BITS Pilani
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Machine Learning
DSECL ZG565

Support Vector Machines –II

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Topics to be covered

- Soft Margin SVM
- Nonlinear SVM
- Kernel Trick
- SVM Kernels
- Multi-Class Problem
- SVM vs Logistic Regression
- SVM Applications

Linear SVMs: Overview

- **The classifier is a *separating hyperplane.***
- **Most "important" training points are support vectors; they define the decision hyperplane (unlike other algorithms like linear regression, ANN etc. where all training points determine decision hyperplane)**
- **Quadratic optimization algorithms can identify which training points $\mathbf{x}_i$ are support vectors with non-zero Lagrangian multipliers α_i.**

Find $\alpha_1 \ldots \alpha_N$ such that

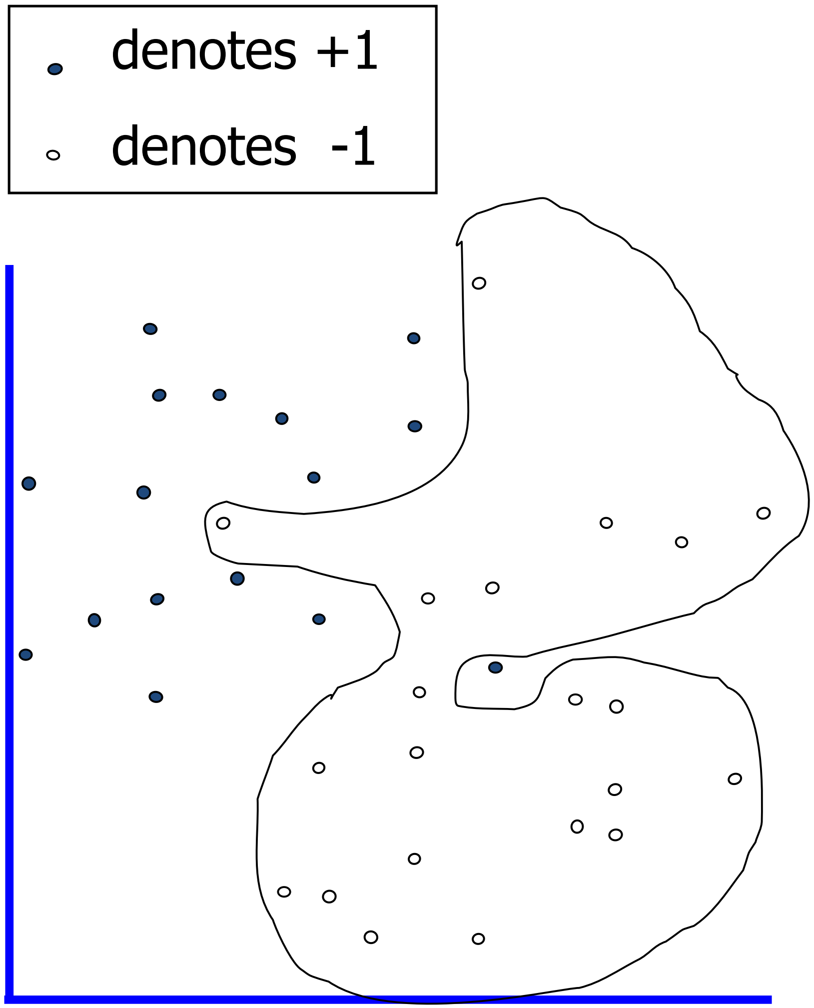
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\left(\sum_i \sum_j \alpha_i \alpha_j y_i y_j \mathbf{x_i} \cdot \mathbf{x_j}\right)$ is maximized and

(1) $\Sigma\alpha_i y_i = 0$

(2) $\boldsymbol{\alpha_i \geq 0}$ **for all** $\boldsymbol{\alpha_i}$

$$f(\mathbf{x}) = \Sigma\alpha_i y_i \mathbf{x_i}^T\mathbf{x} + b$$

Dataset with noise



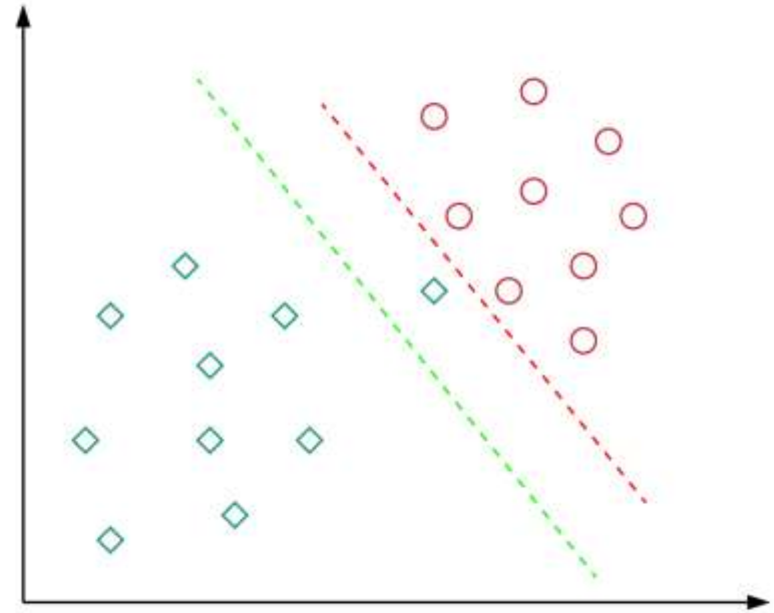
- **Hard Margin:** **So far we require all data points be classified correctly**

  - No training error

- **What if the training set is noisy?**

Motivation : Softmargin

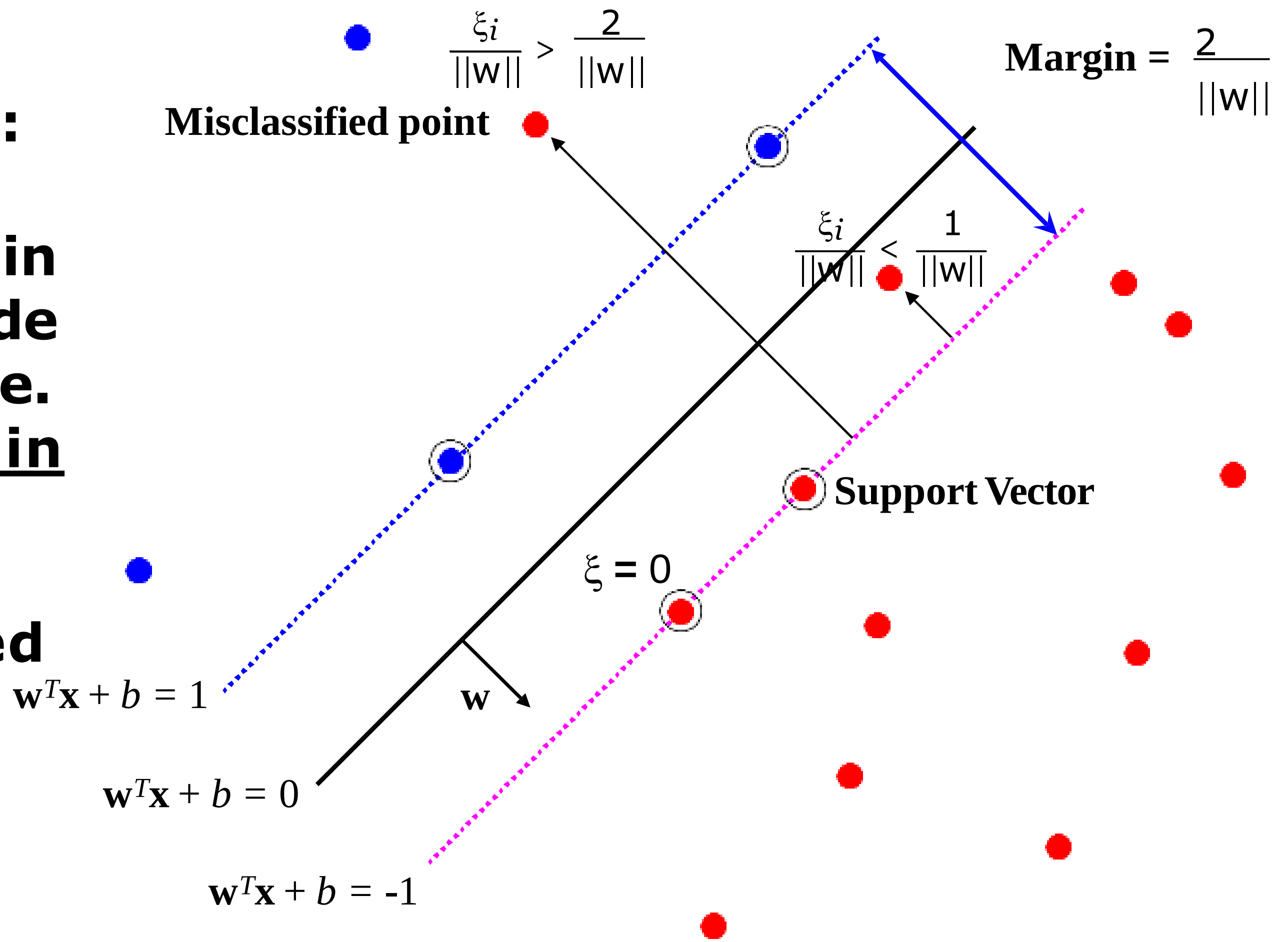
- Almost all real-world applications have data that is linearly inseparable.
- When data *is* linearly separable, choosing perfect decision boundary leads to overfitting



Introduce “slack” variables

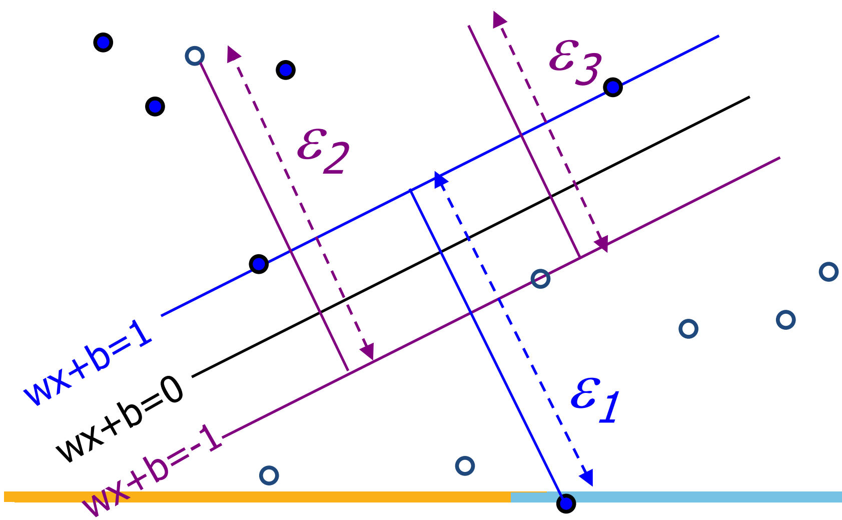
$\xi_i \geq 0$

- **for $0 < \xi \leq 1$: point is between margin and correct side of hyper- plane. This is a <u>margin violation</u>**
- **for $\xi > 1$ point is misclassified**



Soft Margin Classification

- ***Slack variables*** $\boldsymbol{\xi_i}$ **can be added to allow misclassification of difficult or noisy examples.**
- slack variable ξ_i for every data point x_i,
- ξ_i is the distance of x_i from the corresponding class's margin if x_i is on the wrong side of the margin, otherwise zero. **It can be regarded as a measure of confidence**
- Points that are far away from the margin on the wrong side would get more penalty



Soft Margin SVMs

\# data samples

Misclassification cost

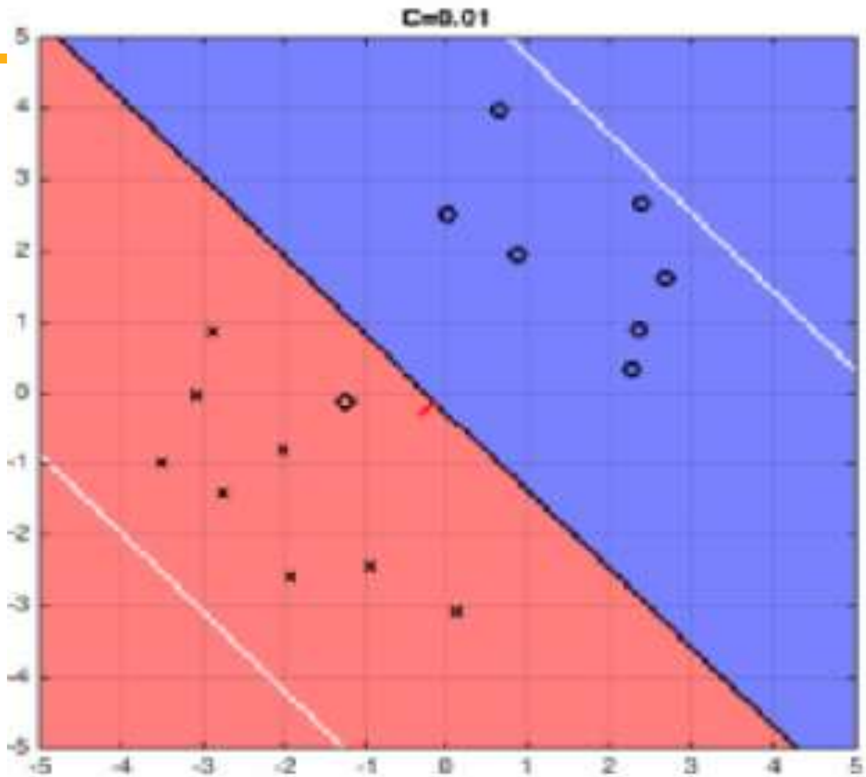
Slack variable

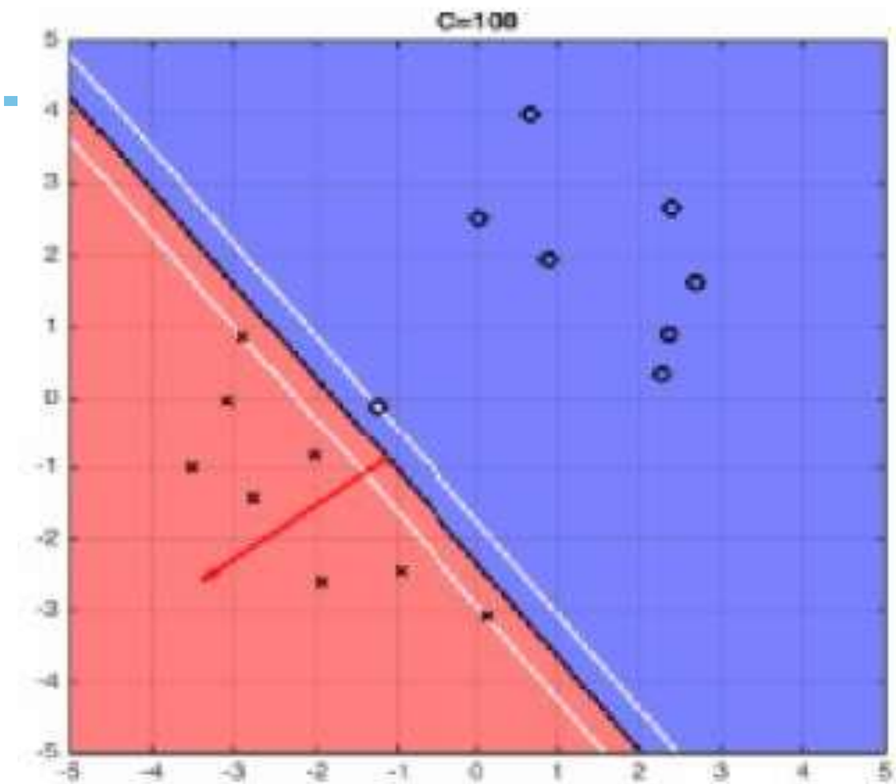
$$\min_{\boldsymbol{w}} \underbrace{\frac{1}{2}\|\boldsymbol{w}\|^2}_{\text{Maximize margin}} + \underbrace{C\sum_{i=1}^{N}\xi_i}_{\text{Minimize misclassification}}$$

The *w* that minimizes…

$$\boxed{\begin{aligned} \text{subject to} \quad & y_i \boldsymbol{w}^T \boldsymbol{x}_i \geq 1 - \xi_i, \\ & \xi_i \geq 0, \quad \forall i = 1, \ldots, N \end{aligned}}$$

Effect of C



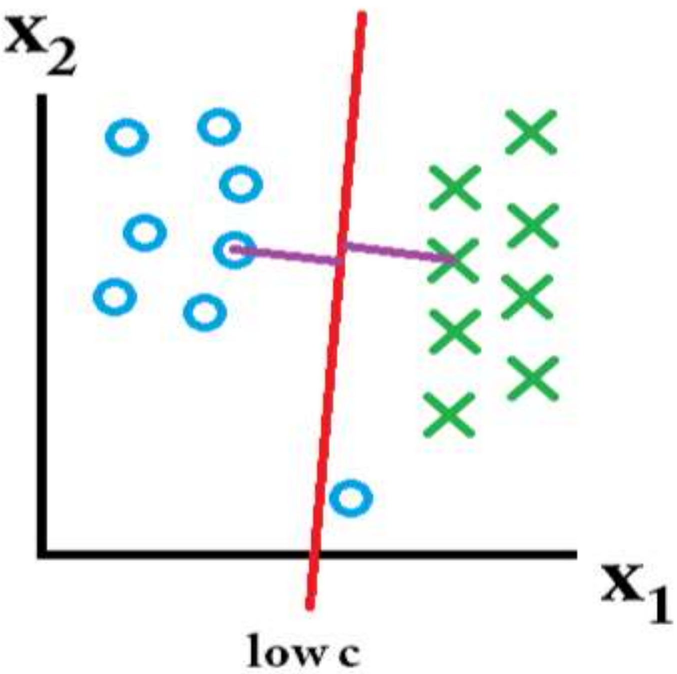


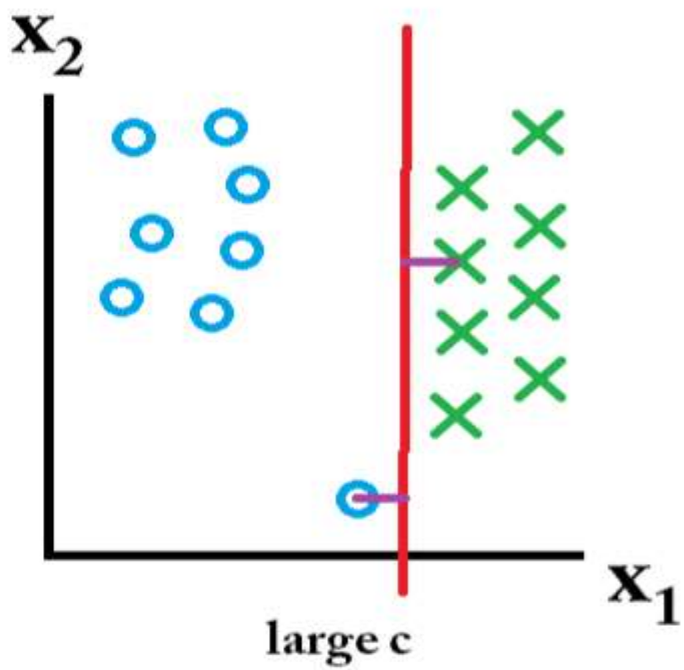
small value of C will cause the optimizer to look for a larger-margin (small penalties) separating hyperplane, even if that hyperplane misclassifies more points.

For large values of C, the optimization will choose a smaller-margin (large penalties) hyperplane if that hyperplane does a better job of getting all the training points classified correctly. C=infinity ->hard margin SVM

Effect of Margin size v/s misclassification cost

– Training set





Misclassification ok, want large margin

Misclassification not ok

classification mistakes are given less importance,

• the focus is more on avoiding misclassification at the expense of keeping the margin small.

SVM Problem

SVM: Optimization

$$\min \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_i \xi_i$$

$$\text{Subject to:} \quad y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i$$

SVM: Training

Input: (X,y), C
Output: alpha for support vectors, b
Hyperparameter : C

SVM: Classification

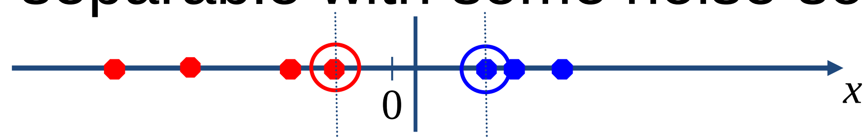
$$sign(\mathbf{w}^T\mathbf{x} + b)$$
$$= sign(\sum_i \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + b)$$

- C parameter tells the SVM optimization how much you want to avoid misclassifying each training example and *C* can be viewed as a way to control overfitting

Nonlinear SVM - kernels

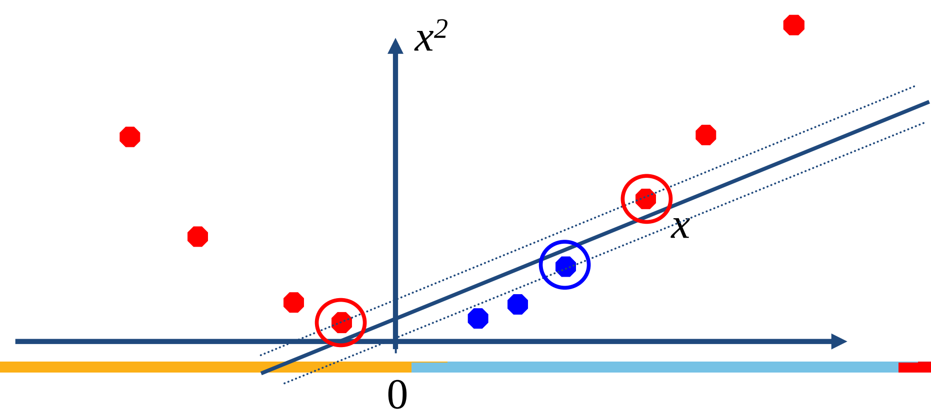
Non-linear SVMs

- What if data is not noisy or having outliers(soft margin can work) but inherently non linear
- Datasets that are linearly separable with some noise soft margin work out great:



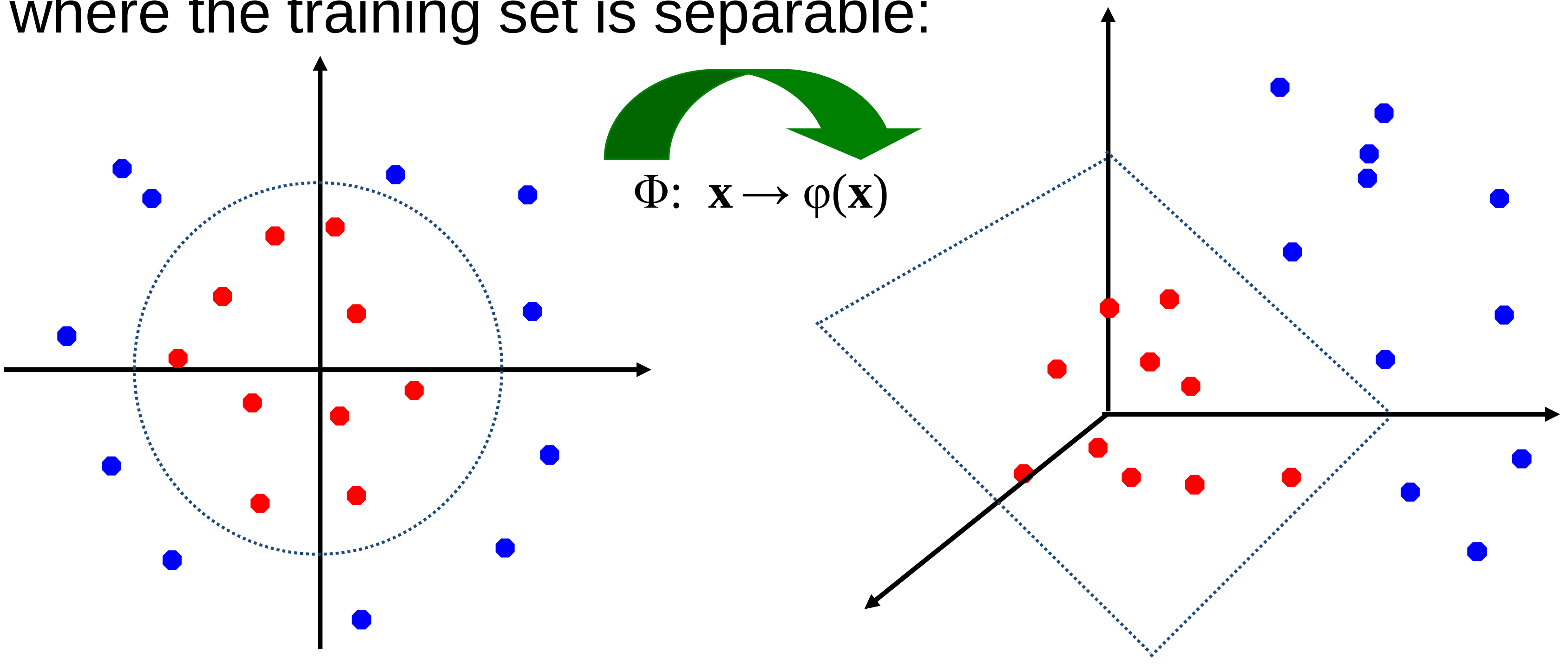
- But what are we going to do if the dataset is just too hard?

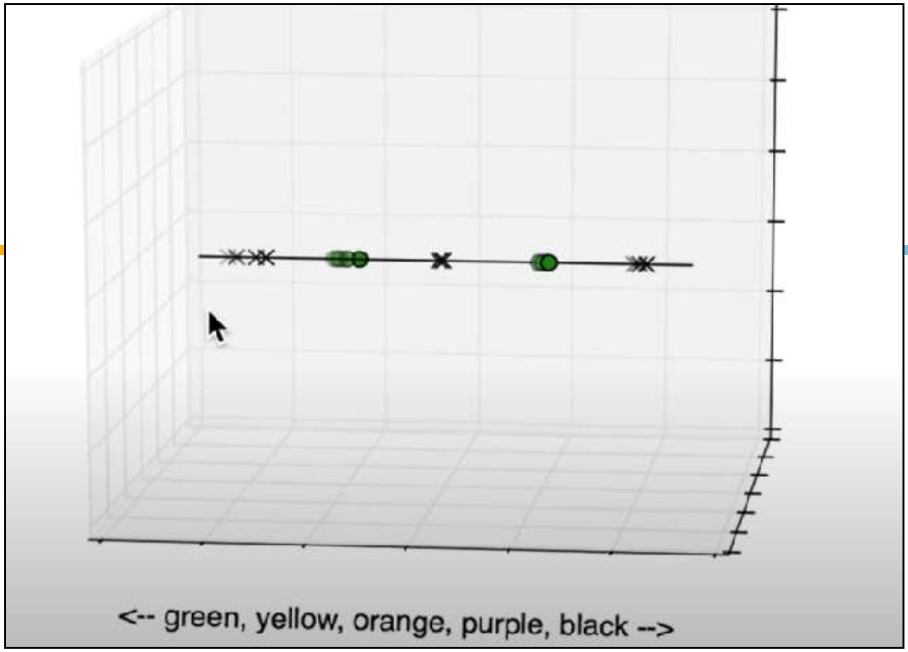
- How about… mapping data to a higher-dimensional space:



Non-linear SVMs: Feature spaces

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

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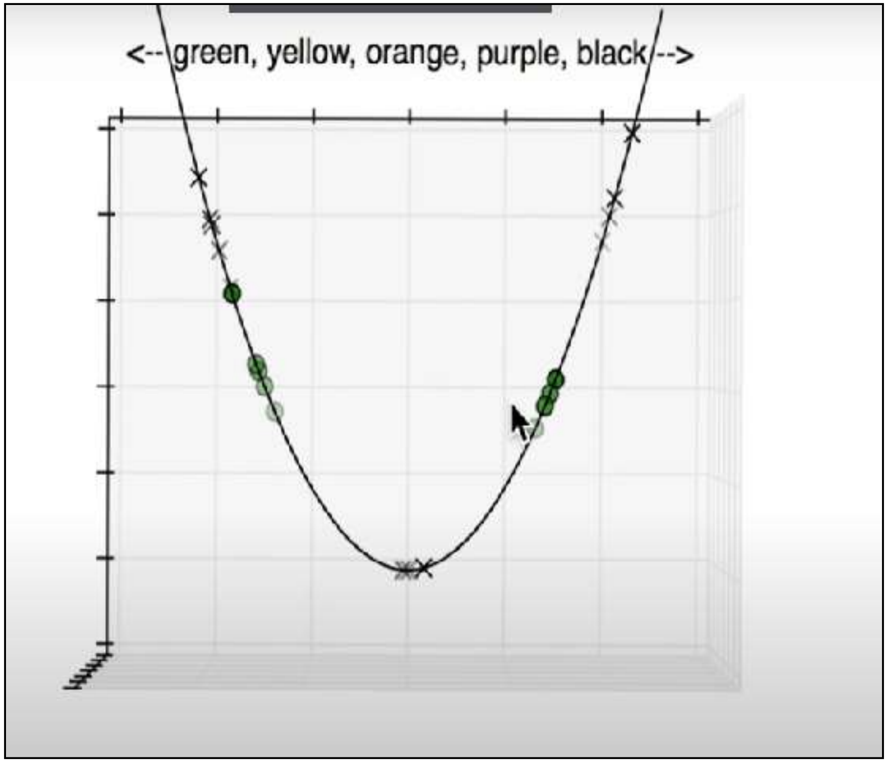
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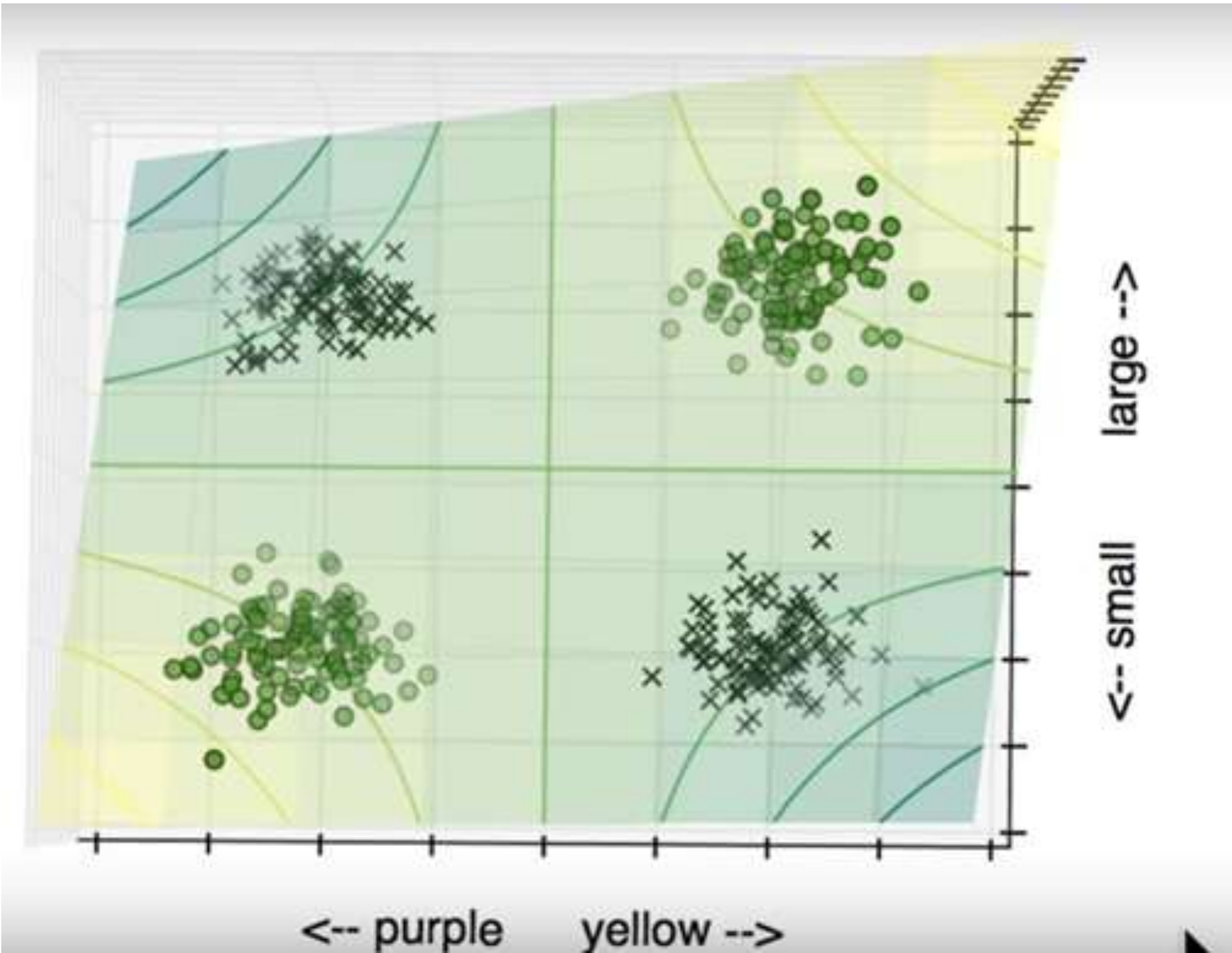
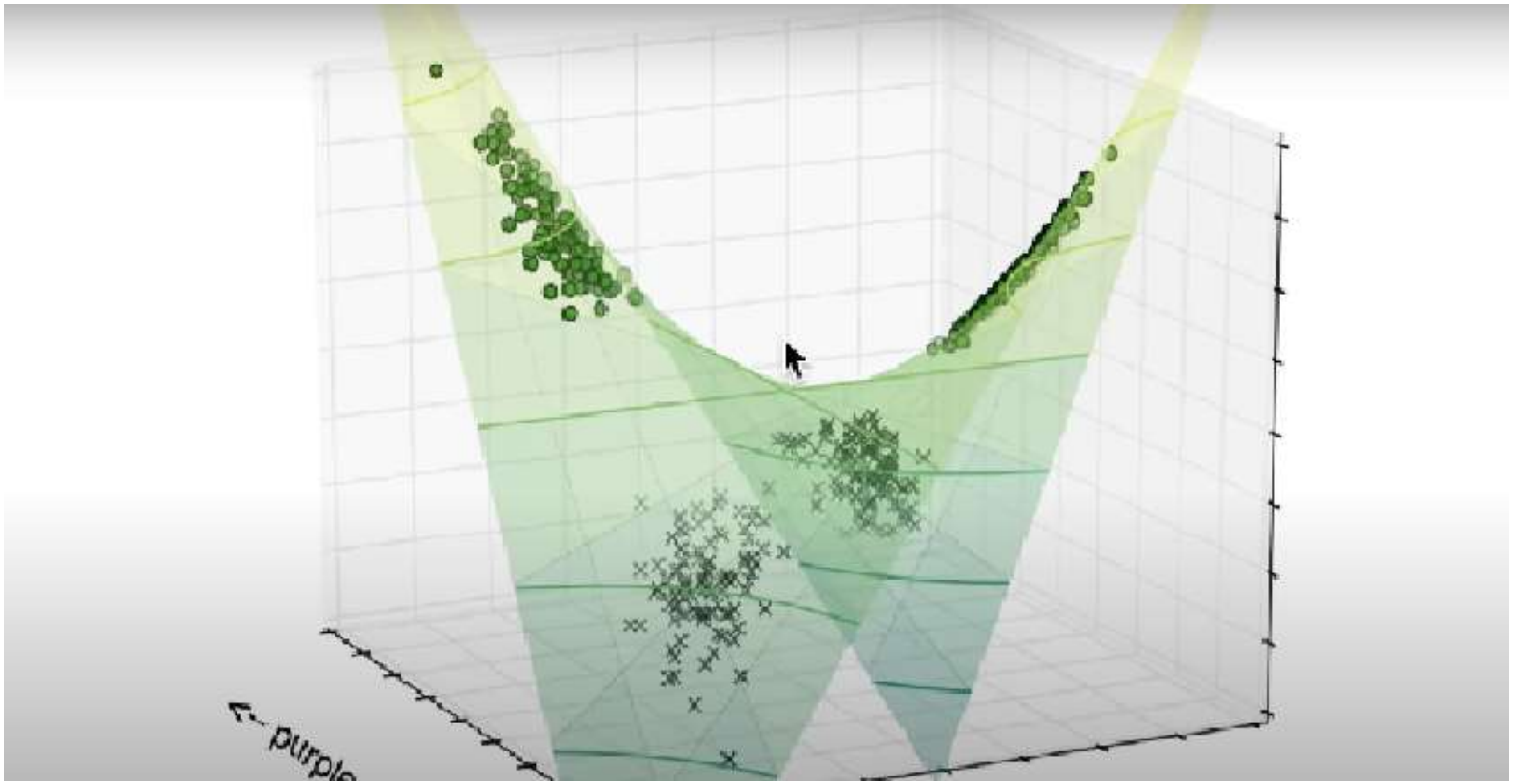
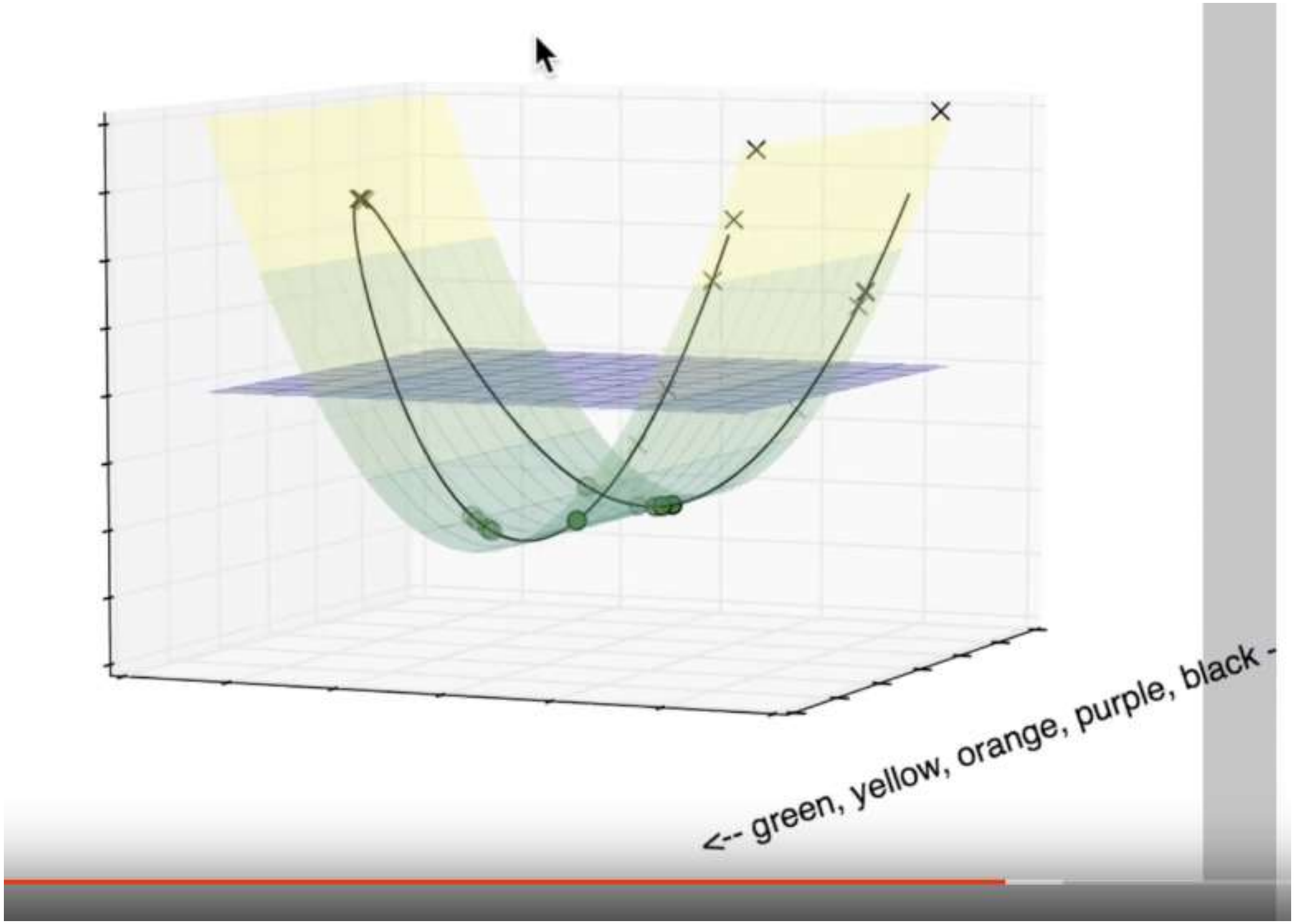
Non-linear SVMs: Feature spaces



Non-linear SVMs: Feature spaces





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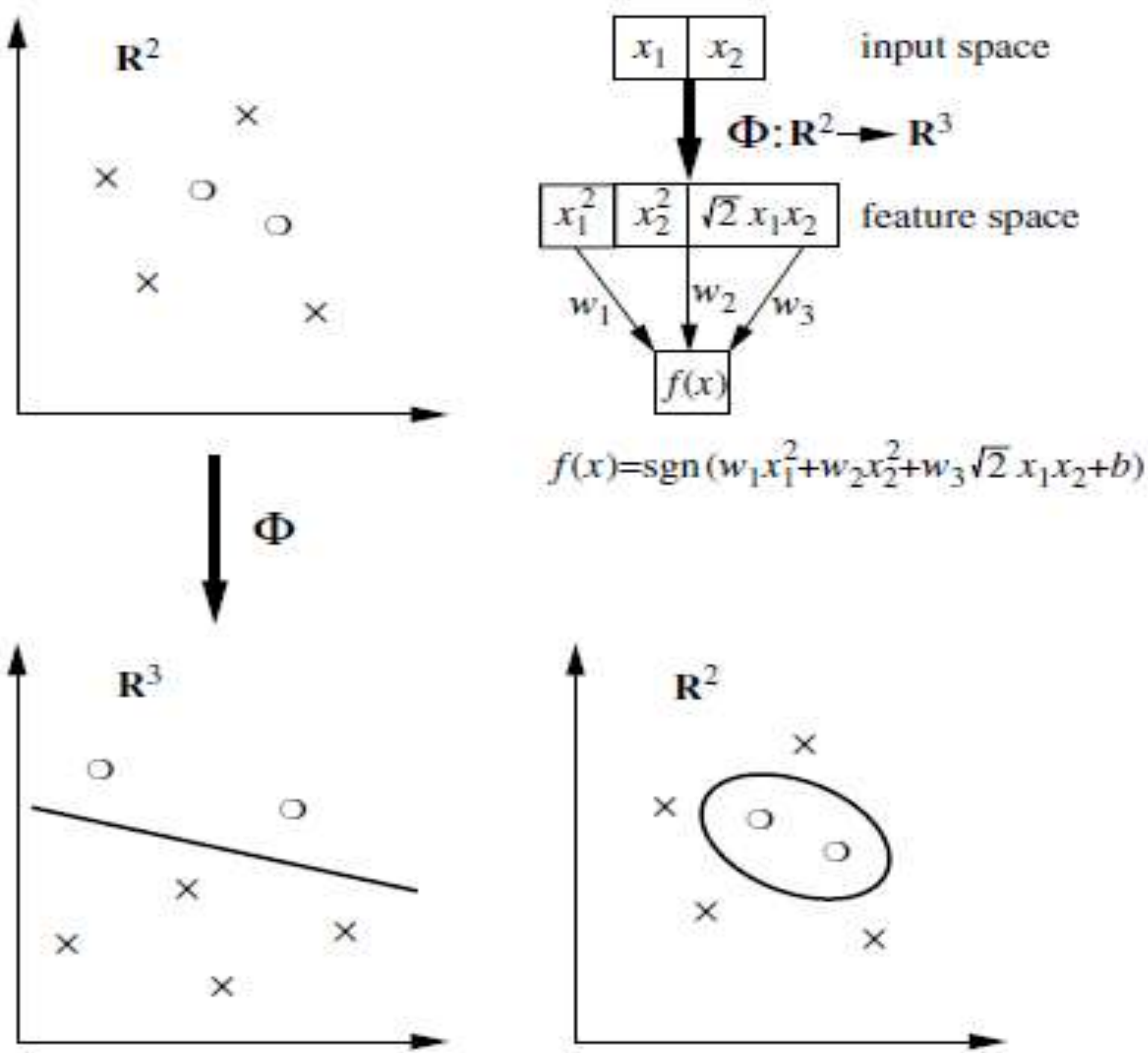
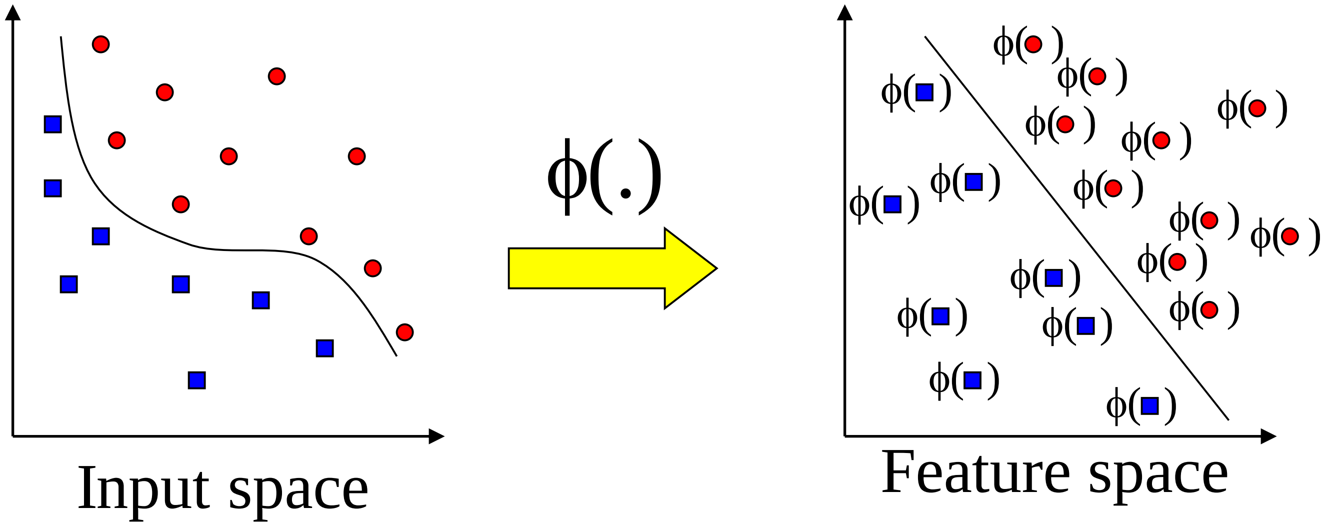
Mapping into a New Feature Space



- Rather than run SVM on x_i, run it on $\Phi(x_i)$
- Find non-linear separator in input space
- What if $\Phi(x_i)$ is really big?
- Use kernels to compute it implicitly!

Transforming the Data



Note: feature space is of higher dimension than the input space in practice

- Computation in the feature space can be costly because it is high dimensional
  - The feature space is typically infinite-dimensional!
- The kernel trick comes to rescue

SVM Kernels

- SVM algorithms use a set of mathematical functions that are defined as the kernel.
- Function of kernel is to take data as input and transform it into the required form.
- Different SVM algorithms use different types of kernel functions. Example *linear, nonlinear, polynomial, and sigmoid etc.*

The "Kernel Trick"

- **The linear classifier relies on dot product between vectors**
  - $\mathbf{x_i}^T \cdot \mathbf{x_j}$
- **If every data point is mapped into high-dimensional space via some transformation Φ: x → φ(x), the dot product becomes:**

$$K(\mathbf{x_i}, \mathbf{x_j}) = \varphi(\mathbf{x_i})^T \, \varphi(\underline{\mathbf{x_j}})$$

- **A *kernel function* is some function that corresponds to an inner product in some expanded feature space.**
- **Computing K(x1,x2) should be efficient, much more so than computing Φ(x1) and Φ(x2)**

Kernel: Example
Polynomial Kernel

Let $\mathbf{p} = [p_1, p_2]^T$ and $\mathbf{q} = [q_1, q_2]^T$ be two samples in 2D.

$$\kappa(\mathbf{p}, \mathbf{q}) = (\mathbf{p}^T \mathbf{q})^2 = ([p_1, p_2]^T [q_1, q_2])^2$$
$$= (p_1 q_1)^2 + (p_2 q_2)^2 + 2 p_1 q_1 p_2 q_2$$

This is equivalent to:

$$\phi(\mathbf{p}) = \phi\left(\begin{array}{c} p_1 \\ p_2 \end{array} \right) = \begin{bmatrix} p_1^2 \\ p_2^2 \\ \sqrt{2} p_1 p_2 \end{bmatrix}$$

Example:

2-dimensional vectors $\mathbf{x}=[x_1 \ \ x_2]$;

let $K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^T\mathbf{x}_j)^2$,

Need to show that $K(\mathbf{x}_i,\mathbf{x}_j)= \boldsymbol{\varphi}(\mathbf{x}_i)^T\boldsymbol{\varphi}(\mathbf{x}_j)$:

$K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^T\mathbf{x}_j)^2$,

$= 1+ x_{i1}^2x_{j1}^2 + 2\, x_{i1}x_{j1}\, x_{i2}x_{j2}+ x_{i2}^2x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_j$

$= [1 \ \ x_{i1}^2 \ \ \sqrt{2}\, x_{i1}x_{i2} \ \ x_{i2}^2 \ \ \sqrt{2}x_{i1} \ \ \sqrt{2}x_{i2}]^T [1 \ \ x_{j1}^2 \ \ \sqrt{2}\, x_{j1}x_{j2} \ \ x_{j2}^2 \ \ \sqrt{2}x_{j1} \ \ \sqrt{2}x_{j2}]$

$= \boldsymbol{\varphi}(\mathbf{x}_i)^T\boldsymbol{\varphi}(\mathbf{x}_j)$,

where $\boldsymbol{\varphi}(\mathbf{x}) = [1 \ \ x_1^2 \ \ \sqrt{2}\, x_1x_2 \ \ x_2^2 \ \ \sqrt{2}x_1 \ \ \sqrt{2}x_2]$

Thus, a kernel function *implicitly* maps data to a high-dimensional space (without the need to compute each $\boldsymbol{\varphi}(\mathbf{x})$ explicitly).

Mercer kernels

What functions are valid kernels that correspond to feature vectors $\varphi(x)$?

Mercer kernels K

- K is continuous
- K is symmetric
- K is positive semi-definite, i.e. $x^T K x \geq 0$ for all x

Ensures optimization is concave maximization

What Functions are Kernels?

1) We can *construct kernels from scratch*:

- For any $\varphi : \mathcal{X} \to \mathbb{R}^m$, $k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathbb{R}^m}$ is a kernel.
- If $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a *distance function*, i.e.
  - $d(x, x') \geq 0$ for all $x, x' \in \mathcal{X}$,
  - $d(x, x') = 0$ only for $x = x'$,
  - $d(x, x') = d(x', x)$ for all $x, x' \in \mathcal{X}$,
  - $d(x, x') \leq d(x, x'') + d(x'', x')$ for all $x, x', x'' \in \mathcal{X}$,

  then $k(x, x') := \exp(-d(x, x'))$ is a kernel.

2) We can *construct kernels from other kernels*:

- if k is a kernel and $\alpha > 0$, then αk and $k + \alpha$ are kernels.
- if k_1, k_2 are kernels, then $k_1 + k_2$ and $k_1 \cdot k_2$ are kernels.

Examples of Kernel Functions

- Linear: $K(\mathbf{x_i},\mathbf{x_j}) = \mathbf{x_i}^T\mathbf{x_j}$

- Polynomial of power p: $K(\mathbf{x_i},\mathbf{x_j}) = (1 + \mathbf{x_i}^T\mathbf{x_j})^p$

- Gaussian (radial-basis function network):

$$K(\mathbf{x_i},\mathbf{x_j}) = \exp\left(-\frac{\|\mathbf{x_i} - \mathbf{x_j}\|^2}{2\sigma^2}\right)$$

- Sigmoid: $K(\mathbf{x_i},\mathbf{x_j}) = \tanh(\beta_0 \mathbf{x_i}^T\mathbf{x_j} + \beta_1)$

Using a Different Kernel in the Dual Optimization Problem

$$f(\mathbf{x}) = \Sigma \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}_j) + b$$

- For example, using the polynomial kernel with d = 4 (including lower-order terms) → $(\langle x_i, x_j \rangle + 1)^4$
- Maximize over α
  - $W(\alpha) = \Sigma_i \alpha_i - 1/2\, \Sigma_{i,j} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$
- Subject to
  - $\alpha_i \geq 0$
  - $\Sigma_i \alpha_i y_i = 0$
- Decision function
  - $f(x) = \text{sign}(\Sigma_i \alpha_i y_i \langle x, x_i \rangle + b)$

These are kernels!

$(\langle x_i, x_j \rangle + 1)^4$

So by the kernel trick,
we just replace them!

Non-linear SVM using kernel

1. Select a kernel function.
2. Compute pairwise kernel values between labeled examples.
3. Use this “kernel matrix” to solve for SVM support vectors & alpha weights.
4. To classify a new example: compute kernel values between new input and support vectors, apply alpha weights, check sign of output.

Nonlinear SVM - Overview

- SVM locates a separating hyperplane in the feature space and classify points in that space
- It does not need to represent the space explicitly, simply by defining a kernel function
- The kernel function plays the role of the dot product in the feature space.

Multi-Class Problem

Instead of just two classes, we now have C classes

- E.g. predict which movie genre a viewer likes best
- Possible answers: action, drama, indie, thriller, etc.

Two approaches:

- One-vs-all
- One-vs-one

Multi-Class Problem

One-vs-all (a.k.a. one-vs-others)

- Train C classifiers
- In each, pos = data from class *i*, neg = data from classes other than *i*
- The class with the most confident prediction wins
- Example:
  - You have 4 classes, train 4 classifiers
  - 1 vs others: score 3.5
  - 2 vs others: score 6.2
  - 3 vs others: score 1.4
  - 4 vs other: score 5.5
  - Final prediction: class 2
- Issues?

Multi-Class Problem

One-vs-one (a.k.a. all-vs-all)

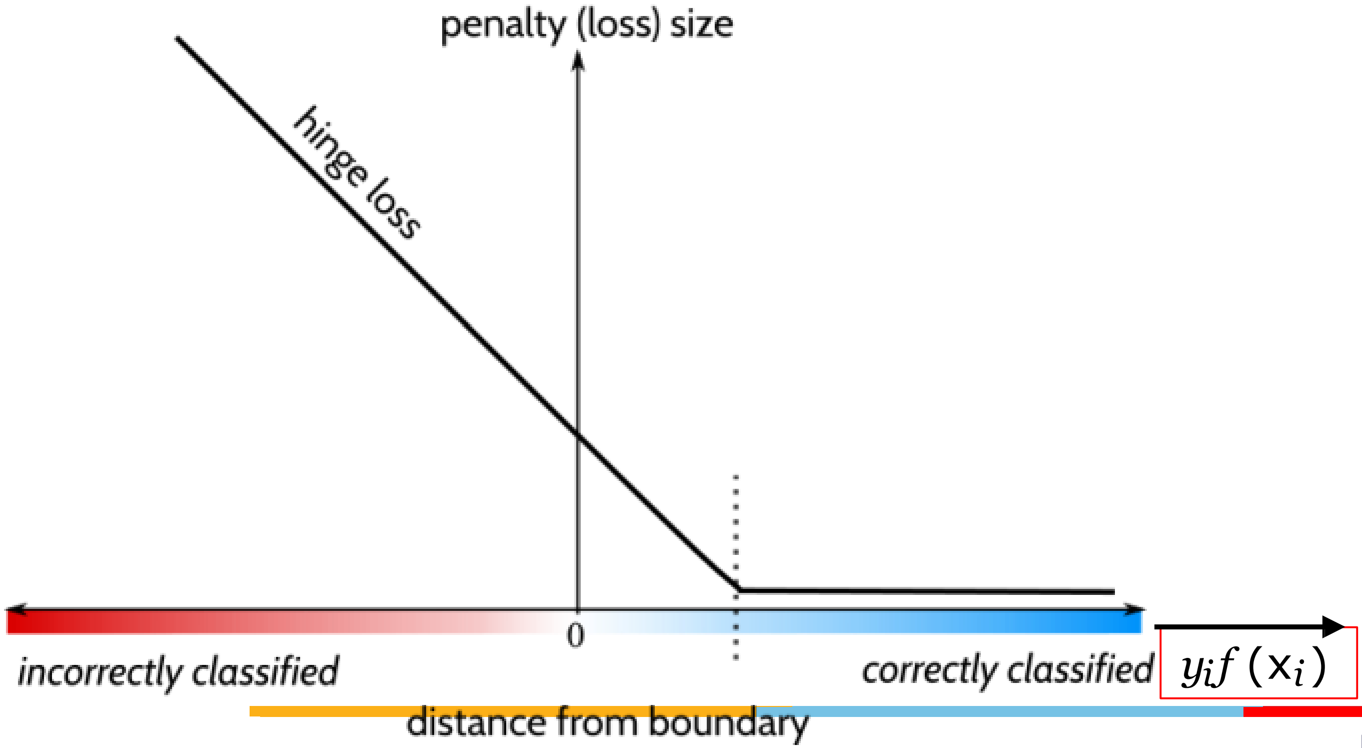
- Train C(C-1)/2 binary classifiers (all pairs of classes)
- They all vote for the label
- Example:
  - You have 4 classes, then train 6 classifiers
  - 1 vs 2, 1 vs 3, 1 vs 4, 2 vs 3, 2 vs 4, 3 vs 4
  - Votes: 1, 1, 4, 2, 4, 4
  - Final prediction is class 4

Slack variable-Hinge loss

$$\xi_j = \text{loss}(f(x_j), y_j)$$

$$f(x_j) = \text{sgn}(\mathbf{w} \cdot \mathrm{x_j} + \mathrm{b})$$

$$\xi_j = (1 - (\mathbf{w} \cdot x_j + b)y_j))_+$$



SVM versus Logistic Regression

- When viewed from the point of view of regularized empirical loss minimization, SVM and logistic regression appear quite similar:

SVM: $$\sum_{i=1}^{n} \left(1 - y_i \left[w_0 + \mathbf{x}_i^T \mathbf{w}_1\right]\right)^+ + \quad \|\mathbf{w}_1\|^2/2$$

Logistic: $$\sum_{i=1}^{n} \overbrace{-\log \sigma\left(y_i \left[w_0 + \mathbf{x}_i^T \mathbf{w}_1\right]\right)}^{-\log P(y_i|\mathbf{x},\mathbf{w})} + \quad \|\mathbf{w}_1\|^2/2$$

where $\sigma(z) = (1 + \exp(-z))^{-1}$ is the logistic function.

SVM versus Logistic Regression

- The difference comes from how we penalize "errors":

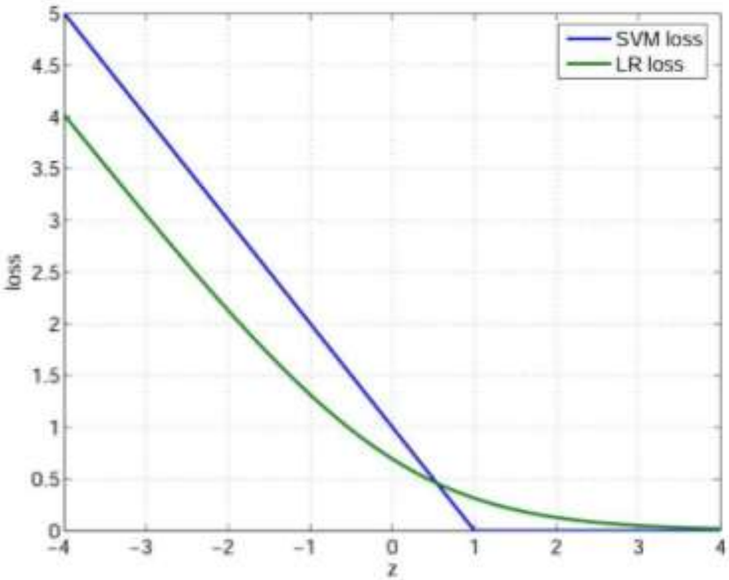
Both: $$\sum_{i=1}^{n} \text{Loss}\Big(\overbrace{y_i\left[w_0 + \mathbf{x}_i^T \mathbf{w}_1\right]}^{z}\Big) + \quad \|\mathbf{w}_1\|^2/2$$

- SVM:

$$\text{Loss}(z) = (1 - z)^+$$

- Regularized logistic reg:

$$\text{Loss}(z) = \log(1 + \exp(-z))$$



SVM versus Logistic Regression

- Logistic regression focuses on maximizing the probability of the data. The farther the data lies from the separating hyperplane (on the correct side), the happier LR is
- An SVM tries to find the separating hyperplane that maximizes the distance of the closest points to the margin (the support vectors). If a point is not a support vector, it doesn't really matter.

SVM versus Logistic Regression

- LR gives calibrated probabilities that can be interpreted as confidence in a decision.
- LR gives us an unconstrained, smooth objective
- LR can be (straightforwardly) used within Bayesian models.
- SVMs don't penalize examples for which the correct decision is made with sufficient confidence. This may be good for generalization.
- SVMs have a nice dual form, giving sparse solutions when using the kernel trick (better scalability).

Properties of SVM

- Flexibility in choosing a similarity function
- Sparseness of solution when dealing with large data sets
  - Only support vectors are used to specify the separating hyperplane
  - Therefore SVM also called sparse kernel machine.
- Ability to handle large feature spaces
  - complexity does not depend on the dimensionality of the feature space
- Overfitting can be controlled by soft margin approach
- Nice math property: a simple convex optimization problem which is guaranteed to converge to a single global solution
- Feature Selection

Strengths of SVMs

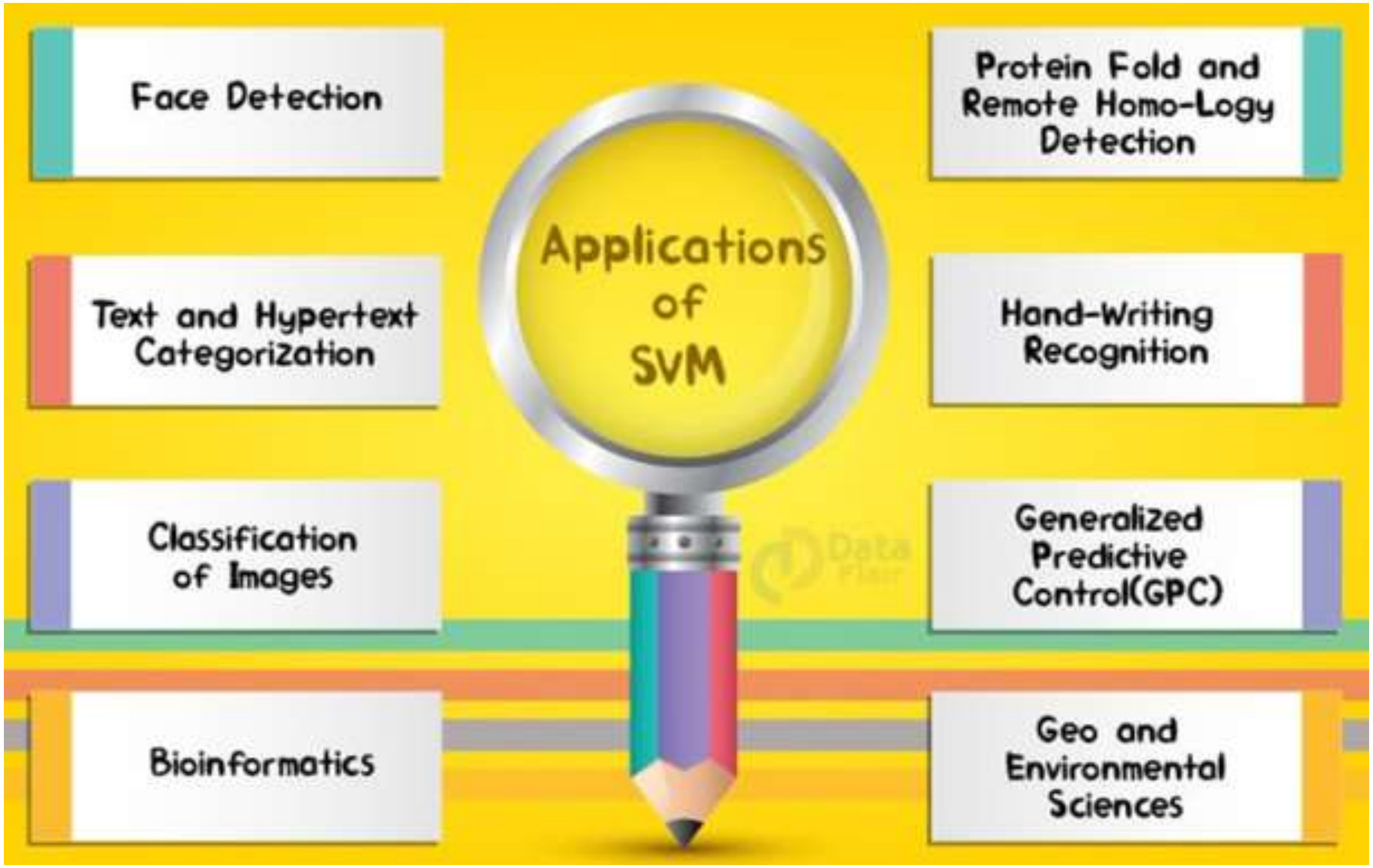
- Good generalization in theory
- Good generalization in practice
- Work well with few training instances
- Find globally best model
- Efficient algorithms
- Amenable to the kernel trick
- Although the SVM based classification (i.e., training time) is extremely slow, the result, is however highly accurate. Further, testing an unknown data is very fast.

Some Issues

- **Sensitive to noise**
  - A relatively small number of mislabeled examples can dramatically decrease the performance
- **Choice of kernel**
  - Gaussian or polynomial kernel is default
  - if ineffective, more elaborate kernels are needed
  - domain experts can give assistance in formulating appropriate similarity measures
- **Choice of kernel parameters**
  - e.g. σ in Gaussian kernel
  - σ is the distance between closest points with different classifications
  - In the absence of reliable criteria, applications rely on the use of a validation set or cross-validation to set such parameters.
- **Optimization criterion – Hard margin v.s. Soft margin**
  - a lengthy series of experiments in which various parameters are tested
- **Large data sets.**
  - Calculating the kernel is expensive.

SVM Applications

SVM has been used successfully in many real-world problems



Application : Text Categorization

- Task: The classification of natural text (or hypertext) documents into a fixed number of predefined categories based on their content.

  A document can be assigned to more than one category, so this can be viewed as a series of binary classification problems, one for each category

Text Categorization using SVM

- **The distance between two documents is $\phi(x)\cdot\phi(z)$**

- **$K(x,z) = \phi(x)\cdot\phi(z)$ is a valid kernel, SVM can be used with $K(x,z)$ for discrimination.**

- **Why SVM?**

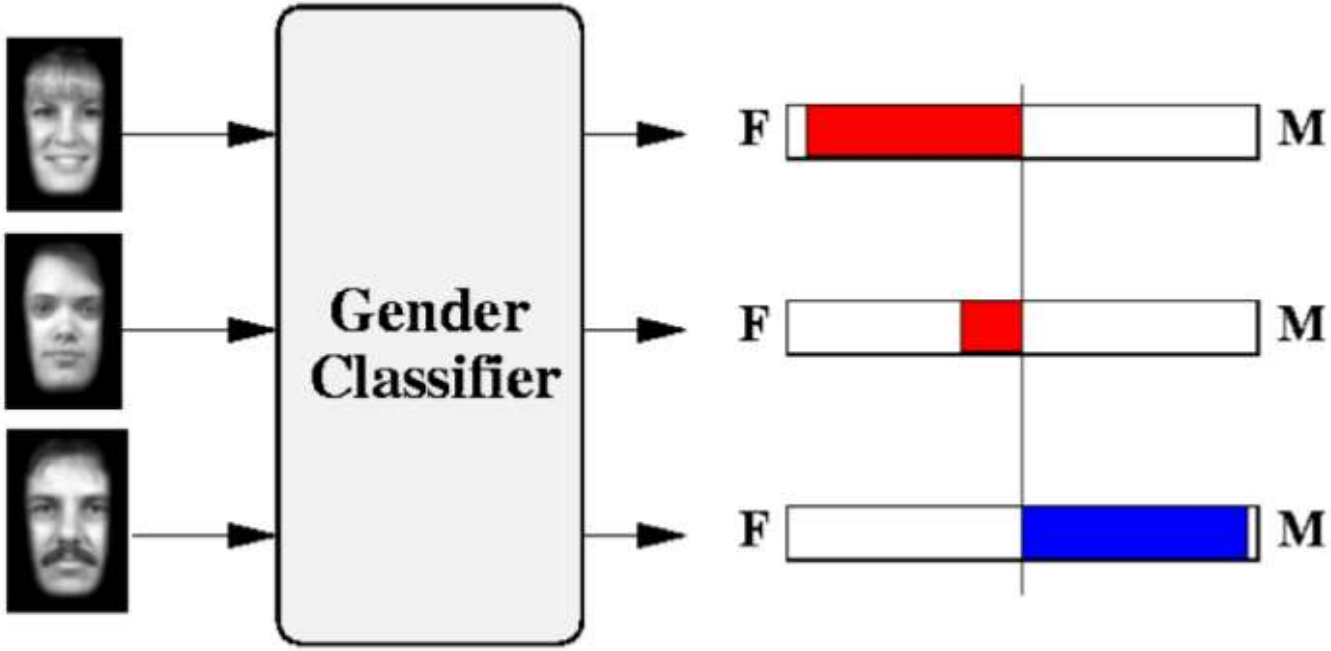
-High dimensional input space

-Few irrelevant features (dense concept)

-Sparse document vectors (sparse instances)

-Text categorization problems are linearly separable

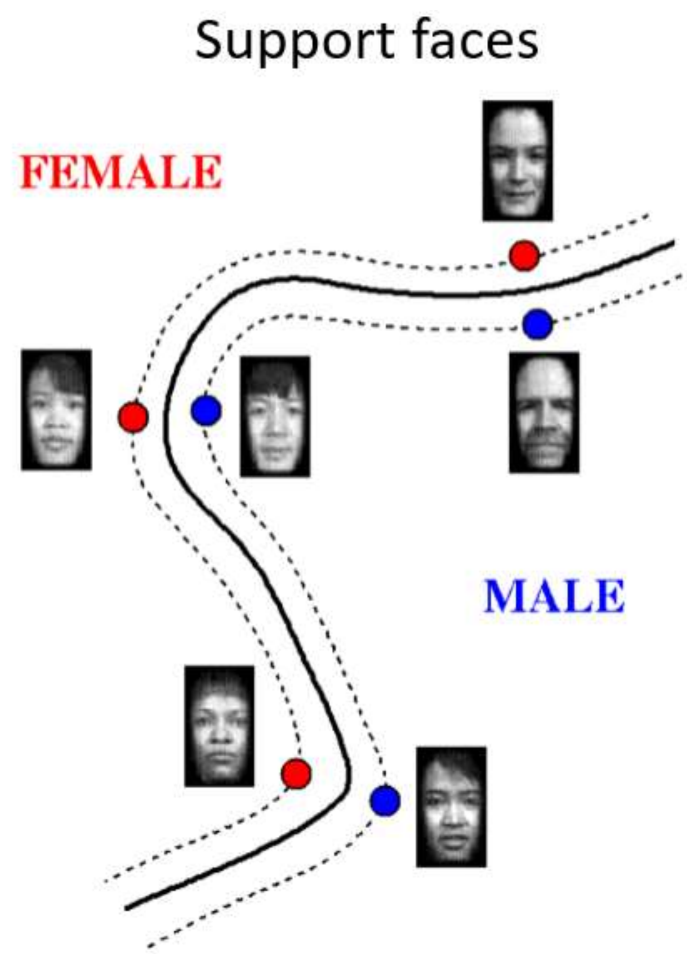
Learning Gender from image with SVM



Moghaddam and Yang, Learning Gender with Support Faces, TPAMI 2002

Moghaddam and Yang, Face & Gesture 2000

Support faces



Summary

SVM Points to remember

- Primal and Dual optimization problems
- Kernel functions
- Support Vector Machines
  - Maximizing margin
  - Derivation of SVM formulation
  - Slack variables and hinge loss
- Relationship between SVMs and logistic regression
  - 0/1 loss
  - Hinge loss
  - Log loss

Hard Margin versus Soft Margin

- **Hard Margin:**

Find $\mathbf{w}$ and b such that

$\mathbf{\Phi(w)} = \frac{\mathbf{1}}{\mathbf{2}}\,\mathbf{w}^{\mathrm{T}}\mathbf{w}$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$

$y_i\,(\mathbf{w^T x_i} + \mathrm{b}) \geq 1$

- **Soft Margin incorporating slack variables:**

Find $\mathbf{w}$ and b such that

$\mathbf{\Phi(w)} = \frac{\mathbf{1}}{\mathbf{2}}\,\mathbf{w}^{\mathrm{T}}\mathbf{w} + C\,\Sigma\,\xi_i$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$

$y_i\,(\mathbf{w^T x_i} + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$ for all i

- **Corresponding Lagrangian function**

$$L = \frac{1}{2}\|\vec{w}\|^2 + C\sum_i \xi_i + \sum_i \lambda_i (y_i(\vec{w}\,.\,\vec{x}_i + b) - 1 + \xi_i)$$

Soft Margin Vs Hard margin Classification – Solution

The dual problem

Find $\alpha_1 \ldots \alpha_N$ such that

$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i}^{\mathbf{T}}\mathbf{x_j}$ is maximized and

(1) $\Sigma\alpha_i y_i = 0$

(2) $\mathbf{0 \leq \alpha_i \leq C}$ **for all** $\boldsymbol{\alpha_i}$

Solution to the dual problem

$f(\mathbf{x}) = \Sigma\alpha_i y_i \mathbf{x_i}^{\mathbf{T}}\mathbf{x} + b$

$\mathbf{w} = \Sigma\alpha_i y_i \mathbf{x_i}$

$\boldsymbol{b = y_k(1- \xi_k) - \mathrm{w}^{\mathrm{T}}\mathrm{x}_k}$ **where** $\boldsymbol{k = \mathrm{argmax}\ \alpha_k{}'}$

Find $\alpha_1 \ldots \alpha_N$ such that

The dual problem

$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\left(\sum_i \sum_j \alpha_i \alpha_j y_i y_j \mathbf{x_i} \cdot \mathbf{x_j} \right)$ is maximized and

(1) $\Sigma\alpha_i y_i = 0$

(2) $\boldsymbol{\alpha_i \geq 0}$ **for all** $\boldsymbol{\alpha_i}$

Solution to the dual problem

$\mathrm{w} = \Sigma\, \alpha_i y_i \mathrm{x_i}$

$\mathbf{b} = y_i - \mathbf{W.x_i}$

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

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Thank You