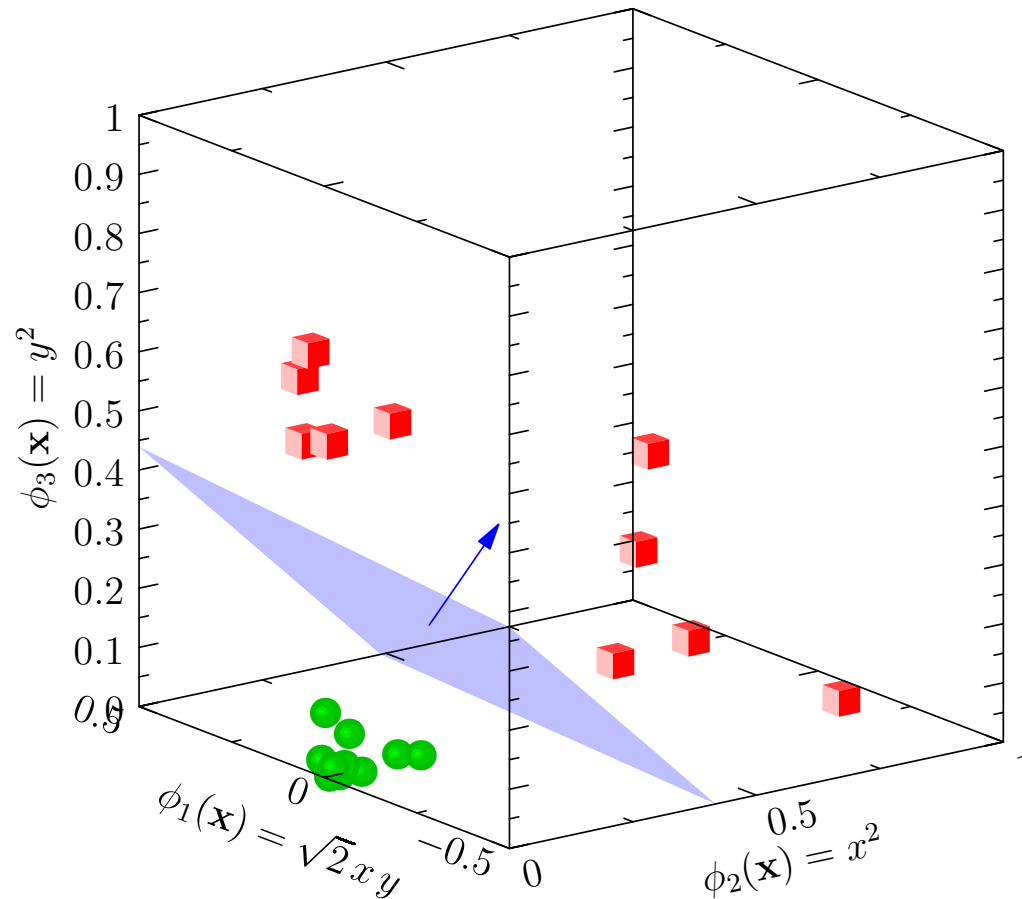# Advanced Machine Learning
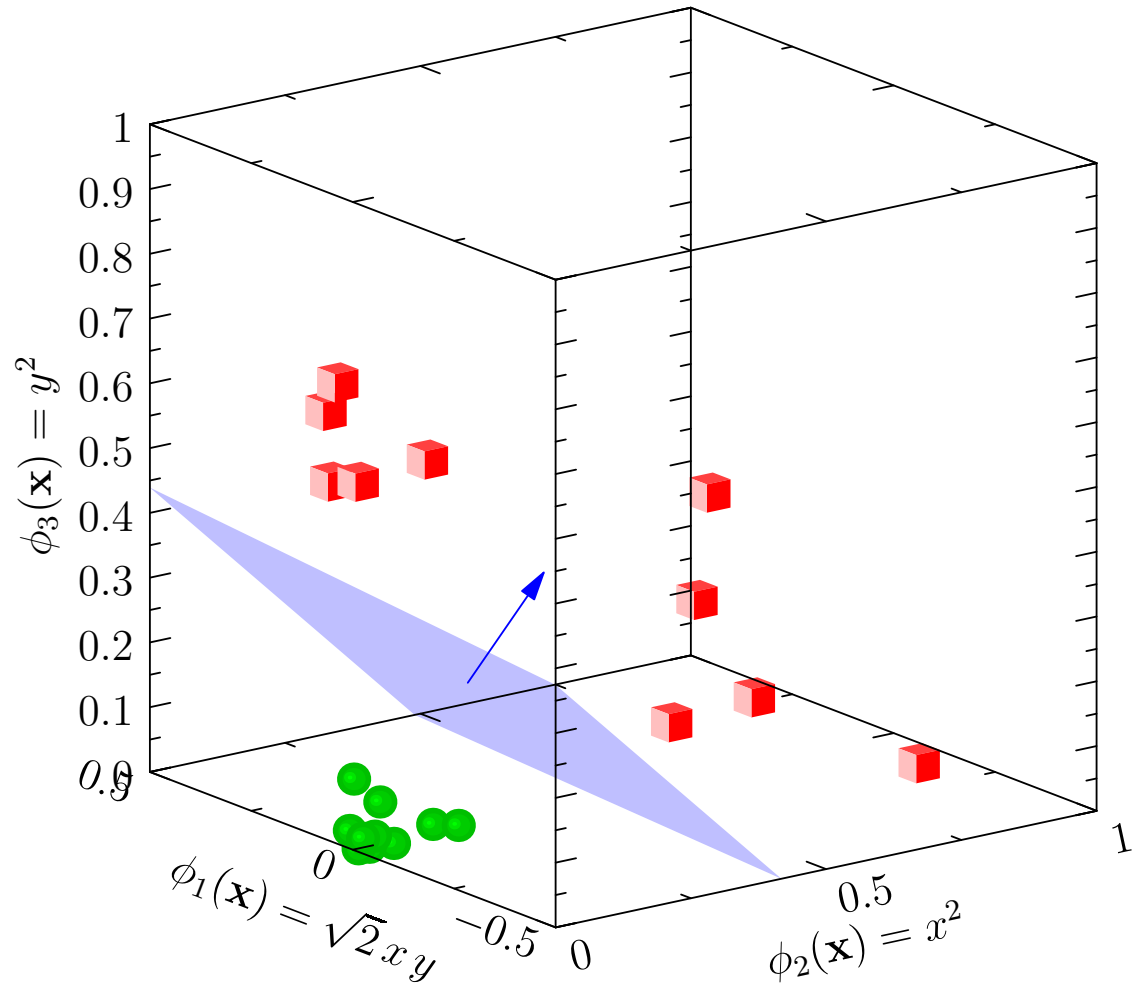
Kernel Trick

The Kernel Trick, SVMs, Regression

Outline

1. **The Kernel Trick**

2. Positive Semi-Definite Kernels

3. Kernel Properties

4. Beyond Classification

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

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

- subject to $\sum_{k=1}^{m} y_k \alpha_k = 0$ and $0 \le \alpha_k (\le C)$

- But since $K(\boldsymbol{x}_k, \boldsymbol{x}_l) = \left\langle \boldsymbol{\phi}(\boldsymbol{x}_k), \boldsymbol{\phi}(\boldsymbol{x}_l) \right\rangle$ 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

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

- In the dual representation this becomes

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

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

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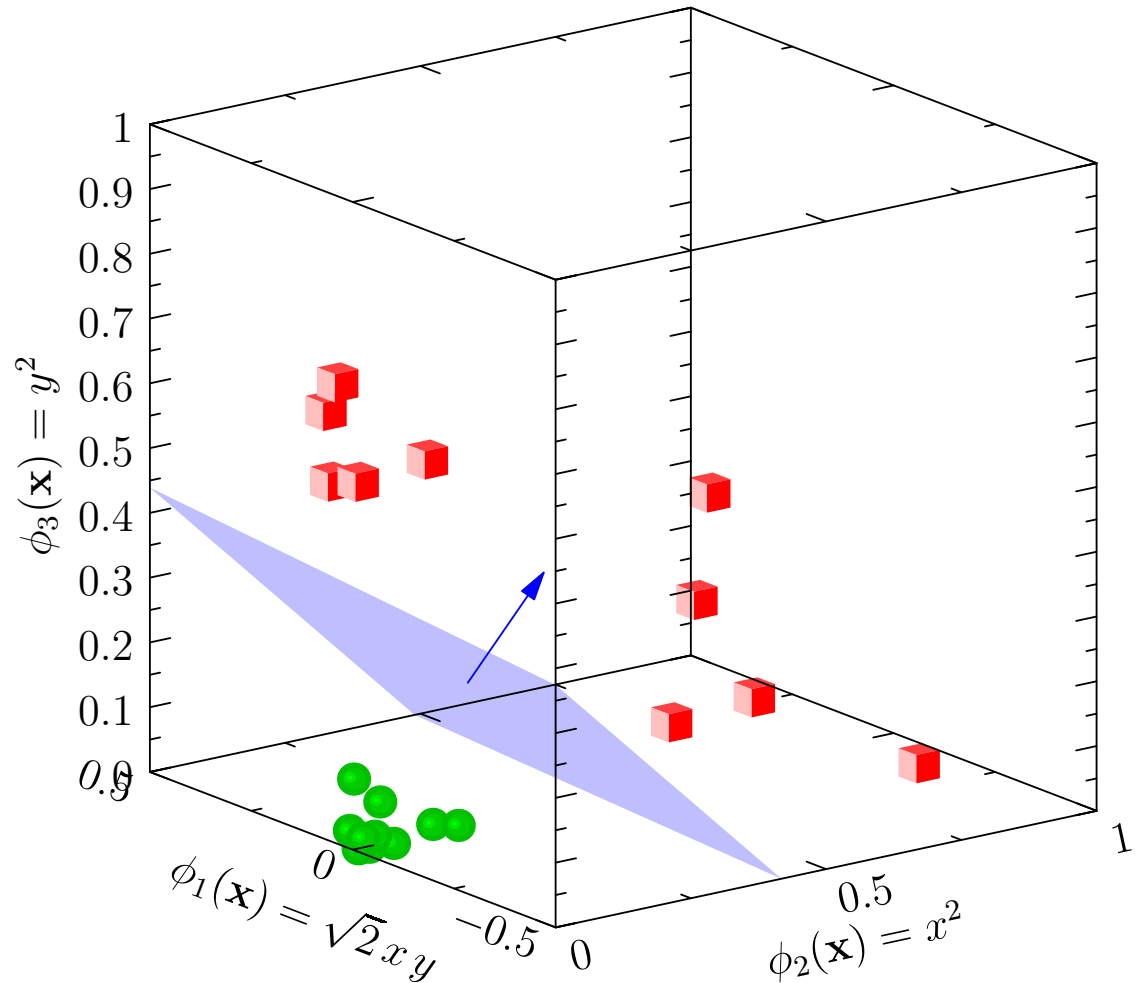
Recap on Eigen Systems

- 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 $\mathbf{M}\boldsymbol{v}^{(k)} = \lambda^{(k)}\boldsymbol{v}^{(k)}$

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

- 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

$$\boldsymbol{v} = \begin{pmatrix} 0.0512 \\ 0.529 \\ 0.0512 \\ 0.617 \\ 1.06 \\ 0.749 \\ 0.703 \\ 8 \\ 0.703 \end{pmatrix}$$
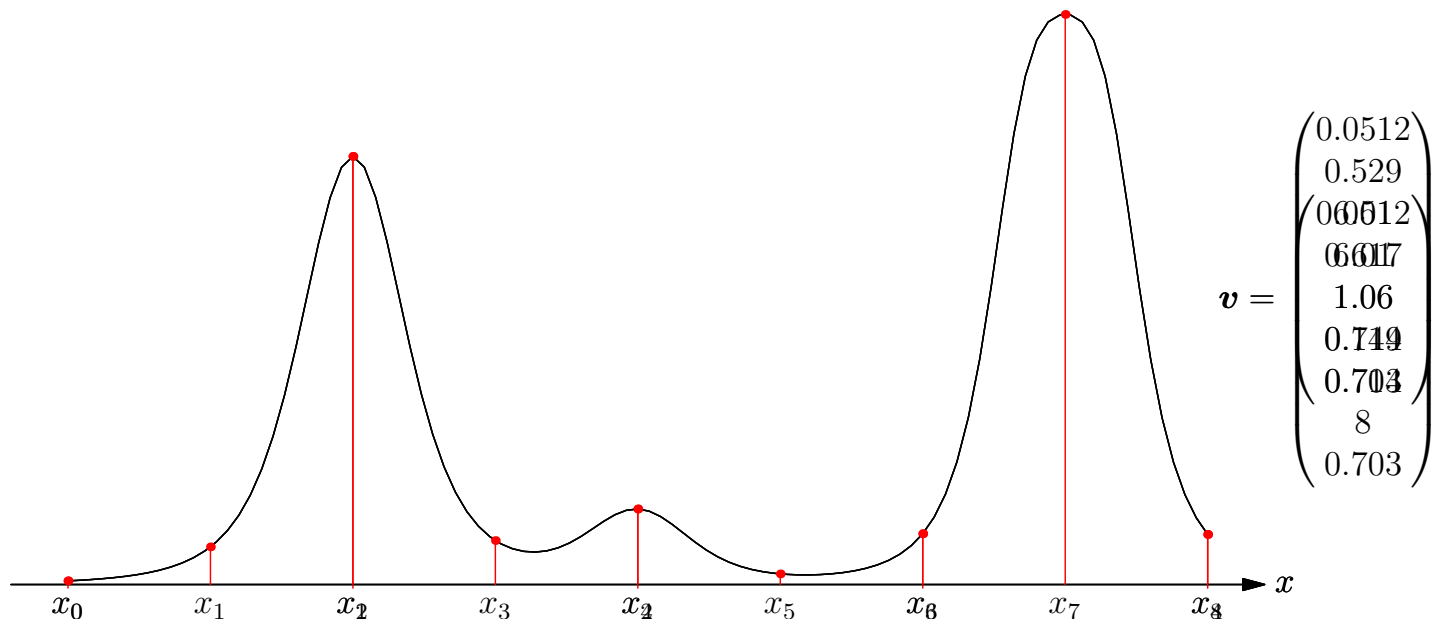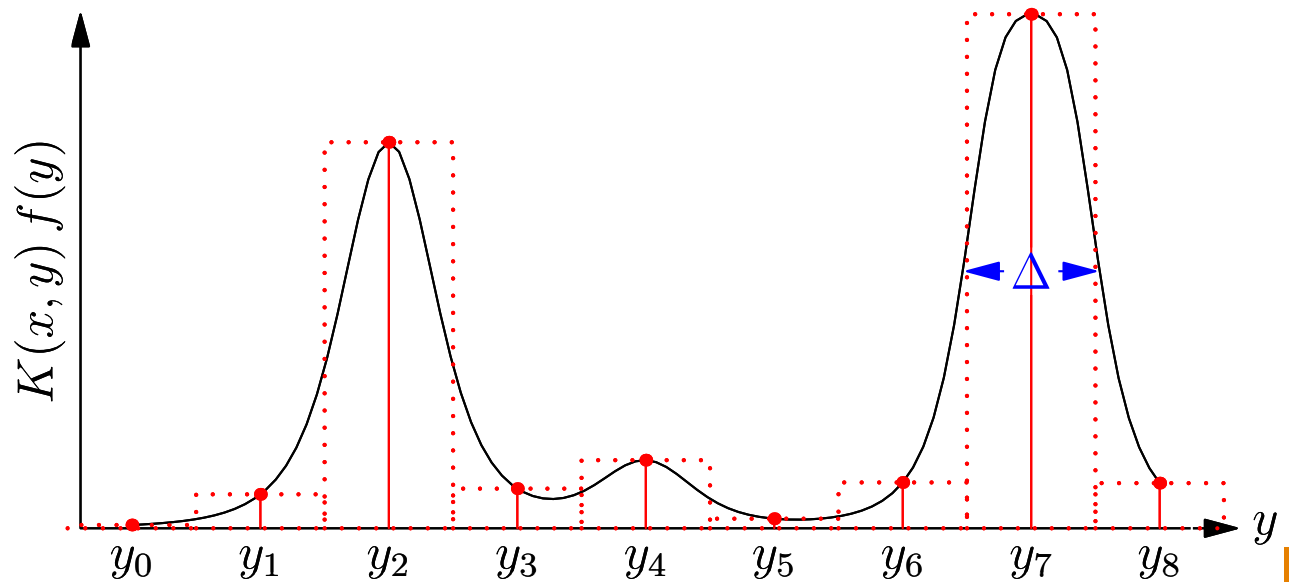
- In the limit where the number of sample points goes to infinity the vector more closely approximates a function

- 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 $\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}) \rangle = \|\phi(\boldsymbol{x})\|^2$ 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

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3. **Kernel Properties**

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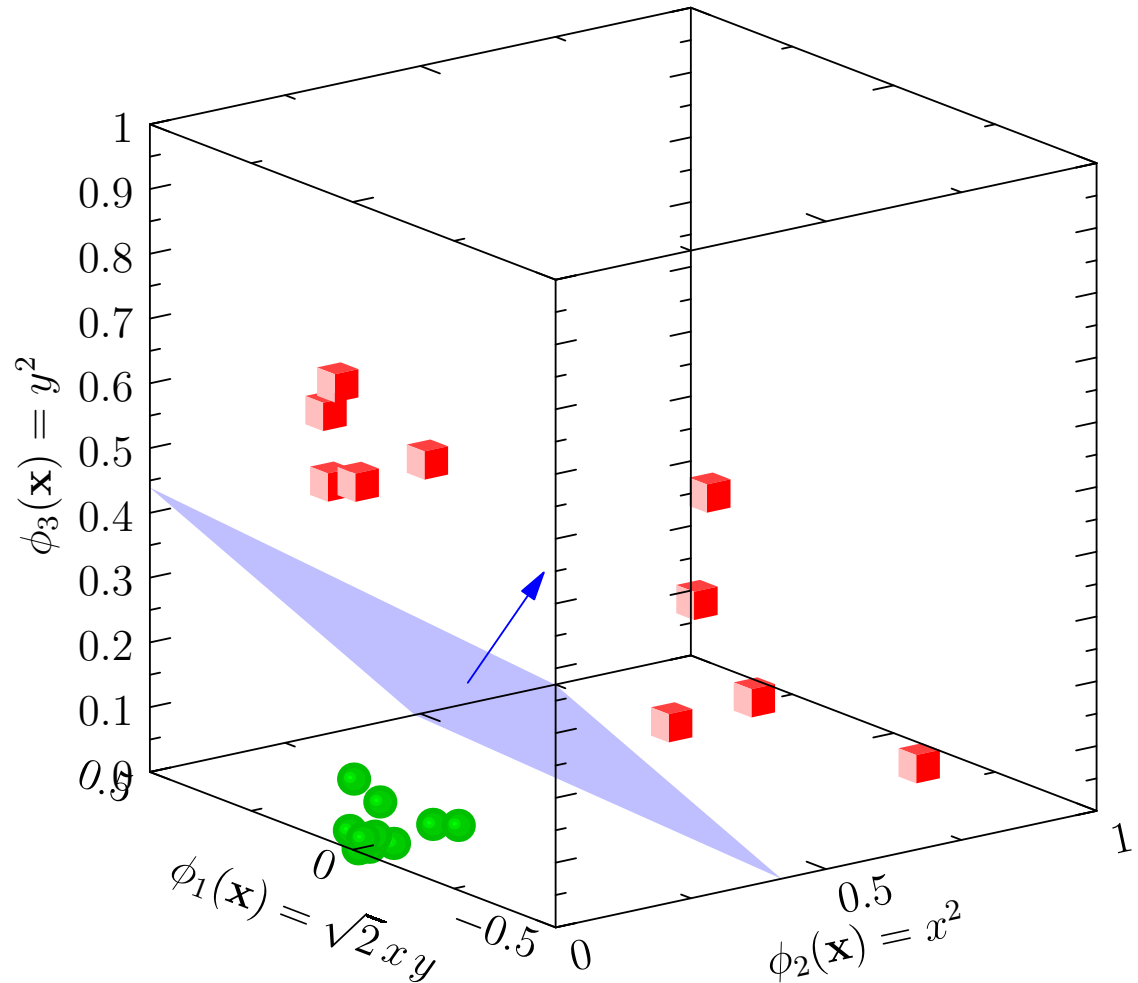
Positive Semi-Definite Kernels

- 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

$$K_3(\boldsymbol{x}, \boldsymbol{y}) = \sum_{i,j} \phi_i^{(1)}(\boldsymbol{x}) \phi_i^{(1)}(\boldsymbol{y}) \phi_j^{(2)}(\boldsymbol{x}) \phi_j^{(2)}(\boldsymbol{y})$$

$$= \sum_{i,j} \phi_{ij}^{(3)}(\boldsymbol{x}) \phi_{ij}^{(3)}(\boldsymbol{y}) = \left\langle \boldsymbol{\phi}^{(3)}(\boldsymbol{x}), \boldsymbol{\phi}^{(3)}(\boldsymbol{y}) \right\rangle$$

  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 $x^\top y = \langle x, y \rangle$ is a valid kernel because it is an inner product of functions $\phi(x) = x$

- For $\gamma > 0$ we have $2\gamma x^\top y \succeq 0$

- Thus $\exp(2\gamma x^\top y) \succeq 0$

- If $K(x, y) \succeq 0$ then $g(x) K(x, y) g(y) \succeq 0$

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

where $f(x) g(x) = h(x)$

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

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

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

- $K(s,t) = 2$ ("$\texttt{tat}$" and "$\texttt{ati}$")

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
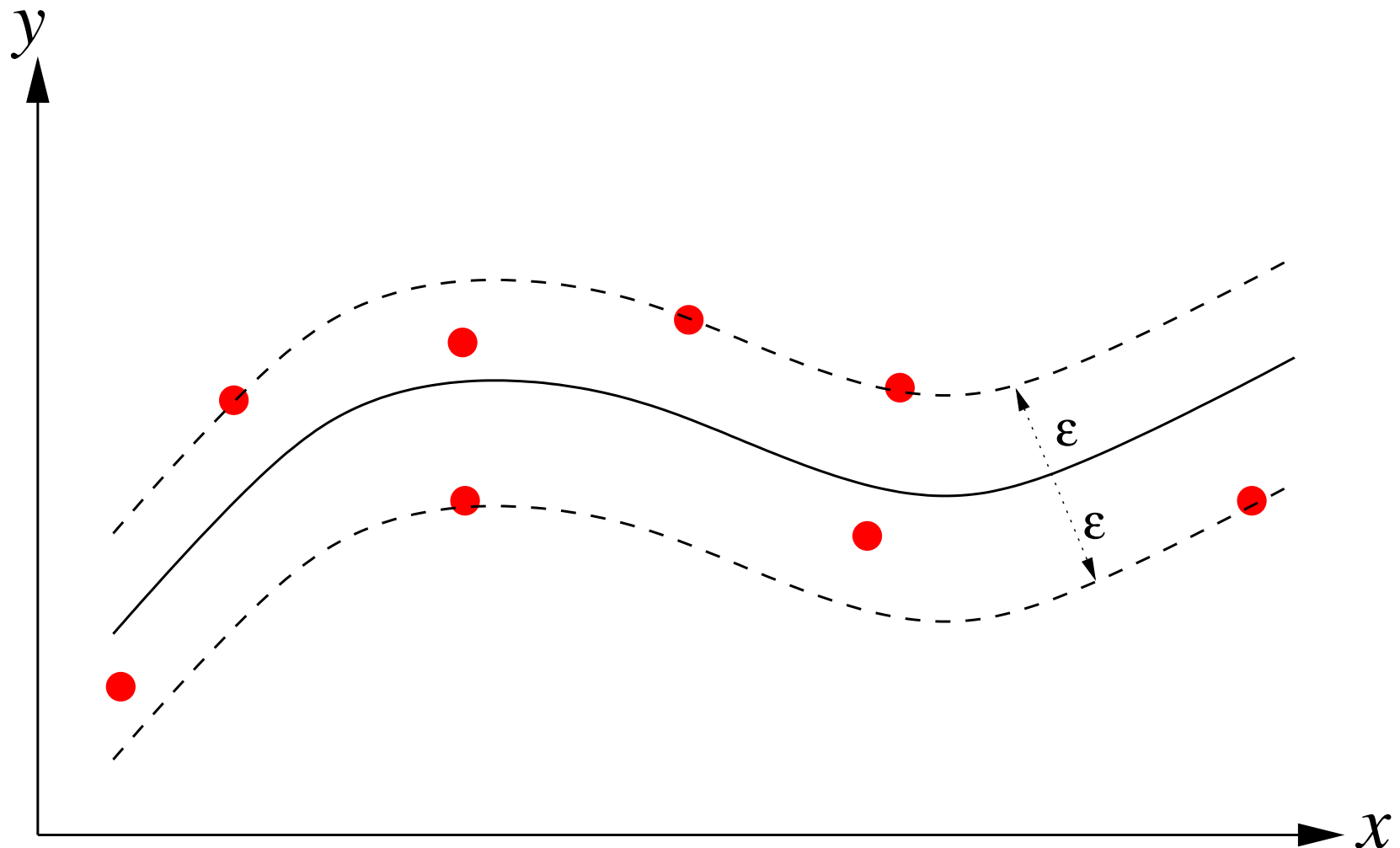

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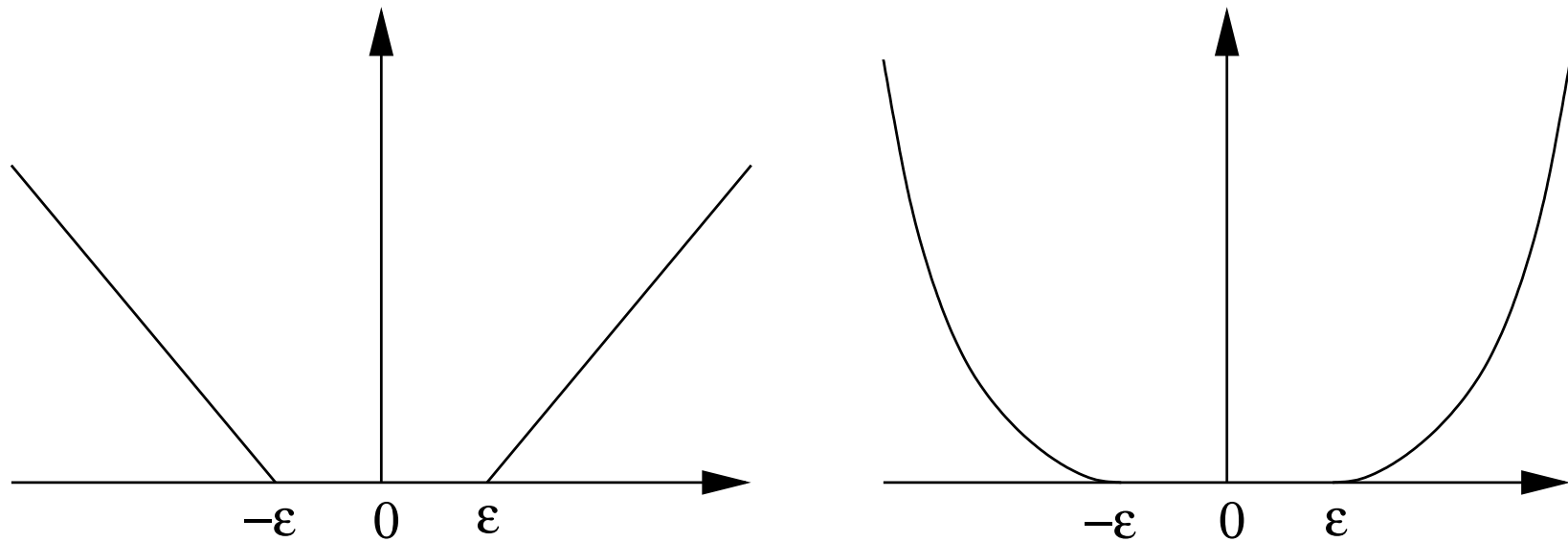
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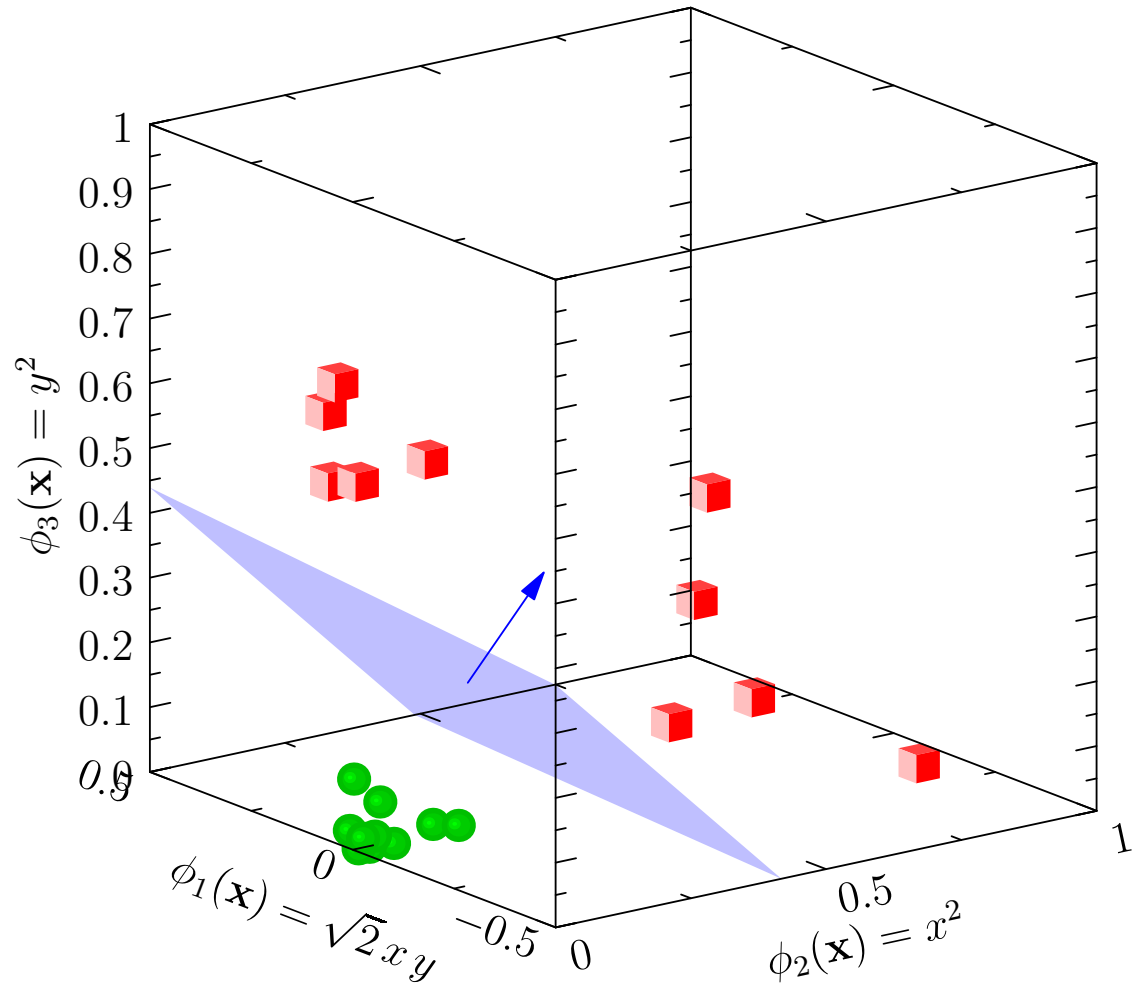
Regression with Margins

- 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▮