Supervised Learning

Classification

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March 24, 2015

Supervised Learning

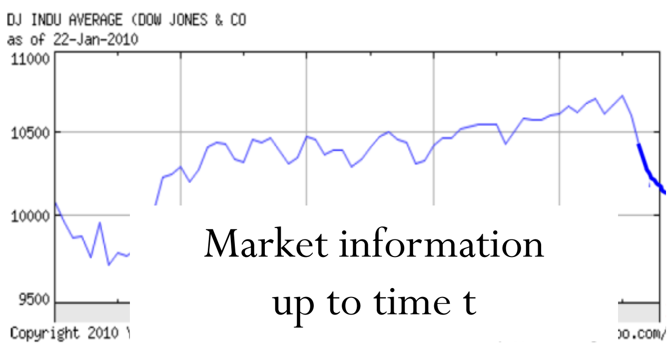
- Task: learn a predictive function $h: \mathcal{X} \rightarrow \mathcal{Y}$

Feature space $\mathcal{X}$

Label space $\mathcal{Y}$

Words in documents

“Sports”
“News”
“Politics”
…



Market information up to time t

Share price
“$ 20.50”

- “Experience” or training data:

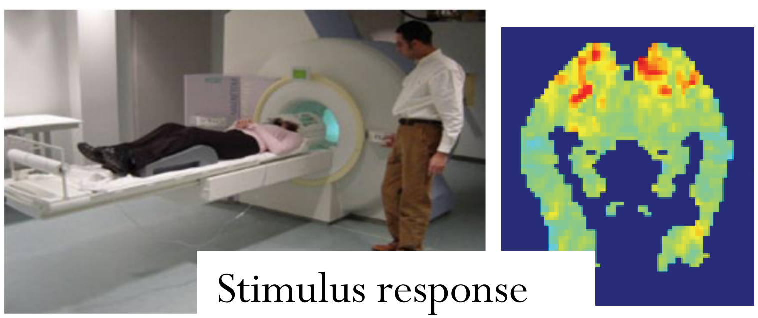
$$\{< \mathrm{x}_d, y_d >\}_{d=1}^{D}, \ \mathrm{x}_d \in \mathcal{X}, y_d \in \mathcal{Y}$$

Supervised Learning – classification

Feature space $\mathcal{X}$ | **Label** space $\mathcal{Y}$

Words in documents

“Sports”
“News”
“Politics”
…



Stimulus response

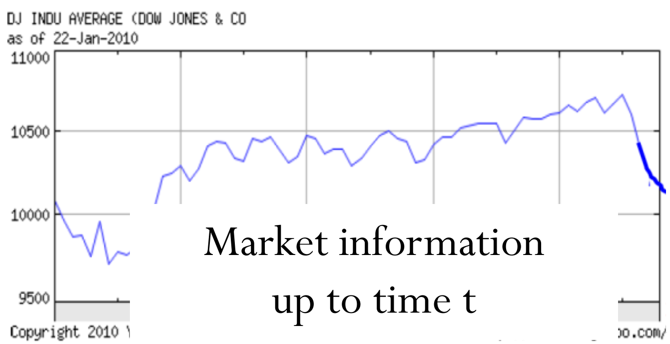
“Tool”
“Animal”
…

Discrete Labels

Supervised Learning – regression

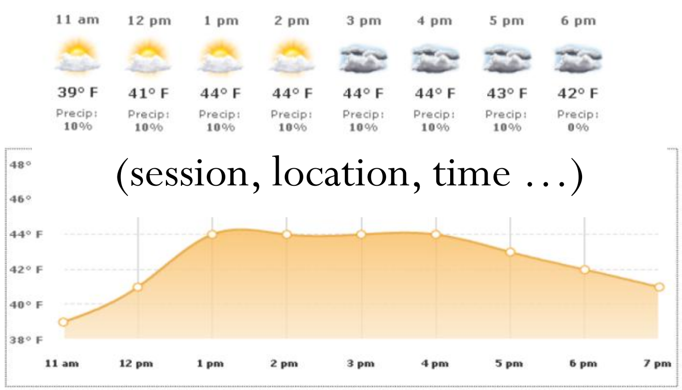
Feature space $\mathcal{X}$

Label space $\mathcal{Y}$



Market information
up to time t

Share price
"$ 20.50"

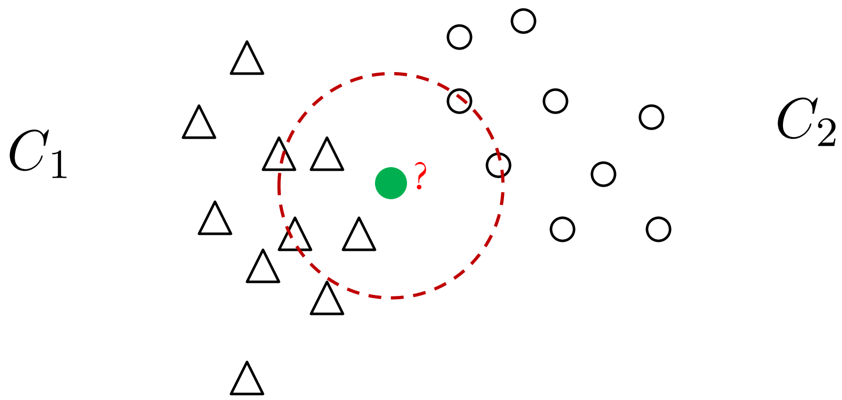


(session, location, time ...)

Temperature
"42° F"

Continuous Labels

How to learn a classifier?



K-NN: a Non-parametric approach

Properties of K-NN

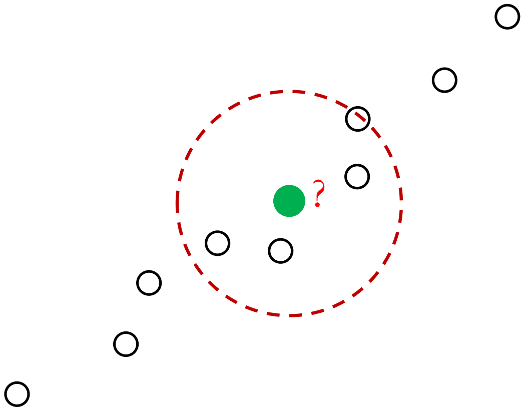
- Simple
- Strong consistency results:
  - With infinite data, the error rate of K-NN is at most twice the optimal error rate (i.e., Bayes error rate)

- **Note**: Bayes error rate – the minimum achievable error rate given the distribution of the data

Issues of K-NN

- Computationally intensive for large training sets
  - Clever nearest neighbor search helps
- Selection of K
- Distance metric matters a lot
  - Aware of the metric learning field

K-NN for regression

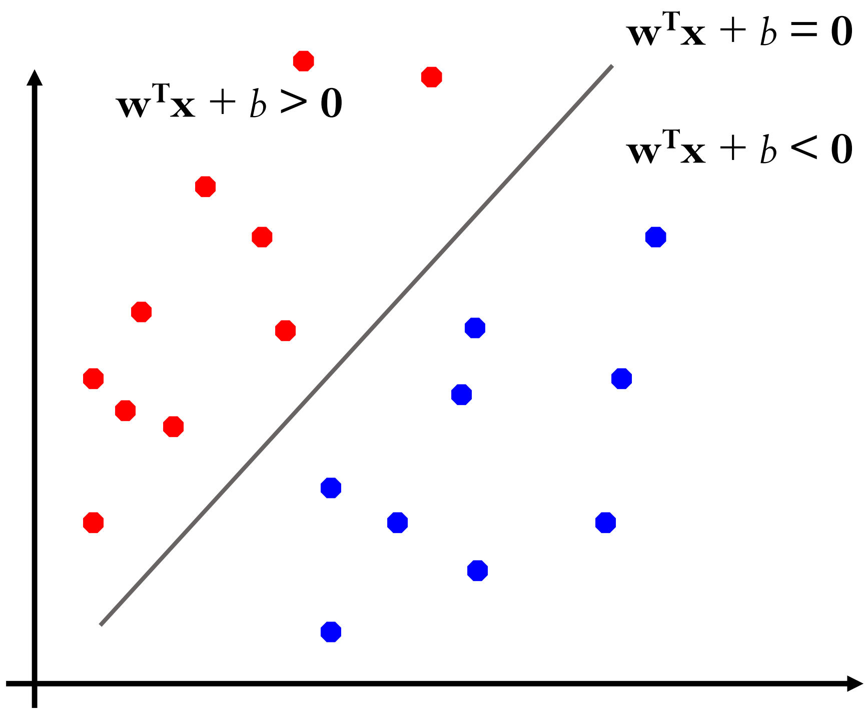


$$\hat{y} = \sum_{i \in \mathcal{N}_K} \frac{1}{dist(\mathbf{x}, \mathbf{x}_i)} y_i$$

A weighted average is an estimate; where the weight is the inverse distance

A Parametric Method

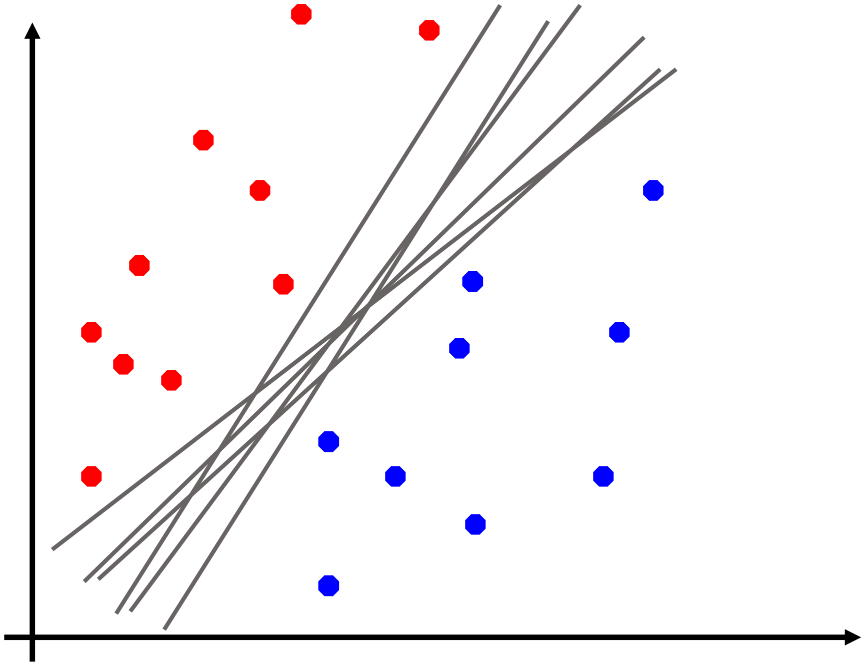
- Binary classification can be viewed as the task of separating classes in feature space:



$$f(\mathbf{x}) = \mathrm{sign}(\mathbf{w}^{\mathrm{T}}\mathbf{x} + b)$$

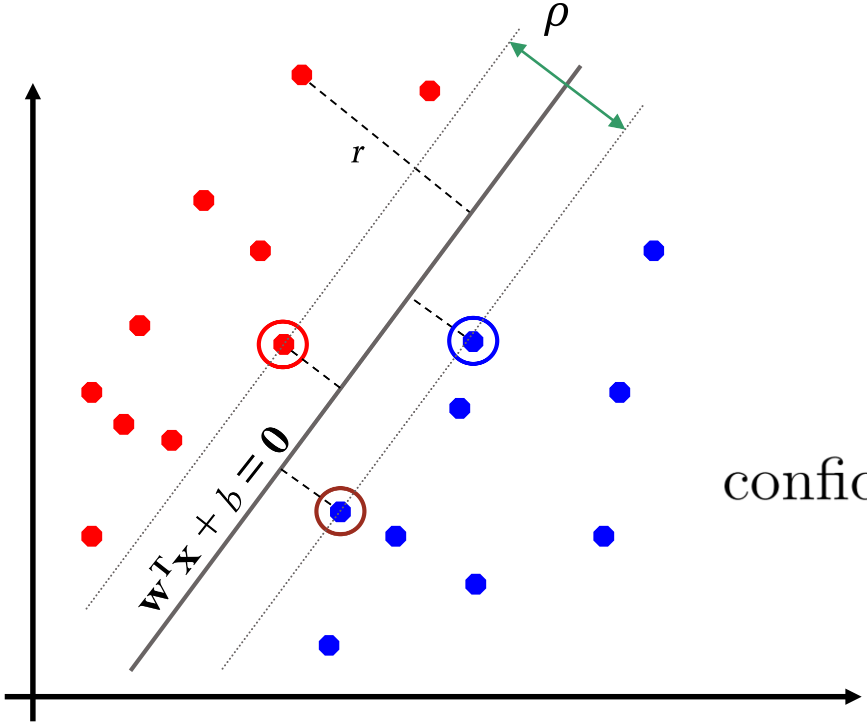
Linear Separators

- Which of the linear separators is optimal?



Classification Margin

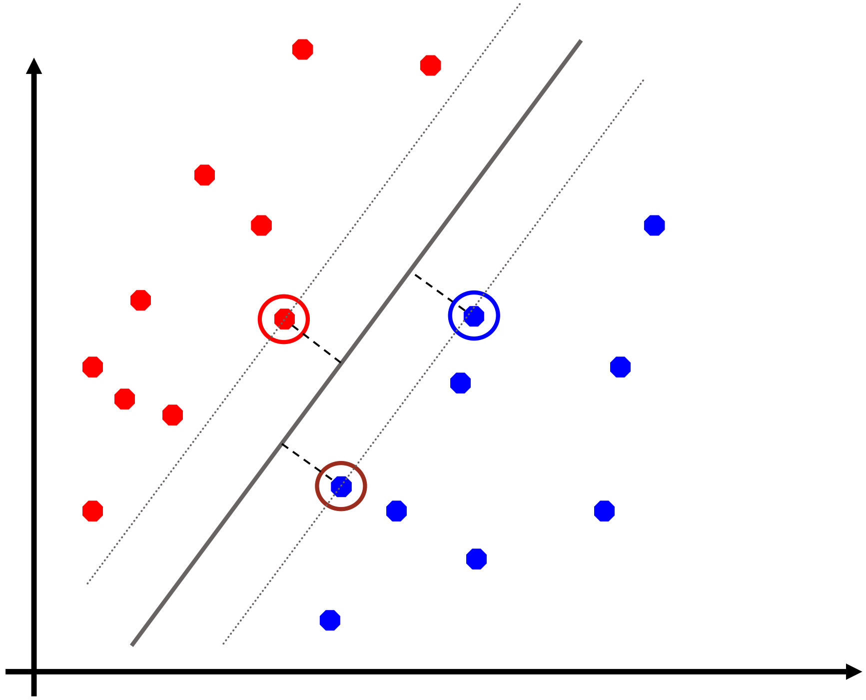
- Distance from example $\mathbf{x}_i$ to the separator is $r = \dfrac{|\mathbf{w}^\top \mathbf{x}_i + b|}{\|\mathbf{w}\|}$
- Examples closest to the hyperplane are ***support vectors***.
- ***Margin*** ρ of the separator is the distance between supporting hyperplanes.



confidence $:= y_i(\mathbf{w}^\top \mathbf{x}_i + b)$

Max-margin Classification

- Maximizing the margin is good according to intuition and PAC theory.
- Implies that only support vectors matter; other training examples are ignorable.



Linear SVM

- Let training set $\{(\mathbf{x}_i, y_i)\}_{i=1}^N,\ \mathbf{x}_i \in \mathbb{R}^d,\ y_i \in \{-1, +1\}$ be separated by a hyperplane with margin ρ. Then for each training example $(\mathbf{x}_i, y_i)$:

$$\begin{aligned} &\mathbf{w}^{\mathbf{T}}\mathbf{x}_i + b \leq -\rho/2 \quad \text{if } y_i = -1 \\ &\mathbf{w}^{\mathbf{T}}\mathbf{x}_i + b \geq \rho/2 \quad \text{if } y_i = 1 \end{aligned} \quad \Leftrightarrow \quad y_i(\mathbf{w}^{\mathbf{T}}\mathbf{x}_i + b) \geq \rho/2$$

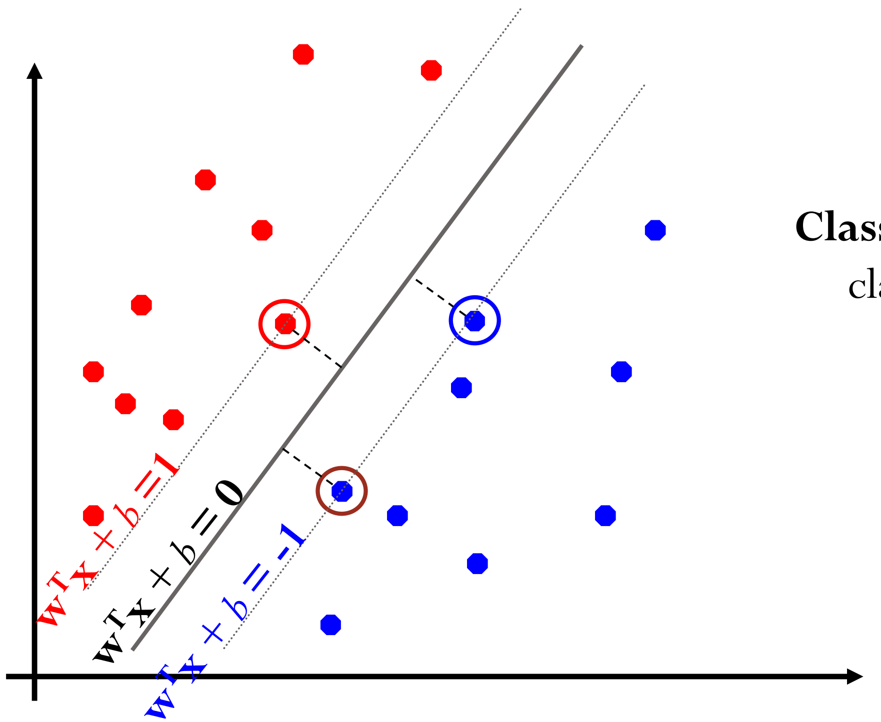
- For support vector $\mathbf{x}_s$ the above inequality is an equality. After rescaling $\mathbf{w}$ and b by $\rho/2$, we obtain that distance between each $\mathbf{x}_s$ and the hyperplane is

$$r = \frac{y_s(\mathbf{w}^\top \mathbf{x}_s + b)}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|}$$

Linear SVM

- Then the margin can be expressed through (rescaled) **w** and b as:

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



Classification rule:

classify as: **+1** **if** $\mathbf{w}^\top\mathbf{x} + b \geq 1$

-1 **if** $\mathbf{w}^\top\mathbf{x} + b \leq -1$

universe explodes if $|\mathbf{w}^\top\mathbf{x} + b| < 1$

Observations

- We can assume b=0

Classification rule:

classify as:	**+1**	**if**	$\mathbf{w}^\top \mathbf{x} + b \geq 1$
	- 1	**if**	$\mathbf{w}^\top \mathbf{x} + b \leq -1$
	universe explodes	if	$\lvert \mathbf{w}^\top \mathbf{x} + b \rvert < 1$

- This is the same as:

$$y_i \mathbf{w}^\top \mathbf{x}_i \geq 1, \ \forall i = 1, \ldots, N$$

The Primal Hard SVM

- Given training dataset: $D = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$
- Assume that D is linearly separable

$$\begin{aligned} \hat{\mathbf{w}} &= \arg\min_{\mathbf{w}} \frac{1}{2}\|\mathbf{w}\|^2 \\ \text{s.t.:} &\quad y_i \mathbf{w}^\top \mathbf{x}_i \geq 1, \ \forall i = 1, \ldots, N \end{aligned}$$

- Prediction:

$$f(\mathbf{x}; \hat{\mathbf{w}}) = \operatorname{sign}(\hat{\mathbf{w}}^\top \mathbf{x})$$

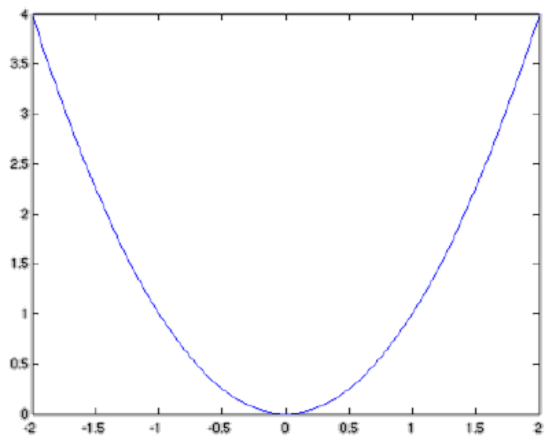
This is a QP problem (d-dimensional)

(Quadratic cost function, linear constraints)

Constrained Optimization

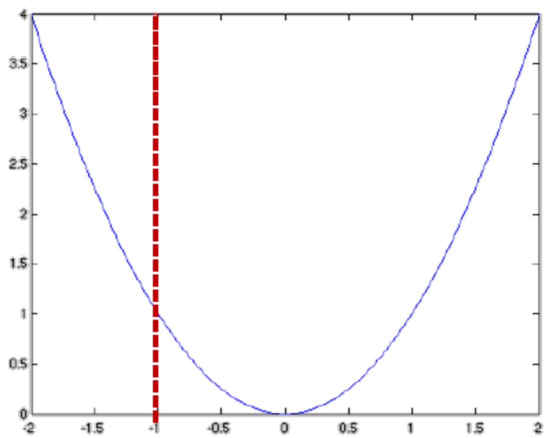
$$\min_x \; x^2$$
$$\text{s.t.} \quad x \geq b$$

$$\min_x \; x^2$$



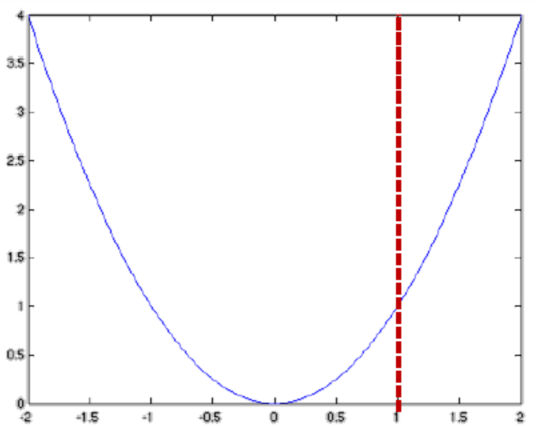
$$x^* = 0$$

$$\min_x \; x^2$$
$$\text{s.t.} \quad x \geq -1$$



$$x^* = 0$$

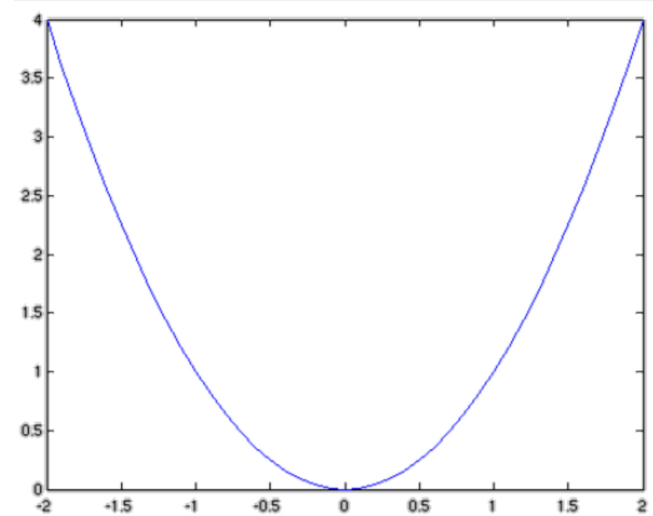
$$\min_x \; x^2$$
$$\text{s.t.} \quad x \geq 1$$



$$x^* = 1$$

Lagrange Multiplier

$$\min_x \; x^2$$
$$\text{s.t.} \quad x \geq b$$



- Move the constraint to objective function – Lagrangian

$$L(x, \alpha) = x^2 - \alpha(x - b), \quad \text{s.t.: } \alpha \geq 0$$

- Solve:

$$\min_x \max_\alpha \quad L(x, \alpha)$$
$$\text{s.t.:} \quad \alpha \geq 0$$

Constraint is active when $\alpha > 0$

Lagrange Multiplier – dual variables

- Solving:

$$\min_x \max_\alpha \quad L(x,\alpha) = x^2 - \alpha(x-b)$$
$$\text{s.t.:} \quad \alpha \geq 0$$

- We get:

$$\frac{\partial L}{\partial x} = 0 \Rightarrow x^* = \frac{\alpha}{2}$$

$$\frac{\partial L}{\partial \alpha} = 0 \Rightarrow \alpha^* = \max(2b, 0)$$

When $\alpha > 0$, constraint is tight

From Primal to Dual

- Primal problem:

$$\begin{aligned}\hat{\mathbf{w}} &= \arg\min_{\mathbf{w}} \frac{1}{2}\|\mathbf{w}\|^2 \\ \text{s.t.:} \quad & y_i \mathbf{w}^\top \mathbf{x}_i \geq 1, \;\; \forall i = 1, \ldots, N\end{aligned}$$

- Lagrange function:

$$L(\mathbf{w}, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N} \alpha_i \left(y_i \mathbf{w}^\top \mathbf{x}_i - 1 \right)$$

$$\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_N)^\top \geq 0$$

The Lagrange Problem

$$L(\mathbf{w}, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N} \alpha_i \left(y_i \mathbf{w}^\top \mathbf{x}_i - 1\right)$$

- The Lagrange problem:

$$(\hat{\mathbf{w}}, \hat{\boldsymbol{\alpha}}) = \arg\min_{\mathbf{w}} \max_{\boldsymbol{\alpha}} L(\mathbf{w}, \boldsymbol{\alpha})$$

$$0 = \frac{\partial L(\mathbf{w}, \boldsymbol{\alpha})}{\partial \mathbf{w}}\Big|_{\hat{\mathbf{w}}} = \hat{\mathbf{w}} - \sum_i \alpha_i y_i \mathbf{x}_i$$

$$\Rightarrow \hat{\mathbf{w}} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$$

The Dual Problem

$$L(\mathbf{w}, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N} \alpha_i \left(y_i \mathbf{w}^\top \mathbf{x}_i - 1\right)$$

$$\Rightarrow \hat{\mathbf{w}} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$$

$$\Rightarrow L(\hat{\mathbf{w}}, \boldsymbol{\alpha}) = \frac{1}{2}\|\hat{\mathbf{w}}\|^2 - \sum_{i} \alpha_i \left(y_i \hat{\mathbf{w}}^\top \mathbf{x}_i - 1\right)$$

$$= \frac{1}{2}\|\sum_{i} \alpha_i y_i \mathbf{x}_i\|^2 + \boldsymbol{\alpha}^\top \mathbf{1} - \sum_{i} \alpha_i y_i \left(\sum_{j} \alpha_j y_j \mathbf{x}_j\right)^\top \mathbf{x}_i$$

$$= \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}^\top \mathbf{Y} G \mathbf{Y} \boldsymbol{\alpha}$$

$$\mathbf{Y} := diag(y_1, \ldots, y_N)$$

$G \in \mathbb{R}^{N \times N}$, where $G_{ij} := \mathbf{x}_i^\top \mathbf{x}_j$ Gram matrix

The Dual Hard SVM

$$\mathbf{Y} := diag(y_1, \ldots, y_N)$$

$$G \in \mathbb{R}^{N \times N}, \text{ where } G_{ij} := \mathbf{x}_i^\top \mathbf{x}_j \quad \text{Gram matrix}$$

$$\hat{\boldsymbol{\alpha}} = \arg\max_{\boldsymbol{\alpha}} \; \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2} \boldsymbol{\alpha}^\top \mathbf{Y} G \mathbf{Y} \boldsymbol{\alpha}$$

$$\text{s.t.: } \alpha_i \geq 0, \; \forall i = 1, \ldots, N$$

- Optimal solution:

$$\hat{\mathbf{w}} = \sum_{i=1}^{N} \hat{\alpha}_i y_i \mathbf{x}_i$$

- Prediction:

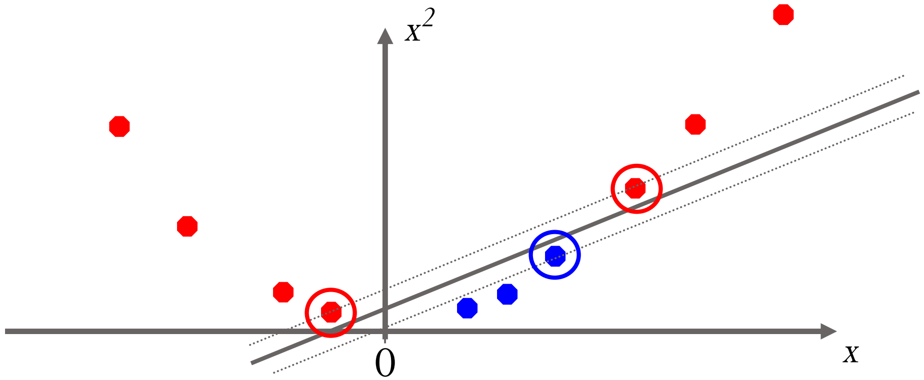
$$f(\mathbf{x}; \hat{\mathbf{w}}) = \text{sign}\left(\hat{\mathbf{w}}^\top \mathbf{x}\right) = \text{sign}\left(\sum_{i=1}^{N} \hat{\alpha}_i y_i \mathbf{x}_i^\top \mathbf{x}\right)$$

The Problem with Hard SVM

- It assumes samples are linearly separable …
- How about if the data is not linearly separable?

The Problem with Hard SVM

- If the data is not linearly separable, adding new features might make it linearly separable



- Now drop this "augmented" data into our linear SVM!

The Problem with Hard SVM

- It assumes samples are linearly separable

- Solutions:
  - User feature transformation to a higher-dim space
    - Overfitting ☹
  - Soft margin SVM instead of hard SVM
    - Next slides

Hard SVM

- The hard SVM problem can be rewritten:

$$
\begin{aligned}
\hat{\mathbf{w}} &= \arg\min_{\mathbf{w}} \frac{1}{2}\|\mathbf{w}\|^2 \\
\text{s.t.:} \quad & y_i \mathbf{w}^\top \mathbf{x}_i > 0, \ \forall i = 1, \ldots, N
\end{aligned}
$$

$$
\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \frac{\lambda}{2}\|\mathbf{w}\|^2 + \sum_{i=1}^{N} \ell_{0-\infty}(y_i \mathbf{w}^\top \mathbf{x}_i)
$$

$$
\text{where } \ell_{0-\infty}(b) = \begin{cases} \infty & if \ b < 0 \\ 0 & if \ b > 0 \end{cases}
$$

From Hard to Soft Constraints

- Instead of using hard constraints (linearly separable)

$$\hat{\mathbf{w}}_{hard} \quad = \quad \arg\min_{\mathbf{w}} \frac{\lambda}{2}\|\mathbf{w}\|^2 + \sum_{i=1}^{N} \ell_{0-\infty}(y_i \mathbf{w}^\top \mathbf{x}_i)$$

- We can try to solve the soft version of it:
  - The loss is only 1 instead of ∞ if misclassify an instance

$$\hat{\mathbf{w}}_{soft} \quad = \quad \arg\min_{\mathbf{w}} \frac{1}{2}\|\mathbf{w}\|^2 + \sum_{i=1}^{N} \ell_{0-1}(y_i \mathbf{w}^\top \mathbf{x}_i)$$

$$\text{where } \ell_{0-1}(b) = \begin{cases} 1 & if\ \ b < 0 \\ 0 & if\ \ b > 0 \end{cases}$$

Problems with 0/1 loss

$$\hat{\mathbf{w}}_{soft} \quad = \quad \arg\min_{\mathbf{w}} \frac{\lambda}{2}\|\mathbf{w}\|^2 + \sum_{i=1}^{N} \ell_{0-1}(y_i \mathbf{w}^\top \mathbf{x}_i)$$

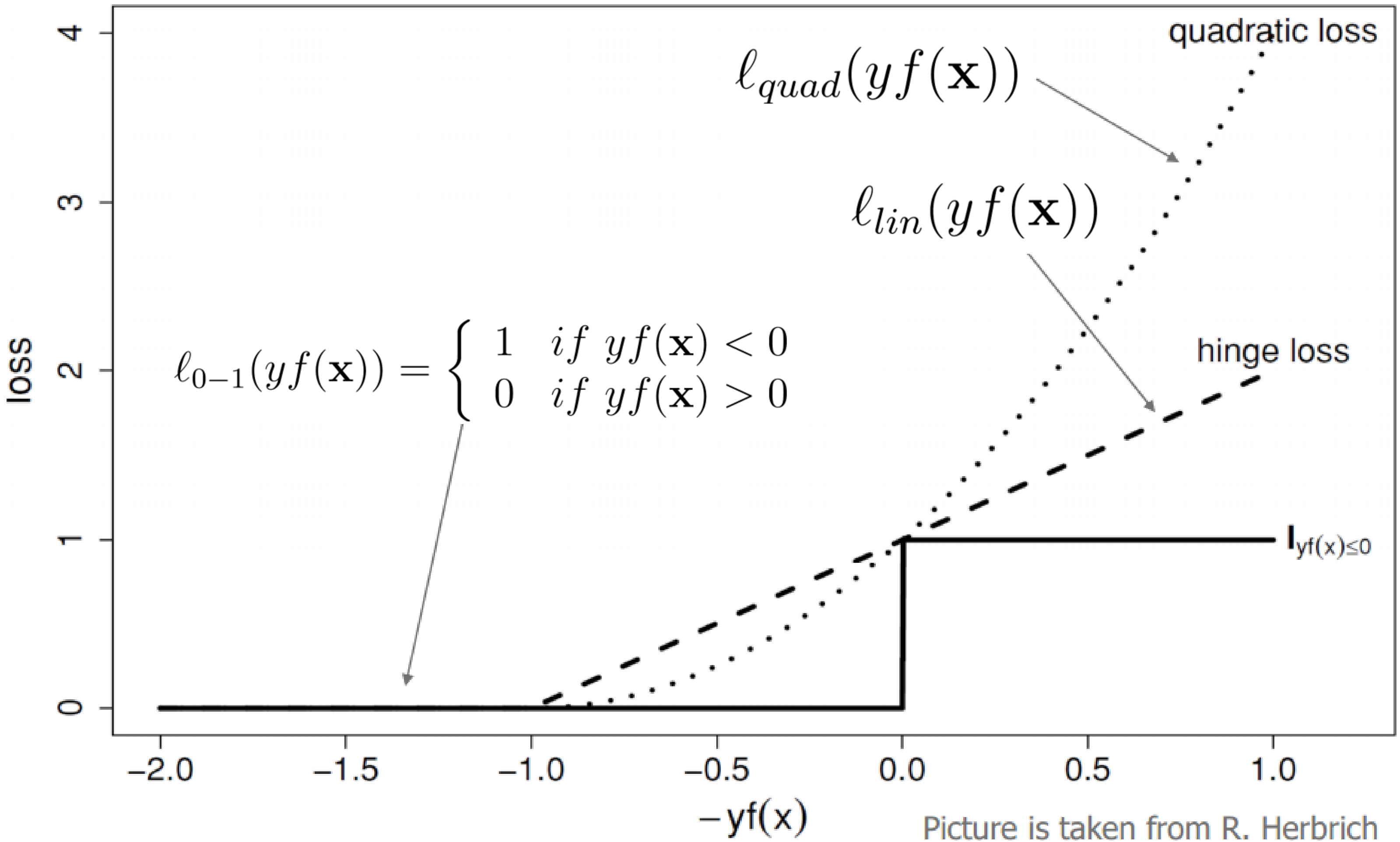
$$\text{where } \ell_{0-1}(b) = \begin{cases} 1 & if\ b < 0 \\ 0 & if\ b > 0 \end{cases}$$

- It is not convex in $y\mathbf{w}^\top\mathbf{x}$
  - It is not convex in $\mathbf{w}$, either

- We like convex functions …

Approximation of the step function

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



Picture is taken from R. Herbrich

Approximation of 0/1 loss

- Piecewise linear approximation (hinge loss, convex, nonsmooth)

$$\ell_{lin}(yf(\mathbf{x})) = \max(0, 1 - yf(\mathbf{x}))$$

  - we want $yf(\mathbf{x}) > 1$

- Quadratic approximation (square-loss, convex, smooth)

$$\ell_{quad}(yf(\mathbf{x})) = \max(0, 1 - yf(\mathbf{x}))^2$$

- Huber loss (combine the above two, convex, smooth)

$$\ell_{Huber}(yf(\mathbf{x})) = \begin{cases} 1 - yf(\mathbf{x}) & if \;\; yf(\mathbf{x}) < 0 \\ \max(0, 1 - yf(\mathbf{x}))^2 & if \;\; yf(\mathbf{x}) \geq 0 \end{cases}$$

The Hinge loss approximation of 0/1 loss

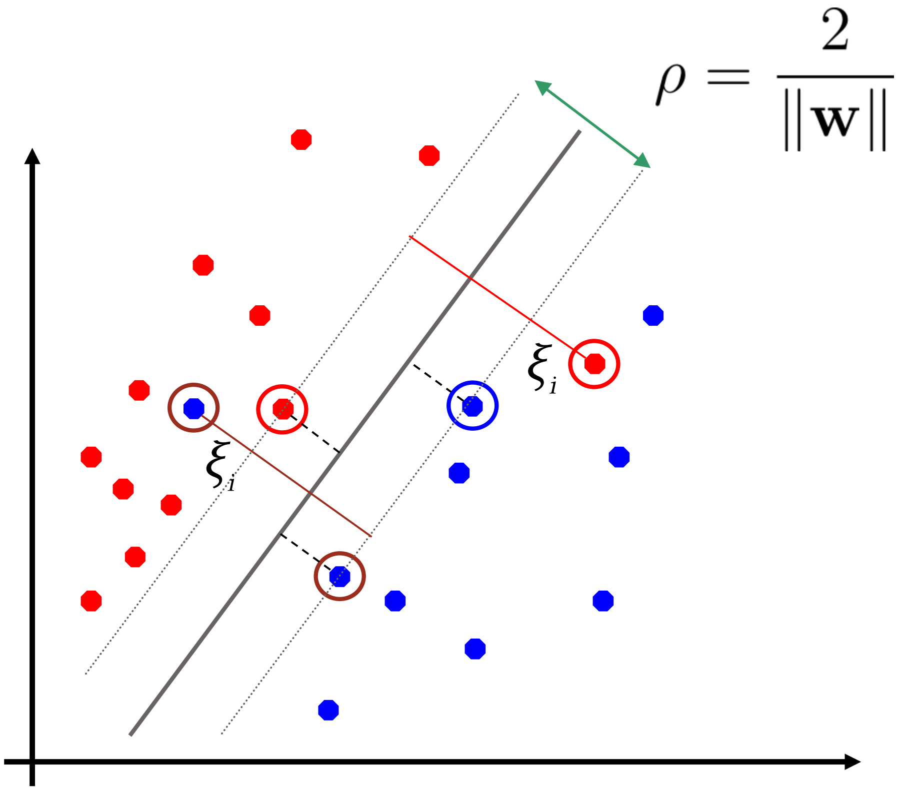
$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \frac{\lambda}{2}\|\mathbf{w}\|^2 + \sum_{i=1}^{N} \ell_{lin}(y_i \mathbf{w}^\top \mathbf{x}_i)$$

- where:

$$\begin{aligned}\ell_{lin}(y_i \mathbf{w}^\top \mathbf{x}_i) &= \max(0, 1 - y_i \mathbf{w}^\top \mathbf{x}_i) \\ &\geq \ell_{0-1}(y_i \mathbf{w}^\top \mathbf{x}_i)\end{aligned}$$

- The hinge loss upper bounds the 0/1 loss

Geometric interpretation: slack variables



$$\xi_i := \ell_{lin}(y_i \mathbf{w}^\top \mathbf{x}_i) = \max(0, 1 - y_i \mathbf{w}^\top \mathbf{x}_i)$$

The Primal Soft SVM problem

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \frac{\lambda}{2}\|\mathbf{w}\|^2 + \sum_{i=1}^{N} \xi_i$$

$$\text{where } \xi_i := \ell_{lin}(y_i \mathbf{w}^\top \mathbf{x}_i) = \max(0, 1 - y_i \mathbf{w}^\top \mathbf{x}_i)$$

- Equivalently:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w},\boldsymbol{\xi}} \frac{\lambda}{2}\|\mathbf{w}\|^2 + \sum_{i=1}^{N} \xi_i$$

$$\text{s.t.:} \quad y_i \mathbf{w}^\top \mathbf{x}_i \geq 1 - \xi_i, \;\; \forall i = 1, \ldots, N$$

$$\xi_i \geq 0, \;\; \forall i = 1, \ldots, N$$

The Primal Soft SVM problem

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w},\boldsymbol{\xi}} \frac{\lambda}{2}\|\mathbf{w}\|^2 + \sum_{i=1}^{N} \xi_i$$

$$\text{s.t.:} \quad y_i \mathbf{w}^\top \mathbf{x}_i \geq 1 - \xi_i, \ \forall i = 1, \ldots, N$$

$$\xi_i \geq 0, \ \forall i = 1, \ldots, N$$

- Equivalently:

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

$$C = \frac{1}{\lambda}$$

Dual Soft SVM (using hinge loss)

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

$$\text{s.t.:} \quad y_i\mathbf{w}^\top\mathbf{x}_i \geq 1 - \xi_i, \ \forall i = 1,\ldots,N$$

$$\xi_i \geq 0, \ \forall i = 1,\ldots,N$$

- Lagrange multipliers

$$\boldsymbol{\alpha} \geq 0, \ \boldsymbol{\beta} \geq 0$$

- Lagrange function

$$L(\mathbf{w},\boldsymbol{\xi},\boldsymbol{\alpha},\boldsymbol{\beta}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i \xi_i - \sum_i \alpha_i(y_i\mathbf{w}^\top\mathbf{x}_i - 1 + \xi_i) - \sum_i \beta_i\xi_i$$

$$\boxed{\min_{\mathbf{w},\boldsymbol{\xi}} \max_{\boldsymbol{\alpha},\boldsymbol{\beta}} L(\mathbf{w},\boldsymbol{\xi},\boldsymbol{\alpha},\boldsymbol{\beta})}$$

Dual Soft SVM (using hinge loss)

$$L(\mathbf{w}, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{2}\|\mathbf{w}\|^2 + C\boldsymbol{\xi}^\top \mathbf{1} - \sum_i \alpha_i y_i \mathbf{w}^\top \mathbf{x}_i + \boldsymbol{\alpha}^\top \mathbf{1} - \boldsymbol{\xi}^\top(\boldsymbol{\alpha} + \boldsymbol{\beta})$$

- We get:

$$0 = \frac{\partial L}{\partial \mathbf{w}}\Big|_{\hat{\mathbf{w}}} \quad \Rightarrow \hat{\mathbf{w}} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$$

$$0 = \frac{\partial L}{\partial \boldsymbol{\xi}}\Big|_{\hat{\boldsymbol{\xi}}} \quad \Rightarrow \boldsymbol{\beta} = C\mathbf{1} - \boldsymbol{\alpha} \geq 0$$

$$\Rightarrow 0 \leq \boldsymbol{\alpha} \leq C\mathbf{1}$$

- Dual problem:

$$(\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}}) = \underset{0 \leq \boldsymbol{\alpha} \leq C\mathbf{1}; 0 \leq \boldsymbol{\beta}}{\operatorname{argmax}} \; L(\hat{\mathbf{w}}, \hat{\boldsymbol{\xi}}, \boldsymbol{\alpha}, \boldsymbol{\beta})$$

$$\hat{\boldsymbol{\alpha}} = \underset{0 \leq \boldsymbol{\alpha} \leq C\mathbf{1}}{\operatorname{argmax}} \, \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}^\top \mathbf{Y} G \mathbf{Y} \boldsymbol{\alpha}$$

Dual Soft SVM (using hinge loss)

$$\mathbf{Y} := diag(y_1, \ldots, y_N)$$

$$G \in \mathbb{R}^{N \times N}, \text{ where } G_{ij} := \mathbf{x}_i^\top \mathbf{x}_j \quad \text{Gram matrix}$$

$$\hat{\boldsymbol{\alpha}} = \underset{0 \le \boldsymbol{\alpha} \le C\mathbf{1}}{\operatorname{argmax}} \, \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2} \boldsymbol{\alpha}^\top \mathbf{Y} G \mathbf{Y} \boldsymbol{\alpha}$$

- This is the same as the dual hard SVM problem, except that we have additional constraints

SVM in the dual space

- Solve the dual problem

$$\hat{\boldsymbol{\alpha}} = \underset{0 \le \boldsymbol{\alpha} \le C\mathbf{1}}{\operatorname{argmax}} \, \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2} \boldsymbol{\alpha}^\top \mathbf{Y} G \mathbf{Y} \boldsymbol{\alpha}$$

- The primal solution

$$\Rightarrow \hat{\mathbf{w}} = \sum_{i=1}^{N} \hat{\alpha}_i y_i \mathbf{x}_i$$

- Prediction

$$f(\mathbf{x}; \hat{\mathbf{w}}) = \operatorname{sign}\left(\hat{\mathbf{w}}^\top \mathbf{x}\right) = \operatorname{sign}\left(\sum_{i=1}^{N} \hat{\alpha}_i y_i \mathbf{x}_i^\top \mathbf{x}\right)$$

Why it is called Support Vector Machines?

- Hard-SVM:

$$L(\mathbf{w}, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N} \alpha_i \left(y_i \mathbf{w}^\top \mathbf{x}_i - 1\right)$$

$$\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_N)^\top \geq 0$$

- KKT conditions (complementary slackness condition):

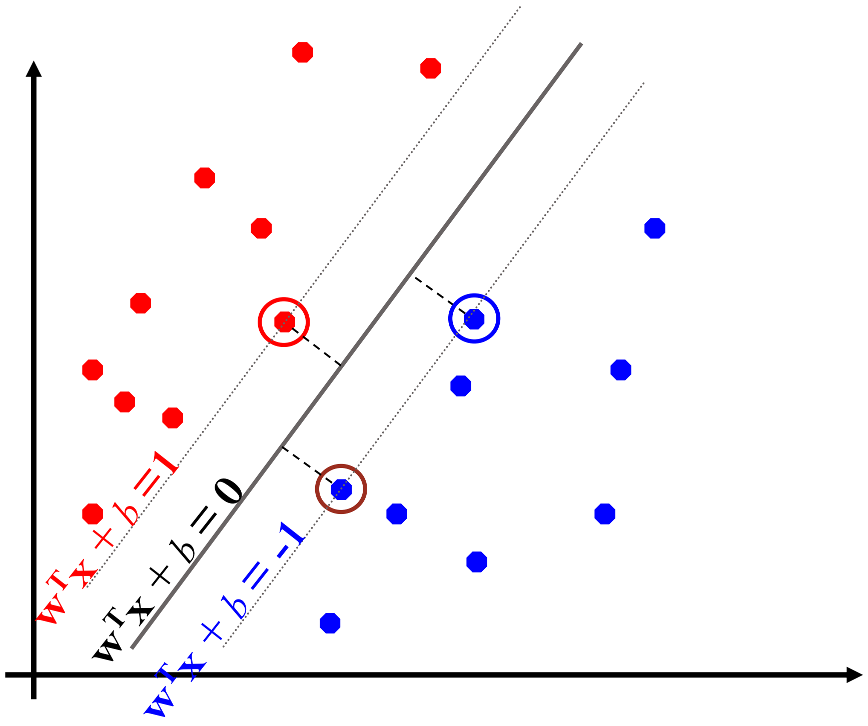
$$\forall i: \;\; \hat{\alpha}_i \left(y_i \hat{\mathbf{w}}^\top \mathbf{x}_i - 1\right) = 0$$

$$\hat{\alpha}_i = 0 \quad OR \quad \hat{\alpha}_i > 0 \Rightarrow y_i \hat{\mathbf{w}}^\top \mathbf{x}_i = 1$$

$\mathbf{x}_i$ is on the margin line! SUPPORT VECTORS

Why it is called Support Vector Machines?

- Hard SVM:



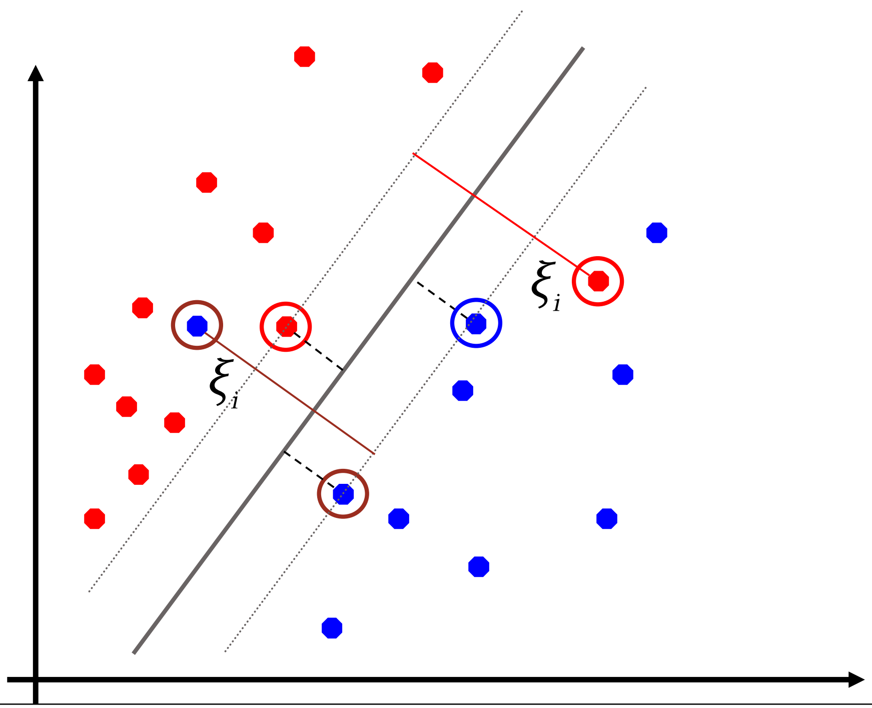
- Only need to store support vectors to predict labels of test data

Support vectors in Soft SVM

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

$$\text{s.t.:}\quad y_i\mathbf{w}^\top\mathbf{x}_i \geq 1-\xi_i,\ \forall i=1,\ldots,N$$

$$\xi_i \geq 0,\ \forall i=1,\ldots,N$$



- Margin support vectors

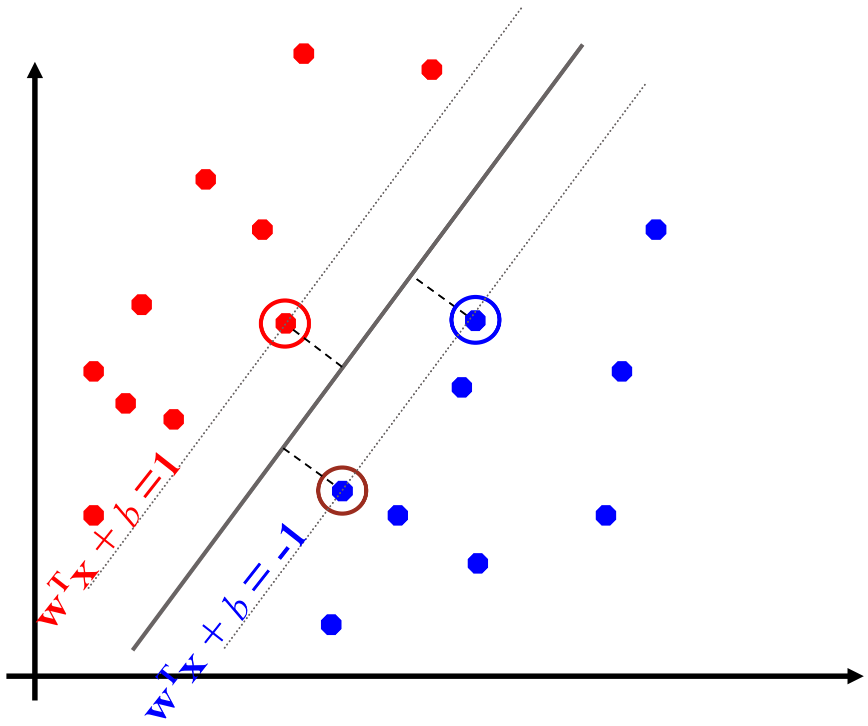
$$y_i\mathbf{w}^\top\mathbf{x}_i = 1$$

- Nonmargin support vectors

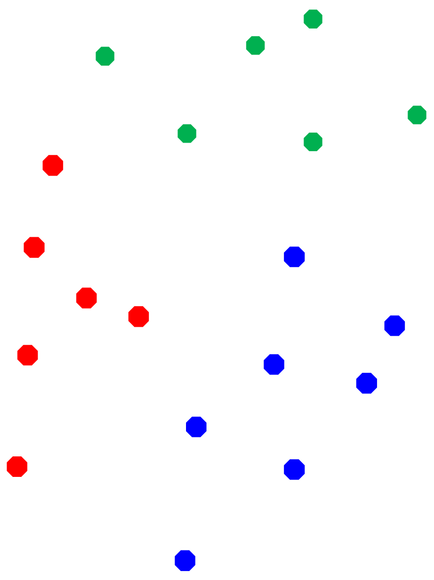
$$\xi_i > 0$$

Dual Sparsity

- Only few Lagrange multipliers (dual variables) α_i can be non-zero

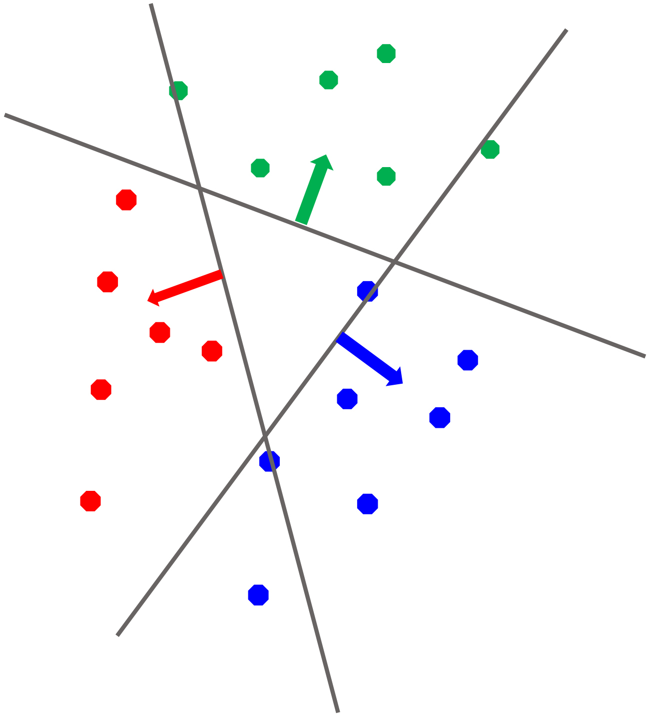


What about multiple classes?



One vs All

- Learn multiple binary classifiers separately:
  - class k vs. rest $(\mathbf{w}_k, b_k)_{k=1,2,3}$



- Prediction: $$\hat{y} = \underset{k}{\operatorname{argmax}}(\mathbf{w}_k^\top \mathbf{x} + b_k)$$

Problems with One vs All?

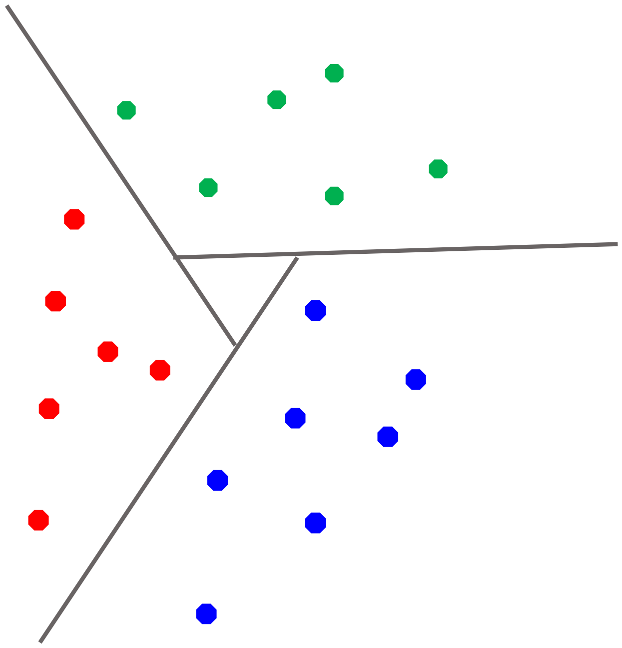
$$\hat{y} = \underset{k}{\operatorname{argmax}}(\mathbf{w}_k^\top \mathbf{x} + b_k)$$

- (1) The weights may not be based on the same scale
  - Note: $(a\mathbf{w}_k)^\top \mathbf{x} + (ab_k)$ is also a solution

- (2) Imbalance issue when learning each binary classifier
  - Much more negatives than positives

One vs One

- Learn K(K-1)/2 binary classifiers

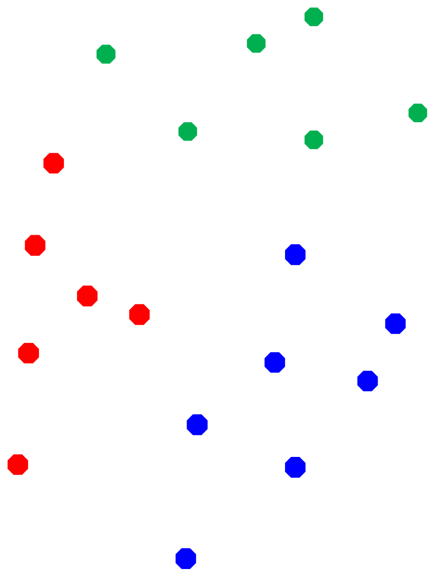


- Prediction:
  - Majority voting
- Ambiguity issue!

Learning 1 Joint Classifier

- Simultaneously learn 3 sets of weights $(\mathbf{w}_k, b_k)_{k=1,2,3}$

$$\hat{y} = \underset{k}{\mathrm{argmax}}(\mathbf{w}_k^\top \mathbf{x} + b_k)$$



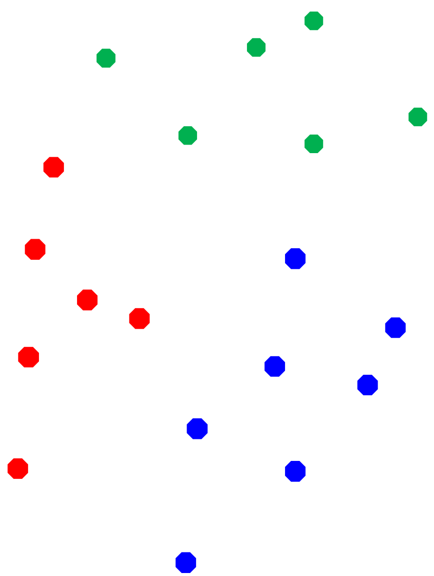
$$\forall i,\ \forall y \neq y_i :$$

$$\mathbf{w}_{y_i}^\top \mathbf{x}_i + b_{y_i} \geq \mathbf{w}_y^\top \mathbf{x}_i + b_y + 1$$

Margin: gap between true class and nearest other class

Learning 1 Joint Classifier

- Simultaneously learn 3 sets of weights $(\mathbf{w}_k, b_k)_{k=1,2,3}$



Joint optimization:

$$\min_{\mathbf{w},b} \; \frac{1}{2}\sum_{y} \|\mathbf{w}_y\|^2 + C\sum_{i=1}^{N}\sum_{y\neq y_i} \xi_{iy}$$

$$\text{s.t.: } \mathbf{w}_{y_i}^\top \mathbf{x}_i + b_{y_i} \geq \mathbf{w}_y^\top \mathbf{x}_i + b_y + 1 - \xi_{iy} \quad \forall i,\ \forall y \neq y_i$$

$$\xi_{iy} \geq 0 \qquad \forall i,\ \forall y \neq y_i$$

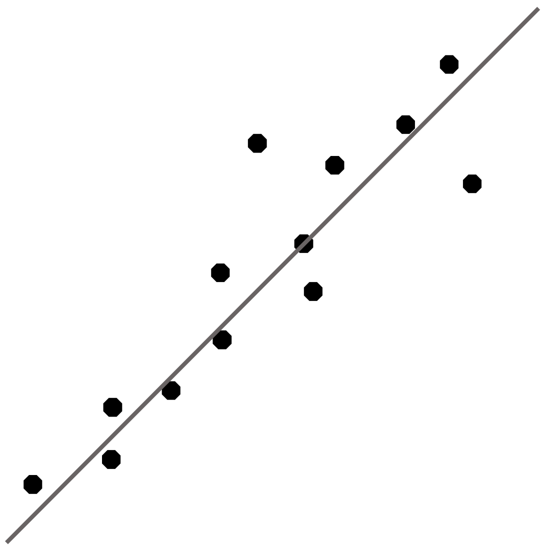
Prediction:

$$\hat{y} = \operatorname*{argmax}_k (\mathbf{w}_k^\top \mathbf{x} + b_k)$$

What you need to know

- Maximizing margin
- Derivation of SVM formulation
- Slack variables and hinge loss
- Relationship between
  - 0/1 loss
  - Hinge loss
- Tackling multiple class
  - One vs. All
  - Multiclass SVMs

SVM for Regression



- Training data $(\mathbf{x}_i, y_i), \ \mathbf{x}_i \in \mathbb{R}^d, \ y_i \in \mathbb{R}$
- Still learn a hyper-plane (linear model)
- Squared error is the popular loss

$$\sum_{i=1}^{N} (y_i - \mathbf{w}^\top \mathbf{x}_i)^2$$

  - a smooth function – no sparsity

- A piecewise linear approximation (ϵ -insensitive loss)

$$\sum_{i=1}^{N} \max(0, |y_i - \mathbf{w}^\top \mathbf{x}_i| - \epsilon)$$

SVM in the dual space

- Without offset b:

$$\hat{\boldsymbol{\alpha}} = \operatorname*{argmax}_{\boldsymbol{\alpha}} \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2} \boldsymbol{\alpha}^\top \mathbf{Y} G \mathbf{Y} \boldsymbol{\alpha}$$

$$\text{s.t.: } 0 \leq \boldsymbol{\alpha} \leq C\mathbf{1}$$

- With offset b:

$$\hat{\boldsymbol{\alpha}} = \operatorname*{argmax}_{\boldsymbol{\alpha}} \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2} \boldsymbol{\alpha}^\top \mathbf{Y} G \mathbf{Y} \boldsymbol{\alpha}$$

$$\text{s.t.: } 0 \leq \boldsymbol{\alpha} \leq C\mathbf{1}$$

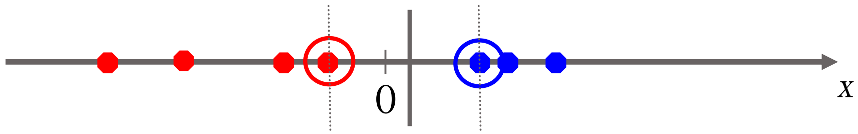
$$\sum_i \alpha_i y_i = 0$$

Why solve the dual SVM?

- The dual problem has simpler constraints
- There some quadratic programming algorithms that can solve the dual fast, especially in high-dimensions (d >> N)
  - See [Bottou & Lin, 2007] for a summary of dual SVM solvers
  - Be aware of the fast algorithms directly solving the primal problem, e.g., cutting-plane, stochastic subgradient, etc.
- More importantly, the **Kernel Trick**!!

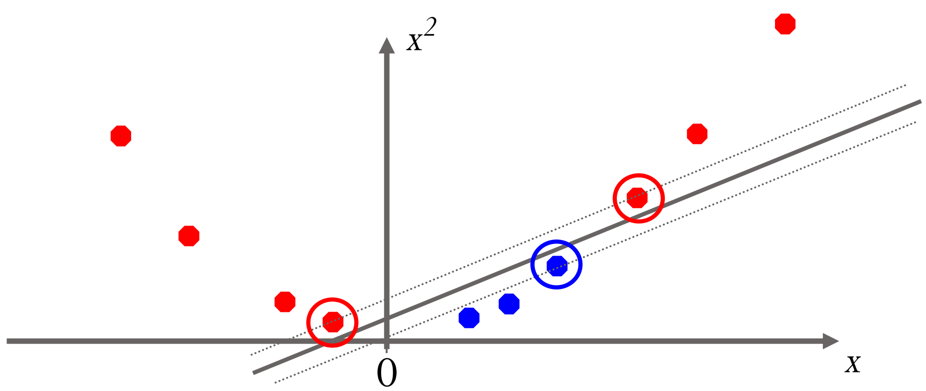
Nonlinear SVM

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



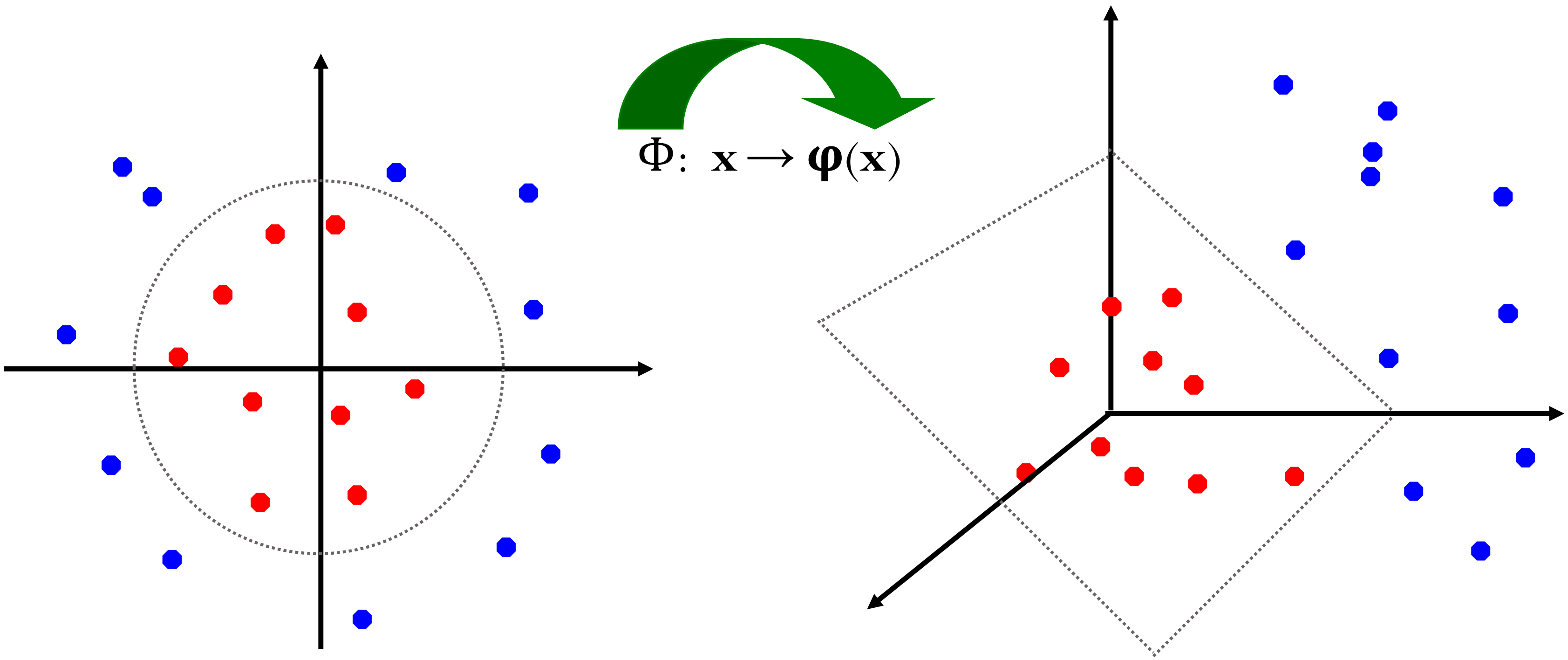
- But what are we going to do if the dataset is just too hard?

- 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:



Dot Product of Polynomials

- Polynomials of degree exactly d: $\Phi(\mathbf{x})$

$$\mathbf{x} = (x_1, x_2)^\top, \quad \mathbf{z} = (z_1, z_2)^\top$$

- d=1:

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

- d=2: $\Phi(\mathbf{x}) = (x_1^2, \sqrt{2} x_1 x_2, x_2^2)^\top$

$$\boxed{\Phi(\mathbf{x})^\top \Phi(\mathbf{x}) = \left(\mathbf{x}^\top \mathbf{z}\right)^2}$$

- In general:

$$\boxed{\Phi(\mathbf{x})^\top \Phi(\mathbf{x}) = \left(\mathbf{x}^\top \mathbf{z}\right)^d = K(\mathbf{x}, \mathbf{z})}$$

The Kernel Trick

- Linear SVM relies on inner product between vectors

$$K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^\top \mathbf{x}_j$$

- If map every data point into high-dimensional space via $\mathbf{\Phi}$: $\mathbf{x} \rightarrow \mathbf{\Phi}(\mathbf{x})$, the inner product becomes:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \Phi(\mathbf{x}_i)^\top \Phi(\mathbf{x}_j)$$

- A *kernel function* is a function that is equivalent to an inner product in some feature space.

- The feature mapping is not explicitly needed as long as we can compute the dot product using some Kernel K

What functions are kernels?

- For some function $K(\mathbf{x}_i,\mathbf{x}_j)$ checking that $K(\mathbf{x}_i,\mathbf{x}_j) = \varphi(\mathbf{x}_i)^\mathrm{T}\varphi(\mathbf{x}_j)$ can be cumbersome.
- Mercer's theorem:

  Every semi-positive definite symmetric function is a kernel

- Semi-positive definite symmetric functions correspond to a semi-positive definite symmetric Gram matrix:

$K =$

$K(\mathbf{x}_1,\mathbf{x}_1)$	$K(\mathbf{x}_1,\mathbf{x}_2)$	$K(\mathbf{x}_1,\mathbf{x}_3)$	…	$K(\mathbf{x}_1,\mathbf{x}_n)$
$K(\mathbf{x}_2,\mathbf{x}_1)$	$K(\mathbf{x}_2,\mathbf{x}_2)$	$K(\mathbf{x}_2,\mathbf{x}_3)$		$K(\mathbf{x}_2,\mathbf{x}_n)$
…	…	…	…	…
$K(\mathbf{x}_n,\mathbf{x}_1)$	$K(\mathbf{x}_n,\mathbf{x}_2)$	$K(\mathbf{x}_n,\mathbf{x}_3)$	…	$K(\mathbf{x}_n,\mathbf{x}_n)$

Example Kernel Functions

- Linear: $K(\mathbf{x}_i,\mathbf{x}_j)= \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j$
  - Mapping Φ: $\mathbf{x} \rightarrow \Phi(\mathbf{x})$, where $\Phi(\mathbf{x})$ is $\mathbf{x}$ itself

- Polynomial of power p: $K(\mathbf{x}_i,\mathbf{x}_j)= (1+ \mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j)^p$
  - Mapping Φ: $\mathbf{x} \rightarrow \Phi(\mathbf{x})$, where $\Phi(\mathbf{x})$ has $\binom{d+p}{p}$ dimensions

- Gaussian (radial-basis function):

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

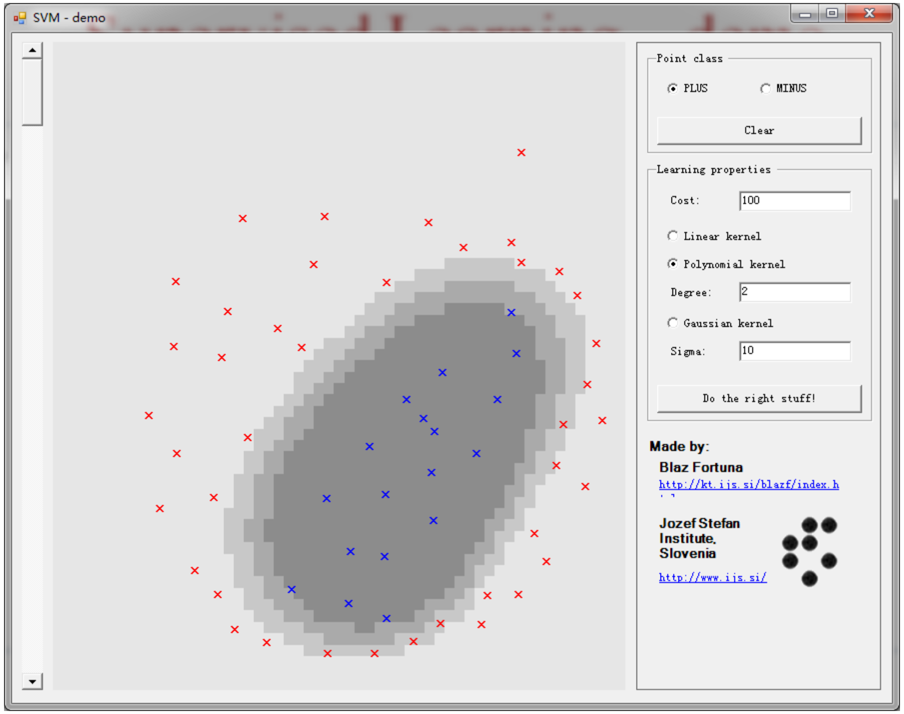
  - Mapping Φ: $\mathbf{x} \rightarrow \Phi(\mathbf{x})$, where $\Phi(\mathbf{x})$ is *infinite-dimensional*: every point is mapped to *a function*; combination of functions for support vectors is the separator.

- Higher-dimensional space still has *intrinsic* dimensionality d, but linear separators in it correspond to *non-linear* separators in original space.

Overfitting

- Huge feature space with kernels, what about overfitting??
  - Maximizing margin leads to a sparse set of support vectors
  - Some interesting theory says that SVMs search for simply hypothesis with a large margin
  - Often robust to overfitting

SVM – demo

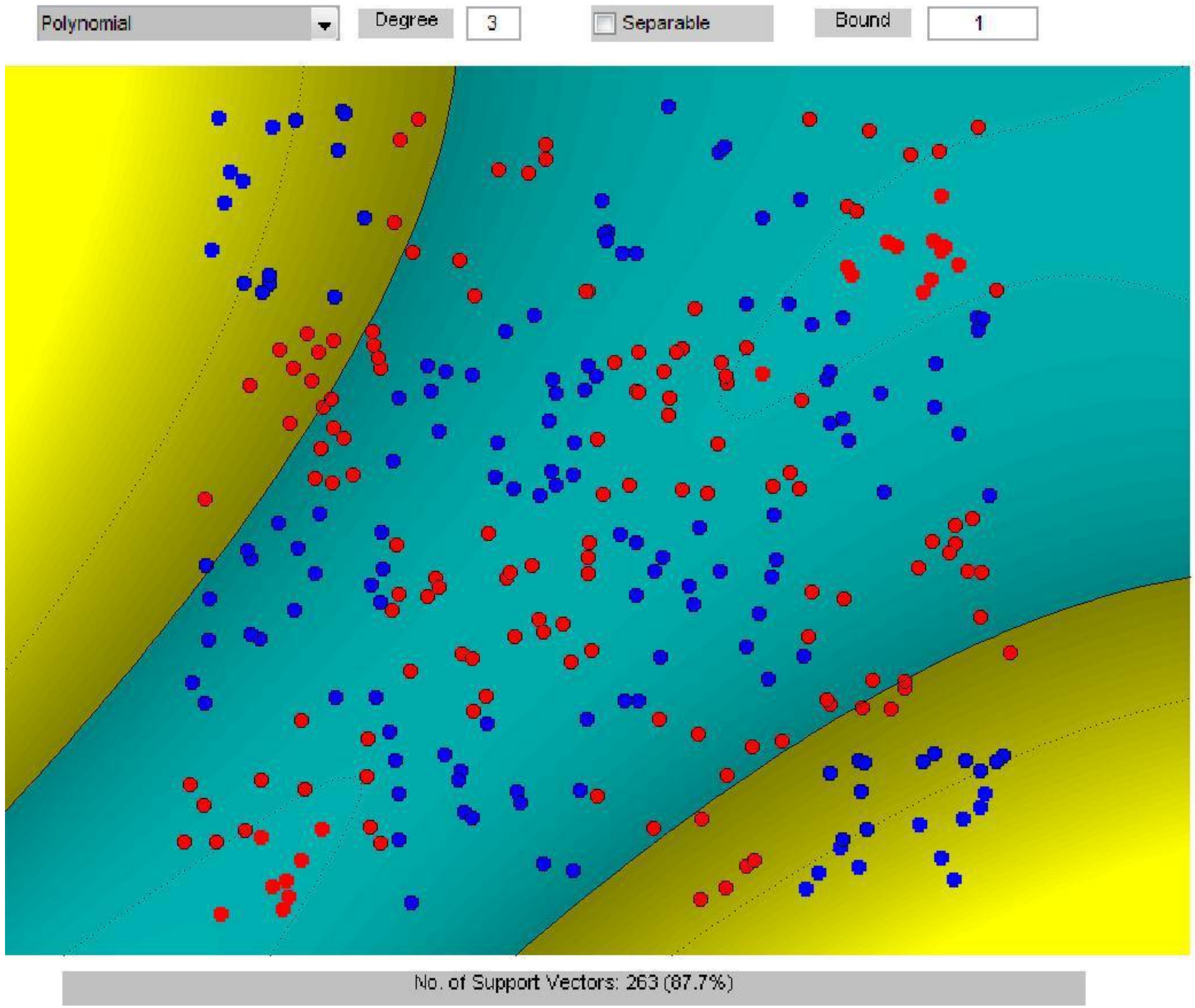


- http://www.isis.ecs.soton.ac.uk/resources/svminfo/

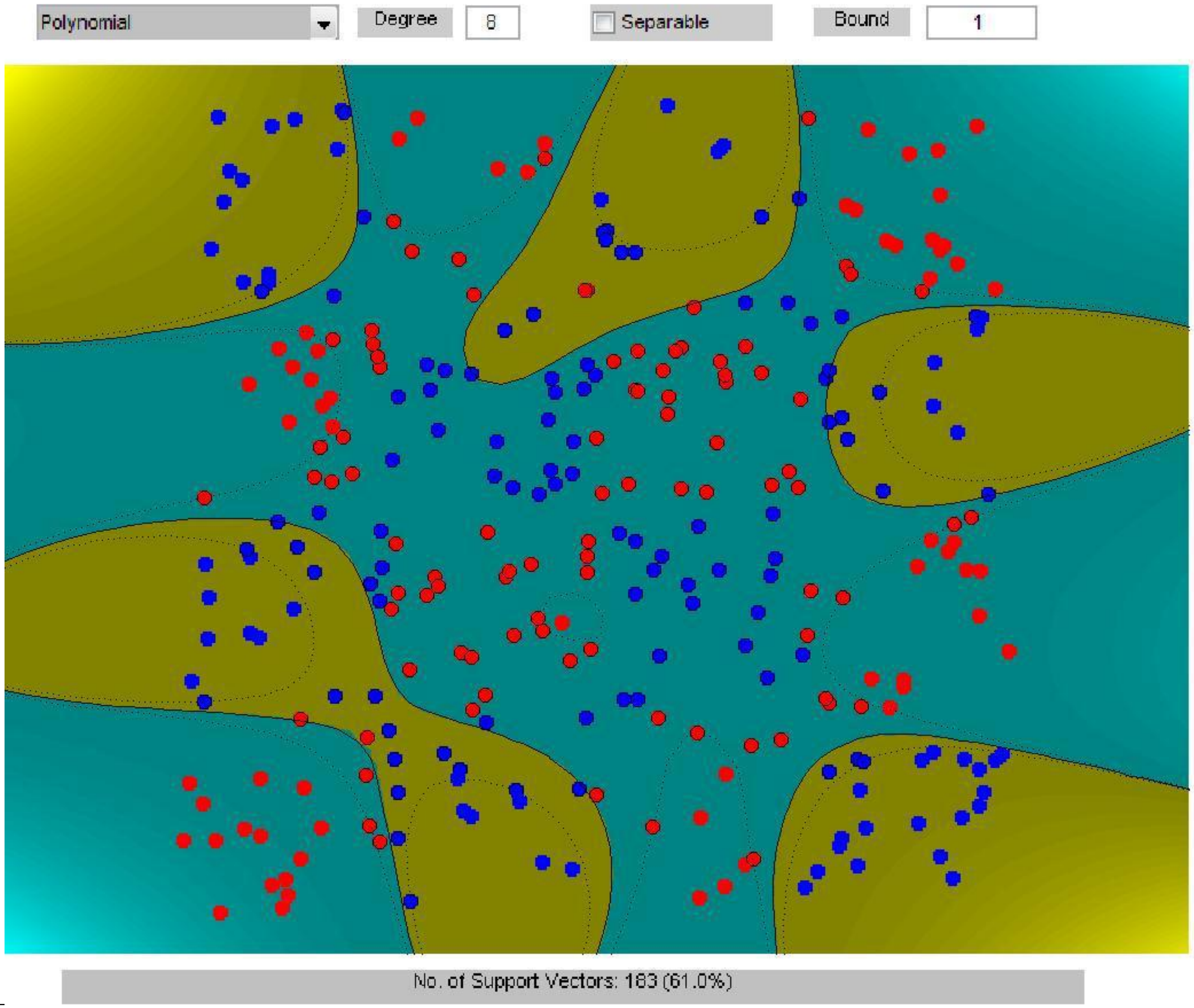
Good ToolKits: [1] SVM-Light: http://svmlight.joachims.org/

[2] LibSVM: http://www.csie.ntu.edu.tw/~cjlin/libsvm/

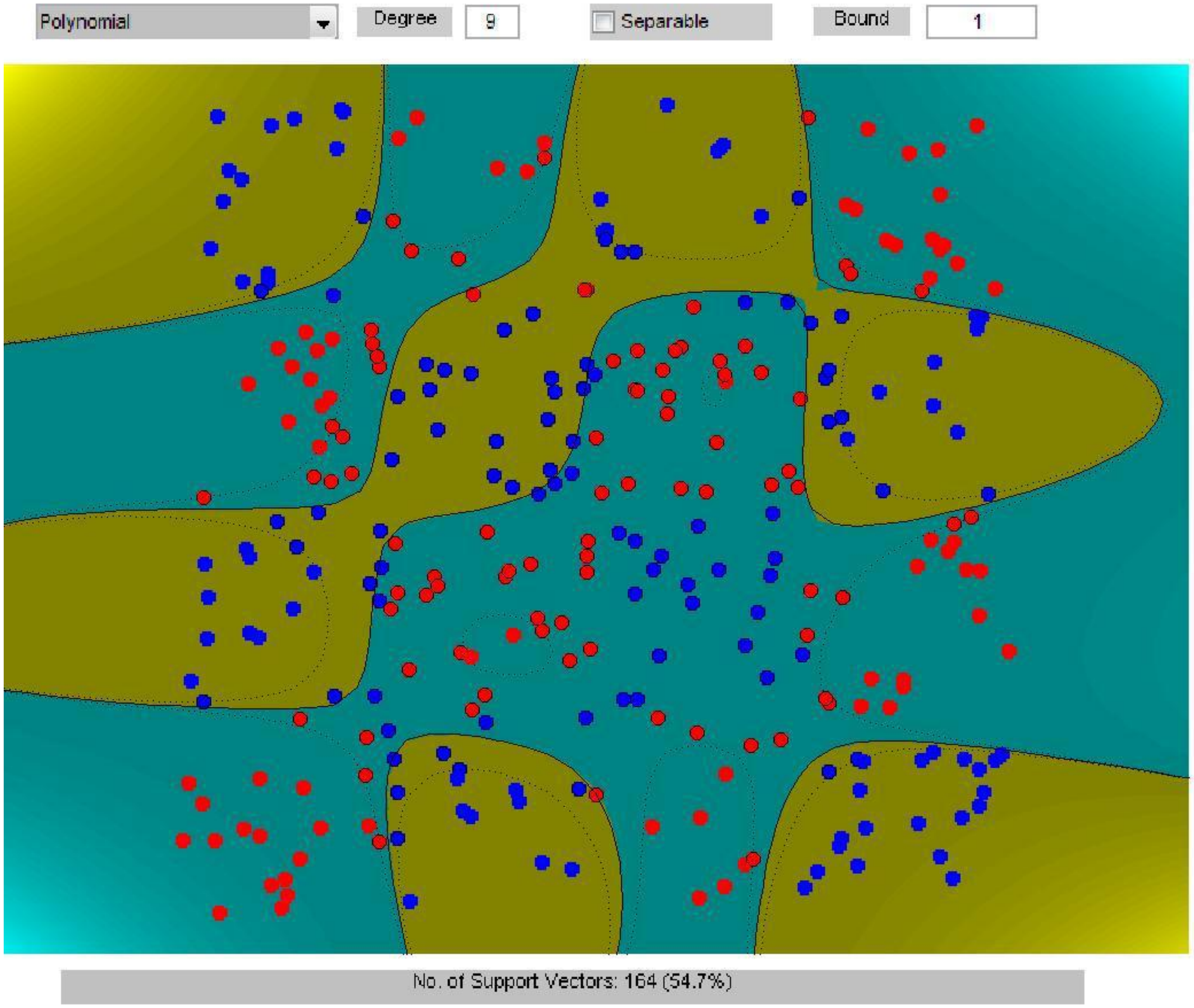
Chessboard dataset, Polynomial kernel



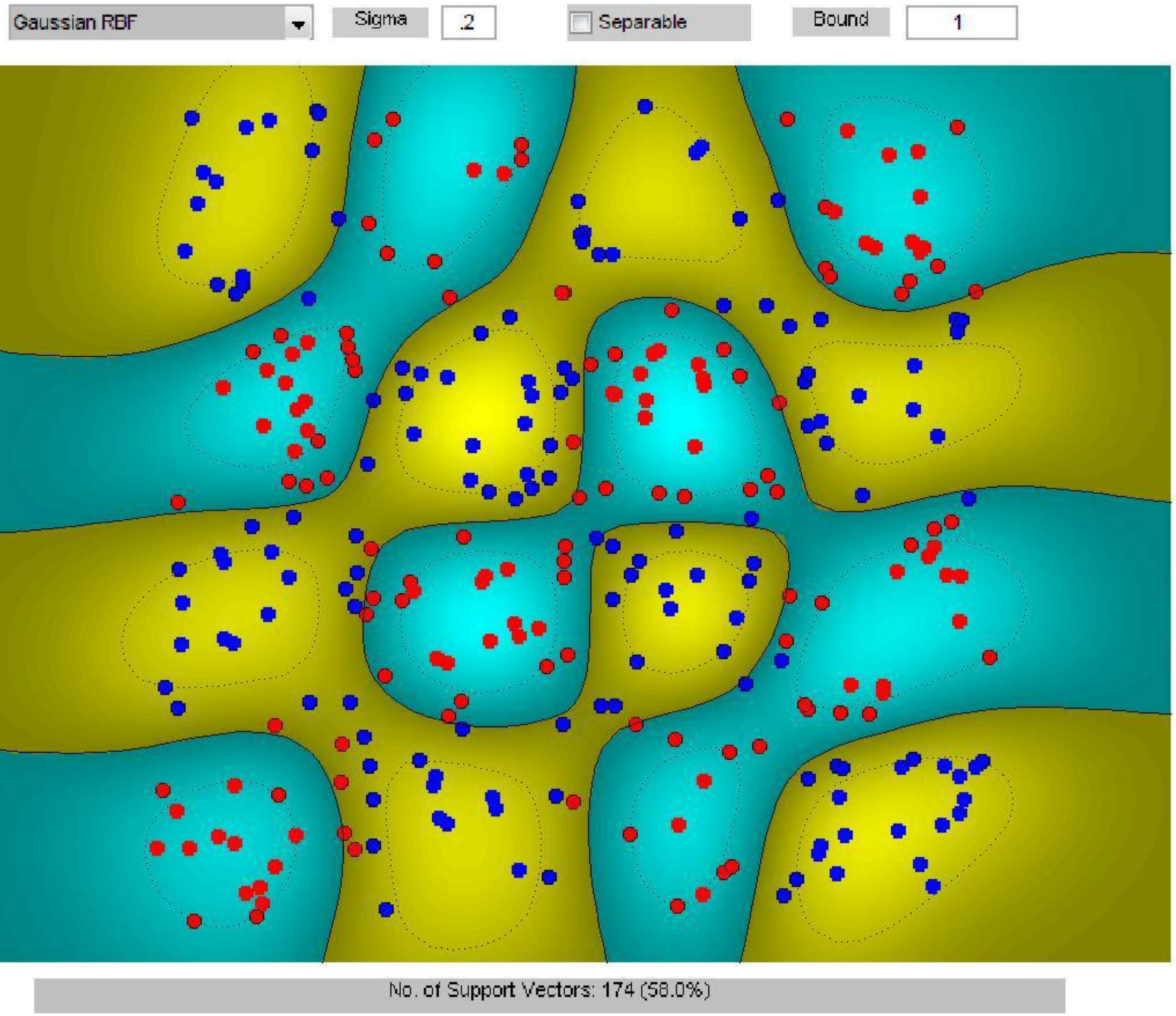
Chessboard dataset, Polynomial kernel



Chessboard dataset, Polynomial kernel



Chessboard dataset, RBF kernel



Advanced topics

- Scalable algorithms to learn SVMs
  - Linear SVMs
    - Linear algorithm, e.g., cutting-plane (2009)
    - Stochastic optimization, e.g., Pegasos (2007)
    - Distributed learning, e.g., divide-and-conquer (2013)
  - Non-linear SVMs
    - Kernel approximation, e.g., using low-rank or random features

- Structured output learning with SVMs
  - Will cover later

- An incomplete list of SVM solvers [Menon, 2010]

Algorithm	Citation	SVM type	Optimization type	Style	Runtime
SMO	[Platt, 1999]	Kernel	Dual QP	Batch	$\Omega(n^2 d)$
$\text{SVM}^{\text{light}}$	[Joachims, 1999]	Kernel	Dual QP	Batch	$\Omega(n^2 d)$
Core Vector Machine	[Tsang et al., 2005, 2007]	SL Kernel	Dual geometry	Batch	$O(s/\rho^4)$
SVM^{perf}	[Joachims, 2006]	Linear	Dual QP	Batch	$O(ns/\lambda\rho^2)$
NORMA	[Kivinen et al., 2004]	Kernel	Primal SGD	Online(-style)	$\tilde{O}(s/\rho^2)$
SVM-SGD	[Bottou, 2007]	Linear	Primal SGD	Online-style	Unknown
Pegasos	[Shalev-Shwartz et al., 2007]	Kernel	Primal SGD/SGP	Online-style	$\tilde{O}(s/\lambda\rho)$
LibLinear	[Hsieh et al., 2008]	Linear	Dual coordinate descent	Batch	$O(nd \cdot \log(1/\rho))$
SGD-QN	[Bordes and Bottou, 2008]	Linear	Primal 2SGD	Online-style	Unknown
FOLOS	[Duchi and Singer, 2008]	Linear	Primal SGP	Online-style	$\tilde{O}(s/\lambda\rho)$
BMRM	[Smola et al., 2007]	Linear	Dual QP	Batch	$O(d/\lambda\rho)$
OCAS	[Franc and Sonnenburg, 2008]	Linear	Primal QP	Batch	$O(nd)$

Validation

- Model selection:
  - Almost invariably, all ML methods have some free parameters
    - The number of neighbors in K-NN
    - The kernel parameters in SVMs

- Performance estimation:
  - Once we have chosen a model, how to estimate its performance?

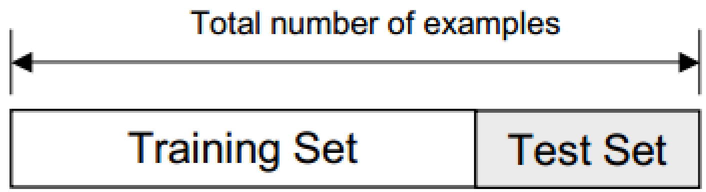
Motivation

- If we had access to an unlimited number of examples, there is a straightforward answer
  - Choose the model with the lowest error rate on the entire population
  - The error rate is the true error rate

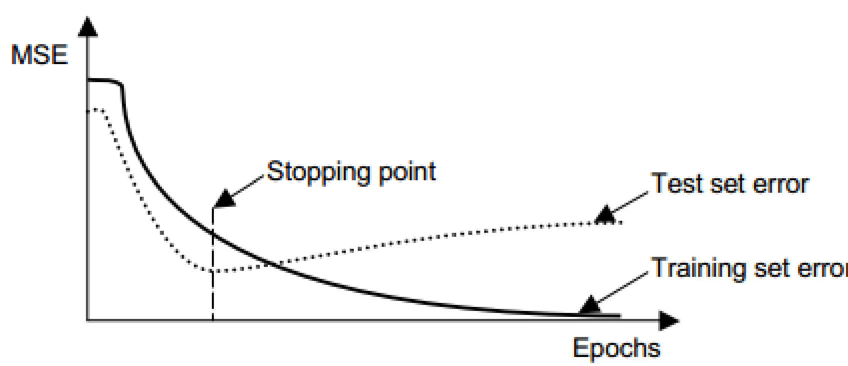
- In practice, we only access to a finite set of examples, usually smaller than we wanted
  - Use all training data to select model => too optimistic!
  - A better approach is to split the training set into disjoint subsets

Holdout Method

- Split dataset into two subsets
  - Training set: used to learn the classifier
  - Test set: used to estimate the error rate of the trained classifier



- E.g.: used to determine a stopping point of an iterative alg.:



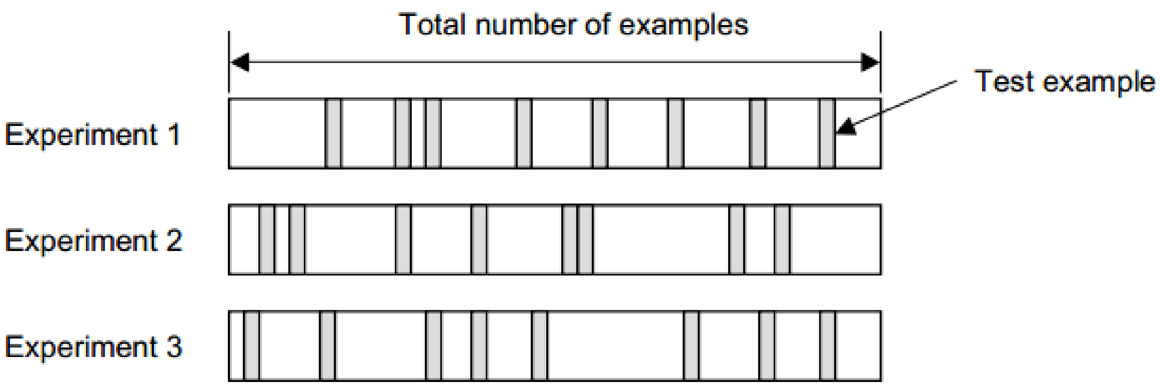
Holdout Method

- Two basic drawbacks
  - In problems with a sparse dataset, we may not be able to afford the "luxury" of setting aside a portion of data for testing
  - A single train-test split may lead to misleading results, e.g., if we happened to get an "unfortunate" split

- Resampling can overcome the limitations, but at the expense of more computations
  - Cross-validation
    - Random subsampling
    - K-fold cross-validation
    - Leave-one-out cross-validation
  - Bootstrap

Random Subsampling

- Performs K data splits of the entire dataset
  - Each split randomly selects a (fixed) no. examples
  - For each split, retrain the classifier with training data, and evaluate on test examples

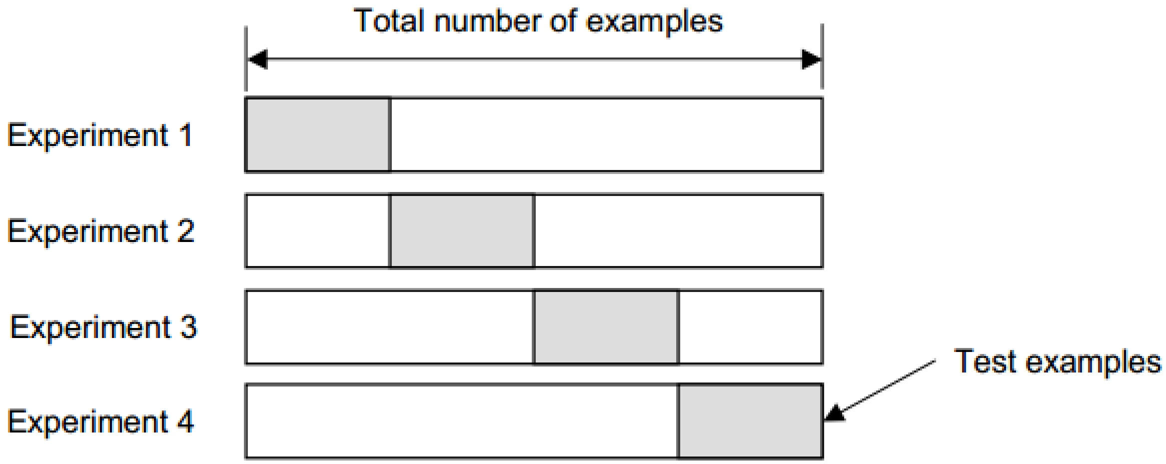


- The true error is estimated as the average

$$E = \frac{1}{K} \sum_{k=1}^{K} E_k$$

K-Fold Cross-validation

- Create a K-fold partition of the dataset
  - For each of K experiments, use K-1 folds for training and the remaining one for testing

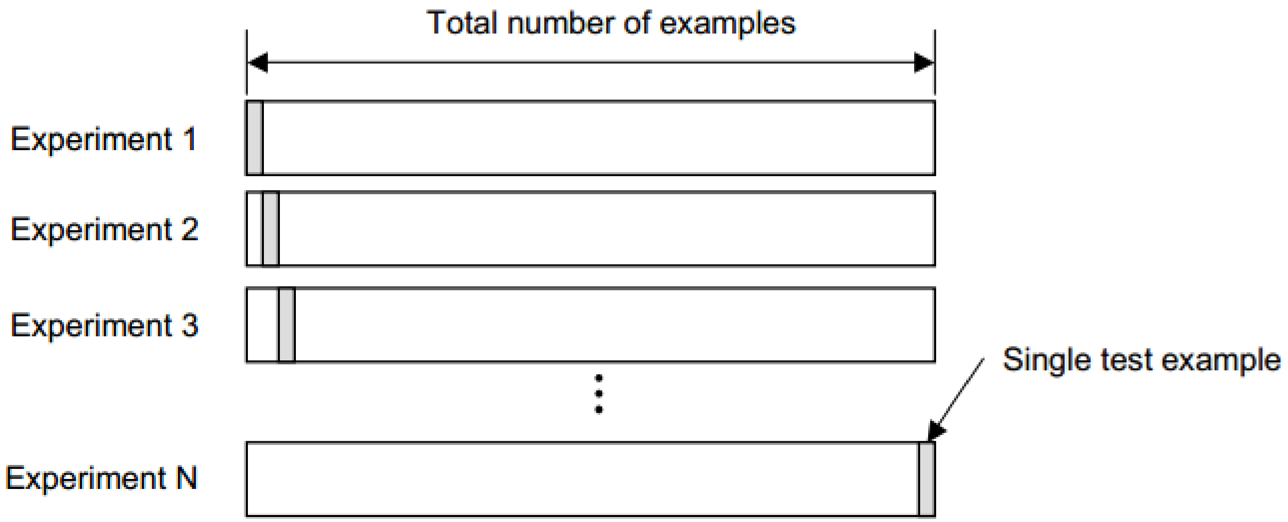


- K-fold CV is similar to random subsampling
  - The advantage of K-fold CV is that all examples are eventually used for both training and testing
- True error is estimated as the average

$$E = \frac{1}{K}\sum_{k=1}^{K} E_k$$

Leave-one-out Cross-Validation

- Leave-one-out CV is the extreme case of K-fold CV, where K=N



$$E = \frac{1}{N}\sum_{k=1}^{N} E_k$$

How many folds are needed?

- With a large number of folds
  - (+) The bias of true error estimate is small (i.e., accurate estimate)
  - (–) The variance of true error estimate is large – the K training sets are too similar to one another
  - (–) The computational time will be large (i.e., many experiments)
- With a small number of folds
  - (+) The computation time is reduced
  - (+) The variance of true error estimate is small
  - (–) The bias of the estimator is large, depending on the learning curve of the classifier
- In practice, a large dataset often needs a small K, while a very sparse dataset often needs a large K
- A common choice for K-fold CV is K=10

Three-way data splits

- If model selection and true error estimates are to be computed simultaneously, the data needs to be divided into 3 disjoint sets
  - **Training set**: used for learning – to fit the parameters of the classifier
  - **Validation set**: used to tune the parameters of a classifier
  - **Test set**: used only to assess the performance of a fully trained classifier