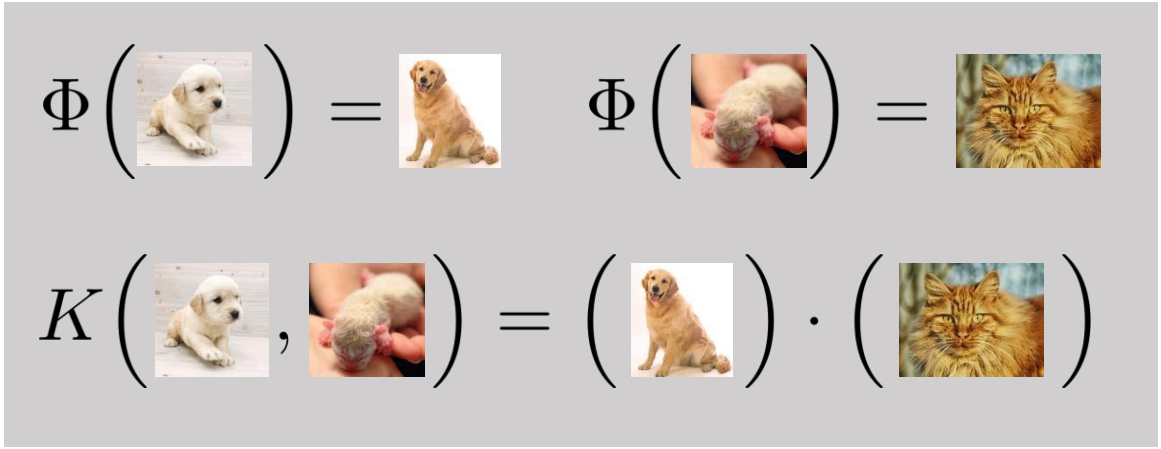


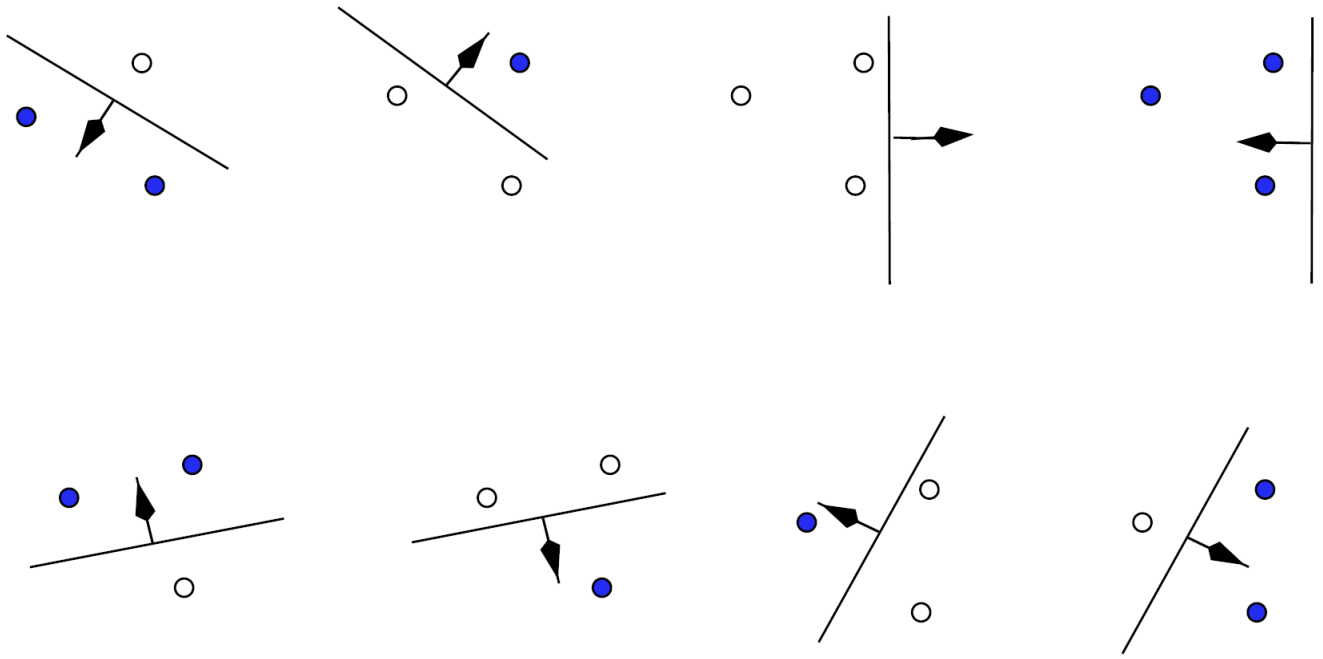
Lecture 2: Kernel-based Learning

Pilsung Kang
School of Industrial Management Engineering
Korea University

AGENDA

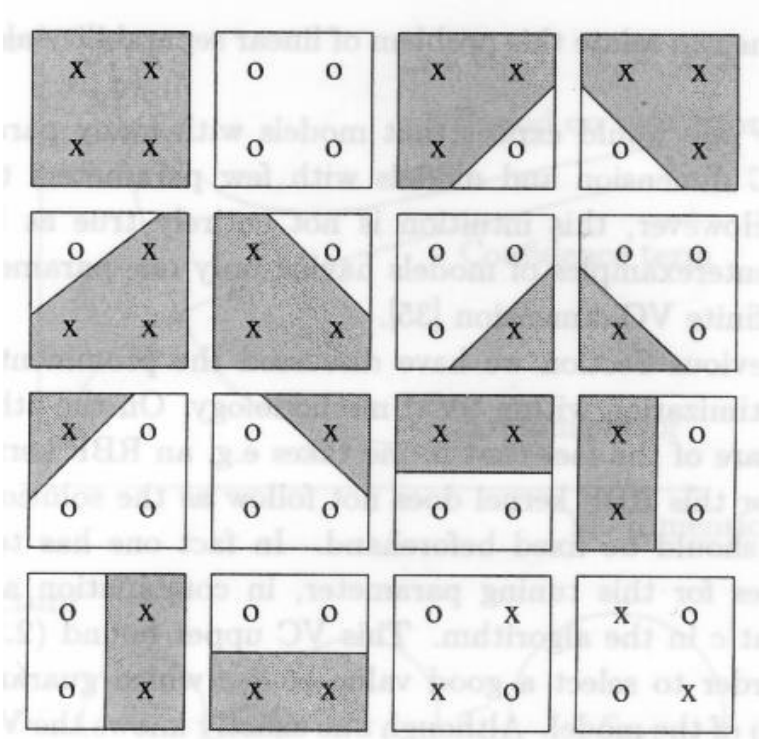
The Concept of Shatter

- Shatter
  - ✓ A set of points is said to be shattered by a class of functions if, no matter how we assign a binary label to each points, a member of the class can perfectly separate them.
    - A linear classifier can shatter (n+1) instances in n-dimensional space



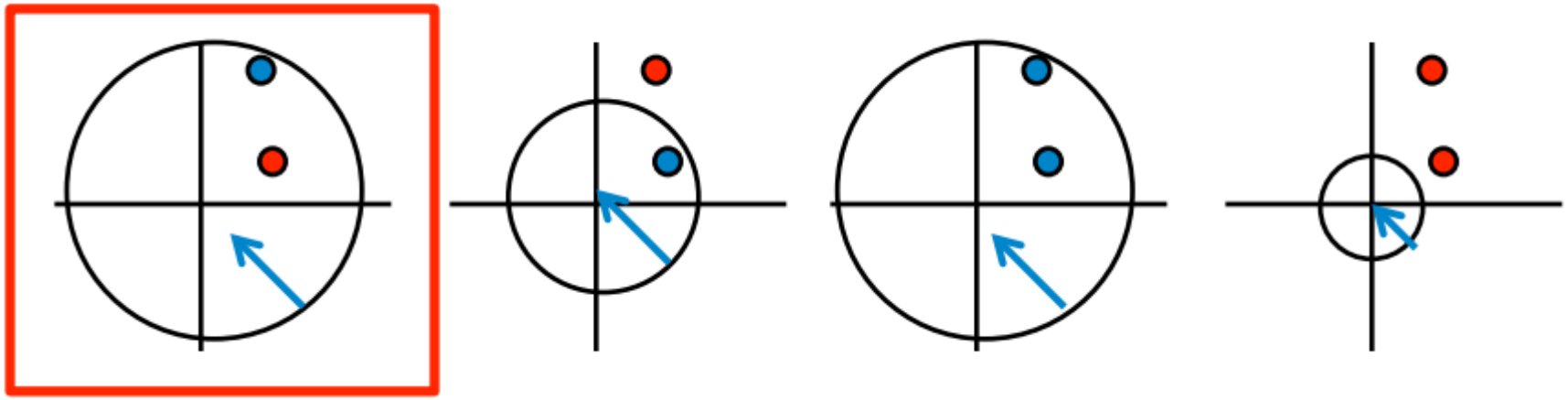
The Concept of Shatter

- Shatter
  - ✓ A set of points is said to be shattered by a class of functions if, no matter how we assign a binary label to each points, a member of the class can perfectly separate them.
    - Can a linear classifier shatter (n+2) instances in n-dimensional space?



The Concept of Shatter

- Shatter
  - ✓ A set of points is said to be shattered by a class of functions if, no matter how we assign a binary label to each points, a member of the class can perfectly separate them.
    - A circle cannot shatter 2 instances in 2-dimensional space

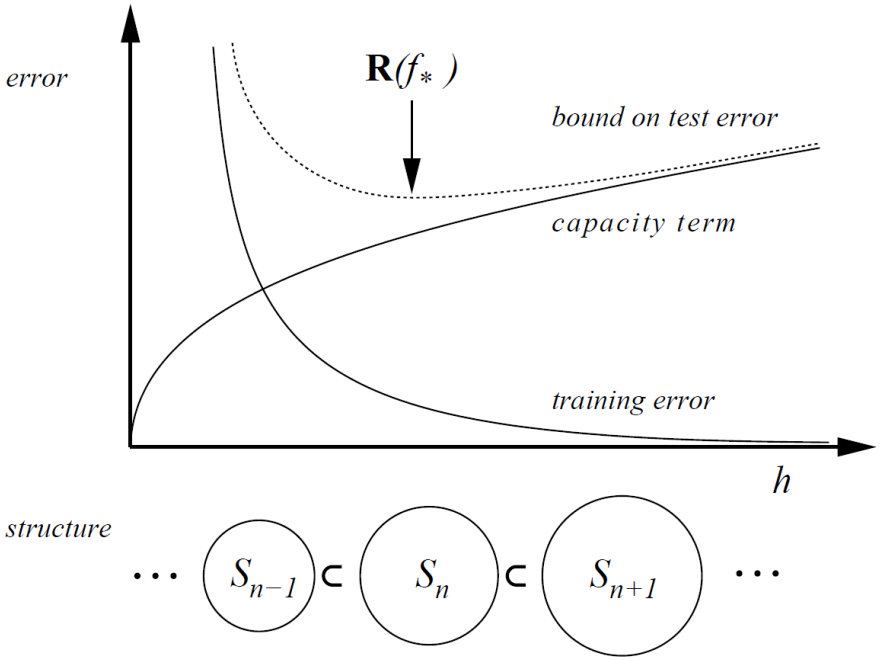


Vapnik-Chervonekis (VC) Dimension

- VC dimension
  - ✓ Measures the capacity of a hypothesis space
  - ✓ Capacity is a measure of complexity and measures the expressive power, richness or flexibility of a set of functions by assessing how wiggly its members can be
  - ✓ The maximum number of points that can be shattered by H is called VC dimension

ERM vs. SRM

- Structural Risk Minimization (SRM)

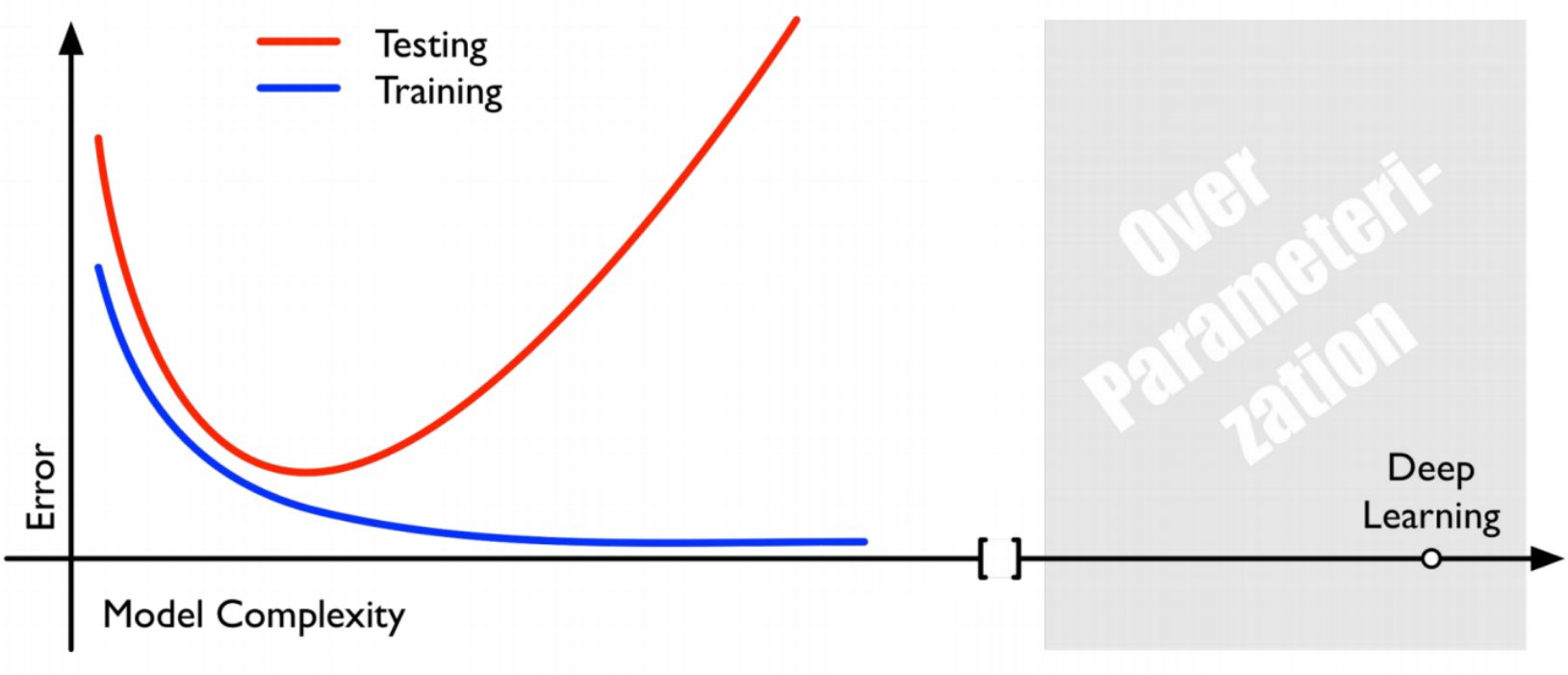


✓ An inductive principle for model selection used for learning from finite training data

✓ Describe a general model of capacity control and provides a trade-off between **hypothesis space complexity (VC dim.)** and the **quality of fitting the training data (empirical error)**

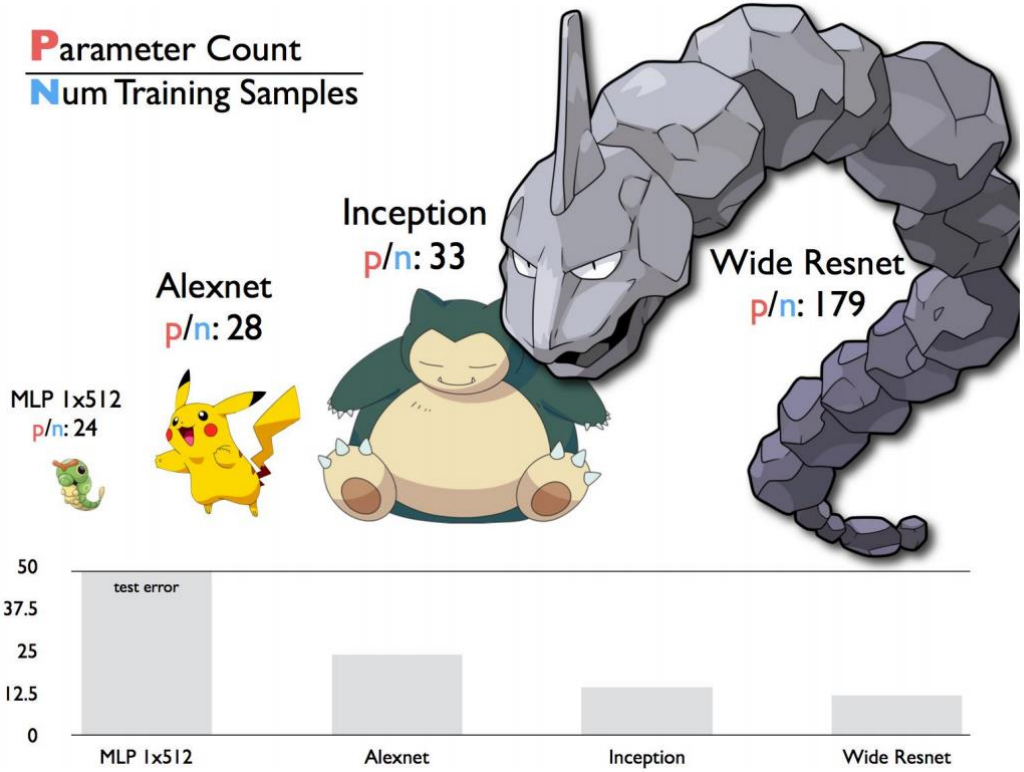
ERM vs. SRM

- Structural Risk Minimization (SRM)
  - ✓ Trade-off between **hypothesis space complexity (VC dim.)** and the **quality of fitting the training data (empirical error)**
  - ✓ Understanding Deep Learning Requires Rethinking Generalization (Zhang et al 2017a, 2017b, 2017c, Park 2017)



ERM vs. SRM

- Structural Risk Minimization (SRM)
  - ✓ Trade-off between **hypothesis space complexity (VC dim.)** and the **quality of fitting the training data (empirical error)**
  - ✓ Understanding Deep Learning Requires Rethinking Generalization (Zhang et al 2017a, 2017b, 2017c, Park 2017)



ERM vs. SRM

- Structural Risk Minimization

Let h denote the VC dimension of the function class F and let R_{emp} be defined as follows using the 0/1 loss.

$$R_{emp}[f] = \frac{1}{n}\sum_{i=1}^{n} L(f(x_i), y_i)$$

For all $\delta > 0$ and $f \in F$ the inequality bounding the risk below holds with probability of at least $1 - \delta$ for $n > h$.

$$R[f] \leq R_{emp}[f] + \sqrt{\frac{h\left(ln\frac{2n}{h} + 1\right) - \ln\left(\frac{\delta}{4}\right)}{n}}$$

Kernel Machine Kids vs. Deep Learning Kids

- Fantastic Four in Deep Learning

Yann Lecun
Facebook AI Director
Professor @NYU

Geoffrey Hinton
Fellow @ Google
Professor @U of Toronto

Yoshua Bengio
Head of MILA

Andrew Ng
Chief Scientist @Baidu
Co-Founder of Coursera
Professor @Stanford Univ.

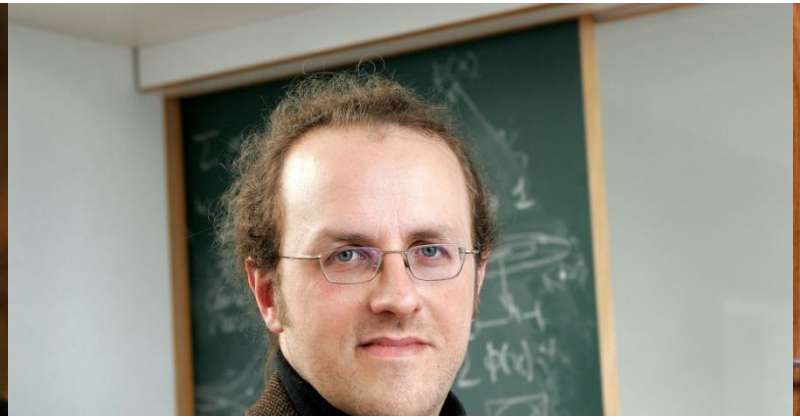
Kernel Machine Kids vs. Deep Learning Kids

- The Three Musketeers in Kernel Machine

Vladimir Vapnik
Professor @RHUL
Book: Statistical Learning Theory

Bernhard Scholkopf
Director of Intelligent Systems
@Max Planck Institute
Book: Learning with Kernels

Alexander J. Smola
Professor @CMU
Book: Advances in Kernel Methods


BIG DATA

Facebook's AI team hires Vladimir Vapnik, father of the popular support vector machine algorithm

JORDAN NOVET @JORDANNOVET NOVEMBER 25, 2014 1:23 PM

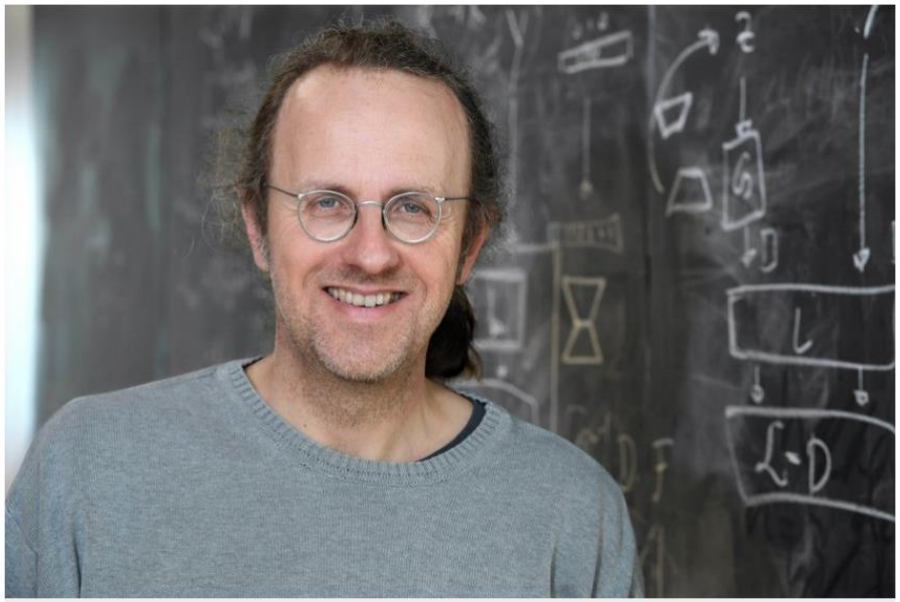
Kernel Machine → Deep Learning

Körber Prize 2019 for Bernhard Schölkopf

This year, the scientific distinction with the highest prize money in Germany goes to the pioneer of artificial intelligence

SEPTEMBER 13, 2019

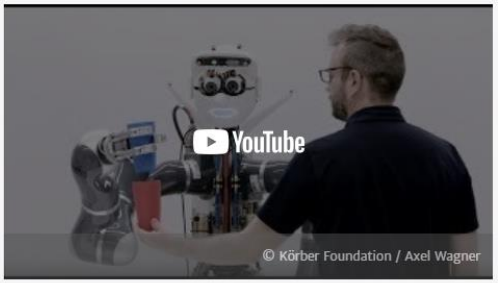
Bernhard Schölkopf, Director at the Max Planck Institute for Intelligent Systems in Tübingen, is honoured with the Körber Prize for European Science 2019. The Körber Foundation awards the prize to honour the computer scientist's contributions to machine learning, which today supplies one of the most important methods of Artificial Intelligence (AI). The Körber Prize includes prize money of one million Euros.



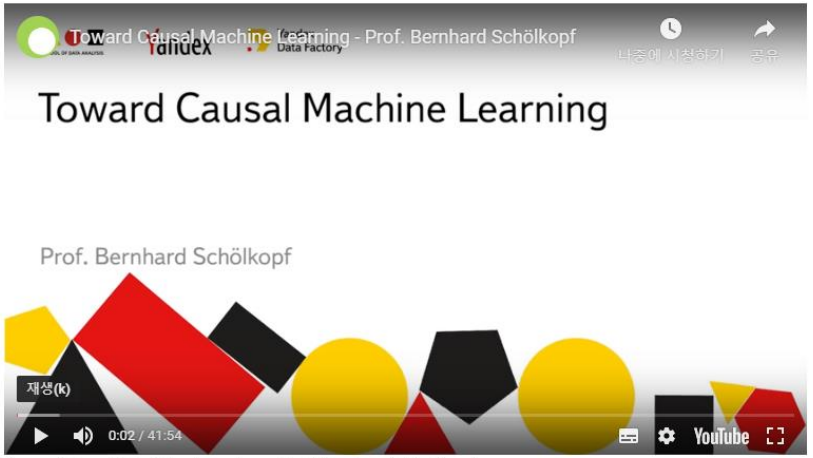
A pioneer of Artificial Intelligence: Bernhard Schölkopf receives the 2019 Körber Prize for European Science.
© David Ausserhofer

https://www.mpg.de/13645470/schoelkopf-koerber-prize

Causal relationships in data



Teaching robots how to learn



Toward Causal Machine Learning – Prof. Bernhard Schölkopf

https://www.youtube.com/watch?time_continue=2&v=ooeRIw3U2zU

Kernel Machine → Deep Learning

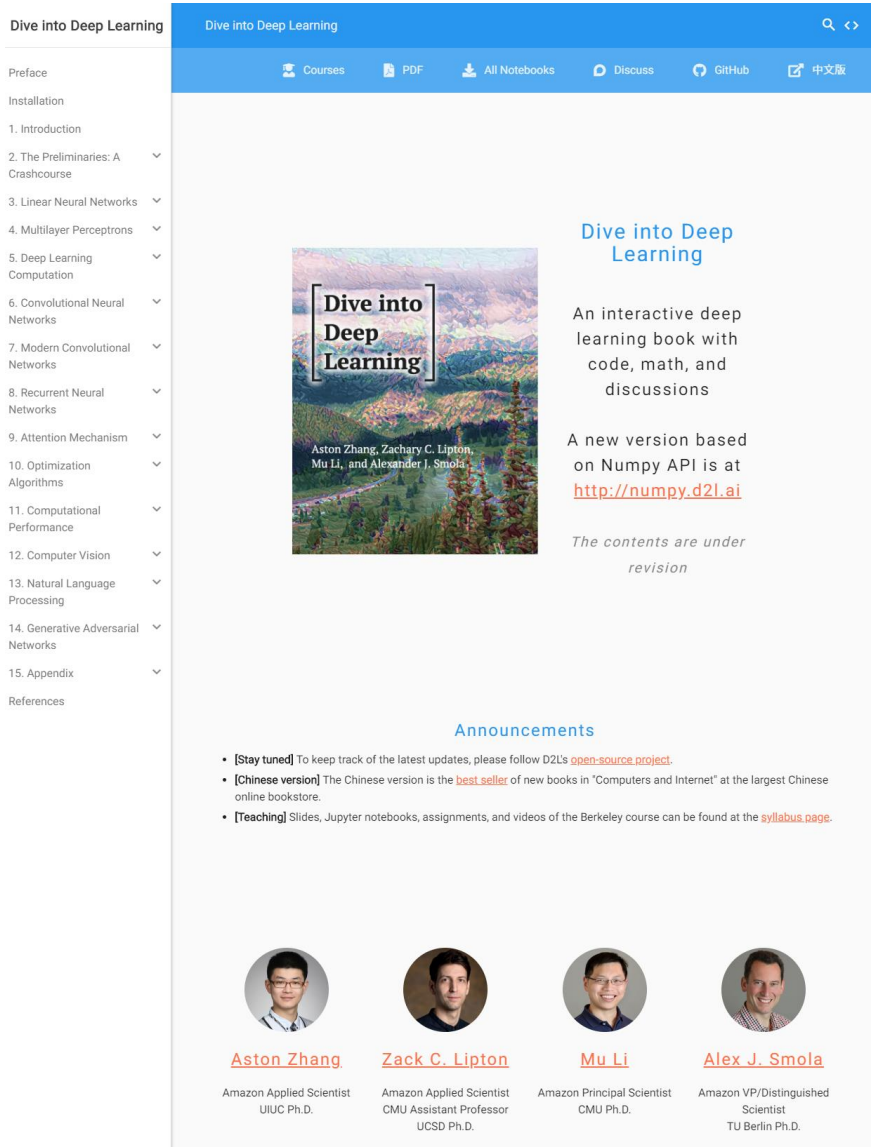
AWS Startups Blog

Alex Smola Showcases the Breadth of AWS's Machine Learning Capabilities at Collision 2018

by Michelle Kung | on 07 MAY 2018 | in Events | Permalink | Share

https://aws.amazon.com/ko/blogs/startups/alex-smola-aws-machine-learning-collision-conference-new-orleans/

훗날 이 말을 한 당사자인 이진영이 은퇴 후 인터뷰에서 밝히길 야잘잘의 진짜 속뜻은 **'야구를 잘하는 사람이 잘하지만 그걸 이겨내기 위해선 자신과 같은 길을 가는 경쟁자들을 어떻게 해야 이길 수 있는지 고민하고 노력하는 것'**라고 밝혔다. 그러니까 재능 말고도 노력도 뒷받침해야 한다는 이야기

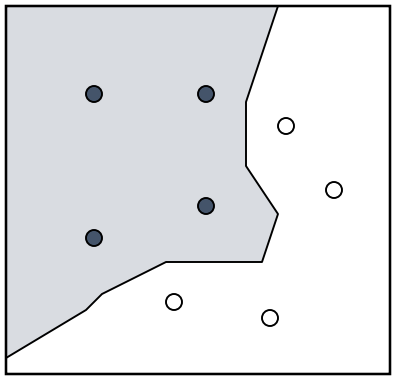


https://www.d2l.ai/

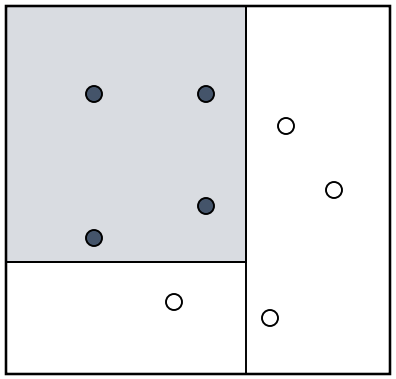
AGENDA

Discriminant Function

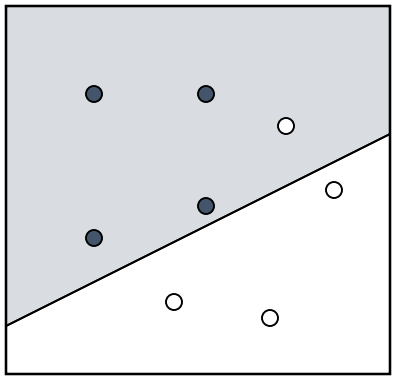
- Discriminant functions in classification



Nearest Neighbor

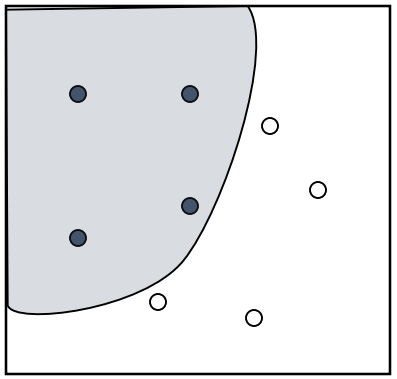


Decision Tree



Linear Functions

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



Nonlinear Functions

Linear Classification

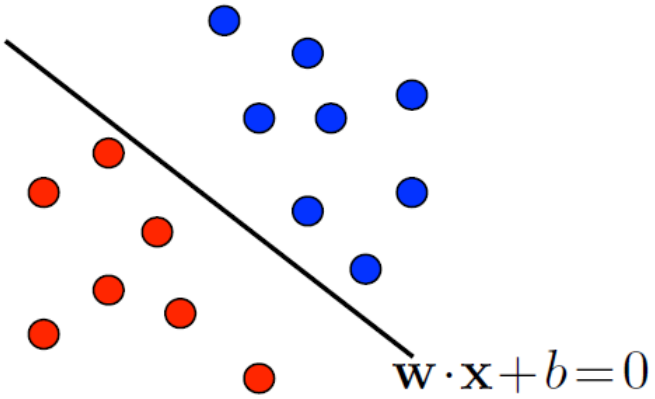
- Binary Classification Problem
  - ✓ Training data: sample drawn i.i.d. from set $X \in R^d$ according to some distribution D

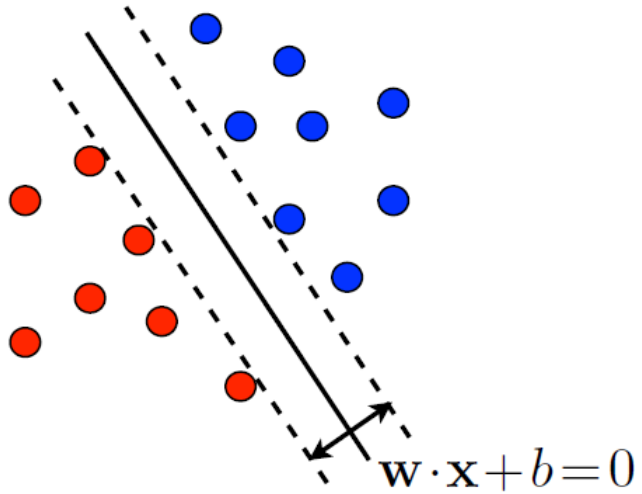
$$S = \Big((x_1, y_1), ..., (x_n, y_n) \Big) \in X \times \{-1, +1\}$$

  - ✓ Problem: find hypothesis $h : X \to \{-1, +1\}$ in *H* (classifier) with small generalization error $R_D(h)$
  - ✓ Linear classifier
    - Hypothesis based on hyperplanes
    - Linear separation in high-dimensional data

Linear Classification

- Binary classification problem

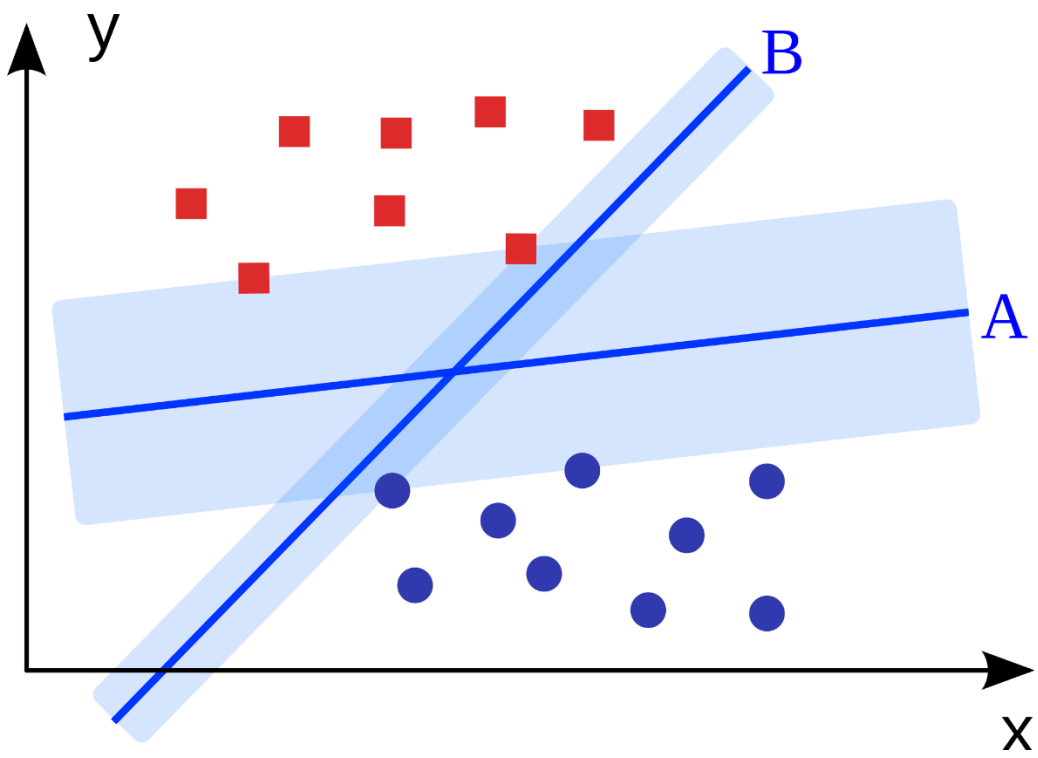




$$H = \{\mathbf{x} \rightarrow sign(\mathbf{w}\cdot\mathbf{x}+b:\ \ \mathbf{w}\in R^d,\ b\in R\}$$

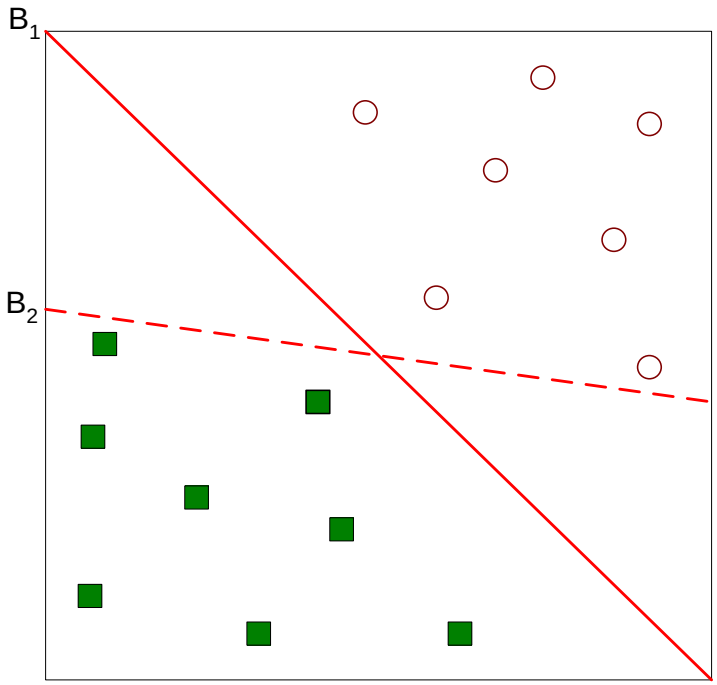
Local Optimum? Global Optimum!

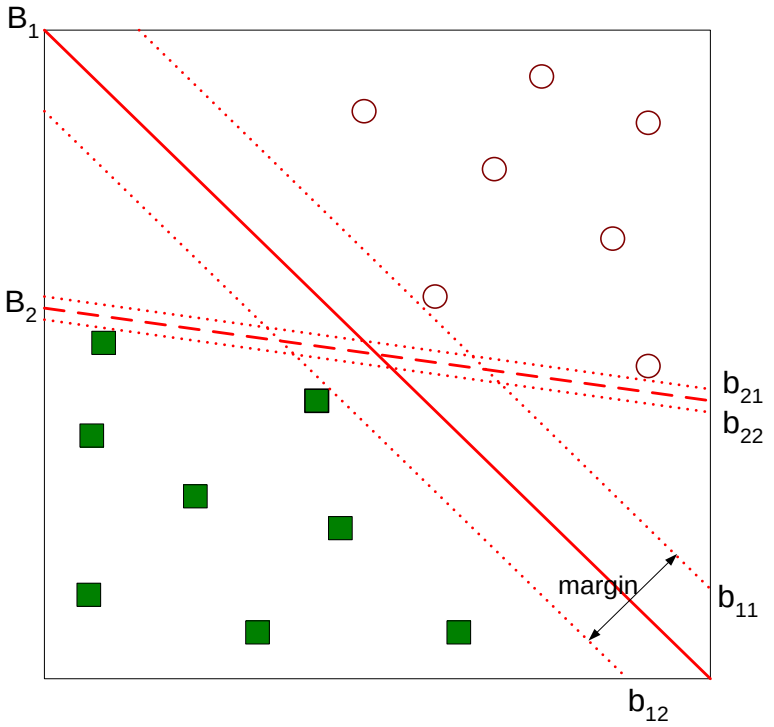
- Which classification boundary is better?
  - ✓ How do you define "better"?



Local Optimum? Global Optimum!

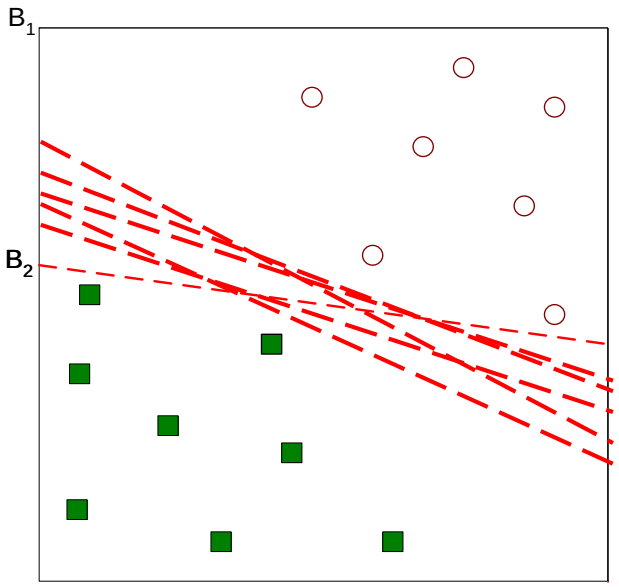
- Which classification boundary is better?
  - ✓ Find the hyperplane that maximizes the margin!

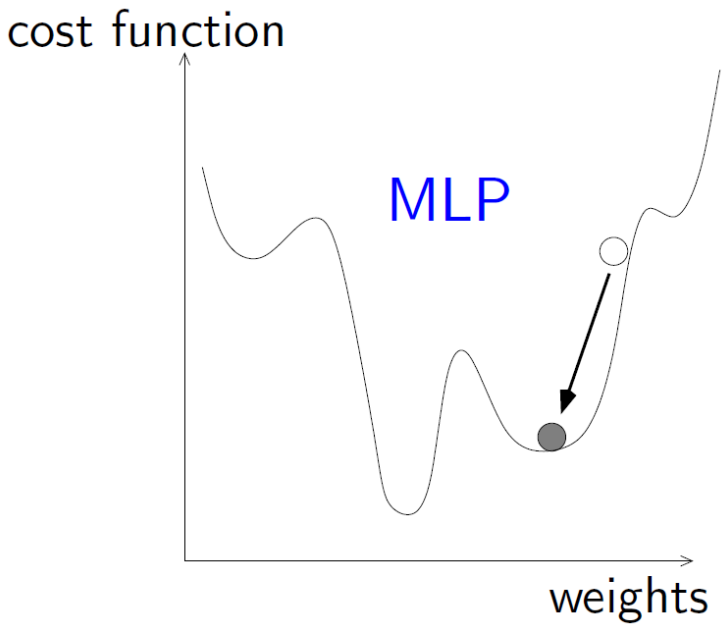




Local Optimum? Global Optimum!

- Artificial neural network (ANN)
  - ✓ Universal approximation of continuous nonlinear functions
  - ✓ Learning from input-output patterns
  - ✓ Parallel network architecture, multiple inputs and outputs
  - ✓ But, existence of many local optimums!



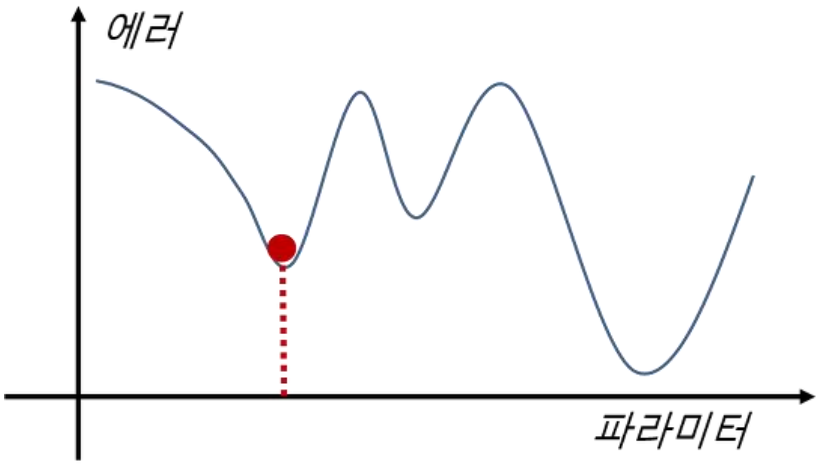


Local Optimum? Global Optimum!

- Artificial neural network (ANN) (cont')
- But!!

Dauphin, Y. N., Pascanu, R., Gulcehre, C., Cho, K., Ganguli, S., & Bengio, Y. (2014). Identifying and attacking the saddle point problem in high-dimensional non-convex optimization. In *Advances in neural information processing systems* (pp. 2933-2941).

이럴 줄 알았는데…



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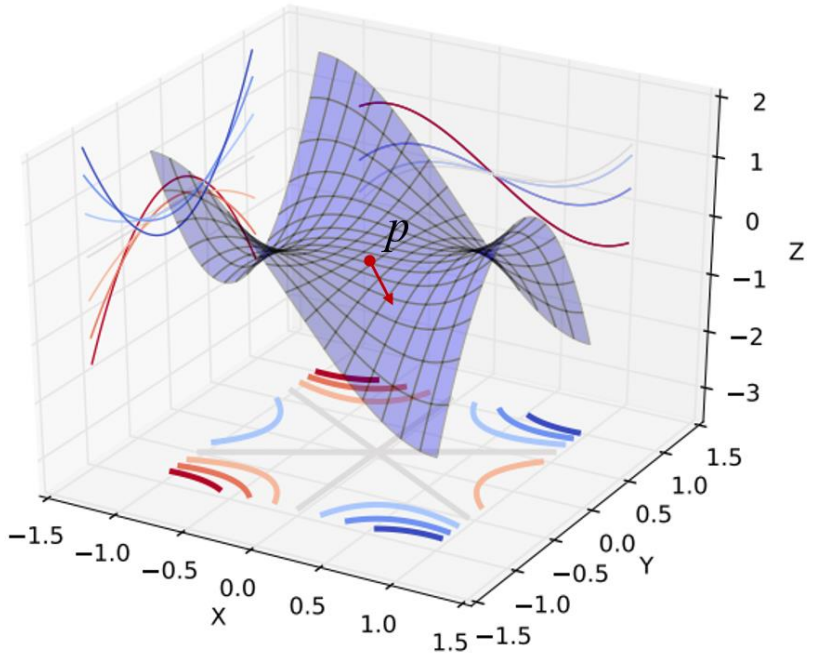
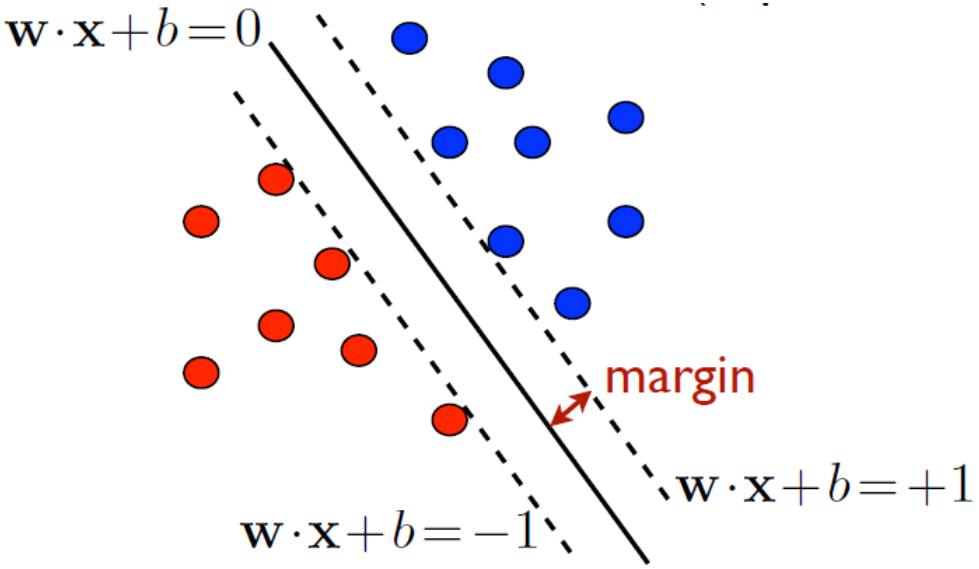
고차원에서 모든 방향으로 gradient가 0인 경우는 거의 없더라…



Support Vector Machine: Formulation

Burges (1998)

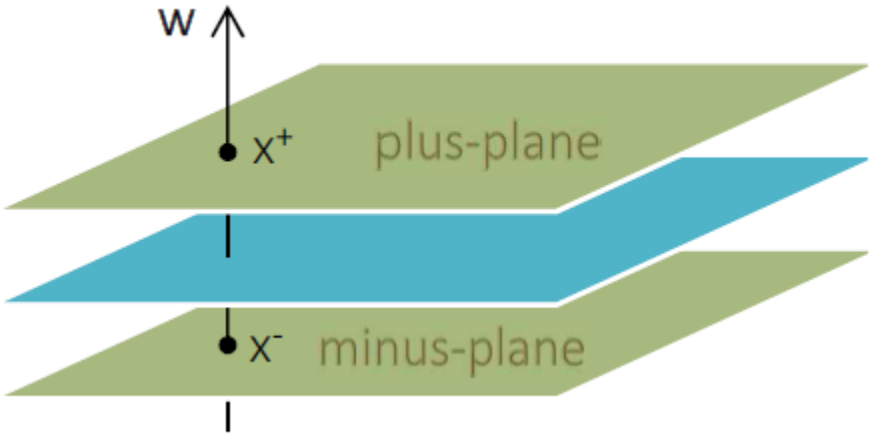
- Optimal hyperplane: Maximize the margin



- Canonical hyperplane: $\mathbf{w}$ and b chosen such that for closest points $|\mathbf{w}\cdot\mathbf{x}+b|=1$.

Support Vector Machine: Formulation

- How to compute the margin?



$$\text{margin} = \frac{1}{||\mathbf{w}||_2}$$

Margin and VC Dimension

- Recall the relationship between margin and VC dimension

The VC dimension of a separating hyperplane with a margin Δ is bounded as follows

$$h \leq min\left(\left\lceil\frac{R^2}{\Delta^2}\right\rceil, D\right) + 1$$

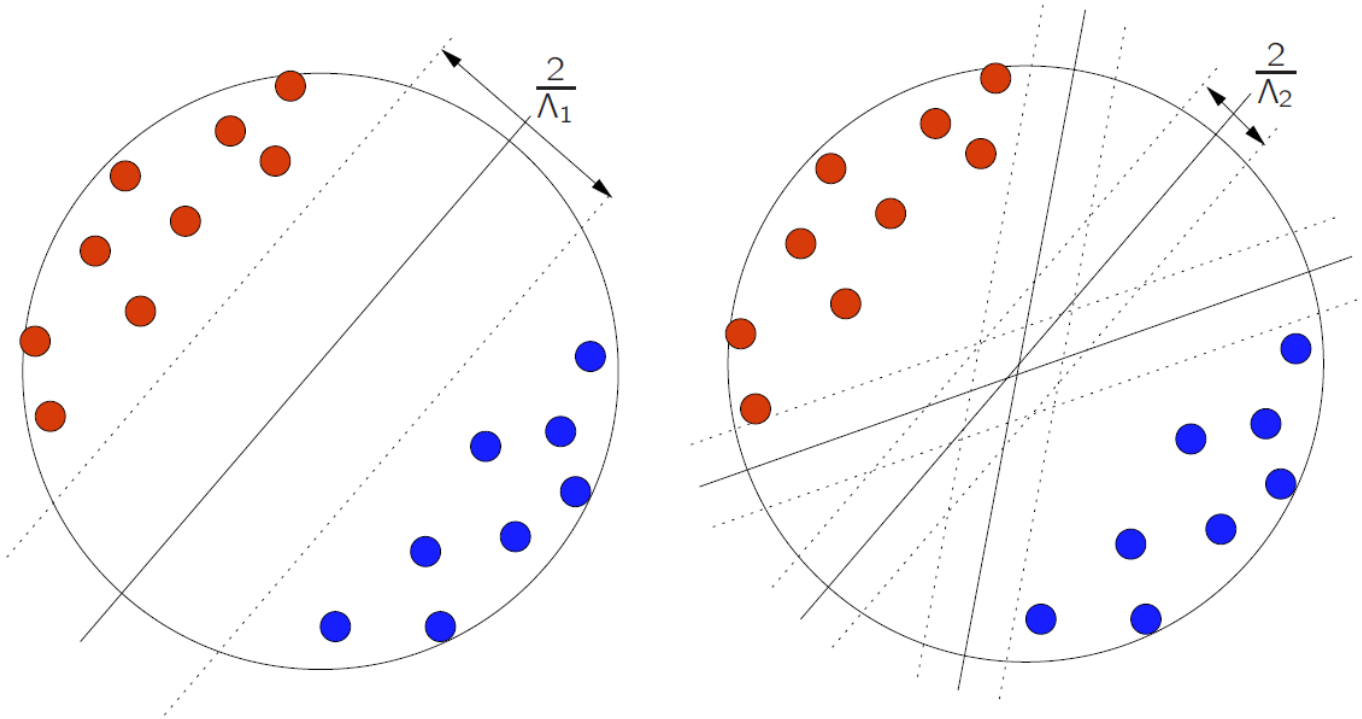
where D is the dimensionality of the input space, and R is the radius of the smallest sphere containing all the input vectors

- Maximizing the margin → Minimizing the VC dimension → Minimizing the Expected Risk

$$R[f] \leq R_{emp}[f] + \sqrt{\frac{h\left(ln\frac{2n}{h} + 1\right) - \ln\left(\frac{\delta}{4}\right)}{n}}$$

Margin and VC Dimension

- An illustrative example



✓ If we choose a hyperplane with a large margin (left), there is only a small number of possibilities to separate the data → lower VC dimension

Support Vector Machine: Cases

- Support Vector Machine Formulation

	Hard margin?	Soft margin?
Linearly separable?	Basic form (Case 1)	Introduce penalty terms (Case 2)
Linearly non-separable?	Utilize Kernel Trick	Introduce penalty terms Utilize Kernel Trick (Case 3)

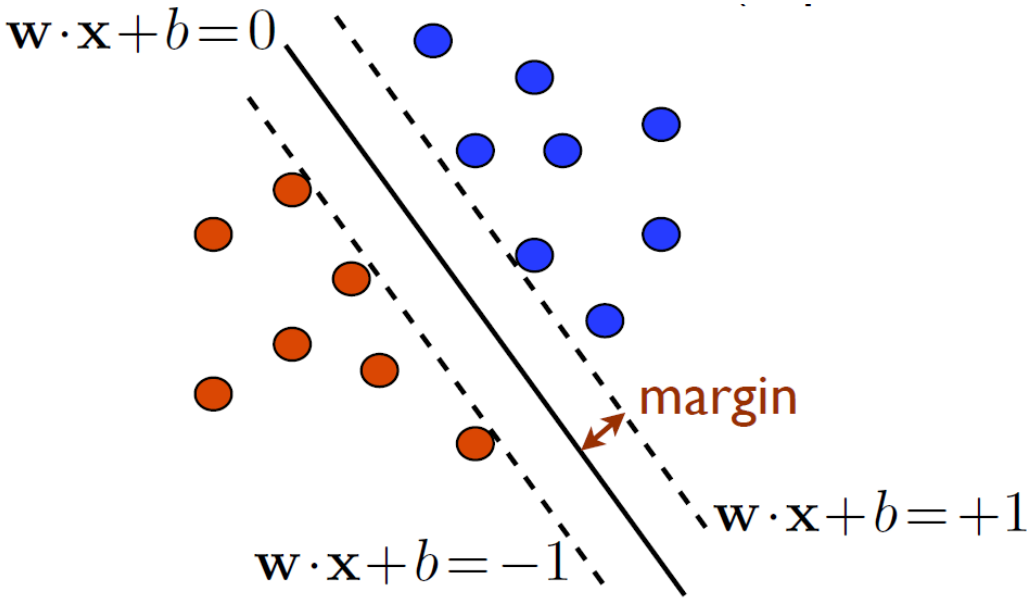
SVM Case 1: Linear Case & Hard Margin

- Optimization Problem
  - ✓ Objective function

$$\min \quad \frac{1}{2}\|\mathbf{w}\|^2$$

  - ✓ Constraints

$$s.t. \quad y_i(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b) \geq 1$$



SVM Case 1: Linear Case & Hard Margin

- Optimization Problem
  - ✓ Lagrangian Problem

$$\min \quad L_P(\mathbf{w}, b, \alpha_i) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N} \alpha_i \left(y_i\left(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b\right) - 1\right)$$

$$s.t. \quad \alpha_i \geq 0$$

  - ✓ KKT conditions

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^{N} \alpha_i \, y_i \mathbf{x}_i \qquad \frac{\partial L_p}{\partial b} = 0 \quad \Rightarrow \quad \sum_{i=1}^{N} \alpha_i y_i = 0$$

SVM Case 1: Linear Case & Hard Margin

- From Primal to Dual

$$\min \quad L_P(\mathbf{w}, b, \alpha_i) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N} \alpha_i \left(y_i\left(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b\right) - 1\right)$$
$$s.t. \quad \alpha_i \geq 0$$

$$\max \quad L_D(\alpha_i) = \sum_{i=1}^{N} \alpha_i \; - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^{\mathrm{T}}\mathbf{x}_j$$
$$s.t. \sum_{i=1}^{N} \alpha_i y_i = 0 \quad and \quad \alpha_i \geq 0$$

- Solution

$$f(\mathbf{x}_{new}) = sign\left(\sum_{i=1}^{N} \alpha_i y_i \, \mathbf{x}_i^{\mathrm{T}}\mathbf{x}_{new} + b\right)$$

SVM Case 1: Linear Case & Hard Margin

- From KKT condition, we know that

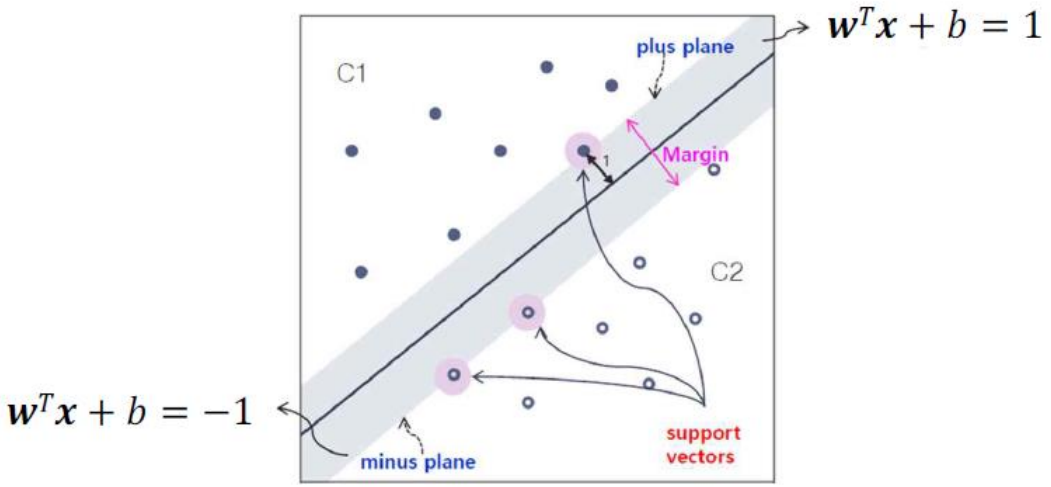
$$\alpha_i\left(y_i\left(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b\right) - 1\right) = 0$$

✓ Thus, the only support vectors have $\alpha_i \neq 0$

✓ The solution has the form

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i\, y_i \mathbf{x}_i = \sum_{i \in SV}^{N} \alpha_i\, y_i \mathbf{x}_i$$

✓ b can be computed by $y_i\left(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b\right) - 1 = 0$ with a support vector $\mathbf{x}_i$



SVM Case 1: Linear Case & Hard Margin

- Compute the margin
  - ✓ Since the SVs lie on the marginal hyperplanes, for any support vector $\mathbf{x}_i$, $\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b = y_i$

$$b = y_i - \sum_{i=1}^{N} \alpha_i y_i (\mathbf{x}_j, \mathbf{x}_i)$$

  - ✓ Multiplying both sides by $\alpha_i y_i$ and taking the sum leads to

$$\sum_{i=1}^{N} \alpha_i y_i b = \sum_{i=1}^{N} \alpha_i y_i^2 - \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j (\mathbf{x}_i, \mathbf{x}_j)$$

  - ✓ Using the fact that $y_i^2 = 1$

$$0 = \sum_{i=1}^{N} \alpha_i - \mathbf{w}^{\mathrm{T}}\mathbf{w}$$

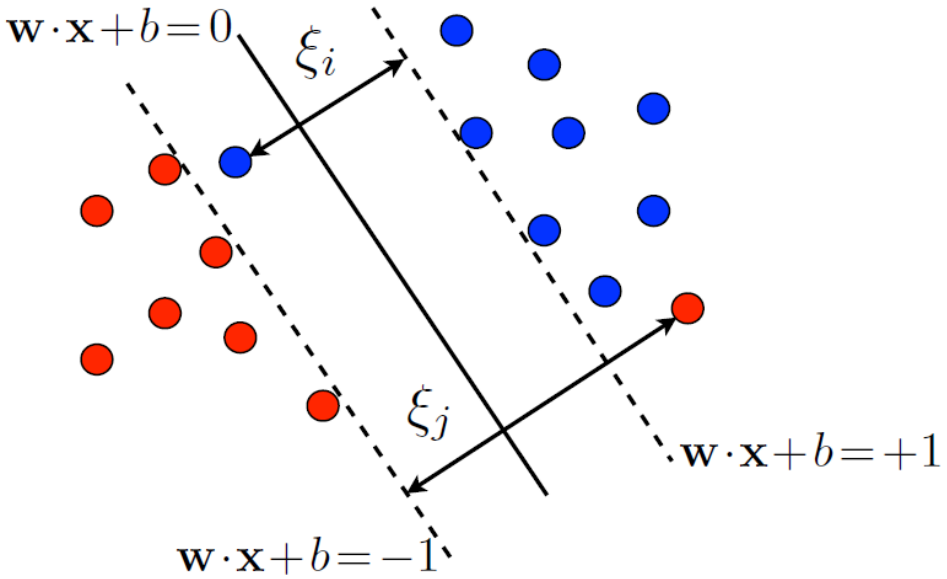
$$\rho^2 = \frac{1}{\|\mathbf{w}\|_2^2} = \frac{1}{\sum_{i=1}^{N} \alpha_i} = \frac{1}{\|\boldsymbol{\alpha}\|_1}$$

SVM Case 2: Linear Case & Soft Margin

- Optimization Problem (C-SVM)
  - ✓ Objective function
  - ✓ Constraints

$$\min \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\xi_i$$

$$s.t. \;\; y_i\left(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b\right) \geq 1 - \xi_i, \xi_i \geq 0, \;\; \forall i$$



SVM Case 2: Linear Case & Soft Margin

- Optimization Problem
  - ✓ Lagrangian Problem

$$\min \quad L_P(\mathbf{w}, b, \alpha_i) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\xi_i - \sum_{i=1}^{N}\alpha_i\left(y_i\left(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b\right) - 1 + \xi_i\right) - \sum_{i=1}^{N}\mu_i\xi_i$$

$$s.t. \quad \alpha_i \geq 0$$

  - ✓ KKT conditions

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^{N}\alpha_i\, y_i\mathbf{x}_i \qquad \frac{\partial L_p}{\partial b} = 0 \quad \Rightarrow \quad \sum_{i=1}^{N}\alpha_i y_i = 0$$

$$\frac{\partial L_p}{\partial \xi_i} = 0 \quad \Rightarrow \quad C - \alpha_i - \mu_i = 0$$

SVM Case 2: Linear Case & Soft Margin

- From Primal to Dual

$$\min \quad L_P(\mathbf{w}, b, \alpha_i) = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\xi_i - \sum_{i=1}^{N}\alpha_i\left(y_i\left(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b\right) - 1 + \xi_i\right) - \sum_{i=1}^{N}\mu_i\xi_i$$
$$s.t. \quad \alpha_i \geq 0$$

$$\max \quad L_D(\alpha_i) = \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j \mathbf{x}_i^{\mathrm{T}}\mathbf{x}_j$$
$$s.t. \quad \sum_{i=1}^{N}\alpha_i y_i = 0 \quad and \quad 0 \leq \alpha_i \leq C$$

- Solution
  - ✓ Only requires support vectors

$$f(\mathbf{x}_{new}) = sign\left(\sum_{i=1}^{N}\alpha_i y_i\, \mathbf{x}_i^{\mathrm{T}}\mathbf{x}_{new} + b\right)$$

SVM Case 2: Linear Case & Soft Margin

- From KKT condition, we know that

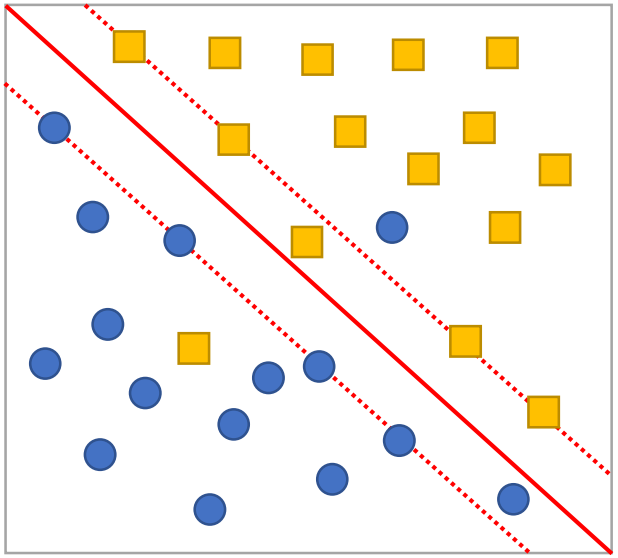
$$\alpha_i \left(y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 + \xi_i \right) = 0$$

✓ Thus, the only support vectors have $\alpha_i \neq 0$

✓ In addition,

$$C - \alpha_i - \mu_i = 0 \quad \& \quad \mu_i \xi_i = 0$$

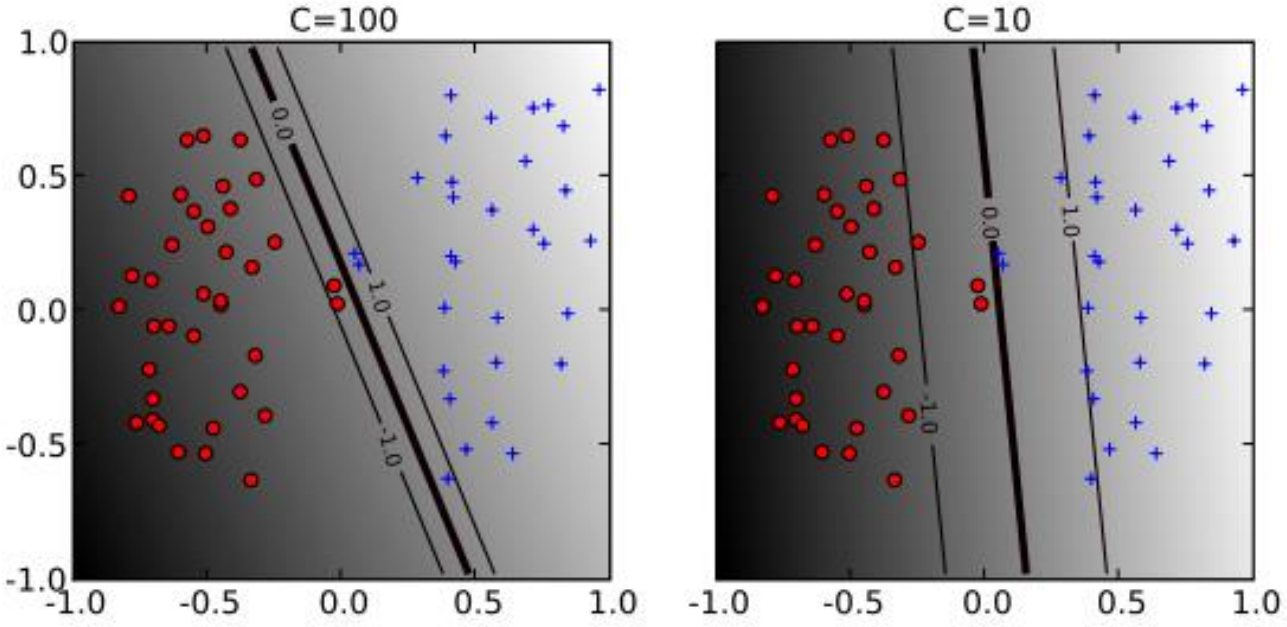
- Case 1: $\alpha_i = 0$ → non-support vectors
- Case 2: $0 < \alpha_i < C$ → support vectors on the margin
- Case 3: $\alpha_i = C$ → support vectors outside the margin



SVM Case 2: Linear Case & Soft Margin

- Regularization cost C
  - ✓ Large C: narrow margin with a few support vectors
  - ✓ Small C: wide margin with many support vectors

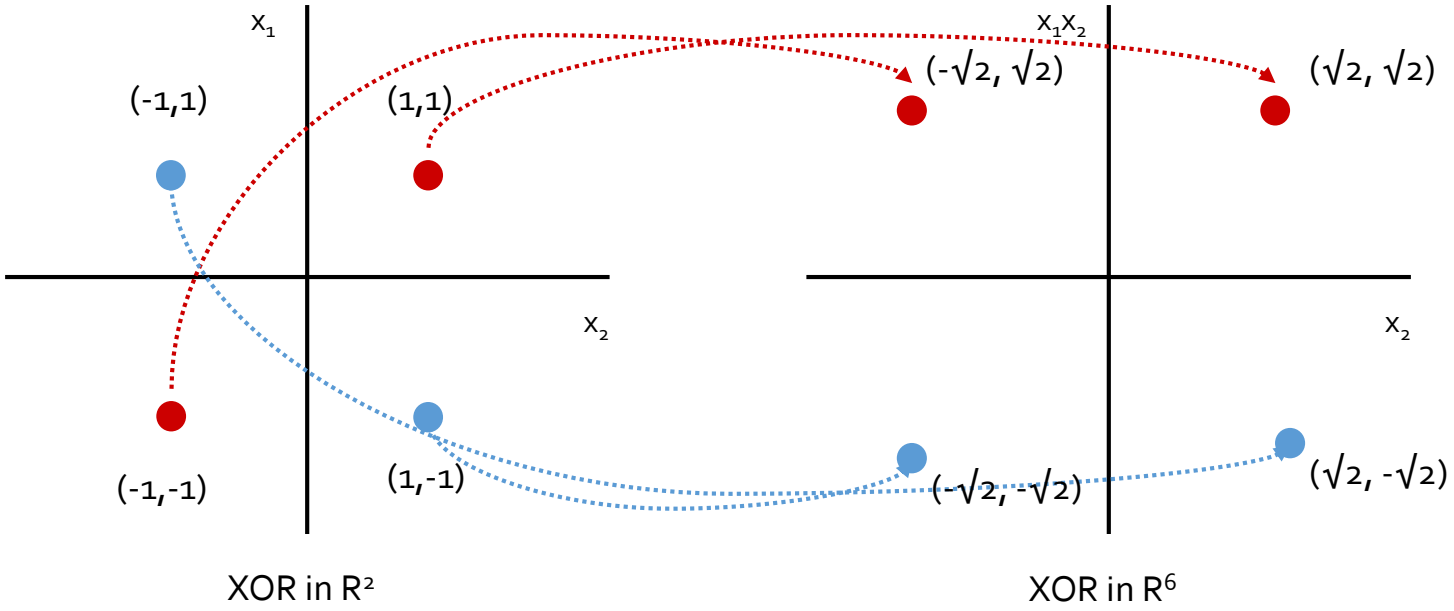
$$\min \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\xi_i$$



SVM Case 3: Non-linear Case & Soft Margin

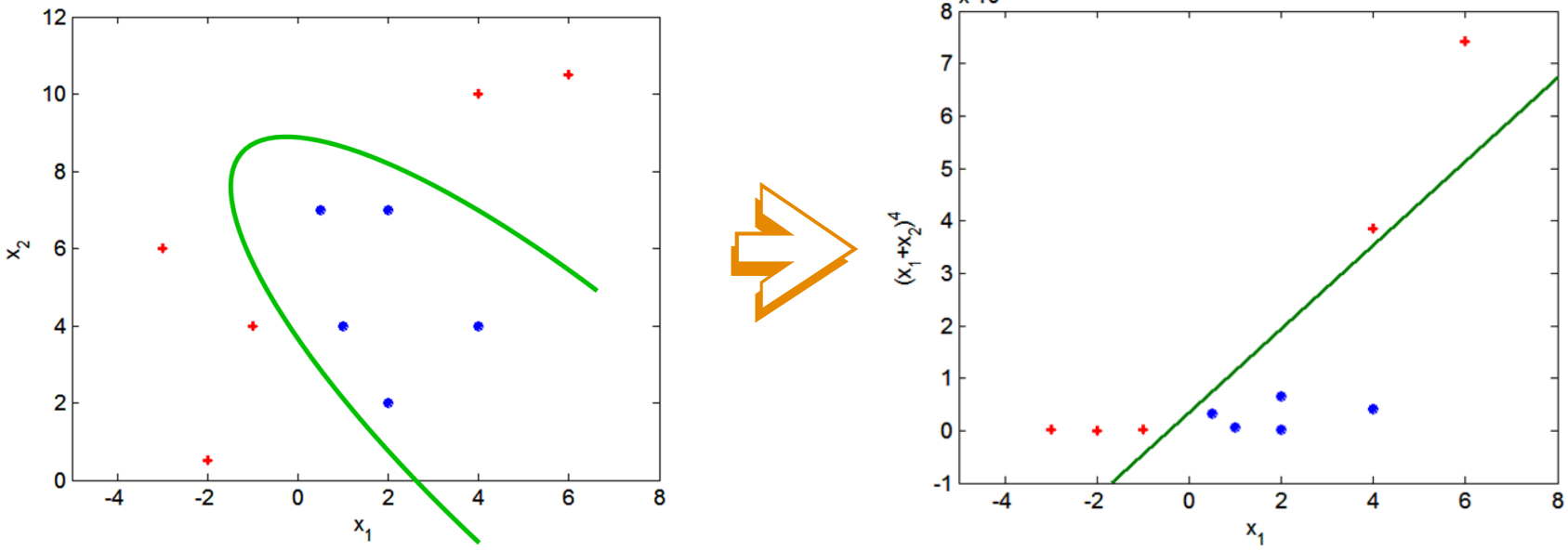
- What if the decision boundary is not linear?
  - ✓ Use a mapping function $\Phi(\mathrm{x})$ to transform an input vector from a lower dimensional space into a higher dimensional space

$$\Phi : (\mathbf{x}_1, \mathbf{x}_2) \rightarrow (\mathbf{x}_1^2, \mathbf{x}_2^2, \sqrt{2}\mathbf{x}_1, \sqrt{2}\mathbf{x}_2, \sqrt{2}\mathbf{x}_1\mathbf{x}_2, 1)$$



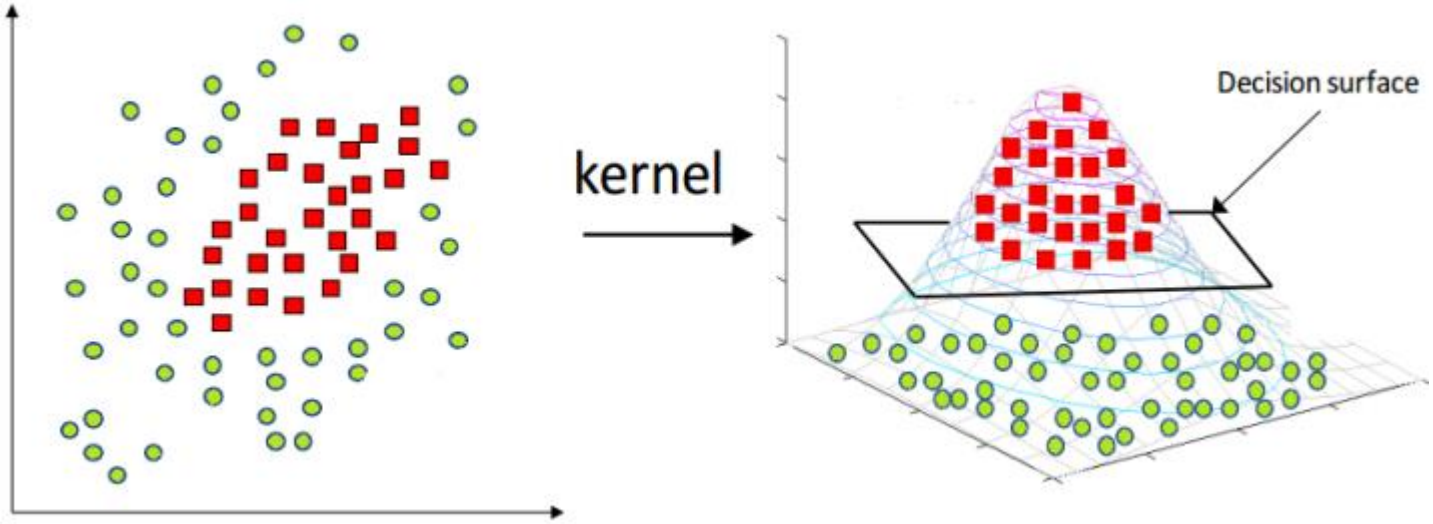
SVM Case 3: Non-linear Case & Soft Margin

- What if the decision boundary is not linear?
  - ✓ Transform an input vector into a higher feature vector



SVM Case 3: Non-linear Case & Soft Margin

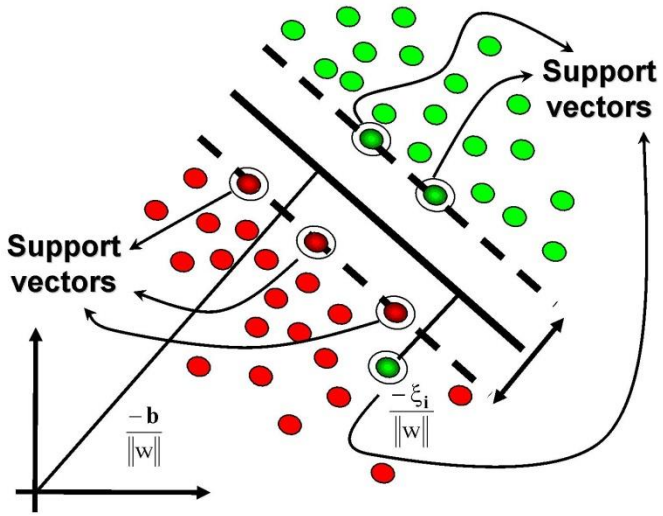
- What if the decision boundary is not linear?
  - ✓ Transform an input vector into a higher feature vector

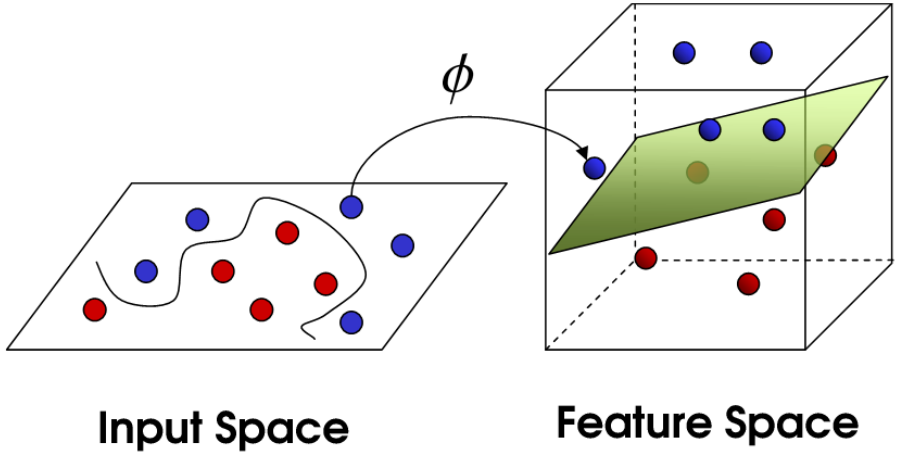


http://blog.hackerearth.com/simple-tutorial-svm-parameter-tuning-python-r

SVM Case 3: Non-linear Case & Soft Margin

- Goal: To find the best hyperplane that maximizes the margin and minimize the misclassification error
  - ✓ **Large margin**: preserve the generalization ability
  - ✓ **Flexible**: can generate an arbitrary shape of boundary in the input space

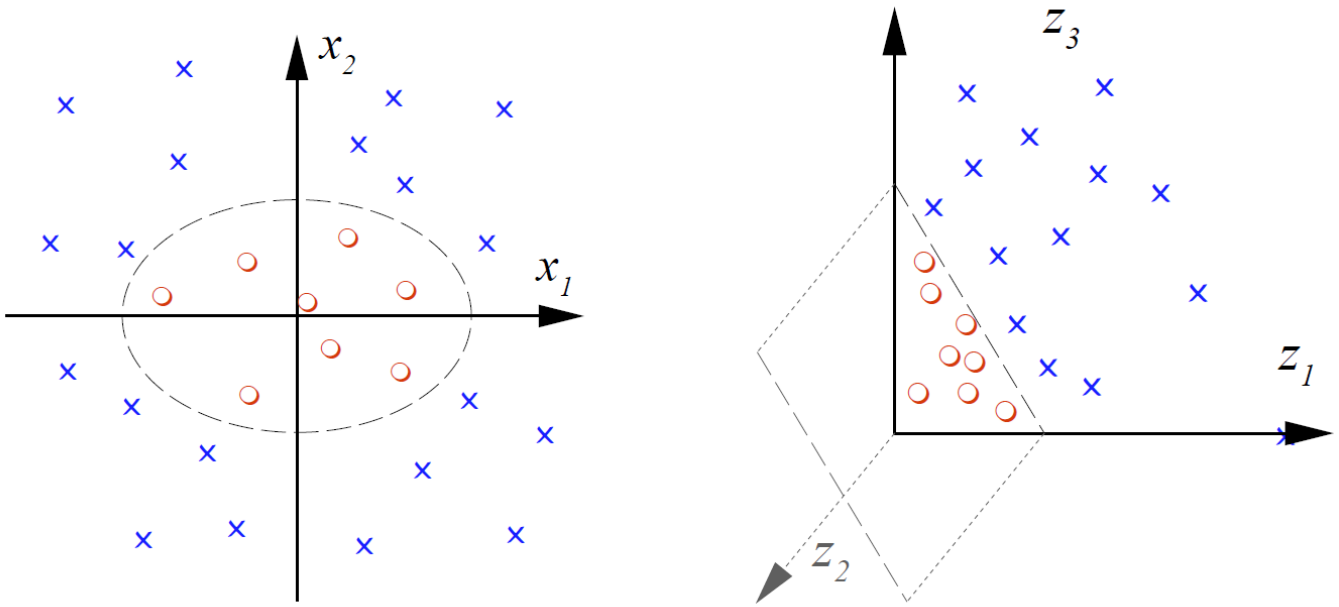




SVM Case 3: Non-linear Case & Soft Margin

- Goal: To find the best hyperplance that maximizes the margin and minimize the misclassification error
  - ✓ **Large margin**: preserve the generalization ability
  - ✓ **Flexible**: can generate an arbitrary shape of boundary in the input space

$$\Phi : \mathbb{R}^2 \rightarrow \mathbb{R}^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2}\, x_1 x_2, x_2^2)$$



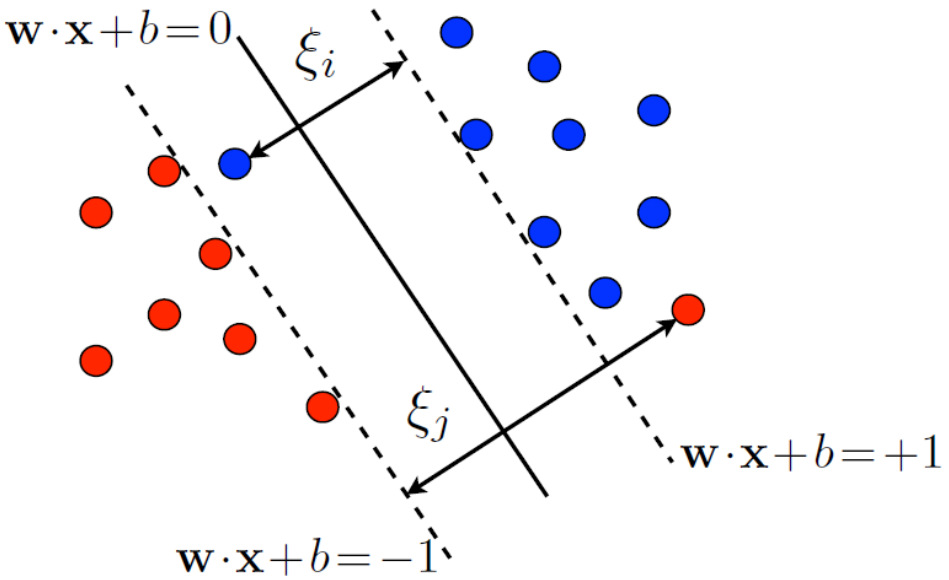
SVM Case 3: Non-linear Case & Soft Margin

- Optimization Problem (C-SVM)
  - ✓ Objective function

$$\min \quad \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{N}\xi_i$$

  - ✓ Constraints

$$s.t. \quad y_i(\mathbf{w}^T\Phi(\mathbf{x}_i) + b) \geq 1 - \xi_i, \quad \xi_i \geq 0, \quad \forall i$$



SVM Case 3: Non-linear Case & Soft Margin

- Optimization Problem (C-SVM)
  - ✓ Lagrangian Problem

$$\min \quad L_P(\mathbf{w}, b, \alpha_i) = \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n}\xi_i$$

$$-\sum_{i=1}^{n}\alpha_i\left(y_i(\mathbf{w}^T\Phi(\mathbf{x}_i)+b)-1+\xi_i\right)-\sum_{i=1}^{n}\mu_i\xi_i$$

  - ✓ KKT condition

$$\frac{\partial L_P}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w} = \sum_{i=1}^{n}\alpha_i y_i \Phi(\mathbf{x}_i) \qquad \frac{\partial L_P}{\partial b} = 0 \Rightarrow \sum_{i=1}^{n}\alpha_i y_i = 0$$

$$\frac{\partial L_P}{\partial \xi_i} = 0 \Rightarrow C - \alpha_i - \mu_i = 0$$

SVM Case 3: Non-linear Case & Soft Margin

✓ Lagrangian Problem (Primal)

$$\min \quad L_P(\mathbf{w}, b, \alpha_i) = \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n}\xi_i$$

$$-\sum_{i=1}^{n}\alpha_i\left(y_i(\mathbf{w}^T\Phi(\mathbf{x}_i)+b)-1+\xi_i\right)-\sum_{i=1}^{n}\mu_i\xi_i$$

✓ Lagrangian Problem (Dual)

$$\max \quad L_D = \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \Phi(\mathbf{x}_i)^T\Phi(\mathbf{x}_j)$$

$$s.t. \quad \sum_{i=1}^{n}\alpha_i y_i = 0 \quad and \quad 0 \le \alpha_i \le C$$

SVM Case 3: Non-linear Case & Soft Margin

- How to find a mapping function Φ?
  - ✓ Introduce a Kernel Trick

$$\max \quad L_D = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \Phi(\mathbf{x}_i)^T \Phi(\mathbf{x}_j)$$

$$s.t. \quad \sum_{i=1}^{n} \alpha_i y_i = 0 \quad and \quad 0 \leq \alpha_i \leq C$$

$$\max \quad L_D = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$s.t. \quad \sum_{i=1}^{n} \alpha_i y_i = 0 \quad and \quad 0 \leq \alpha_i \leq C$$

Kernel Trick

- Generalized inner product

Given two points $\mathbf{x}$ and $\mathbf{x}' \in \mathcal{X}$, we need $\mathbf{z}^\intercal \mathbf{z}'$

Let $\mathbf{z}^\intercal \mathbf{z}' = K(\mathbf{x}, \mathbf{x}')$ (the kernel) "inner product" of $\mathbf{x}$ and $\mathbf{x}'$

Example: $\mathbf{x} = (x_1, x_2) \longrightarrow$ 2nd-order Φ

$$\mathbf{z} = \Phi(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)$$

$$K(\mathbf{x}, \mathbf{x}') = \mathbf{z}^\intercal \mathbf{z}' = 1 + x_1 x'_1 + x_2 x'_2 + x_1^2 x'^2_1 + x_2^2 x'^2_2 + x_1 x'_1 x_2 x'_2$$

Kernel Trick

- Kernel Trick

Can we compute $K(\mathbf{x}, \mathbf{x}')$ **without** transforming $\mathbf{x}$ and $\mathbf{x}'$?

Example: Consider $K(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^\intercal \mathbf{x}')^2 = (1 + x_1 x'_1 + x_2 x'_2)^2$

$$= 1 + x_1^2 x'^2_1 + x_2^2 x'^2_2 + 2x_1 x'_1 + 2x_2 x'_2 + 2x_1 x'_1 x_2 x'_2$$

This is an inner product!

$$(1 , x_1^2 , x_2^2 , \sqrt{2}\, x_1 , \sqrt{2}\, x_2 , \sqrt{2}\, x_1 x_2)$$

$$(1 , x'^2_1 , x'^2_2 , \sqrt{2} x'_1 , \sqrt{2} x'_2 , \sqrt{2} x'_1 x'_2)$$

Kernel Trick

- Polynomial Kernel

$\mathcal{X} = \mathbb{R}^d$ and $\Phi : \mathcal{X} \to \mathcal{Z}$ is polynomial of order Q

The "equivalent" kernel $K(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^\intercal \mathbf{x}')^Q$

$$= (1 + x_1 x'_1 + x_2 x'_2 + \cdots + x_d x'_d)^Q$$

Compare for $d = 10$ and $Q = 100$

Can adjust scale: $K(\mathbf{x}, \mathbf{x}') = (a\mathbf{x}^\intercal \mathbf{x}' + b)^Q$

Kernel Trick

- Gaussian (RBF) Kernel

If $K(\mathbf{x}, \mathbf{x}')$ is an inner product in some space $\mathcal{Z}$, we are good.

Example: $K(\mathbf{x}, \mathbf{x}') = \exp\left(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2\right)$

Infinite-dimensional $\mathcal{Z}$: take simple case

$$K(x, x') = \exp\left(-(x - x')^2\right)$$

$$= \exp\left(-x^2\right) \exp\left(-x'^2\right) \underbrace{\sum_{k=0}^{\infty} \frac{2^k (x)^k (x')^k}{k!}}_{\exp(2xx')}$$

Taylor expansion of exponential function

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \text{ for all } x$$

Kernel Trick

- Idea
  - ✓ Define K: $X \times X \rightarrow R$, called Kernel, such that

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

  - ✓ K is often interpreted as a similarity measure

- Benefits
  - ✓ Efficiency
    - K is often more efficient to compute than Φ and the dot product
  - ✓ Flexibility
    - K can be chosen arbitrarily so long as the existence of Φ is guaranteed (Mercer's condition)

Kernel Trick

- Conditions on Kernel functions

For any symmetric function K: $\mathrm{X} \times \mathrm{X} \rightarrow R$ which is square integrable (L_2-space) in $\mathrm{X} \times \mathrm{X}$ and which satisfies

$$\int_{\mathrm{X}\times\mathrm{X}} f(\mathbf{x}) K(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') dx dx' \geq 0 \text{ for all } f \in L_2(\mathrm{X})$$

there exist functions $\phi_i : \mathrm{X} \rightarrow R$ and numbers $\lambda_i \geq 0$ such that

$$K(\mathbf{x}, \mathbf{x}') = \sum_i \lambda_i \phi_i(\mathbf{x}) \phi_i(\mathbf{x}') \text{ for all } \mathbf{x}, \mathbf{x}' \in \mathrm{X}$$

- Interpretation
  - ✓ Double integral is the continuous version of a vector-matrix-vector multiplication

$$\sum_i \sum_j K(\mathbf{x}_i, \mathbf{x}_j) \alpha_i \alpha_j \geq 0$$

Kernel Trick

- Conditions on Kernel functions

$K(\mathbf{x}, \mathbf{x}')$ is a valid kernel iff

1. It is symmetric and **2.** The matrix:

$$\begin{bmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & K(\mathbf{x}_1, \mathbf{x}_2) & \dots & K(\mathbf{x}_1, \mathbf{x}_N) \\ K(\mathbf{x}_2, \mathbf{x}_1) & K(\mathbf{x}_2, \mathbf{x}_2) & \dots & K(\mathbf{x}_2, \mathbf{x}_N) \\ \dots & \dots & \dots & \dots \\ K(\mathbf{x}_N, \mathbf{x}_1) & K(\mathbf{x}_N, \mathbf{x}_2) & \dots & K(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}$$

is **positive semi-definite**

for any $\mathbf{x}_1, \cdots, \mathbf{x}_N$ (Mercer's condition)

Kernel Trick

- Type of Kernel Functions
  - ✓ Polynomial

$$K(x, y) = (x \cdot y + c)^d, \quad c > 0$$

  - ✓ Gaussian (RBF)

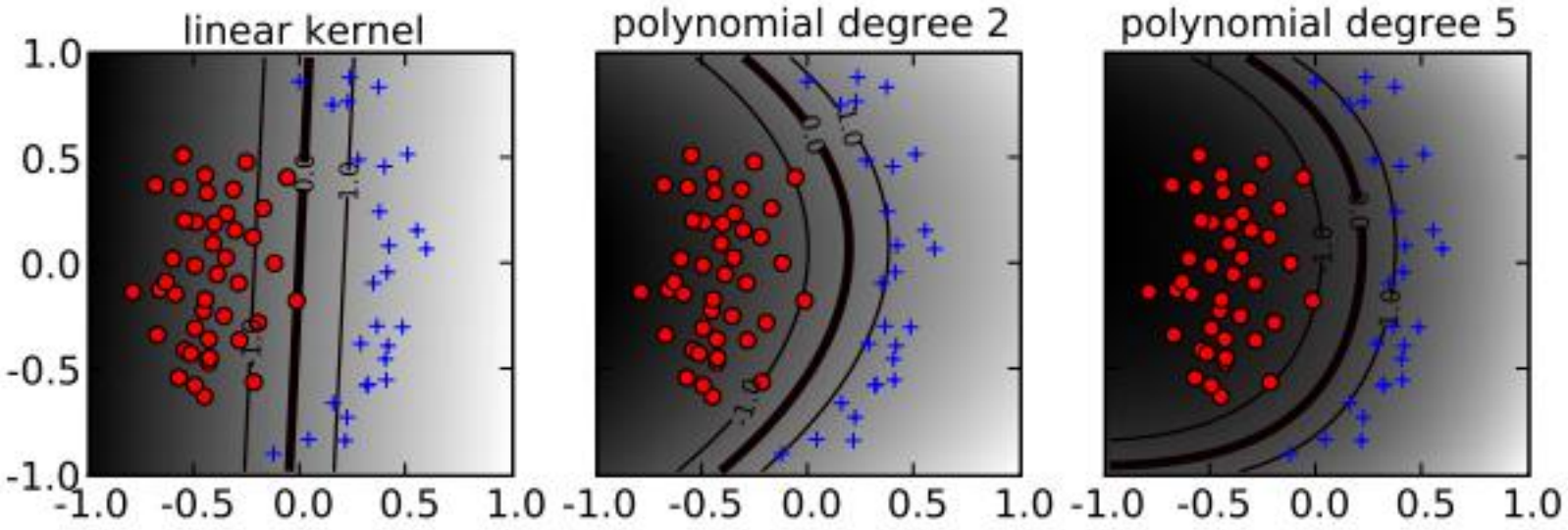
$$K(x, y) = \exp\Big(- \frac{||x - y||^2}{2\sigma^2} \Big), \quad \sigma \neq 0$$

  - ✓ Sigmoid

$$K(x, y) = \tanh(a(x \cdot y) + b), \quad a, b \geq 0$$

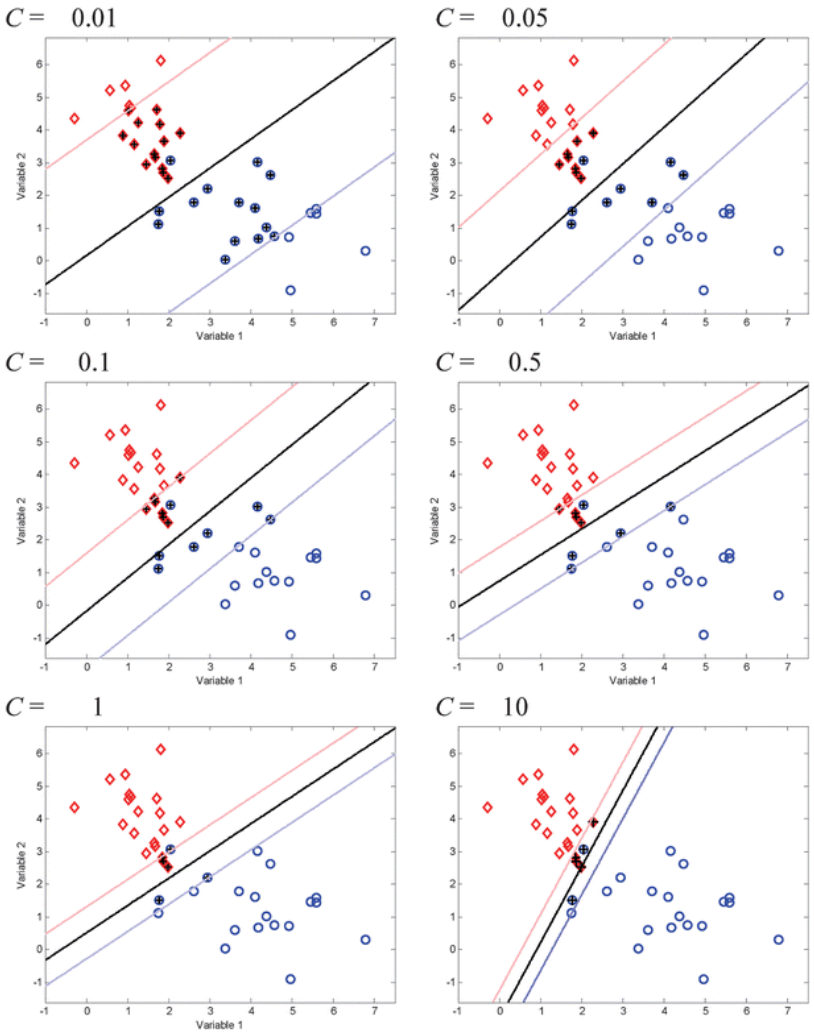
Effects of Different Kernels

- Decision boundary for different kernels
  - ✓ Linear kernel: only generate linear decision boundary
  - ✓ Non-linear kernel: can generate complex shape of decision boundary
  - ✓ Gaussian(RBF) kernel is commonly used



Effects of Different Costs

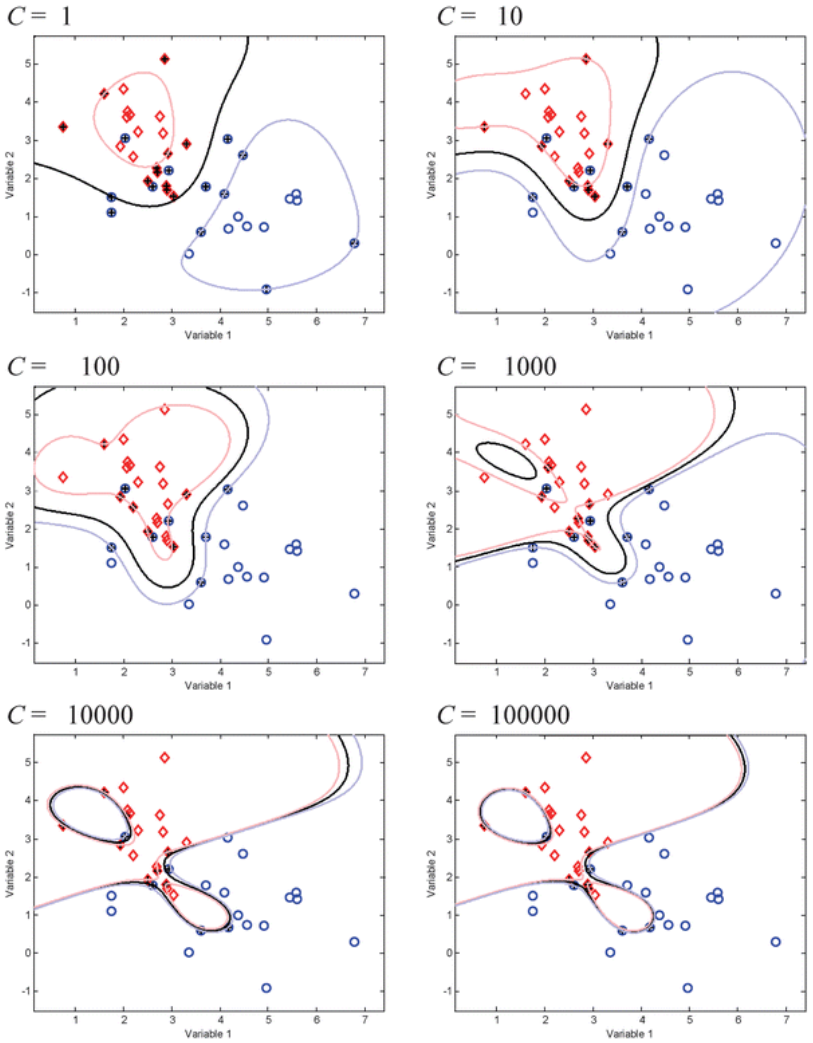
- Margins and SVs with different cost values (Linear kernel)



http://pubs.rsc.org/-/content/articlehtml/2010/an/b918972f

Effects of Different Costs

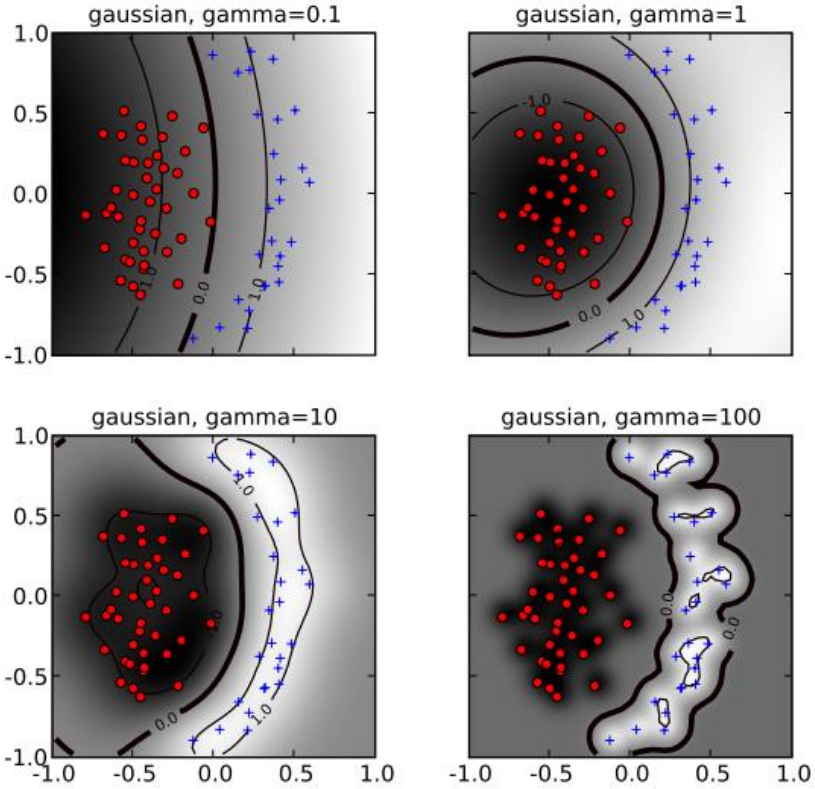
- Margins and SVs with different cost values (RBF kernel)

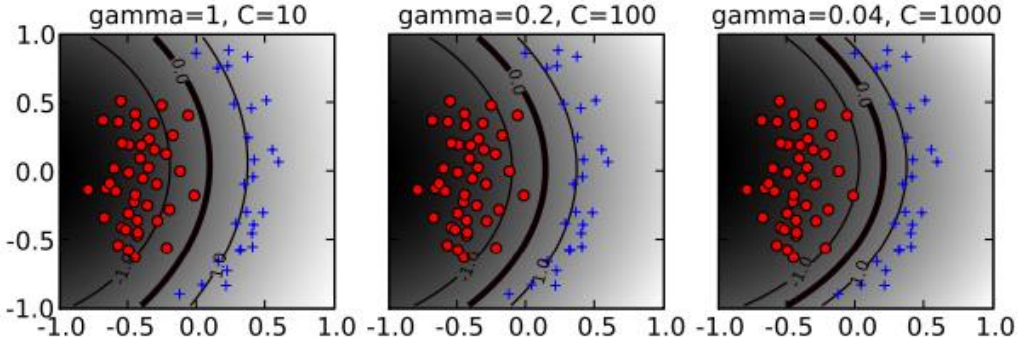


http://pubs.rsc.org/-/content/articlehtml/2010/an/b918972f

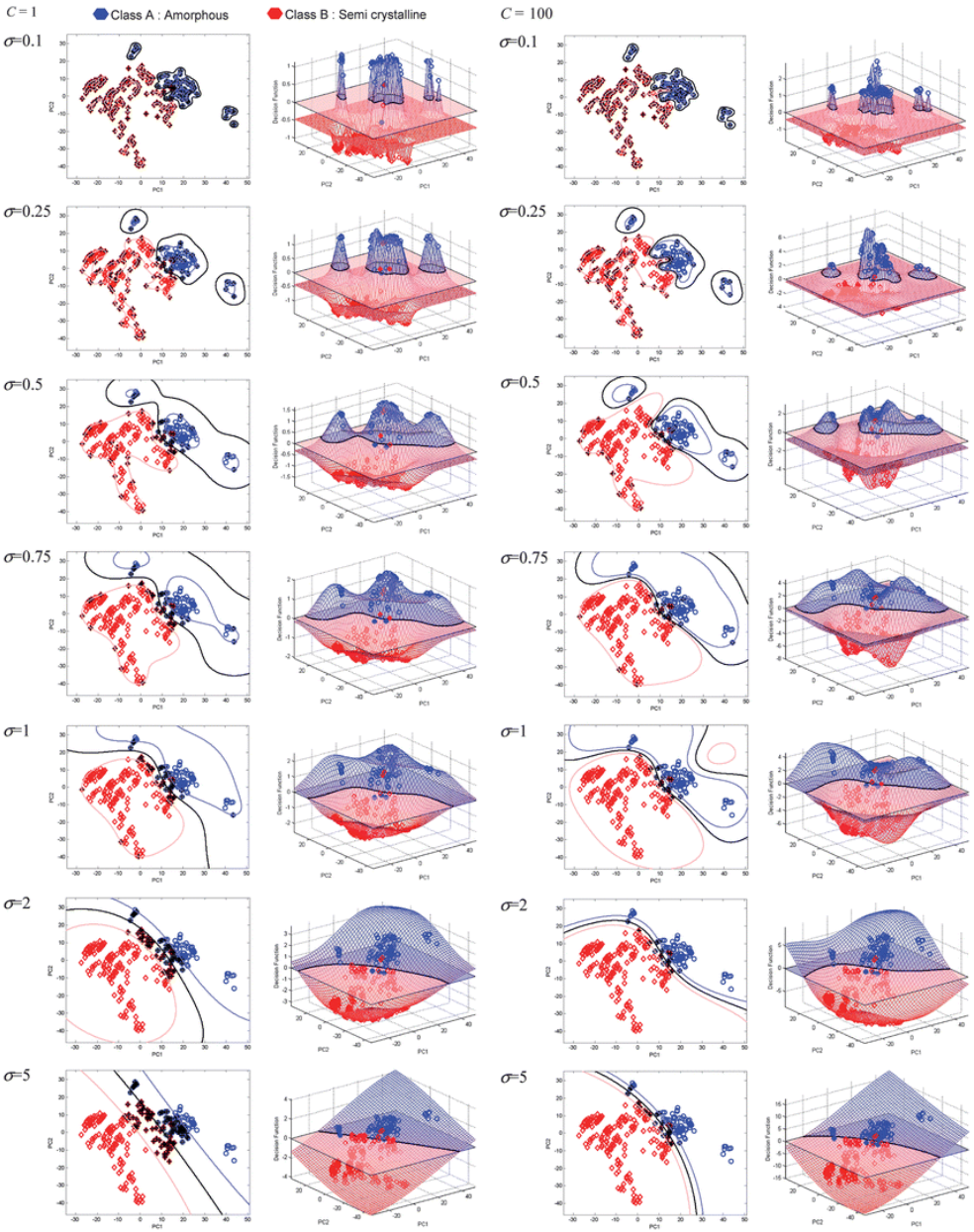
Effects of Different Kernels

- Kernel width (sigma) for RBF Kernel
  - ✓ The smaller the sigma, the more complicated decision boundary is generated
  - ✓ In many libraries, gamma (=1/sigma^2) is commonly used





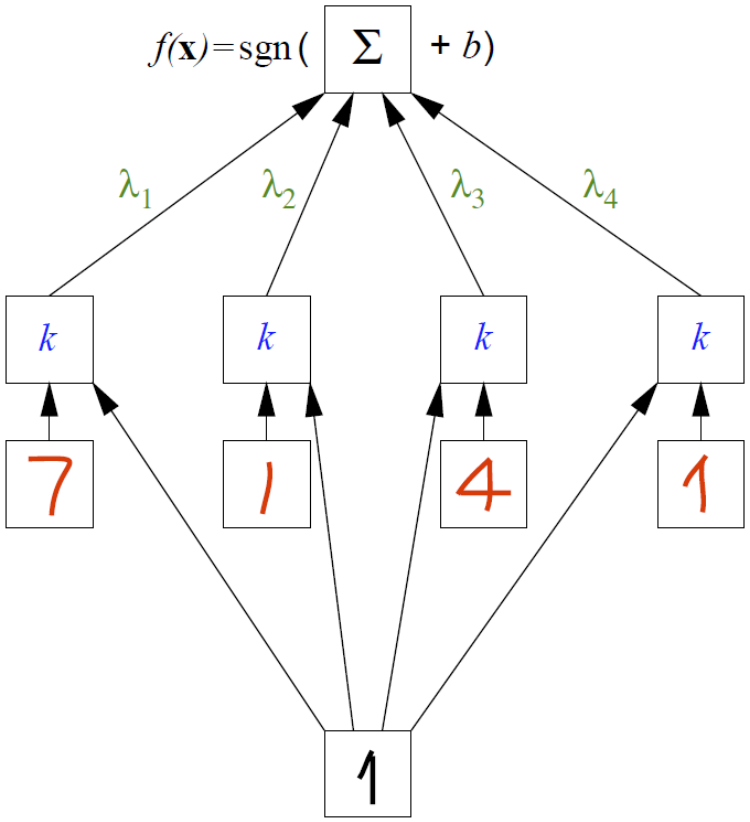
Effects of Kernels and Misclassification Cost



SVM Architecture

- Class decision for a new instance **x**

$$f(\mathbf{x}) = sign\left(\sum_{i=1}^{N} \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}) + b\right)$$



classification $f(\mathbf{x})=\text{sgn}\left(\sum \lambda_i k(\mathbf{x},\mathbf{x}_i) + b\right)$

weights

comparison: $k(\mathbf{x},\mathbf{x}_i)$, e.g. $k(\mathbf{x},\mathbf{x}_i)=(\mathbf{x}\cdot\mathbf{x}_i)^d$

$k(\mathbf{x},\mathbf{x}_i)=\exp(-\|\mathbf{x}-\mathbf{x}_i\|^2 / c)$

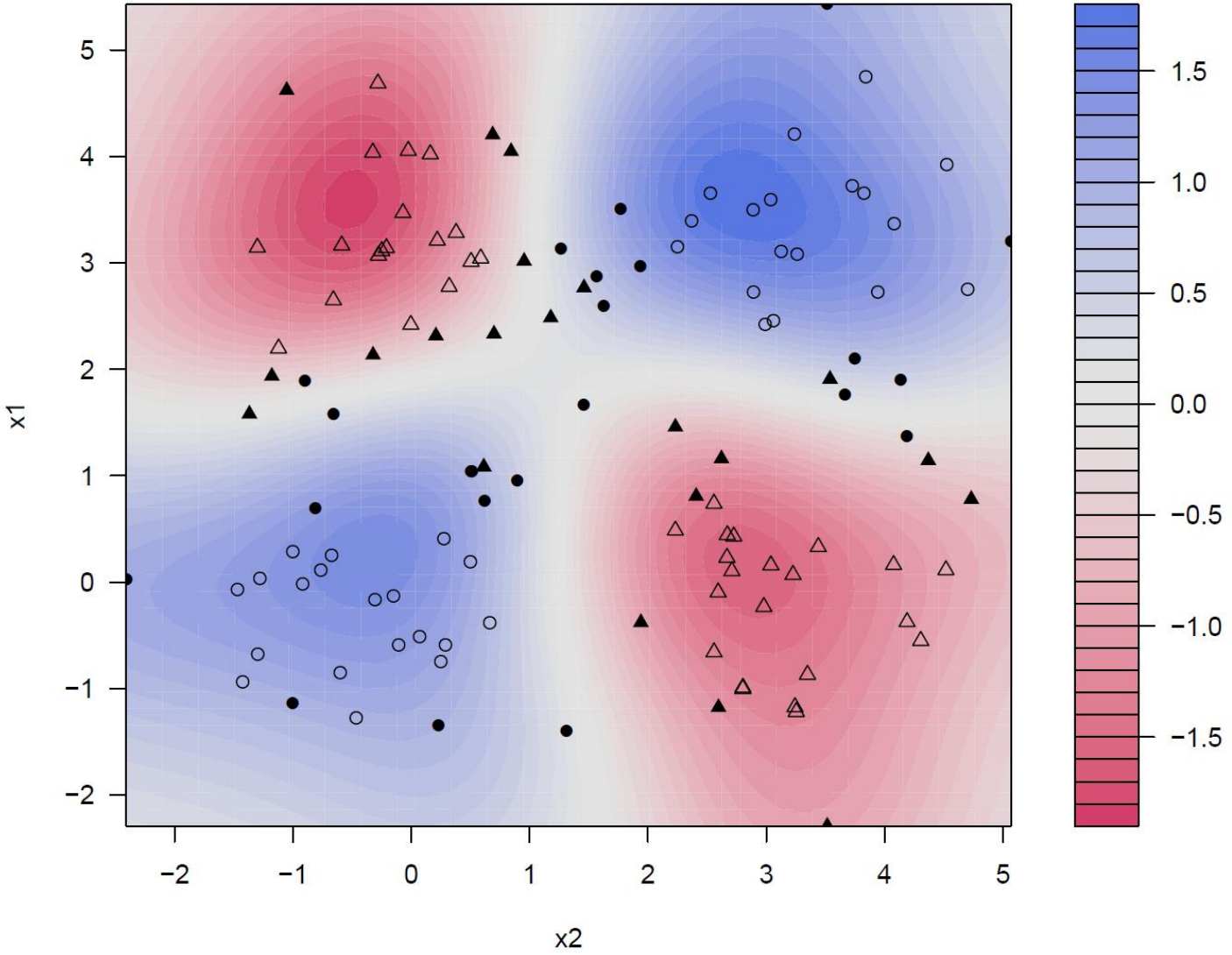
support vectors $\mathbf{x}_1 \ldots \mathbf{x}_4$

$k(\mathbf{x},\mathbf{x}_i)=\tanh(\kappa(\mathbf{x}\cdot\mathbf{x}_i)+\theta)$

input vector **x**

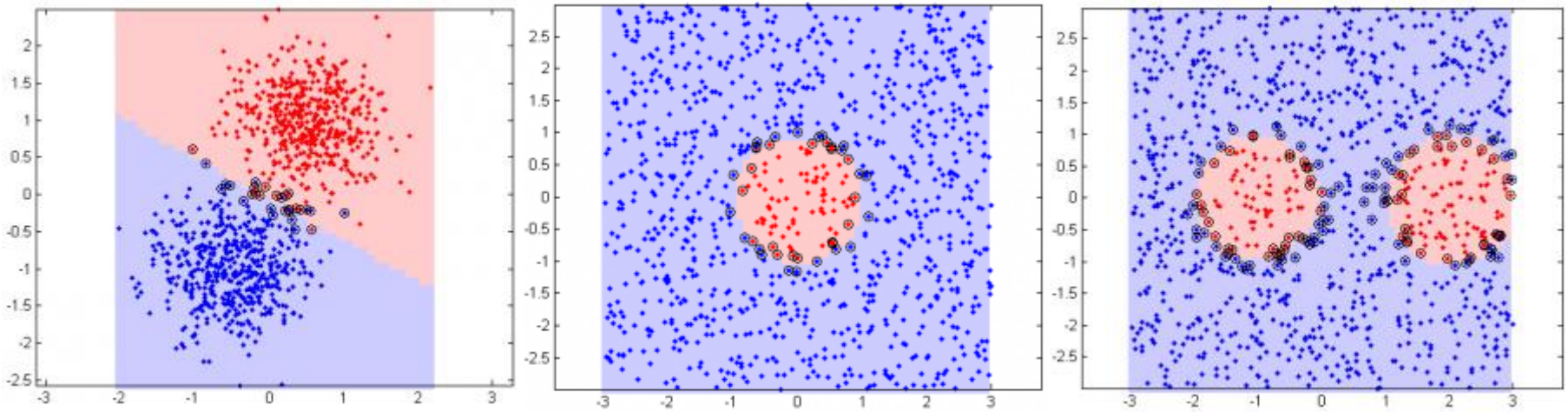
SVM Decision Boundary & Support Vectors

- XOR Problem



SVM Decision Boundary & Support Vectors

- Other examples

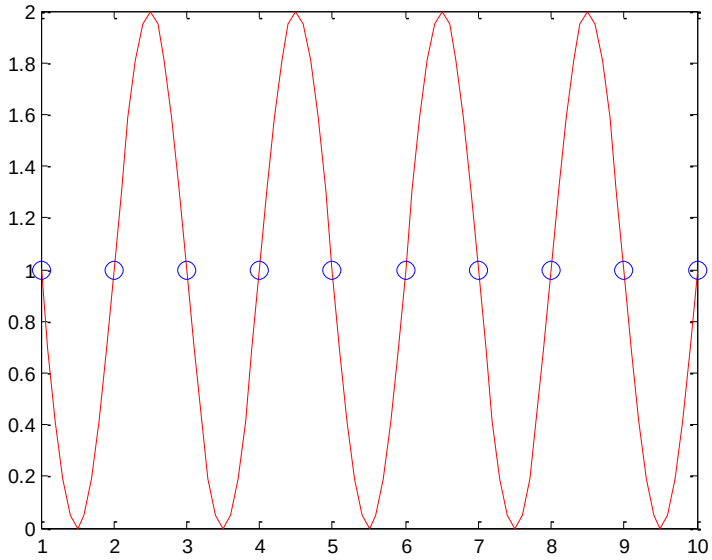


http://www.alivelearn.net/?p=912

AGENDA

Fitting Function

- Two objectives of function fitting
  - ✓ To fit a function, we minimize an error measure, called also loss function
  - ✓ We also like the function to be simple
    - Fewest basis functions
    - Simplest basis functions
    - Flatness is desirable

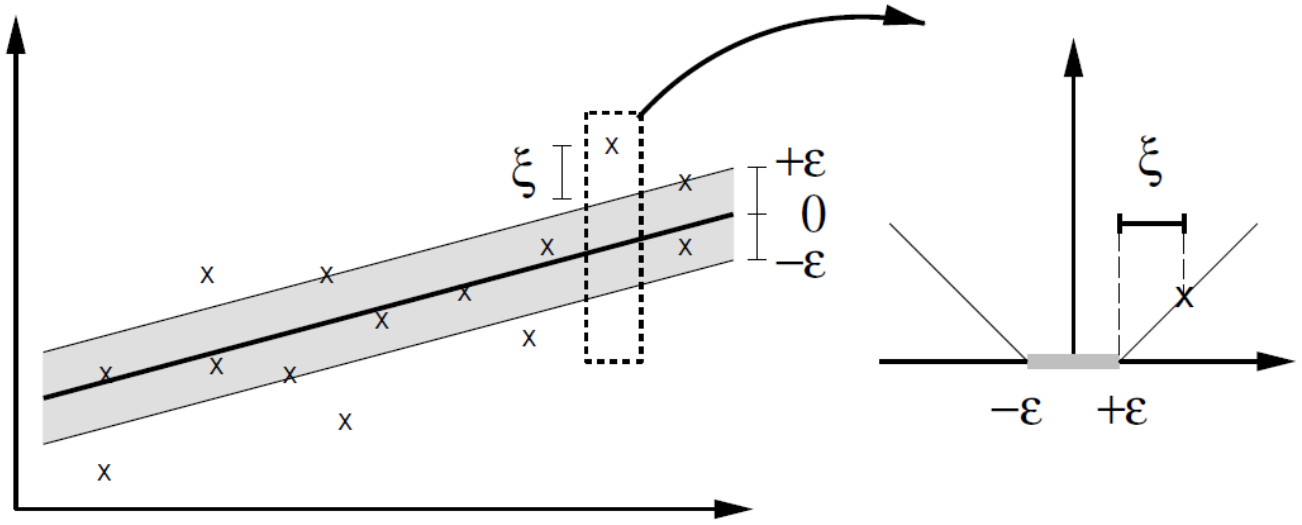


Why not draw a flat line rather than a sine function?

Support Vector Regression (SVR)

Smola and Scholkopf (2004)

- Combine loss function and flatness as a single objective
  - ✓ SVM was developed in the 1960s
  - ✓ Its extension to regression, i.e. SVR, is developed in 1997
- ε-SVR
  - ✓ Loss function



Support Vector Regression (SVR)

- SVR Formulation
  - ✓ Estimating a linear regression

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

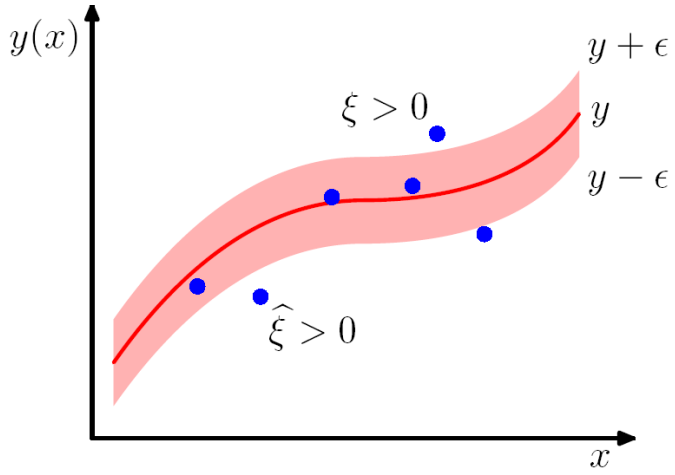
  - ✓ with precision ε by minimizing

$$\min \quad \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n}(\xi_i + \xi_i^*)$$

$$s.t. \quad (\mathbf{w}^T\mathbf{x}_i + b) - y_i \leq \epsilon + \xi_i$$

$$y_i - (\mathbf{w}^T\mathbf{x}_i + b) \leq \epsilon + \xi_i^*$$

$$\xi_i,\ \xi_i^* \geq 0$$



Support Vector Regression (SVR)

- Primal Lagrangian

$$L_P = \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{n}(\xi_i + \xi_i^*) - \sum_{i=1}^{n}(\eta_i\xi_i + \eta_i^*\xi_i^*)$$

$$-\sum_{i=1}^{n}\alpha_i(\epsilon + \xi_i + y_i - \mathbf{w}^T\mathbf{x}_i - b) - \sum_{i=1}^{n}\alpha_i^*(\epsilon + \xi_i^* - y_i + \mathbf{w}^T\mathbf{x}_i + b)$$

$$\alpha_i^{(*)}, \eta_i^{(*)} \geq 0$$

- Take the derivative w.r.t. b, w, ξ

$$\frac{\partial L}{\partial b} = \sum_{i=1}^{n}(\alpha_i - \alpha_i^*) = 0 \qquad \frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{n}(\alpha_i^* - \alpha_i)\mathbf{x}_i = 0$$

$$\frac{\partial L}{\partial \xi_i^{(*)}} = C - \alpha_i^{(*)} - \eta_i^{(*)}$$

Support Vector Regression (SVR)

- Dual Lagrangian Problem

$$L_D = -\frac{1}{2}\sum_{i,j=1}^{n}(\alpha_i^* - \alpha_i)(\alpha_j^* - \alpha_j)\mathbf{x}_i^T\mathbf{x}_j - \epsilon\sum_{i,j=1}^{n}(\alpha_i + \alpha_i^*) + \sum_{i,j=1}^{n} y_i(\alpha_i^* - \alpha_i)$$

$$s.t. \sum_{i=1}^{n}(\alpha_i - \alpha_i^*) = 0, \quad \alpha_i, \alpha_i^* \in [0, C]$$

- Decision Function

$$\mathbf{w} = \sum_{i=1}^{n}(\alpha_i^* - \alpha_i)\mathbf{x}_i \quad \Rightarrow \quad f(\mathbf{x}) = \sum_{i=1}^{n}(\alpha_i^* - \alpha_i)\mathbf{x}_i^T\mathbf{x} + b$$

Support Vector Regression (SVR)

- Dual Lagrangian Problem with Kernel Trick

$$L_D = -\frac{1}{2}\sum_{i,j=1}^{n}(\alpha_i^* - \alpha_i)(\alpha_j^* - \alpha_j)K(\mathbf{x}_i, \mathbf{x}_j) - \epsilon\sum_{i,j=1}^{n}(\alpha_i^* + \alpha_i) + \sum_{i,j=1}^{n} y_i(\alpha_i^* - \alpha_i)$$

$$s.t. \sum_{i=1}^{n}(\alpha_i - \alpha_i^*) = 0, \quad \alpha_i, \alpha_i^* \in [0, C]$$

- Decision Function

$$\mathbf{w} = \sum_{i=1}^{n}(\alpha_i^* - \alpha_i)\Phi(\mathbf{x}_i) \quad \Rightarrow \quad f(\mathbf{x}) = \sum_{i=1}^{n}(\alpha_i^* - \alpha_i)K(\mathbf{x}_i, \mathbf{x}) + b$$

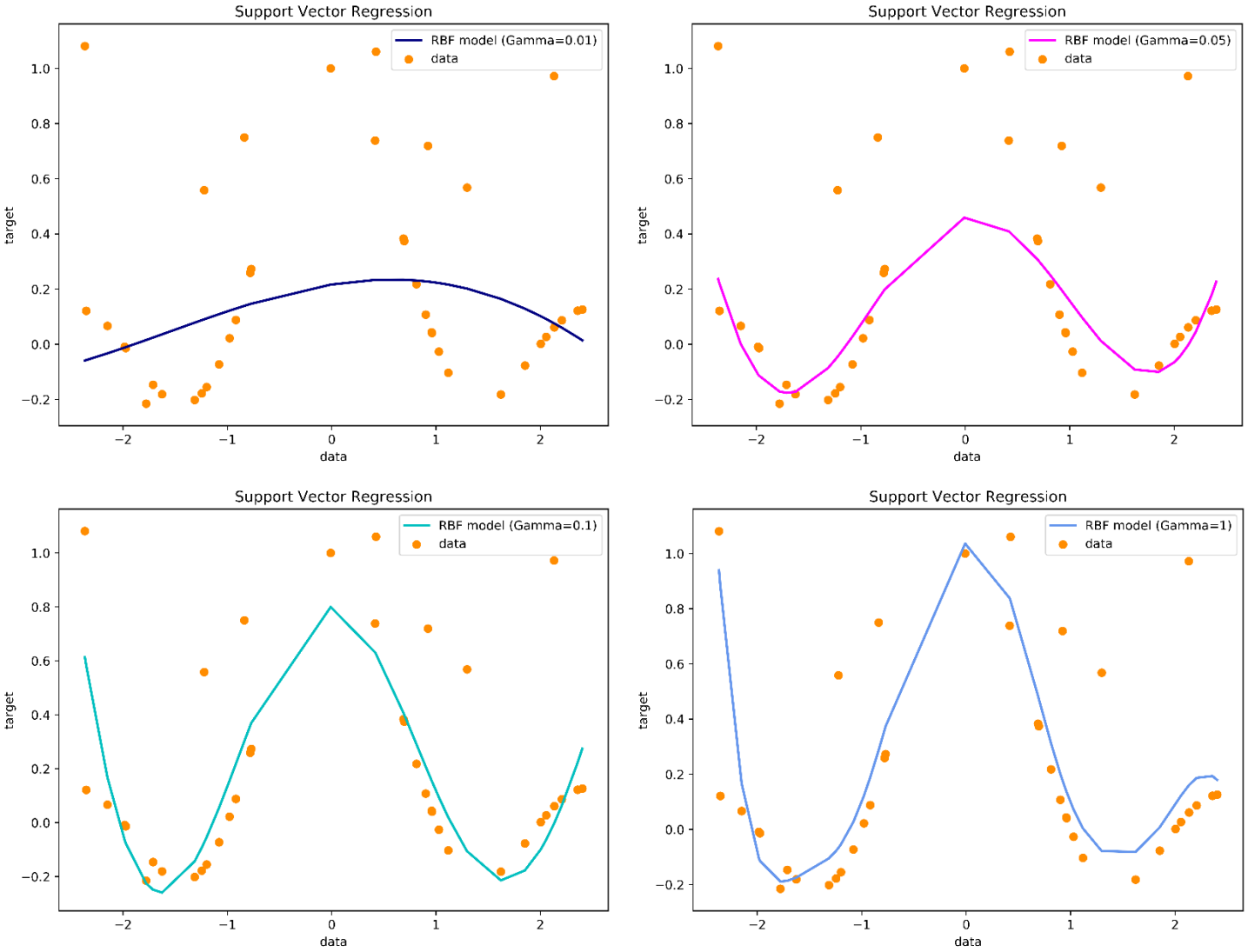
Support Vector Regression (SVR)

- Various Loss Functions for SVR

	loss function	density model
ε–insensitive	$c(\xi) = \lvert\xi\rvert_\varepsilon$	$p(\xi) = \frac{1}{2(1+\varepsilon)} \exp(-\lvert\xi\rvert_\varepsilon)$
Laplacian	$c(\xi) = \lvert\xi\rvert$	$p(\xi) = \frac{1}{2} \exp(-\lvert\xi\rvert)$
Gaussian	$c(\xi) = \frac{1}{2}\xi^2$	$p(\xi) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{\xi^2}{2})$
Huber's robust loss	$c(\xi) = \begin{cases} \frac{1}{2\sigma}(\xi)^2 & \text{if } \lvert\xi\rvert \le \sigma \\ \lvert\xi\rvert - \frac{\sigma}{2} & \text{otherwise} \end{cases}$	$p(\xi) \propto \begin{cases} \exp(-\frac{\xi^2}{2\sigma}) & \text{if } \lvert\xi\rvert \le \sigma \\ \exp(\frac{\sigma}{2} - \lvert\xi\rvert) & \text{otherwise} \end{cases}$
Polynomial	$c(\xi) = \frac{1}{p}\lvert\xi\rvert^p$	$p(\xi) = \frac{p}{2\Gamma(1/p)} \exp(-\lvert\xi\rvert^p)$
Piecewise polynomial	$c(\xi) = \begin{cases} \frac{1}{p\sigma^{p-1}}(\xi)^p & \text{if } \lvert\xi\rvert \le \sigma \\ \lvert\xi\rvert - \sigma\frac{p-1}{p} & \text{otherwise} \end{cases}$	$p(\xi) \propto \begin{cases} \exp(-\frac{\xi^p}{p\sigma^{p-1}}) & \text{if } \lvert\xi\rvert \le \sigma \\ \exp(\sigma\frac{p-1}{p} - \lvert\xi\rvert) & \text{otherwise} \end{cases}$

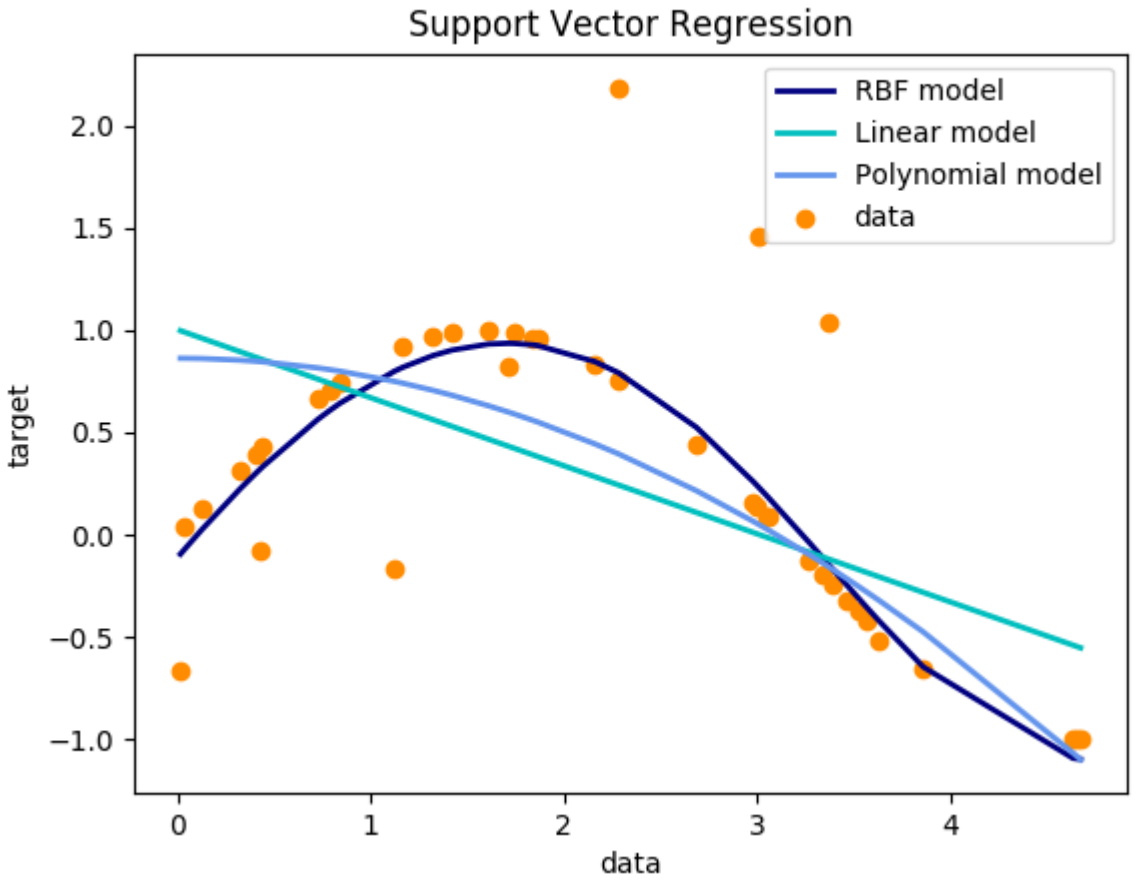
Support Vector Regression (SVR)

- Fitted functions with different ε



Support Vector Regression (SVR)

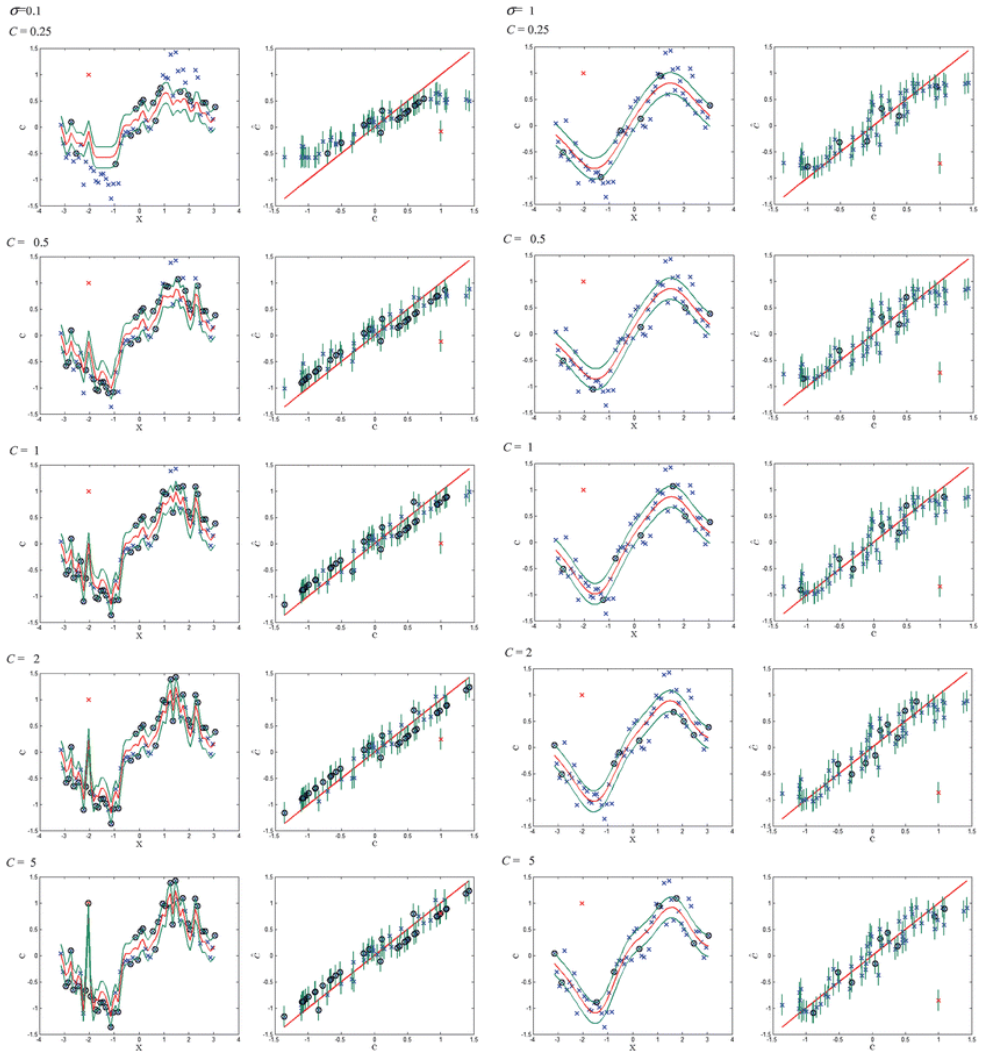
- Fitted function with different Kernel functions



http://scikit-learn.org/stable/auto_examples/svm/plot_svm_regression.html#sphx-glr-auto-examples-svm-plot-svm-regression-py

Support Vector Regression (SVR)

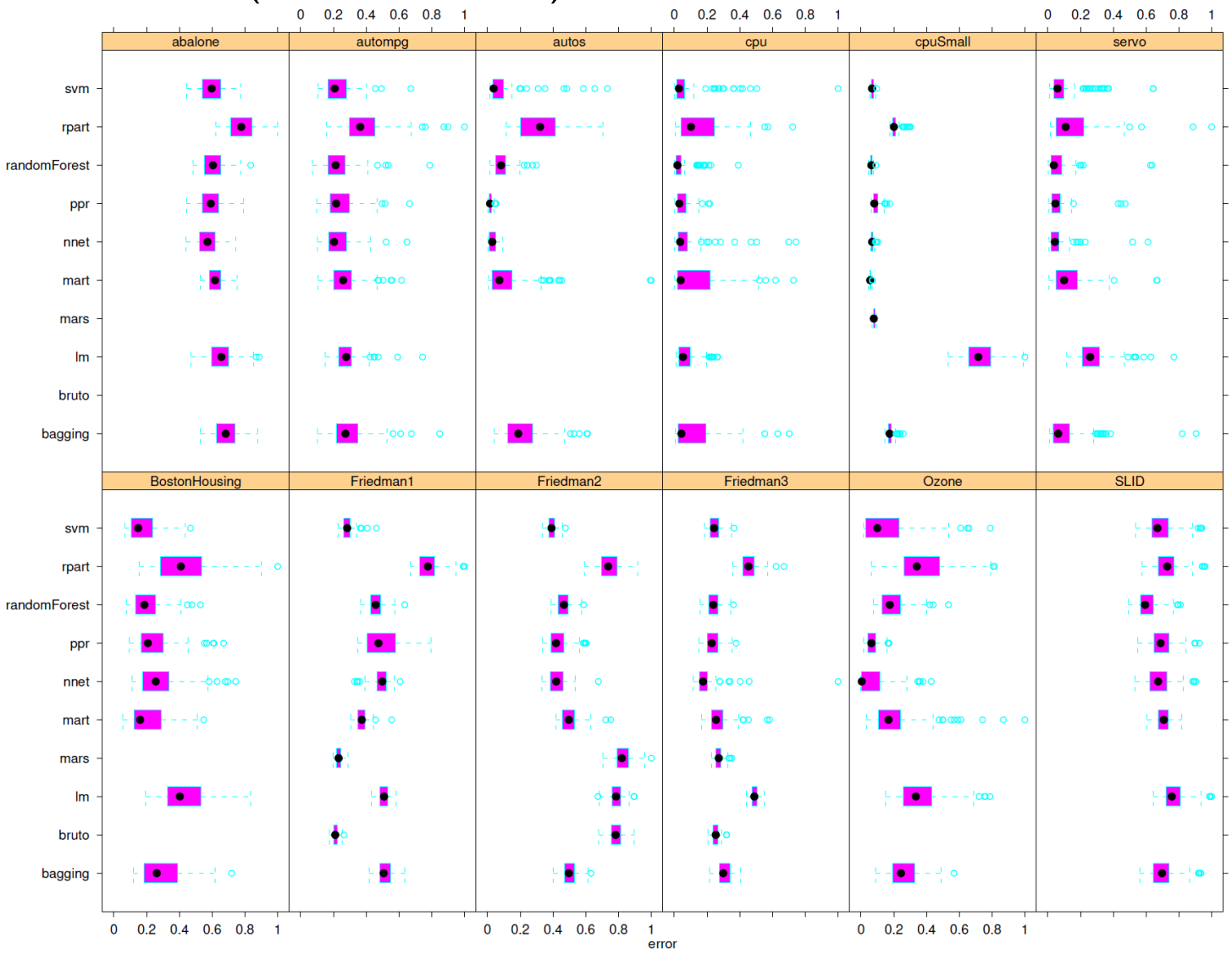
- SVR with different sigma and cost combinations



http://pubs.rsc.org/-/content/articlehtml/2010/an/b918972f

Support Vector Regression (SVR)

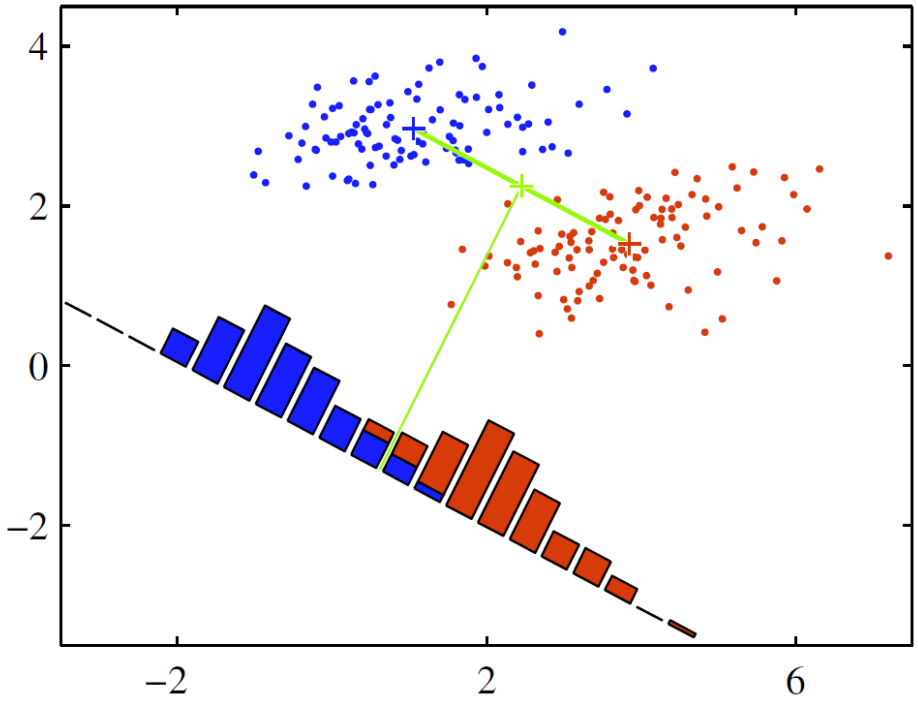
- SVR Performance (in terms of MSE)

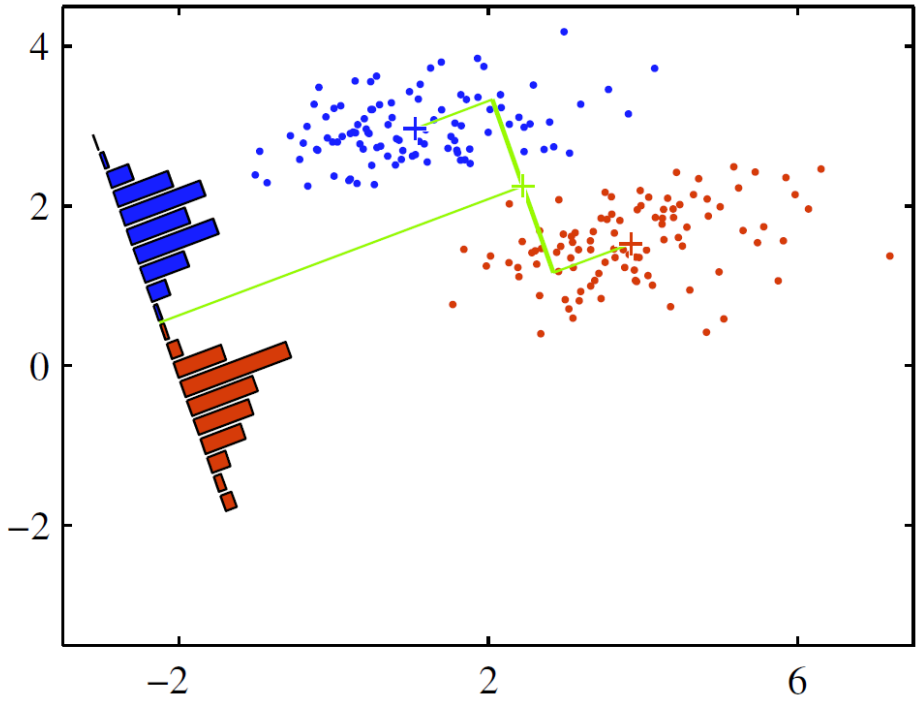


AGENDA

Linear Discriminant Analysis

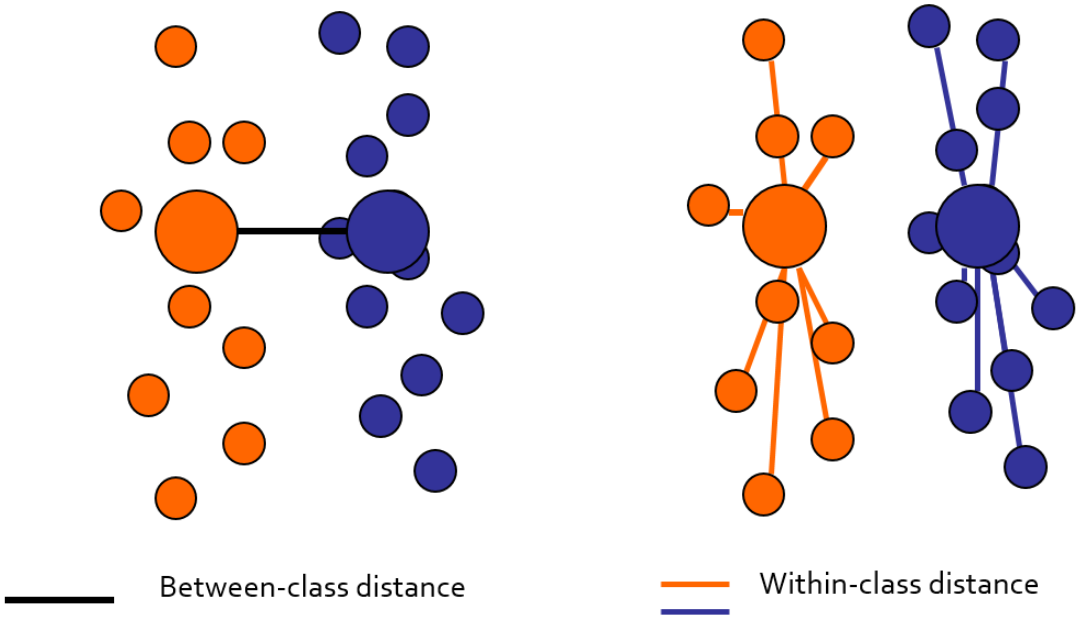
- LDA
  - ✓ Find a line to which two classes are well separated after projection





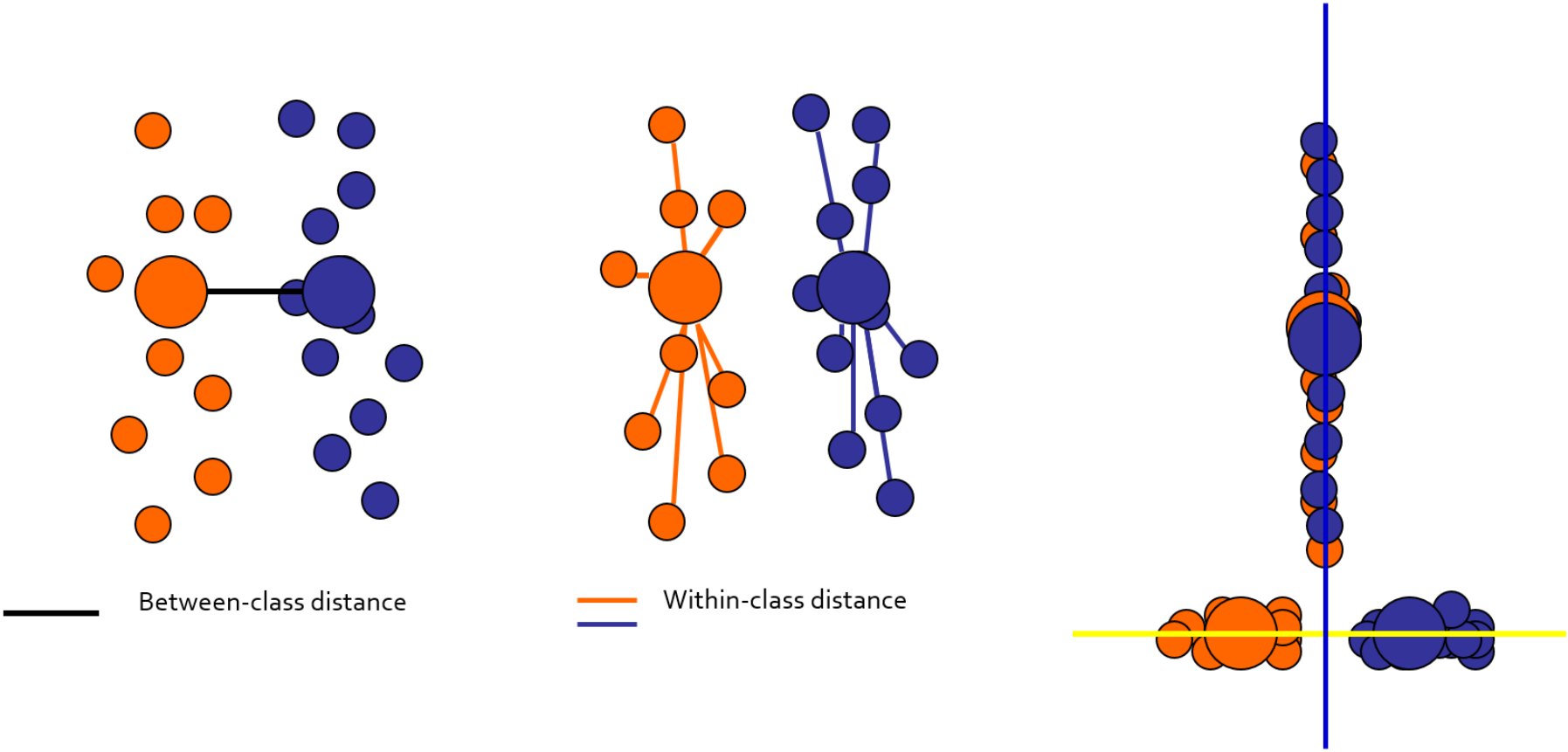
Linear Discriminant Analysis

- Two type of class distances
  - ✓ Between-class distance
    - Distance between the centroids of different classes
  - ✓ Within-class distance
    - Accumulated distance of an instance to the centroid of its class



Linear Discriminant Analysis

- (Fisher's) Linear Discriminant Analysis
  - ✓ Find most discriminant projection by maximizing between-class distance (variance) and minimizing within-class distance (variance)



Linear Discriminant Analysis

- Fisher's LDA (cont')
  - ✓ Take the D-dimensional input vector x and project it down to one dim.

$$y = \mathbf{w}^T \mathbf{x}$$

  - ✓ Consider a two-class problem in which there are N_1 & N_2 observations in C_1 and C_2, respectively.

$$\mathbf{m}_1 = \frac{1}{N_1} \sum_{n \in C_1} \mathbf{x}_n, \quad \mathbf{m}_2 = \frac{1}{N_2} \sum_{n \in C_2} \mathbf{x}_n$$

  - ✓ Objective 1: Choose w to maximize the separation of the projected class means (between class variance)

$$m_2 - m_1 = \mathbf{w}^T (\mathbf{m}_2 - \mathbf{m}_1), \quad m_k = \mathbf{w}^T \mathbf{m}_k$$

Linear Discriminant Analysis

- Fisher's LDA (cont')
  - ✓ Objective 2: Choose w to minimize the variance in each class after projection (within class variance)

$$s_k^2 = \sum_{n \in C_k} (y_n - m_k)^2$$

  - ✓ Fisher's criterion
    - The ratio of the between-class variance to the within-class variance

$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2} = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

$$\mathbf{S}_B = (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^T$$

$$\mathbf{S}_W = \sum_{n \in C_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^T + \sum_{n \in C_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^T$$

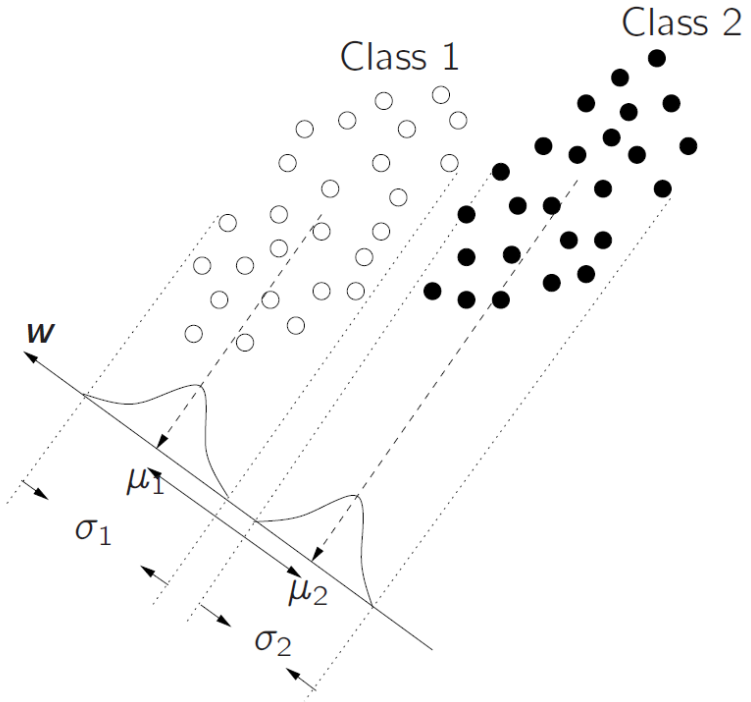
Linear Discriminant Analysis

- Fisher's LDA (cont')
  - ✓ Find w
    - Differentiating the Fisher's criterion w.r.t. w, then $J(\mathrm{w})$ is maximized when

$$(\mathbf{w}^T\mathbf{S}_B\mathbf{w})\mathbf{S}_W\mathbf{w} = (\mathbf{w}^T\mathbf{S}_W\mathbf{w})\mathbf{S}_B\mathbf{w}$$

    - $S_B w$ is always in the direction of $(m_2\text{-}m_1)$
    - Can drop the scalar factor $(w^T S_B w)$ and $(w^T S_W w)$
    - Then, obtain *Fisher's linear discriminant*

$$\mathbf{w} \propto \mathbf{S}_W^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$



Kernel Fisher Discriminant (KFD)

Mika (2002)

- Extend the LDA formulation by introducing kernels
  - ✓ KFD formulation
    - The full covariance of a dataset **Z** in the feature space by

$$\mathbf{C}^{\Phi} = \frac{1}{N}\sum_{n=1}^{N}(\Phi(\mathbf{x}_n) - \mathbf{m}^{\Phi})(\Phi(\mathbf{x}_n) - \mathbf{m}^{\Phi})^T, \quad \mathbf{m}^{\Phi} = \frac{1}{N}\sum_{n=1}^{N}\Phi(\mathbf{x}_n)$$

    - The within-class variance and the between-class variance in the feature space are given by

$$\mathbf{S}_W^{\Phi} = \sum_{i=1,2}\sum_{n=1}^{N_i}(\Phi(\mathbf{x}_n^i) - \mathbf{m}_i^{\Phi})(\Phi(\mathbf{x}_n^i) - \mathbf{m}_i^{\Phi})^T$$

$$\mathbf{S}_B = (\mathbf{m}_2^{\Phi} - \mathbf{m}_1^{\Phi})(\mathbf{m}_2^{\Phi} - \mathbf{m}_1^{\Phi})^T \qquad \mathbf{m}_i^{\Phi} = \frac{1}{N_i}\sum_{j=1}^{N_i}\Phi(\mathbf{x}_j^i)$$

Kernel Fisher Discriminant (KFD)

Mika (2002)

- Extend the LDA formulation by introducing kernels
  - ✓ Objective functions

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B^{\Phi} \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W^{\Phi} \mathbf{w}}$$

  - ✓ Projected vector

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n \Phi(\mathbf{x}_n), \quad \alpha_n \in R$$

  - ✓ Projected mean

$$\mathbf{w}^T \mathbf{m}_i^{\Phi} = \frac{1}{N_i} \sum_{n=1}^{N} \sum_{k=1}^{N_i} \alpha_n (\Phi(\mathbf{x}_n) \cdot \Phi(\mathbf{x}_k^i)) = \frac{1}{N_i} \sum_{n=1}^{N} \sum_{k=1}^{N_i} \alpha_n \mathbf{K}(\mathbf{x}_n, \mathbf{x}_k^i) = \boldsymbol{\alpha}^T \boldsymbol{\mu}_i$$

$$(\boldsymbol{\mu}_i)_n = \frac{1}{N_i} \sum_{k=1}^{N_i} \mathbf{K}(\mathbf{x}_n, \mathbf{x}_k^i)$$

Kernel Fisher Discriminant (KFD)

Mika (2002)

- Extend the LDA formulation by introducing kernels
  - ✓ Objective function (Numerator)

$$\mathbf{w}^T \mathbf{S}_B^\Phi \mathbf{w} = \mathbf{w}^T (\mathbf{m}_2^\Phi - \mathbf{m}_1^\Phi)(\mathbf{m}_2^\Phi - \mathbf{m}_1^\Phi)^T \mathbf{w}$$

$$= \boldsymbol{\alpha}^T (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^T \boldsymbol{\alpha}$$

$$= \boldsymbol{\alpha}^T \mathbf{M} \boldsymbol{\alpha}, \quad \text{where} \quad \mathbf{M} = (\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)^T$$

Kernel Fisher Discriminant (KFD)

Mika (2002)

- Extend the LDA formulation by introducing kernels
  - ✓ Objective function (Denominator)

$$\mathbf{w}^T \mathbf{S}_W^\Phi \mathbf{w} = \left(\sum_{i=1}^{N} \alpha_i \Phi(\mathbf{x}_i) \right) \left(\sum_{j=1,2} \sum_{n=1}^{N_i} (\Phi(\mathbf{x}_n^j) - \mathbf{m}_j^\Phi)(\Phi(\mathbf{x}_n^j) - \mathbf{m}_j^\Phi)^T \right) \sum_{k=1}^{N} \alpha_k \Phi(\mathbf{x}_k)$$

$$= \sum_{j=1,2} \sum_{i=1}^{N} \sum_{n=1}^{N_j} \sum_{k=1}^{N} \left(\alpha_i \Phi(\mathbf{x}_i) \left(\Phi(\mathbf{x}_n^j) - \mathbf{m}_j^\Phi \right) \left(\Phi(\mathbf{x}_n^j) - \mathbf{m}_j^\Phi \right)^T \alpha_k \Phi(\mathbf{x}_k) \right)$$

$$= \sum_{j=1,2} \sum_{i=1}^{N} \sum_{n=1}^{N_j} \sum_{k=1}^{N} \left(\alpha_i \mathbf{K}(\mathbf{x}_i, \mathbf{x}_n^j) - \frac{1}{N_j} \sum_{p=1}^{N_j} \alpha_i \mathbf{K}(\mathbf{x}_i, \mathbf{x}_p^j) \right) \times$$

$$\left(\alpha_k \mathbf{K}(\mathbf{x}_k, \mathbf{x}_n^j) - \frac{1}{N_j} \sum_{q=1}^{N_j} \alpha_k \mathbf{K}(\mathbf{x}_k, \mathbf{x}_q^j) \right)$$

Kernel Fisher Discriminant (KFD)

Mika (2002)

- Extend the LDA formulation by introducing kernels
  - ✓ Objective function (Denominator)

$$\sum_{j=1,2}\sum_{i=1}^{N}\sum_{n=1}^{N_j}\sum_{k=1}^{N}\left(\alpha_i\mathbf{K}(\mathbf{x}_i,\mathbf{x}_n^j)-\frac{1}{N_j}\sum_{p=1}^{N_j}\alpha_i\mathbf{K}(\mathbf{x}_i,\mathbf{x}_p^j)\right)\left(\alpha_k\mathbf{K}(\mathbf{x}_k,\mathbf{x}_n^j)-\frac{1}{N_j}\sum_{q=1}^{N_j}\alpha_k\mathbf{K}(\mathbf{x}_k,\mathbf{x}_q^j)\right)$$

$$=\sum_{j=1,2}\left(\sum_{i=1}^{N}\sum_{n=1}^{N_j}\sum_{k=1}^{N}\left(\alpha_i\alpha_k\mathbf{K}(\mathbf{x}_i,\mathbf{x}_n^j)\mathbf{K}(\mathbf{x}_k,\mathbf{x}_n^j)-\frac{2\alpha_i\alpha_k}{N_j}\sum_{p=1}^{N_j}\mathbf{K}(\mathbf{x}_i,\mathbf{x}_n^j)\mathbf{K}(\mathbf{x}_k,\mathbf{x}_p^j)\right.\right.$$

$$\left.\left.+\frac{\alpha_i\alpha_k}{N_j^2}\sum_{p=1}^{N_j}\sum_{q=1}^{N_j}\mathbf{K}(\mathbf{x}_i,\mathbf{x}_p^j)\mathbf{K}(\mathbf{x}_k,\mathbf{x}_q^j)\right)\right)$$

$$=\sum_{j=1,2}\left(\sum_{i=1}^{N}\sum_{n=1}^{N_j}\sum_{k=1}^{N}\left(\alpha_i\alpha_k\mathbf{K}(\mathbf{x}_i,\mathbf{x}_n^j)\mathbf{K}(\mathbf{x}_k,\mathbf{x}_n^j)-\frac{\alpha_i\alpha_k}{N_j}\sum_{p=1}^{N_j}\mathbf{K}(\mathbf{x}_i,\mathbf{x}_n^j)\mathbf{K}(\mathbf{x}_k,\mathbf{x}_p^j)\right)\right)$$

Kernel Fisher Discriminant (KFD)

Mika (2002)

- Extend the LDA formulation by introducing kernels
  - ✓ Objective function (Denominator)

$$\sum_{j=1,2}\left(\sum_{i=1}^{N}\sum_{n=1}^{N_j}\sum_{k=1}^{N}\left(\alpha_i\alpha_k\mathbf{K}(\mathbf{x}_i,\mathbf{x}_n^j)\mathbf{K}(\mathbf{x}_k,\mathbf{x}_n^j)-\frac{\alpha_i\alpha_k}{N_j}\sum_{p=1}^{N_j}\mathbf{K}(\mathbf{x}_i,\mathbf{x}_n^j)\mathbf{K}(\mathbf{x}_k,\mathbf{x}_p^j)\right)\right)$$

$$=\sum_{j=1,2}\boldsymbol{\alpha}^T\mathbf{K}_j\mathbf{K}_j^T\boldsymbol{\alpha}-\boldsymbol{\alpha}^T\mathbf{K}_j\mathbf{1}_{N_j}\mathbf{K}_j^T\boldsymbol{\alpha}$$

$$=\boldsymbol{\alpha}^T\mathbf{N}\boldsymbol{\alpha},\quad\text{where}\quad\mathbf{N}=\sum_{j=1,2}\mathbf{K}_j(\mathbf{I}-\mathbf{1}_{N_j})\mathbf{K}_j^T$$

  - ✓ $\mathbf{1}_{N_j}$: Gram matrix with the size of N_j by N_j with all elements equal to $1/N_j$

Kernel Fisher Discriminant (KFD)

Mika (2002)

- Extend the LDA formulation by introducing kernels
  - ✓ Objective function

$$J(\boldsymbol{\alpha}) = \frac{\boldsymbol{\alpha}^T \mathbf{M} \boldsymbol{\alpha}}{\boldsymbol{\alpha}^T \mathbf{N} \boldsymbol{\alpha}}$$

  - ✓ Take the first derivative and set it equal to 0

$$\left(\boldsymbol{\alpha}^T \mathbf{M} \boldsymbol{\alpha}\right) \mathbf{N} \boldsymbol{\alpha} = \left(\boldsymbol{\alpha}^T \mathbf{N} \boldsymbol{\alpha}\right) \mathbf{M} \boldsymbol{\alpha}$$

  - ✓ Since $\mathbf{M}\boldsymbol{\alpha} = (\mathbf{M}_2 - \mathbf{M}_1)(\mathbf{M}_2 - \mathbf{M}_1)^T \boldsymbol{\alpha} = \lambda(\mathbf{M}_2 - \mathbf{M}_1)$,

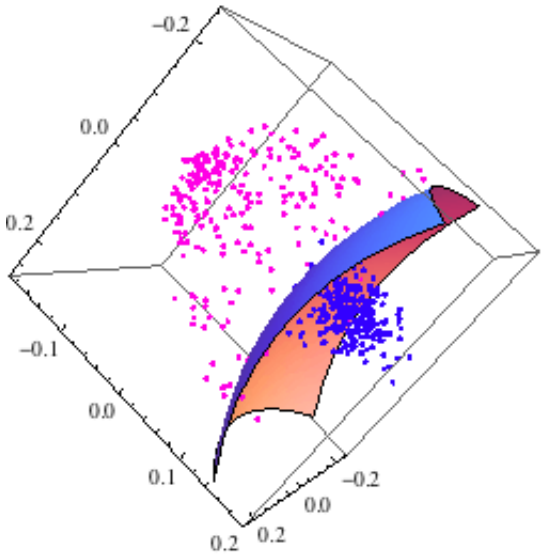
$$\boldsymbol{\alpha} = \mathbf{N}^{-1}(\mathbf{M}_2 - \mathbf{M}_1)$$

  - ✓ Given the solution for α, the projection of a new data point is given by

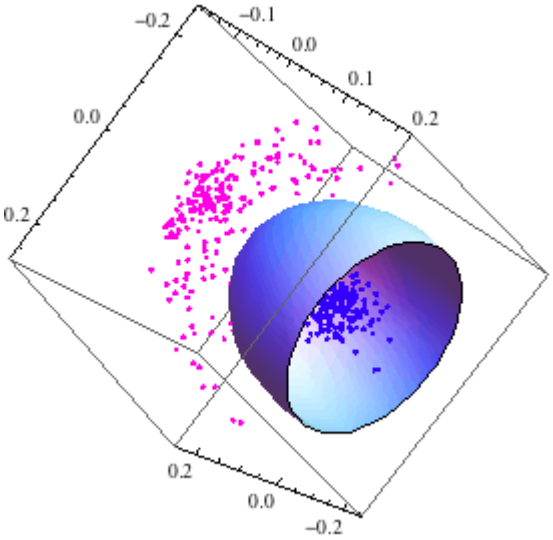
$$y(\mathbf{x}) = \left(\mathbf{w} \cdot \Phi(\mathbf{x})\right) = \sum_{n=1}^{N} \alpha_n \mathbf{K}(\mathbf{x}_n, \mathbf{x})$$

KFD Example

- KFD with a polynomial kernel



- KFD with a RBF (Gaussian) kernel



http://www.mathematica-journal.com/2011/07/fisher-discrimination-with-kernels/

KFD Performance

- Classification Performance
  - ✓ Benchmark data sets

	dimensionality	Size of training set	test set
Banana	2	400	4900
B.Cancer	9	200	77
Diabetes	8	468	300
German	20	700	300
Heart	13	170	100
Ringnorm	20	400	7000
F.Sonar	9	666	400
Thyroid	5	140	75
Titanic	3	150	2051
Waveform	21	400	4600

KFD Performance

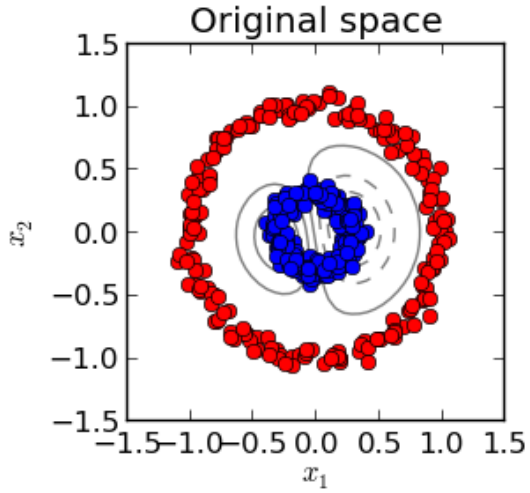
- Classification Performance
  - ✓ Classification accuracy

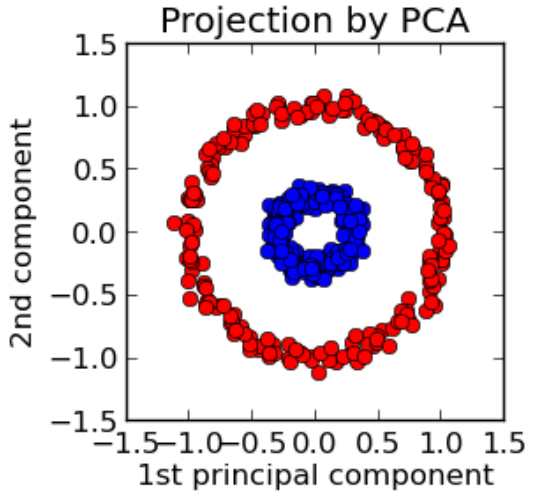
	RBF	AB	AB_R	SVM	KFD
Banana	**10.8±0.06**	12.3±0.07	*10.9±0.04*	11.5±0.07	**10.8±0.05**
B.Cancer	27.6±0.47	30.4±0.47	26.5±0.45	*26.0±0.47*	**25.8±0.46**
Diabetes	24.3±0.19	26.5±0.23	23.8±0.18	*23.5±0.17*	**23.2±0.16**
German	24.7±0.24	27.5±0.25	24.3±0.21	**23.6±0.21**	*23.7±0.22*
Heart	17.6±0.33	20.3±0.34	16.5±0.35	**16.0±0.33**	*16.1±0.34*
Ringnorm	1.7±0.02	1.9±0.03	*1.6±0.01*	1.7±0.01	**1.5±0.01**
F.Sonar	34.4±0.20	35.7±0.18	34.2±0.22	**32.4±0.18**	*33.2±0.17*
Thyroid	4.5±0.21	*4.4±0.22*	4.6±0.22	4.8±0.22	**4.2±0.21**
Titanic	23.3±0.13	*22.6±0.12*	*22.6±0.12*	**22.4±0.10**	23.2±0.20
Waveform	10.7±0.11	10.8±0.06	**9.8±0.08**	*9.9±0.04*	*9.9±0.04*
Average	18.0%	20.2%	17.5%	17.2%	17.2%

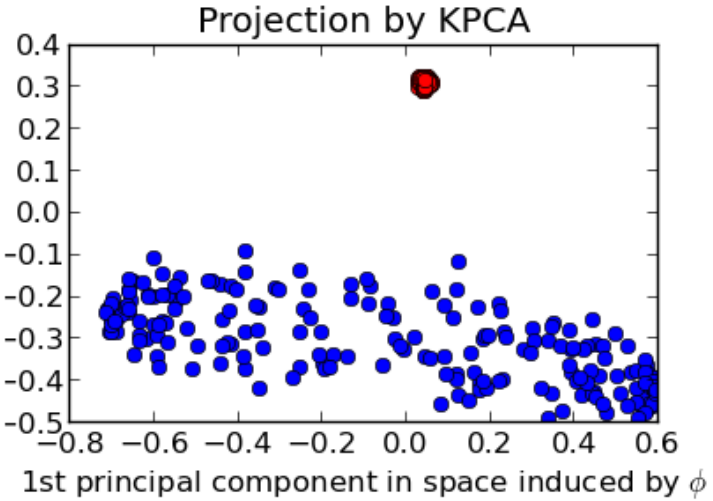
AGENDA

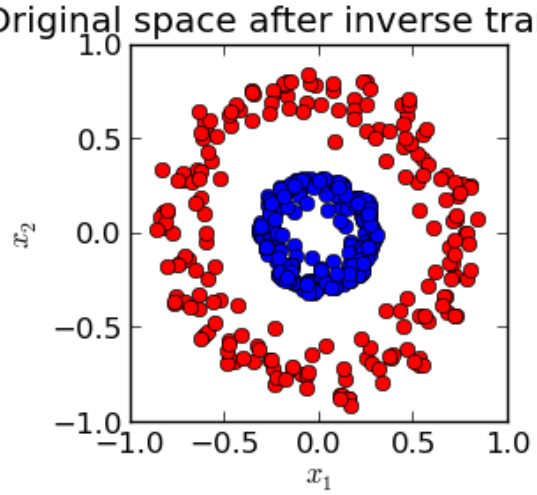
Kernel PCA

- What if the embedding is not linear?





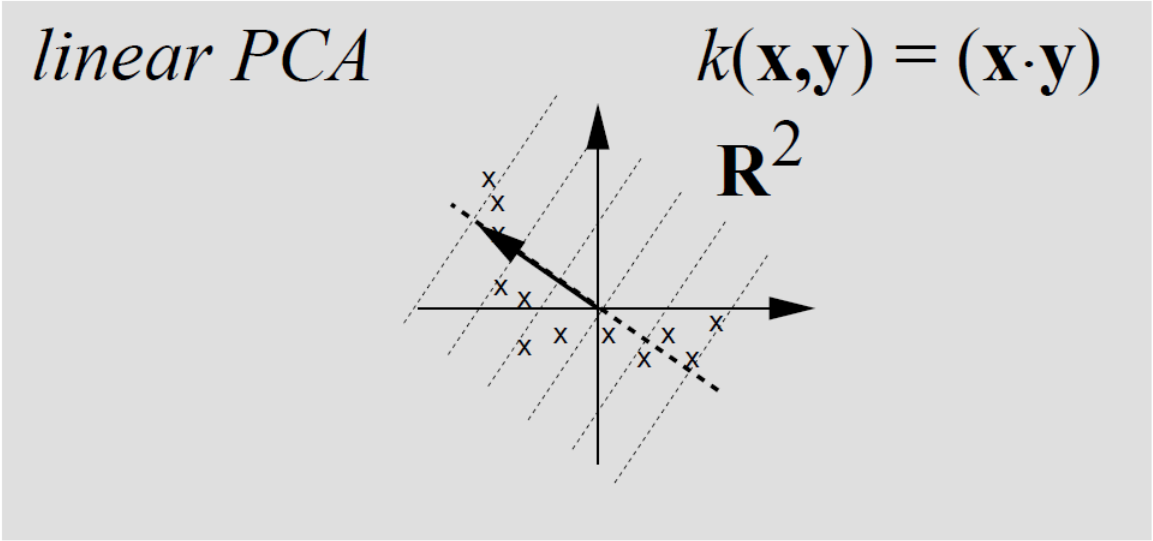


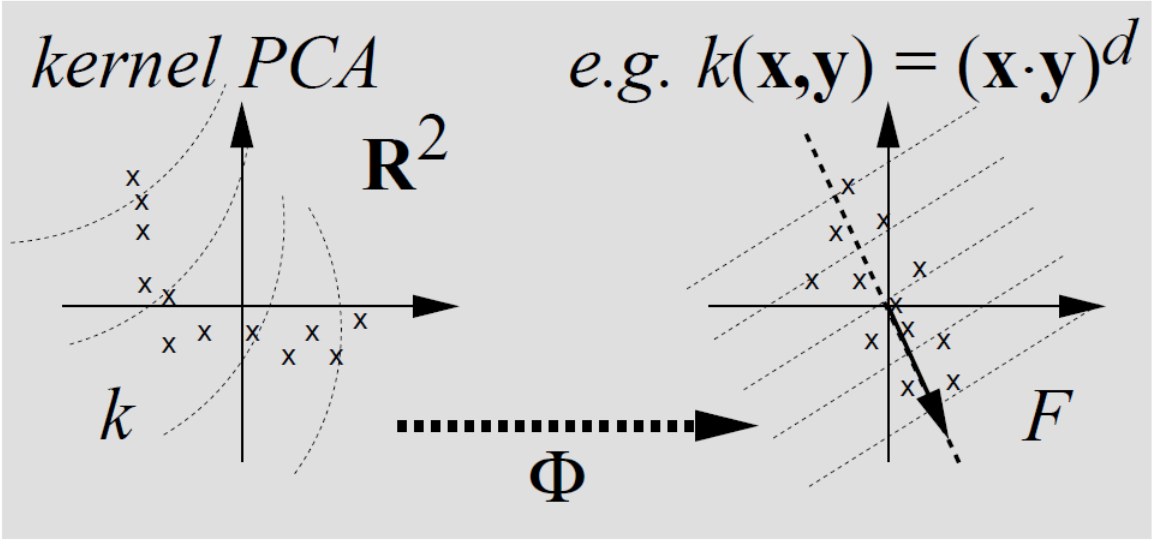


Kernel PCA

Schölkopf et al. (1998)

- Motivation





Kernel PCA

- Kernel PCA Procedure
  - ✓ Assumption: the projected new features have zero mean

$$\mathbf{m}^{\Phi} = \frac{1}{N}\sum_{i=1}^{N}\Phi(\mathbf{x}_i) = \mathbf{0}$$

  - ✓ The covariance matrix of the projected features is M by M, calculated by

$$\mathbf{C}^{\Phi} = \frac{1}{N}\sum_{i=1}^{N}(\Phi(\mathbf{x}_i) - \mathbf{m}^{\Phi})(\Phi(\mathbf{x}_i) - \mathbf{m}^{\Phi})^T = \frac{1}{N}\sum_{i=1}^{N}\Phi(\mathbf{x}_i)\Phi(\mathbf{x}_i)^T$$

  - ✓ Its eigenvalues and eigenvectors are given by

$$\mathbf{C}^{\Phi}\mathbf{v}_k = \lambda_k\mathbf{v}_k$$

    - where k = 1. 2. …, M.

Kernel PCA

- Kernel PCA Procedure
  - ✓ From the previous two equations, we have

$$\frac{1}{N}\sum_{i=1}^{N}\Phi(\mathbf{x}_i)\left(\Phi(\mathbf{x}_i)^T\mathbf{v}_k\right) = \lambda_k\mathbf{v}_k$$

  - ✓ which can be rewritten as

$$\mathbf{v}_k = \frac{1}{N}\sum_{i=1}^{N}\alpha_{ki}\Phi(\mathbf{x}_i)$$

  - ✓ By substituting v_k above, we have

$$\frac{1}{N}\sum_{i=1}^{N}\Phi(\mathbf{x}_i)\Phi(\mathbf{x}_i)^T\sum_{j=1}^{N}\alpha_{kj}\Phi(\mathbf{x}_j) = \lambda_k\sum_{i=1}^{N}\alpha_{kj}\Phi(\mathbf{x}_i)$$

Kernel PCA

✓ If we define the kernel function

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

✓ And multiply both side of the last equation in the previous page by $\Phi(\mathbf{x}_l)$

$$\frac{1}{N} \sum_{i=1}^{N} \Phi(\mathbf{x}_l)^T \Phi(\mathbf{x}_i) \sum_{j=1}^{N} \alpha_{kj} \Phi(\mathbf{x}_i)^T \Phi(\mathbf{x}_j) = \lambda_k \sum_{i=1}^{N} \alpha_{kj} \Phi(\mathbf{x}_l)^T \Phi(\mathbf{x}_i)$$

$$\frac{1}{N} \sum_{i=1}^{N} \mathbf{K}(\mathbf{x}_l, \mathbf{x}_i) \sum_{j=1}^{N} \alpha_{kj} \mathbf{K}(\mathbf{x}_i, \mathbf{x}_j) = \lambda_k \sum_{i=1}^{N} \alpha_{kj} \mathbf{K}(\mathbf{x}_l, \mathbf{x}_i)$$

✓ Then, we can use the matrix notation

$$\mathbf{K}^2 \boldsymbol{\alpha}_k = \lambda_k N \mathbf{K} \boldsymbol{\alpha}_k$$

- Where $\boldsymbol{\alpha}_k$ is the N-dimensional column vector $\boldsymbol{\alpha}_k = (\alpha_{k1}, \alpha_{k2}, \cdots, \alpha_{kN})^T$

Kernel PCA

✓ The eigenvector problem becomes

$$\mathbf{K}\boldsymbol{\alpha}_k = \lambda_k N \boldsymbol{\alpha}_k$$

✓ And the resulting kernel PCA can be calculated using

$$y_k(\mathbf{x}) = \Phi(\mathbf{x})^T \mathbf{v}_k = \sum_{i=1}^{N} \alpha_{ki} \mathbf{K}(\mathbf{x}, \mathbf{x}_i)$$

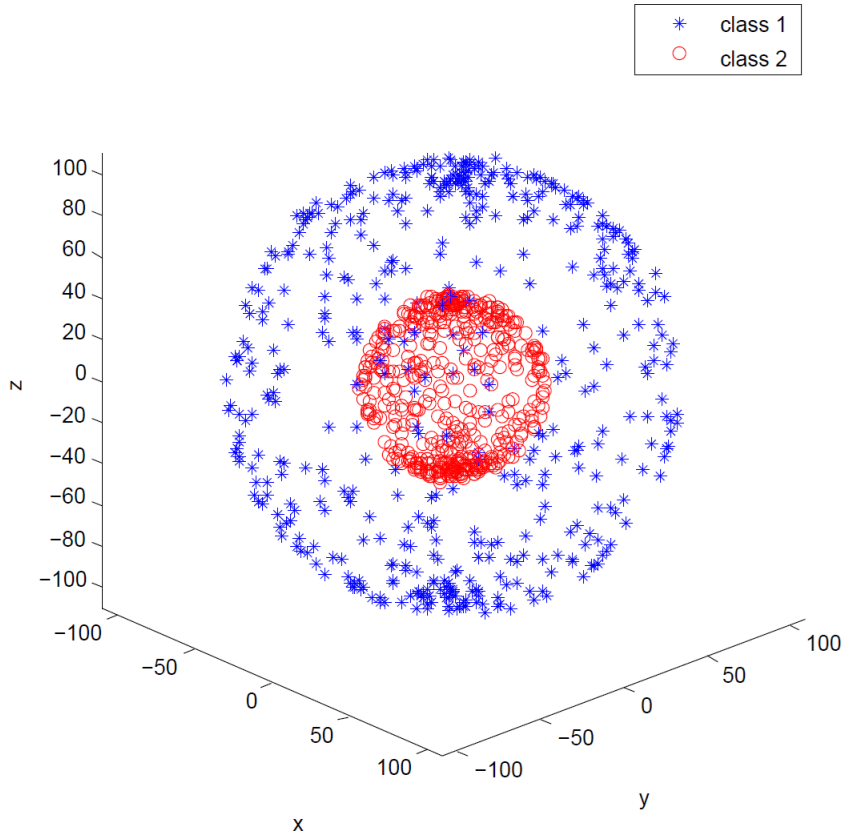
✓ If the projected dataset does not have zero mean, use the Gram matrix

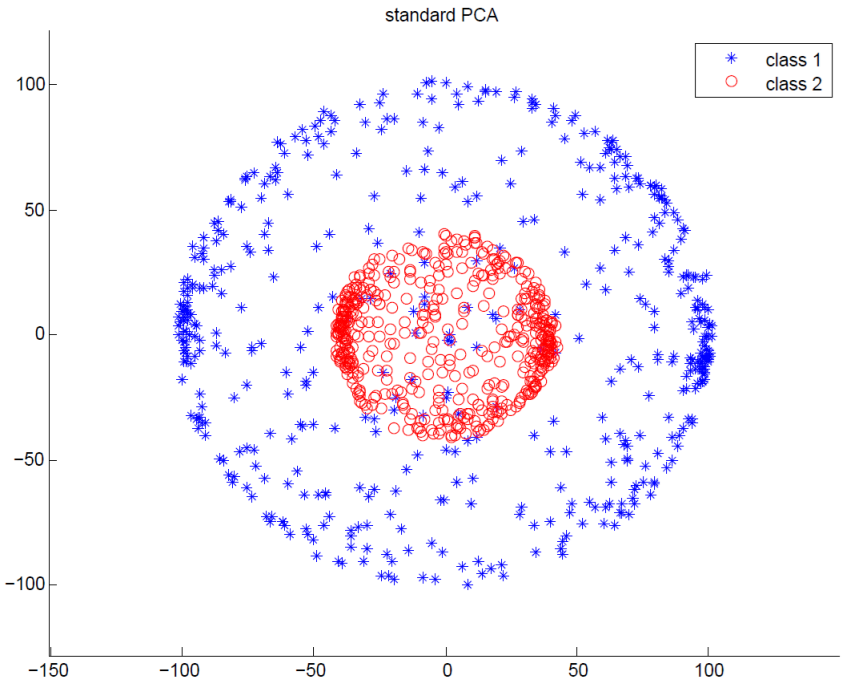
$$\begin{aligned}\widetilde{\mathbf{K}} &= (\mathbf{I} - \mathbf{1}_N)\mathbf{K}(\mathbf{I} - \mathbf{1}_N) \\ &= \mathbf{K} - \mathbf{1}_N\mathbf{K} - \mathbf{K}\mathbf{1}_N + \mathbf{1}_N\mathbf{K}\mathbf{1}_N\end{aligned}$$

- Where $\mathbf{1}_N$ is the N by N matrix with all elements equal to 1/N

Kernel PCA

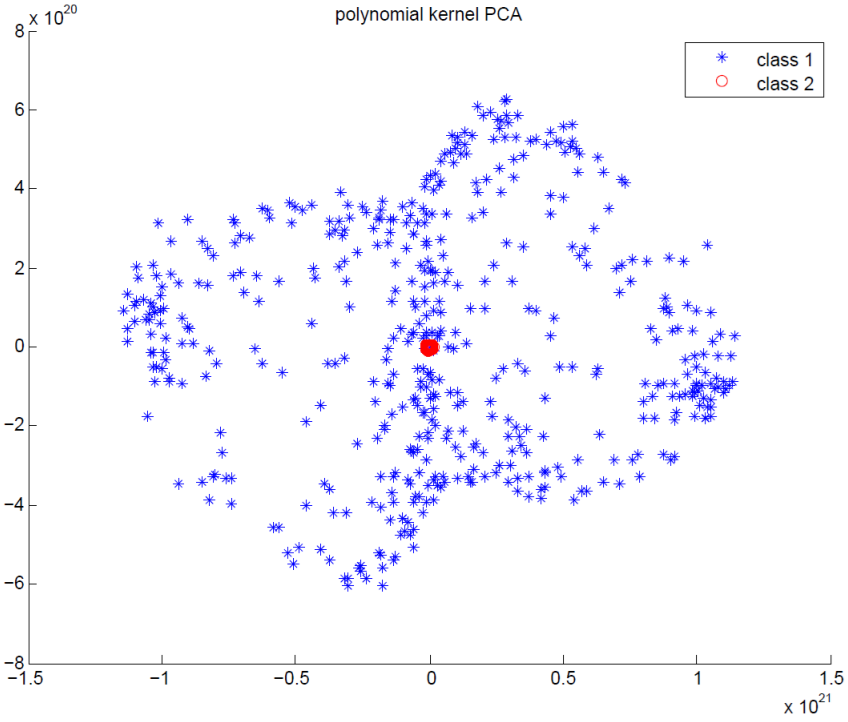
- PCA for two sphere sets

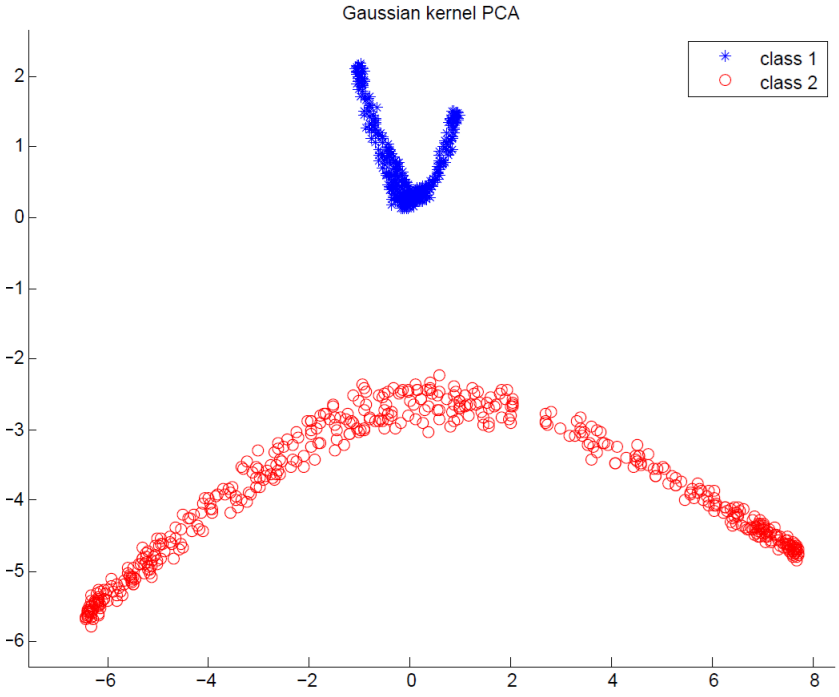




Kernel PCA

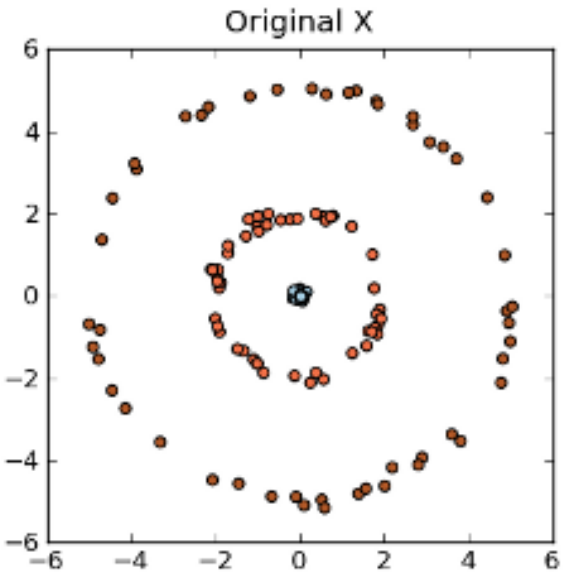
- KPCA for two sphere sets

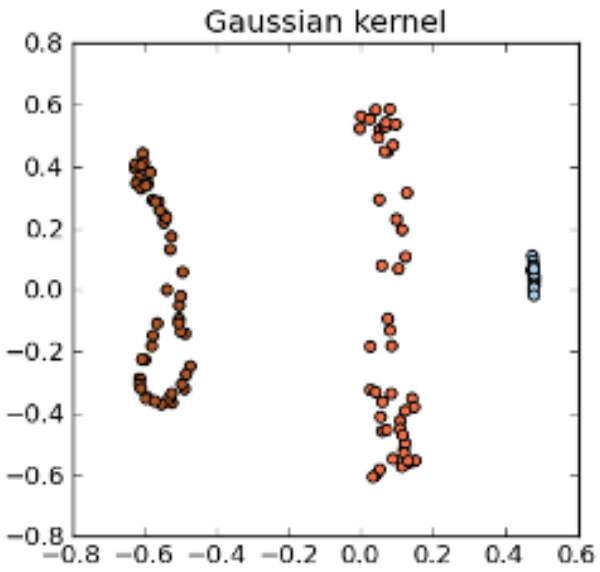


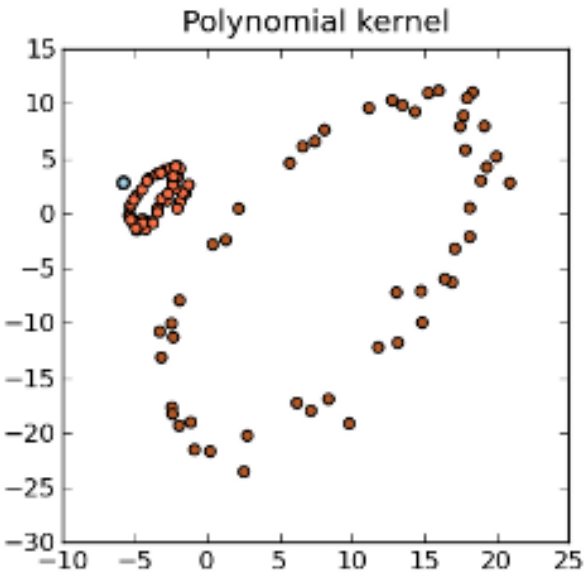


Kernel PCA

- Projection result according to different kernel types

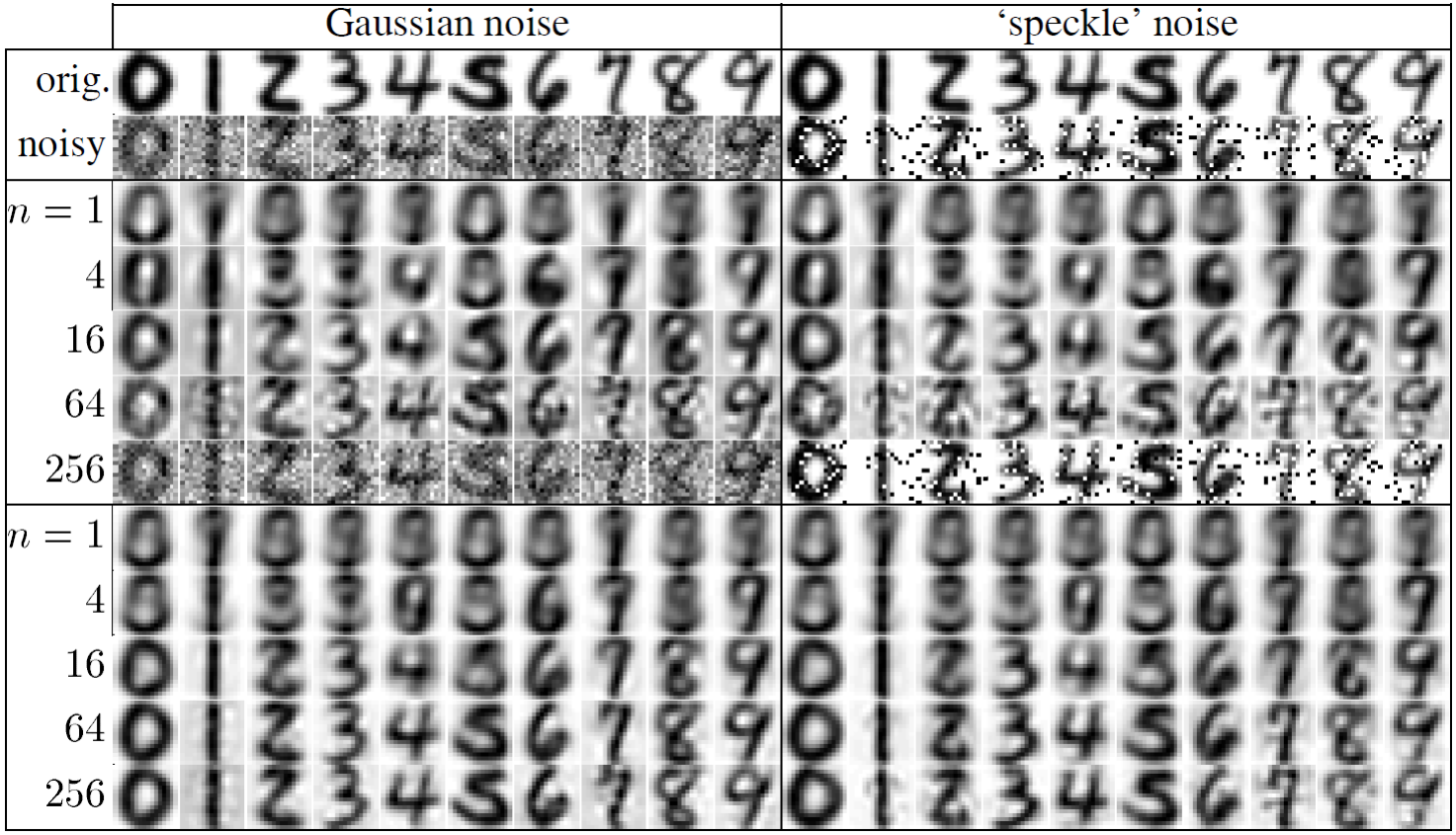






Kernel PCA: Application

- De-noising images




Q & A

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