Neural Networks and Learning Systems
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Lecture 9

Kernel methods

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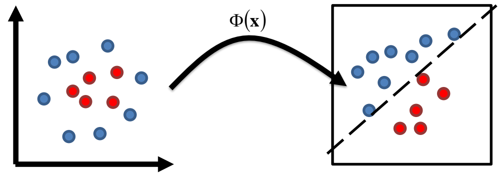
Introduction

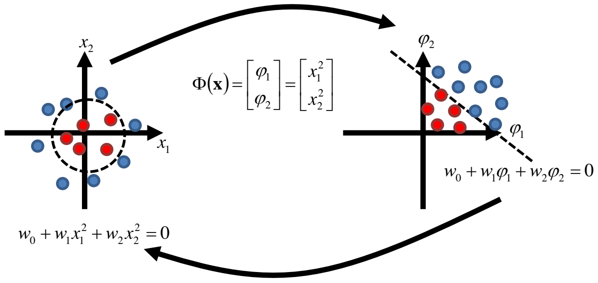
- We have seen nonlinear mappings of input features to a new feature space:
  - Hidden layer in a neural network
  - Base classifiers in ensemble learning



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



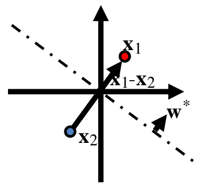
Kernel methods

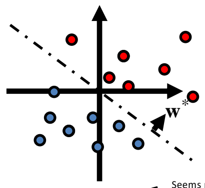
A general approach to making linear methods non-linear.

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

Consider a linear classifier

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





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

Seems plausible that the optimal direction can be expressed as a linear combination of the training data!

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

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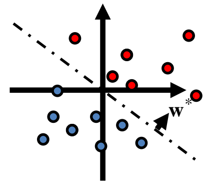
Linear classifier in scalar product form

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

$\alpha_0 = w_0$

Scalar products between training data and the new sample

$\mathbf{w}$ is expressed as a linear combination of the training data



For the bias weight

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

(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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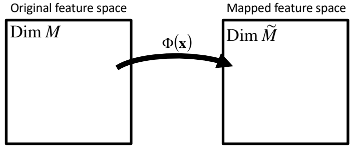
Non-linear mappings

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



(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 <u>two</u> 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 $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ $\qquad \Phi(\mathbf{x}) = \begin{bmatrix} x_1^2 \\ x_1x_2 \\ x_2^2 \end{bmatrix}$

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

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

$$\kappa(\mathbf{x},\mathbf{z}) = (\mathbf{x}^T\mathbf{z})^2 = (x_1z_1 + x_2z_2)^2 = (x_1^2z_1^2 + 2x_1x_2z_1z_2 + x_2^2z_2^2) = \underbrace{\begin{pmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{pmatrix}^T \begin{pmatrix} z_1^2 \\ \sqrt{2}z_1z_2 \\ z_2^2 \end{pmatrix}}_{\Phi(\mathbf{x})^T\Phi(\mathbf{z})}$$

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, $x_2^2x_9^3$,….)
- 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

$$\left.\begin{array}{l} \mathbf{x}\cdot\mathbf{z} = \mathbf{z}\cdot\mathbf{x} \\ a\mathbf{x}\cdot b\mathbf{z} = ab(\mathbf{x}\cdot\mathbf{z}) \\ \mathbf{x}\cdot(\mathbf{z}_1 + \mathbf{z}_2) = \mathbf{x}\cdot\mathbf{z}_1 + \mathbf{x}\cdot\mathbf{z}_2 \\ \vdots \end{array}\right\} \text{Properties of a scalar product}$$

Polynomial kernels

$$\kappa(\mathbf{x}_i,\mathbf{x}_j) = (1 + \mathbf{x}_i^T\mathbf{x}_j)^d$$

Gaussian kernel

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

Sigmoid kernel

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

Many other kernels, see for example:
http://crsouza.com/2010/03/17/kernel-functions-for-machine-learning-applications/

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Summary so far and open questions

- We assumed 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

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

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Example: Kernel perceptron algorithm

Gradient descent:

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

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

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

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

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Example: Kernel perceptron algorithm

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

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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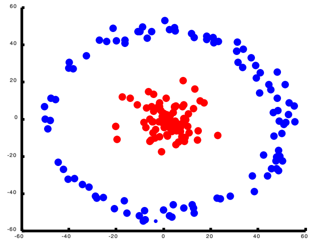
Kernel Perceptron example



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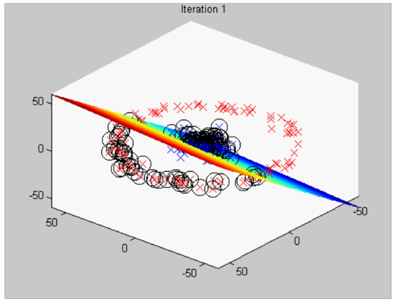
Kernel Perceptron example, cont

Movie!



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

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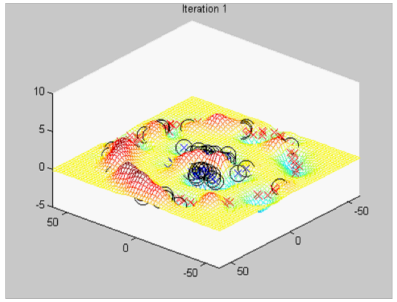
Kernel Perceptron example, cont

Movie!



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

Gaussian kernel with σ=10 $\kappa(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2} \right)$

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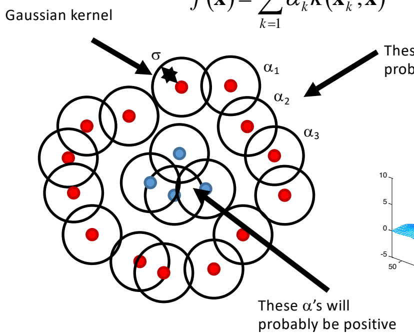
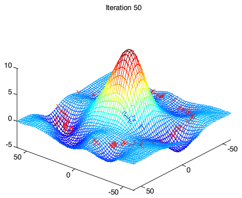
Structure of the classification function

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

Weighted distance to all training samples





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Kernelization of linear methods

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

Perceptron, LDA, SVM: Linear classifiers

PCA: Linear structure discovery methods

k-means: Clustering

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

Number of parameters equals the number of training samples

Have to store all training samples

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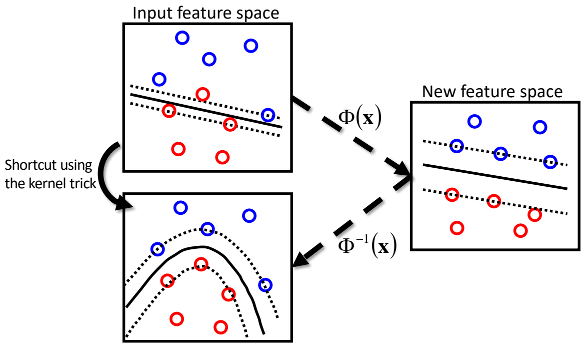
Nonlinear SVM



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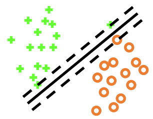
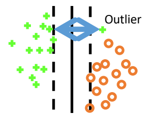
Kernelizing the linear SVM



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

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

Assume again that $\mathbf{w} = \sum_{j=1}^{N} \alpha_j \mathbf{w}_j$



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

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

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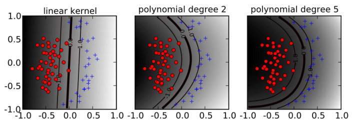
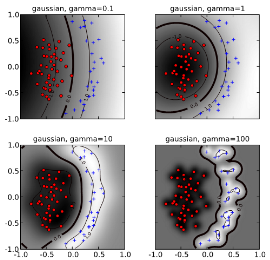
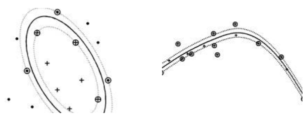
Nonlinear SVM - Examples





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



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

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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.
- Must store the support vectors, which can be many.
- Classification slower than, for example, boosting.

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

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Kernel PCA

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

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Kernel-PCA

$\mathbf{X}\mathbf{X}^T\mathbf{e} = \lambda\mathbf{e}$ 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!

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Kernel-PCA

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

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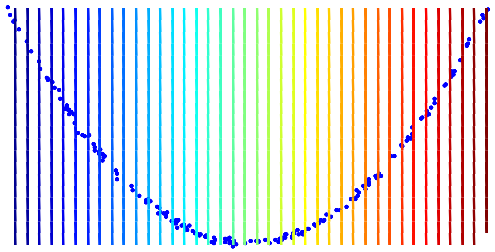
Linear PCA



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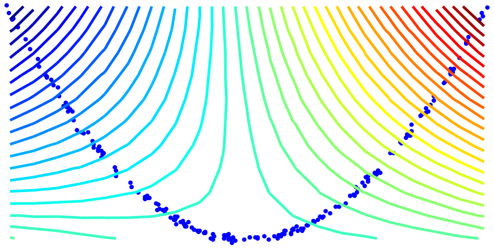
KPCA with quadratic kernel



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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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