EECS 545: Machine Learning

Lecture 8. Kernel methods

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Outline

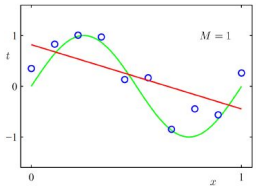
- Kernel methods: Motivation
- Kernel functions
- Kernel trick
  - Converting a ML model (objective function, prediction function, etc.) expressed with feature vectors to kernel functions
  - Kernel trick for linear regression
- Constructing (valid) kernels
- Kernel regression
  - Simple application of kernel method

Linear regression

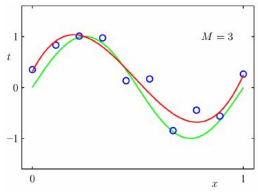
- Example: 1D regression
  - one input x, one output h(x)
- Linear model $h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$ can only produce straight lines through origin
- Not very flexible/powerful
- How do we deal with this?

Feature mappings

- Replace $x \to (1, x)$



- Replace $x \to (1, x, x^2, x^3)$



Linear regression with (nonlinear) features

- Linear regression model

$$h(\mathbf{x}, \mathbf{w}) = \mathbf{w}^\top \phi(\mathbf{x}) = \sum_{j=0}^{M} w_j \phi_j(\mathbf{x})$$

- Least-squares with L2 regression

$$J(\mathbf{w}) = \frac{1}{2} \sum_{n=0}^{N} (\mathbf{w}^\top \phi(\mathbf{x}^{(n)}) - y^{(n)})^2 + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w}$$

- Closed form solution: $N \times M$

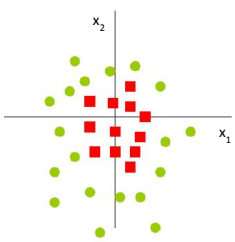
$$\mathbf{w} = (\underbrace{\Phi^\top \Phi}_{M \times N} + \lambda \mathbf{I})^{-1} \mathbf{y}$$

This is nice, but…

- What features to use?
- Computational complexity
  - Φ: *N***M* matrix
    - *N*: the number of examples
    - *M*: the number of features
  - Need to invert $\Phi^\top \Phi$ (*M***M*) matrix
  - Computational complexity scales with O(M^3)

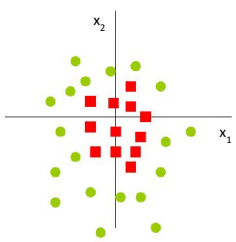
Linear classifiers

- No linear separating plane
- Linear classifiers not very flexible/powerful
- Can we do better?



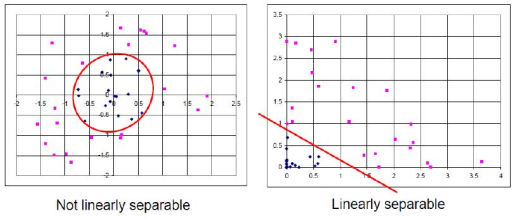
Linear classifiers with nonlinear features

- Add distance to origin $(x_1^2 + x_2^2)^{1/2}$ (L^2) as a third feature
- Data now lives on a parabolic surface in 3D.
- Linear separation in 3D feature space.
- In original feature space, decision boundary is an ellipse



Linear classifiers with nonlinear features

- Another way: Replace $x_1 \rightarrow x_1^2, \quad x_2 \rightarrow x_2^2$



Not linearly separable Linearly separable

  - Different expansions make the problem solvable with linear methods.

Linear classifiers with nonlinear features

- Data has been mapped to a new, higher dimensional space
- Alternative way to think about this: data still lives in original space, but the definition of *distance* or *inner product* has been changed

Classifiers with nonlinear features

- We have been mapping each data point x through a fixed non-linear mapping to get a feature vector $\phi(\mathbf{x})$
  - The feature vector extracts important properties from **x**.
  - E.g., polynomial combinations of the original features, up to some order
  - It may make many regression/classification problems easier.
- Unfortunately, the feature vector may be high-dimensional, even infinite-dimensional.
  - Problems: computational complexity

Kernels to the rescue (kernel trick)

- Embed data in a high dimensional space, and use simple models (linear relations) in this space.
- Use algorithms that do not need the coordinates of the embedded points, but only pairwise inner products
- Compute these inner products efficiently using a kernel

Kernel functions

- A kernel function ***k*(x,x')** is intended to represent the similarity between **x** and **x'**.
- A popular way to express similarity is as the inner product of feature vectors: $k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^\top \phi(\mathbf{x}')$
- We *define* a kernel function ***k*(x,x')** as one that can be expressed as an inner product, but we may not need to compute it that way.
- This definition immediately leads to symmetricity of kernels:

$$k(\mathbf{x}, \mathbf{x}') = k(\mathbf{x}', \mathbf{x})$$

Example: 2D input data

- Inner product between two vectors (x_1, x_2) and (z_1, z_2)

$$k(\mathbf{x}, \mathbf{z}) = \mathbf{x}^\top \mathbf{z} = x_1 z_1 + x_2 z_2$$

- Let's replace this by its square

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z})^2 = x_1^2 z_1^2 + x_2^2 z_2^2 + 2 x_1 x_2 z_1 z_2$$

- This is the same as inner product between

$$(x_1^2, \sqrt{2} x_1 x_2, x_2^2) \quad \text{and} \quad (z_1^2, \sqrt{2} z_1 z_2, z_2^2)$$

  - Or between

$$(x_1^2, x_1 x_2, x_1 x_2, x_2^2) \quad \text{and} \quad (z_1^2, z_1 z_2, z_1 z_2, z_2^2)$$

  - Note: solution is not unique.

Example: 2D input data

- Consider higher-order polynomial of degree p:

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z})^p = \left(\sum_{j=1}^{M} x_j z_j \right)^p$$

$$= \sum_{(j_1, j_2, \cdots, j_M): \sum_k j_k = p} \binom{p}{j_1, j_2, \cdots, j_M} (x_1 z_1)^{j_1} (x_2 z_2)^{j_2}, \cdots, (x_M z_M)^{j_M}$$

- Feature mapping:

$$\phi(\mathbf{x}) = \left[\cdots, \sqrt{\binom{p}{j_1, j_2, \cdots, j_M}} x_1^{j_1} x_2^{j_2}, \cdots, x_M^{j_M}, \cdots \right]^\top$$

  - All monomials of degree *p*

Example: 2D input data

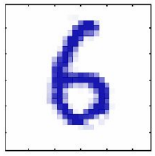
- Inhomogeneous polynomial up to degree p:

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z} + c)^p = \left(\sum_{j=1}^{M} x_j z_j + c \right)^p, \quad c > 0$$

- Feature mapping:
  - All monomials of degree <= p

Example: handwritten digits images

- Take the pixel values and compute
$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z} + 1)^p$$
  - Here **x** is 28*28 = 784 dimensional



- You need to compute the inner product in the space of all monomials up to degree *p*.
- For dim(**x**)=784 and p=4 a 16-billion dimensional space!

Kernel trick

- Kernels allow you to achieve a high-dimensional feature space which is desirable for better separability for classes, i.e., classification performance.
- Crucially, we don't have to compute the high-dimensional feature explicitly, the inner product of the features are computed directly via the kernel function.
- Many algorithms can be expressed completely in terms of kernels k(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.

$$k(\mathbf{x}, \mathbf{z}) = (\underbrace{\mathbf{x}^\top \mathbf{z}}_{784\ \text{dim}} + 1)^4 = \underbrace{\phi(\mathbf{x})^\top \phi(\mathbf{z})}_{16\ \text{billion dim}}$$

Kernel trick

- The kernel trick represents the problem formulation and its solutions entirely in terms of kernels (this is called "**dual** representation").
- The elements of the Gram matrix $K = \Phi\Phi^\top$

$$K_{nm} = \phi(\mathbf{x}^{(n)})^\top \phi(\mathbf{x}^{(m)}) = k(\mathbf{x}^{(n)}, \mathbf{x}^{(m)})$$

- These represent the pairwise similarities among all the observed feature vectors.
  - Assumption: 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 *cannot* 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:

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

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

Example: mean

- Can you determine the mean of data in the mapped feature space through kernel operations only?
  - A: No, you cannot compute any point explicitly

$$\phi_s = \frac{1}{N} \sum_{i=1}^{N} \phi(\mathbf{x}^{(i)})$$

Example: distance to the mean

- Mean of data points given by: $\phi_s = \frac{1}{N} \sum_{i=1}^{N} \phi(\mathbf{x}^{(i)})$
  - **cannot** be computed with kernel functions only
- Distance to mean:
  - **can** be computed with kernel functions only

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

Kernel trick for linear regression

- Recall regression problems with error function

$$J(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \left\{ \mathbf{w}^\top \phi\left(x^{(n)}\right) - y^{(n)} \right\}^2 + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w}$$

- *J*(w) is minimized at

$$\mathbf{w}_{\mathrm{ML}} = \left(\lambda \mathbf{I} + \Phi^\top \Phi\right)^{-1} \Phi^\top \mathbf{y}$$

- Recall the *N* x *M* design matrix that is central to this solution.
- We can approach the solution a different way

Recap: the design matrix

- The design matrix is an *N* x *M* matrix, applying
  - the *M* basis functions (*M*: number of columns)
  - to *N* data points (*N*: number of rows)

$$\Phi = \begin{pmatrix} \phi_0(\mathbf{x}^{(1)}) & \phi_1(\mathbf{x}^{(1)}) & \cdots & \phi_{M-1}(\mathbf{x}^{(1)}) \\ \phi_0(\mathbf{x}^{(2)}) & \phi_1(\mathbf{x}^{(2)}) & \cdots & \phi_{M-1}(\mathbf{x}^{(2)}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}^{(N)}) & \phi_1(\mathbf{x}^{(N)}) & \cdots & \phi_{M-1}(\mathbf{x}^{(N)}) \end{pmatrix}$$

$$\Phi\mathbf{w} \approx \mathbf{y}$$

The gram matrix

- For regression, a key term is the *M* x *M* matrix

$$\Phi^\top\Phi$$ "covariance"

- Here, we will use the *N* x *N Gram* matrix

$$\mathbf{K} = \Phi\Phi^\top$$ "pairwise similarity"

- Note that $K_{nm} = \phi(\mathbf{x}^{(n)})^\top\phi(\mathbf{x}^{(m)}) = k(\mathbf{x}^{(n)}, \mathbf{x}^{(m)})$
  - the pairwise similarities of all the data points in the training set
- Note that kernel methods use only K, not **Φ**

Kernel trick for linear regression

- Objective: $J(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{\mathbf{w}^\top\phi(x^{(n)}) - y^{(n)}\}^2 + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}$
- Another way to minimize *J*(w) is to set $\nabla_{\mathbf{w}}J(\mathbf{w}) = 0$

$$\nabla_{\mathbf{w}}J(\mathbf{w}) = \sum_{n=1}^{N}\{\mathbf{w}^\top\phi(x^{(n)}) - y^{(n)}\}\phi(x^{(n)}) + \lambda\mathbf{w} = 0$$

$$\Rightarrow \mathbf{w} = -\frac{1}{\lambda}\sum_{n=1}^{N}\left\{\mathbf{w}^\top\phi\left(\mathbf{x}^{(n)}\right) - y^{(n)}\right\}\phi(\mathbf{x}^{(n)}) = \sum_{n=1}^{N}a_n\phi(\mathbf{x}^{(n)}) = \Phi^\top\mathbf{a}$$

  - where $a_n = -\frac{1}{\lambda}\left\{\mathbf{w}^\top\phi\left(\mathbf{x}^{(n)}\right) - y^{(n)}\right\}$ (scalar)
- Let a be the **dual** parameter, instead of w.
- Transform *J*(w) to *J*(a) by substituting

$$\mathbf{w} = \Phi^\top\mathbf{a}$$ $\left[\phi(\mathbf{x}^{(1)}) \cdots \phi(\mathbf{x}^{(N)})\right]\begin{bmatrix} a^{(1)} \\ \vdots \\ a^{(N)} \end{bmatrix}$

Kernel trick for linear regression

- Objective function $J(\mathbf{w}) = \underbrace{\frac{1}{2}\sum_{n=1}^{N}\left\{\mathbf{w}^\top\phi\left(x^{(n)}\right) - y^{(n)}\right\}^2}_{\frac{1}{2}\mathbf{w}^\top\Phi^\top\Phi\mathbf{w} - \mathbf{w}^\top\Phi^\top\mathbf{y} + \frac{1}{2}\mathbf{y}^\top\mathbf{y}} + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}$
- Substitute $\mathbf{w} = \Phi^\top\mathbf{a}$

$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^\top\Phi\Phi^\top\Phi\Phi^\top\mathbf{a} - \mathbf{a}^\top\Phi\Phi^\top\mathbf{y} + \frac{1}{2}\mathbf{y}^\top\mathbf{y} + \frac{\lambda}{2}\mathbf{a}^\top\Phi\Phi^\top\mathbf{a}$$
$$= \frac{1}{2}\mathbf{a}^\top\mathbf{K}\mathbf{K}\mathbf{a} - \mathbf{a}^\top\mathbf{K}\mathbf{y} + \frac{1}{2}\mathbf{y}^\top\mathbf{y} + \frac{\lambda}{2}\mathbf{a}^\top\mathbf{K}\mathbf{a}$$ $\mathbf{K} = \Phi\Phi^\top$

- Setting the gradient w.r.t. *a* to zero:

$$\nabla_{\mathbf{a}}J(\mathbf{a}) = \mathbf{K}\mathbf{K}\mathbf{a} - \mathbf{K}\mathbf{y} + \lambda\mathbf{K}\mathbf{a} = 0$$
$$(\mathbf{K} + \lambda\mathbf{I})\mathbf{a} = \mathbf{K}\mathbf{y}$$ simplify (K is invertible)

- Solution (closed form):

$$\mathbf{a} = (\mathbf{K} + \lambda\mathbf{I}_N)^{-1}\mathbf{y}$$

Kernel trick for linear regression

- Objective function $J(\mathbf{w}) = \underbrace{\frac{1}{2}\sum_{n=1}^{N}\left\{\mathbf{w}^\top\phi\left(x^{(n)}\right) - y^{(n)}\right\}^2}_{\frac{1}{2}\mathbf{w}^\top\Phi^\top\Phi\mathbf{w} - \mathbf{w}^\top\Phi^\top\mathbf{y} + \frac{1}{2}\mathbf{y}^\top\mathbf{y}} + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}$
- Substitute $\mathbf{w} = \Phi^\top\mathbf{a}$

$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^\top\Phi\Phi^\top\Phi\Phi^\top\mathbf{a} - \mathbf{a}^\top\Phi\Phi^\top\mathbf{y} + \frac{1}{2}\mathbf{y}^\top\mathbf{y} + \frac{\lambda}{2}\mathbf{a}^\top\Phi\Phi^\top\mathbf{a}$$
$$= \frac{1}{2}\mathbf{a}^\top\mathbf{K}\mathbf{K}\mathbf{a} - \mathbf{a}^\top\mathbf{K}\mathbf{y} + \frac{1}{2}\mathbf{y}^\top\mathbf{y} + \frac{\lambda}{2}\mathbf{a}^\top\mathbf{K}\mathbf{a}$$ $\mathbf{K} = \Phi\Phi^\top$

- Solution (closed form): $\mathbf{a} = (\mathbf{K} + \lambda\mathbf{I}_N)^{-1}\mathbf{y}$
- Prediction for any arbitrary input *x*:

$$h(\mathbf{x}) = \mathbf{w}^\top\phi(\mathbf{x}) = \phi(\mathbf{x})^\top\mathbf{w} = \phi(\mathbf{x})^\top\Phi^\top\mathbf{a} = (\Phi\phi(\mathbf{x}))^\top\mathbf{a} = \sum_{n=1}^{N}a_n k(\mathbf{x}^{(n)}, \mathbf{x})$$
$$= k(\mathbf{x})^\top(\mathbf{K} + \lambda\mathbf{I}_N)^{-1}\mathbf{y}$$

definition: $k(\mathbf{x}) = \left[k(\mathbf{x}^{(1)}, \mathbf{x}), \cdots, k(\mathbf{x}^{(N)}, \mathbf{x})\right]^\top$

Kernel trick for linear regression

- Transform *J*(w) to *J*(a) by using $\mathbf{w} = \Phi^\top\mathbf{a}$ and the *Gram* matrix $\mathbf{K} = \Phi\Phi^\top$
- Find **a** to minimize *J*(a): $\mathbf{a} = (\mathbf{K} + \lambda\mathbf{I}_N)^{-1}\mathbf{y}$
- For predictions (for query point/test example **x**):

$$h(\mathbf{x}) = \phi(\mathbf{x})^\top\mathbf{w} = \phi(\mathbf{x})^\top\Phi^\top\mathbf{a} = k(\mathbf{x})^\top(\mathbf{K} + \lambda\mathbf{I}_N)^{-1}\mathbf{y}$$

  - where $k(\mathbf{x}) = \left[k(\mathbf{x}^{(1)}, \mathbf{x}), \cdots, k(\mathbf{x}^{(N)}, \mathbf{x})\right]^\top$
- This method is called ***Kernel Ridge Regression***.

Primal versus Dual

- Primal: $\mathbf{w} = \left(\Phi^\top\Phi + \lambda\mathbf{I}_M\right)^{-1}\Phi^\top\mathbf{y}$
- Dual: $\mathbf{a} = (\mathbf{K} + \lambda\mathbf{I}_N)^{-1}\mathbf{y}$
- Primal: invert *M* by *M* matrix (*M* = dim feature space), w vector of length *M*
  - cheaper because usually *N* > *M*, but you need to explicitly construct features.
- Dual: invert *N* by *N* matrix (*N* = number of data points)
  - can use the kernel trick (embed into very high dimensional feature space)
  - Use kernels *k*(x,x') to represent similarity.
  - Kernels can be defined over vectors, images, sequences, graphs, text, etc.

Constructing valid kernels

- One can do *kernel engineering* to create kernels for particular purposes, expressing different kinds of similarity.
- How do we verify that a kernel is valid?
- Three methods (for verification):
  1. Direct construction with feature vectors
  2. Mercer Theorem
  3. Composition of kernels with pre-defined rules

Constructing valid kernels: Method 1
Explicit Construction by defining feature vectors

- Method 1: One way is to define the feature space mapping $\phi(\mathbf{x})$ and show that the kernel function represents the inner product of feature vectors:

$$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^\top \phi(\mathbf{x}') = \sum_{i=1}^{M} \phi_i(\mathbf{x})\phi_i(\mathbf{x}')$$

Constructing valid kernels: Method 1
Explicit Construction by defining feature vectors

- Suppose we define a kernel function directly, such as

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z})^2$$

- In 2D, we can explicitly identify the feature map

$$\phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

  – such that

$$k(\mathbf{x}, \mathbf{z}) = \phi(\mathbf{x})^\top \phi(\mathbf{z})$$

- Explicit feature mappings can be very complex.
  – Kernels help us avoid that complexity.

Constructing valid kernels: Method 2
Mercer Theorem

- A simpler way to test without having to construct ϕ(x)
- Use the necessary and sufficient condition (Mercer Theorem) that for a function k(x,x') to be a inner product (valid) kernel:
  – the Gram matrix **K**, whose elements are given by $k(\mathbf{x}^{(n)}, \mathbf{x}^{(m)})$, should be positive semidefinite for all possible choices of the data set {x(n)}
  – I.e., **K** is positive semidefinite:

$$\mathbf{a}^\top \mathbf{K}\mathbf{a} = \sum_{i=1}^{N}\sum_{j=1}^{N} a_i K_{i,j} a_j \geq 0 \quad \forall \mathbf{a} \in \mathbb{R}^N$$

Constructing valid kernels: Method 3
Using Pre-Defined Rules

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

$$k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x})k_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}')$$
$$k(\mathbf{x}, \mathbf{x}') = \exp(k_1(\mathbf{x}, \mathbf{x}'))$$
$$k(\mathbf{x}, \mathbf{x}') = \exp(-\|\mathbf{x} - \mathbf{x}'\|^2/2\sigma^2)$$

  – **Prove** that these are valid kernels (homework)

Constructing valid kernels: Method 3
Using Pre-Defined Rules

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$, the following new kernels will also be valid:

(build kernel from kernels)

$$k(\mathbf{x}, \mathbf{x}') = ck_1(\mathbf{x}, \mathbf{x}') \quad (6.13)$$
$$k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x})k_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}') \quad (6.14)$$
$$k(\mathbf{x}, \mathbf{x}') = q(k_1(\mathbf{x}, \mathbf{x}')) \quad (6.15)$$
$$k(\mathbf{x}, \mathbf{x}') = \exp(k_1(\mathbf{x}, \mathbf{x}')) \quad (6.16)$$
$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') \quad (6.17)$$
$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}') \quad (6.18)$$
$$k(\mathbf{x}, \mathbf{x}') = k_3(\phi(\mathbf{x}), \phi(\mathbf{x}')) \quad (6.19)$$
$$k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^\top \mathbf{A}\mathbf{x}' \quad (6.20)$$
$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b) \quad (6.21)$$
$$k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a)k_b(\mathbf{x}_b, \mathbf{x}'_b) \quad (6.22)$$

where $c > 0$ is a constant, $f(\cdot)$ is any function, $q(\cdot)$ is a polynomial with nonnegative coefficients, $\phi(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$, $k_3(\cdot, \cdot)$ is a valid kernel in $\mathbb{R}^M$, $\mathbf{A}$ is a symmetric positive semidefinite matrix, $\mathbf{x}_a$ and $\mathbf{x}_b$ are variables (not necessarily disjoint) with $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$, and k_a and k_b are valid kernel functions over their respective spaces.

Most popular kernels

- Simple Polynomial Kernel (terms of degree 2)

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z})^2$$

- Generalized Polynomial kernel - degree M

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z} + c)^M, \quad c > 0$$

- Gaussian Kernels

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

Gaussian kernel

- Not related to Gaussian pdf
- Translation invariant (depends only on distance between points)
- Corresponds to an infinitely dimensional space! (PRML ex6.11)

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

Kernel regression

Kernel regression

- Recall k-nearest neighbor regression:

$$k(\mathbf{x}) = \frac{1}{k} \sum_{(\mathbf{x}',y') \in \mathrm{KNN}(\mathbf{x})} y'$$

- Kernel regression:

$$h(\mathbf{x}) = \frac{\sum_i k(\mathbf{x}, \mathbf{x}^{(i)}) y^{(i)}}{\sum_j k(\mathbf{x}, \mathbf{x}^{(j)})} = \frac{1}{Z} \sum_i k(\mathbf{x}, \mathbf{x}^{(i)}) y^{(i)}$$

$$\text{where} \quad Z = \sum_j k(\mathbf{x}, \mathbf{x}^{(j)})$$

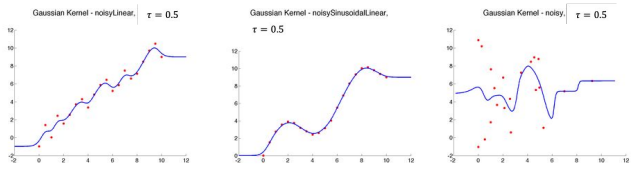
- Weighted average of training responses where weight is proportional to the similarity with the corresponding feature.

Kernel regression

- Can use different kinds of kernels as they capture similarity between features differently.
  - Popular: Gaussian kernel with width τ:

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\tau^2}\right)$$

- Examples



Kernels for classification

- We can just as easily use kernels for classification as well.
- Assume $y_i \in \{-1, +1\}$, return output as weighted majority:

$$h(\mathbf{x}) = \mathrm{sign}\left(\sum_{i=1}^{N} k(\mathbf{x}, \mathbf{x}^{(i)}) y^{(i)}\right)$$

- Compare it to k-nearest neighbor classification:

$$h(\mathbf{x}) = \mathrm{sign}\left(\frac{1}{k} \sum_{(\mathbf{x}',y') \in \mathrm{KNN}(\mathbf{x})} y'\right)$$

Locally-weighted Linear Regression vs. Kernel regression

- Suppose we want to predict y given a query x.
- Locally-weighted linear regression
  - 1. Fit **w** to minimize $\sum_i r^{(i)} (y^{(i)} - \mathbf{w}^\top \phi(\mathbf{x}^{(i)}))^2 \leftarrow \mathbf{w} = (\Phi^\top R \Phi)^{-1} \Phi^\top R \mathbf{y}$
  - 2. Output $\mathbf{w}^\top \phi(\mathbf{x}^{(i)})$
  - Standard choice: $r^{(i)} = \exp\left(-\frac{\|\mathbf{x}^{(i)} - \mathbf{x}\|^2}{2\tau^2}\right)$

R is a diagonal matrix with $R_{i,i} = \frac{1}{2} r^{(i)}$

τ: "kernel width"

- Kernel regression (Using Gaussian kernel)
  - output: $\frac{\sum_i \kappa(\mathbf{x}, \mathbf{x}^{(i)}) y^{(i)}}{\sum_i \kappa(\mathbf{x}, \mathbf{x}^{(i)})}$

    where $\kappa(\mathbf{x}, \mathbf{x}^{(i)}) = \exp\left(\frac{\|\mathbf{x}^{(i)} - \mathbf{x}\|^2}{2\tau}\right)$

More generally, any distance metric (other than L2 or Euclidean distance) can be used.
Also, more general types of kernel function can be used.