Lecture 9: Support Vector Machines II

Reading: Section 12.3

GU4241/GR5241 Statistical Machine Learning

Linxi Liu
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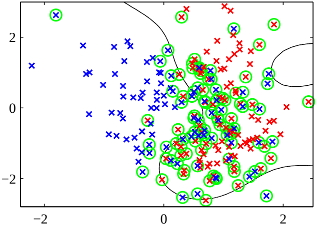
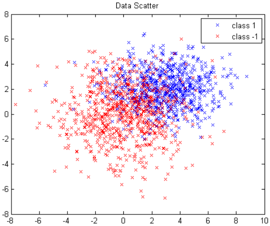
Motivation

More realistic data





Motivation: Kernels

Idea

- The SVM uses the scalar product $\langle \mathbf{x}, \tilde{\mathbf{x}}_i \rangle$ as a measure of similarity between $\mathbf{x}$ and $\tilde{\mathbf{x}}_i$, and of distance to the hyperplane.
- Since the scalar product is linear, the SVM is a linear method.
- By using a *nonlinear* function instead, we can make the classifier nonlinear.

Kernels in Detail

- Scalar product can be regarded as a two-argument function

$$\langle\, .\, ,\, .\,\rangle : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$$

- We will replace this function with a function $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ and substitute

$$k(\mathbf{x}, \mathbf{x}') \qquad \text{for every occurrence of} \qquad \langle \mathbf{x}, \mathbf{x}' \rangle$$

  in the SVM formula.
- Under certain conditions on k, all optimization/classification results for the SVM still hold. Functions that satisfy these conditions are called **kernel functions**.

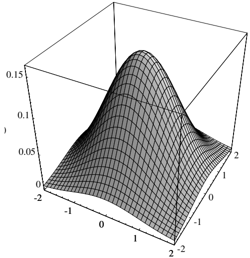
The Most Popular Kernel

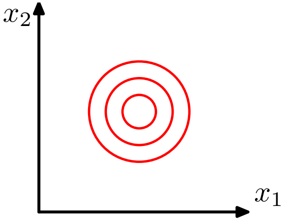
RBF Kernel

$$k_{\mathsf{RBF}}(\mathbf{x}, \mathbf{x}') := \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|_2^2}{2\sigma^2}\right) \qquad \text{for some } \sigma \in \mathbb{R}_+$$

is called an **RBF kernel** (RBF = radial basis function). The parameter σ is called **bandwidth**.
Other names for k_{RBF}: Gaussian kernel, squared-exponential kernel.

If we fix $\mathbf{x}'$, the function $k_{\mathsf{RBF}}(\,.\,, \mathbf{x}')$ is (up to scaling) a spherical Gaussian density on $\mathbb{R}^d$, with mean $\mathbf{x}'$ and standard deviation σ.





contours (d=2)

Choosing a kernel

Theory

To define a kernel:

- We have to define a function of two arguments and prove that it is a kernel.
- This is done by checking a set of necessary and sufficient conditions known as "Mercer's theorem".

Practice

The data analyst does not define a kernel, but tries some well-known standard kernels until one seems to work. Most common choices:

- The RBF kernel.
- The "linear kernel" $k_{\mathsf{SP}}(\mathbf{x}, \mathbf{x}') = \langle \mathbf{x}, \mathbf{x}' \rangle$, i.e. the standard, linear SVM.

Once kernel is chosen

- Classifier can be trained by solving the optimization problem using standard software.
- SVM software packages include implementations of most common kernels.

Which Functions work as Kernels?

Formal definition

A function $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is called a **kernel** on $\mathbb{R}^d$ if there is *some* function $\phi : \mathbb{R}^d \to \mathcal{F}$ into *some* space $\mathcal{F}$ with scalar product $\langle\, .\, ,\, .\, \rangle_{\mathcal{F}}$ such that

$$k(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle_{\mathcal{F}} \qquad \text{for all } \mathbf{x}, \mathbf{x}' \in \mathbb{R}^d \,.$$

In other words

- k is a kernel if it can be interpreted as a scalar product on some other space.
- If we substitute $k(\mathbf{x}, \mathbf{x}')$ for $\langle \mathbf{x}, \mathbf{x}' \rangle$ in all SVM equations, we implicitly train a *linear* SVM on the space $\mathcal{F}$.
- The SVM still works: It still uses scalar products, just on another space.

The mapping ϕ

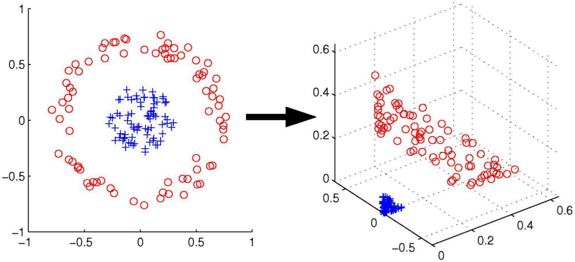
- ϕ has to transform the data into data on which a linear SVM works well.
- This is usually achieved by choosing $\mathcal{F}$ as a higher-dimensional space than $\mathbb{R}^d$.

Mapping into Higher Dimensions

Example

How can a map into higher dimensions make class boundary (more) linear?
Consider

$$\phi : \mathbb{R}^2 \to \mathbb{R}^3 \qquad \text{where} \qquad \phi\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} := \begin{pmatrix} x_1^2 \\ 2x_1x_2 \\ x_2^2 \end{pmatrix}$$



Mapping into Higher Dimensions

Problem

In previous example: We have to know what the data looks like to choose ϕ!

Solution

- Choose high dimension h for $\mathcal{F}$.
- Choose components ϕ_i of $\phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \ldots, \phi_h(\mathbf{x}))$ as different nonlinear mappings.
- If two points differ in $\mathbb{R}^d$, some of the nonlinear mappings will amplify differences.

The RBF kernel is an extreme case

- The function k_{RBF} can be shown to be a kernel, however:
- $\mathcal{F}$ is infinite-dimensional for this kernel.

Determining whether k is a kernel

Mercer's theorem

A mathematical result called *Mercer's theorem* states that, if the function k is positive, i.e.

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} k(\mathbf{x}, \mathbf{x}') f(\mathbf{x}) f(\mathbf{x}') d\mathbf{x} d\mathbf{x}' \geq 0$$

for all functions f, then it can be written as

$$k(\mathbf{x}, \mathbf{x}') = \sum_{j=1}^{\infty} \lambda_j \phi_j(\mathbf{x}) \phi_j(\mathbf{x}') \ .$$

The ϕ_j are functions $\mathbb{R}^d \to \mathbb{R}$ and $\lambda_i \geq 0$. This means the (possibly infinite) vector $\phi(\mathbf{x}) = (\sqrt{\lambda_1}\phi_1(\mathbf{x}), \sqrt{\lambda_2}\phi_2(\mathbf{x}), \ldots)$ is a feature map.

Kernel arithmetic

Various functions of kernels are again kernels: If k_1 and k_2 are kernels, then e.g.

$$k_1 + k_2 \qquad\qquad k_1 \cdot k_2 \qquad\qquad \text{const.} \cdot k_1$$

are again kernels.

The Kernel Trick

Kernels in general

- Many linear machine learning and statistics algorithms can be "kernelized".
- The only conditions are:
  1. The algorithm uses a scalar product.
  2. In all relevant equations, the data (and all other elements of $\mathbb{R}^d$) appear *only inside a scalar product*.
- This approach to making algorithms non-linear is known as the "kernel trick".

Kernel SVM

Optimization problem

$$\min_{\mathbf{v}_{\mathsf{H}}, c} \quad \|\mathbf{v}_{\mathsf{H}}\|_{\mathcal{F}}^2 + \gamma \sum_{i=1}^{n} \xi^2$$

$$\text{s.t.} \quad \tilde{y}_i(\langle \mathbf{v}_{\mathsf{H}}, \phi(\tilde{\mathbf{x}}_i) \rangle_{\mathcal{F}} - c) \geq 1 - \xi_i \quad \text{and } \xi_i \geq 0$$

Note: $\mathbf{v}_{\mathsf{H}}$ now lives in $\mathcal{F}$, and $\| \, . \, \|_{\mathcal{F}}$ and $\langle \, . \, , \, . \, \rangle_{\mathcal{F}}$ are norm and scalar product on $\mathcal{F}$.

Dual optimization problem

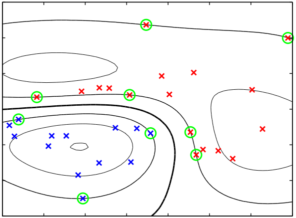
$$\max_{\boldsymbol{\alpha} \in \mathbb{R}^n} \quad W(\boldsymbol{\alpha}) := \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j \tilde{y}_i \tilde{y}_j \left(k(\tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_j) + \frac{1}{\gamma} \mathbb{I}\{i = j\} \right)$$

$$\text{s.t.} \quad \sum_{i=1}^{n} \tilde{y}_i \alpha_i = 0 \quad \text{and} \quad \alpha_i \geq 0$$

Classifier

$$f(\mathbf{x}) = \operatorname{sgn} \left(\sum_{i=1}^{n} \tilde{y}_i \alpha_i^* k(\tilde{\mathbf{x}}_i, \mathbf{x}) - c \right)$$

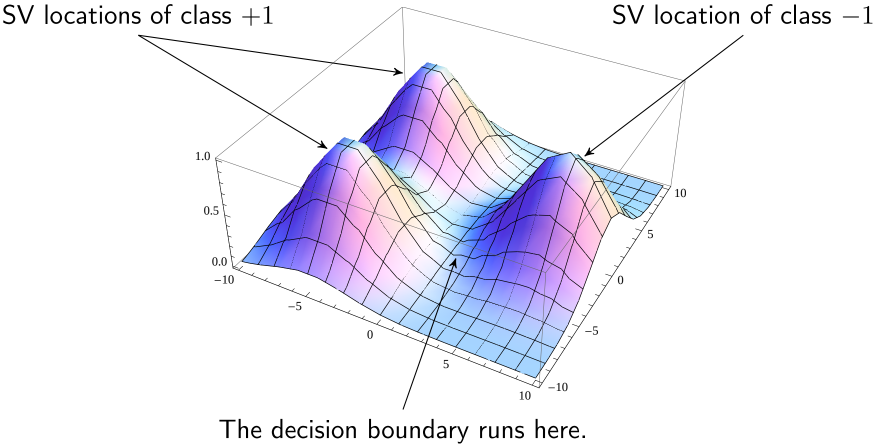
SVM with RBF Kernel



$$f(\mathbf{x}) = \text{sign}\left(\sum_{i=1}^{n} y_i \alpha_i^* k_{\textsf{RBF}}(\mathbf{x}_i, \mathbf{x})\right)$$

- Circled points are support vectors. The the two contour lines running through support vectors are the nonlinear counterparts of the convex hulls.
- The thick black line is the classifier.
- Think of a Gaussian-shaped function $k_{\textsf{RBF}}(\,.\,, \mathbf{x}')$ centered at each support vector $\mathbf{x}'$. These functions add up to a function surface over $\mathbb{R}^2$.
- The lines in the image are contour lines of this surface. The classifier runs along the bottom of the "valley" between the two classes.
- Smoothness of the contours is controlled by σ

Decision Boundary with RBF Kernel



The decision boundary of the classifier coincides with the set of points where the surfaces for class $+1$ and class -1 have equal value.

Summary: SVMs

Basic SVM

- Linear classifier for linearly separable data.
- Positions of affine hyperplane is determined by maximizing margin.
- Maximizing the margin is a convex optimization problem.

Full-fledged SVM

Ingredient	Purpose
Maximum margin	Good generalization properties
Slack variables	Overlapping classes
	Robustness against outliers
Kernel	Nonlinear decision boundary

Use in practice

- Software packages (e.g. libsvm, SVMLite)
- Choose a kernel function (e.g. RBF)
- Cross-validate margin parameter γ and kernel parameters (e.g. bandwidth)