$\LaTeX$ command declarations here.

In [1]:
```
# plotting
%matplotlib inline
from matplotlib import pyplot as plt;
import matplotlib as mpl;
from mpl_toolkits.mplot3d import Axes3D

# scientific
import numpy as np;
import scipy as scp;
import scipy.stats;

# python
import random;

# rise config
from notebook.services.config import ConfigManager
cm = ConfigManager()
cm.update('livereveal', {
              'theme': 'simple',
              'start_slideshow_at': 'selected',
              'transition':'fade',
              'scroll':False
})

# scikit-learn
from sklearn import svm
from sklearn.linear_model import Ridge
from sklearn.preprocessing import PolynomialFeatures
from sklearn.pipeline import make_pipeline
from sklearn.grid_search import GridSearchCV
from sklearn.learning_curve import learning_curve
from sklearn.kernel_ridge import KernelRidge

# math
from __future__ import division
```

EECS 545: Machine Learning

Lecture 08: Kernel Methods, Part I

- Instructor: **Jacob Abernethy**
- Date: February 8, 2016

Lecture Exposition Credit: Benjamin Bray, Saket Dewangan

Outline

- Perceptron Algorithm
- Recap Classification Algorithms
- Kernel Methods
  - Kernel functions
  - Kernel trick
  - Constructing kernels

Perceptron Algorithm

- The *Perceptron*, perhaps the oldest "learning algorithm", goes back to Rosenblatt in the 1960s
- The Perceptron is the most basic model of a training a linear predictor with sequential update steps:

INIT: set $\mathbf{w}_1 = \mathbf{0}$;

FOR: $t = 1, 2, \ldots$

- Observe $\mathbf{x}_t$, predict $\hat{y}_t = \text{sign}(\mathbf{w}_t^\top \phi(\mathbf{x}_t))$
- Receive $y_t \in \{-1, 1\}$, update: $\mathbf{w}_{t+1} = \begin{cases} \mathbf{w}_t, & \text{if } y_t \mathbf{w}_t^\top \phi(\mathbf{x}_t) > 0 \\ \mathbf{w}_t + y_t \phi(\mathbf{x}_t), & \text{otherwise.} \end{cases}$

Perceptron is just Stochastic Gradient Descent

- Perceptron update:

$$\mathbf{w}_{t+1} = \begin{cases} \mathbf{w}_t, & \text{if } y_t \mathbf{w}_t^\top \phi(\mathbf{x}_t) > 0 \\ \mathbf{w}_t + y_t \phi(\mathbf{x}_t), & \text{otherwise.} \end{cases}$$

- This is just SGD on the following error func.:

$$E(\mathbf{w}) := \sum_{t=1}^{n} \max(0, -y_t \mathbf{w}^\top \phi(\mathbf{x}_t))$$

- Notice the "step size" is $\eta = 1$! This is atypical.
- Perceptron was (originally) viewed as building block of the *neural network* (NN). Indeed, NN often called the MultiLayerPerceptron (MLP).

Perceptron has a magical property

- If problem is *linearly separable*, i.e. a hyperplane separates positives/negatives, then Perceptron *will find a separating* $\mathbf{w}^*$.
- **Theorem**:
  - Assume that $\|\mathbf{x}_t\| \leq 1$ for all t
  - Assume $\exists \mathbf{w}$, with $\|\mathbf{w}\|_2 = 1$, such that for all $(\mathbf{x}_t, y_t)$ that $y_t \mathbf{w}^\top \phi(\mathbf{x}_t) > \gamma$ for some $\gamma > 0$.
  - Then the Perceptron algorithm will find some $\mathbf{w}^*$ which perfectly classifies all examples
  - The number of updates/mistakes in learning is bounded by $\frac{1}{\gamma^2}$
- This is a *margin bound*, notice that it depends on γ not the dimension of $\phi(\mathbf{x})$

Proof Sketch: (See learning theory lecture notes (http://web.eecs.umich.edu/~jabernet/eecs598course/fall2015/web/notes/lec16_110515.pdf) for full details.)

Let $\mathbf{w}_*$ be perfect classifier scaled by $\frac{1}{\gamma}$. \begin{align} \frac{1}{\gamma^2} = \norm{\vec{w}*}^2 & \ge \norm{\vec{w} - \mathbf 0}^2 - \norm{\vec{w}_ - \vec{w}{T+1}} \nonumber \ & = \sum{t=1}^T \norm{\vec{w}* - \vec{w}{t}}^2 - \norm{\vec{w}* - \vec{w}{t+1}}^2 \ & = \sum{t:y_t(\vec{w}_t^\top \vec{x}_t)<0} \norm{\vec{w} - \vec{w}{t}}^2 - \norm{\vec{w} - (\vec{w}t + y_t \vec{x}_t)}^2 \ & = \sum{t:yt(\vec{w}_t^\top \vec{x}_t)<0} 2 \left(\underbrace{y_t (\vec{w}*^{\top}\vec{x}t)}{\ge 1} \underbrace{- yt (\vec{w}_t^{\top}\vec{x}_t)}{\ge 0} \right) \underbrace{- yt^2 \norm{\vec{x}_t}^2}{\ge -1} \ & \ge \sum_{t:y_t(\vec{w}_t^\top \vec{x}_t)<0} 1 \quad = \quad \text{#mistakes[Perceptron]} \end{align}

A Recap of Classification Methods

- **Logistic Regression**
  - Provides model for $P(y|x, w)$ using sigmoid
  - No explicit model for $P(x|w)$ or $P(x|y, w)$
- **Naive Bayes**
  - Provides a full model for $P(x, y|w)$
  - Assumes independence between features *conditioned on* target y
  - Typically requires discrete data (can generalize to continuous spaces)
  - ML estimates are pretty straightforward

A Recap of Classification Methods

- **Gaussian Discriminant Analysis**
  - Gives full model $P(x|y, w)$ via *multivariate Gaussian*
  - Requires estimating μ, Σ for each class
  - When we include additional assumption that all class covariances matrices are identical, we get *Linear Discriminant Analysis*, and decision threshold becomes linear. (**Exercise:** why?)
- **Perceptron**
  - No probability model on x, y, w
  - Can prove algorithmic benefits (i.e. guaranteed convergence) under *margin assumption*

Break!!

References

This lecture draws upon the following resources:

- **[MLAPP]** Murphy, Kevin. *Machine Learning: A Probabilistic Perspective* (https://mitpress.mit.edu/books/machine-learning-0). 2012.
- **[PRML]** Bishop, Christopher. *Pattern Recognition and Machine Learning* (http://www.springer.com/us/book/9780387310732). 2006.
- **[CS229]** Ng, Andrew. CS 229: Machine Learning (http://cs229.stanford.edu/). Autumn 2015.
  - Lecture Notes 03: Support Vector Machines & Kernels (http://cs229.stanford.edu/notes/cs229-notes3.pdf)

Feature Mapping: Linear Regression

(recall Lectures 04 & 05)

Review: Feature Mapping

Our models so far employ a nonlinear **feature mapping** $\phi : \mathcal{X} \mapsto \mathbb{R}^M$

- in general, features are nonlinear functions of the data
- each feature $\phi_j(x)$ extracts important properties from x

Allows us to use *linear* methods for *nonlinear* tasks.

- For example, **polynomial features** for linear regression...

Linear Regression: Polynomial Features

Problem: Linear model $y(x) = w^T x$ can only produce straight lines through the origin.

- Not very flexible / powerful
- Can't handle nonlinearities

Solution: Polynomial Regression

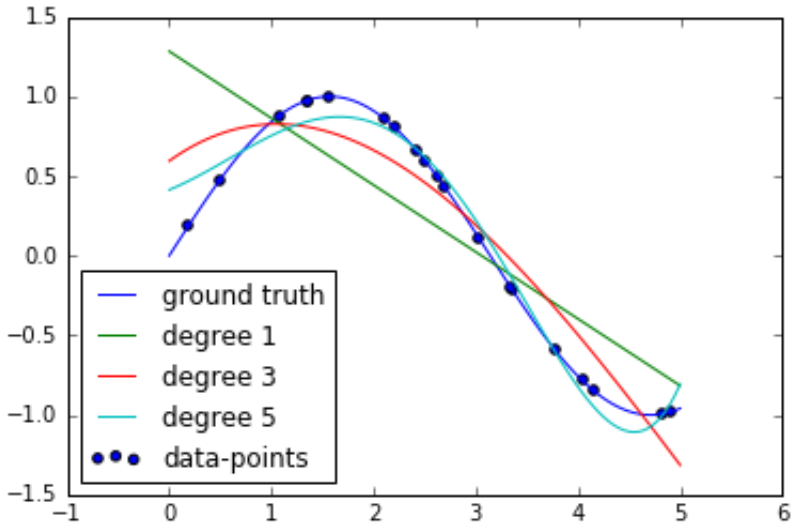
- Replace x by $\phi(x) = \begin{bmatrix} 1 & x & x^2 & \cdots & x^p \end{bmatrix}^T$
- The feature mapping ϕ is nonlinear

Linear Regression: Polynomial Features

In [2]:
```
def poly_reg_example(fn):
    # generate random points
    x = np.random.random(20) * 5;
    y = fn(x);
    # format into matrix
    X = x[:, np.newaxis];

    # plot ground truth
    x_plot = np.linspace(0,5,100)[:, np.newaxis];
    plt.plot(x_plot, fn(x_plot), label="ground truth")
    plt.scatter(x, y, label="data-points")

    # polynomial regression for degree 1,3 and 5
    for degree in [1, 3, 5]:
        model = make_pipeline(PolynomialFeatures(degree), Ridge())
        model.fit(X, y)
        y_plot = model.predict(x_plot)
        plt.plot(x_plot, y_plot, label="degree %d" % degree)

    plt.legend(loc='lower left')
    plt.show()
```

Linear Regression: Polynomial Features

In [3]:
```
# ground truth:  function to be approximated
def fn(x): return np.sin(x);

# plot
poly_reg_example(fn);
```



Linear Regression: Nonlinear Features

Linear Regression Model

$$y(x, w) = w^T \phi(x) = \sum_{j=0}^{M} w_j \cdot \phi_j(x)$$

Least-squares with L-2 regularization

$$J(w) = \frac{1}{2} \sum_{n=1}^{N} (w^T \phi(x_n) - t_n)^2 + \frac{\lambda}{2} w^T w$$

Closed-form Solution

$$w = (\phi^T \phi + \lambda I)^{-1} \phi^T \cdot t$$

This is neat, but...

How do I choose a feature mapping $\phi(x)$?

- Manually? Learn features?

With N examples and M features,

- design matrix is $\Phi \in \mathbb{R}^{N \times M}$
- linear regression requires inverting $\Phi^T \Phi \in \mathbb{R}^{M \times M}$
- computational complexity of $O(M^3)$

Feature Mapping: Linear Classifiers

(recall Lectures 06 & 07)

Linear Classifiers: Review

Recall: Linear (binary) classifiers separate data with a **hyperplane** in feature space,

$$h(x) = \begin{cases} 1 & \text{if } w^T \phi(x) > 0 \\ 0 & \text{otherwise} \end{cases}$$

Examples: Differ only in how the weights w are learned.

- Logistic regression
- Linear Discriminant Analysis
- Fisher's Linear Discriminant
- Perceptron Learning

Feature Mapping: Example

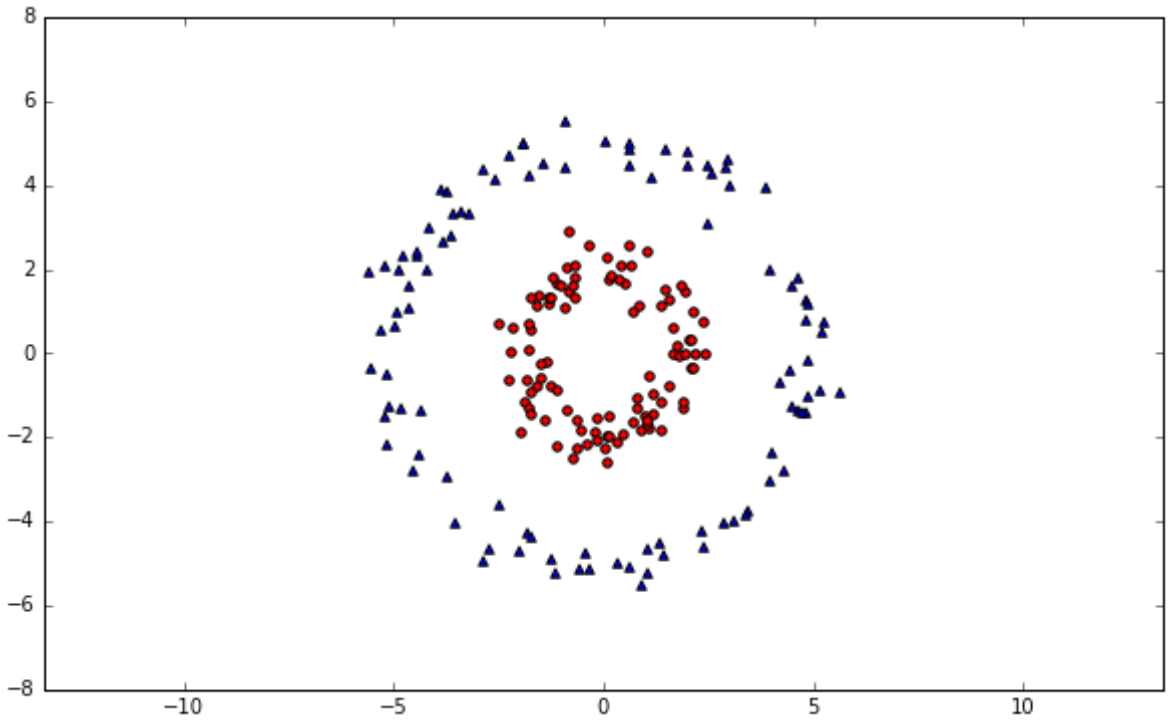
In [4]:
```
def get_circular_data(n):
    # sample outer circle
    theta0 = np.random.random(n) * 2 * np.pi;
    r0 = 2 + np.random.randn(n) / 3;
    # sample inner circle
    theta1 = np.random.random(n) * 2 * np.pi;
    r1 = 5 + np.random.randn(n) / 3;
    # join data
    x0 = r0 * [np.cos(theta0), np.sin(theta0)];
    x1 = r1 * [np.cos(theta1), np.sin(theta1)];
    return x0, x1;

def plot_circular_data(n):
    # get data
    x0, x1 = get_circular_data(n);

    # plot
    plt.figure(figsize=(10,6))
    plt.scatter(*x0, c="r")
    plt.scatter(*x1, c="b", marker="^")
    plt.axis("equal");

def plot_circular_3d(n):
    # get data
    x0, x1 = get_circular_data(n);

    # plot
    fig = plt.figure(figsize=(10,6));
    ax = fig.add_subplot(111, projection='3d');
    # plot 3d points
    ax.scatter(*x0, np.linalg.norm(x0, axis=0)**2, c="r")
    ax.scatter(*x1, np.linalg.norm(x1, axis=0)**2, c="b", marke
r="^");
    # set camera
    ax.view_init(elev=20, azim=45);

def plot_circular_squared(n):
    # get data
    x0, x1 = get_circular_data(n);

    # plot
    plt.figure(figsize=(10,6))
    plt.scatter(*(x0**2), c="r")
    plt.scatter(*(x1**2), c="b", marker="^")
    plt.axis("equal");
```

Feature Mapping: Example

Problem: The following data is **not** linearly separable.

- Every linear classifier will fail.

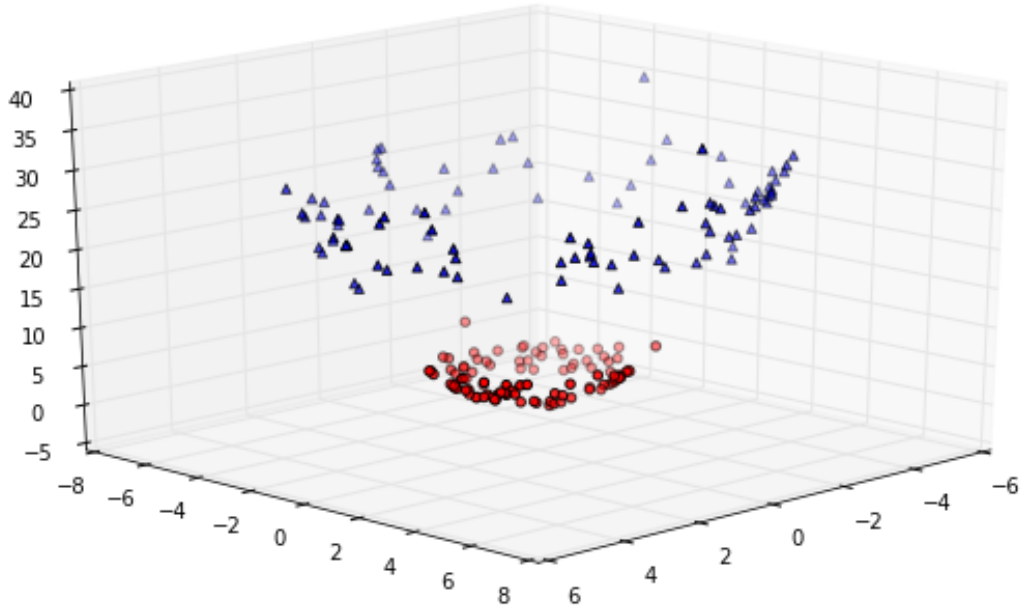
```
In [5]: plot_circular_data(100);
```



Feature Mapping: Example

Solution 1: Add squared-distance-to-origin $(x_1^2 + x_2^2)$ as third feature.

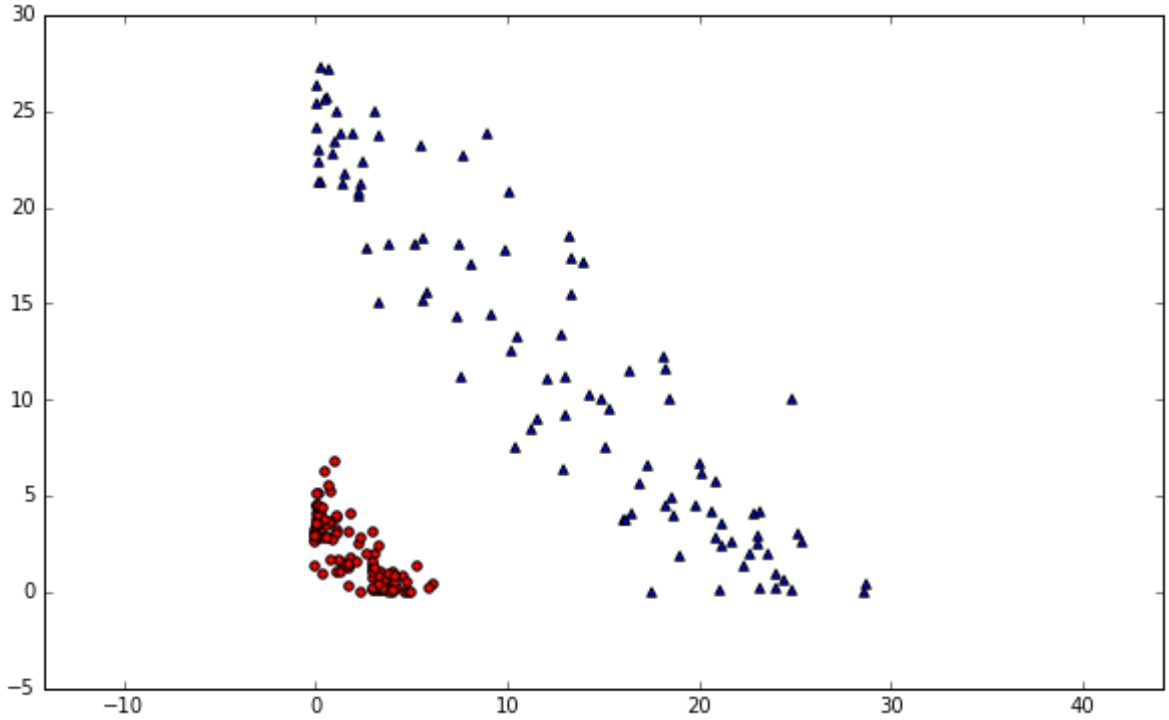
In [6]:
```
plot_circular_3d(100);
```



Feature Mapping: Example

Solution 2: Replace (x_1, x_2) with (x_1^2, x_2^2)

In [7]:
```
plot_circular_squared(100);
```



Feature Mapping: Linear Classifiers

Data has been mapped via ϕ to a new, higher-dimensional (possibly infinite!) space

- Certain *representations* are better for certain problems

Alternatively, the data still lives in original space, but the definition of **distance** or **inner product** has changed.

- Certain *inner products* are better for certain problems

Feature Mapping: Linear Classifiers

Unfortunately, higher-dimensional features come at a price!

- We can't possibly manage infinite-dimensional $\phi(x)$!
- Computational complexity blows up.

Kernel methods to the rescue!

Kernel Functions

> Uses content from **[PRML]** and Wikipedia, "Kernel Method" (https://en.wikipedia.org/wiki/Kernel_method)

Kernel Methods: Intro

Many algorithms depend on the data only through pairwise **inner products** between data points,

$$\langle x_1, x_2 \rangle = x_2^T x_1$$

Inner products can be replaced by **Kernel Functions**, capturing more general notions of *similarity*.

- No longer need coordinates!

Kernel Functions: Definition

A **kernel function** $\kappa(x, x')$ is intended to measure the similarity between x and x'.

- So far, we have used the standard inner product in the **transformed space**,
$$\kappa(x, x') = \phi(x)^T \phi(x')$$
- In general, $\kappa(x, x')$ is any symmetric positive-semidefinite function. This means that for every set $x_1, \ldots, x_n$, the matrix $[\kappa(x_i, x_j)]_{i,j \in [n]}$ is a PSD matrix.

Kernel Functions: Implicit Feature Map

For every valid kernel function $\kappa(x, x')$,

- there is an implicit feature mapping $\phi(x)$
- corresponding to an inner product $\phi(x)^T \phi(x')$ in some high-dimensional feature space

This *incredible* result follows from **Mercer's Theorem**,

- Generalizes the fact that *every positive-definite matrix corresponds to an inner product*
- For more info, see Hsing & Eubank 2015, "Theoretical Foundations of Functional Data Analysis" (http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470016914.html)

Kernel Functions: Simple Example

Kernel: For $x = (x_1, x_2)$ and $z = (z_1, z_2)$, define
$$\begin{aligned} \kappa(x, z) &= (x^T z)^2 \\ &= (x_1 z_1 + x_2 z_2)^2 \\ &= x_1^2 z_1^2 + 2 x_1 z_1 x_2 z_2 + x_2^2 z_2^2 \end{aligned}$$

Mapping: Equivalent to the standard inner product when either
$$\phi(x) = (x_1^2, \sqrt{2} x_1 x_2, x_2^2)$$
$$\phi(x) = (x_1^2, x_1 x_2, x_1 x_2, x_2^2)$$

> Implicit mapping is **not** unique!

Kernel Functions: Polynomial Example

Kernel: Higher-order polynomial of degree p,

$$\kappa(x, z) = (x^T z)^p = \left(\sum_{k=1}^{M} x_k z_k \right)^p$$

Mapping: Implicit feature vector $\phi(x)$ contains all monomials of degree p

Kernel Functions: Polynomial Example

Kernel: Inhomogeneous polynomial up to degree p, for $c > 0$,

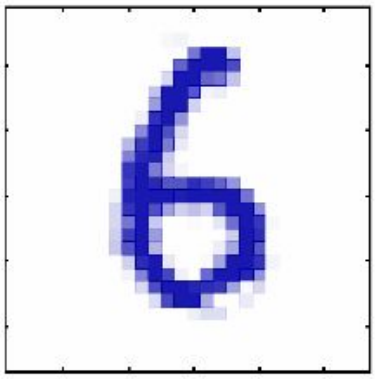
$$\kappa(x, z) = (x^T z + c)^p = \left(c + \sum_{k=1}^{M} x_k z_k \right)^p$$

Mapping: Implicit feature vector $\phi(x)$ contains all monomials of degree $\leq p$

Example: Handwritten Digits

Take the pixel values and compute $\kappa(x, z) = (x^T z + 1)^p$

- here, $x = 28 \times 28 = 784$ pixels



You can compute the inner product in the space of all monomials up to degree p

- (for $dim(x) = 784$ and $p = 4$ a $16G$ dimensional space!)

The Kernel Trick

- By using different definitions for inner product, we can compute inner products in a high dimensional space, with only the computational complexity of a low dimensional space.
- Many algorithms can be expressed completely in terms of kernels $\kappa(x, x')$, rather than other operations on x.
- In this case, you can replace one kernel with another, and get a new algorithm that works over a different domain.

Dual Representation and Kernel Trick

- The dual representation, and its solutions, are entirely written in terms of kernels.
- The elements of the Gram matrix $K = \Phi\Phi^T$

$$K_{ij} = \kappa(x_i, x_j) = \phi(x_i)^T \phi(x_j)$$

- These represent the pairwise similarities among all the observed feature vectors.
  - We may be able to compute the kernels more efficiently than the feature vectors.

Kernel Substitution

- To use the kernel trick, we must formulate (training and test) algorithms purely in terms of inner products between data points
- We can *not* access the coordinates of points in the high-dimensional feature space
- This seems a huge limitation, but it turns out that quite a lot can be done

Example: Distance

Distance between samples can be expressed in inner products:

$$\begin{aligned} \|\phi(x) - \phi(z)\|^2 &= \langle \phi(x) - \phi(z), \phi(x) - \phi(z) \rangle \\ &= \langle \phi(x), \phi(x) \rangle - 2\langle \phi(x), \phi(z) \rangle + \langle \phi(z), \phi(z) \rangle \\ &= \kappa(x, x) - 2\kappa(x, z) + \kappa(z, z) \end{aligned}$$

Nothing stops you from doing **k-nearest neighbor searches** in high dimensional spaces

> (Phew!!)

Example: Mean

Question: Can you determine the mean of data in the mapped feature space through kernel operations only?

Answer: No, you cannot compute any point explicitly.

Example: Distance to the Mean

- Mean of data points given by: $\phi(s) = \frac{1}{N} \sum_{i=1}^{N} \phi(x_i)$
- Distance to the mean:

$$\begin{aligned} \|\phi(x) - \phi_s\|^2 &= \langle \phi(x) - \phi_s, \phi(x) - \phi_s \rangle \\ &= \langle \phi(x), \phi(x) \rangle - 2\langle \phi(x), \phi_s \rangle + \langle \phi_s, \phi_s \rangle \\ &= \kappa(x, x) - \frac{2}{N} \sum_{i=1}^{N} \kappa(x, x_i) + \frac{1}{N^2} \sum_{j=1}^{N} \sum_{i=1}^{N} \kappa(x_i, x_j) \end{aligned}$$

Constructing Kernels

Method 1: Explicitly define a feature space mapping $\phi(x)$ and use **inner product kernel**

$$\kappa(x, x') = \phi(x)^T \phi(x') = \sum_{i=1}^{M} \phi_i(x) \phi_i(x')$$

Constructing Kernels

Method 2: Explicitly define a kernel $\kappa(x, x')$ and identify the implicit feature map, e.g.

$$\kappa(x, z) = (x^T z)^2 \qquad \Longrightarrow \qquad \phi(x) = (x_1^2, \sqrt{2} x_1 x_2, x_2^2)$$

> Kernels help us avoid the complexity of explicit feature mappings.

Constructing Kernels

Method 3: Define a similarity function $\kappa(x, x')$ and use **Mercer's Condition** to verify that an implicit feature map *exists* without finding it.

- Define the Gram matrix K to have elements $K_{nm} = \kappa(x_n, x_m)$
- K must **positive semidefinite** for all possible choices of the data set $\{x_n\}$

$$a^T K a \equiv \sum_i \sum_j a_i K_{ij} a_j \geq 0 \quad \forall\, a \in \mathbb{R}^n$$

Constructing Kernels: Building Blocks

There are a number of axioms that help us construct new, more complex kernels, from simpler known kernels.

- Check out **[PRML]** Chapter 6
- Prove these as an exercise!

For example, the following are kernels:

$$\kappa(x, x') = f(x)\kappa_1(x, x')f(x')$$
$$\kappa(x, x') = \exp(\kappa_1(x, x'))$$
$$\kappa(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right)$$

Popular Kernel Functions

Simple Polynomial Kernel (terms of degree 2)

$$\kappa(x, z) = (x^T z)^2$$

Generalized Polynomial Kernel (degree M)

$$\kappa(x, z) = (x^T z + c)^M, c > 0$$

Gaussian Kernels

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

Gaussian Kernel

> **Not related to Gaussian pdf!**

- Translation invariant (depends only on distance between points)
- Corresponds to an infinitely dimensional space!
  - **Important:** Do PRML Exercise 6.11