Neural Networks and Learning Systems
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Lecture 7
Kernel methods

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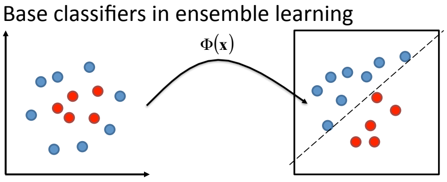
Introduction

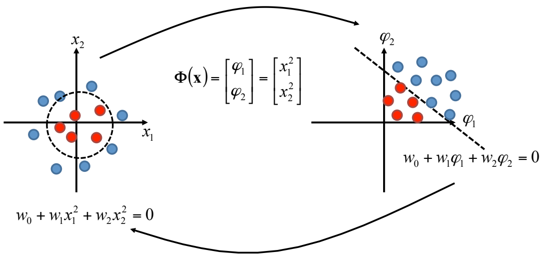
- We have seen nonlinear mappings of input features to a new feature space:
  - Hidden layer in a neural network
  - Base classifiers in ensemble learning



Cover's theorem: The probability that classes are linearly separable increases when the features are nonlinearly mapped to a higher dimensional feature space.

(*cf. the extreme case of putting each sample in a dimension of its own!*)

Nonlinear mapping example



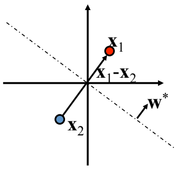
Kernel methods

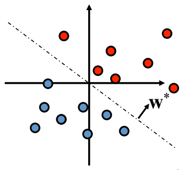
A general approach to making linear methods non-linear.

The name *kernel* refers to positive definite kernels in operator theory mathematics.

Consider a linear classifier

$$f(\mathbf{x};\mathbf{w}) = \mathbf{w}^T\mathbf{x} + w_0$$





$$\mathbf{w}^* = 1.0\mathbf{x}_1 - 1.0\mathbf{x}_2$$

Seems plausible that the optimal direction can be expressed like this!

$$\mathbf{w}^* = \sum_{n=1}^{N} \alpha_n \mathbf{x}_n$$

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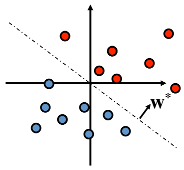
Linear classifier in scalar product form

$$\left.\begin{aligned} f(\mathbf{x};\mathbf{w}) &= \mathbf{w}^T\mathbf{x} + w_0 \\ \mathbf{w} &= \sum_{n=1}^{N} \alpha_n \mathbf{x}_n \end{aligned}\right\} \quad f(\mathbf{x};\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n \mathbf{x}_n^T \mathbf{x} + \alpha_0$$

$\alpha_0 = w_0$

Scalar product = distance and angle between the vectors



For the bias weight

(i) $f(\mathbf{x};\mathbf{w}) = \mathbf{w}^T\mathbf{x}$ $\quad \mathbf{x} \leftarrow \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix}$

(ii) $f(\mathbf{x};\boldsymbol{\alpha}) = \sum_{n=0}^{N} \alpha_n \mathbf{x}_n^T \mathbf{x}$

Add a dummy training example $\mathbf{x}_0 = \begin{bmatrix} 1 \\ \mathbf{0} \end{bmatrix}$ for α_0.

NOTE: Classifier form (ii) must store all training examples for the classification, whereas form (i) must not.

Is there any advantage of form (ii)?

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Scalar product

a.k.a. dot product or inner product

Usual Euclidian space

$$\boxed{\mathbf{x}\cdot\mathbf{z} = \mathbf{x}^T\mathbf{z} = \|\mathbf{x}\|\|\mathbf{z}\|\cos(\theta)}$$

$$\mathbf{x}^T\mathbf{x} = \|\mathbf{x}\|^2 \Rightarrow \|\mathbf{x}\| = \sqrt{\mathbf{x}^T\mathbf{x}}$$

$$\|\mathbf{x}-\mathbf{z}\|^2 = (\mathbf{x}-\mathbf{z})^T(\mathbf{x}-\mathbf{z}) = \mathbf{x}^T\mathbf{x} - 2\mathbf{x}^T\mathbf{z} + \mathbf{z}^T\mathbf{z}$$

Vector lengths and distances between points are determined by the scalar product.

$$\cos(\theta) = \frac{\mathbf{x}^T\mathbf{z}}{\sqrt{\mathbf{x}^T\mathbf{x}}\sqrt{\mathbf{z}^T\mathbf{z}}}$$

$\mathbf{x}^T\mathbf{z} = 0 \Leftrightarrow \mathbf{x}$ and $\mathbf{z}$ orthogonal

Angles are determined by the scalar product.

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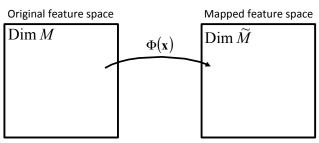
Non-linear mappings

$$\Phi(\mathbf{x}): R^M \rightarrow R^{\tilde{M}}, \text{ with } \tilde{M} > M$$



(i) $f(\mathbf{x};\mathbf{w}) = \mathbf{w}^T\mathbf{x}$

(ii) $f(\mathbf{x};\boldsymbol{\alpha}) = \sum_{n=0}^{N} \alpha_n \mathbf{x}_n^T \mathbf{x}$

(i) $f(\mathbf{x};\mathbf{w}) = \mathbf{w}^T\Phi(\mathbf{x})$

(ii) $f(\mathbf{x};\boldsymbol{\alpha}) = \sum_{n=0}^{N} \alpha_n \Phi(\mathbf{x}_n)^T \Phi(\mathbf{x})$

Examples: $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

$$\Phi(\mathbf{x}) = \begin{bmatrix} x_1^2 \\ x_1x_2 \\ x_2^2 \end{bmatrix}$$

$$\Phi(\mathbf{x}) = \begin{bmatrix} \cos(x_1) \\ \sin(x_2) \\ x_2e^{-x_1} \\ x_2^{1000} \end{bmatrix}$$

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Explicit and implicit mapping

Classifier form (ii) offers two different ways of defining $\Phi(\mathbf{x})$!

$$f(\mathbf{x};\boldsymbol{\alpha}) = \sum_{n=0}^{N} \alpha_n \Phi(\mathbf{x}_n)^T \Phi(\mathbf{x})$$

Reminder: We only need the scalar product!

Explicit: Do the actual mapping, for example $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ $\quad \Phi(\mathbf{x}) = \begin{bmatrix} x_1^2 \\ x_1 x_2 \\ x_2^2 \end{bmatrix}$

Definition

But this is only an intermediate vector that we do not really need.

Implicit: Define the new feature space by defining the scalar product in that space, i.e., how distances and angles are measured. For example:

$$\kappa(\mathbf{x},\mathbf{z}) = \Phi(\mathbf{x})^T \Phi(\mathbf{z}) = (\mathbf{x}^T \mathbf{z})^2$$

Kernel function Definition

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Explicit and implicit mappings are equivalent

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad \mathbf{z} = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$$

$$\kappa(\mathbf{x},\mathbf{z}) = (\mathbf{x}^T\mathbf{z})^2 = (x_1 z_1 + x_2 z_2)^2 = (x_1^2 z_1^2 + 2x_1x_2z_1z_2 + x_2^2 z_2^2) = \underbrace{\begin{pmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{pmatrix}^T \begin{pmatrix} z_1^2 \\ \sqrt{2}z_1z_2 \\ z_2^2 \end{pmatrix}}_{\Phi(\mathbf{x})^T \Phi(\mathbf{z})}$$

Define!

The kernel function $\kappa(\mathbf{x},\mathbf{z}) = (\mathbf{x}^T\mathbf{z})^2$ defines the same space as the explicit mapping $\mathbf{x} \rightarrow \Phi(\mathbf{x})$.

Only in some special cases can we find the explicit mapping function from the implicit kernel function!

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Why not always use explicit mappings?

- Assume we have 20 input features….
- Create all polynomial combinations up to degree 5 (e.g., x_1, x_1^5, $x_2^2 x_9^3$,….)
- Generates a new feature space with dimension > 50,000!
- For example, PCA in new space: Eigendecomposition of a 50,000 x 50,000 matrix.

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The kernel function

$$\boxed{\mathbf{x} \cdot \mathbf{z} = \mathbf{x}^T \mathbf{z}}$$

Needs to define a valid scalar product in some space

$\mathbf{x} \cdot \mathbf{z} = \mathbf{z} \cdot \mathbf{x}$

$a\mathbf{x} \cdot b\mathbf{z} = ab(\mathbf{x} \cdot \mathbf{z})$

$\mathbf{x} \cdot (\mathbf{z}_1 + \mathbf{z}_2) = \mathbf{x} \cdot \mathbf{z}_1 + \mathbf{x} \cdot \mathbf{z}_2$

⋮

Properties of a scalar product

Polynomial kernels	Gaussian kernel	Sigmoid kernel
$\kappa(\mathbf{x}_i,\mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^d$	$\kappa(\mathbf{x}_i,\mathbf{x}_j) = \exp\left(-\frac{\lVert \mathbf{x}_i - \mathbf{x}_j \rVert^2}{2\sigma^2}\right)$	$\kappa(\mathbf{x}_i,\mathbf{x}_j) = \tanh(\mathbf{x}_i^T \mathbf{x}_j)$

Includes all monomials up to degree d, e.g., for d=2: 1, x_1, x_2, x_1^2, x_1x_2, x_2^2

Many other kernels, see for example: http://crsouza.blogspot.com/2010/03/kernel-functions-for-machine-learning.html

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Summary so far and open questions

- Assume that the optimal solution for a linear classifier can be expressed as: $\mathbf{w} = \sum_{n=1}^{N} \alpha_n \mathbf{x}_n$ This must be verified!
- The linear classifier can then be expressed as:
$$f(\mathbf{x};\boldsymbol{\alpha}) = \sum_{n=0}^{N} \alpha_n \mathbf{x}_n^T \mathbf{x}$$ How do we find the α's?
- Apply the linear classifier in a higher-dimensional space by defining its scalar product via the kernel function
$$\kappa(\mathbf{x},\mathbf{z}) = \Phi(\mathbf{x})^T \Phi(\mathbf{z})$$
$$f(\mathbf{x};\boldsymbol{\alpha}) = \sum_{n=0}^{N} \alpha_n \kappa(\mathbf{x}_n, \mathbf{x})$$ How do we select the kernel function?

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Example: Linear perceptron with square error cost

From lecture 2!

Minimize the following cost function

$$\varepsilon(\mathbf{w}) = \sum_{i=1}^{N} \left(\mathbf{w}^T \mathbf{x}_i - y_i\right)^2$$

N = # training samples
$y_i \in \{-1,1\}$ depending on the class of training sample *i*

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Example: Linear perceptron algorithm

From lecture 2!

$$\varepsilon(\mathbf{w}) = \sum_{i=1}^{N} \left(\mathbf{w}^T \mathbf{x}_i - y_i\right)^2$$

$$\frac{\partial \varepsilon}{\partial \mathbf{w}} = 2\sum_{i=1}^{N} \left(\mathbf{w}^T \mathbf{x}_i - y_i\right)\mathbf{x}_i$$

Gradient descent:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \frac{\partial \varepsilon}{\partial \mathbf{w}} = \mathbf{w}_t - \eta \sum_{i=1}^{N} \left(\mathbf{w}_t^T \mathbf{x}_i - y_i\right)\mathbf{x}_i \quad (\text{Eq.}1)$$

Algorithm:
1. Start with a random **w**
2. Iterate Eq. 1 until convergence

$$\mathbf{w}^* = \sum_{i=1}^{N} \alpha_i \mathbf{x}_i \text{ as } t \to \infty$$

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Example: Kernel perceptron algorithm

Gradient descent:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \sum_{i=1}^{N} \left(\mathbf{w}_t^T \mathbf{x}_i - y_i\right)\mathbf{x}_i$$ Original space

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \sum_{i=1}^{N} \underbrace{\left(\mathbf{w}_t^T \Phi(\mathbf{x}_i) - y_i\right)}_{\beta_{t,i}} \Phi(\mathbf{x}_i)$$ Mapped space

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \sum_{i=1}^{N} \beta_{t,i} \Phi(\mathbf{x}_i)$$

$$\mathbf{w}^* = \sum_{i=1}^{N} \alpha_i \Phi(\mathbf{x}_i) \text{ as } t \to \infty$$

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Example: Kernel perceptron algorithm

$$\left.\begin{array}{l}\varepsilon(\mathbf{w}) = \sum_{i=1}^{N}\left(y_i - \mathbf{w}^T\Phi(\mathbf{x}_i)\right)^2 \\ \mathbf{w} = \sum_{i=1}^{N}\alpha_i\Phi(\mathbf{x}_i)\end{array}\right\} \varepsilon(\boldsymbol{\alpha}) = \sum_{i=1}^{N}\left(y_i - \sum_{j=1}^{N}\alpha_j \underline{\Phi(\mathbf{x}_j)^T\Phi(\mathbf{x}_i)}\right)^2 = \sum_{i=1}^{N}\left(y_i - \sum_{j=1}^{N}\alpha_j \underline{\kappa(\mathbf{x}_j,\mathbf{x}_i)}\right)^2$$

Kernel trick!

Gradient:

$$\frac{\partial\varepsilon}{\partial\alpha_k} = -2\sum_{i=1}^{N}\left(y_i - \sum_{j=1}^{N}\alpha_j\kappa(\mathbf{x}_j,\mathbf{x}_i)\right)\kappa(\mathbf{x}_k,\mathbf{x}_i)$$

Gradient descent in α!

$$\boxed{\alpha_{k,t+1} = \alpha_{k,t} - \eta\frac{\partial\varepsilon}{\partial\alpha_k}}$$

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Example: Kernel perceptron summary

1. Showed that $\mathbf{w}^* = \sum_{i=1}^{N}\alpha_i\Phi(\mathbf{x}_i)$
2. Cost function in α: $\varepsilon(\boldsymbol{\alpha}) = \sum_{i=1}^{N}\left(y_i - \sum_{j=1}^{N}\alpha_j\Phi(\mathbf{x}_j)^T\Phi(\mathbf{x}_i)\right)^2$
3. Choose kernel function: $\kappa(\mathbf{x}_j,\mathbf{x}_i) = \Phi(\mathbf{x}_j)^T\Phi(\mathbf{x}_i)$
4. Gradient descent in α: $\alpha_{k,t+1} = \alpha_{k,t} - \eta\frac{\partial\varepsilon}{\partial\alpha_k}$
5. Apply classifier: $f(\mathbf{x};\boldsymbol{\alpha}) = \sum_{i=0}^{N}\alpha_i\kappa(\mathbf{x}_i,\mathbf{x})$

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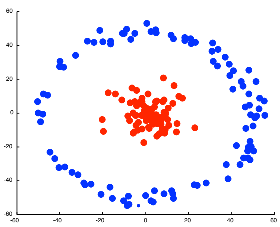
Kernel Perceptron example



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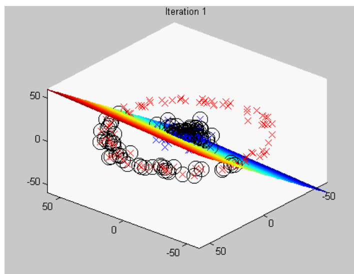
Kernel Perceptron example, cont

Movie!



The original linear perceptron algorithm will not work because the classes are not linearly separable

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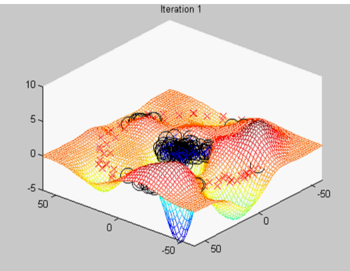
Kernel Perceptron example, cont

Movie!



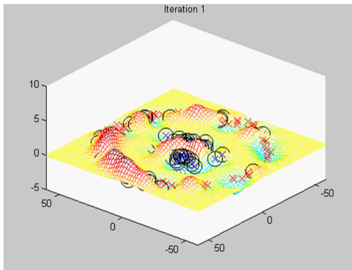
The surface shows the value of $\sum_{k=1}^{N} \alpha_k \kappa(\mathbf{x}_k, \mathbf{x})$ for different **x**.

Gaussian kernel with σ=10

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

Kernel Perceptron example, cont

Movie!



The surface shows the value of $\sum_{k=1}^{N} \alpha_k \kappa(\mathbf{x}_k, \mathbf{x})$ for different **x**.

Gaussian kernel with σ=10

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

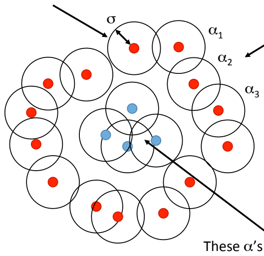
Structure of the classification function

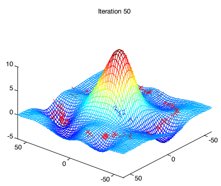
$$f(\mathbf{x}) = \sum_{k=1}^{N} \alpha_k \kappa(\mathbf{x}_k, \mathbf{x})$$

Weighted distance to all training samples

Gaussian kernel

These α's will probably be negative





These α's will probably be positive

Kernelization of linear methods

- Perceptron
- LDA
- SVM
- PCA
- k-means

Linear classifiers

Linear structure discovery methods

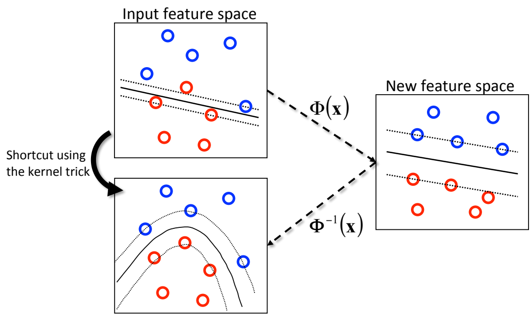
Clustering

Number of parameters equals the number of training samples

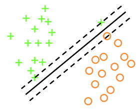
$$f(\mathbf{x}) = \sum_{k=1}^{N} \alpha_k \kappa(\mathbf{x}_k, \mathbf{x})$$

Have to store all training samples

Nonlinear SVM

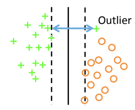


Kernelizing the linear SVM



$$\min_{\mathbf{w}} \mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{N}\xi_i$$

subject to $y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1 - \xi_i$



Assume that we can show that $\mathbf{w} = \sum_{i=1}^{N}\alpha_i\mathbf{x}_i$

$$\min_{\boldsymbol{\alpha}} \sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j\underline{\mathbf{x}_i^T\mathbf{x}_j} + C\xi_i$$

subject to $y_i(\sum_{j=1}^{N}\alpha_n\underline{\mathbf{x}_i^T\mathbf{x}_j} + \alpha_0) \geq 1 - \xi_i$

Nonlinear SVM

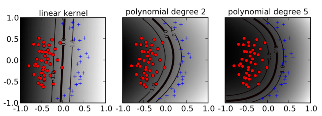
$$\min_{\boldsymbol{\alpha}} \sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j\kappa(\mathbf{x}_i, \mathbf{x}_j) + C\xi_i$$

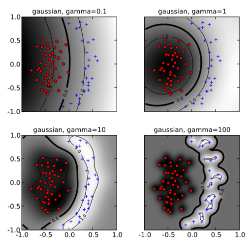
subject to $y_i(\sum_{j=1}^{N}\alpha_n\kappa(\mathbf{x}_i, \mathbf{x}_j) + \alpha_0) \geq 1 - \xi_i$

C: Trade-off parameter between the importance of a low error on the training data vs. finding wide margins that may give better generalization on test data.

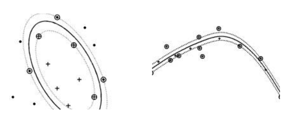
κ(.,.): Kernel function that determines the non-linear mapping. May contain additional parameters such as the width of a Gaussian kernel.

Nonlinear SVM - Examples





Source: A. Ben-Hur & J. Weston
A User's Guide to Support Vector Machines



Source: http://www.support-vector-machines.org/

SVM recipe

- Find a good software library, e.g., LIBSVM or SVM-Light.
- Normalize features, e.g., to the interval [-1,1] or [0,1]
- Choose a Gaussian kernel function
- Choose the width of the Gaussian kernel (σ) and the trade-off parameter *C* using cross-validation.

$$C = 2^{-5}, 2^{-3}, \ldots, 2^{15}$$
$$\sigma = 2^{-4}, 2^{-3}, \ldots, 2^{2} \longleftarrow \text{Depends on the scaling of the data}$$

Training data	Training data	Test data
Training data	Test data	Training data
Test data	Training data	Training data

Hsu et al.
A Practical Guide to Support Vector Classification

Nonlinear SVM - Summary

- Brings two clever and independent concepts together:
  - Large margin principle for good generalization
  - Kernel trick for making linear methods nonlinear
- Cost function ”landscape” less complex than in, e.g., neural network training.
- By many considered to be the state-of-the-art classifier around.
- Must store the support vectors, which can be many.
- Classification slower than, for example, boosting.

$$f(\mathbf{x}) = \sum_{k=1}^{N} \alpha_k \kappa(\mathbf{x}_k, \mathbf{x})$$

Kernel PCA

- Non-linear version of PCA.
- PCA can be written in terms of scalar products.
- Use the ”kernel trick”.

Kernel-PCA

$\mathbf{XX}^T\mathbf{e} = \lambda\mathbf{e}$ Ordinary PCA

Multiply from left with $\mathbf{X}^T$:

$$\mathbf{X}^T\mathbf{X}\underbrace{\mathbf{X}^T\mathbf{e}}_{\mathbf{f}} = \lambda\underbrace{\mathbf{X}^T\mathbf{e}}_{\mathbf{f}} \quad \rightarrow \mathbf{X}^T\mathbf{X}\mathbf{f} = \lambda\mathbf{f}$$

Eigen value problem on an inner product matrix
i.e. with coeficients defined by scalar products!

Kernel-PCA

- Similarly, PCA can be performed on any kernel matrix $\mathbf{K}$ whose components k_{ij} are defined by a kernel function $k_{ij} = \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j) = k(\mathbf{x}_i, \mathbf{x}_j)$
- The principal components are linear in the feature space but non-linear in the input space.

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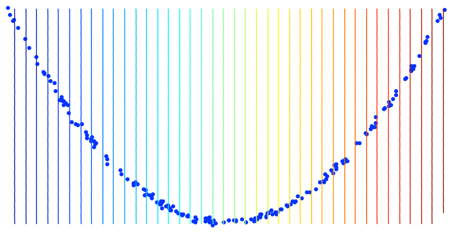
Linear PCA



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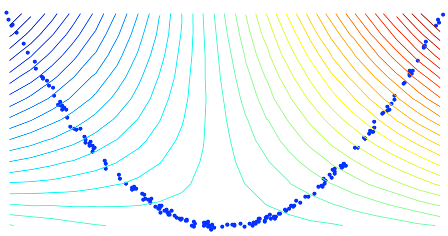
KPCA with quadratic kernel



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Kernels – Pros and cons

- Well understood linear methods carried out in a high-dimensional space where linear separability is more likely.
- Can achieve good performance

- How to choose the kernel and the kernel parameters?
- Have to store the training data.
- Need all combinations of training samples: (# samples)^2
- Training and classification can be computationally intensive

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Some math concepts you'll see when reading about kernel methods

- **Mercer's theorem (1909)**
  Tells us when a kernel function represents a valid scalar product (in some space).
- **Reproducing Kernel Hilbert Spaces (RKHS)**
  Theory about the space for which our kernel is actually the scalar product.
- **Representer theorem**
  Tells us for which optimization problems the solution is a linear combination of the input vectors.

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