Kernel methods for classification

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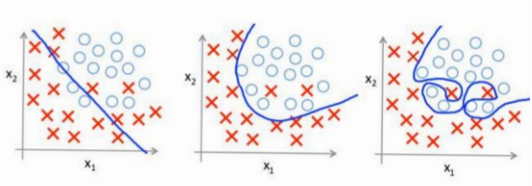
An example

3 classifiers trained over the dataset shown in the figure



Which one will perfom better over a different **test** dataset?
There is a tradeoff between:

- Training error / test error (generalization error, aka out-of-sample error)
- Bias/variance of the model/classifier

Statististical Learning Theory places these ideas in a mathematical framework, characterizing the properties of learning machines

Statistical Learning

- Supervised binary classification problem

$$f(\mathbf{x}) : \mathcal{X} \rightarrow \{\pm 1\}$$

- Training dataset: $(\mathcal{X}, \mathcal{Y}) = \{(\mathbf{x}_i, y_i)\}$
- **Loss function**: $l(\mathbf{x}, y, f)$ (e.g., $l(\mathbf{x}, y, f) = \frac{1}{2}|f(\mathbf{x}) - y|$)
- A good classifier should minimize the **risk or test error**

$$R[f] = \int \frac{1}{2}|f(\mathbf{x}) - y| dP(\mathbf{x}, y)$$

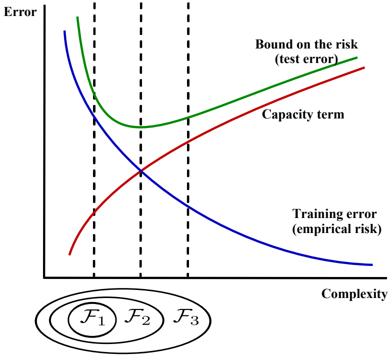
- As we are only given the training data, we can minimize only the **empirical risk or training error**

$$R_{emp}[f] = \sum_{i=1}^{n} \frac{1}{2}|f(\mathbf{x}_i) - y_i|$$

- The test error can be bounded as

$$R[f] \leq R_{emp}[f] + \phi(f)$$

where $\phi(f)$ is a capacity term that measures the complexity of the set of functions from which f is chosen
- It is imperative to restrict the set of functions $f(\mathbf{x})$



Structural Risk Minimization o **Regularized Empirical Risk Minimization**: To minimize a regularized version of the training error

$$\text{minimize} \quad R_{emp}[f] + \lambda\Omega(f),$$

where $\Omega(f)$ measures the complexity of the classifier (learning machine) and λ is the regularization parameter

- $\lambda \uparrow$ Simple models/class. boundaries
- $\lambda \downarrow$ More complex models/class. boundaries (**overfitting** risk)

Typically λ is estimated by cross-validation

Introducción

- Many machine learning algorithms (still) need a suitable **feature space** to perform satisfactorily
- Dimensionality reduction techniques (PCA/LDA) are routinely used in many applications

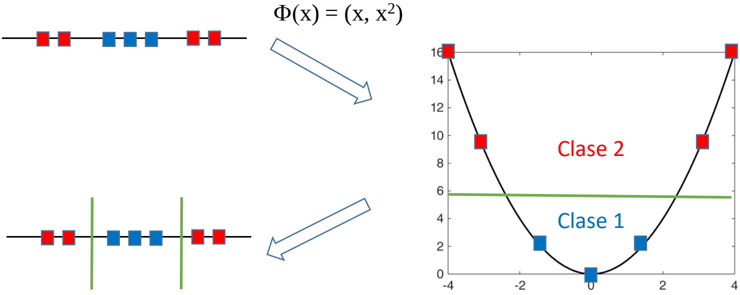
$$\mathbf{x}_i \in \mathcal{R}^d \longrightarrow \mathbf{W}\mathbf{x}_i \in \mathcal{R}^r, \qquad r < d$$

- Kernel methods follow a different approach: map the data to a higher dimensionality space

$$\mathbf{x}_i \in \mathcal{R}^d \longrightarrow \Phi(\mathbf{x}_i) \in \mathcal{R}^r, \qquad r >> d$$

Why?

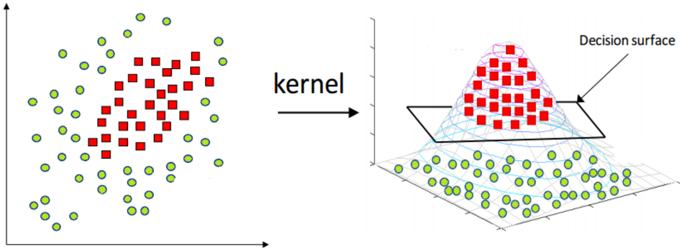
- Let's consider a simple binary 1D classification problem
- Training dataset: { -4, -3, -1, 0, 1, 3, 4 }



- $\Phi(x) = [x, x^2]^T$ produces a linearly separable problem in a 2D feature space

- In practice, there is no need to know the mapping $\Phi(\mathbf{x})$ explicitly
- We just need its **kernel** function

$$K(\mathbf{x}, \mathbf{x}') = \langle \Phi(\mathbf{x}), \Phi(\mathbf{x}') \rangle = \Phi(\mathbf{x})^T \Phi(\mathbf{x}')$$



- Kernel methods obtain a linear solution in the feature space, which becomes a nonlinear solution in the input space

Support Vector Machine (SVM)

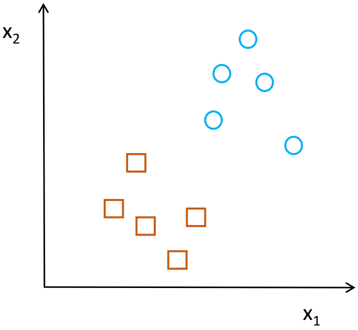
- The Support Vector Machine **SVM** is the most popular kernel machine for classification
- It solves a linear classification problem in the feature space applying the SRM principle

$$\min_{f(\cdot)\in\mathcal{F}} \quad \sum_{i=1}^{n} \frac{1}{2}|f(\mathbf{x}_i) - y_i| + \lambda\Omega(f)$$

- Let's start with the linear SVM working in the input space
  - $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$: **Optimal Hyperplane**

Linear SVM

- Binary classification problem: $\{(\mathbf{x}_i, y_i = \pm 1)\}$
- Linear classifier: $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b = \langle \mathbf{w}, \mathbf{x} \rangle + b$
- Linearly separable data: $y_i(\mathbf{w}^T\mathbf{x} + b) \geq 0,\ i = 1, \ldots, n$



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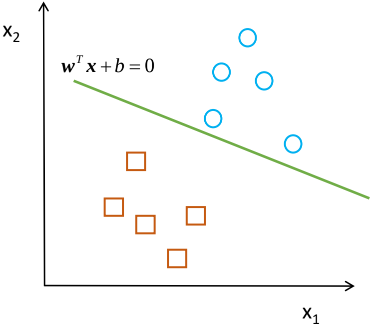

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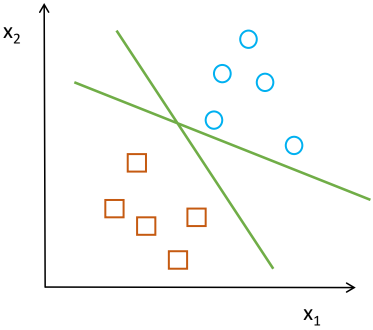

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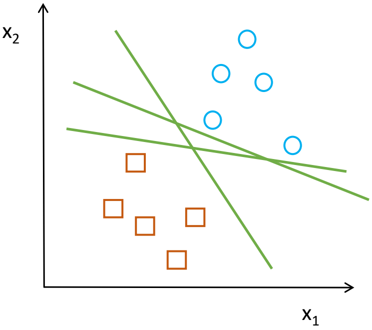
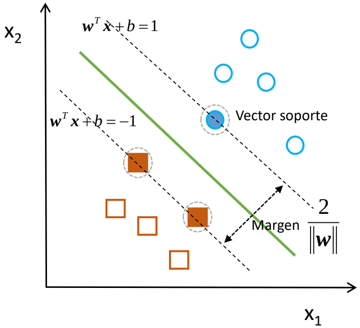


- Scale $\mathbf{w}$ and b so that the closest points to the hyperplane satisfy:

$$|\mathbf{w}^T\mathbf{x} + b| = 1 \implies y_i(\mathbf{w}^T\mathbf{x} + b) \geq 1, \ \forall i$$

- The optimal hyperplane maximizes the **margin**



- The support vectors $\mathbf{w}^T\mathbf{x}_j + b = \pm 1$ determine the optimal, or maximum margin, hyperplane

Optimization problem

$$
\begin{aligned}
\min_{\mathbf{w},b} \quad & \frac{1}{2}||\mathbf{w}||^2 \\
\text{s.t.} \quad & y_i\left(\mathbf{w}^T\mathbf{x}_i + b\right) \geq 1, \quad \forall i
\end{aligned}
$$

It is a **convex** problem → the solution is unique

Solution

- The Lagrangian is

$$\mathcal{L}(\mathbf{w}, b, \alpha) = \frac{1}{2}||\mathbf{w}||^2 + \sum_{i=1}^{n} \alpha_i \left(1 - y_i \left(\mathbf{w}^T \mathbf{x}_i + b\right)\right)$$

- Strong duality $\Rightarrow$ KKT optimality
  1. The optimal hyperplane is a linear combination of the input patterns

$$\nabla \mathcal{L}_{\mathbf{w}}(\mathbf{w}, b, \alpha) = \mathbf{w} + \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = 0 \Rightarrow \boxed{\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i}$$

  2. The optimal hyperplane only depends on a few (closest) patterns: the support vectors

$$\alpha_i \left(1 - y_i(\mathbf{w}^T \mathbf{x}_i + b)\right) = 0, \forall i \quad \Rightarrow \quad y_i(\mathbf{w}^T \mathbf{x}_i + b) = 1$$

  3. The bias b can be found from any support vector

Substituting $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$ in the Lagrangian, we obtain the **dual problem**, which is the problem we actually solve

$$\begin{array}{ll} \min\limits_{\boldsymbol{\alpha}} & \frac{1}{2}\sum_i \sum_j \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j - \sum_i \alpha_i \\ \text{s.t.} & \sum_i \alpha_i y_i = 0, \\ & \alpha_i \geq 0, \quad \forall i \end{array}$$

Defining $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)^T$, $\mathbf{1} = (1, \ldots, 1)^T$, $\mathbf{Y} = \operatorname{diag}(y_1, \ldots, y_n)$ and the $n \times n$ matrix $\mathbf{K}$ with elements $k(i,j) = \mathbf{x}_i^T \mathbf{x}_j = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$, the problem can be written as

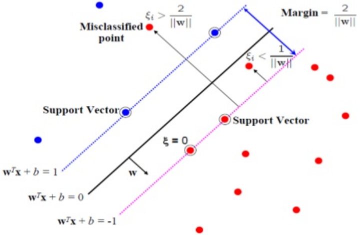
QP (Quadratic Programming) Problem

$$\begin{array}{ll} \min\limits_{\boldsymbol{\alpha}} & \frac{1}{2}\boldsymbol{\alpha}^T \mathbf{YKY} \boldsymbol{\alpha} - \mathbf{1}^T \boldsymbol{\alpha} \\ \text{s.t.} & \boldsymbol{\alpha}^T \mathbf{y} = 0, \\ & \boldsymbol{\alpha} \geq 0 \end{array}$$

Soft-margin SVM

- Non-linearly separable classes
- We introduce **slack variables** into the optimization problem to allow for classification errors: ξ_i
- Regularization parameter $C \rightarrow$ penalty
- Still a QP problem

$$
\begin{aligned}
\min_{\mathbf{w},b} \quad & \frac{1}{2}||\mathbf{w}||^2 + C\sum_i \xi_i \\
\text{s.t.} \quad & y_i\left(\mathbf{w}^T\mathbf{x}_i + b\right) \geq 1 - \xi_i, \quad \forall i \\
& \xi_i \geq 0 \quad \forall i
\end{aligned}
$$



Non-linear SVM

- The input patterns are mapped to a higher dimensionality (probably ∞) feature space: $\mathbf{x}_i \rightarrow \Phi(\mathbf{x}_i)$
- We solve a linear SVM problem in the feature space
- Optimal hyperplane in the feature space

$$\mathbf{w} = \sum_i \alpha_i y_i \Phi(\mathbf{x}_i)$$

- Same dual problem

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \quad & \tfrac{1}{2}\boldsymbol{\alpha}^T \mathbf{YKY}\boldsymbol{\alpha} - \mathbf{1}^T\boldsymbol{\alpha} \\ \text{s.t.} \quad & \boldsymbol{\alpha}^T \mathbf{y} = 0, \\ & 0 \leq \boldsymbol{\alpha} \leq C \end{aligned}$$

but now the $n \times n$ kernel matrix $\mathbf{K}$ has elements

$$k(i,j) = \Phi(\mathbf{x}_i)^T \Phi(\mathbf{x}_j) = \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_i) \rangle$$

- A linear classifier in the feature space

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

- But a nonlinear classifier in the input space
- The decision function can be expressed in terms of the kernel function

$$\begin{aligned} f(\mathbf{x}) &= \underbrace{\left(\sum_i \alpha_i y_i \Phi(\mathbf{x}_i) \right)^T}_{\mathbf{w}^T} \Phi(\mathbf{x}) + b \\ &= \sum_i \alpha_i y_i \Phi(\mathbf{x}_i)^T \Phi(\mathbf{x}) + b = \sum_i \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}) + b \end{aligned}$$

- This is the **kernel trick**!

Example: polynomial kernel

- Consider a problem with 2D patterns $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$
- And the following polynomial mapping to a feature 3D space

$$\Phi(\mathbf{x}) = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1 x_2 \end{bmatrix}$$

- The corresponding kernel function is

$$\begin{aligned} k(\mathbf{x}, \mathbf{y}) = & \quad \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle = \Phi(\mathbf{x})^T \Phi(\mathbf{y}) = \\ = & \quad x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 y_1 x_2 y_2 \end{aligned}$$

Kernel functions

Mercer Theorem (informal statement)

Any function $k(\cdot, \cdot)$ that produces a positive definite kernel matrix $\mathbf{K}$ for any training dataset

$$\mathbf{x}^T \mathbf{K} \mathbf{x} \geq 0, \qquad \forall \mathbf{x},$$

induces an inner product in a Hilbert space (feature space). That is,

$$k(\mathbf{x}_i, \mathbf{x}_j) = \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle = \Phi(\mathbf{x}_i)^T \Phi(\mathbf{x}_j)$$

- Note that the mapping $\Phi(\mathbf{x})$ does not have to be known
- As long as we choose a positive definite kernel $\Rightarrow$ QP dual problem

Kernels

- **Linear**

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

- **Polynomial** (parameters p y c)

$$k(\mathbf{x}_i, \mathbf{x}_j) = \left(\mathbf{x}_i^T \mathbf{x}_j + c\right)^p$$

- **Gaussian** (parameter σ^2)

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

- Let $k_1(\mathbf{x}, \mathbf{y})$ and $k_2(\mathbf{x}, \mathbf{y})$ be kernels, then the following functions are also kernels
  1. $k_1(\mathbf{x}, \mathbf{y}) + k_2(\mathbf{x}, \mathbf{y})$
  2. $k_1(\mathbf{x}, \mathbf{y}) k_2(\mathbf{x}, \mathbf{y})$
  3. $\exp(k_1(\mathbf{x}, \mathbf{y}))$
- The sigmoid function $\mathtt{tanh}\left(\mathbf{x}^T \mathbf{y} + b\right)$ is not a valid kernel

String kernel

It is also possible to define kernel functions over non-vectorial or non-Euclidean spaces (e.g., text strings)

- Given two sequences

$$\begin{aligned} s &= statistics \\ t &= computation \end{aligned}$$

- Generate all substrings of a given length (e.g., 3)

$$\begin{aligned} s &\rightarrow \{sta, tat, ati, tis, ist, sti, tic, ics\} \\ t &\rightarrow \{com, omp, mpu, put, uta, tat, ati, tio, ion\} \end{aligned}$$

- A string kernel can defined counting the number of common substrings

$$k(s,t) = 2$$

Other kernels can be defined over structured data: text (bag of words), graphs, times series, etc

Kernel matrix

The input to any kernel method is the kernel matrix

$$\mathbf{K} = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & k(\mathbf{x}_1, \mathbf{x}_2) & \cdots & k(\mathbf{x}_1, \mathbf{x}_n) \\ k(\mathbf{x}_2, \mathbf{x}_1) & k(\mathbf{x}_2, \mathbf{x}_2) & \cdots & k(\mathbf{x}_2, \mathbf{x}_n) \\ \vdots & \ddots & \ddots & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & k(\mathbf{x}_n, \mathbf{x}_2) & \cdots & k(\mathbf{x}_n, \mathbf{x}_n) \end{bmatrix}$$

- It is a Grammian matrix: matrix of inner products
- $k(\mathbf{x}_i, \mathbf{x}_j)$ measures the similarity between patterns
- $n \times n$ matrix: storage and computational complexities when $n \uparrow\uparrow$

The Gaussian kernel

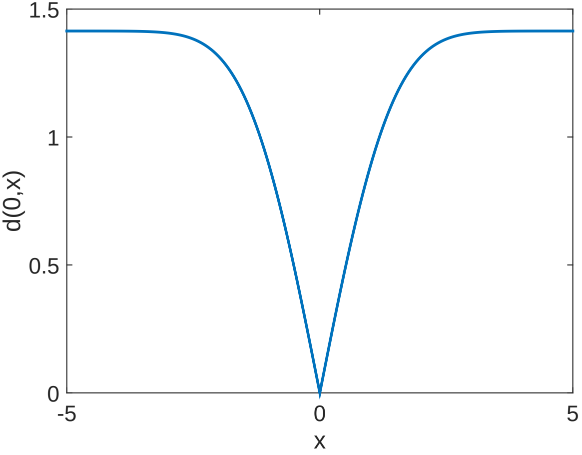
- The Gaussian kernel is an inner product in an infinite-dimensional feature space

$$k(\mathbf{x},\mathbf{y}) = \Phi(\mathbf{x})^T\Phi(\mathbf{y}) = e^{-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}}$$

- The distance between $\Phi(\mathbf{x})$ and $\Phi(\mathbf{y})$ is

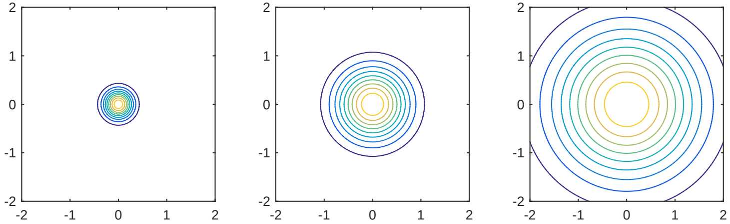
$$\begin{aligned} d(\Phi(\mathbf{x}),\Phi(\mathbf{y})) &= \sqrt{\|\Phi(\mathbf{x})-\Phi(\mathbf{y})\|^2} = \sqrt{2\left(1-e^{-\frac{\|\mathbf{x}-\mathbf{y}\|^2}{2\sigma^2}}\right)} \\ &= \sqrt{2\left(1-k(\mathbf{x},\mathbf{y})\right)} \end{aligned}$$

Example 1D, $\sigma^2 = 1$



Example 2D

$\sigma^2 = 0,2$ $\sigma^2 = 0{,}5$ $\sigma^2 = 1$



- $\sigma^2 \downarrow\downarrow$ local distance: all points beyond a given radius are at the same distance (equally far apart)
- $\sigma^2 \uparrow\uparrow$ global distance: like a linear kernel

Hyperparameters

- SVM with Gaussian kernel

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \quad & \tfrac{1}{2}\boldsymbol{\alpha}^T \mathbf{YKY}\boldsymbol{\alpha} - \mathbf{1}^T\boldsymbol{\alpha} \\ \text{s.t.} \quad & \boldsymbol{\alpha}^T\mathbf{y} = 0, \\ & 0 \leq \boldsymbol{\alpha} \leq C \end{aligned}$$

$$k(\mathbf{x}_i, \mathbf{x}_j) = e^{-\gamma\|\mathbf{x}-\mathbf{y}\|^2}$$

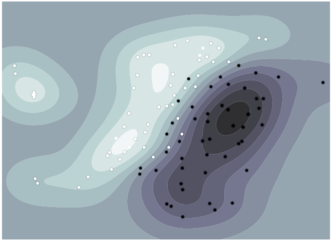
  where $\gamma = \frac{1}{2\sigma^2}$
- Choosing suitable hyperparameters γ and C is essential to get good performance
- Typically, there are selected by **cross-validation**

Regularization parameter: C

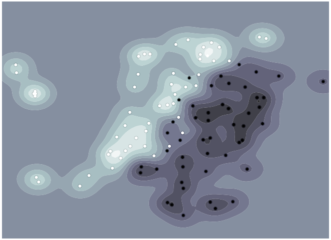
- C establishes a compromise between training error and model complexity
- $C\downarrow$ simple model, large training error, smooth decision boundary
- $C\uparrow$ complex model, small training error, non-smooth decision boundary, **overfitting** risk

Example

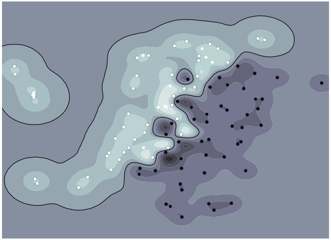
$C = 0.001$



$C = 0.01$



$C = 100$



Kernel size: γ

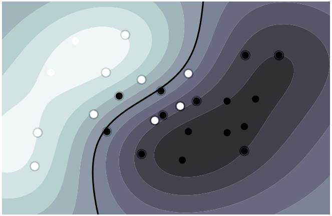
- The kernel size λ (a.k.a. bandwidth) controls how fast $k(\mathbf{x}, \mathbf{y}) \to 0$ as a function of the pairwise distance
- Recall that the SVM decision function for a new pattern $\mathbf{x}$ is

$$f(\mathbf{x}) = \sum_i \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}) + b \underset{C_0}{\overset{C_1}{\gtrless}} 0$$

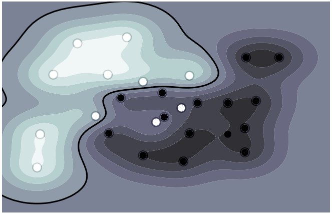
- $\gamma \downarrow$ large overlap among Gaussians, smooth decision boundary
- $\gamma \uparrow$ all patterns tend to be orthogonal to each other **overfitting**

Example

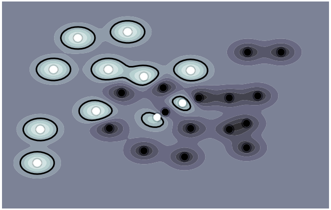
$\gamma = 0.001$



$\gamma = 0.01$

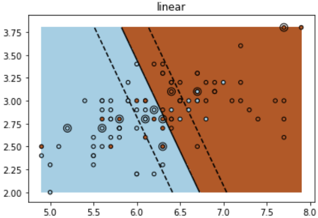


$\gamma = 100$

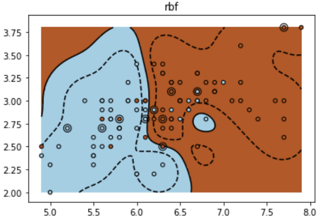


Kernel comparison

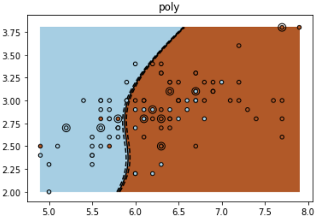
Linear $C = 1$



Gaussian $C = 1, \gamma = 10$



Polynomial $C = 1, \mathrm{order} = 10$



SVM solvers

- QP problem $\rightarrow$ **Interior Point Methods**
  1. Memory requirements for $\mathbf{K}$: $\mathcal{O}(n^2)$
  2. Slow convergence, computational complexity $\mathcal{O}(n^3)$
- More efficient (and scalable) algorithms exist
- **Sequential Minimal Optimization (SMO)**: it solves a sequence of smaller subproblems
- **LIBSVM**:
  - Standard SVM package
  - It applies a version of SMO
  - Interfaces in R, Matlab, Python,...

Multi-class SVM

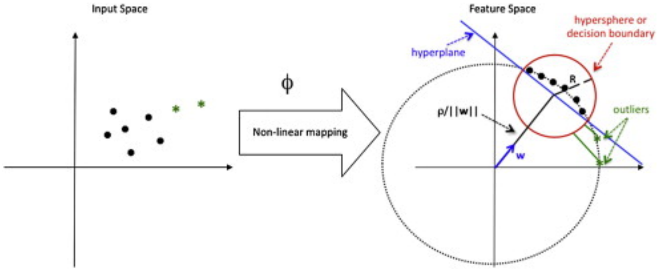
- Standard methodology: **One-Versus-All**
- For a problem with K classes we solve K independent binary problems
- Each SVM is trained to separate one class from the others
- With a new test pattern, $\mathbf{x}$, the k-th SVM outputs a score

$$f^k(\mathbf{x}) = \sum_i \alpha_i^k y_i^k k(\mathbf{x}_i^k, \mathbf{x}) + b^k, \qquad k = 1, \ldots, K$$

- The class finally assigned to $\mathbf{x}$ is the one providing a highest score

$$k^* = \underset{k}{\operatorname{argmax}}\, f^k(\mathbf{x})$$

One-class SVM



- Goal: to find an SVM that encloses most of the data
- Outlier/Novelty detection
- We can separate normal data from outliers in the feature space through
  - A hyperplane (see figure)
  - A hypersphere

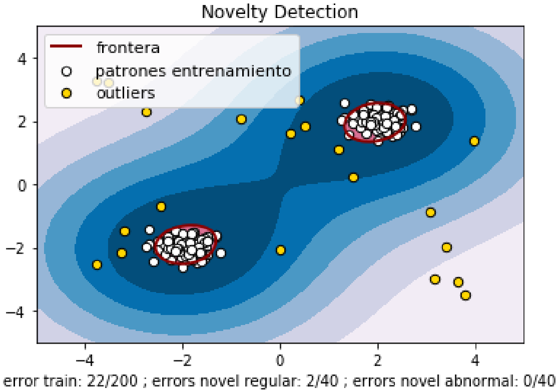
One-class SVM

$$\begin{aligned} \min_{\mathbf{w},\xi_i,\rho} \quad & \frac{1}{2}||\mathbf{w}||^2 + \frac{1}{\nu n}\sum_{i=1}^{n} \xi_i - \rho \\ \text{s.t.} \quad & \mathbf{w}^T\Phi(\mathbf{x}_i) \geq \rho - \xi_i, \qquad \forall i \\ & \xi_i \geq 0 \qquad \forall i \end{aligned}$$

- Dual problem equivalent to that of a conventional SVM
- The parameter ν characterizes the solution $\rightarrow$ **ν-SVM**
  - An upper bound on the fraction of outliers
  - A lower bound on the fraction of support vectors

Example

- ν-SVM, Gaussian kernel, $\gamma = 0{,}1$, $\nu = 0{,}1$



Conclusions

- SVM: one of the most popular learning machines
- Derived from the Structural Risk Minimization principle
- QP problem: unique minimum, well-defined problem
- A kernel (measuring the similarity between patterns)+ regularization parameter + hyperparameters
- Sparse solution: it admits an expansion in terms of a few patterns (support vectors)
- Still competitive results in a number of applications