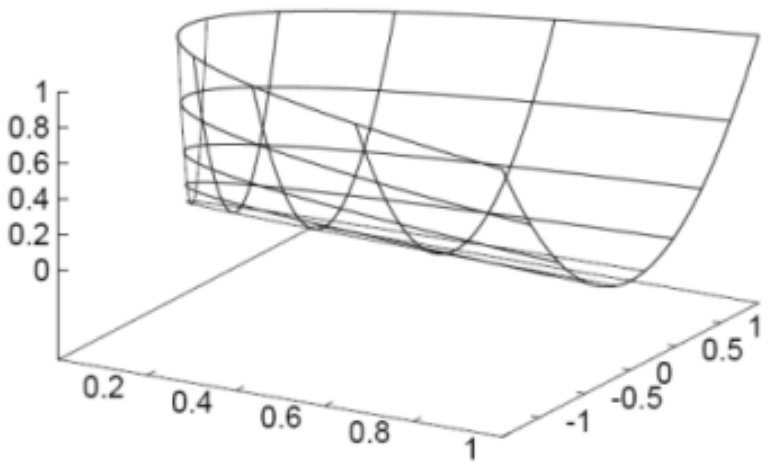
Introduction to Supervised Learning



Week 3:
Support Vector Machines

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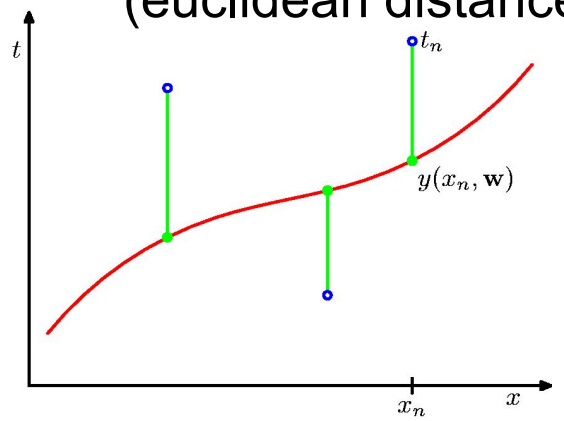
Lecture outline

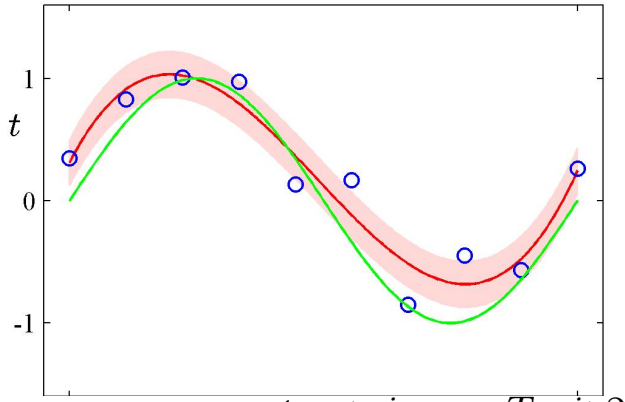
- Introduction to Support Vector Machines
  - Geometric margins
  - Training criterion & hinge loss
- Large margins and generalization
- Optimization
- Kernels
- Applications to vision

Our path so far (week 1-2)

Week 1 - regression: geometric (euclidean distance)

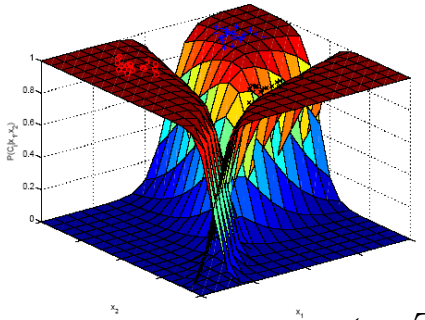


Week 2: probabilistic interpretation



$$P(y^i|\mathbf{x}^i) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^i - \mathbf{w}^T\mathbf{x}^i)^2}{2\sigma^2}\right)$$

Week 2: switch to classification

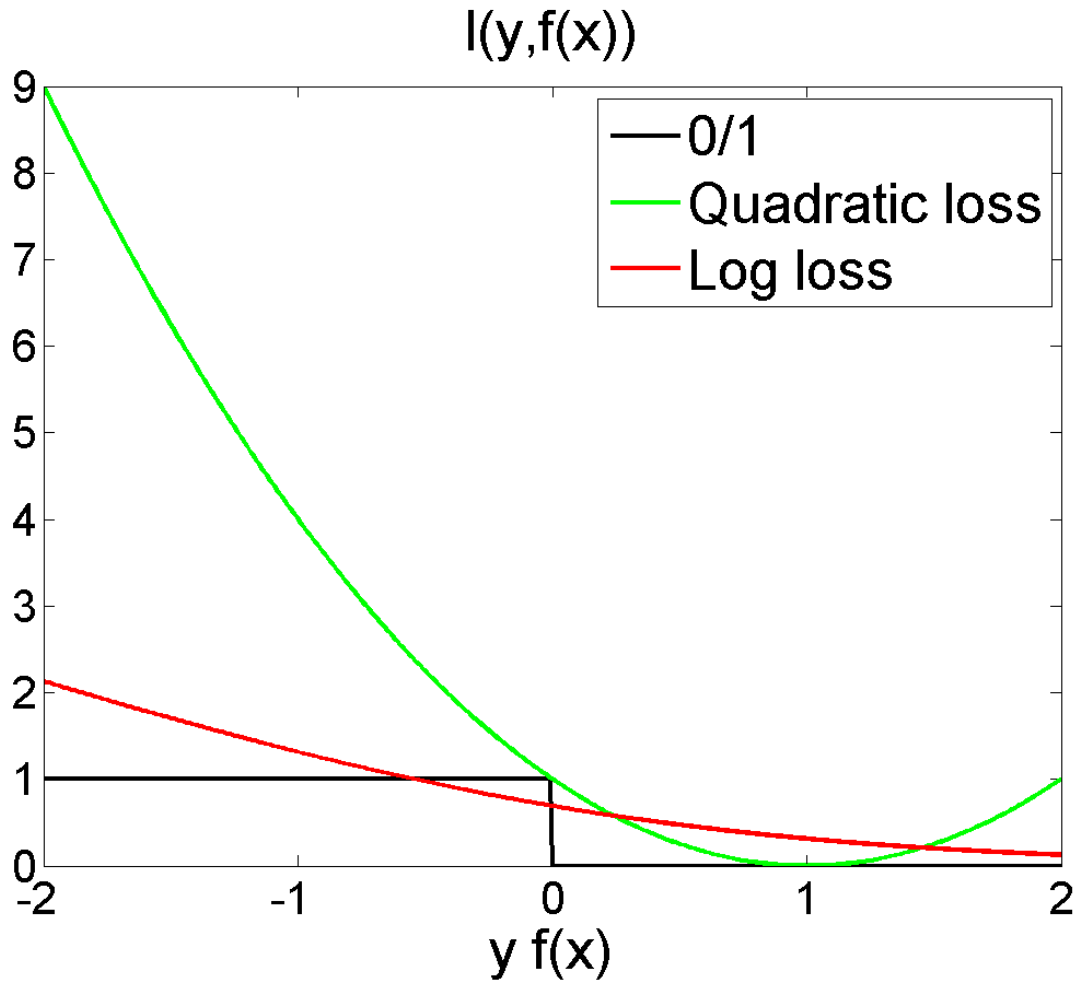


$$P(y^i|\mathbf{x}^i) = \frac{\exp(\mathbf{w}_c^T\mathbf{x})}{\sum_{c'=1}^{C}\exp(\mathbf{w}_{c'}^T\mathbf{x})}$$

?

geometry + classification?

Week 2: log loss vs. quadratic loss



Quadratic loss

$$l(y, f(x)) = (1 - yf(x))^2$$

Log loss

$$l(y, f(x)) = \log(1 + \exp(-yf(x)))$$

Do we need the logistic loss?

Week 2: Useful criterion for training classifiers

Maybe we can quickly hack an easy algorithm

Least squares: Gauss, 1795

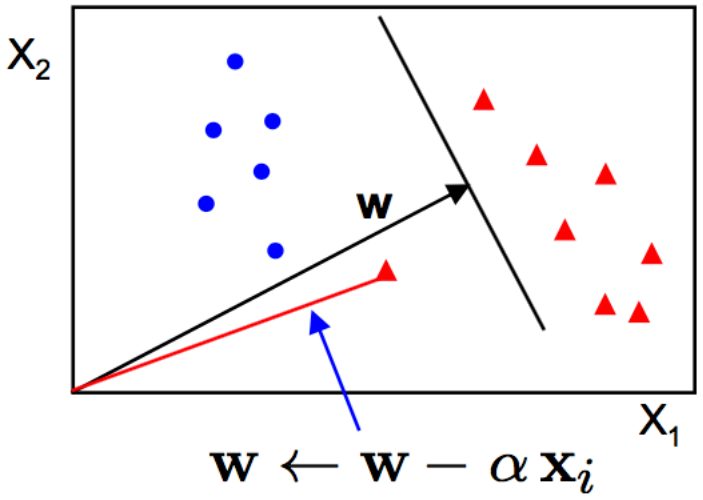
Logistic Regression: Cox, 1958

Perceptrons, Minsky & Papert, 1969

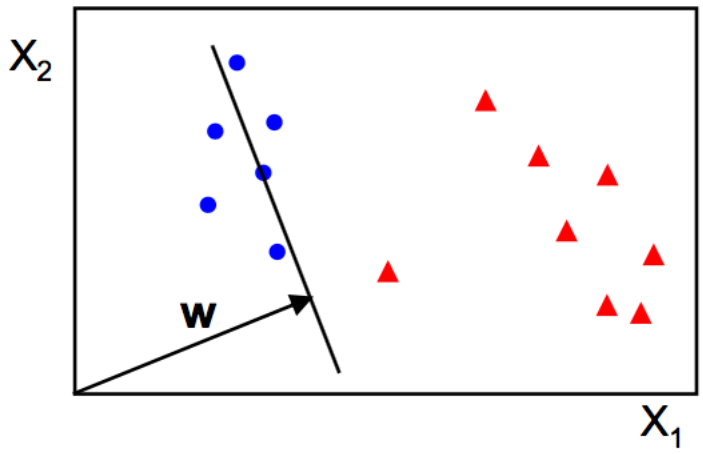
Perceptron algorithm

- Initialize $\mathbf{w} = 0$
- Cycle though the data points $\{ \mathbf{x}_i, y_i \}$
  - if $\mathbf{x}_i$ is misclassified then $\mathbf{w} \leftarrow \mathbf{w} + \alpha \, \text{sign}(f(\mathbf{x}_i)) \, \mathbf{x}_i$
- Until all the data is correctly classified

before update



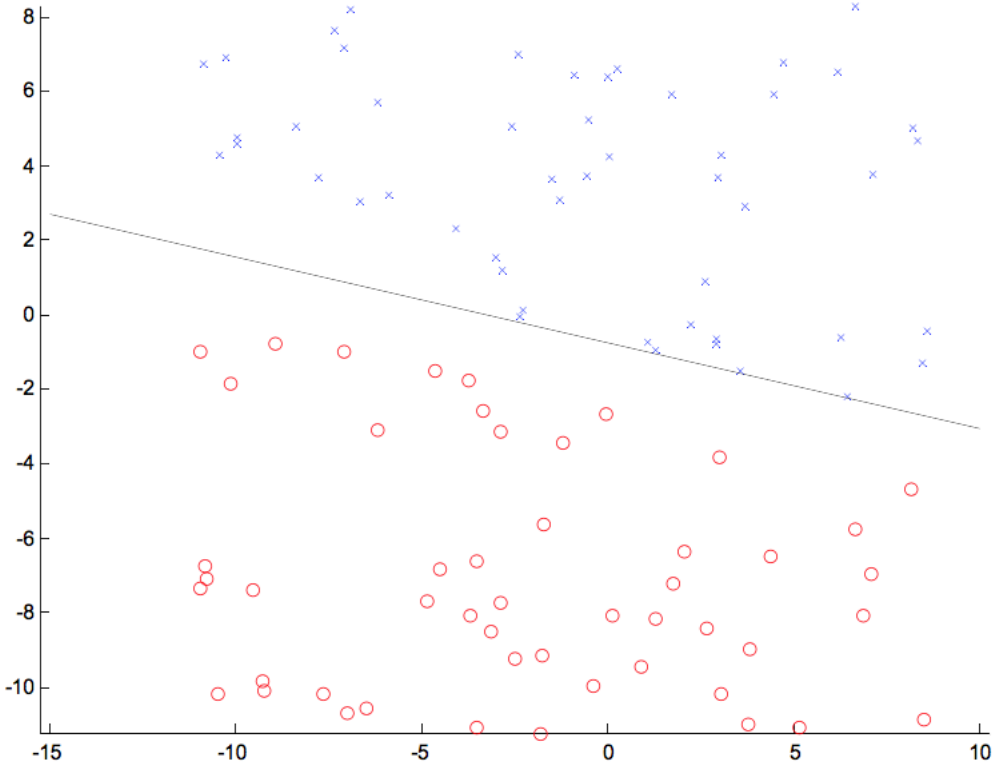
after update



after convergence $\mathbf{w} = \sum_i^N \alpha_i \mathbf{x}_i$

Perceptron algorithm (first 'neural network')

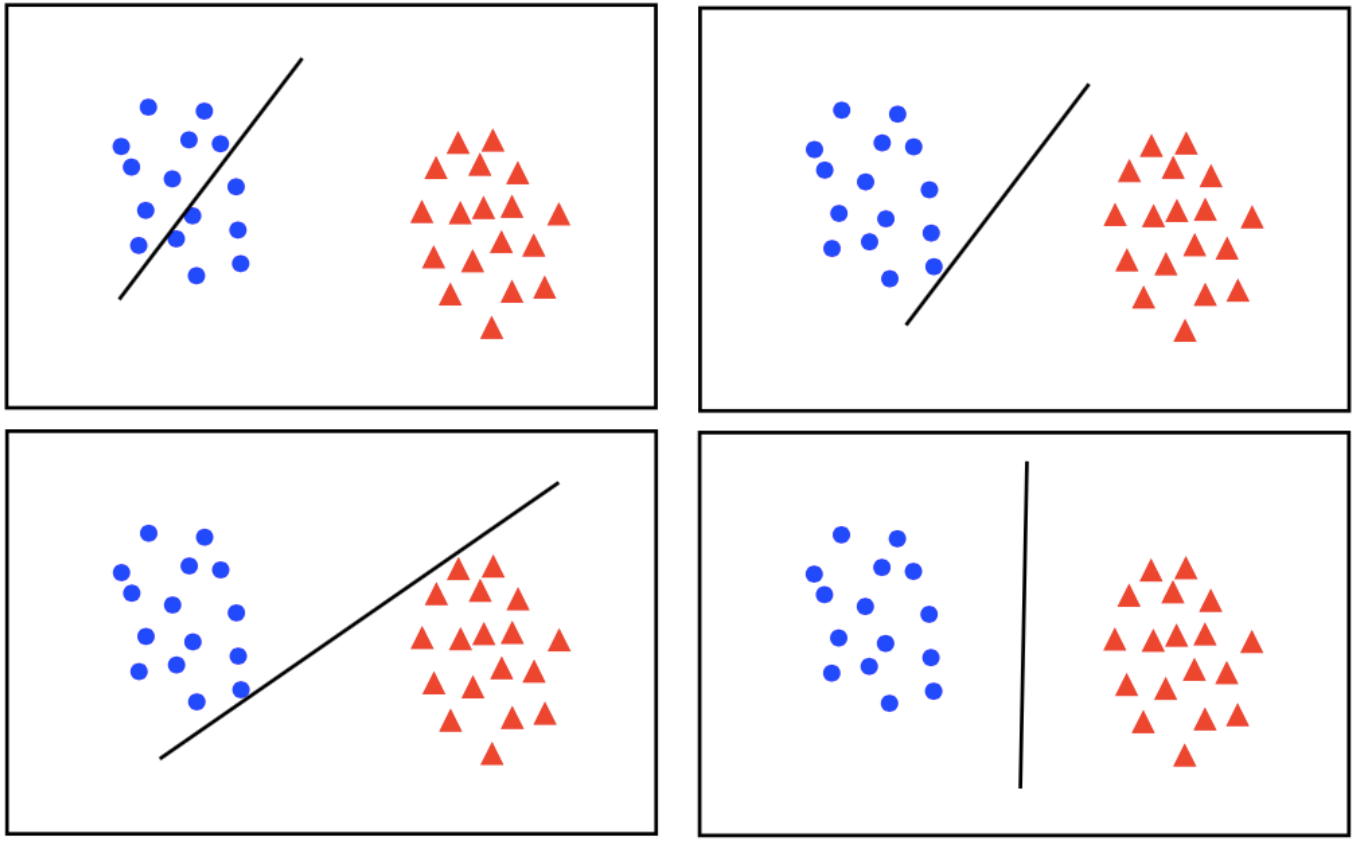
Perceptron example



- if the data is linearly separable, then the algorithm will converge
- convergence can be slow …
- separating line close to training data

This lecture: push it far away!

Which classifier is best?



All points should lie **clearly** on the correct side of the boundary

How can we quantify this?

How can we enforce this?

Functional Margins

Consider Logistic Regression:

$$P(y = 1|\mathbf{x}; \mathbf{w}) = g(\mathbf{w}^T\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T\mathbf{x})}$$

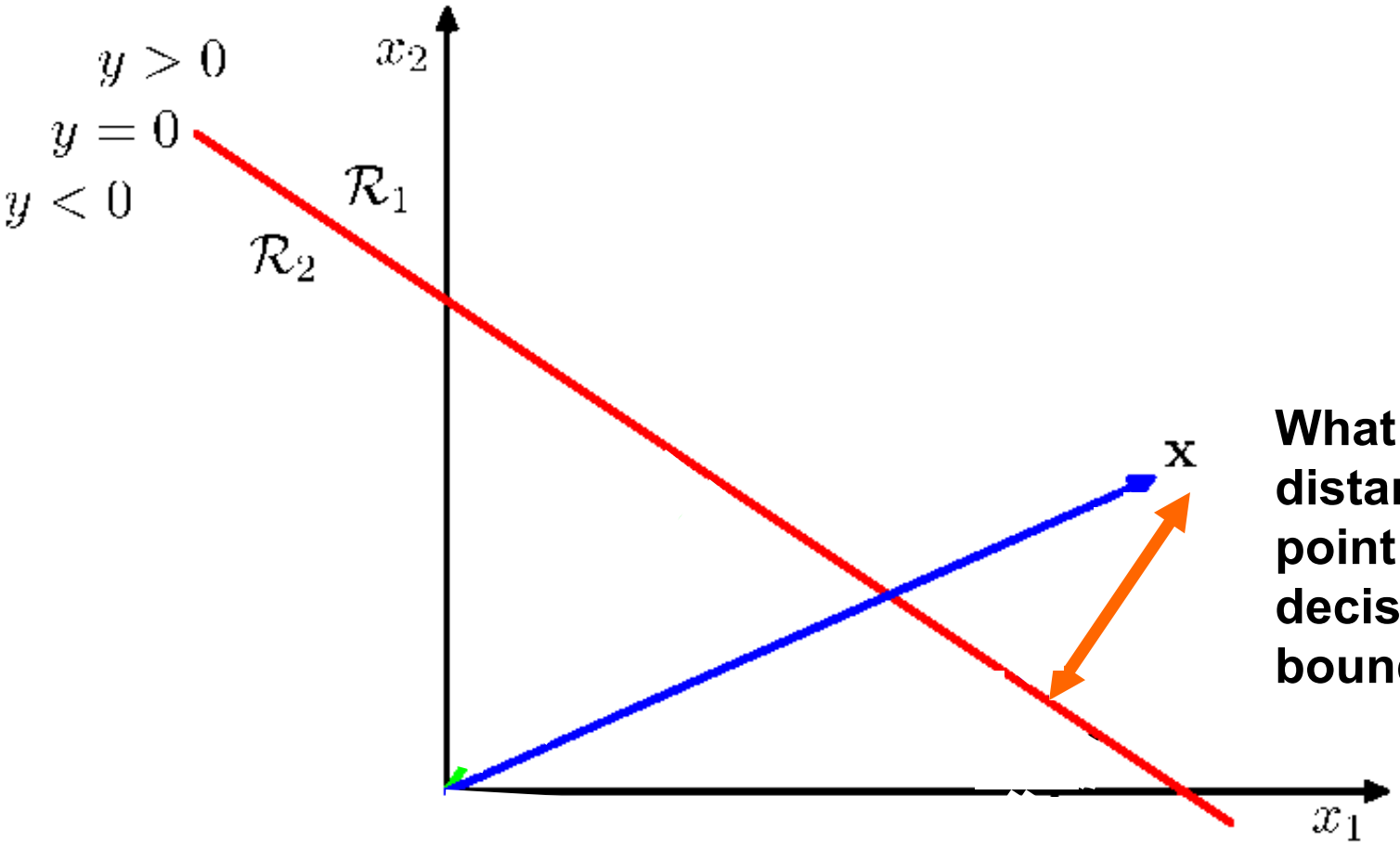
Ideally:
$$\mathbf{w}^T\mathbf{x}^i \gg 0, \quad \text{if} \quad y^i = 1$$
$$\mathbf{w}^T\mathbf{x}^i \ll 0, \quad \text{if} \quad y^i = -1$$

Put together: $y^i(\mathbf{w}^T\mathbf{x}^i) \gg 0$

`functional margin'

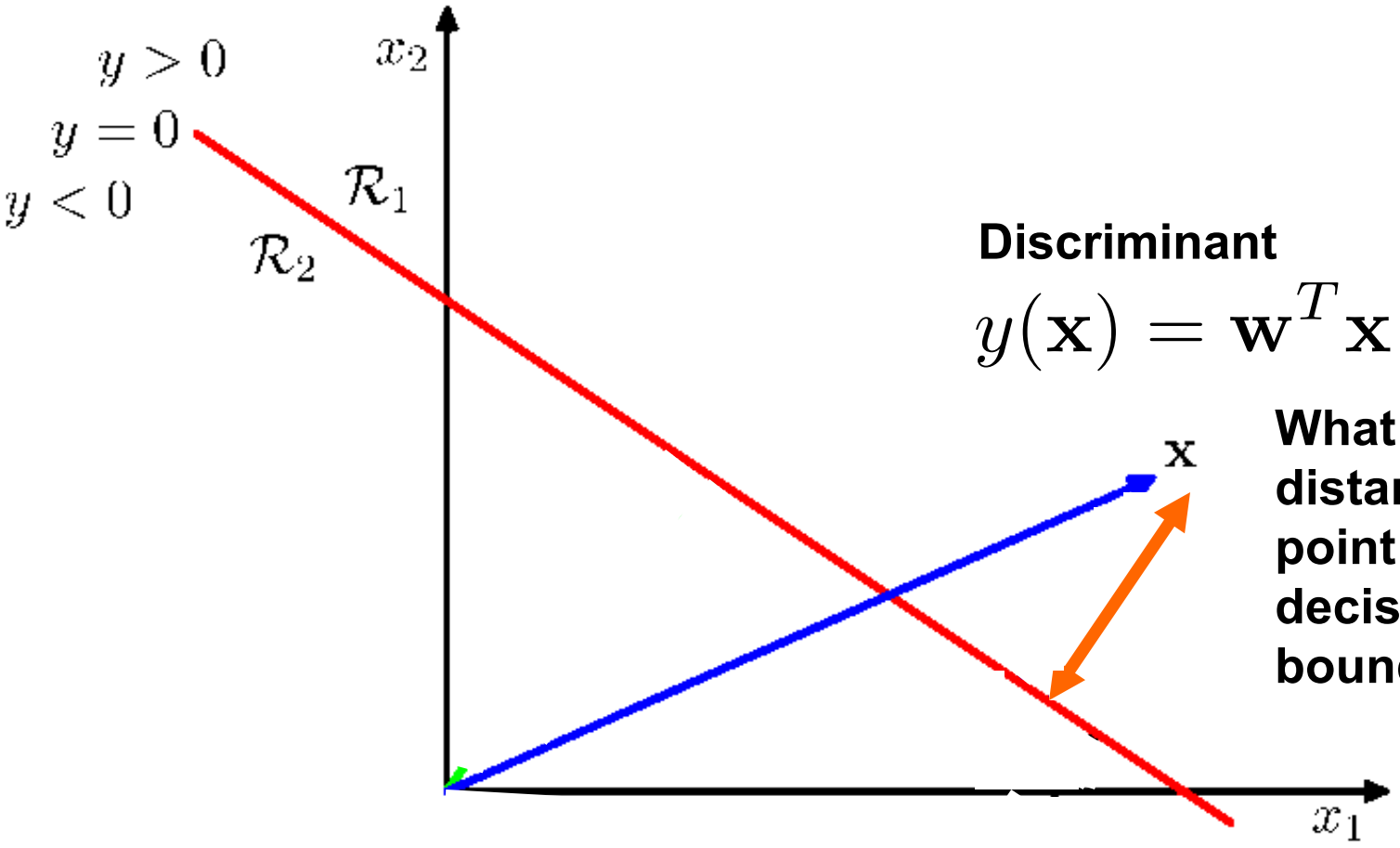
Problem: scaling **w** changes functional margin, but not decision boundary

Geometric Margins



What is the distance of this point from the decision boundary?

Geometric Margins

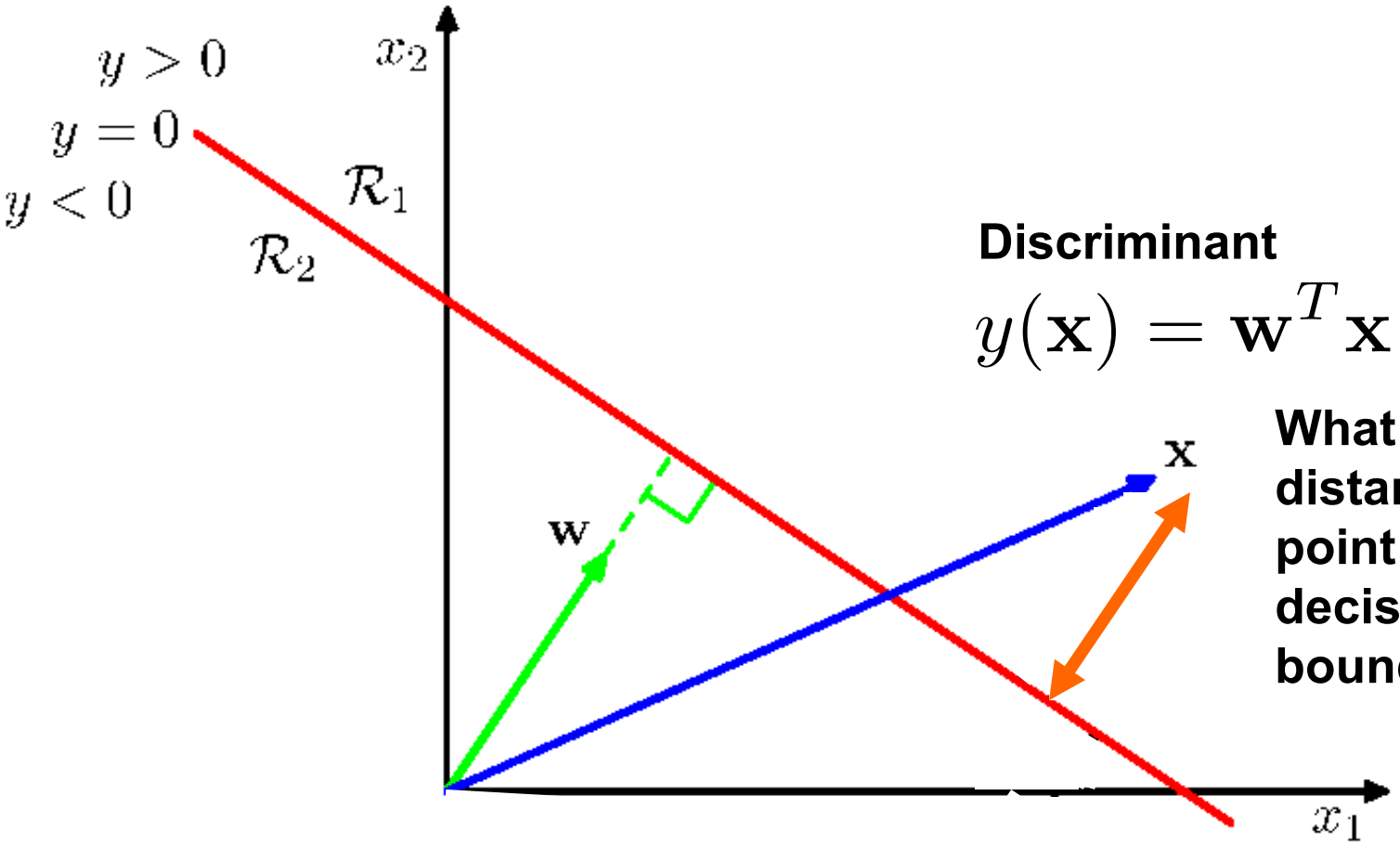


Discriminant

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

What is the distance of this point from the decision boundary?

Geometric Margins



Discriminant

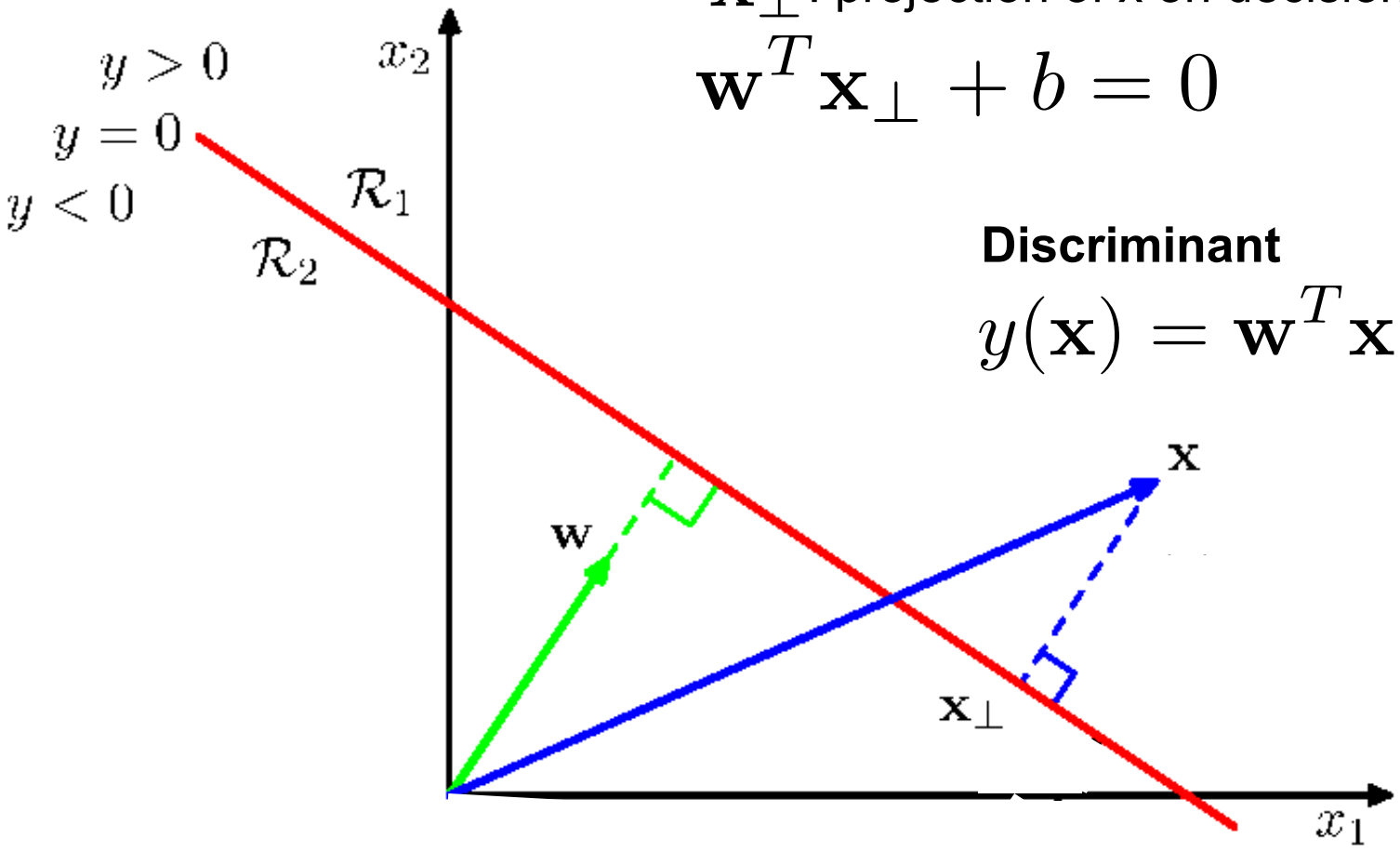
$$y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$

What is the distance of this point from the decision boundary?

Geometric Margins

$\mathbf{x}_\perp$: projection of x on decision boundary

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

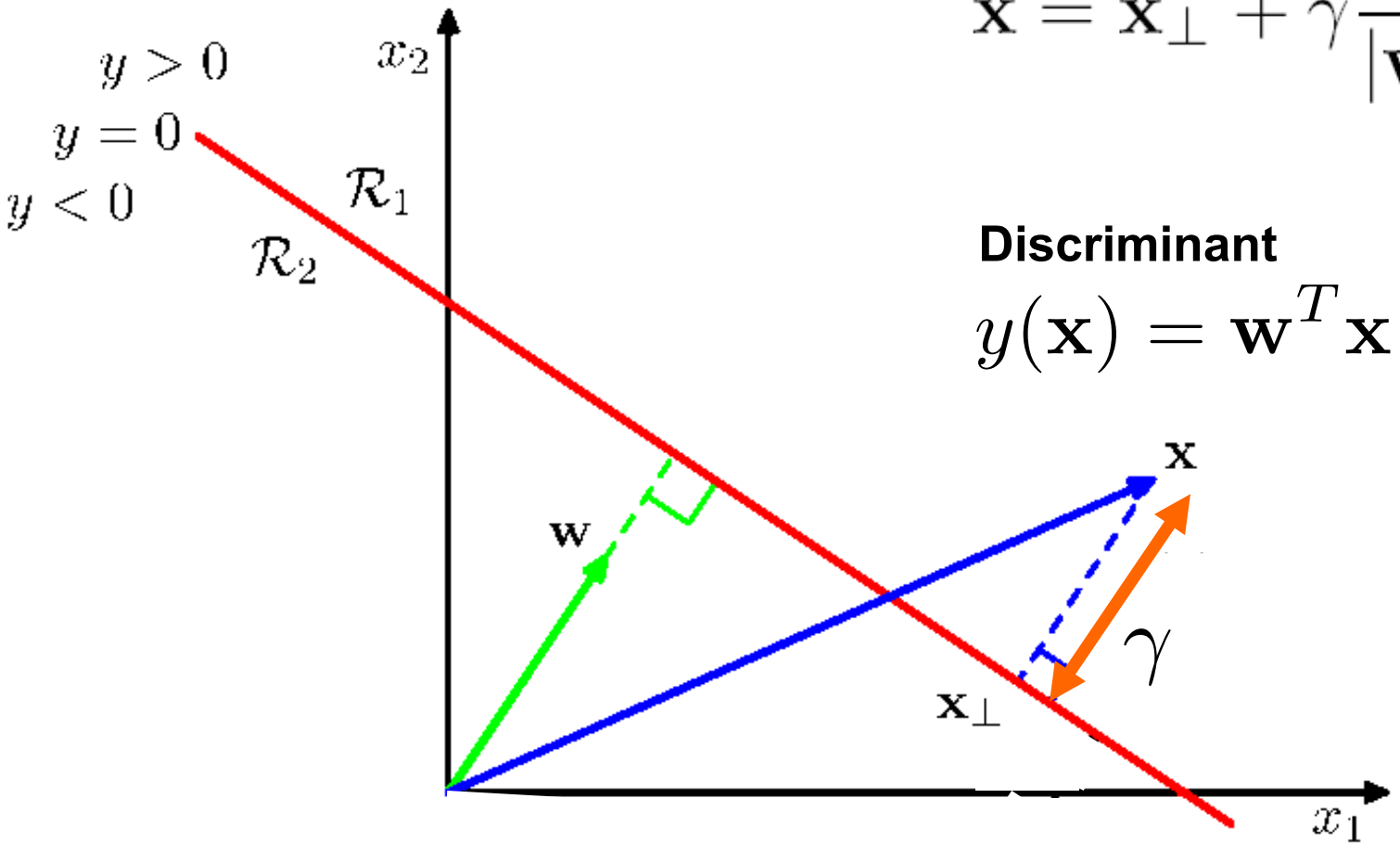


Discriminant

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

Geometric Margins

$$\mathbf{x} = \mathbf{x}_\perp + \gamma \frac{\mathbf{w}}{|\mathbf{w}|}$$



Discriminant

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

Geometric Margins

Point = projection + distance* direction

$$\mathbf{x} = \mathbf{x}_\perp + \gamma \frac{\mathbf{w}}{|\mathbf{w}|}$$

Note: γ is independent of |w|

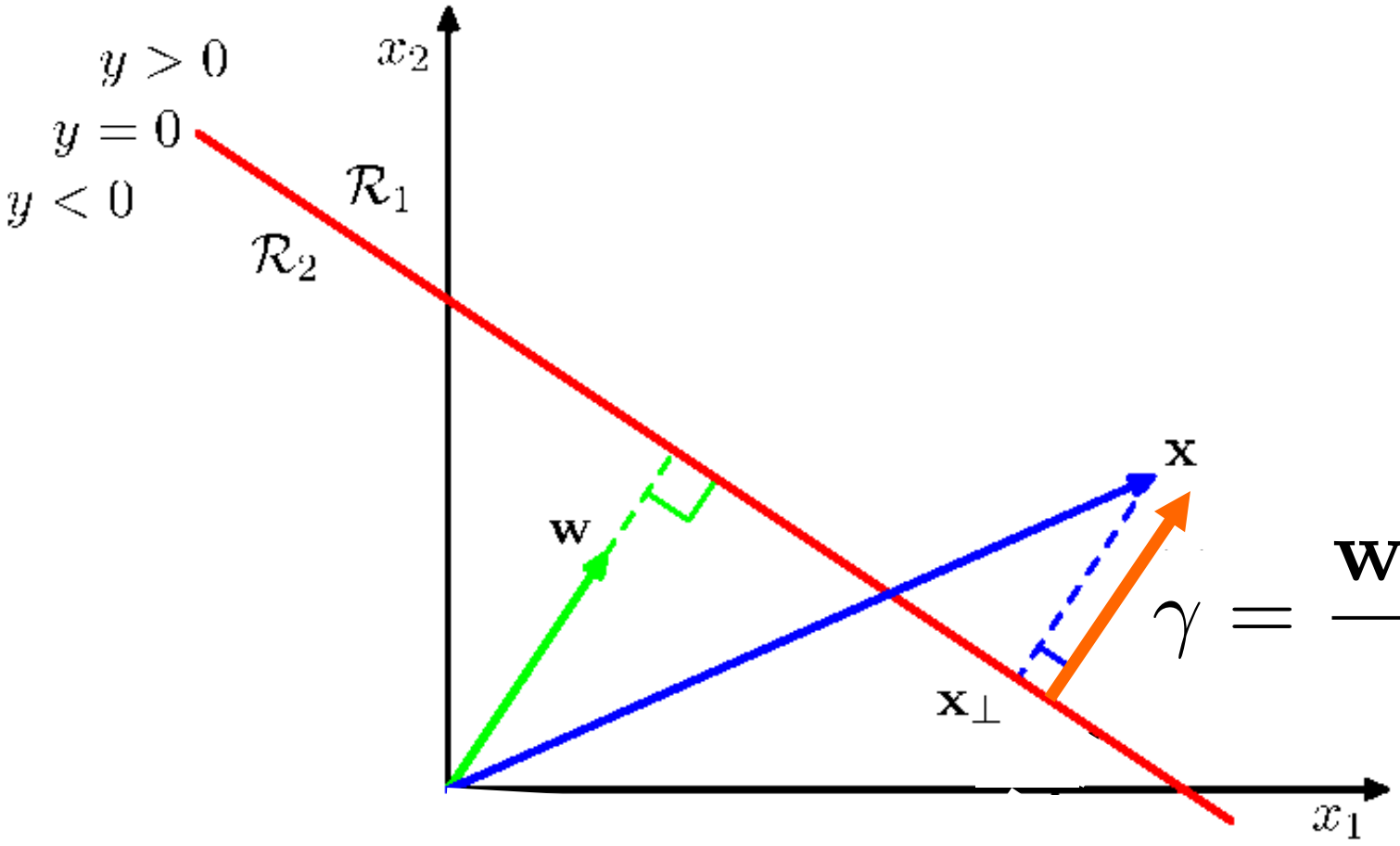
Multiply: $$\mathbf{w}^T\mathbf{x} = \mathbf{w}^T\mathbf{x}_\perp + \mathbf{w}^T\gamma \frac{\mathbf{w}}{|\mathbf{w}|}$$

Rewrite ($\mathbf{w}^T\mathbf{x}_\perp + b = 0$) :

$$\mathbf{w}^T\mathbf{x} = -b + \gamma|\mathbf{w}|$$

Solve for γ: $$\gamma = \frac{\mathbf{w}^T\mathbf{x} + b}{|\mathbf{w}|} = \frac{\mathbf{w}^T}{|\mathbf{w}|}\mathbf{x} + \frac{b}{|\mathbf{w}|}$$

Geometric Margins

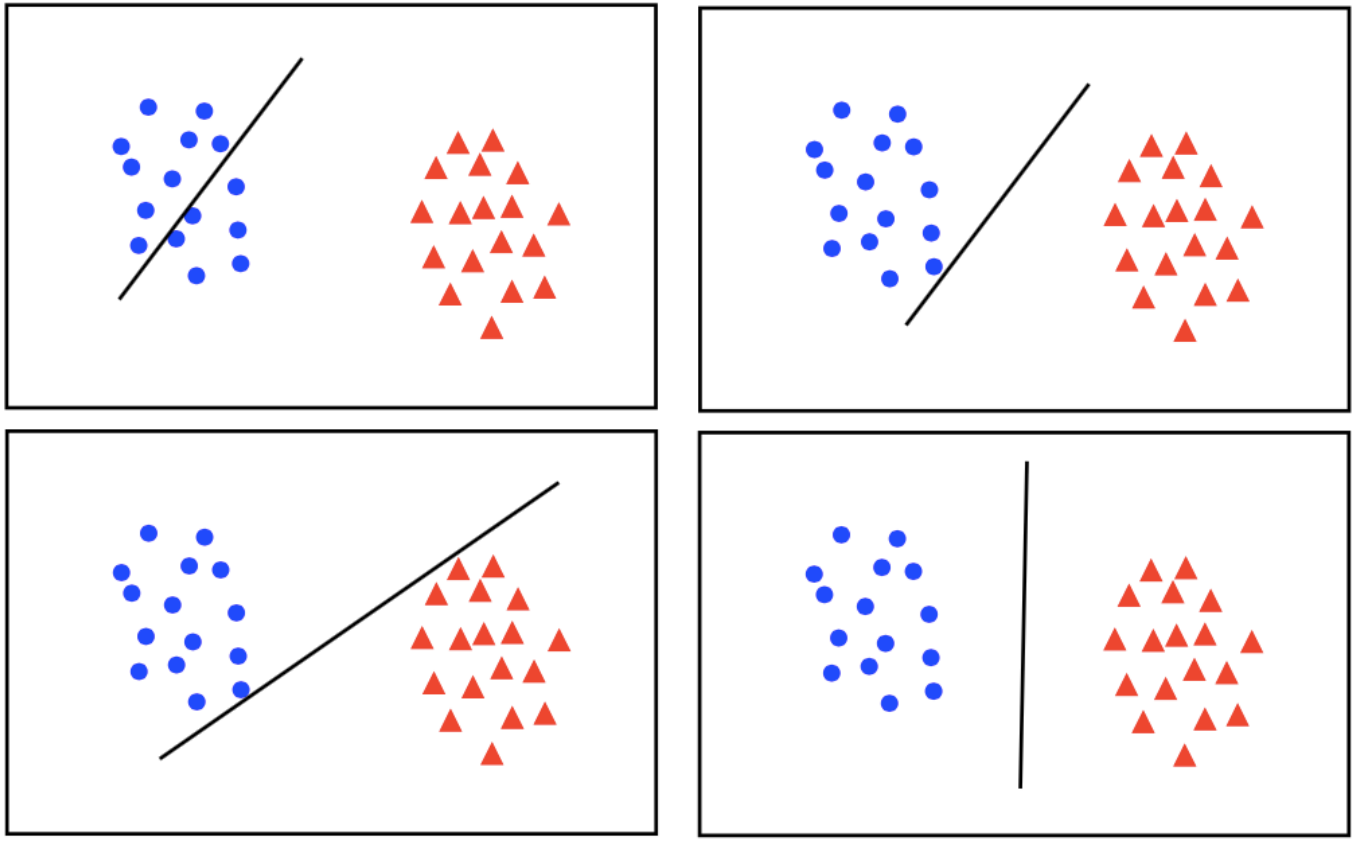


$$\gamma = \frac{\mathbf{w}^T\mathbf{x} + b}{|\mathbf{w}|}$$

Geometric Margin: $\gamma^i = y^i \left(\frac{\mathbf{w}^T}{|\mathbf{w}|}\mathbf{x}^i + \frac{b}{|\mathbf{w}|} \right)$

(positive if x is on the correct size of the decision boundary)

Which classifier is best?



All points should lie **clearly** on the correct side of the boundary

How can we quantify this? (large margins!)

How can we enforce this?

Lecture outline

- Introduction to Support Vector Machines
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- Large margins and generalization
- Optimization
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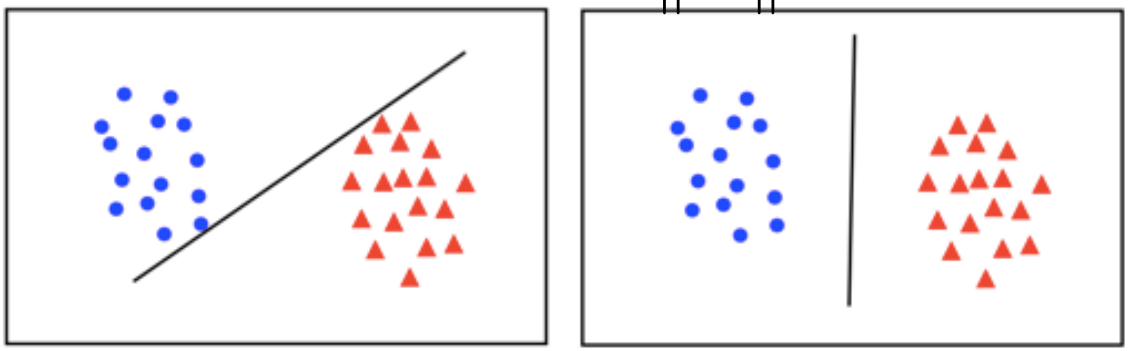
What should we be optimizing?

Training set: $\{(\mathbf{x}^1, y^1), \ldots, (\mathbf{x}^N, y^N)\}$

Candidate parameter vector: $(\mathbf{w}, b)$

Related margins: $\gamma^i = y^i \dfrac{\mathbf{w}^T \mathbf{x}^i + b}{\|\mathbf{w}\|}$



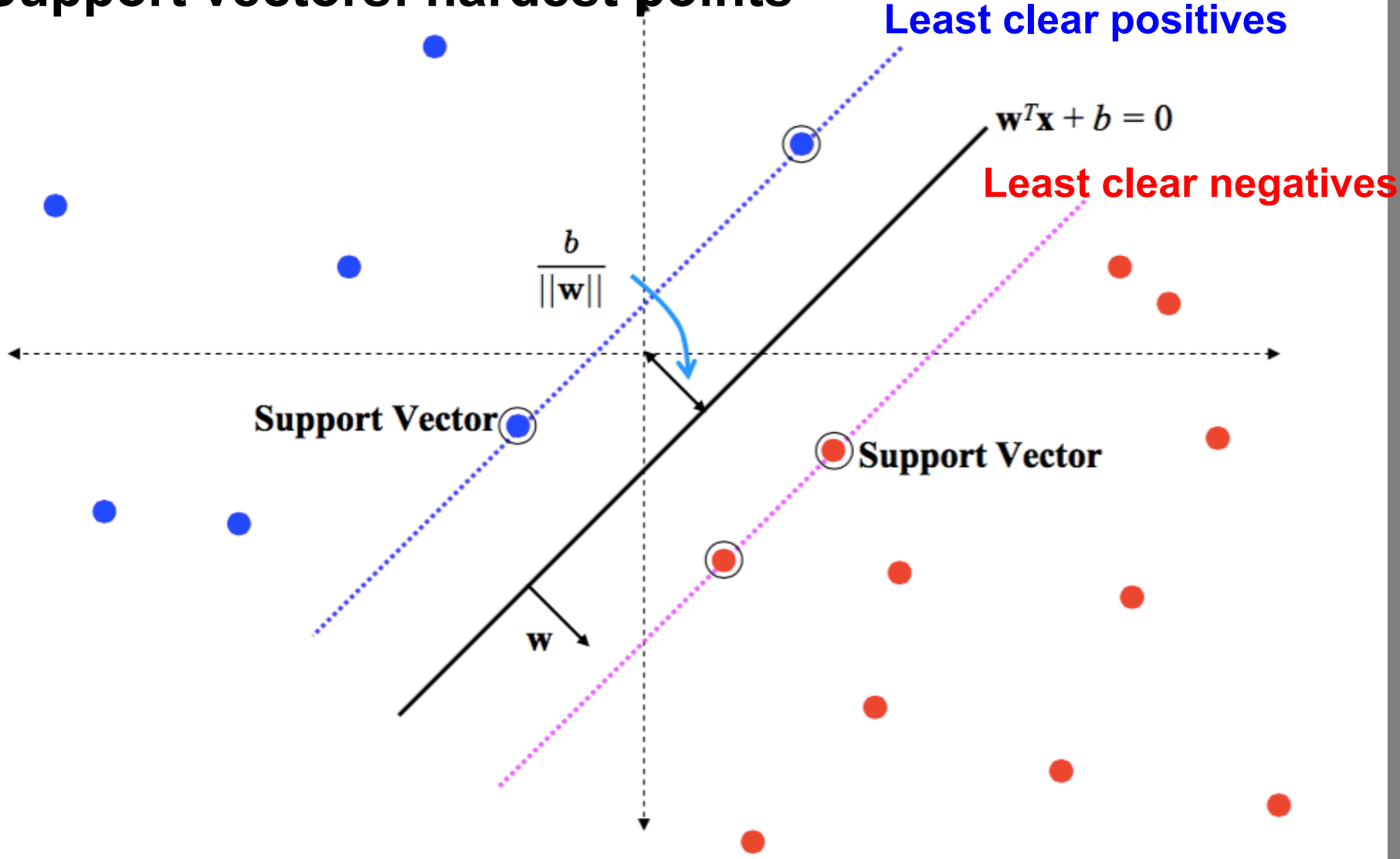
Should we be optimizing the mean, max, min margin?

All points should lie **clearly** on the correct side of the boundary

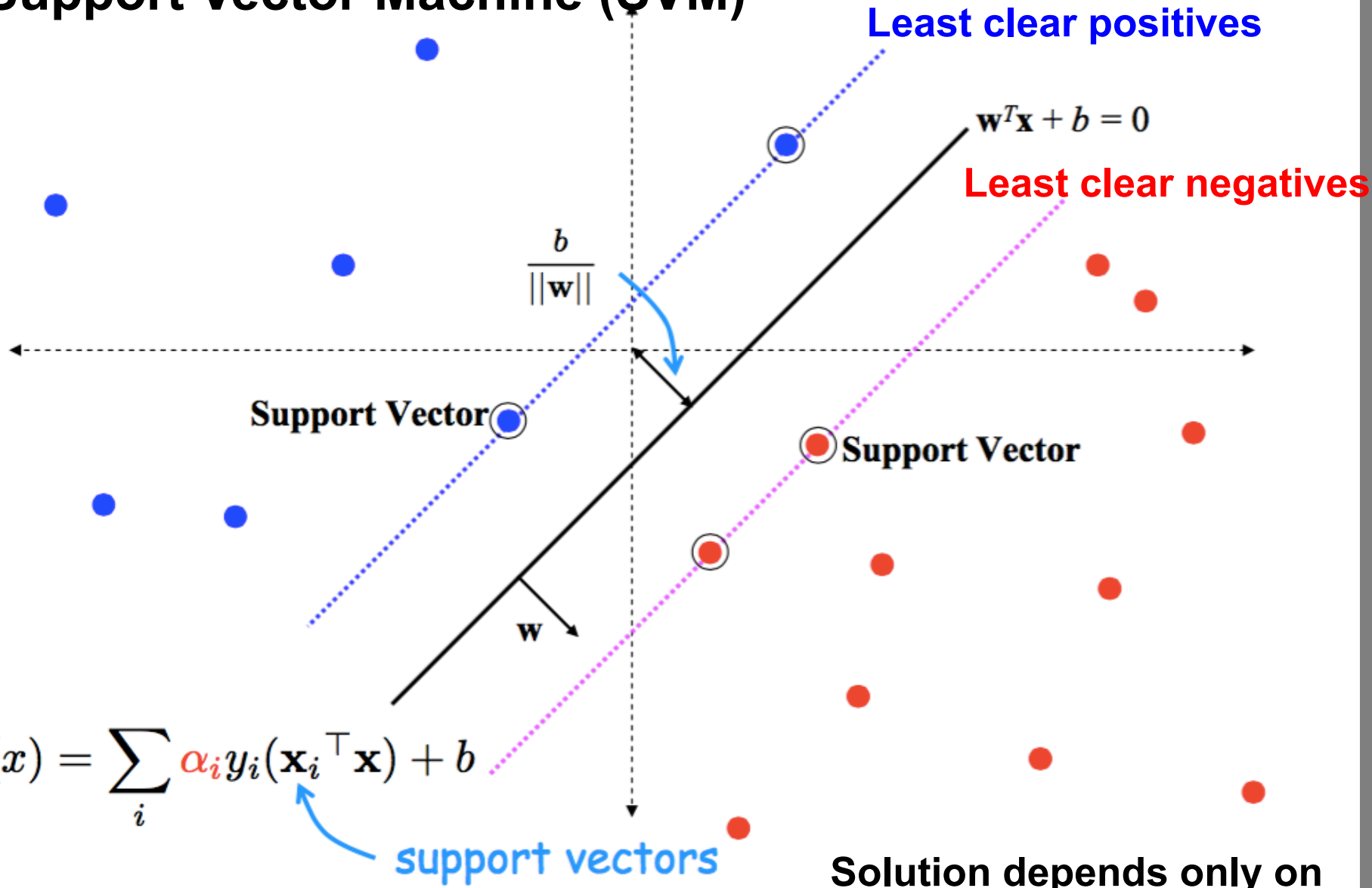
1) Take points that do not lie clearly on the correct side

2) Make sure they do

Support vectors: hardest points



Support Vector Machine (SVM)



Solution depends only on hardest points

SVM, sketch of 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

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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 of derivation

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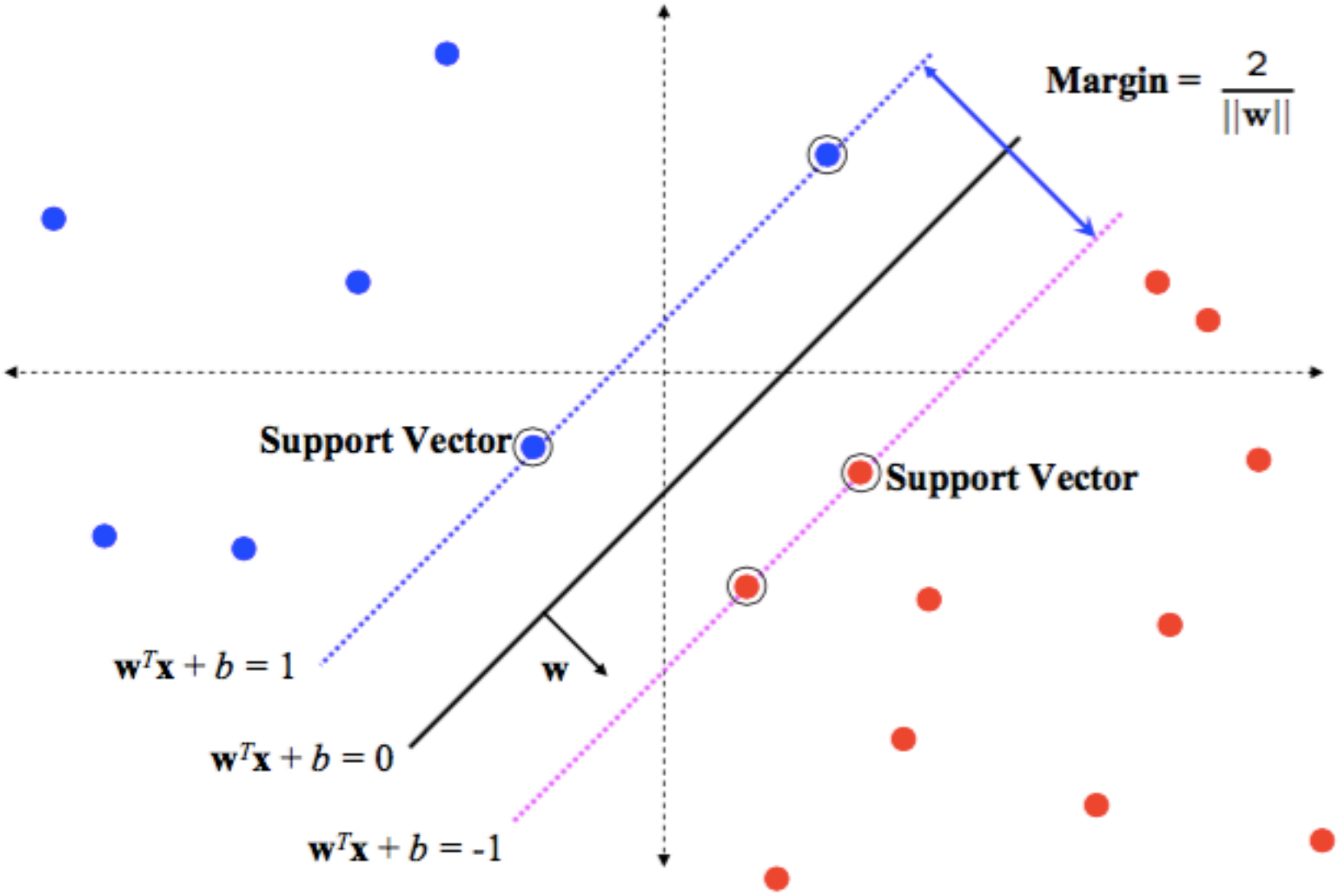
- Choose normalization such that $\mathbf{w}^\top \mathbf{x}_+ + b = +1$ and $\mathbf{w}^\top \mathbf{x}_- + b = -1$ for the positive and negative support vectors respectively

- Then the margin is given by

$$\frac{\mathbf{w}^\top \left(\mathbf{x}_+ - \mathbf{x}_-\right)}{||\mathbf{w}||} = \frac{2}{||\mathbf{w}||}$$

Support Vector Machine (SVM)



Representer theorem

Objective: find **w** that maximizes the margin subject to margin constraints

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

$$\text{s.t.} \quad y^i \left(\mathbf{w}^T \mathbf{x}^i + b\right) \geq 1 \quad \forall i$$

Equivalently:

$$\min_{\mathbf{w}} \|\mathbf{w}\|^2$$

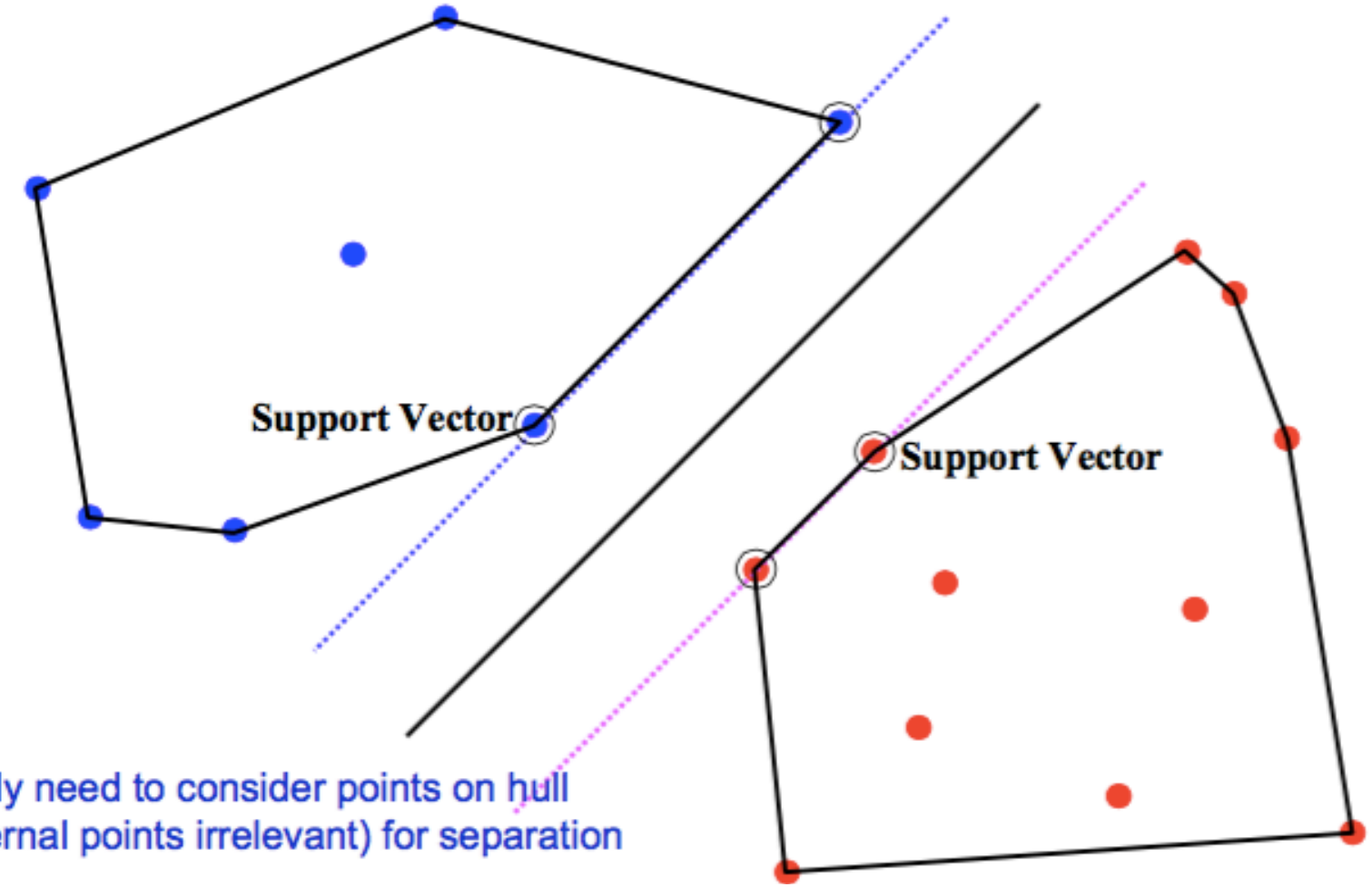
$$\text{s.t.} \quad y^i \left(\mathbf{w}^T \mathbf{x}^i + b\right) \geq 1 \quad \forall i$$

Representer Theorem: $\mathbf{w}^* = \sum_{i=1}^{N} \alpha^i \left(y^i \mathbf{x}^i\right)$

Geometric algorithm

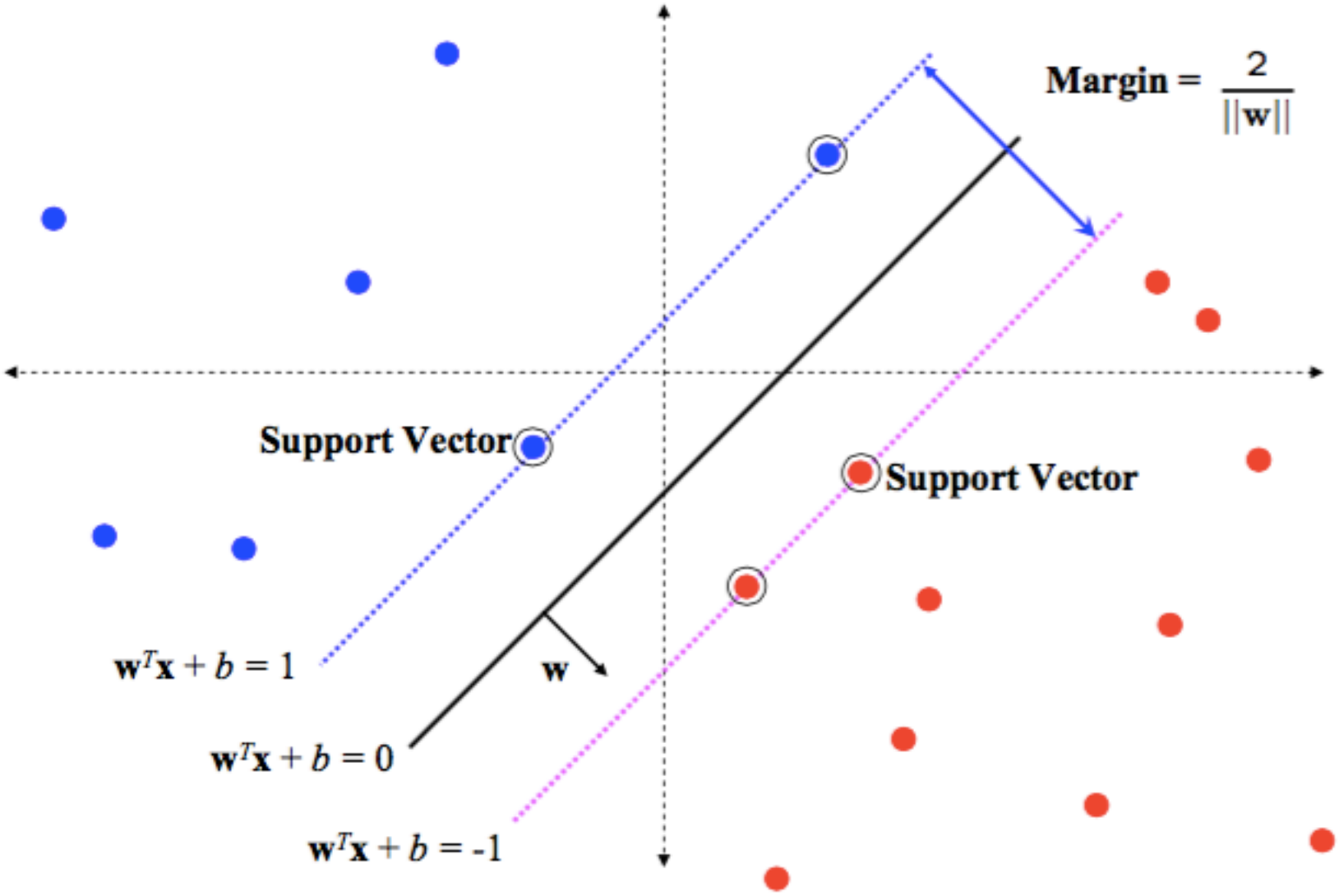
- Compute the convex hull of the positive points, and the convex hull of the negative points
- For each pair of points, one on positive hull and the other on the negative hull, compute the margin
- Choose the largest margin

Intuitive justification of theorem



• only need to consider points on hull
(internal points irrelevant) for separation

Support Vector Machine (SVM)



Primal and dual problems

Primal, in terms of **w:**

$$\min_{\mathbf{w}} \|\mathbf{w}\|^2$$
$$\text{s.t.}: \quad y^i(\mathbf{w}^T\mathbf{x}^i + b) \geq 1, \quad \forall i$$

But: $\|\mathbf{w}^*\|^2 = \langle \mathbf{w}^*, \mathbf{w}^* \rangle$

$$\mathbf{w}^* = \sum_{i=1}^{N} \alpha^i \left(y^i \mathbf{x}^i\right)$$
$$= \left\langle \sum_{i=1}^{N} \alpha^i y^i \mathbf{x}^i, \sum_{j=1}^{N} \alpha^j y^j \mathbf{x}^j \right\rangle = \sum_{i=1}^{N}\sum_{j=1}^{N} \alpha^i \alpha^j y^i y^j \langle \mathbf{x}^i, \mathbf{x}^j \rangle$$

Dual, in terms of $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_N)$:

$$\min_{\boldsymbol{\alpha}} \sum_{i=1}^{N}\sum_{j=1}^{N} \alpha^i \alpha^j y^i y^j \langle \mathbf{x}^i, \mathbf{x}^j \rangle$$
$$\text{s.t.}: \quad y^i \left(\sum_{j=1}^{N} \alpha^j y^j \langle \mathbf{x}^j, \mathbf{x}^i \rangle + b \right) \geq 1, \quad i = 1, \ldots, N$$

Primal vs dual

Primal:
$$\min_{\mathbf{w}} \|\mathbf{w}\|^2 \qquad \mathbf{w} \in \mathbb{R}^D \rightarrow O(D^3)$$
$$\text{s.t. :} \quad y^i(\mathbf{w}^T\mathbf{x}^i + b) \geq 1, \quad \forall i$$

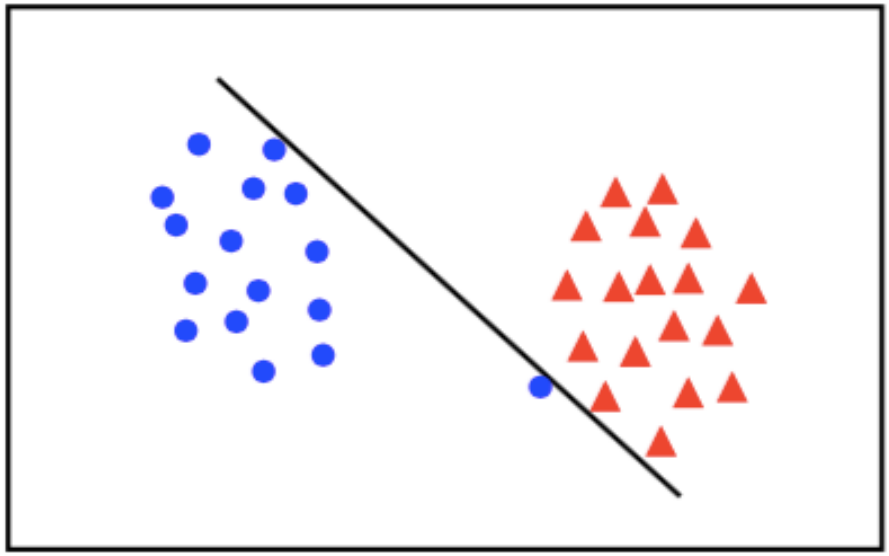
Dual:
$$\min_{\boldsymbol{\alpha}} \sum_{i=1}^{N}\sum_{j=1}^{N} \alpha^i \alpha^j y^i y^j \langle \mathbf{x}^i, \mathbf{x}^j \rangle \qquad \boldsymbol{\alpha} \in \mathbb{R}^N \rightarrow O(N^3)$$
$$\text{s.t. :} \quad y^i \left(\sum_{j=1}^{N} \alpha^j y^j \langle \mathbf{x}^j, \mathbf{x}^i \rangle + b \right) \geq 1, \quad \forall i$$

Dual can be faster if N<D!

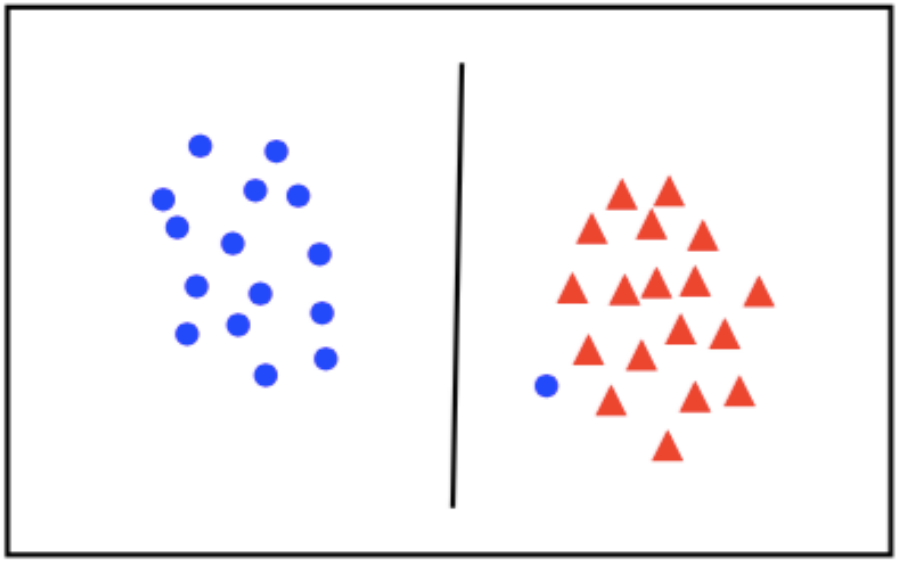
Primal and dual classifier forms:
$$f(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle + b = \sum_{i=1}^{N} \alpha^i y^i \langle \mathbf{x}^i, \mathbf{x} \rangle + b$$

Dual form involves only inner products of features (=> kernel trick)

What is the “best” decision plane?



All points on the correct side!



But this looks better overall!

Best: understood at test time

Maybe we could sacrifice classifying some training points correctly

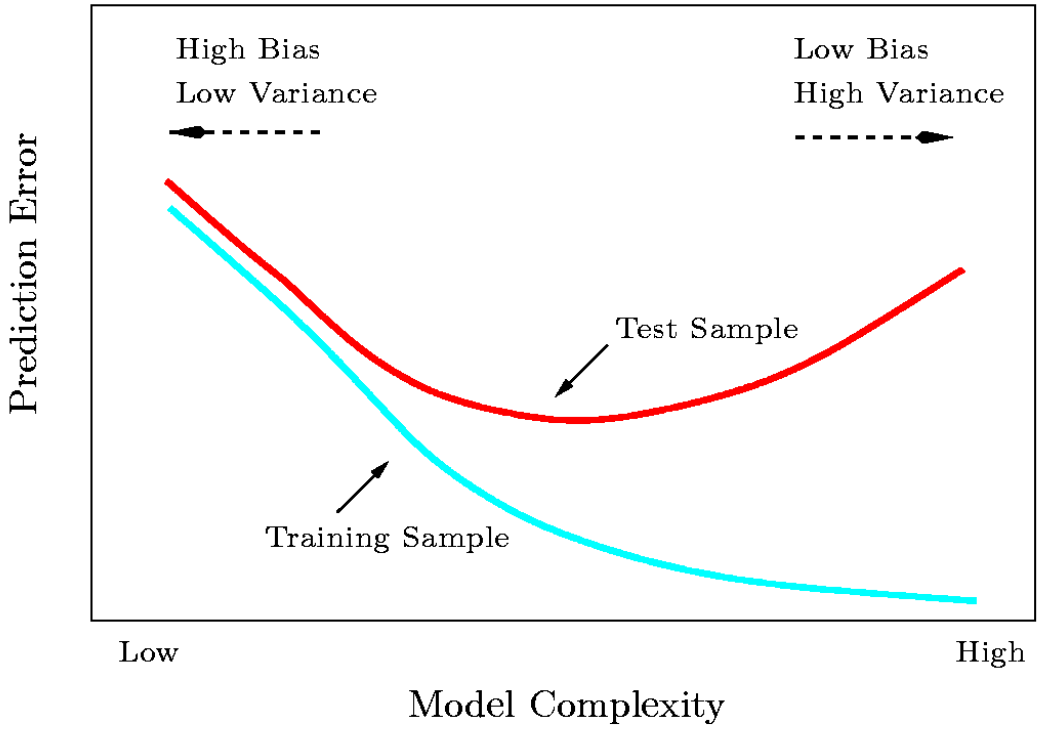
Tuning the model's complexity

A flexible model approximates the target function well in the training set

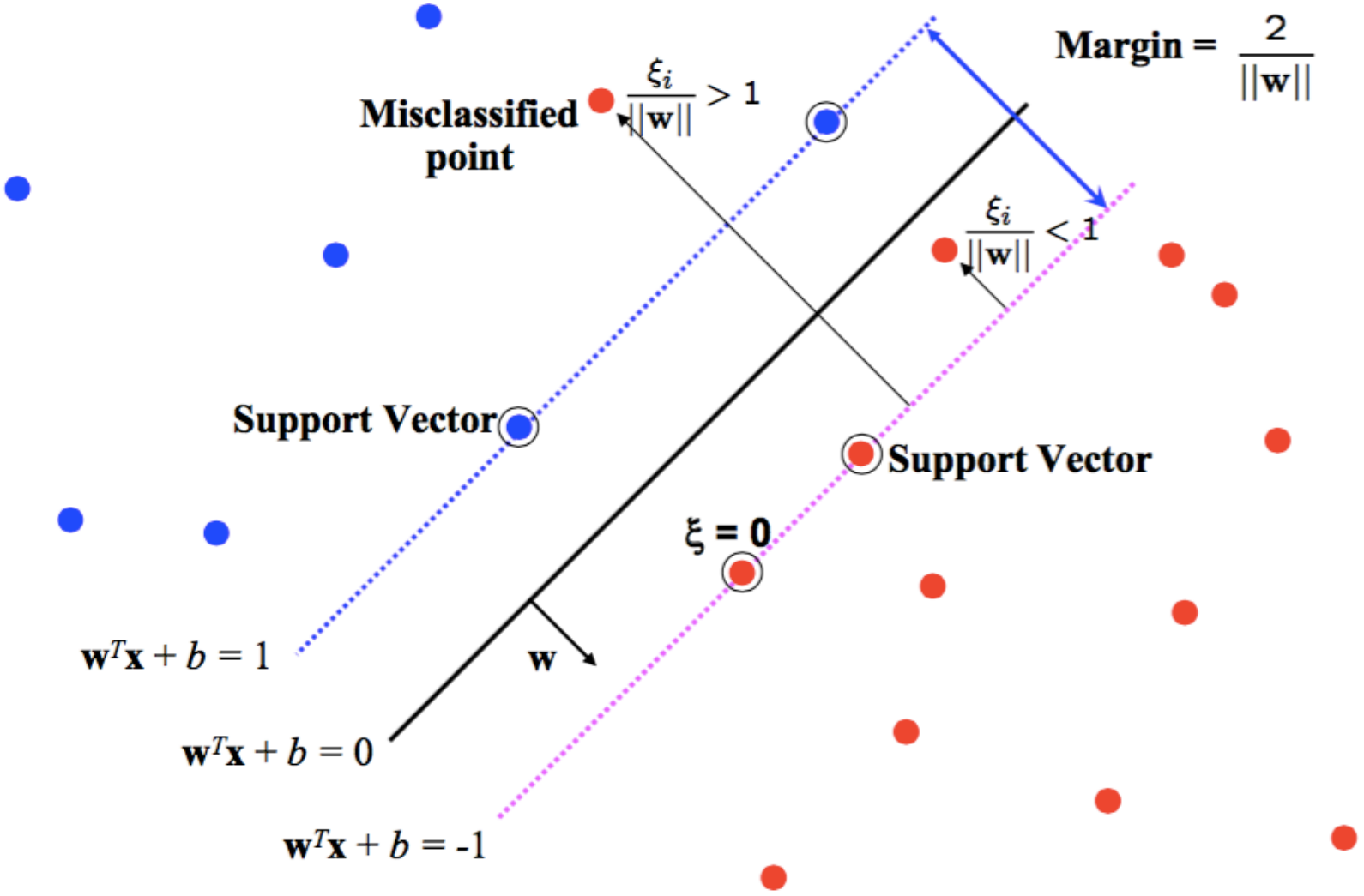
but can "overtrain" and have poor performance on the test set ("variance")

A rigid model's performance is more predictable in the test set

but the model may not be good even on the training set ("bias")



Slack variables: let us make (but also pay) some errors



Objective for non-separable data

$$\min_{\mathbf{w},\boldsymbol{\xi}} \|\mathbf{w}\|^2 + C\sum_{i=1}^{N} \xi^i$$

newcomers

$$\text{s.t.}: \quad y^i(\mathbf{w}^T\mathbf{x}^i + b) \geq 1 - \xi^i \quad \forall i$$

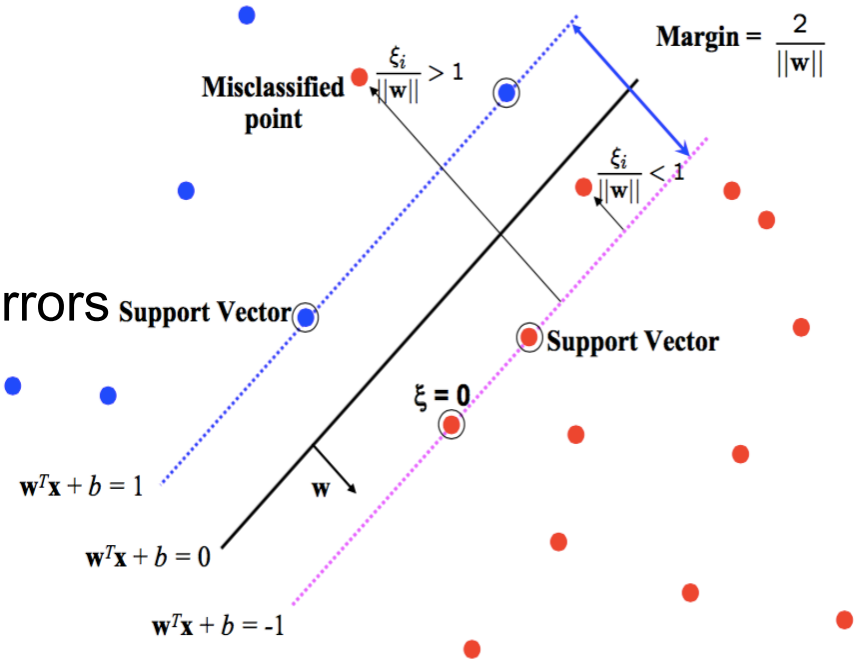
$$\xi^i \geq 0, \quad \forall i$$

misclassification when ξ>1

$\sum_i \xi^i$:upper bound on number of errors

C: hyperparameter

(cross-validation!)



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

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

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 is equivalent to

$$\xi_i = [1 - y_i f(\mathbf{x}_i)]_+$$

where $[.]_+$ indicates the positive part. Hence the optimization problem is equivalent to

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

Loss function

Optimization problem:

$$\min_{\mathbf{w},b} \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\xi^i$$

$$s.t. \quad y^i(\mathbf{w}^T x^i + b) \geq 1 - \xi^i$$

$$\xi^i \geq 0$$

Rewrite constraint: $y^i h_{\mathbf{w},b}(\mathbf{x}) \geq 1 - \xi^i$

Compact form:

$$\xi^i = [1 - y^i h_{\mathbf{w},b}(\mathbf{x})]_+$$

$$= \max(1 - y^i h_{\mathbf{w},b}(\mathbf{x}), 0)$$

What if we plug that in the optimization objective?

Loss function

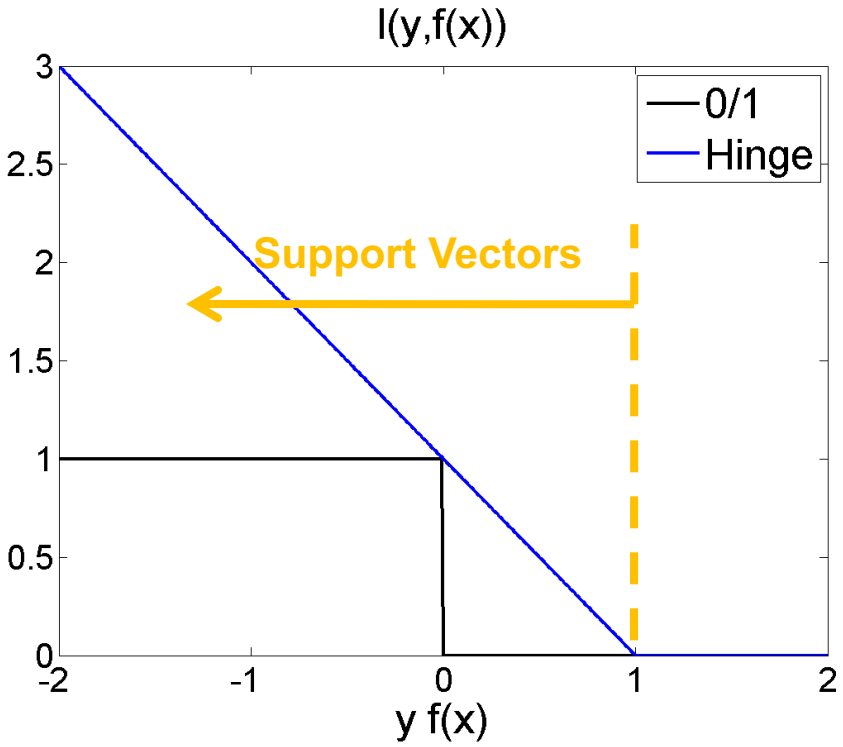
Optimization problem:

$$L(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\max(0, 1 - y^i h_{\mathbf{w},b}(x^i))$$

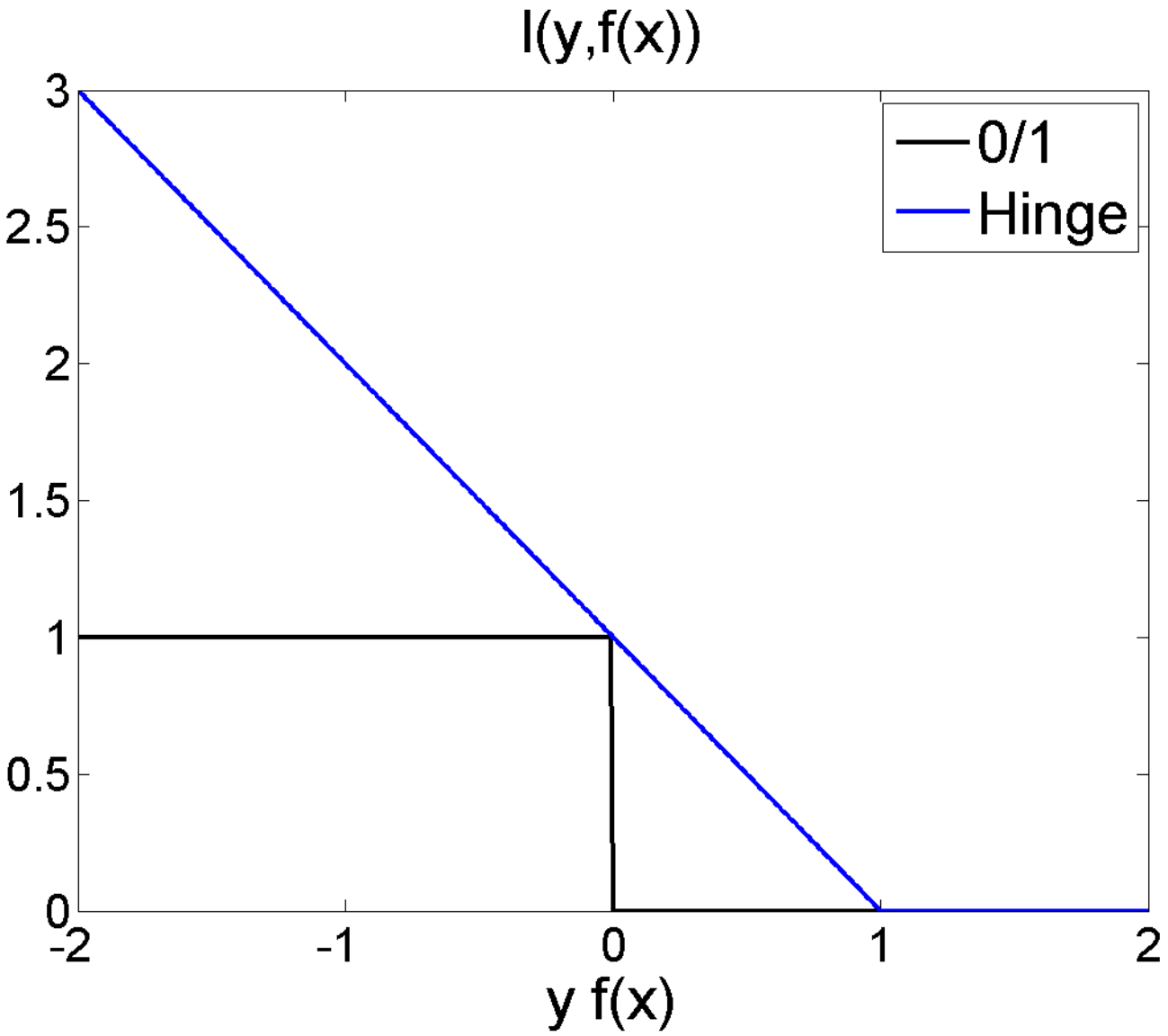
$$\propto \lambda\|\mathbf{w}\|^2 + \sum_{i=1}^{N}\underbrace{\max(0, 1 - y^i h_{\mathbf{w},b}(x^i))}_{l(y^i, x^i)}$$

regularizer **additive loss**

Hinge loss:

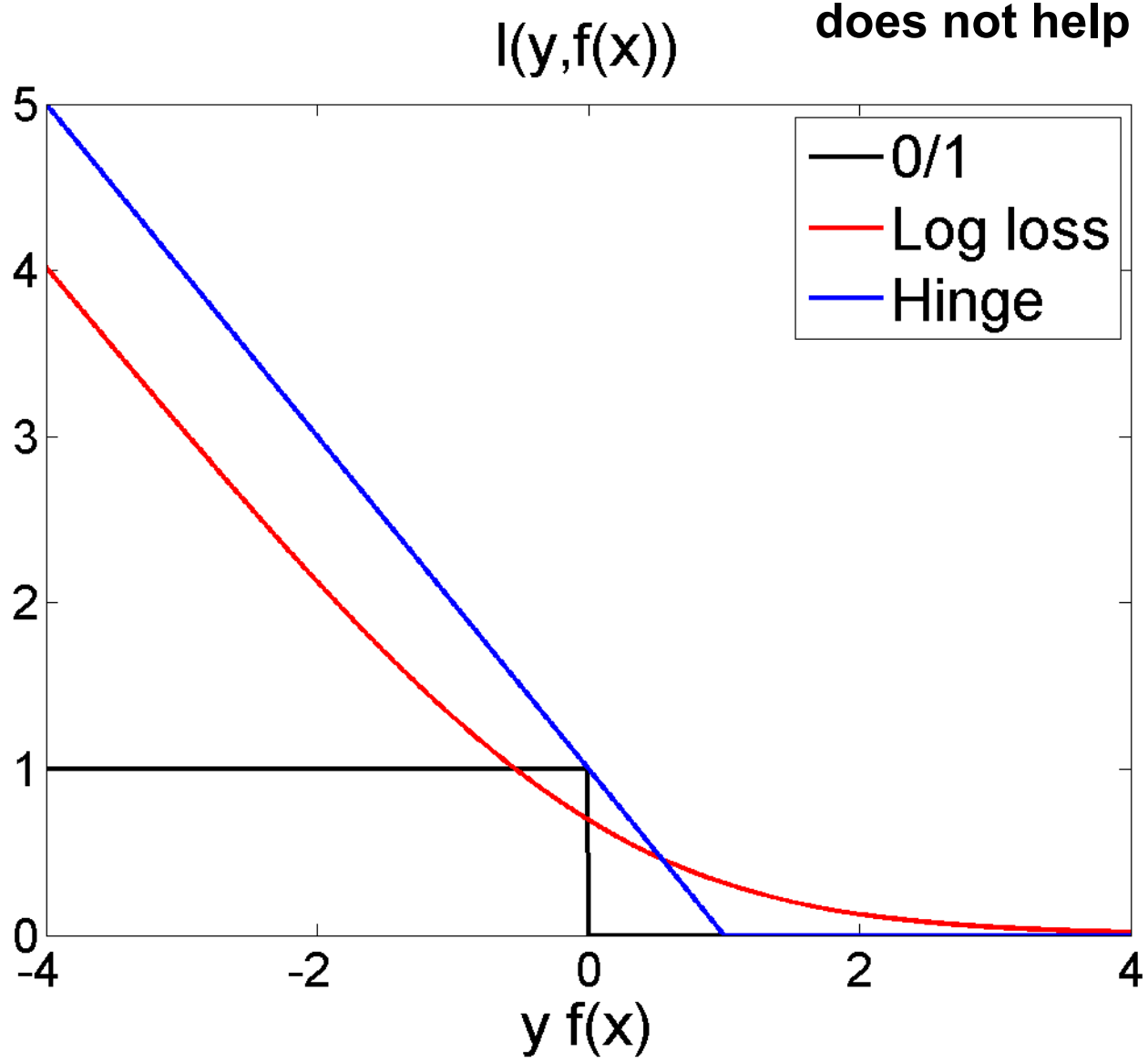


Hinge loss

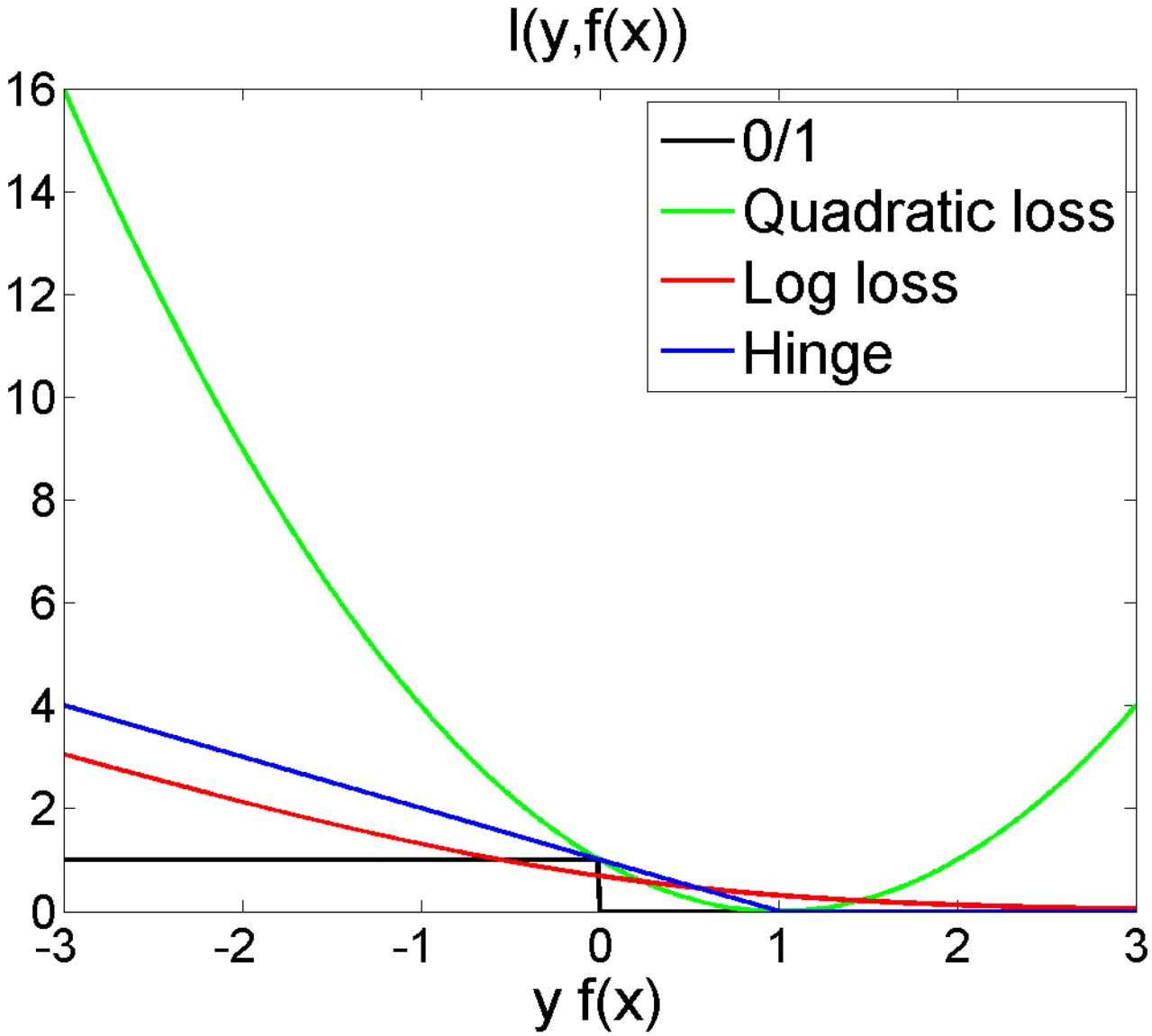


Hinge loss vs log-loss

getting larger than 1: does not harm, but also does not help



Hinge loss vs log-loss vs quadratic



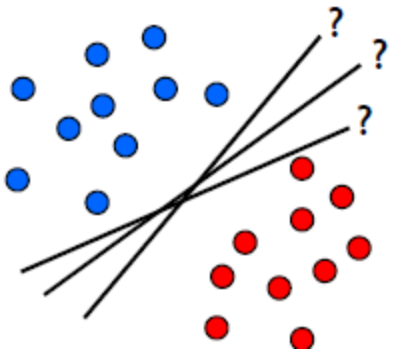
Lecture outline

- Recap
- Large margins and generalization
- Optimization
- Kernels
- Applications to vision

Generalization Error

- What is model complexity?
  - Number of parameters, magnitude of discriminant w?
  - Analyze complexity of hypothesis class

- Linear classifiers:
  - Different decision boundaries
    - Different generalization performance
  - Test error > training error
  - Which line gives smallest test error?



Learning Theory

- V. Vapnik, 1968
  - Mainstream Statistics: Large-sample analysis (`in the limit')
  - Pattern Recognition: Small sample properties

- Distribution-free bounds on worst performance

Empirical and Actual risk

- **Empirical risk**
  - Measured on the training/validation set

$$R_{emp}(\alpha) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, f(\mathbf{x}_i; \alpha))$$

- **Actual risk (= Expected risk)**
  - Expectation of the error on *all* data.

$$R(\alpha) = \int L(y_i, f(\mathbf{x}; \alpha)) dP_{X,Y}(\mathbf{x}, y)$$

  - $P_{X,Y}(\mathbf{x}, y)$ is the probability distribution of $(\mathbf{x},y)$. It is fixed, but typically unknown.

Actual and Empirical Risk

- Idea
  - Compute an upper bound on the actual risk based on the empirical risk

$$R(\alpha) \leq R_{emp}(\alpha) + \epsilon(N, p^*, h)$$

  - where

N: number of training examples

p^*: probability that the bound is correct

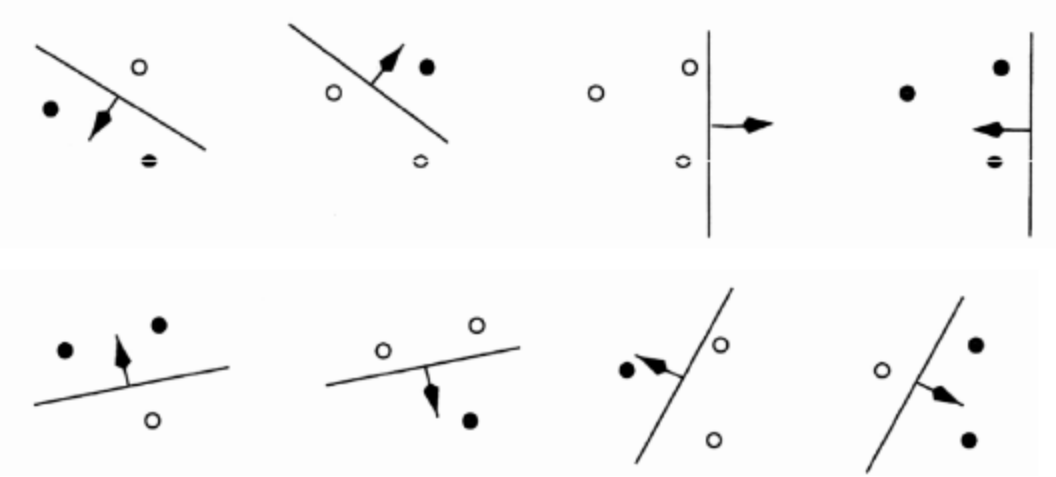
h: capacity of the learning machine ("VC-dimension")

Vapnik Chervonenkis (VC) Dimension

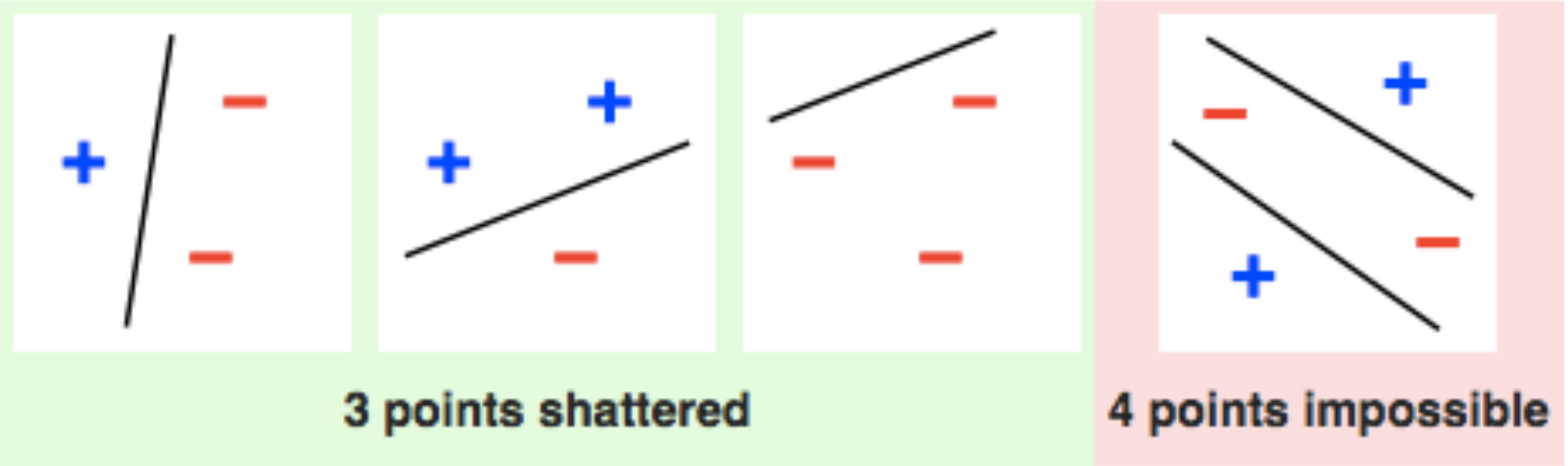
- Shattering: *If a given set of ℓ points can be labeled in all possible 2^ℓ ways, and for each labeling, a member of the set $\{f(\alpha)\}$ can be found which correctly assigns those labels, we say that the set of points is shattered by the set of functions.*

- VC dimension *The VC dimension for the set of functions $\{f(\alpha)\}$ is defined as the maximum number of training points that can be shattered by $\{f(\alpha)\}$.*

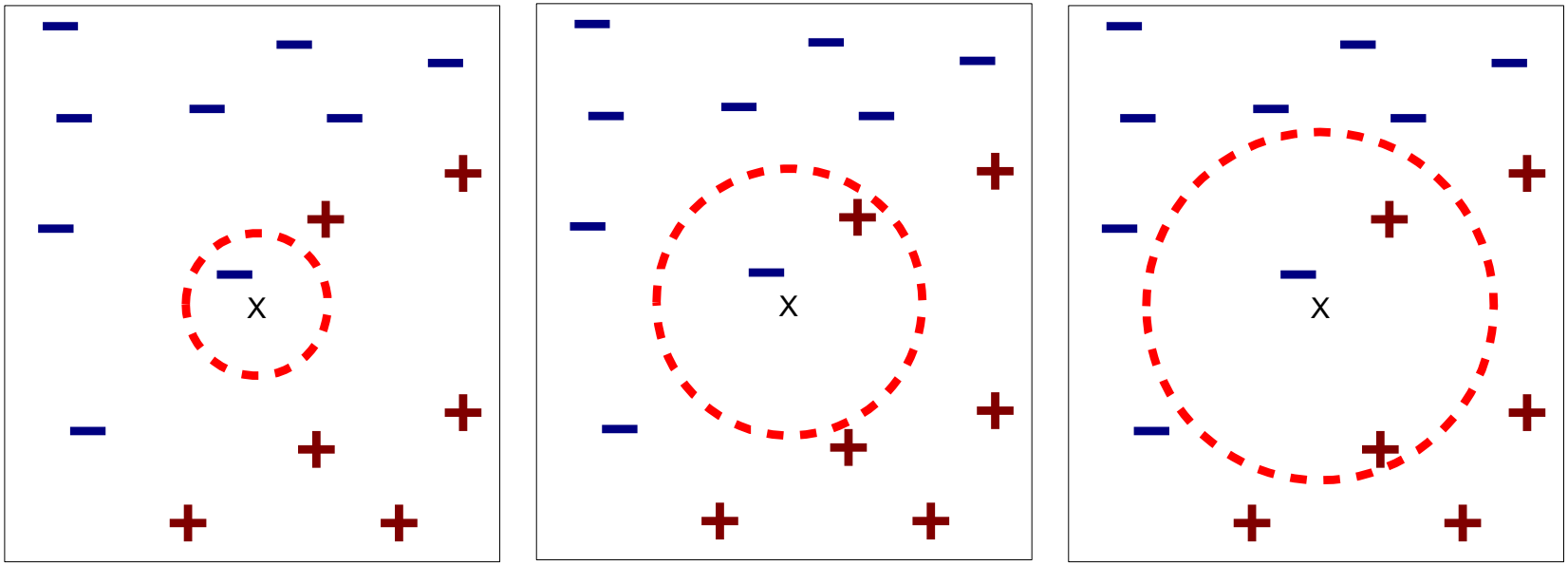
- Example



Arbitrary linear classifier in N-dimensions: VC-dim= N+1



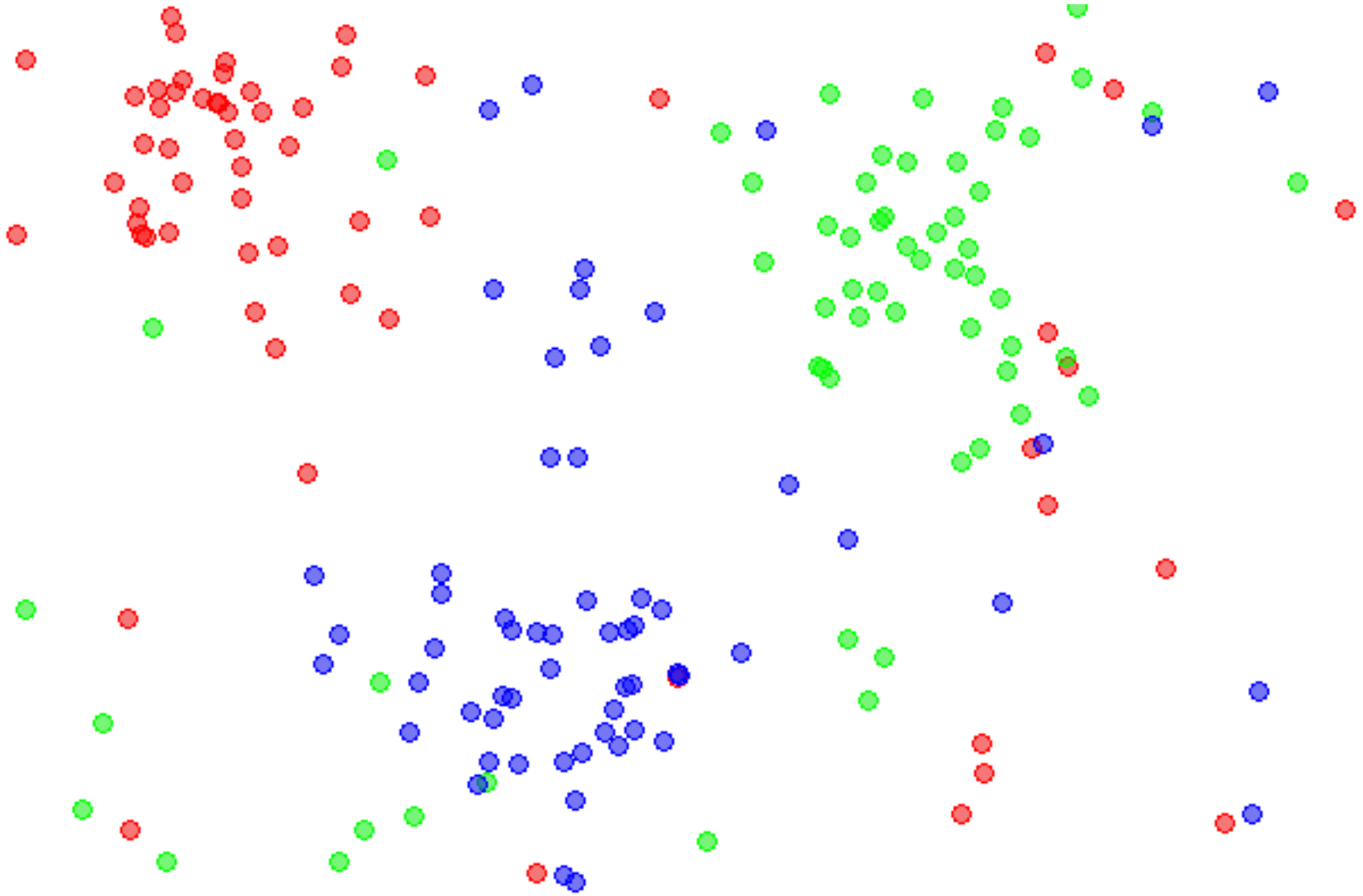
Reminder: K-nearest neighbor classifier



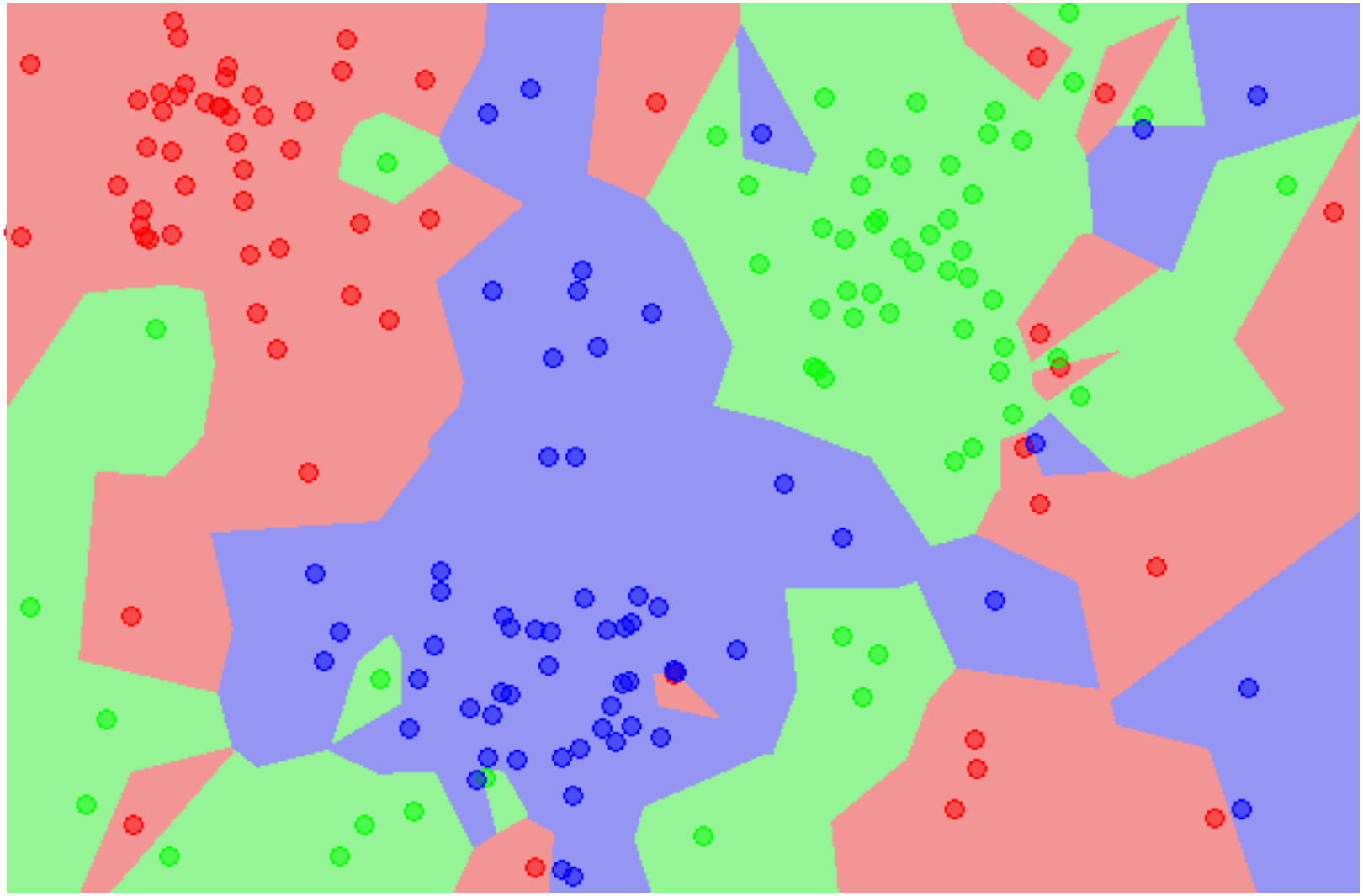
(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

- **Compute distance to other training records**
- **Identify *K* nearest neighbors**
- **Take majority vote**

Training data for NN classifier (in R^2)

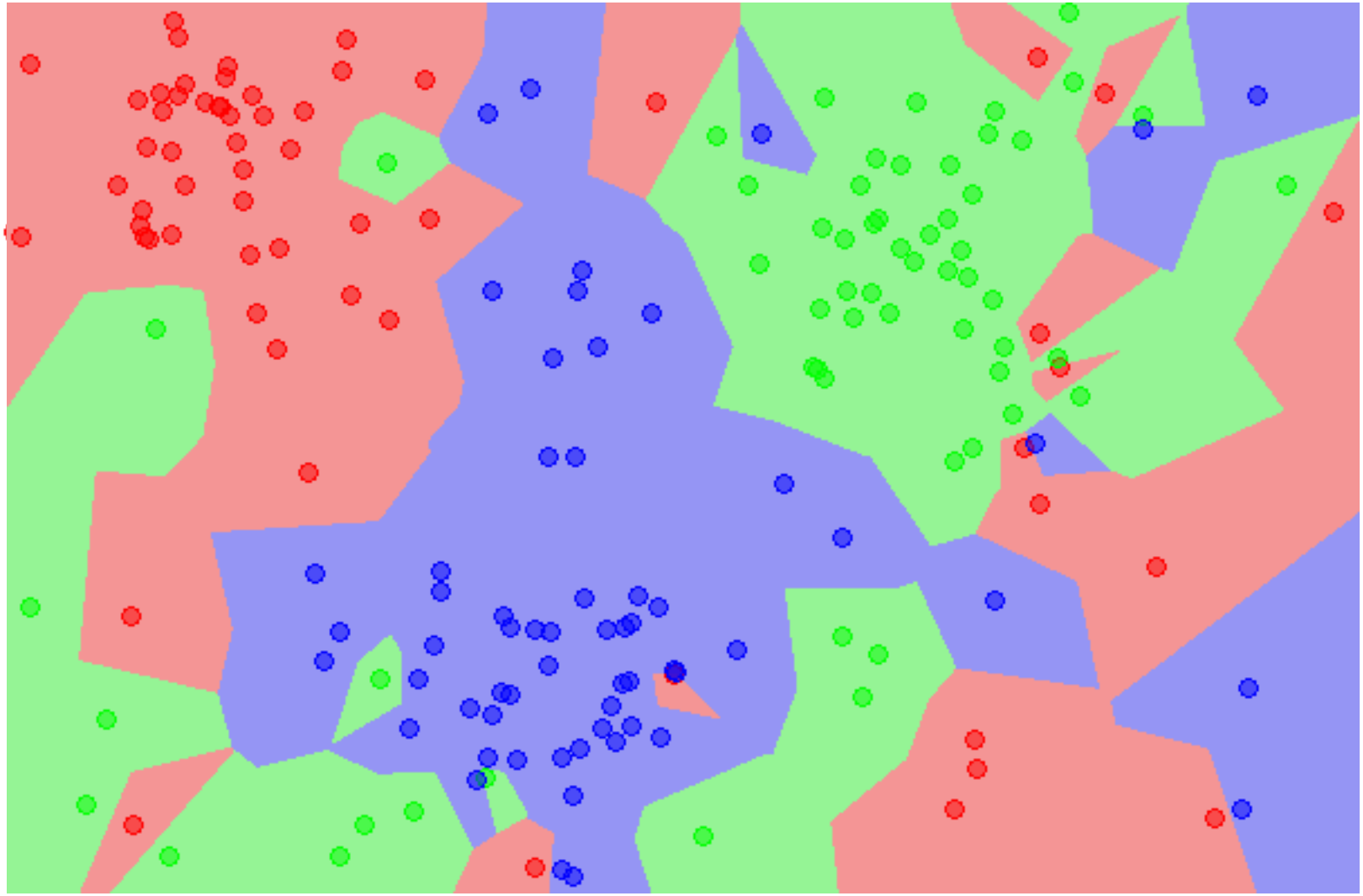


1-nn classifier prediction (in R^2)



What is the VC dimension of this classifier?

1-nn classifier prediction (in R^2)



What is the VC dimension of this classifier?

Large Margins & VC Dimension

- Vapnik: *The class of optimal linear separators has VC dimension h bounded from above as*

$$h \leq \min\left\{\left\lceil \frac{D^2}{\rho^2} \right\rceil, m_0\right\} + 1$$

where ρ is the margin, D is the diameter of the smallest sphere that can enclose all of the training examples, and m_0 is the dimensionality.

- If we maximize the margins, feature dimensionality does not matter

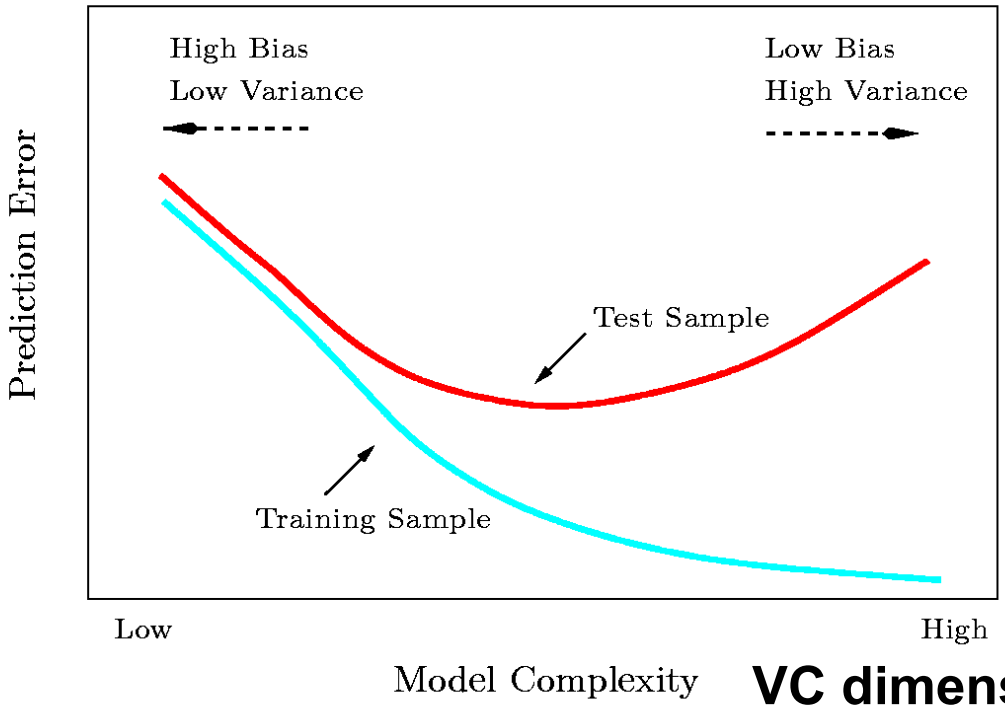
Tuning the model's complexity

A flexible model approximates the target function well in the training set

A rigid model's performance is more predictable in the test set

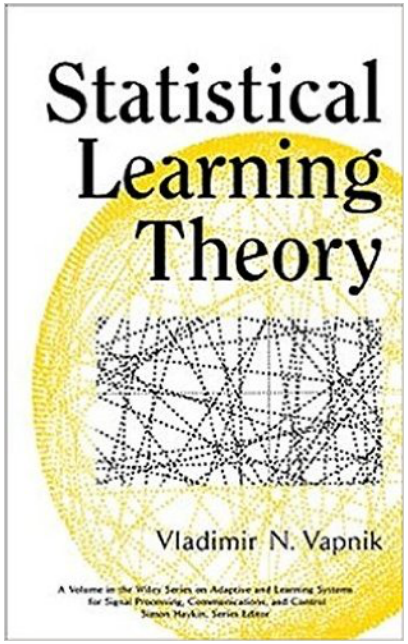
- With probability $(1\text{-}\eta)$, the following bound holds

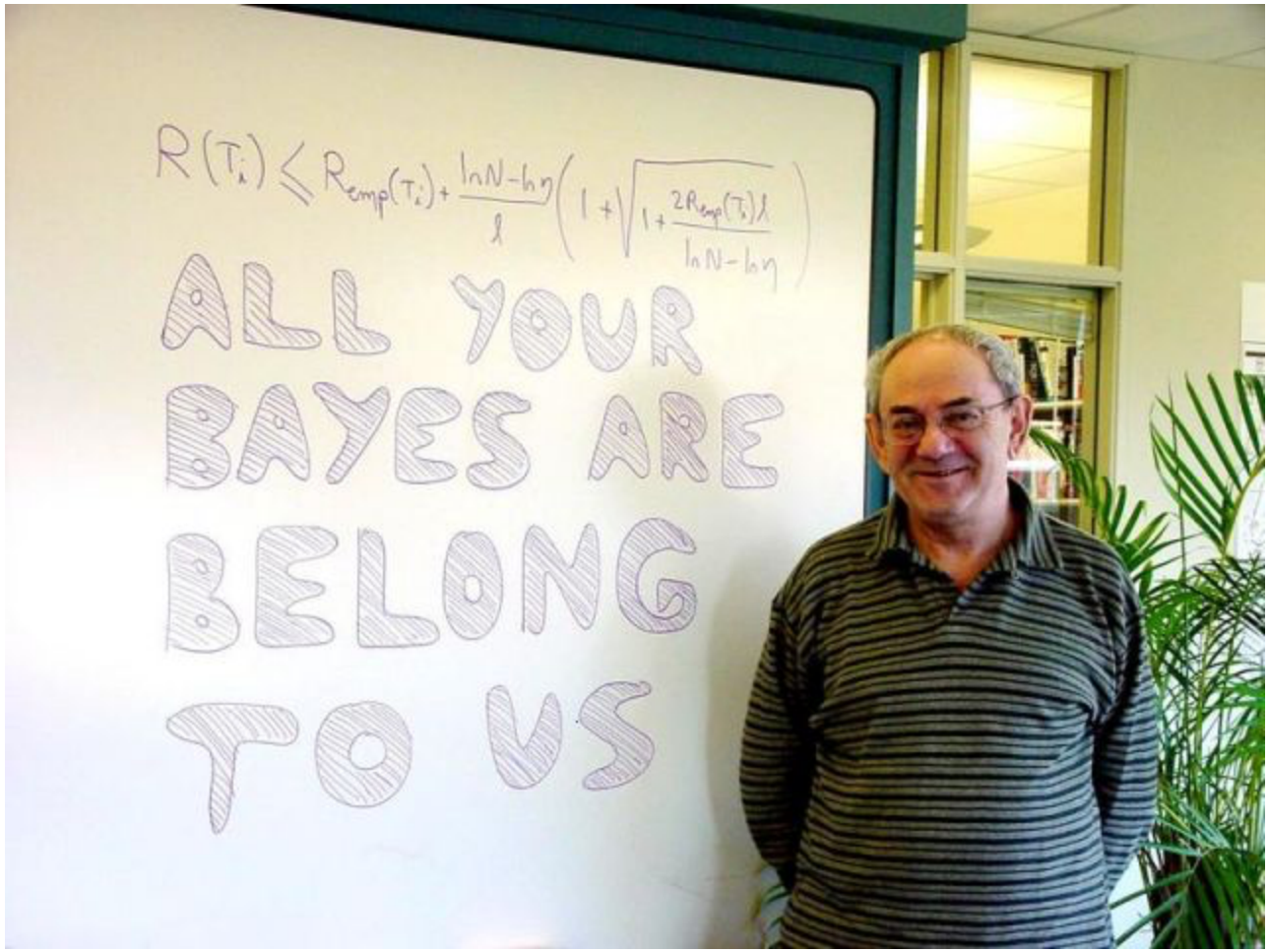
$$R(\alpha) \leq R_{emp}(\alpha) + \underbrace{\sqrt{\frac{h(\log(2N/h)+1) - \log(\eta/4)}{N}}}_{\text{"VC confidence"}}$$



VC dimension

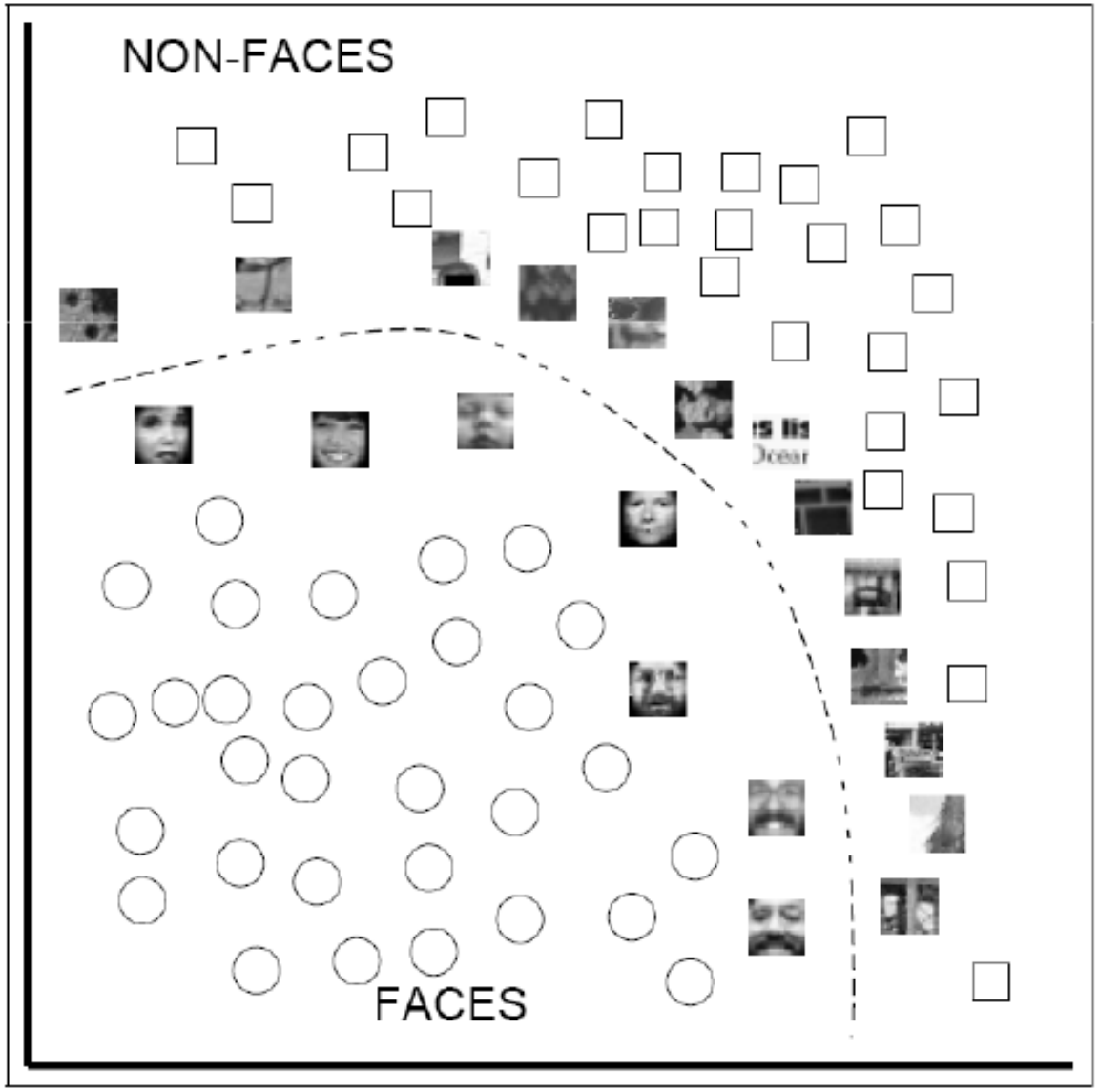
“There’s nothing more practical than a good theory”



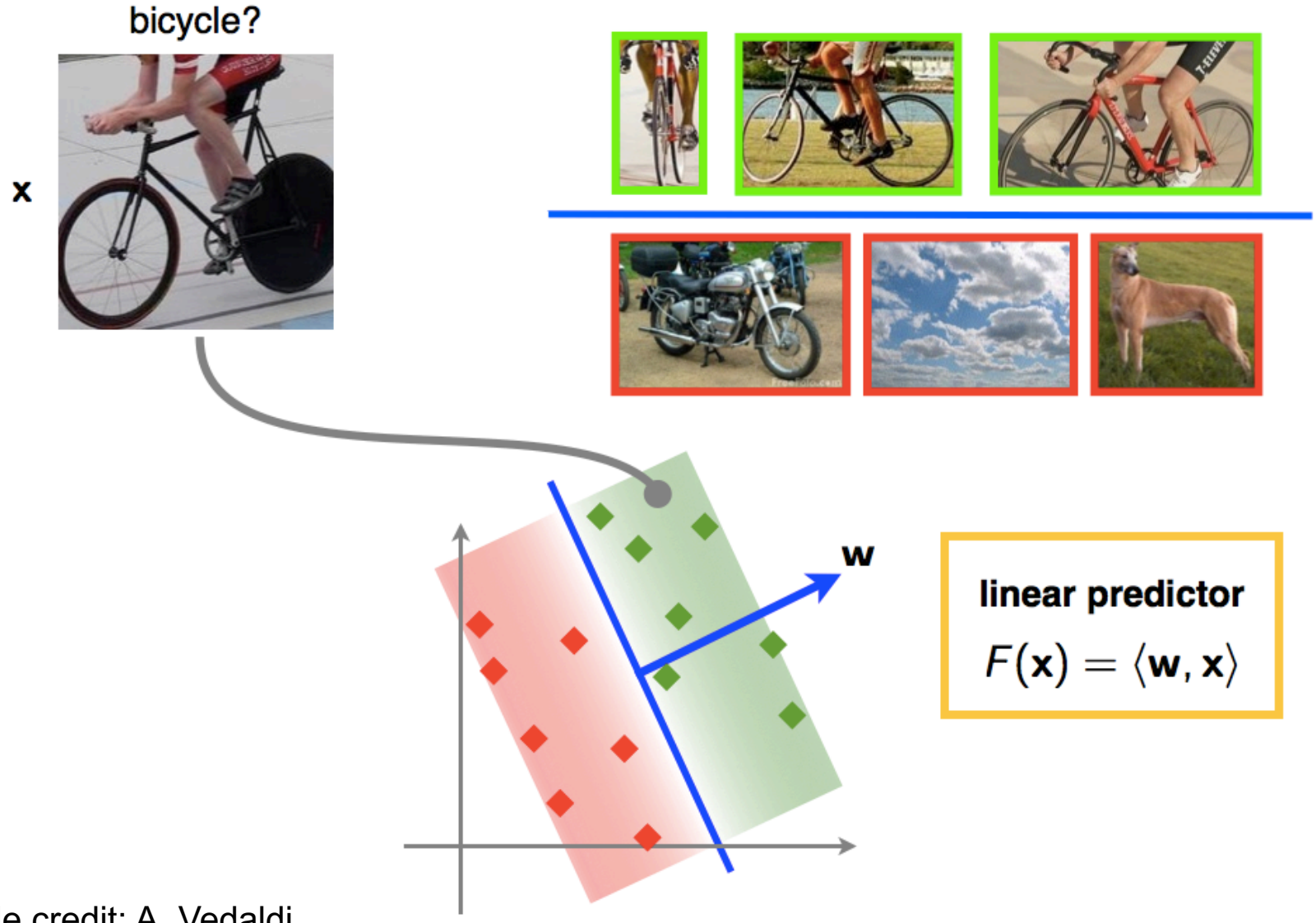


“There’s nothing more practical than a good theory”

Support vectors for Faces (P&P 98)



SVMs in computer vision



Slide credit: A. Vedaldi

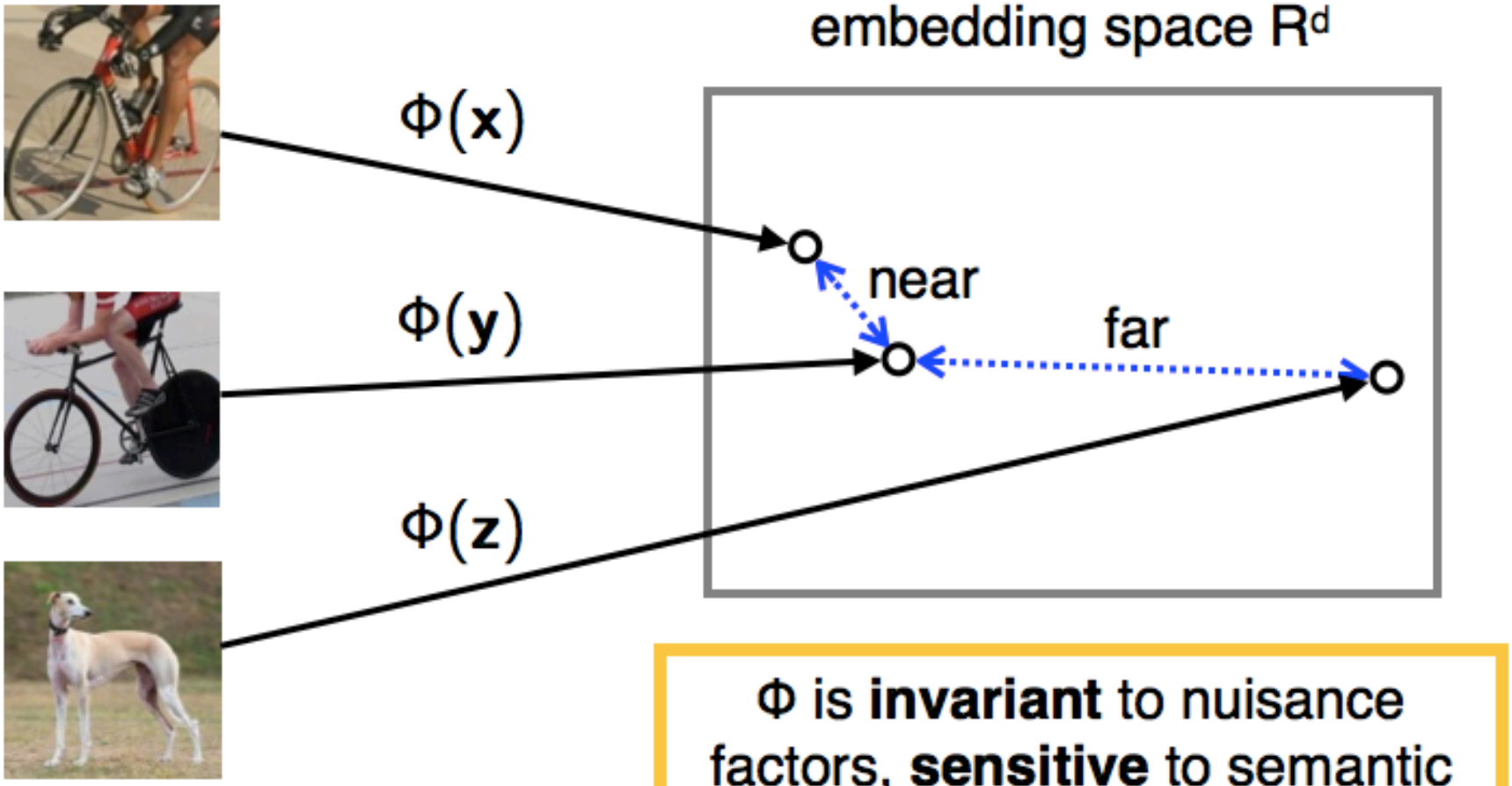
Image features

$\mathbf{x}$ 

encoder Φ → representation $\Phi(\mathbf{x}) \in \mathbb{R}^d$

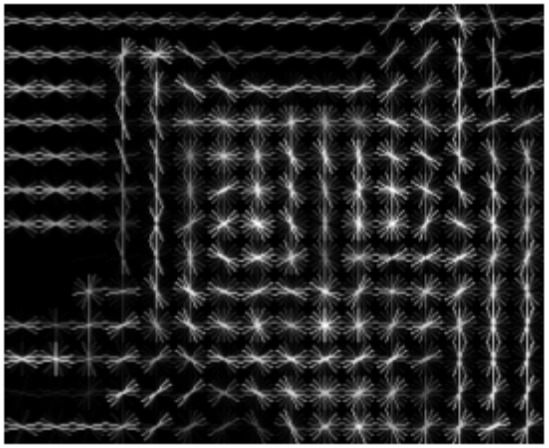
Slides: A. Vedaldi, http://www.robots.ox.ac.uk/~vedaldi/assets/teach/vedaldi14bmvc-tutorial.pdf

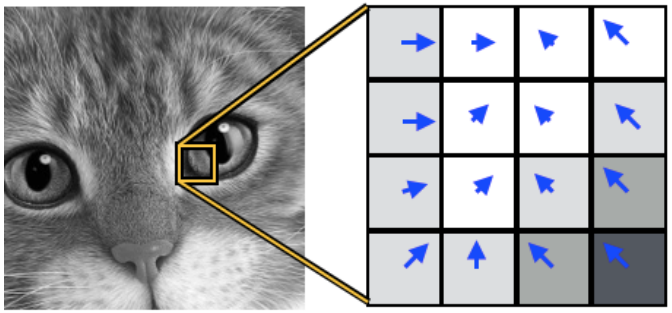
Desirable feature properties

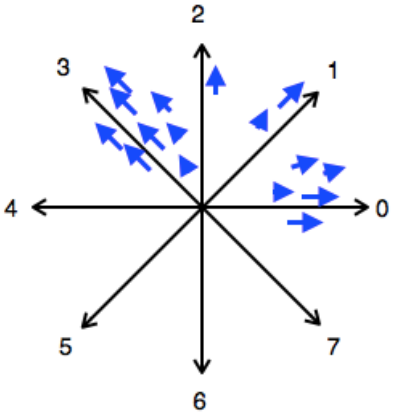


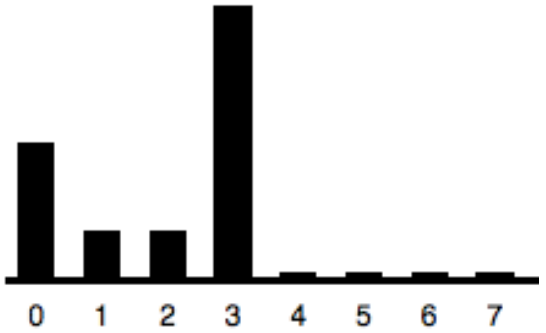
Slide credit: A. Vedaldi

Histogram of Gradient (HOG)/SIFT Features





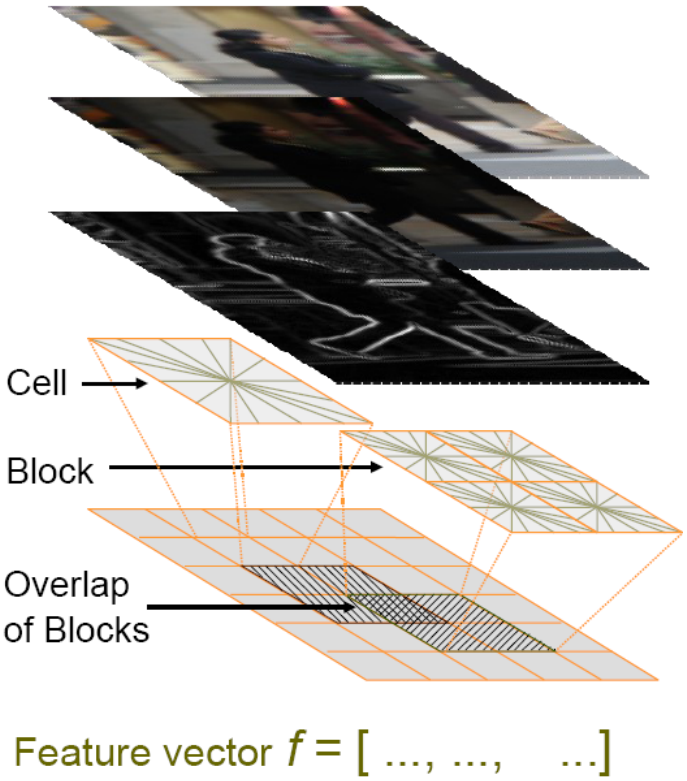




Slide credit: A. Vedaldi

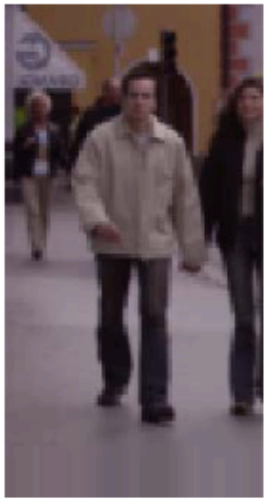
Dalal and Triggs, ICCV 2005

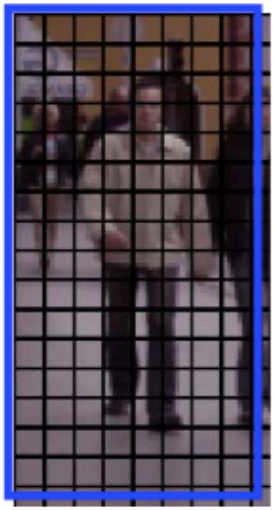
- Histogram of Oriented Gradient (HOG) features
- Highly accurate detection using linear SVM



HOG features for pedestrians

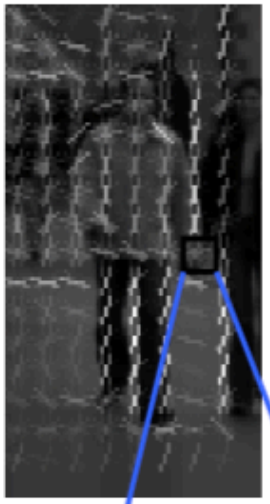
image



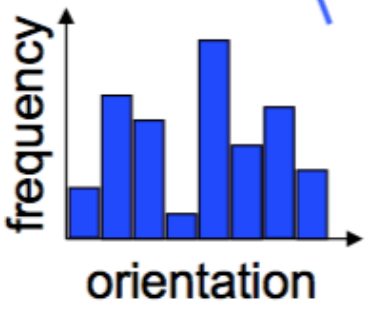


dominant direction

HOG

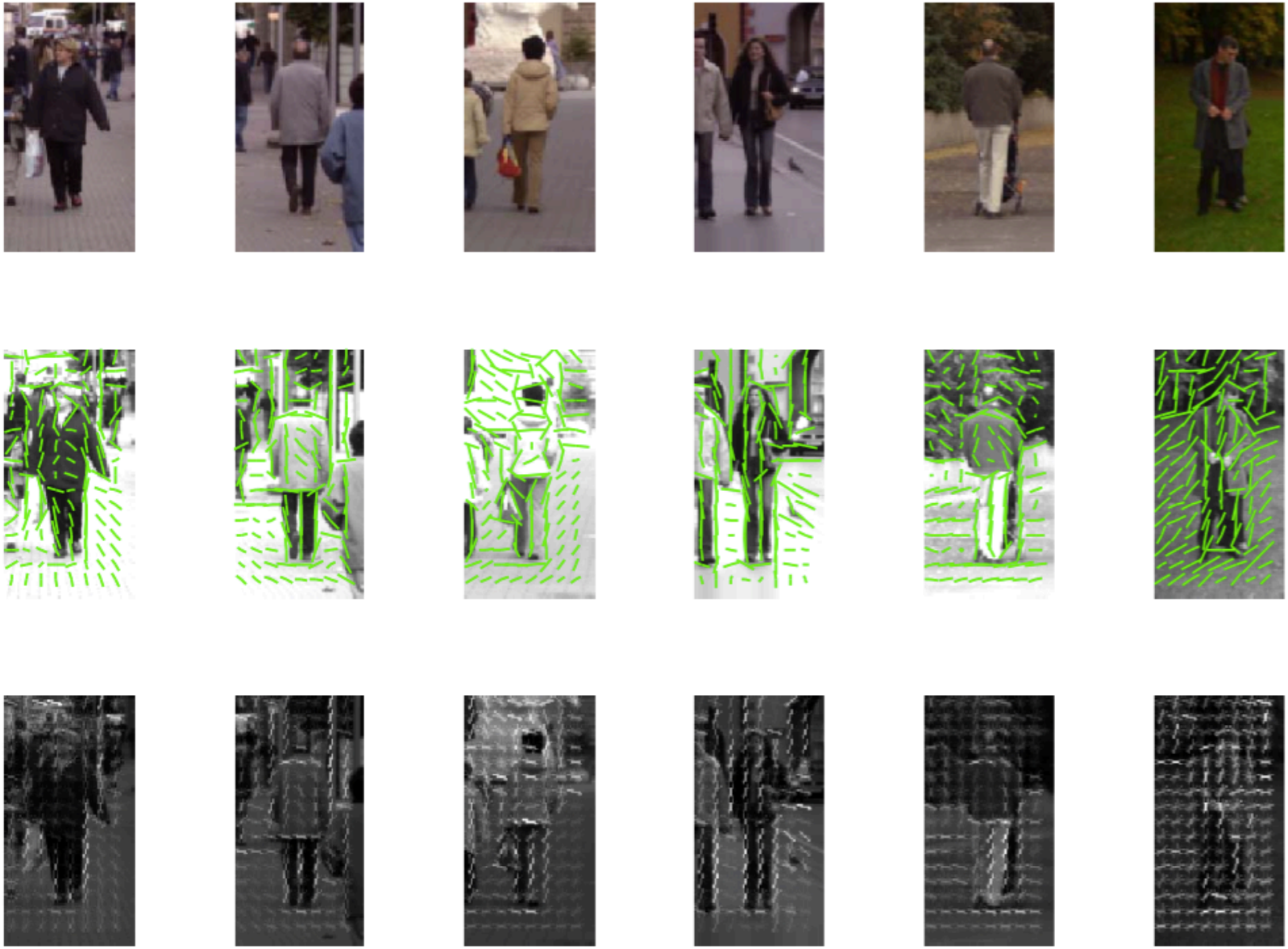


- tile window into 8 x 8 pixel cells
- each cell represented by HOG



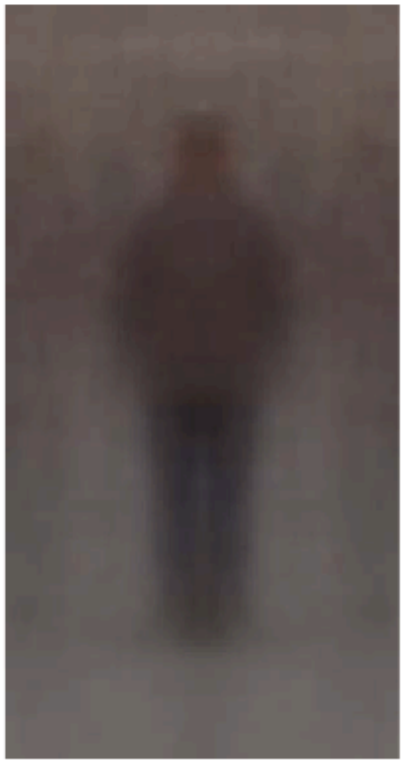
Feature vector dimension = 16 x 8 (for tiling) x 8 (orientations) = 1024

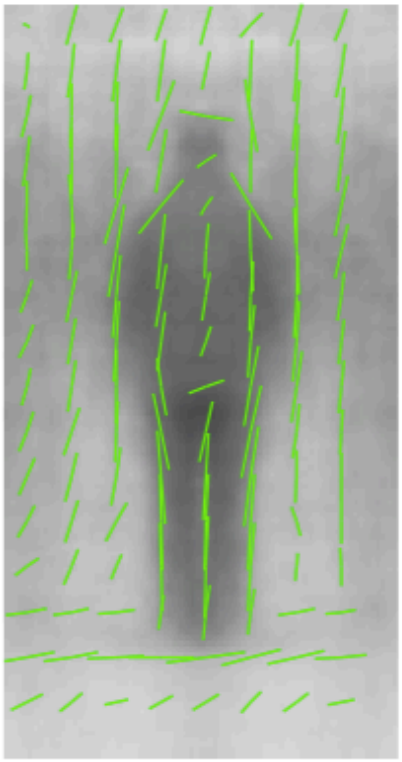
SVMs and Pedestrians

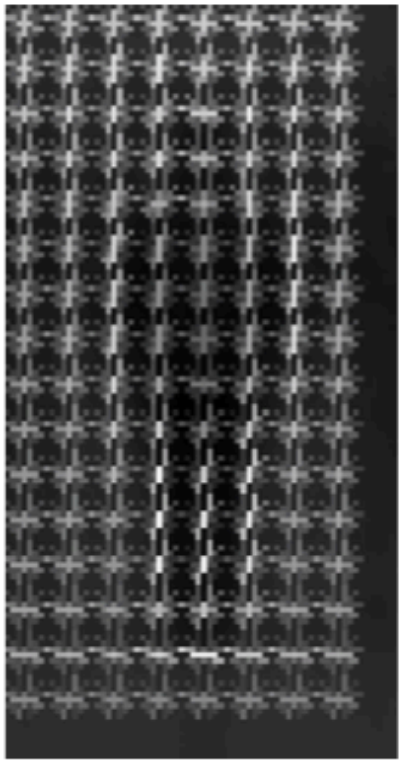


SVMs and Pedestrians

Averaged examples





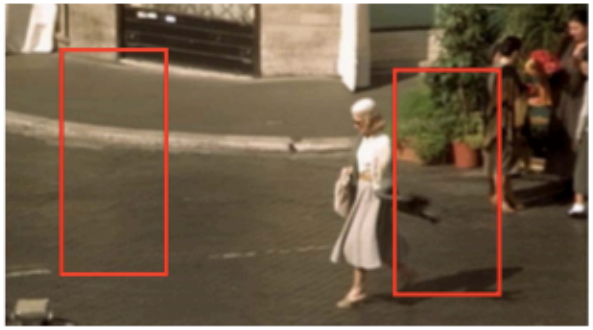


SVMs and Pedestrians

- Positive data – 1208 positive window examples




- Negative data – 1218 negative window examples (initially)

Training (Learning)

- Represent each example window by a HOG feature vector

$$\mathbf{x}_i \in \mathbb{R}^d, \text{ with } d = 1024$$

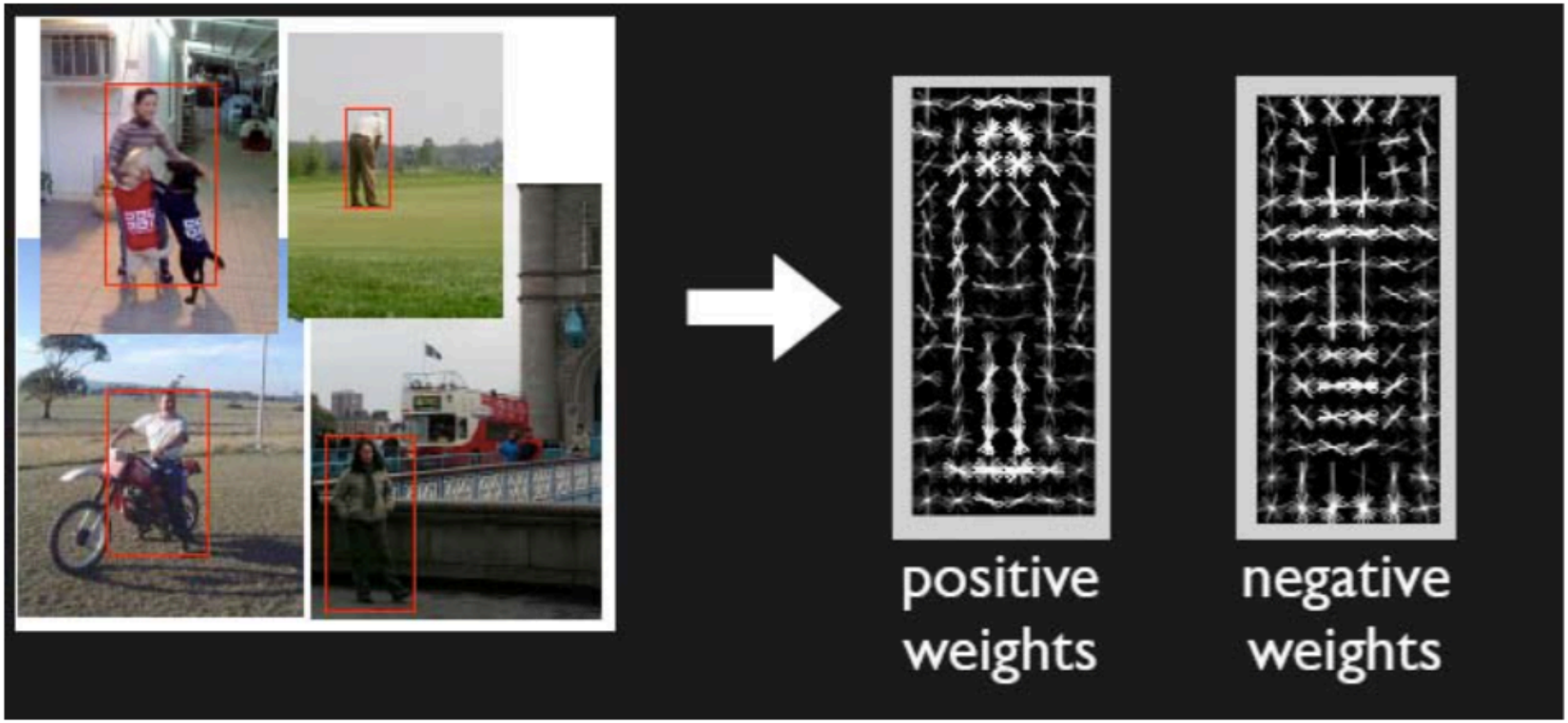
- Train a SVM classifier

Testing (Detection)

- Sliding window classifier

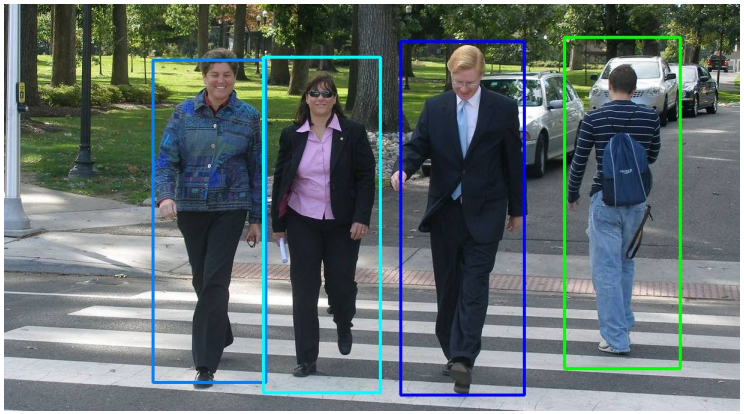
$$f(x) = \sum_i \alpha_i y_i (\mathbf{x}_i{}^\top \mathbf{x}) + b$$

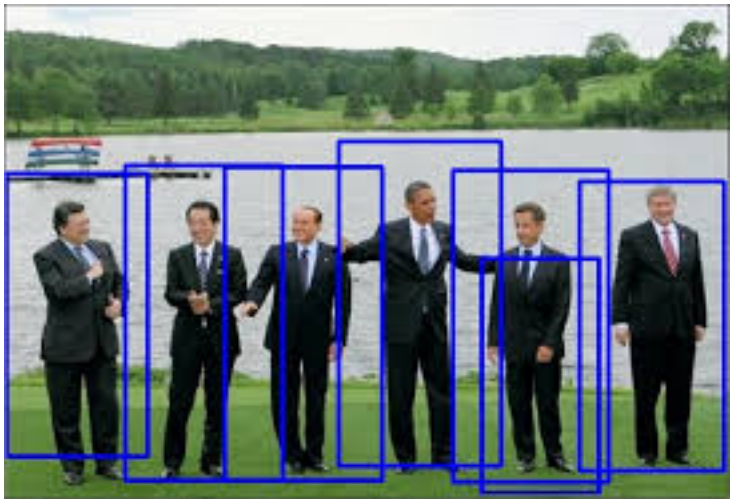
$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

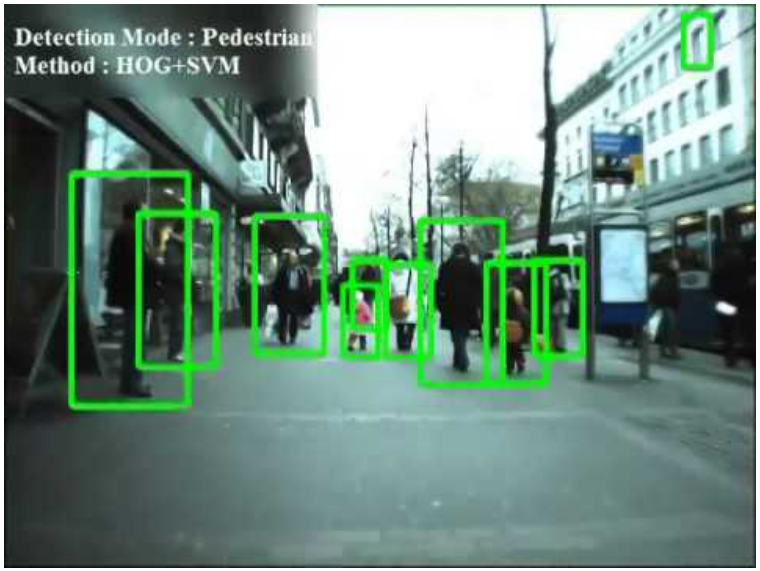


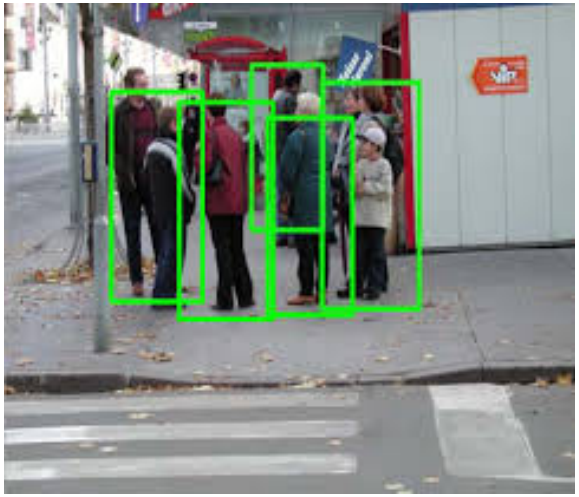
Dalal and Triggs, CVPR 2005

Pedestrian detection: almost done in 2005

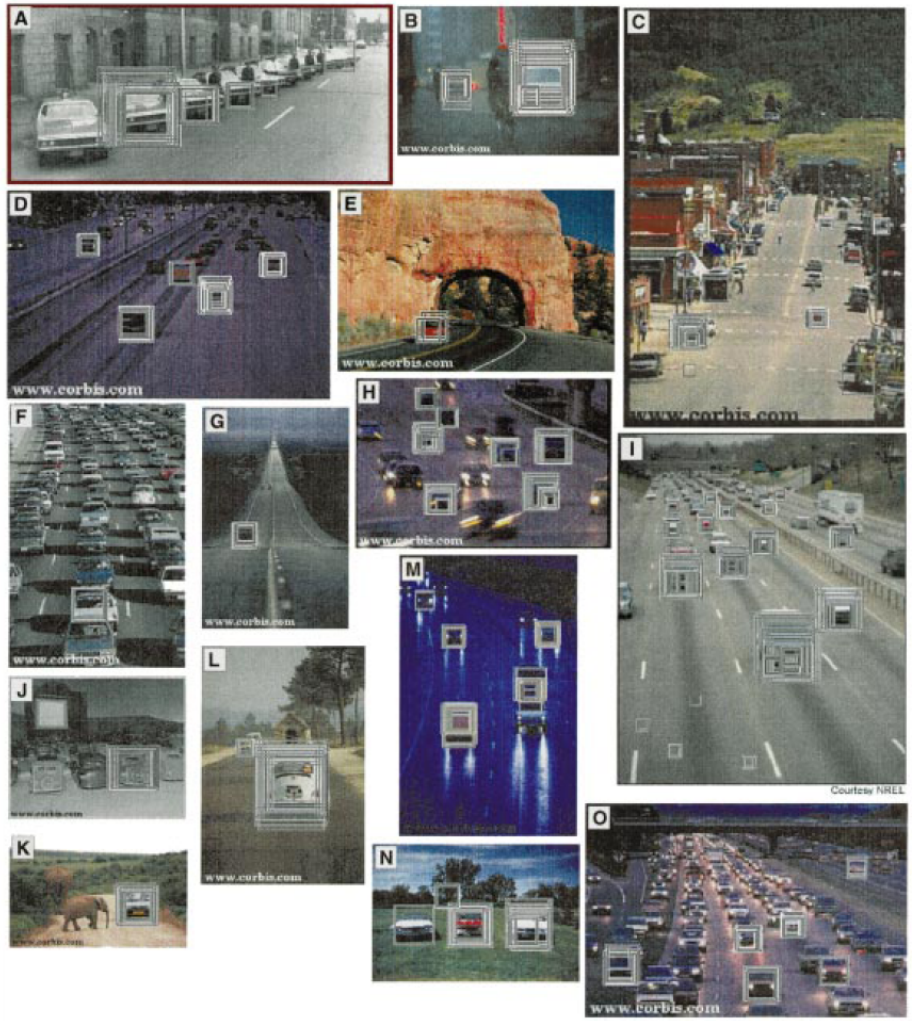








Papageorgiou & Poggio (1998)



Lecture outline

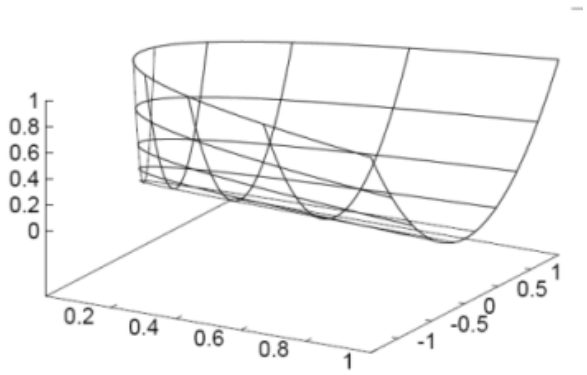
Recap

Large margins and generalization

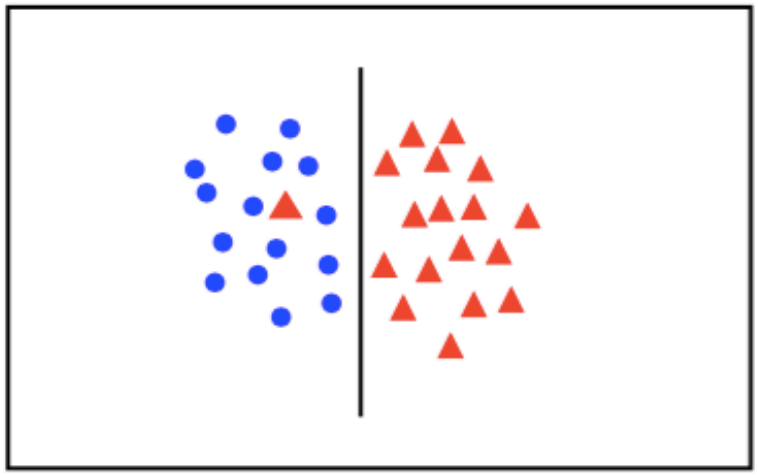
Optimization

Kernels

Applications to vision



Non-separable data

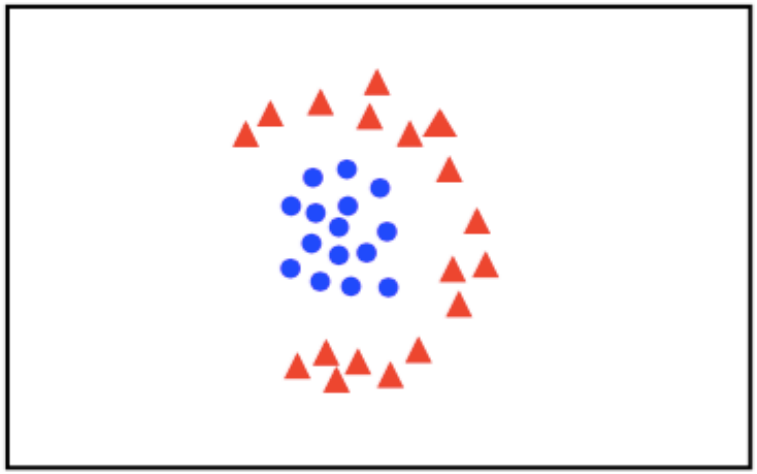


- introduce slack variables

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

subject to

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

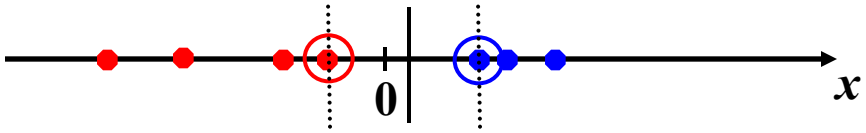


- linear classifier not appropriate

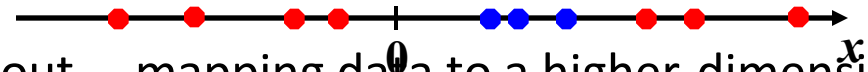
??

Non-linear SVMs

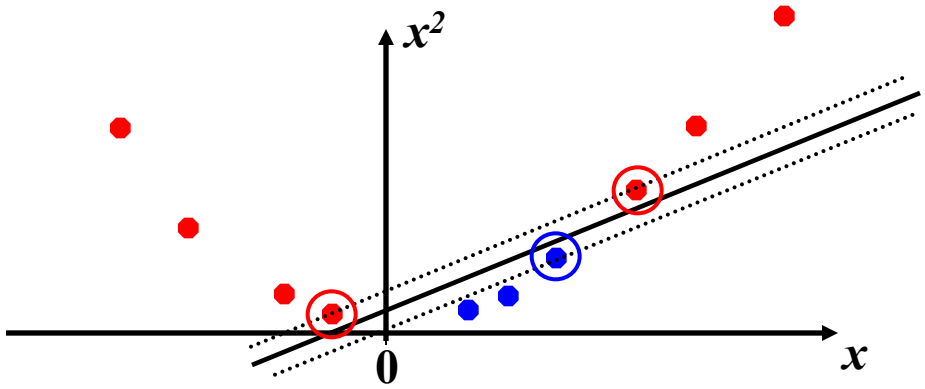
- Datasets that are linearly separable (with some noise) work out great:



- But what are we going to do if the dataset is just too hard?

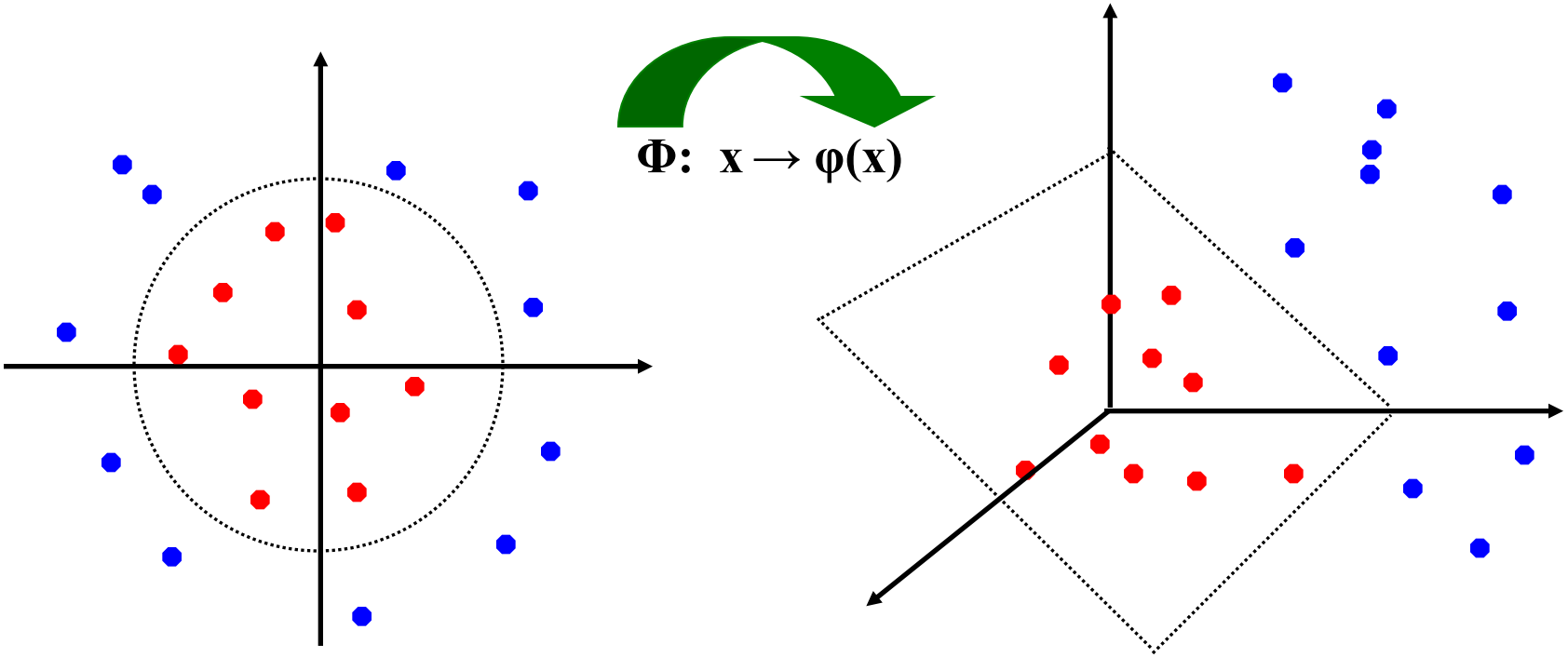


- How about … mapping data to a higher-dimensional space:

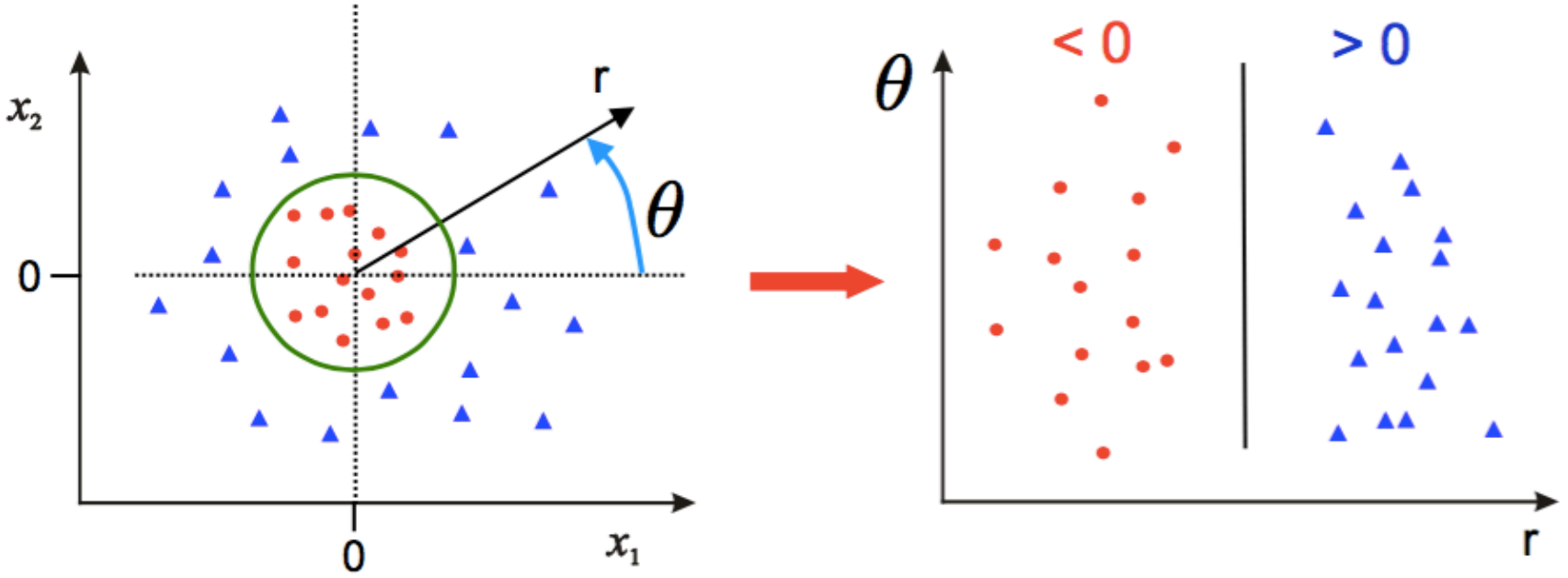


Non-linear SVMs: Feature spaces

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:



Solution by inspection: hand-crafted features

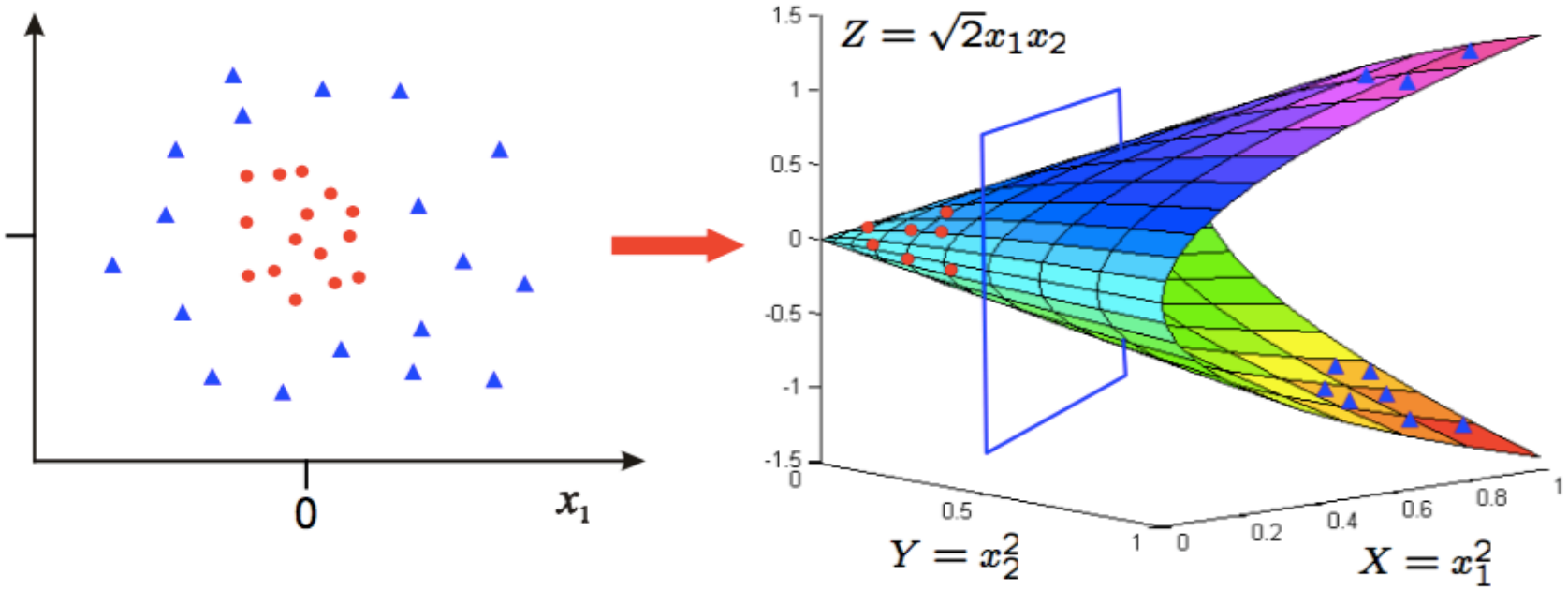


- Data is linearly separable in polar coordinates
- Acts non-linearly in original space

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

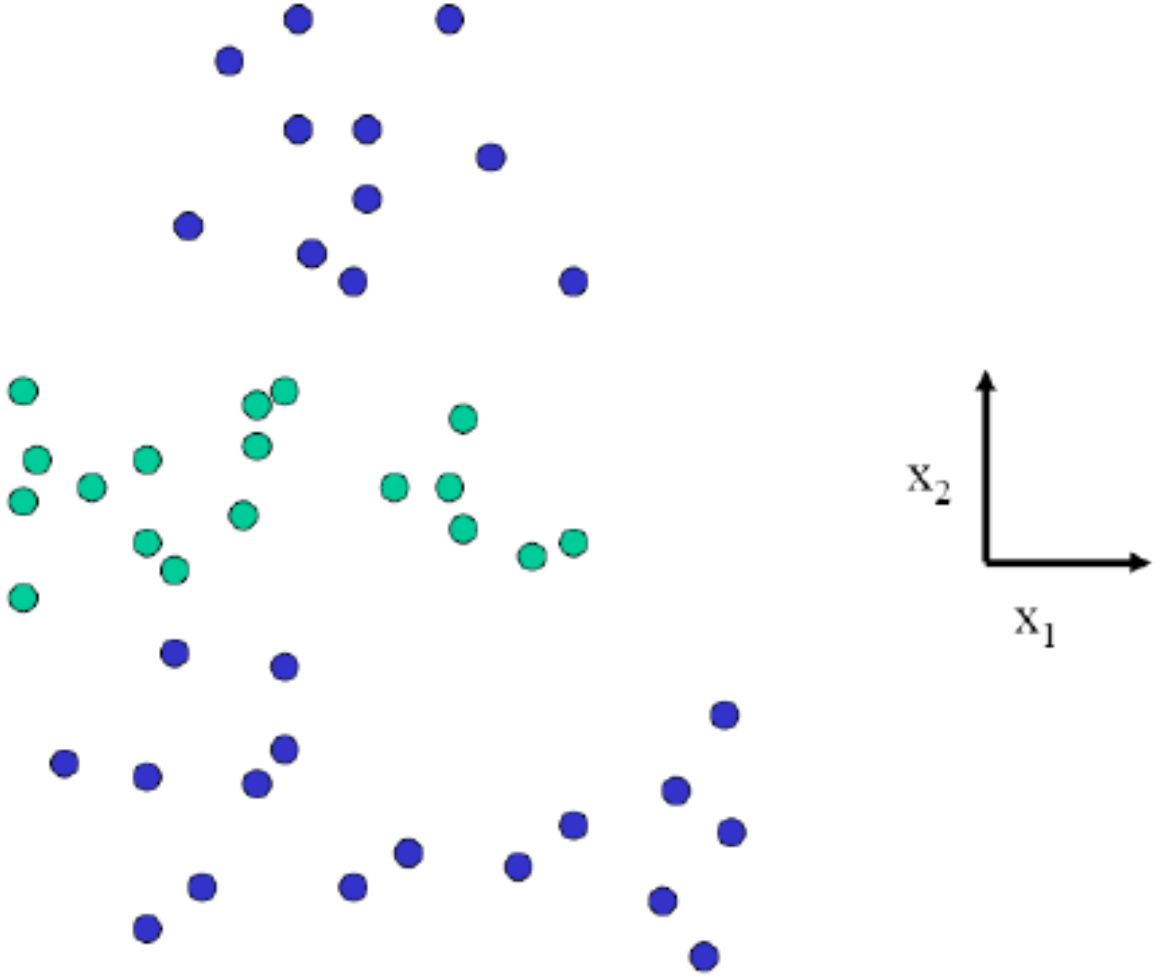
More general method

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

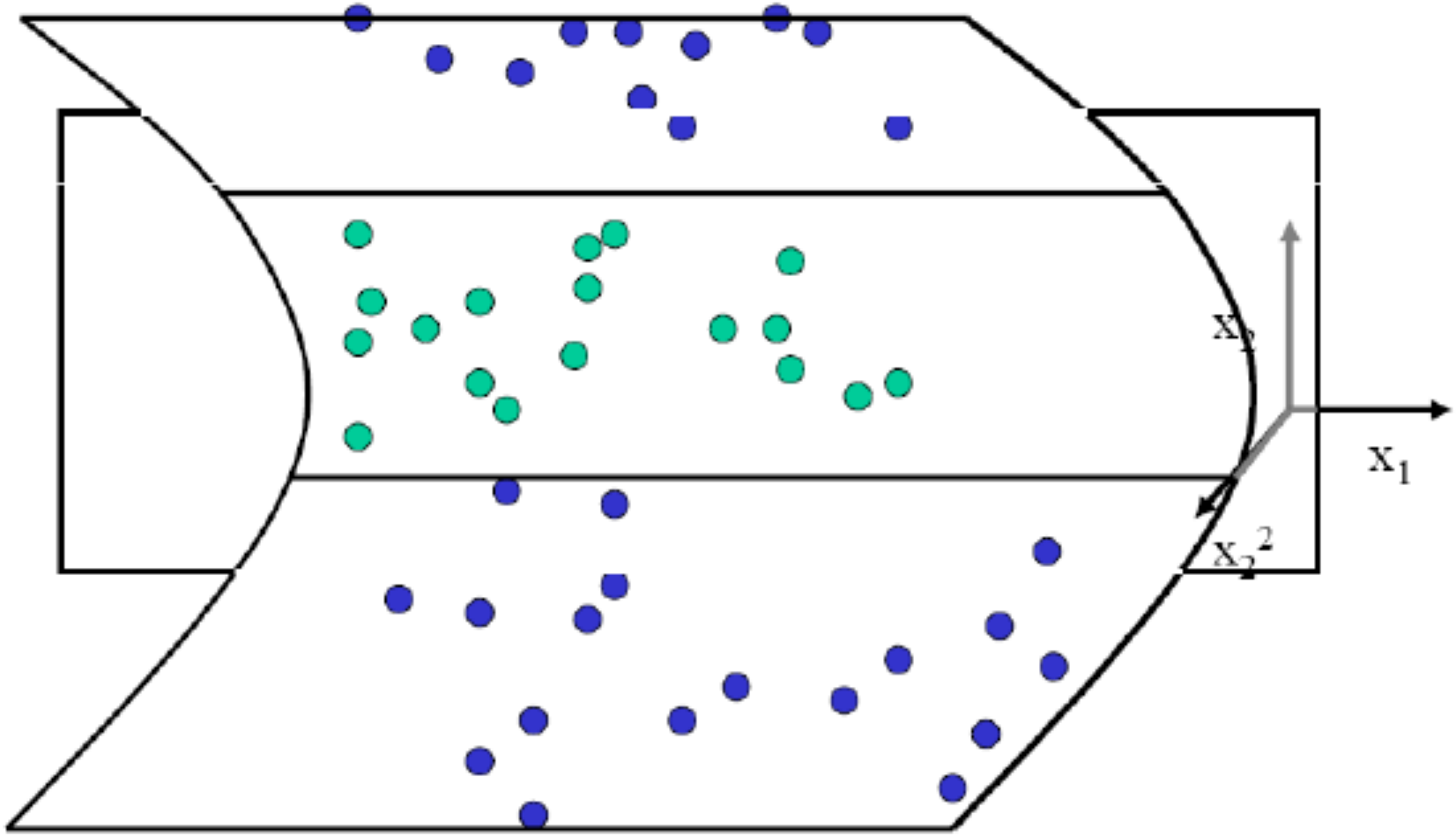


- Data is linearly separable in 3D
- This means that the problem can still be solved by a linear classifier

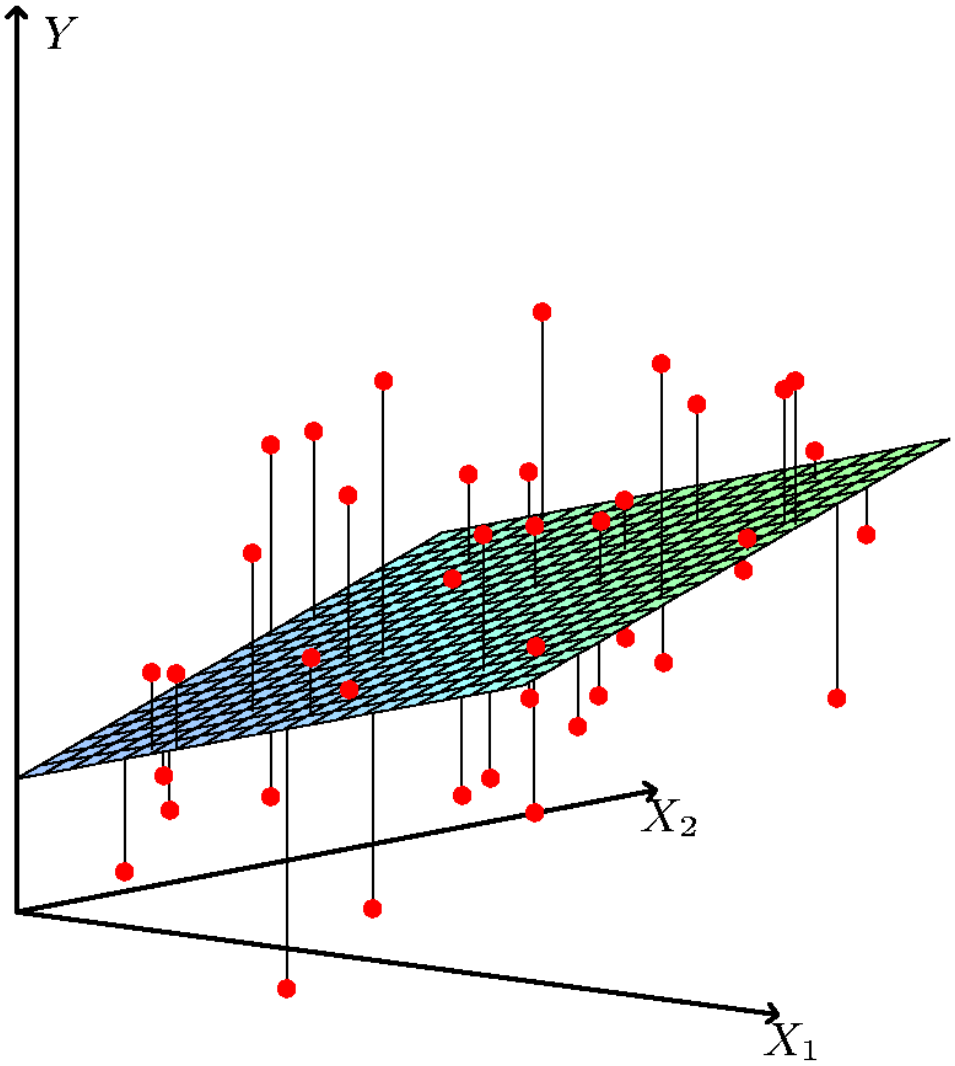
Nonseparable in 2D



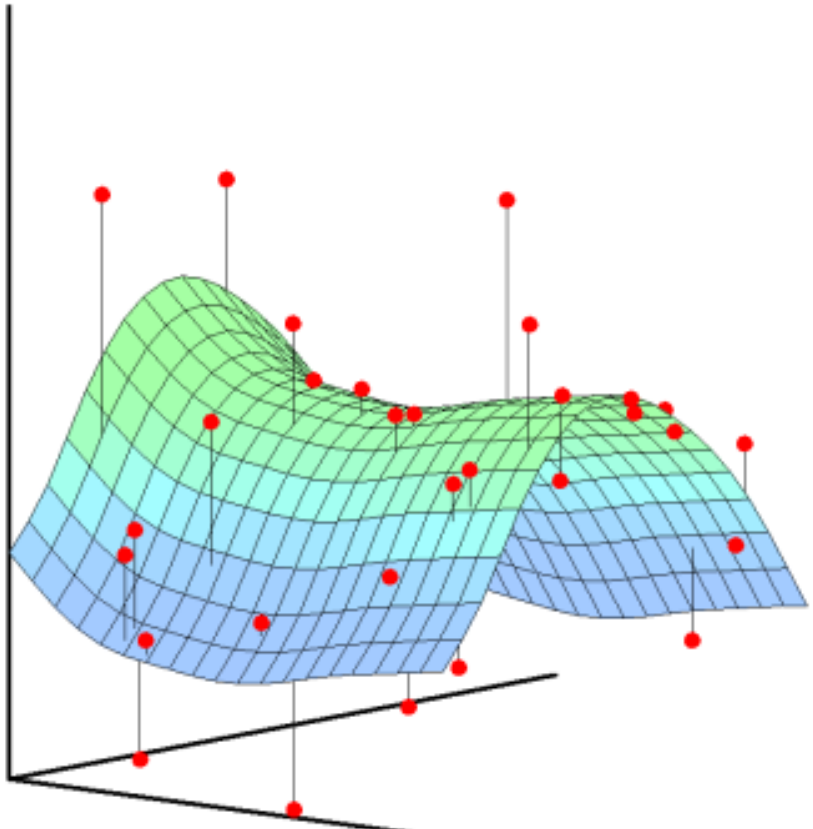
Separable in 3D



Linear regression



Nonlinear regression



$$\mathbf{x} \rightarrow \boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} \phi_1(\mathbf{x}) \\ \vdots \\ \phi_M(\mathbf{x}) \end{bmatrix}$$

Example: second-order polynomials

$$\mathbf{x} = (x_1, x_2)$$

$$\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ (x_1)^2 \\ (x_2)^2 \\ x_1 x_2 \end{bmatrix}$$

$$\langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}) \rangle = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2 + w_5 x_1 x_2$$

Non-linear Classifiers

So far, decision is based on the sign of $y = \mathbf{w}^T \mathbf{x}$

Use non-linear transformation, φ(x) of our data, x

e.g. $\mathbf{x} = (x_1, x_2)$ $\quad \boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ (x_1)^2 \\ (x_2)^2 \\ x_1 x_2 \end{bmatrix}$

Discriminant:

$$\langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}) \rangle = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2 + w_5 x_1 x_2$$

Non-linear in x, linear in φ(x)

Dual form of SVM & kernel trick

Optimization:

$$\min_{\boldsymbol{\alpha}} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha^i \alpha^j y^i y^j \langle \mathbf{x}^i, \mathbf{x}^j \rangle$$

$$\text{s.t.}: \; y^i \left(\sum_{j=1}^{N} \alpha^j y^j \langle \mathbf{x}^j, \mathbf{x}^i \rangle + b \right) \geq 1, \quad \forall i$$

$$\boldsymbol{\alpha} \in \mathbb{R}^N \rightarrow O(N^3)$$

Primal and dual classifier forms:

$$f(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle + b = \sum_{i=1}^{N} \alpha^i y^i \langle \mathbf{x}^i, \mathbf{x} \rangle + b$$

What if we replace **x** with **φ(x)?**

Everything involves only inner products!

Rewrite everything in terms of Kernel

$$K(\mathbf{x}, \mathbf{y}) = \langle \boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{y}) \rangle$$

Dual form of SVM & kernel trick

Optimization: $$\min_{\boldsymbol{\alpha}} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha^i \alpha^j y^i y^j \; K\left(\mathbf{x}^i, \mathbf{x}^j\right)$$

$$\text{s.t.}: \; y^i \left(\sum_{j=1}^{N} \alpha^j y^j K(\mathbf{x}^j, \mathbf{x}^i) + b \right) \geq 1, \quad i = 1, \ldots, N$$

Dual classifier form:

$$f(\mathbf{x}) = \sum_{i=1}^{N} \alpha^i y^i K(\mathbf{x}^i, \mathbf{x}) + b$$

$$= \sum_{\{i:\alpha^i \neq 0\}} w^i K(\mathbf{x}^i, \mathbf{x}) + b, \quad w^i = y^i \alpha^i$$

Compare with general nonlinear form: $$f(\mathbf{x}) = \sum_{k} w_k \phi_k(\mathbf{x})$$

N nonlinear functions – smart choice of sparse coefficients

`Kernel trick'

Consider: $\boldsymbol{\phi}(\mathbf{x}) = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ 1 \end{bmatrix}$

We then have: $\langle \boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{y}) \rangle =$

$$= x_1^2y_1^2 + 2x_1x_2y_1y_2 + x_2^2y_2^2 + 2x_1y_1 + 2x_2y_2 + 1$$

$$= (x_1y_1 + x_2y_2 + 1)^2$$

$$= (\mathbf{x}^T\mathbf{y} + 1)^2 \quad \doteq K(\mathbf{x}, \mathbf{y})$$

Polynomial Kernel $K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T\mathbf{y} + 1)^p$

Kernel: linear complexity in D (dimensions of **x,y**), constant in p

Feature space complexity: much higher

Condition for kernel trick: 'Mercer' kernel

- Given some arbitrary function $k(\mathbf{x}_i, \mathbf{x}_j)$, how do we know if it corresponds to a scalar product $\Phi(\mathbf{x}_i)^\top \Phi(\mathbf{x}_j)$ in some space?

- Mercer kernels: if $k(,)$ satisfies:
  - Symmetric $k(\mathbf{x}_i, \mathbf{x}_j) = k(\mathbf{x}_j, \mathbf{x}_i)$
  - Positive definite, $\boldsymbol{\alpha}^\top \mathtt{K} \boldsymbol{\alpha} \geq 0$ for all $\boldsymbol{\alpha} \in \mathbb{R}^N$, where $\mathtt{K}$ is the $N \times N$ Gram matrix with entries $\mathtt{K}_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$.

  then $k(,)$ is a valid kernel.

Mercer Kernel Examples

Linear kernel

$$K(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \mathbf{y}$$

Polynomial kernel

$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T \mathbf{y} + 1)^p$$

Radial Basis Function (a.k.a. Gaussian) kernel

$$K(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{1}{2\sigma^2}\|\mathbf{x} - \mathbf{y}\|^2\right)$$

Underlying feature dimension: **Infinite**

RBF kernel SVM

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

RBF kernel SVM (next week's assignment)

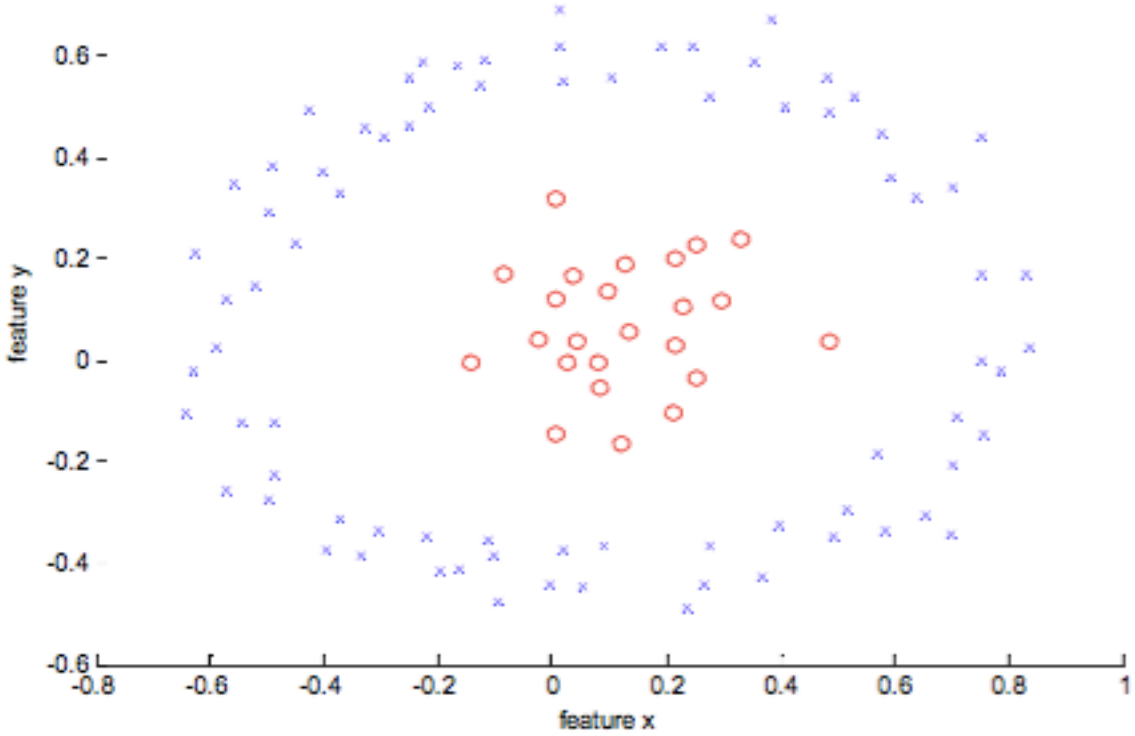
$$f(\mathbf{x}) = \sum_{i=1}^{N} \alpha^i y^i K(\mathbf{x}^i, \mathbf{x}) + b$$

$$= \sum_{\{i:\alpha^i \neq 0\}} \alpha^i y^i K(\mathbf{x}^i, \mathbf{x}) + b$$

$$= \sum_{\{i:\alpha^i \neq 0\}} w^i \exp\left(-\frac{1}{2\sigma^2}\|\mathbf{x}^i - \mathbf{x}\|_2^2\right) + b$$

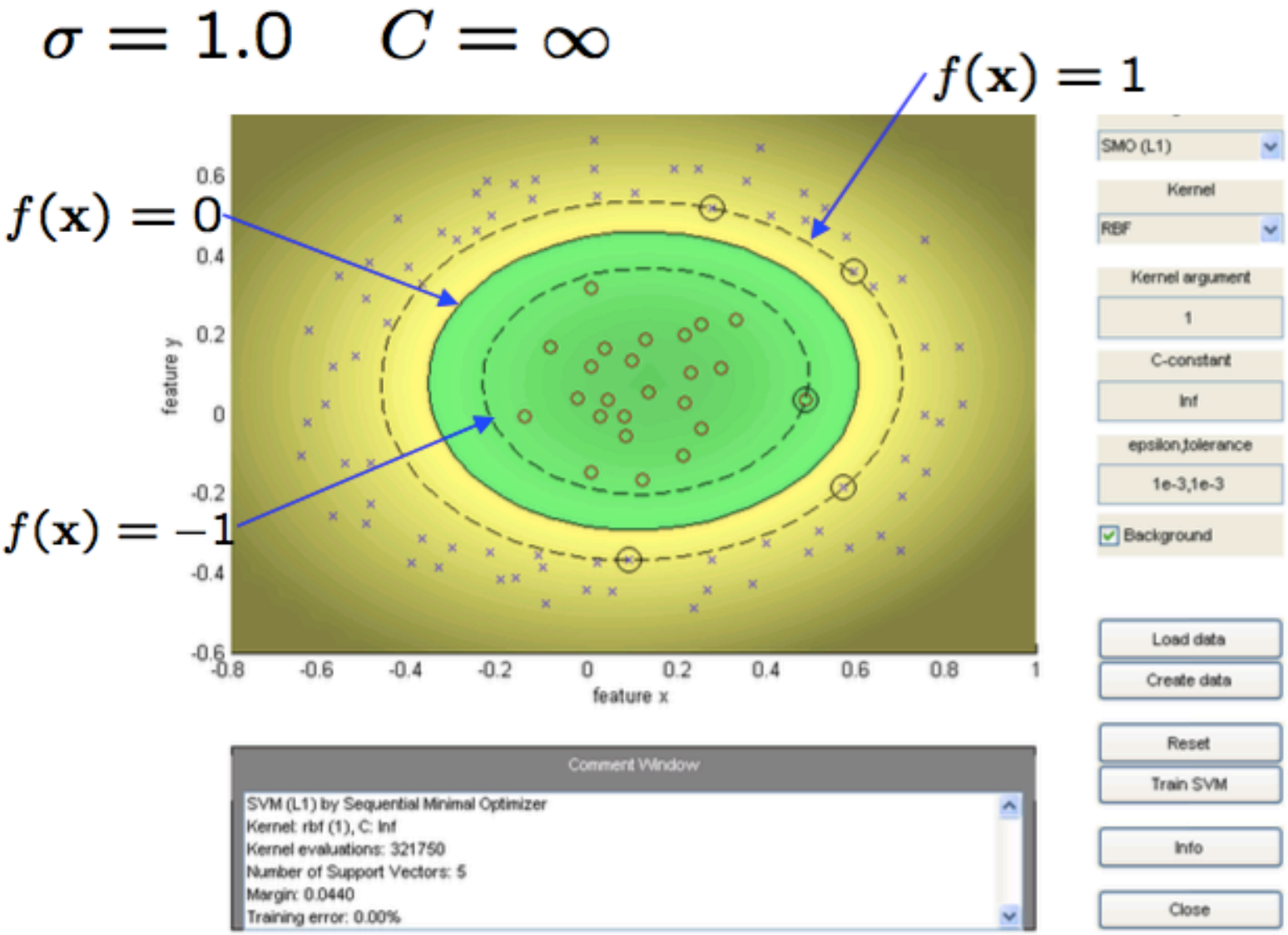
Discriminant form: sum of bumps centered on training points

RBF-SVM example



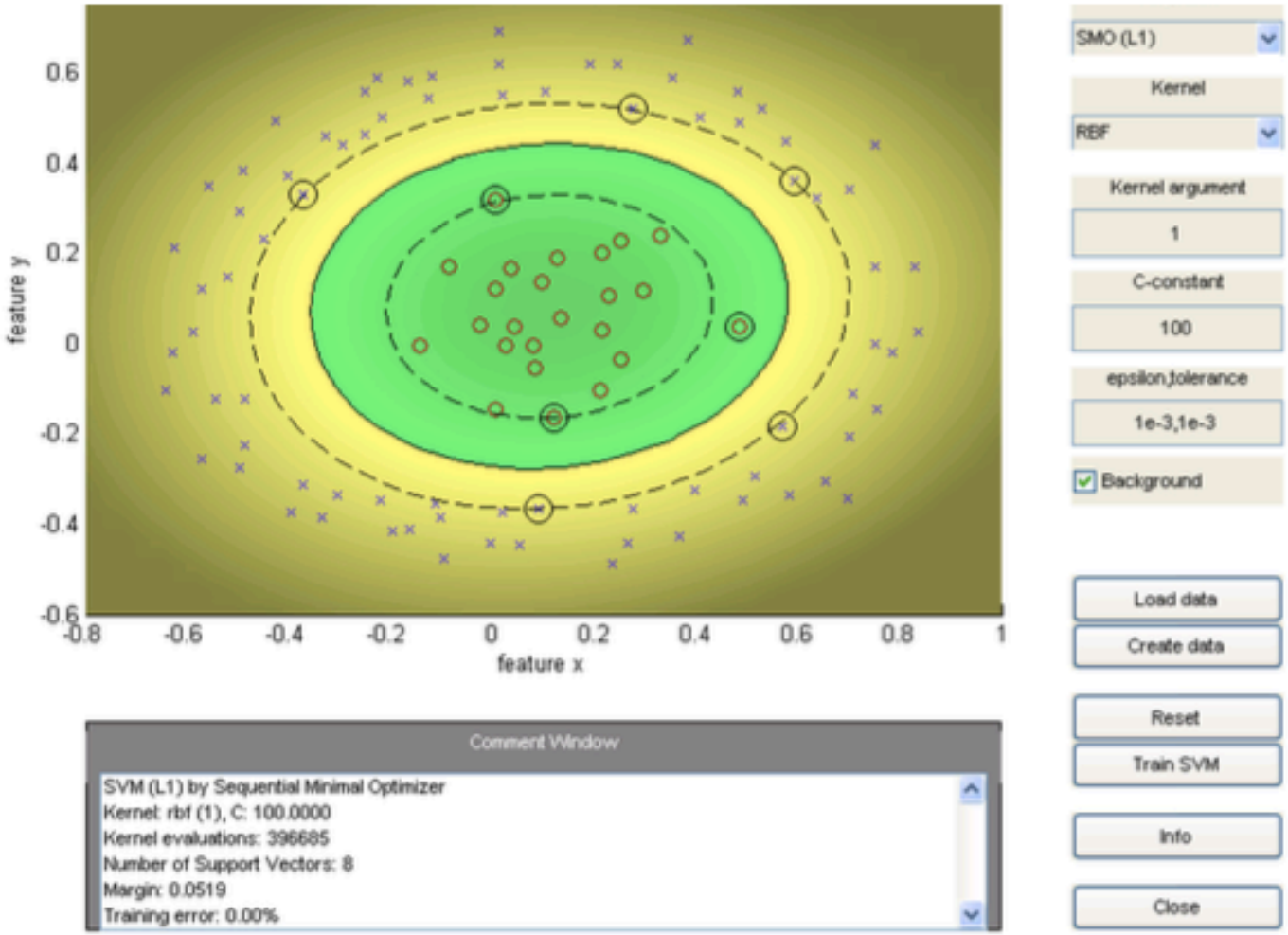
- data is not linearly separable in original feature space

RBF-SVM example



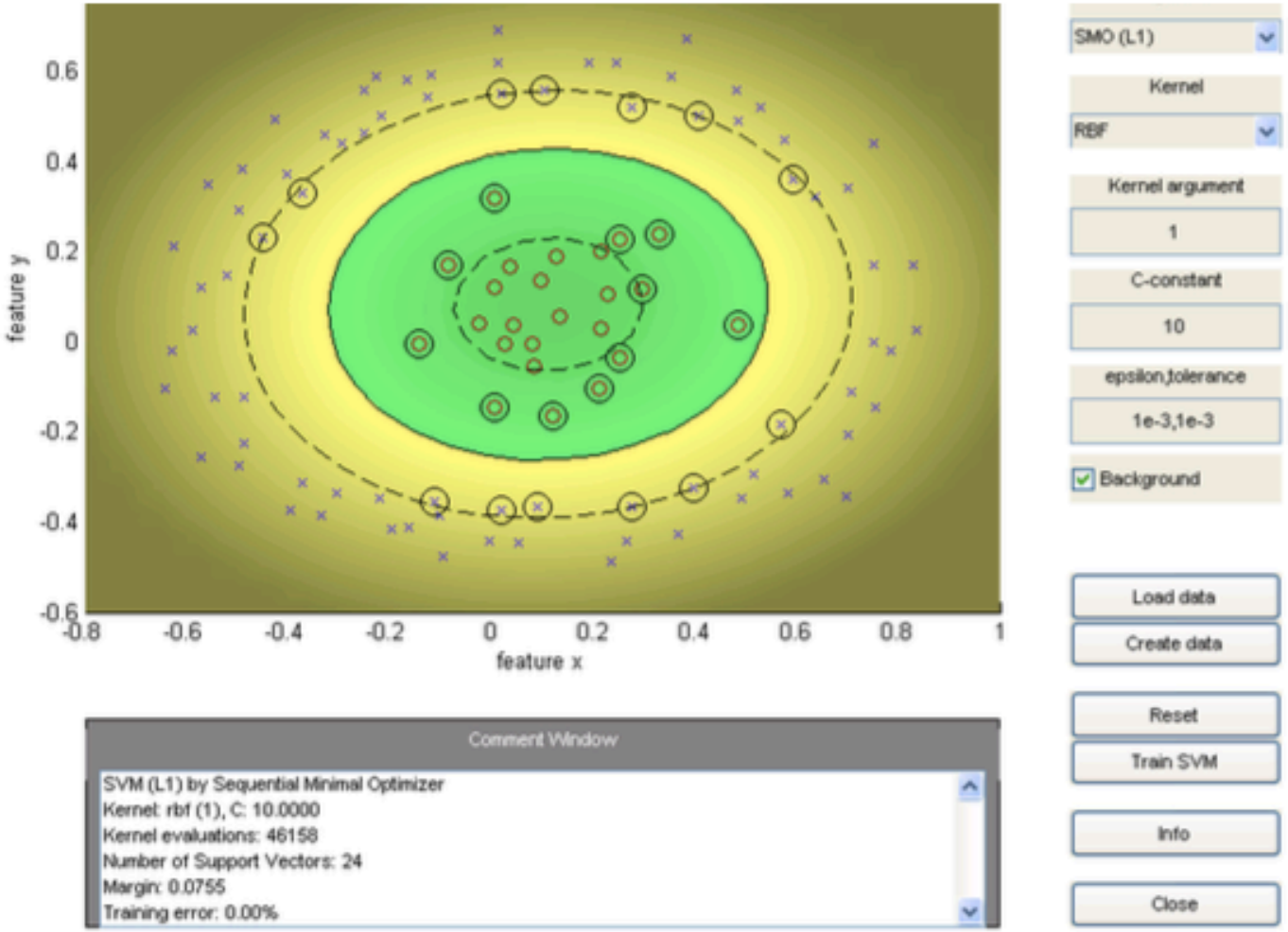
RBF-SVM example

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



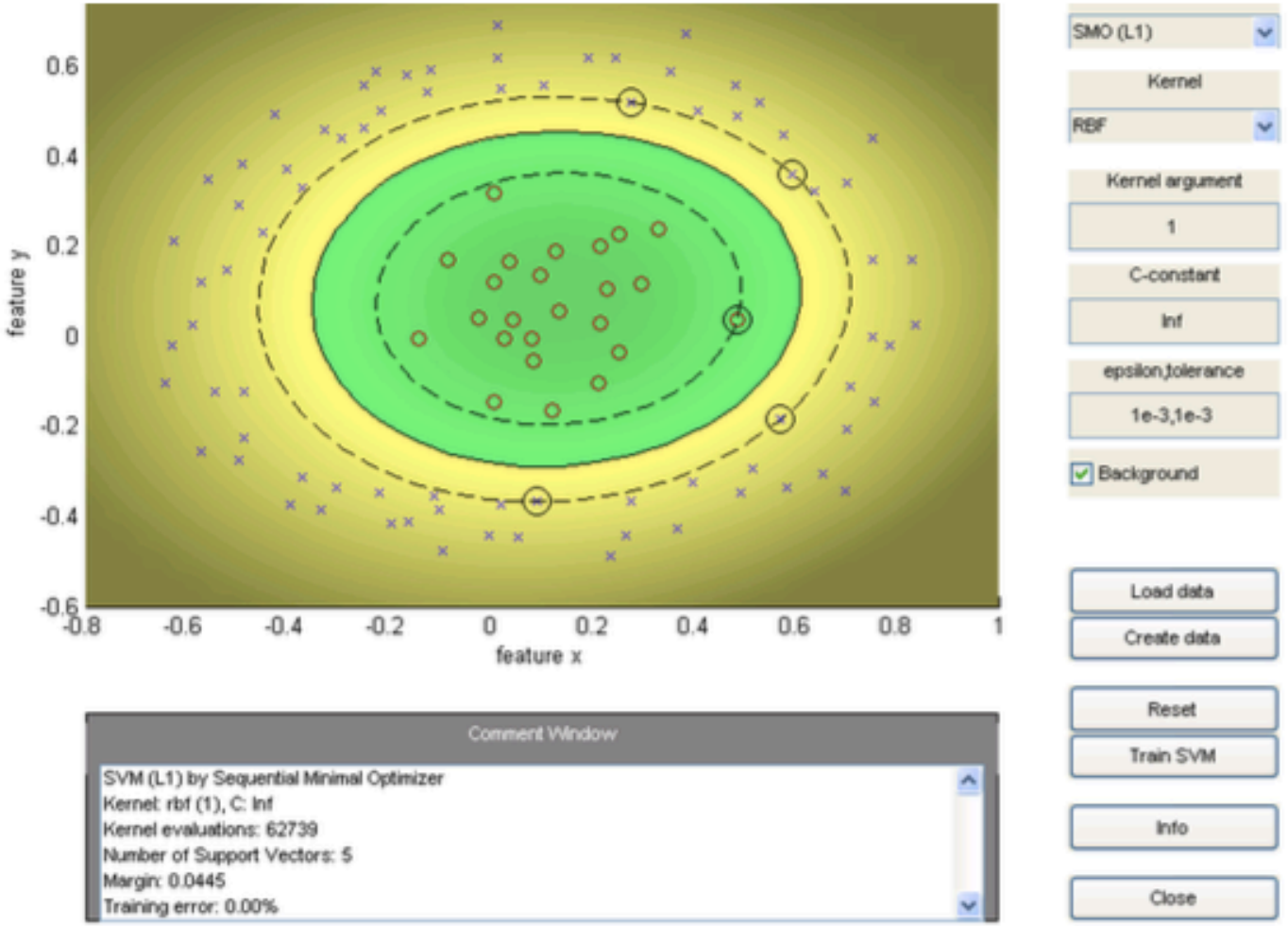
RBF-SVM example

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



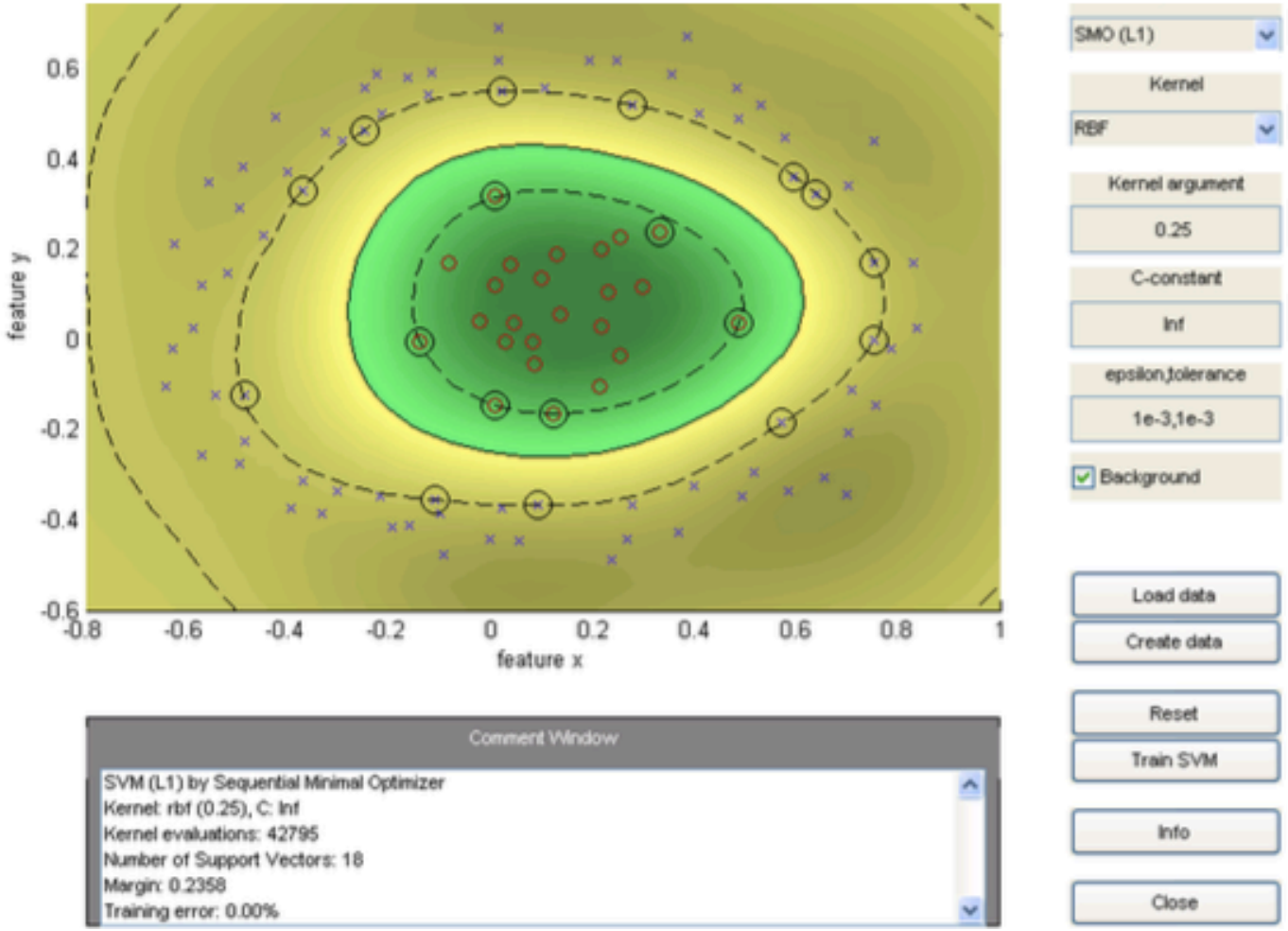
RBF-SVM example

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



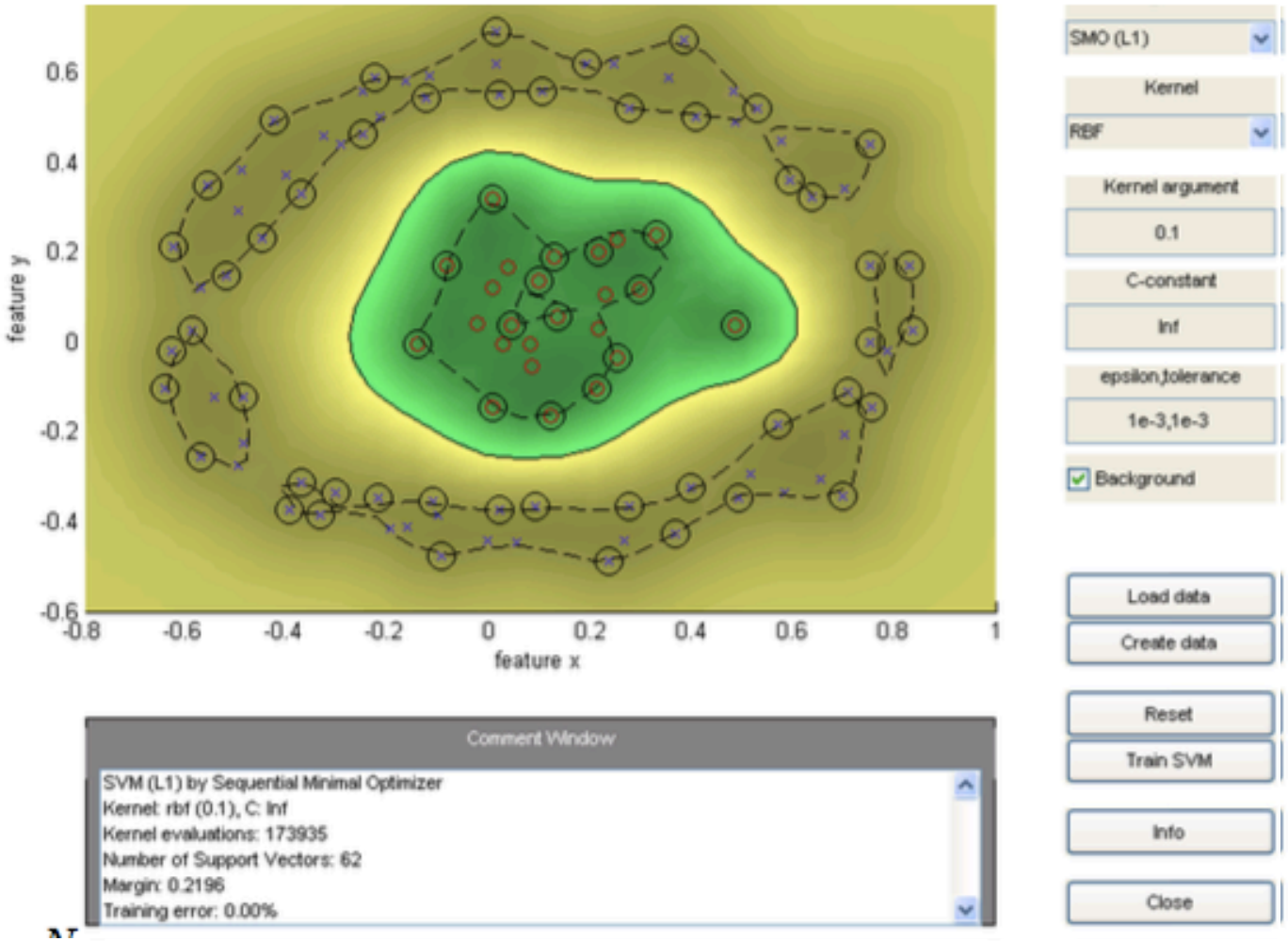
RBF-SVM example

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

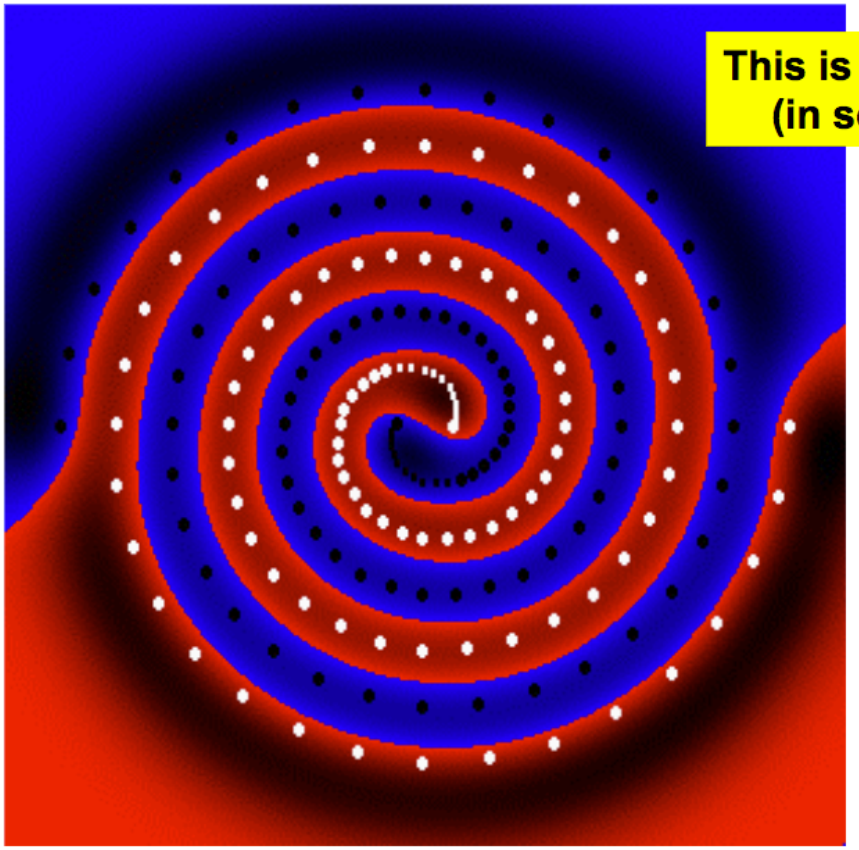


RBF-SVM example

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

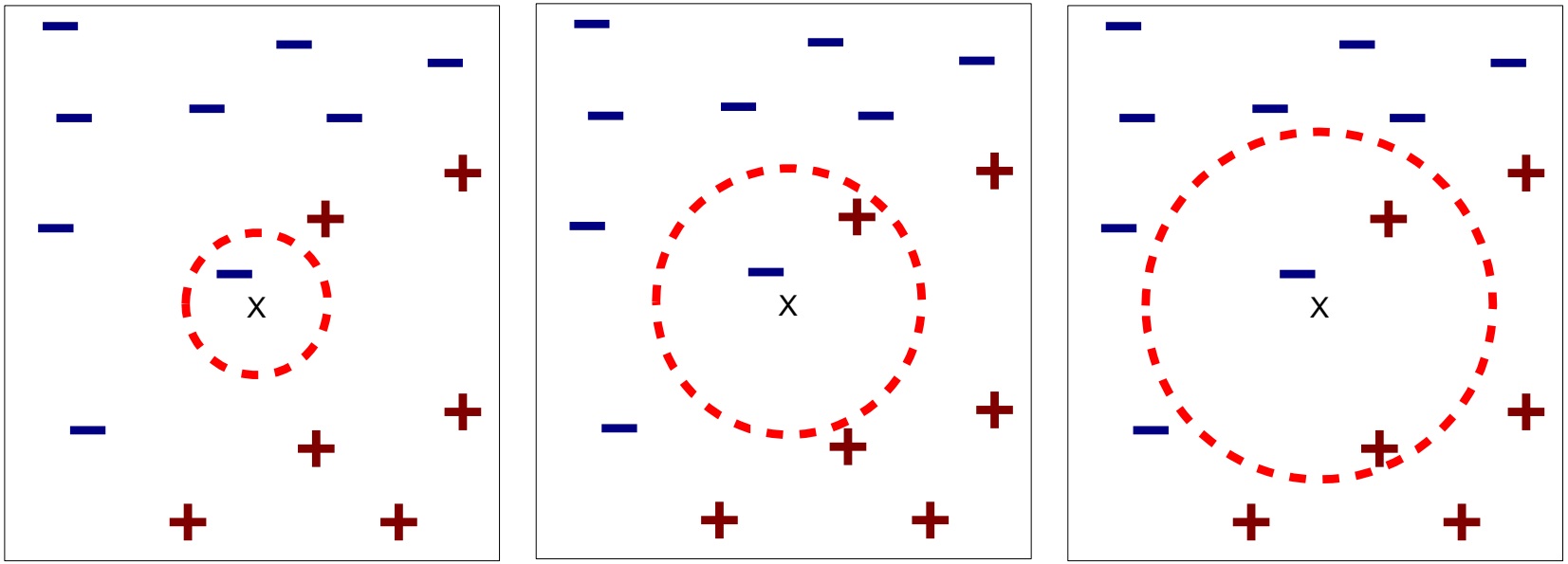


All of the flexibility you may need is there



www.kernel-methods.net

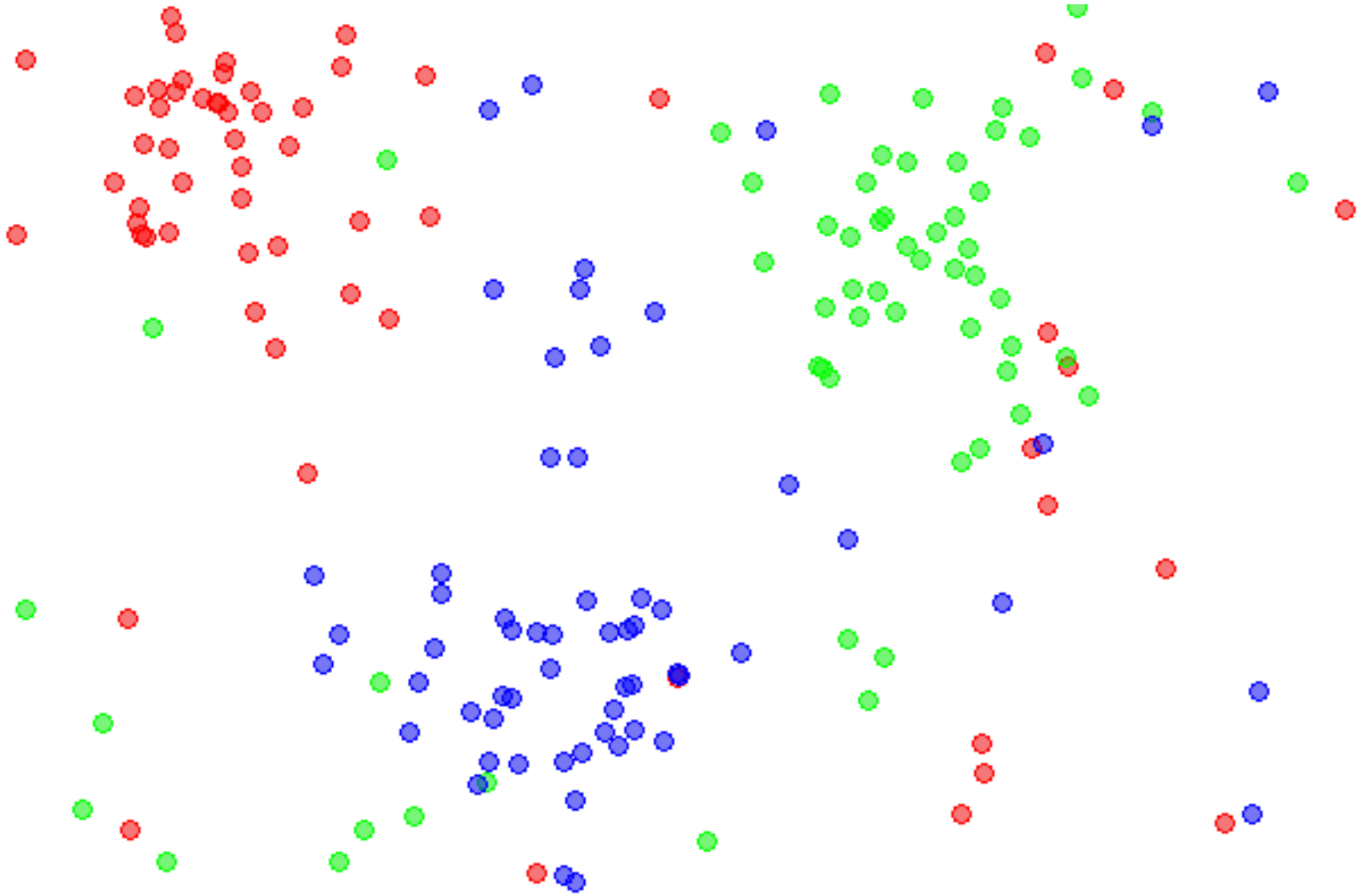
Reminder: K-nearest neighbor classifier



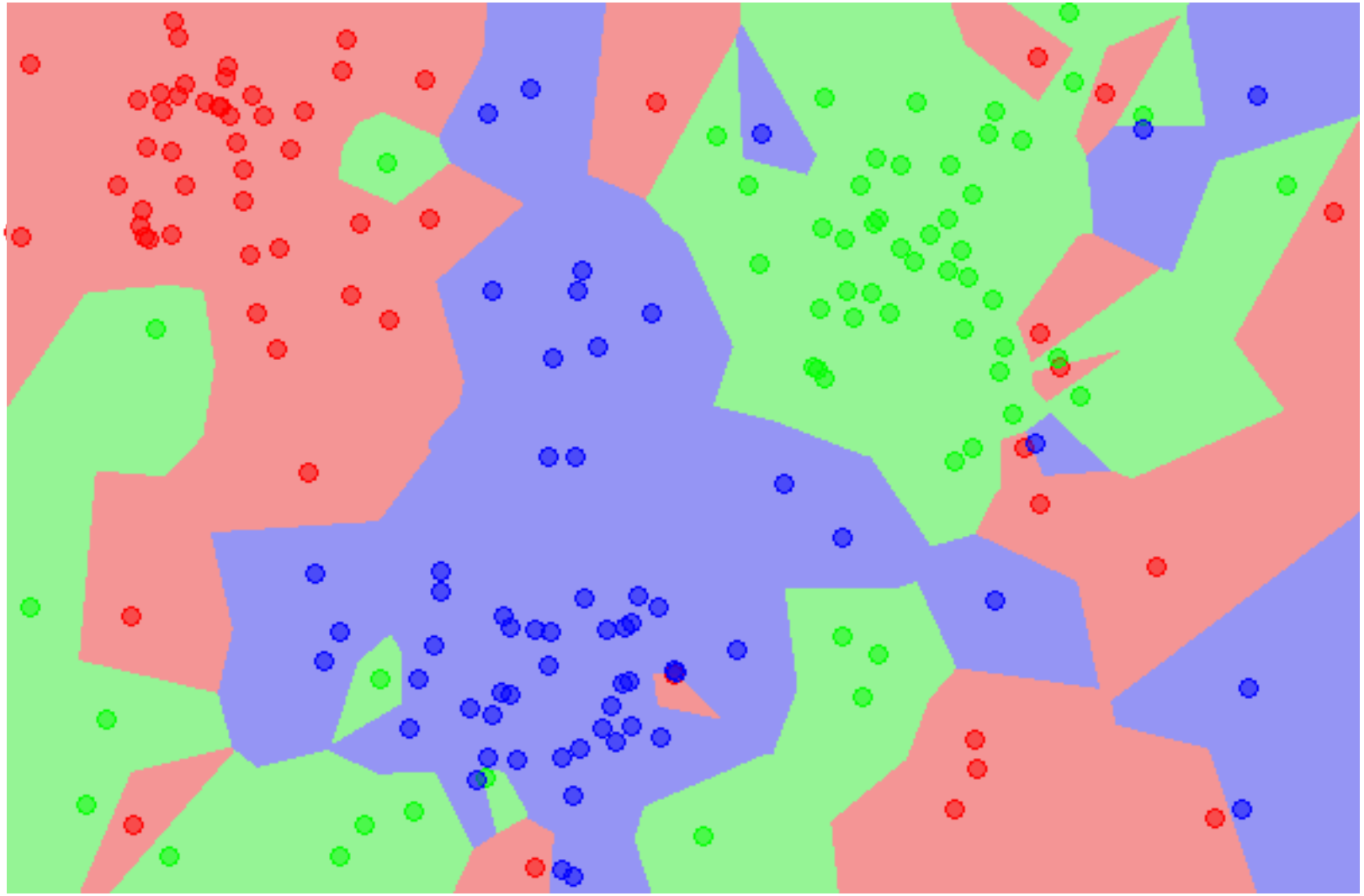
(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

- **Compute distance to other training records**
- **Identify *K* nearest neighbors**
- **Take majority vote**

Training data for NN classifier (in R^2)



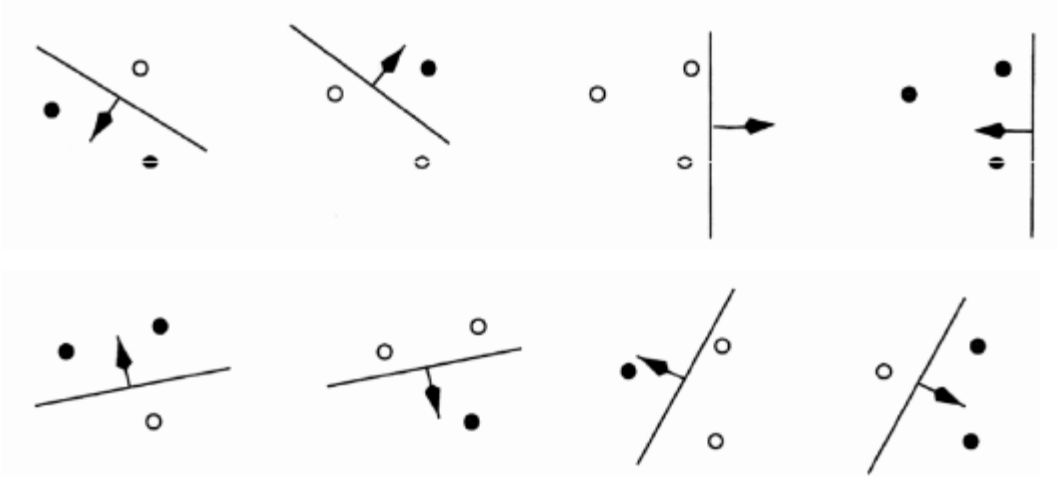
1-nn classifier prediction (in R^2)



VC dimension of 1-nearest neighbor classifier?

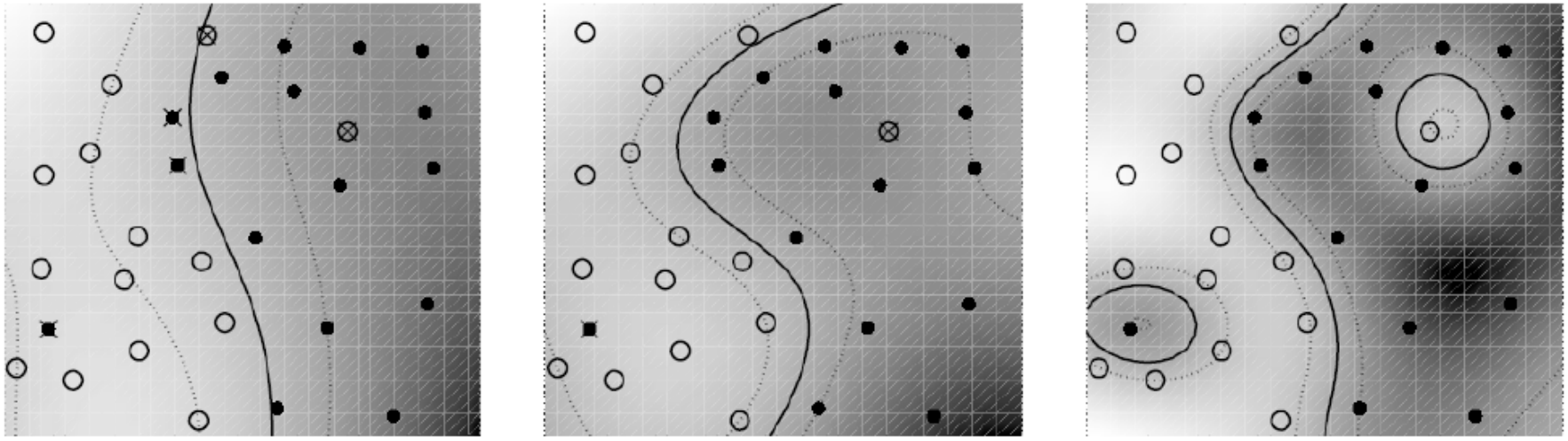
The VC dimension for the set of functions $\{f(\alpha)\}$ is defined as the maximum number of training points that can be shattered by $\{f(\alpha)\}$.

- **VC dimension of N-dimensional linear classifier: N+1**



- **VC dimension of 1-NN: infinite**

Large margins for nonlinear classifiers



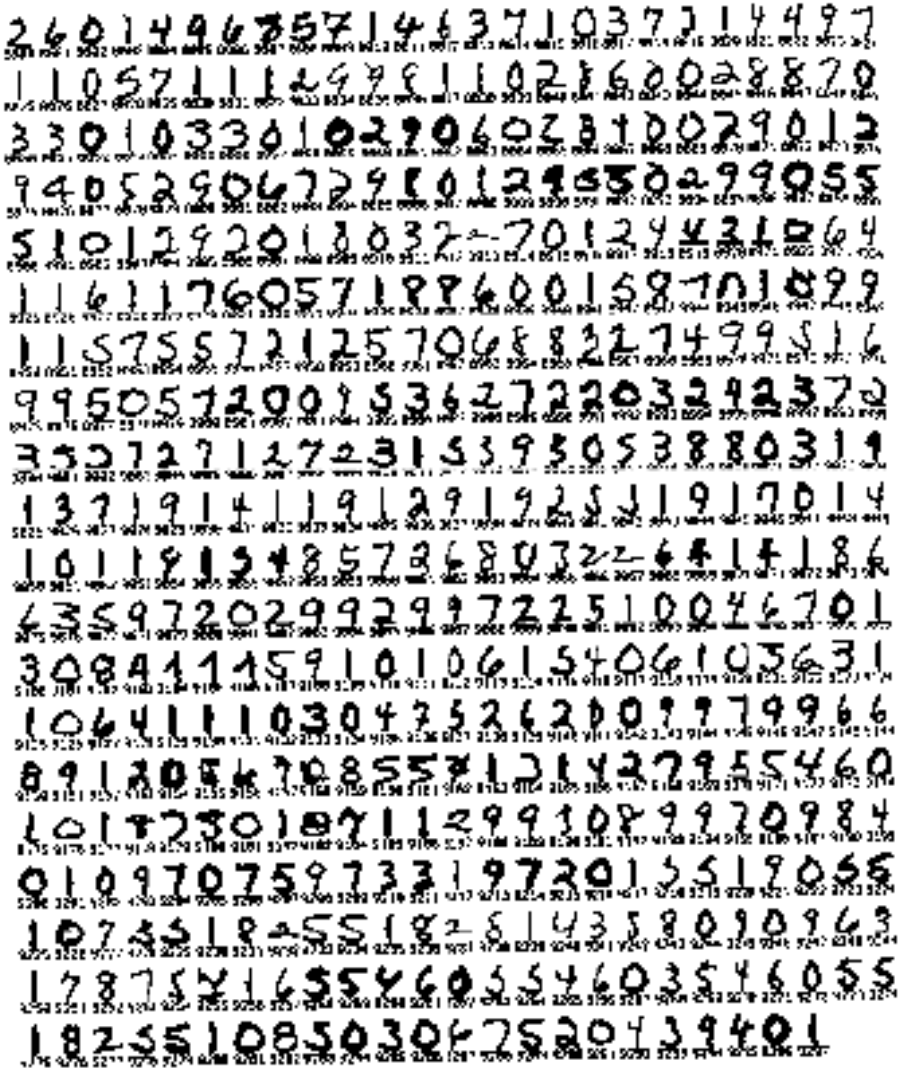
RBF Kernel width (σ)

Margin size: determined by both σ and regularizer

We can slide between a linear and a Nearest-Neighbor classifier!

Guyon & Vapnik, 1995

- Handwritten digit recognition
  - US Postal Service Database
  - Standard benchmark task for many learning algorithms



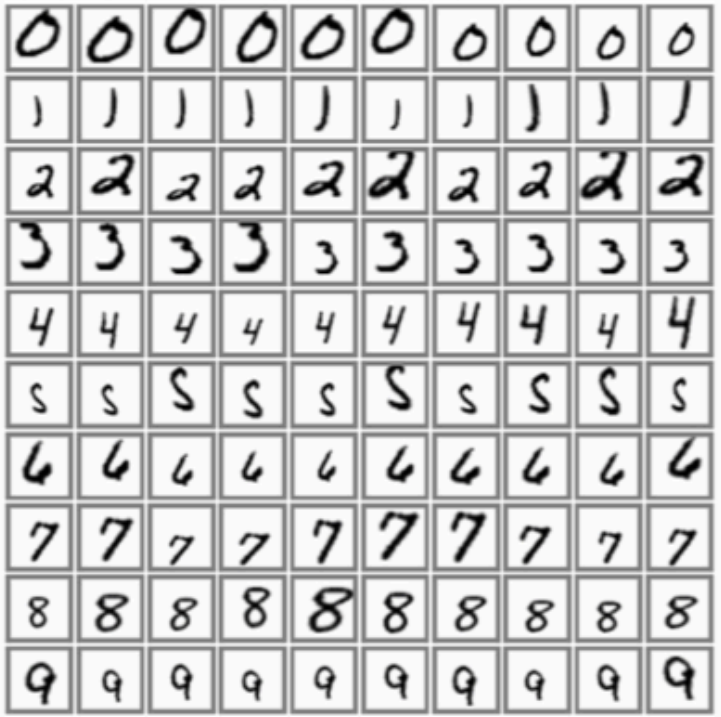
Application: Handwritten digit recognition

- Feature vectors: each image is 28 x 28 pixels. Rearrange as a 784-vector **x**

- Training: learn k=10 two-class 1 vs the rest SVM classifiers $f_k(\mathbf{x})$

- Classification: choose class with most positive score

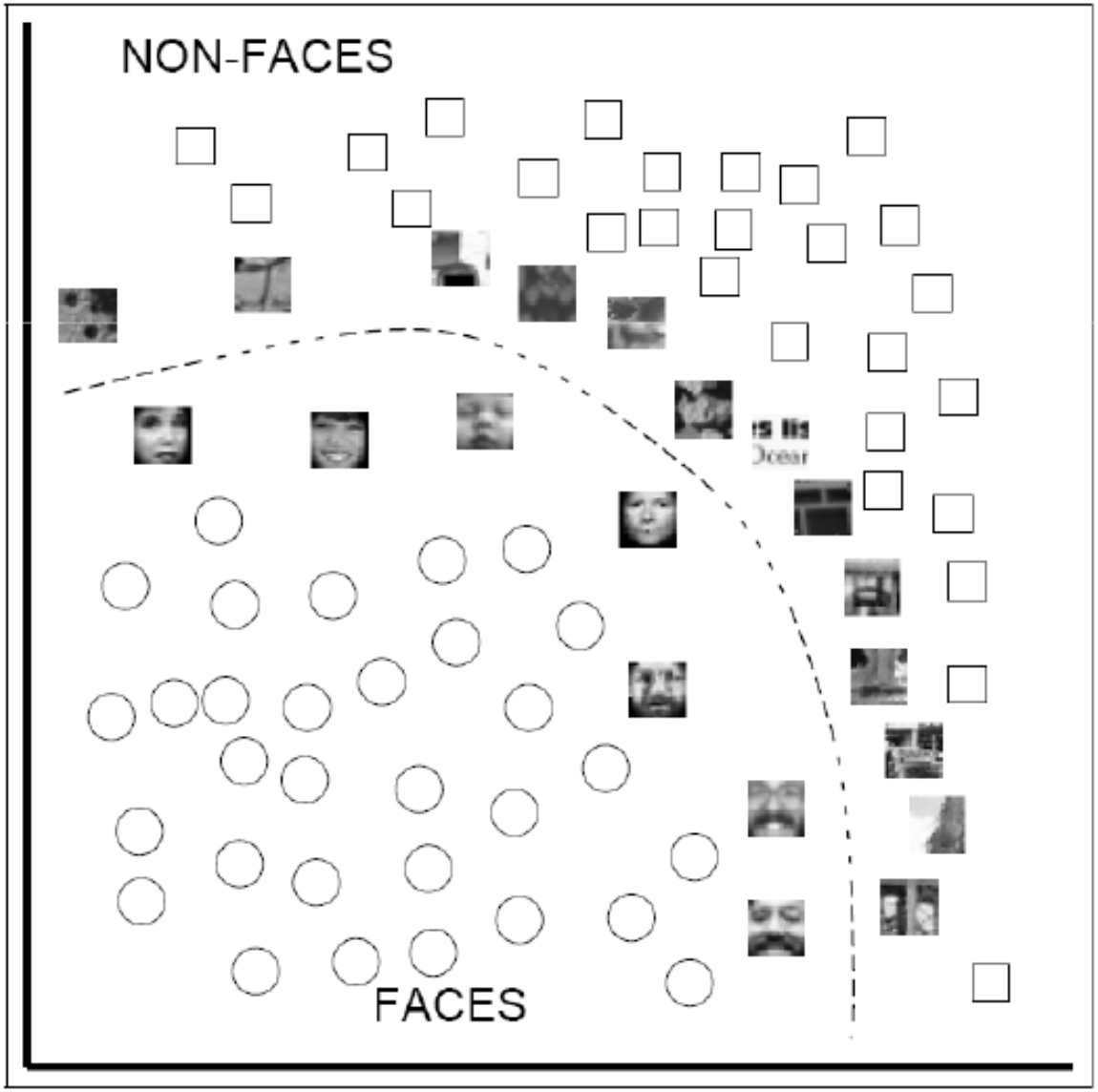
$$f(\mathbf{x}) = \max_k f_k(\mathbf{x})$$



Guyon & Vapnik 1995

- USPS benchmark
  - 2.5% error: human performance
- Different learning algorithms
  - 16.2% error: Decision tree (C4.5)
  - 5.9% error: (best) 2-layer Neural Network
  - 5.1% error: LeNet 1 - (massively hand-tuned) 5-layer network
- Different SVMs
  - 4.0% error: Polynomial kernel (p=3, 274 support vectors)
  - 4.1% error: Gaussian kernel (σ=0.3, 291 support vectors)

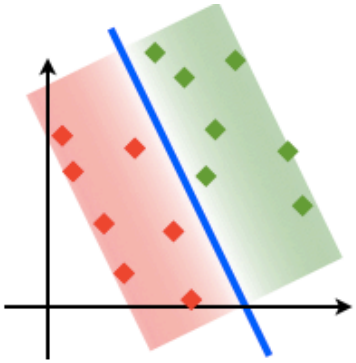
Support vectors for Faces (P&P 98)



Linear vs. Nonlinear

Linear SVM

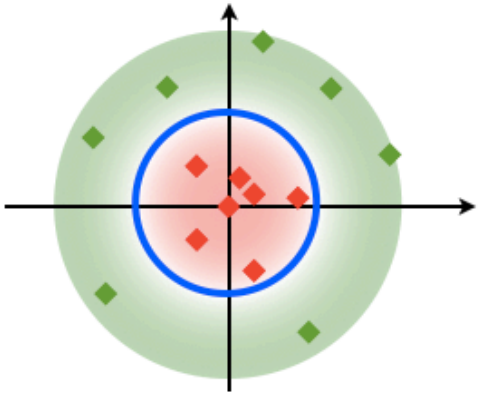
✔ fast
✘ restrictive



$$F(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle$$

Non-linear SVM

✘ much slower
✔ powerful



$$F(\mathbf{x}) = \sum_{i=1}^{N} \alpha_i K(\mathbf{x}, \mathbf{x}_i)$$

Slide credit: A. Vedaldi

Other kernels

- From http://www.kernel-methods.net/kernels.html

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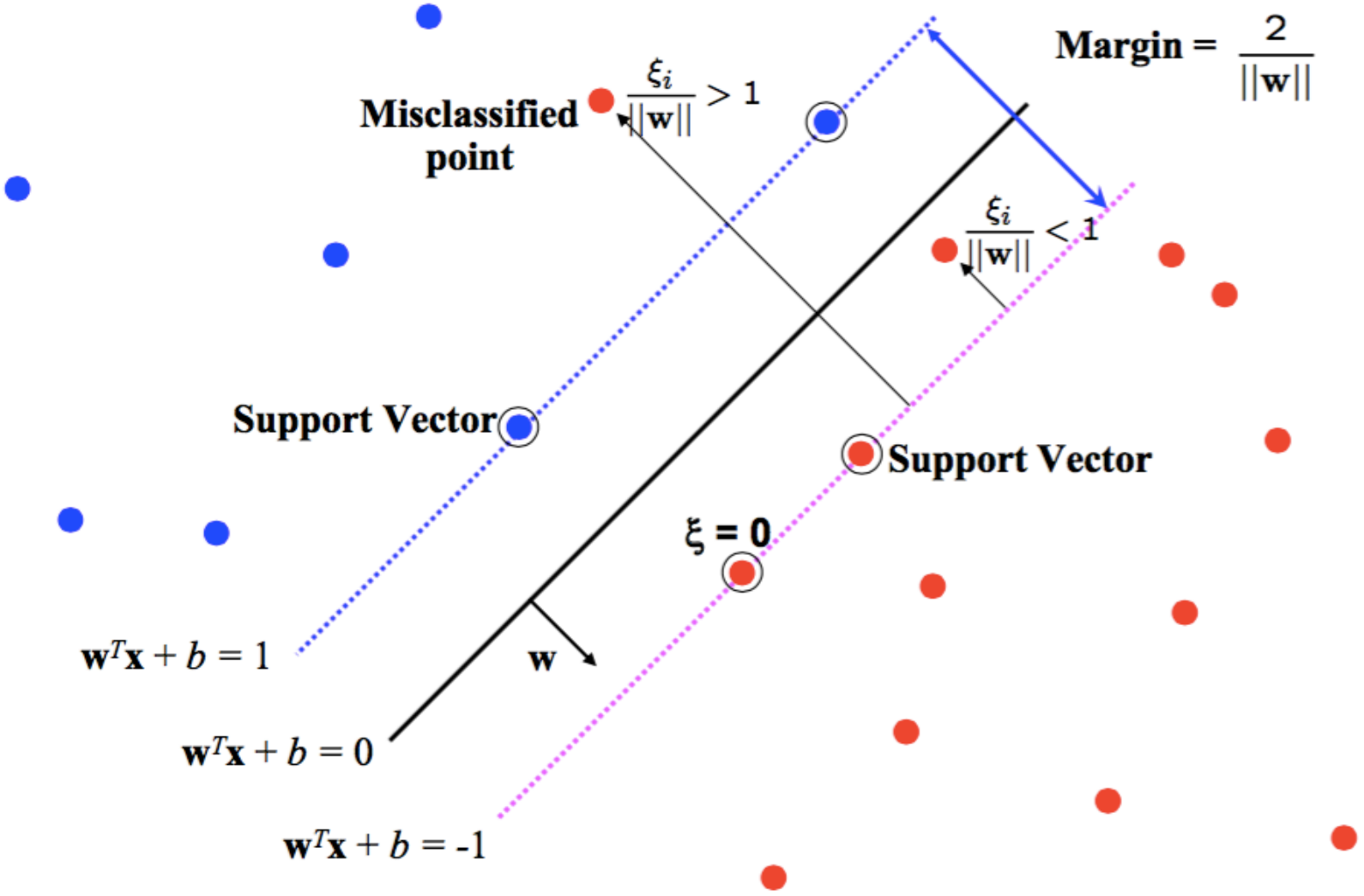
Text Classification: Examples

- Classify news stories as *World, US, Business, SciTech, Sports, Entertainment, Health, Other*
- Add MeSH terms to Medline abstracts
  - e.g. “Conscious Sedation” [E03.250]
- Classify business names by industry.
- Classify student essays as *A,B,C,D,* or *F.*
- Classify email as *Spam, Other.*
- Classify email to tech staff as *Mac, Windows, ..., Other.*
- Classify pdf files as *ResearchPaper, Other*
- Classify documents as *WrittenByReagan, GhostWritten*
- Classify movie reviews as *Favorable,Unfavorable,Neutral.*
- Classify technical papers as *Interesting, Uninteresting.*
- Classify jokes as *Funny, NotFunny.*
- Classify web sites of companies by Standard Industrial Classification (SIC) code.

Slack variables: let us make (but also pay) some errors



Objective for non-separable data

$$\min_{\mathbf{w},\boldsymbol{\xi}} \|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\xi^i$$

newcomers

$$\text{s.t.}: \quad y^i(\mathbf{w}^T\mathbf{x}^i + b) \geq 1 - \xi^i \quad \forall i$$

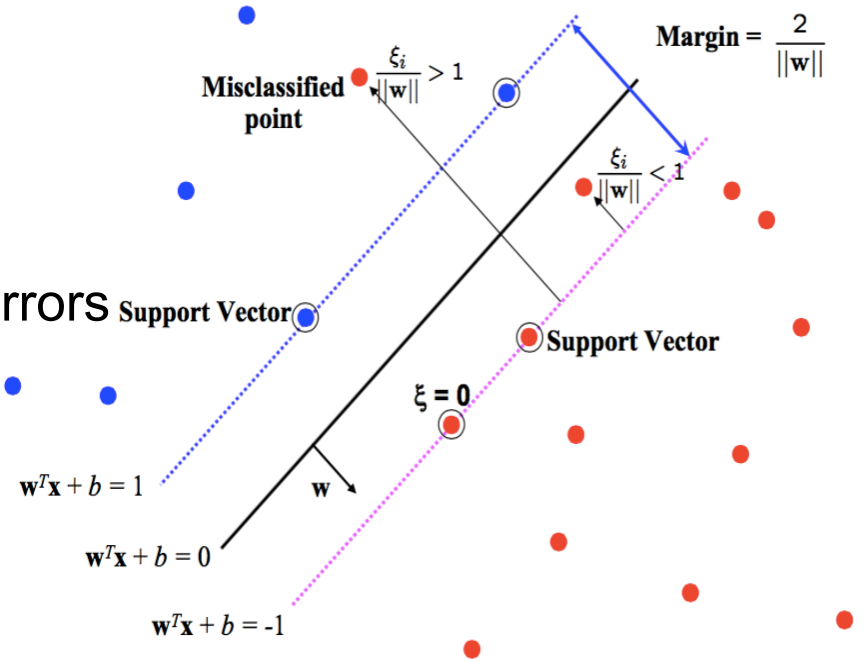
$$\xi^i \geq 0, \quad \forall i$$

misclassification when ξ>1

$\sum_i \xi^i$:upper bound on number of errors

C: hyperparameter

(cross-validation!)



Support Vectors

From complementary slackness (KKT) $\mu_i g_i(x) = 0$

where $g_i(x) = 1 - y^i(\mathbf{w}^T x^i + b) \quad (\leq 0)$

Therefore: $\mu_i \neq 0 \rightarrow y^i(\mathbf{w}^T x^i + b) = 1$

Interpretation: μ is nonzero only for points on the margin (hardest points)

From mimimum w.r.t. w: $\mathbf{w}^* = \sum_{i=1}^{M} \mu_i y^i x^i$

Interpretation: only points on the margin contribute to the solution

- **`Support Vectors'**

Intuitively ok: we want to maximize the margins of the hardest cases

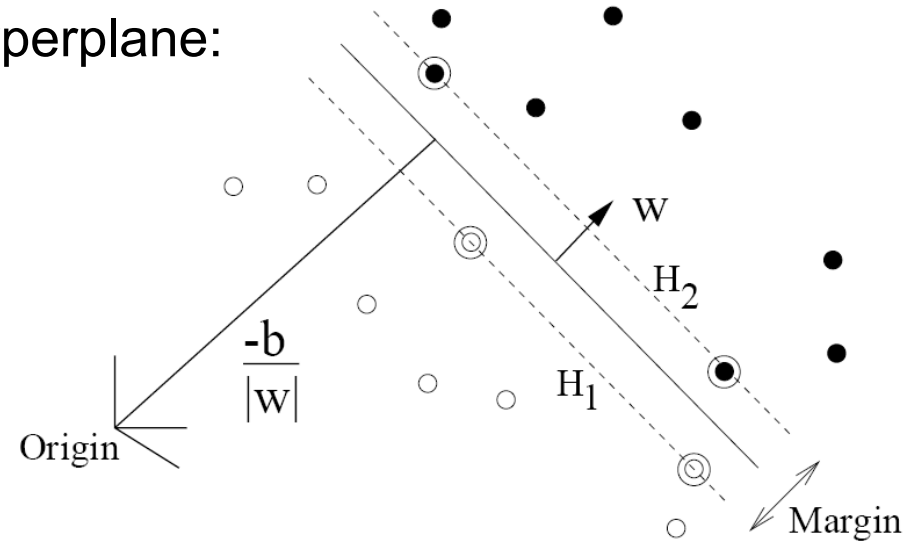
Decision Hyperplanes & Support Vectors

Use support vectors to determine b^*:

$$y^i(\mathbf{w}^T x^i + b) = 1, \quad \forall i \in S$$

$$b^* = \frac{1}{N_S} \sum_{i \in S} (y^i - \mathbf{w}^T x^i)$$

Support Vector Machine decision hyperplane:



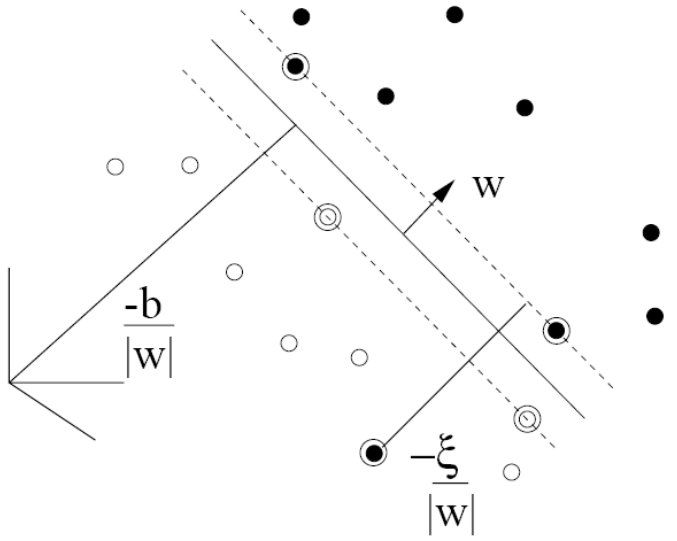
Non-separable data

Primal:

$$\min_{\mathbf{w},b} \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{M}\xi^i$$

$$s.t. \quad y^i(\mathbf{w}^T x^i + b) \geq 1 - \xi^i$$

$$\xi^i \geq 0$$



Lagrangian:

$$L(\mathbf{w}, b, \xi, \mu, \nu) = \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{M}\xi^i - \sum_{i=1}^{M}\mu_i[y^i(\mathbf{w}^T x + b) - 1 + \xi] - \sum_{i=1}^{M}\nu_i\xi_i$$

Dual:

$$\max_{\mu} \quad \sum_{i=1}^{M}\mu_i - \frac{1}{2}\sum_{i=1}^{M}\sum_{j=1}^{M} y^i y^j \mu_i \mu_j < x^i, x^j >$$

$$s.t. \quad 0 \leq \mu_i \leq C$$

$$\sum_{i=1}^{M}\mu_i y^i = 0$$

$$\mu_i \geq 0, \quad \forall i$$

$$\nu_i \geq 0, \quad \forall i$$

KKT conditions – nonseparable case

$$
\begin{aligned}
C - \mu^i - \nu^i &= 0 && (1)\\
y^i(<\mathbf{x}^i, \mathbf{w}> + b) - 1 + \xi^i &\geq 0 && (2)\\
\mu^i \left[y^i(<\mathbf{x}^i, \mathbf{w}> + b) - 1 + \xi^i\right] &= 0 && (3)\\
\nu^i \xi^i &= 0 && (4)\\
\xi^i &\geq 0 && (5)\\
\mu^i &\geq 0 && (6)\\
\nu^i &\geq 0 && (7)
\end{aligned}
$$

Complementary slackness

Complementary slackness

Case analysis:

$$y^i(<\mathbf{x}^i, \mathbf{w}> + b) > 1 \xrightarrow{3:\xi^i \geq 0} \mu_i = 0$$

$$y^i(<\mathbf{x}^i, \mathbf{w}> + b) < 1 \xrightarrow{2:\xi^i > 0 \rightarrow 4:\nu^i = 0 \rightarrow 1:} \mu_i = C$$

$$y^i(<\mathbf{x}^i, \mathbf{w}> + b) = 1 \xrightarrow{3:\mu^i \xi^i = 0 \rightarrow 1:} \mu_i \in [0, C]$$

Interpretation: influence, μ, of any training point is bounded in [0,C]

Hinge Loss

$$
\begin{aligned}
C - \mu^i - \nu^i &= 0 \qquad (1)\\
\mu^i \left[y^i (< \mathbf{x}^i, \mathbf{w} > + b) - 1 + \xi^i \right] &= 0 \qquad (3)\\
\nu^i \xi^i &= 0 \qquad (4)\\
\xi^i &\geq 0 \qquad (5)
\end{aligned}
$$

$$\mu^i \neq 0 \overset{(3)}{\rightarrow} \xi^i = 1 - y^i (< \mathbf{x}^i, \mathbf{w} > + b)$$

$$\mu^i = 0 \overset{(1)}{\rightarrow} \nu^i = C \quad \overset{(4)}{\rightarrow} \xi^i = 0$$

$$\xi^i = \max(0, 1 - y^i (< \mathbf{x}^i, \mathbf{w} > + b))$$

$$
\begin{aligned}
\min_{\mathbf{w},b} \quad & \frac{1}{2}\|\mathbf{w}\|^2 + C \sum_{i=1}^{M} \xi^i \\
s.t. \quad & y^i (\mathbf{w}^T x^i + b) \geq 1 - \xi^i \\
& \xi^i \geq 0
\end{aligned}
\quad \Longleftrightarrow \quad
L(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|^2 + C \sum_{i=1}^{N} \max(0, 1 - y^i h_{\mathbf{w},b}(x^i))
$$

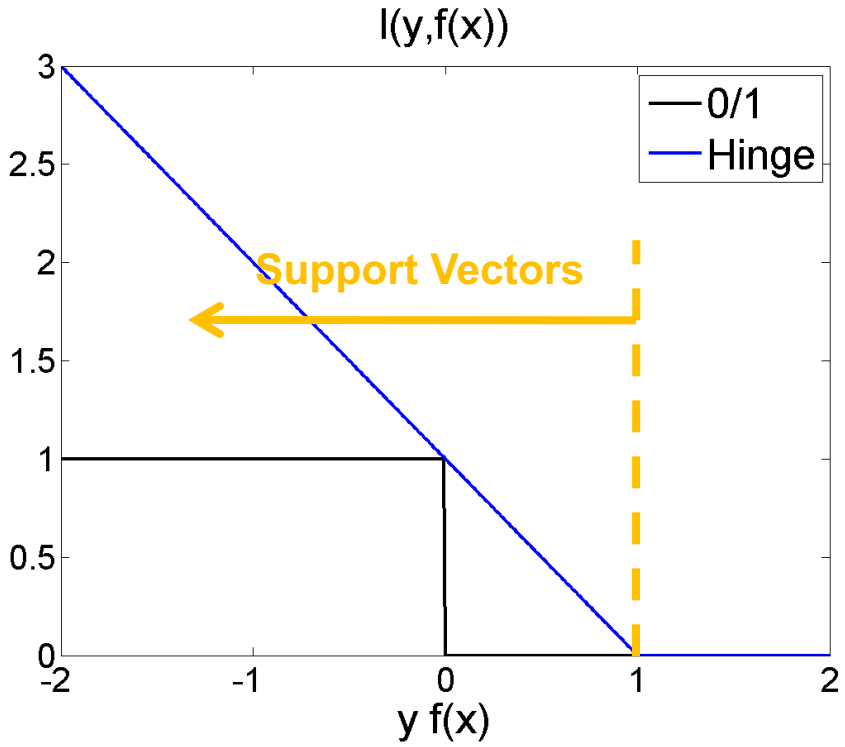
Loss function for SVM training

Optimization problem:

$$L(\mathbf{w}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\max(0, 1 - y^i h_{\mathbf{w},b}(x^i))$$

$$\propto \lambda\|\mathbf{w}\|^2 + \sum_{i=1}^{N}\underbrace{\max(0, 1 - y^i h_{\mathbf{w},b}(x^i))}_{l(y^i, x^i)}$$

Hinge loss:



Appendix

- Primal and Dual form of SVMs: the full story

References:

S. Boyd and L. Vandeberghe: Convex Optimization (textbook)

C. Burges: A tutorial on SVMs for pattern recognition

Duality

- Constrained optimization problem:

$$\begin{aligned} \min_{w} \quad & f(w) \\ s.t. \quad & h_i(w) = 0, \quad i = 1 \dots l \\ & g_i(w) \leq 0, \quad i = 1 \dots m \end{aligned}$$

- Equivalent to unconstrained problem:

$$\min_{w} \quad f_{uc}(w) = f(w) + \sum_{i=1}^{l} I_0(h_i(w)) + \sum_{i=1}^{m} I_+(g_i(w))$$

$$I_0(x) = \begin{cases} 0, & x = 0 \\ \infty, & x \neq 0 \end{cases}, \qquad I_+(x) = \begin{cases} 0, & x \leq 0 \\ \infty, & x > 0 \end{cases}$$

- Soften constraint terms $I_0(x_i) \rightarrow \lambda_i x_i \qquad I_+(x_i) \rightarrow \mu_i x_i, \mu > 0$

Lagrangian

- Replace hard constraints with soft ones

$$\min_w \quad f_{uc}(w) = f(w) + \sum_{i=1}^{l} I_0(h_i(w)) + \sum_{i=1}^{m} I_+(g_i(w))$$

$$L(w, \lambda, \mu) = f(w) + \sum_{i=1}^{l} \lambda_i h_i(w) + \sum_{i=1}^{m} \mu_i g_i(w), \quad \mu_i > 0 \forall i$$

- Observe that

$$f_{uc}(w) = \max_{\lambda, \mu : \mu_i > 0} L(w, \lambda, \mu)$$

- At an optimum:

$$f(w^*) = \min_w \max_{\lambda, \mu : \mu_i > 0} L(w, \lambda, \mu)$$

Lagrange Dual Function

- Form $$\theta(\lambda, \mu) = \inf_{w} L(w, \lambda, \mu)$$

- θ : lower bound on optimal value of the original problem

$$\begin{aligned} L(w^*, \lambda, \mu) &= f(w^*) + \sum_{i=1}^{l} \lambda_i h_i(w^*) + \sum_{i=1}^{m} \mu_i g_i(w^*) = \\ &\overset{w^*:feasible}{=} f(w^*) + \sum_{i=1}^{l} \lambda_i 0 + \sum_{i=1}^{m} \mu_i \underbrace{g_i(w^*)}_{<0} = \\ &\overset{\mu_i > 0}{\leq} f(w^*) \end{aligned}$$

- Therefore: $$\theta(\lambda, \mu) = \inf_{w} L(w, \lambda, \mu) \leq L(w^*, \lambda, \mu) \leq f(w^*)$$

Dual Problem

- Maximize the lower bound on the cost of the primal

$$\max_{\lambda,\mu} \quad \theta(\lambda,\mu)$$
$$s.t. \quad \mu_i > 0 \quad \forall i$$

- In general:

$$\begin{aligned} d^* &= \max_{\lambda,\mu} \theta(\lambda,\mu) \\ &= \max_{\lambda,\mu:\mu_i>0} \min_{w} L(w,\lambda,\mu) \\ &\leq \min_{w} \max_{\lambda,\mu:\mu_i>0} L(w,\lambda,\mu) \\ &= \min_{w} f_{uc}(w) = p^* \end{aligned}$$

- For convex cost and convex constraints (SVM case): $d^* = p^*$

Complementary Slackness

- Assume $d^* = p^*$
- There exists a feasible solution w^*, λ^*, μ^* to the primal and dual problems, such that $f(w^*) = \theta(\lambda^*, \mu^*)$
- We will have

$$\begin{aligned} f(w^*) &= \theta(\lambda^*, \mu^*) \\ &= \inf_w f(w) + \sum_{i=1}^{l} \lambda_i^* h_i(w) + \sum_{i=1}^{m} \mu_i^* f_i(w) \\ &\leq f(w^*) + \sum_{i=1}^{M} \lambda_i^* h_i(w^*) + \sum_{i=1}^{m} \mu_i^* f_i(w^*) \\ &\leq f(w^*) \end{aligned}$$

- This means $\mu_i^* f_i(w^*) = 0, \quad \forall i$

Karush-Kuhn Tucker (KKT) Conditions

- Solution of the primal problem:
  - minimum of the Lagrangan w.r.t. the primal variables
  - therefore $$\nabla f(w^*) + \sum_{i=1}^{l} \lambda_i \nabla h_i(w^*) + \sum_{i=1}^{m} \nabla f_i(w^*) = 0$$

- Putting all constraints together: KKT conditions

$$\begin{aligned} h_i(w^*) &= 0 \\ f_i(w^*) &\leq 0 \\ \mu_i f_i(w^*) &= 0 \\ \mu_i &\geq 0 \\ \nabla f(w^*) + \sum_{i=1}^{l} \lambda_i \nabla h_i(w^*) + \sum_{i=1}^{m} \nabla f_i(w^*) &= 0 \end{aligned}$$

Problem Lagrangian

Primal:

$$\min_{\mathbf{w},b} \quad \frac{1}{2}|\mathbf{w}|^2$$

$$s.t. \quad -y^i(\mathbf{w}^T x^i + b) + 1 \leq 0, \quad i = 1 \ldots M$$

Lagrangian: $L(\mathbf{w}, b, \mu) = \frac{1}{2}|\mathbf{w}|^2 - \sum_{i=1}^{M} \mu_i [y^i(\mathbf{w}^T x^i + b) - 1] \qquad \mu_i \geq 0$

Optimum w.r.t. $\mathbf{w}$: $0 = \mathbf{w}^* - \sum_{i=1}^{M} \mu_i [y^i x^i] \qquad \mathbf{w}^* = \sum_{i=1}^{M} \mu_i y^i x^i$

Optimum w.r.t. b: $0 = \sum_{i=1}^{M} \mu_i y^i$

Dual for Large-Margin Classifier-I

Plug optimal values into Lagrangian:

$$
\begin{aligned}
\theta(\mu) &= L(\mathbf{w}^*, b^*, \mu) \\
&= \frac{1}{2}|\mathbf{w}^*|^2 - \sum_{i=1}^{M} \mu_i [y^i(\mathbf{w}^{*T} x^i + b) - 1] \\
&= \frac{1}{2}(\sum_{i=1}^{M} \mu_i y^i x^i)^T (\sum_{j=1}^{M} \mu_j y^j x^j) - \sum_{i=1}^{M} \mu_i [y^i((\sum_{j=1}^{M} \mu_j y^j x^j)^T x^i + b) - 1] \\
&= \sum_{i=1}^{M} \mu_i - \frac{1}{2} \sum_{i=1}^{M} \sum_{j=1}^{M} \mu_i \mu_j y^i y^j (x^i)^T (x^j) - b \sum_{i=1}^{M} \mu_i y^i
\end{aligned}
$$

Dual for Large-Margin Classifier-II

Equivalent optimization problem:

$$\max_{\mu} \quad \theta(\mu) = \sum_{i=1}^{M} \mu_i - \frac{1}{2} \sum_{i=1}^{M} \sum_{j=1}^{M} \mu_i \mu_j y^i y^j < x^i, x^j >$$

$$s.t. \quad \mu_i > 0, \quad \forall i$$

$$\sum_{i=1}^{M} \mu_i y^i = 0$$