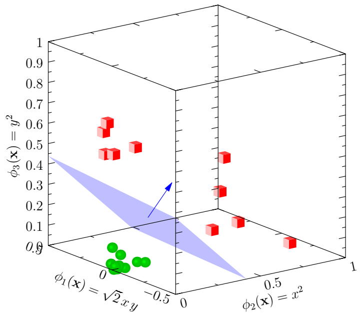
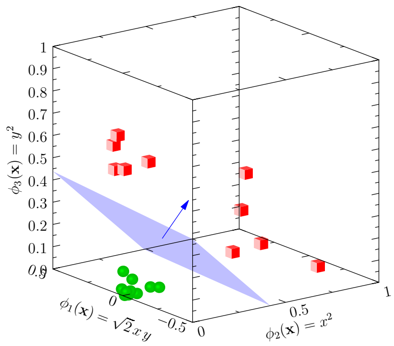
Advanced Machine Learning

Kernel Trick



The Kernel Trick, SVMs, Regression

Outline



SVM Kernels

- SVM Kernels are functions of two variables that can be factorised

$$K(\boldsymbol{x},\boldsymbol{y}) = \langle \boldsymbol{\phi}(\boldsymbol{x}),\boldsymbol{\phi}(\boldsymbol{y})\rangle = \sum_i \phi_i(\boldsymbol{x})\phi_i(\boldsymbol{y})$$

- where $\boldsymbol{\phi}(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}),\phi_2(\boldsymbol{x}),\ldots)^\mathsf{T}$ and $\phi_i(\boldsymbol{x})$ are real valued functions of $\boldsymbol{x}$
- $K(\boldsymbol{x},\boldsymbol{y})$ will be positive semi-definite (because it is an inner-product)
- Furthermore, any positive semi-definite function will factorise
- This factorisation is not always obvious (we return to this later)

Dual Form

- Recall that the dual problem for an SVM is

$$\max_{\boldsymbol{\alpha}} \sum_{k=1}^m \alpha_k - \frac{1}{2}\sum_{k,l=1}^m \alpha_k\alpha_l y_k y_l \langle \boldsymbol{\phi}(\boldsymbol{x}_k),\boldsymbol{\phi}(\boldsymbol{x}_l)\rangle$$

- subject to $\sum_{k=1}^m y_k\alpha_k = 0$ and $0 \le \alpha_k (\le C)$
- But since $K(\boldsymbol{x}_k,\boldsymbol{x}_l) = \langle \boldsymbol{\phi}(\boldsymbol{x}_k),\boldsymbol{\phi}(\boldsymbol{x}_l)\rangle$ the dual problem becomes

$$\max_{\boldsymbol{\alpha}} \sum_{k=1}^m \alpha_k - \frac{1}{2}\sum_{k,l=1}^m \alpha_k\alpha_l y_k y_l K(\boldsymbol{x}_k,\boldsymbol{x}_l)$$

- This is the **kernel trick**—we never have to compute $\boldsymbol{\phi}(\boldsymbol{x})$!

Classifying New Data

- Having trained the SVM we now have to use it
- Given a new input $\boldsymbol{x}$ we decide on the class

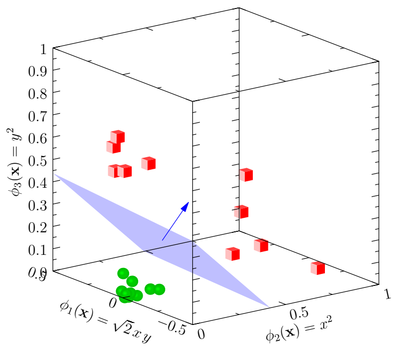
$$y = \mathrm{sgn}(\langle \boldsymbol{w},\boldsymbol{\phi}(\boldsymbol{x})\rangle - b) \qquad \text{but} \qquad \boldsymbol{w} = \sum_{k=1}^m \alpha_k y_k \boldsymbol{\phi}(\boldsymbol{x}_k)$$

- In the dual representation this becomes

$$\mathrm{sgn}\left(\sum_{k=1}^m \alpha_k y_k K(\boldsymbol{x}_k,\boldsymbol{x}) - b\right)$$

where we only need to sum over the non-zero α_k (i.e. the support vectors SVs)

Outline



Recap on Eigen Systems

- Recall for a symmetric $(n \times n)$ matrix $\mathbf{M}$ an eigenvector, $\boldsymbol{v}$

$$\mathbf{M}\boldsymbol{v} = \lambda\boldsymbol{v}$$

- There are n independent eigenvectors $\boldsymbol{v}^{(i)}$ with real eigenvalues $\lambda^{(i)}$
- The eigenvectors are orthogonal so that $\boldsymbol{v}^{(i)\mathsf{T}}\boldsymbol{v}^{(j)} = 0$ if $i \neq j$
- Forming a matrix of eigenvectors $\mathbf{V} = (\boldsymbol{v}^{(1)},\boldsymbol{v}^{(2)},\ldots\boldsymbol{v}^{(n)})$ the matrix satisfies

$$\mathbf{V}^\mathsf{T}\mathbf{V} = \mathbf{V}\mathbf{V}^\mathsf{T} = \mathbf{I}$$

- Such matrices are said to be orthogonal

Eigen Decomposition

- From the eigenvalue equation $\mathbf{M}\boldsymbol{v}^{(k)} = \lambda^{(k)}\boldsymbol{v}^{(k)}$

$$\mathbf{M}\mathbf{V} = \mathbf{V}\boldsymbol{\Lambda} \qquad \text{where} \quad \boldsymbol{\Lambda} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}$$

- Multiplying on the right by $\mathbf{V}^\mathsf{T}$ we get

$$\mathbf{M} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^\mathsf{T} = \sum_{k=1}^n \lambda^{(k)}\boldsymbol{v}^{(k)}\boldsymbol{v}^{(k)\mathsf{T}}$$

Or

$$M_{ij} = \sum_{k=1}^n \lambda^{(k)} v_i^{(k)} v_j^{(k)} = \sum_{k=1}^n u_i^{(k)} u_j^{(k)} = \langle \boldsymbol{u}_i,\boldsymbol{u}_j\rangle$$

$$u_i^{(k)} = \sqrt{\lambda^{(k)}}\, v_i^{(k)}$$

Eigenfunctions

- By analogy for a symmetric function of two variables we can define an *eigenfunction*

$$\int K(\boldsymbol{x},\boldsymbol{y})\psi(\boldsymbol{y})\mathrm{d}\boldsymbol{y} = \lambda\psi(\boldsymbol{x})$$

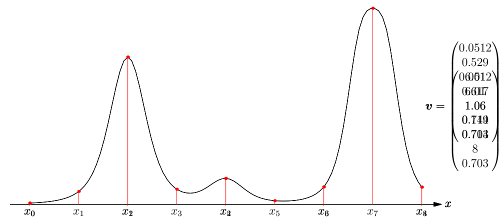
- In general there will be a denumerable set of eigenfunctions $\psi^{(k)}(\boldsymbol{x})$ where

$$K(\boldsymbol{x},\boldsymbol{y}) = \sum_k \lambda^{(k)}\psi^{(k)}(\boldsymbol{x})\psi^{(k)}(\boldsymbol{y})$$

- This is known as Mercer's theorem

Limit Process

- Consider sampling a function at a set of points

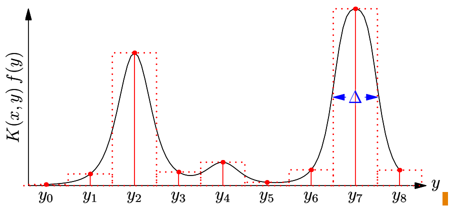


- In the limit where the number of sample points goes to infinity the vector more closely approximates a function
- Instead of the indices being numbers we use $k \leftarrow x_k$

Linear Operators

- Recall a linear function $\mathcal{T}[f(x)]$ can be represented by a kernel

$$\mathcal{T}[f(x)] = \int_{y\in\mathcal{I}} K(x,y)f(y)\mathrm{d}y \approx \Delta\sum_{j=1}^{n} K(x,y_j)f(y_j)$$



This is just a matrix equation with $M_{ij} = \Delta K(x_i,y_j)$

SVM Kernels

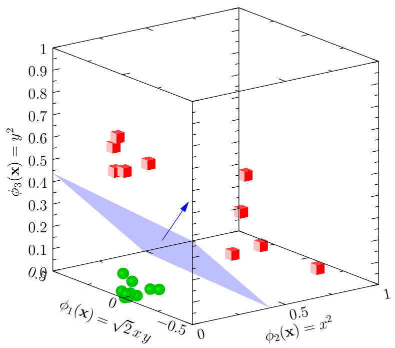
- If we define $\phi^{(k)}(\boldsymbol{x}) = \sqrt{\lambda^{(k)}}\psi^{(k)}(\boldsymbol{x})$ then

$$K(\boldsymbol{x},\boldsymbol{y}) = \sum_k \lambda^{(k)}\psi^{(k)}(\boldsymbol{x})\psi^{(k)}(\boldsymbol{y}) = \sum_k \phi^{(k)}(\boldsymbol{x})\phi^{(k)}(\boldsymbol{y})$$

- This is the definition of a SVM kernel we started with
- Note that for $\phi^{(k)}(\boldsymbol{x})$ to be real $\lambda^{(k)} \geq 0$ for all k
- If $\lambda^{(k)} < 0$ then $\langle\boldsymbol{\phi}(\boldsymbol{x}),\boldsymbol{\phi}(\boldsymbol{x})\rangle = \|\boldsymbol{\phi}(\boldsymbol{x})\|^2$ might be negative and "distance" between points in the extended feature space can be negative!
- If we use a kernel that isn't positive semi-definite then the Hessian of the dual objective function will not be negative semi-definite and there will be a maximum where $\boldsymbol{\alpha}$ diverges

Outline

1. The Kernel Trick
2. Positive Semi-Definite Kernels
3. **Kernel Properties**
4. Beyond Classification



Positive Semi-Definite Kernels

- Kernels (or matrices) that have eigenvalues $\lambda^{(k)} \geq 0$ are called positive semi-definite
- (If the eigenvalues are strictly positive $\lambda^{(k)} > 0$ the kernels or matrices are called positive definite)
- Positive semi-definite kernels can always be decomposed into a sum of real functions

$$K(\boldsymbol{x},\boldsymbol{y}) = \langle\boldsymbol{\phi}(\boldsymbol{x}),\boldsymbol{\phi}(\boldsymbol{y})\rangle$$

Properties of Positive Semi-Definiteness

- Since

$$K(\boldsymbol{x},\boldsymbol{y}) = \langle\boldsymbol{\phi}(\boldsymbol{x}),\boldsymbol{\phi}(\boldsymbol{y})\rangle$$

- An immediate consequence is that for any function $f(\boldsymbol{x})$

$$\begin{aligned}\int f(\boldsymbol{x})K(\boldsymbol{x},\boldsymbol{y})f(\boldsymbol{y})\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} &= \int f(\boldsymbol{x})\langle\boldsymbol{\phi}(\boldsymbol{x}),\boldsymbol{\phi}(\boldsymbol{y})\rangle f(\boldsymbol{y})\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y}\\ &= \left\langle\int f(\boldsymbol{x})\boldsymbol{\phi}(\boldsymbol{x})\mathrm{d}\boldsymbol{x},\int f(\boldsymbol{y})\boldsymbol{\phi}(\boldsymbol{y})\mathrm{d}\boldsymbol{y}\right\rangle\\ &= \left\|\int f(\boldsymbol{x})\boldsymbol{\phi}(\boldsymbol{x})\mathrm{d}\boldsymbol{x}\right\|^2 \geq 0\end{aligned}$$

Positive Semi-Definiteness

- The following statements are equivalent
  - $K(\boldsymbol{x},\boldsymbol{y})$ is positive semi-definite (written $K(\boldsymbol{x},\boldsymbol{y}) \succeq 0$)
  - The eigenvalues of $K(\boldsymbol{x},\boldsymbol{y})$ are non-negative
  - The kernel can be written

$$K(\boldsymbol{x},\boldsymbol{y}) = \langle\boldsymbol{\phi}(\boldsymbol{x}),\boldsymbol{\phi}(\boldsymbol{y})\rangle$$

    where the $\phi^{(k)}(\boldsymbol{x})$'s are real functions
  - For any real function $f(x)$

$$\int f(\boldsymbol{x})K(\boldsymbol{x},\boldsymbol{y})f(\boldsymbol{y})\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} \geq 0$$

Adding Kernels

- We can construct SVM kernels from other kernels
- If $K_1(\boldsymbol{x},\boldsymbol{y})$ and $K_2(\boldsymbol{x},\boldsymbol{y})$ are valid kernels then so is $K_3(\boldsymbol{x},\boldsymbol{y}) = K_1(\boldsymbol{x},\boldsymbol{y}) + K_2(\boldsymbol{x},\boldsymbol{y})$

$$\begin{aligned} Q &= \int f(\boldsymbol{x}) K_3(\boldsymbol{x},\boldsymbol{y}) f(\boldsymbol{y}) \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} \\ &= \int f(\boldsymbol{x}) \left(K_1(\boldsymbol{x},\boldsymbol{y}) + K_2(\boldsymbol{x},\boldsymbol{y})\right) f(\boldsymbol{y}) \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} \\ &= \int f(\boldsymbol{x}) K_1(\boldsymbol{x},\boldsymbol{y}) f(\boldsymbol{y}) \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} + \int f(\boldsymbol{x}) K_2(\boldsymbol{x},\boldsymbol{y}) f(\boldsymbol{y}) \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} \geq 0 \end{aligned}$$

- If $K(\boldsymbol{x},\boldsymbol{y})$ is a valid kernel so is $cK(\boldsymbol{x},\boldsymbol{y})$ for $c > 0$

Product of Kernels

- If $K_1(\boldsymbol{x},\boldsymbol{y})$ and $K_2(\boldsymbol{x},\boldsymbol{y})$ are valid kernels then so is $K_3(\boldsymbol{x},\boldsymbol{y}) = K_1(\boldsymbol{x},\boldsymbol{y}) K_2(\boldsymbol{x},\boldsymbol{y})$
- Writing

$$K_1(\boldsymbol{x},\boldsymbol{y}) = \sum_i \phi_i^{(1)}(\boldsymbol{x})\phi_i^{(1)}(\boldsymbol{y}), \qquad K_2(\boldsymbol{x},\boldsymbol{y}) = \sum_j \phi_j^{(2)}(\boldsymbol{x})\phi_j^{(2)}(\boldsymbol{y})$$

then

$$\begin{aligned} K_3(\boldsymbol{x},\boldsymbol{y}) &= \sum_{i,j} \phi_i^{(1)}(\boldsymbol{x})\phi_i^{(1)}(\boldsymbol{y})\phi_j^{(2)}(\boldsymbol{x})\phi_j^{(2)}(\boldsymbol{y}) \\ &= \sum_{i,j} \phi_{ij}^{(3)}(\boldsymbol{x})\phi_{ij}^{(3)}(\boldsymbol{y}) = \left\langle \boldsymbol{\phi}^{(3)}(\boldsymbol{x}), \boldsymbol{\phi}^{(3)}(\boldsymbol{y}) \right\rangle \end{aligned}$$

where $\phi_{ij}^{(3)}(\boldsymbol{x}) = \phi_i^{(1)}(\boldsymbol{x})\phi_j^{(2)}(\boldsymbol{x})$

Exponentiating Kernels

- If $K(\boldsymbol{x},\boldsymbol{y})$ is a valid kernel so is $K^n(\boldsymbol{x},\boldsymbol{y})$ (by induction)
  - Assume $K(\boldsymbol{x},\boldsymbol{y}) \succeq 0$ this satisfies base case
  - If $K^{n-1}(\boldsymbol{x},\boldsymbol{y}) \succeq 0$ then

$$K^n(\boldsymbol{x},\boldsymbol{y}) = K^{n-1}(\boldsymbol{x},\boldsymbol{y}) K(\boldsymbol{x},\boldsymbol{y}) \succeq 0$$

- and $\exp(K(\boldsymbol{x},\boldsymbol{y}))$ is also a valid kernel since

$$\mathrm{e}^{K(\boldsymbol{x},\boldsymbol{y})} = \sum_{i=1} \frac{1}{i!} K^i(\boldsymbol{x},\boldsymbol{y}) = 1 + K(\boldsymbol{x},\boldsymbol{y}) + \frac{1}{2}K^2(\boldsymbol{x},\boldsymbol{y}) + \cdots$$

but each term in the sum is a kernel

RBF Kernel

- Now $\boldsymbol{x}^\mathsf{T}\boldsymbol{y} = \langle \boldsymbol{x},\boldsymbol{y} \rangle$ is a valid kernel because it is an inner product of functions $\boldsymbol{\phi}(\boldsymbol{x}) = \boldsymbol{x}$
- For $\gamma > 0$ we have $2\gamma\boldsymbol{x}^\mathsf{T}\boldsymbol{y} \succeq 0$
- Thus $\exp(2\gamma\boldsymbol{x}^\mathsf{T}\boldsymbol{y}) \succeq 0$
- If $K(\boldsymbol{x},\boldsymbol{y}) \succeq 0$ then $g(\boldsymbol{x})K(\boldsymbol{x},\boldsymbol{y})g(\boldsymbol{y}) \succeq 0$

$$\int f(\boldsymbol{x})g(\boldsymbol{x})K(\boldsymbol{x},\boldsymbol{y})g(\boldsymbol{y})f(\boldsymbol{y})\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} = \int h(\boldsymbol{x})K(\boldsymbol{x},\boldsymbol{y})h(\boldsymbol{y})\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{y} \geq 0$$

where $f(\boldsymbol{x})g(\boldsymbol{x}) = h(\boldsymbol{x})$

$$\mathrm{e}^{-\gamma\boldsymbol{x}^\mathsf{T}\boldsymbol{x}}\mathrm{e}^{2\gamma\boldsymbol{x}^\mathsf{T}\boldsymbol{y}}\mathrm{e}^{-\gamma\boldsymbol{y}^\mathsf{T}\boldsymbol{y}} = \mathrm{e}^{-\gamma\|\boldsymbol{x}-\boldsymbol{y}\|^2} \succeq 0$$

Other Kernels

- The success of SVMs has meant that researchers try to increase the area of application
- The condition that a SVM kernel must be positive semi-definite is quite restrictive
- There has been a cottage industry of researchers finding smart kernels for solving complicated problems
- The key to finding new kernels is to use the properties of kernels to build more complicated kernels from simpler ones

String Kernels

- One area where SVMs were very important is in document classification
- This requires comparing strings
- There are a large number of kernels developed to do this

Spectrum Kernel

- A simple way to compare documents is to collect a histogram of all occurrences of substrings of length p
- This is known as a p-spectrum
- A p-spectrum kernel counts the number of common substrings

$$\begin{aligned} s &= \texttt{statistics} \qquad \mathcal{S}_3(s) = \{\texttt{sta},\texttt{tat},\texttt{ati},\texttt{tis},\texttt{ist},\texttt{sti},\texttt{tic},\texttt{ics}\} \\ t &= \texttt{computation} \qquad \mathcal{S}_3(t) = \{\texttt{com},\texttt{omp},\texttt{mpu},\texttt{put},\texttt{uta},\texttt{tat},\texttt{ati},\texttt{tio},\texttt{ion}\} \end{aligned}$$

- $K(s,t) = 2$ (“tat” and “ati”)

All Subsequences Kernel

- A more sophisticated kernel is to count all of the common subsequences that occur in two documents
- Naively this would take an exponential amount of time to compute
- Using clever dynamic-programming techniques this can be done relatively efficiently
- This can even be extended to include sub-sequence matches with possible gaps between words

Other Kernel Applications

- String kernels for comparing subsequences are used in bioinformatics
- Kernels have been developed for comparing trees (e.g. for computer program evaluation, XML, etc.)
- Kernels have also been developed for comparing graphs (e.g. for comparing chemicals based on their molecular graph)

Fisher Kernels

- In an attempt to build kernels that capture more domain knowledge, kernels are constructed from other learning machines
- An example of this are "Fisher kernels" whose features come from an Hidden Markov Model (HMM) trained on the data
- These tend to have better discriminative power than the underlying model (HMM), and has a better feature set than a SVM using a generic kernel

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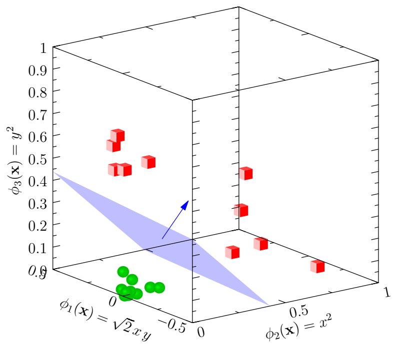
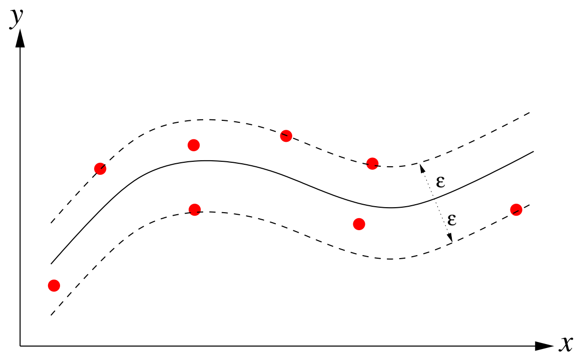


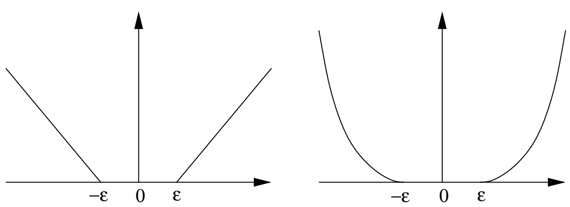
Regression with Margins

- SVMs can be modified to perform regression



Error Functions

- Can introduce slack variables with different errors



- This can be transformed to a quadratic programming problem

Ridge Regression Using Kernels

- We can also solve regression problems without using margins
- To solve a regression problem once again the problem is set up as a quadratic programming problem

$$\min_{\boldsymbol{w}} \lambda \|\boldsymbol{w}\|^2 + \sum_{i=1}^{m} \left(y_i - \boldsymbol{w}^\mathsf{T} \boldsymbol{\phi}(\boldsymbol{x}_i)\right)^2$$

- the $\|\boldsymbol{w}\|^2$ is a regularisation term
- By assuming $\boldsymbol{w} = \sum_i \alpha_i \boldsymbol{\phi}(\boldsymbol{x}_i)$ we obtain a quadratic equation for the α_i's which we can solve

Kernel Methods

- Kernel methods where we project into an extended feature space are used with other linear algorithms
  - Kernel Fisher discriminant analysis (KFDA)
  - Kernel principle component analysis (KPCA)
  - Kernel canonical correlation analysis (KCCA)
  - Gaussian Processes
- These are also extremely powerful machine learning algorithms

Summary

- SVMs require a positive definite kernel function
- These can be built from simpler function
- There was a cottage industry of people creating new kernels for different application
- SVMs are just one example of a host of machine that
  - use the kernel trick
  - often use linear constraints
  - tend to be convex optimisation problems