}(1-z_k) y_k$ 

(Aizerman et al 1964)

Dual logistic regression

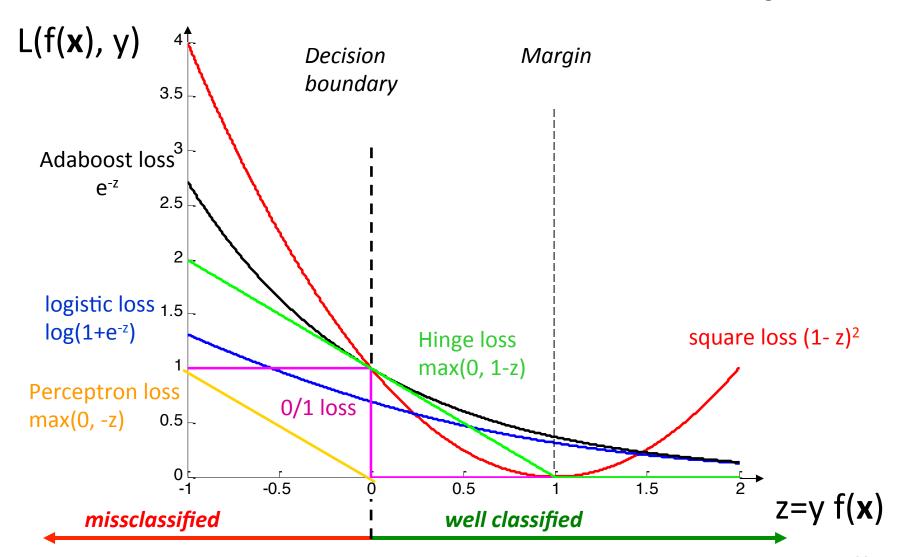
$$\Delta \alpha_k \sim S(-z_k) y_k$$

**Dual LMS** 

$$\Delta \alpha_k \sim (y_k - f(\mathbf{x}^k)) \sim (1 - z_k) y_k$$

#### **Loss Functions**

The risk is the average of the loss.



### Regularized risk minimization

• 
$$f(x) = w \cdot \Phi(x) = \sum_{k} \alpha_{k} k(x^{k}, x)$$

#### • Minimize:

$$R_{reg}[\mathbf{w}] = \sum_{k} L(f(\mathbf{x}^k), y_k) + \lambda \Omega(\mathbf{w})$$

$$\Omega(\mathbf{w}) = \|\mathbf{w}\|^2$$

$$\Omega(\mathbf{w}) = \|\mathbf{w}\|$$

#### Stochastic gradient

$$f(\mathbf{x}) = \sum_{i} w_{i} \Phi_{i}(\mathbf{x}) = \mathbf{w} \cdot \Phi(\mathbf{x}) = \sum_{k} \alpha_{k} k(\mathbf{x}^{k}, \mathbf{x})$$

- 1) Compute  $\partial L/\partial w_i = \partial L/\partial f$ .  $\partial f/\partial w_i = \partial L/\partial f$   $\Phi_i(\mathbf{x})$ 
  - Classification:  $\partial L/\partial w_i = \partial L/\partial z \cdot \partial z/\partial w_i$  with  $z = y f(x) \cdot \partial z/\partial w_i = y \Phi_i(x) \rightarrow \partial L/\partial w_i = \partial L/\partial z \cdot y \Phi_i(x)$
- 2) Compute  $\partial \Omega / \partial w_i$ 
  - $\Omega(\mathbf{w}) = \|\mathbf{w}\|^2 \rightarrow \partial \Omega/\partial \mathbf{w}_i = 2\mathbf{w}_i$
- 3) Compute the negative gradient of  $L(f(\mathbf{x}), \mathbf{y}) + \lambda \Omega(\mathbf{w})$

$$\Delta w_i = -\eta \partial L/\partial f \Phi_i(\mathbf{x}) - \gamma w_i$$

$$\Delta \mathbf{w} = - \eta \partial L / \partial f \Phi(\mathbf{x}) - \gamma \mathbf{w}$$

#### Kernel version

$$\Phi$$
-space version:  $\Delta \mathbf{w} = -\eta \partial L/\partial f \Phi(\mathbf{x})$ 

- Learning  $(\mathbf{x}^k, \mathbf{y}^k)$ :  $\Delta \mathbf{w} = -\eta \partial L/\partial f|_{(\mathbf{x}^k, \mathbf{y}^k)} \Phi(\mathbf{x}^k)$
- $\mathbf{w} = \sum_{k} \alpha_{k} \Phi(\mathbf{x}^{k}), \quad \Delta \mathbf{w} = \Delta \alpha_{k} \Phi(\mathbf{x}^{k})$

$$\Delta \alpha_{\mathbf{k}} = - \eta \partial L / \partial f|_{(\mathbf{x}\mathbf{k}, \, \mathbf{y}\mathbf{k})}$$

$$f(\mathbf{x}) = \sum_{\mathbf{k}} \alpha_{\mathbf{k}} k(\mathbf{x}^{\mathbf{k}}, \mathbf{x})$$

# Kernel version with shrinkage

$$\Phi$$
-space version:  $\Delta \mathbf{w} = -\eta \partial L/\partial f \Phi(\mathbf{x}) - \gamma \mathbf{w}$ 

Learning (x<sup>k</sup>, y<sup>k</sup>):

$$\Delta \mathbf{w} = - \eta \partial L / \partial f|_{(\mathbf{x}^k, \mathbf{y}^k)} \Phi(\mathbf{x}^k) - \gamma \mathbf{w}$$

•  $\mathbf{w} = \sum_{k} \alpha_{k} \Phi(\mathbf{x}^{k}), \quad \Delta \mathbf{w} = \Delta \alpha_{k} \Phi(\mathbf{x}^{k})$ 

$$\Delta\alpha_{k} = -\eta \ \partial L/\partial f|_{(xk, yk)} - \gamma \ \alpha_{k} \qquad \text{for example k}$$
 
$$\Delta\alpha_{h} = -\gamma \ \alpha_{h} \qquad \qquad \text{for other examples}$$

$$f(\mathbf{x}) = \sum_{\mathbf{k}} \alpha_{\mathbf{k}} k(\mathbf{x}^{\mathbf{k}}, \mathbf{x})$$

#### Example: Least Mean Square or LMS

Widrow-Hoff, 1960

• 
$$L_{\text{square\_loss}} = (f(\mathbf{x}) - \mathbf{y})^2$$

• 
$$L/\partial f = 2 (f(x) - y)$$

• 
$$\partial f/\partial w_{i} = \Phi_{i}(\mathbf{x})$$
 for  $f(\mathbf{x}) = \Sigma_{j} w_{j} \Phi_{j}(\mathbf{x})$ 

• 
$$\partial L/\partial w_i = 2 (f(x) - y) \Phi_i(x)$$

Loss variation

• 
$$\Delta w_i = -\eta (f(x) - y) \Phi_i(x) - \gamma w$$

$$\Delta \mathbf{w} = \eta \, (y - f(\mathbf{x})) \, \Phi(\mathbf{x}) - \gamma \, \mathbf{w}$$

$$\Delta \alpha_{k} = \eta \, (y^{k} - f(\mathbf{x}^{k})) - \gamma \, \alpha_{k}$$

$$\Delta \alpha_{h} = -\gamma \, \alpha_{h}$$

LMS learning rule

for example k

# Comparison Hebbs's rule

• 
$$f(x) = w \cdot \Phi(x) = \sum_{k} \alpha_{k} k(x^{k}, x)$$

• Hebb's rule:

$$\Delta w_i = \eta y \Phi_i(x)$$

$$\Delta \alpha_k = \eta y^k$$

• LMS rule:

$$\Delta w_i = \eta (y - f(x)) \Phi_i(x)$$

$$\Delta \alpha_k = \eta (y^k - f(x^k))$$

# Exploiting convexity?

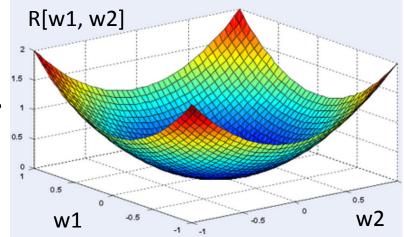
Stochastic gradient does not exploit convexity,

is this the best approach?

Yes for BIG data.

No if either N or d is small.

For regression,
 regularized inverse:

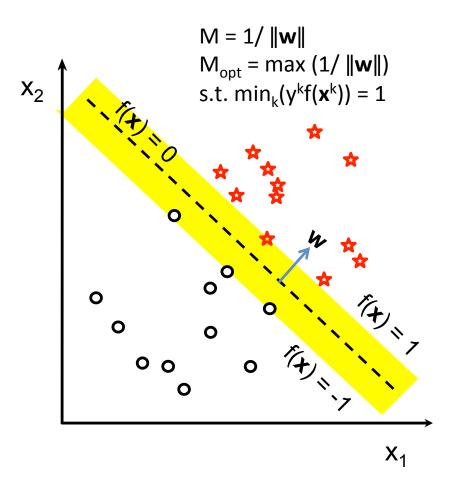


$$\mathbf{w}^{\mathsf{T}} = (\mathsf{X}^{\mathsf{T}}\mathsf{X} + \lambda\mathsf{I})^{-1}\,\mathsf{X}^{\mathsf{T}}\,\mathsf{y}\,\,\mathrm{or}\,\,\mathsf{X}^{\mathsf{T}}\,(\mathsf{X}\,\,\mathsf{X}^{\mathsf{T}} + \lambda\mathsf{I})^{-1}\,\mathsf{y}$$

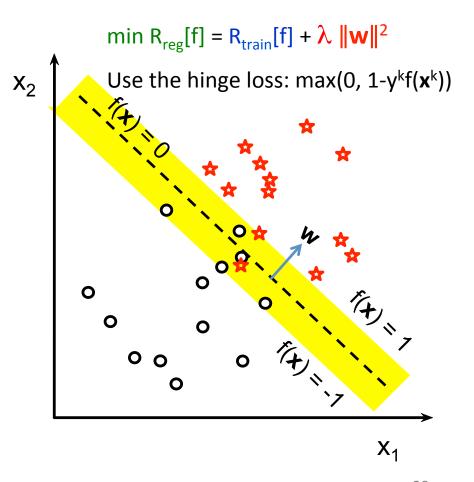
$$\alpha = (\mathsf{K} + \lambda\mathsf{I})^{-1}\,\mathsf{y}$$

#### Classification with optimum margin

#### Hard margin

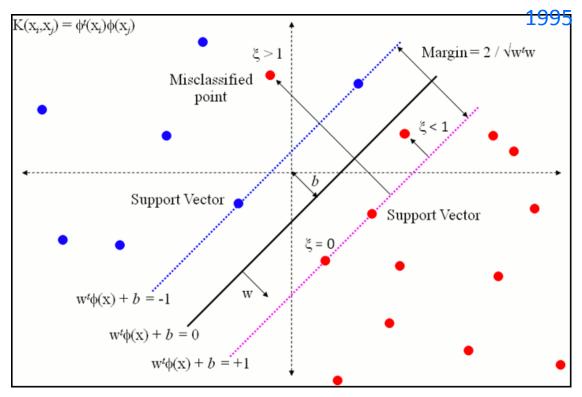


#### Soft margin



### Soft margin

Cortes-Vapnik,



$$\min R_{reg}[f] = R_{train}[f] + \lambda \|\mathbf{w}\|^2$$

Use the hinge loss: 
$$max(0, 1-y^kf(\mathbf{x}^k))$$

min 
$$C \sum_{k=1:N} \xi_k + (1/2) \|\mathbf{w}\|^2$$
  
1-y<sup>k</sup>f( $\mathbf{x}^k$ )  $\leq \xi_k \quad \xi_k > 0$ 

# Standard quadratic programs

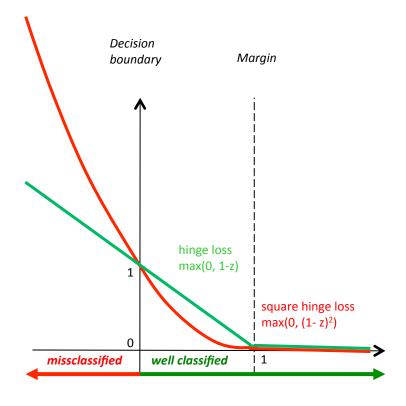
$$f(x) = w \cdot \Phi(x) + b$$

 Soft margin Perceptron-style (with hinge loss)

$$\begin{aligned} & \min_{w,b,\xi} C \sum_{k=1:N} \xi_k + \text{(1/2)} \ \| \boldsymbol{w} \|^2 \\ & y^k f(\boldsymbol{x}^k) - 1 + \xi_k \ge 0 \\ & \xi_k \ge 0 \end{aligned}$$

2) Soft margin RSS-style (with square hinge loss)

$$\begin{aligned} & \min_{\mathbf{w}, \mathbf{b}, \boldsymbol{\xi}} \mathbf{C} \sum_{k=1:N} (\boldsymbol{\xi}_k)^2 + (1/2) \| \mathbf{w} \|^2 \\ & \mathbf{y}^k \mathbf{f}(\mathbf{x}^k) - 1 + \boldsymbol{\xi}_k \ge 0 \\ & \boldsymbol{\xi}_k \ge 0 \end{aligned}$$



# Dual problems (in $\alpha$ space)

• 
$$f(\mathbf{x}) = \sum_{k} \alpha_{k} y_{k} k(\mathbf{x}^{k}, \mathbf{x})$$

$$H = [y_k y_h k(\mathbf{x}^k, \mathbf{x}^h)]$$

1) Hinge loss version:

$$\min_{\alpha} \alpha^{T} \mathbf{1} - (1/2) \alpha^{T} H \alpha$$

$$0 \le \alpha_{k} \le C \text{ box constraint}$$

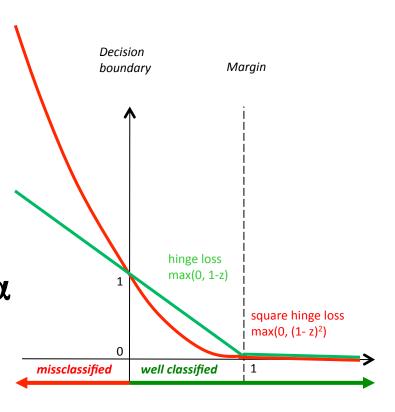
$$\alpha^{T} \mathbf{y} = 0 \text{ bias constraint}$$

2) Square hinge loss version

$$\min_{\alpha} \alpha^{T} \mathbf{1} - (1/2) \alpha^{T} (H + (1/C) I) \alpha$$

$$\alpha_{k} \ge 0$$

$$\alpha^{T} \mathbf{y} = 0 \quad \text{bias constraint}$$



# Dual problems (in $\alpha$ space)

• 
$$f(\mathbf{x}) = \sum_{k} \alpha_{k} k(\mathbf{x}^{k}, \mathbf{x})$$

#### 1) Hinge loss version:

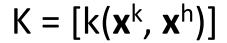
$$\begin{aligned} &\min_{\alpha} \alpha^{\mathsf{T}} \, \mathbf{y} - (1/2) \, \alpha^{\mathsf{T}} \, \mathbf{K} \, \alpha \\ &0 \leq \alpha_{\mathsf{k}} \, \mathsf{y}_{\mathsf{k}} \leq 1/\lambda \quad \mathsf{box} \, \mathsf{constraint} \\ &\alpha^{\mathsf{T}} \, \mathbf{1} = 0 \qquad \qquad \mathsf{bias} \, \mathsf{constraint} \end{aligned}$$

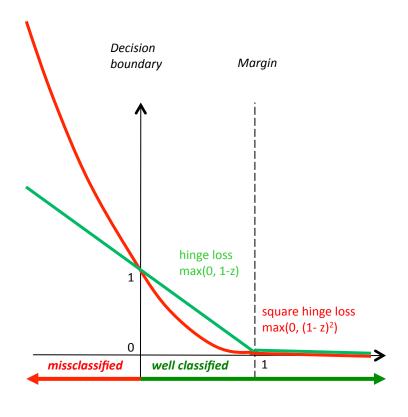
2) Square hinge loss version

$$\min_{\alpha} \alpha^{T} \mathbf{y} - (1/2) \alpha^{T} (K + \lambda I) \alpha$$

$$\alpha_{k} y_{k} \ge 0 \qquad \text{ridge}$$

$$\alpha^{T} \mathbf{1} = 0 \qquad \text{bias constraint}$$





#### Summary

- $f(\mathbf{x}) = \sum_{k=1:N} \alpha_k k(\mathbf{x}, \mathbf{x}_k)$
- Kernel methods are inspired by non-parameteric example-based methods; each example  $\mathbf{x}_k$  votes according to:
  - How similar it is to x measured by  $k(x, x_k)$
  - It weight  $\alpha_k$
- Kernels are "dot products" in a (possibly infinite)  $\Phi$  space.
- The validity of a kernel can be checked with Mercer's condition; there are also kernel composition theorems.
- The weights  $\alpha_k$  can be optimized by gradient descent (for big data) or convex optimization methods.

# Come to my office hours... Wed 2:30-4:30 Soda 329

#### **Next time**

#### **Performance evaluation**

