KERNEL METHODS

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CSE 6390/PSYC 6225 Computational Modeling of Visual Perception

Outline

- Dual representation
- Constructing kernels
- Radial basis functions
- Gaussian processes

Parametric vs Kernel Methods

- In linear **parametric** regression or classification we model target variables t as functions $y(\mathbf{x},\mathbf{w})$ of the input vector $\mathbf{x}$, where $\mathbf{w}$ is a parameter vector.
  1. Estimate $\mathbf{w}$ from the training input vectors $\mathbf{x}_n$ and their associated target variables $\mathbf{t}_n$
  2. Throw away the training data $(\mathbf{x}_n, \mathbf{t}_n)$
  3. Given a new input vector $\mathbf{x}$, estimate the corresponding target variable $\mathbf{t}$, using the learned parameters $\mathbf{w}$:

     $$t \simeq y(x,\mathbf{w})$$

Parametric vs Kernel Methods

- In **kernel** methods we model new data ($\boldsymbol{x}$, $\boldsymbol{t}$) directly as a function of the training data ($\boldsymbol{x}_n$, $\boldsymbol{t}_n$).
  - This means we never throw away the training data.
  - The kernel method allows a high-dimensional (even infinite dimensional) feature space to be used implicitly.

The kernel function

The kernel function $k(\mathbf{x},\mathbf{x}')$ measures the 'similarity' of input vectors $\mathbf{x}$ and $\mathbf{x}'$ as an inner product in a feature space defined by the feature space mapping $\phi(\mathbf{x})$:

$$k(\mathbf{x},\mathbf{x}') = \phi(\mathbf{x})^t \phi(\mathbf{x}')$$

If $k(\mathbf{x},\mathbf{x}') = k(\mathbf{x}-\mathbf{x}')$ we say that the kernel is *stationary*

If $k(\mathbf{x},\mathbf{x}') = k\left(\left\|\mathbf{x}-\mathbf{x}'\right\|\right)$ we call it a *radial basis function*.

Dual Representations

- Many linear models for regression and classification can be reformulated as dual kernel models.
- For example, regularized linear least-squares regression, where the error function is given by:

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

- which has a minimum at

$$\mathbf{w} = -\frac{1}{\lambda}\sum_{n=1}^{N}\left\{\mathbf{w}^t\phi(\mathbf{x}_n) - \mathbf{t}_n\right\}\phi(\mathbf{x}_n)$$

Dual Representations

$$\mathbf{w} = -\frac{1}{\lambda}\sum_{n=1}^{N}\left\{\mathbf{w}^t\phi\left(\mathbf{x}_n\right)-\mathbf{t}_n\right\}\phi\left(\mathbf{x}_n\right)$$

Defining $a_n = -\frac{1}{\lambda}\left\{\mathbf{w}^t\phi\left(\mathbf{x}_n\right)-\mathbf{t}_n\right\}$

we can reexpress $\mathbf{w}$ as

$$\mathbf{w} = \Phi^t\mathbf{a}$$

where $\phi\left(\mathbf{x}_n\right)^t$ is the n^{th} row of Φ

and a_n is the n^{th} element of $\mathbf{a}$

Dual Representations

Substituting, we can express the error function in terms of **a**:

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

which has a minimum at

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

where $\mathbf{K}$ is the Gram matrix $\mathbf{K} = \Phi\Phi^t$ with elements

$$K_{nm} = \phi\left(\mathbf{x}_n\right)^t \phi\left(\mathbf{x}_m\right) = k\left(\mathbf{x}_n, \mathbf{x}_m\right)$$

Dual Representations

Predictions are then given by

$$y(\mathbf{x}) = \mathbf{w}^t \phi(\mathbf{x}) = k(\mathbf{x})^t \left(\mathbf{K} + \lambda \mathbf{I}_N\right)^{-1} \mathbf{t}$$

where $\mathbf{k}(\mathbf{x})$ is the vector with elements $k_n(\mathbf{x}) = k(\mathbf{x}_n, \mathbf{x})$

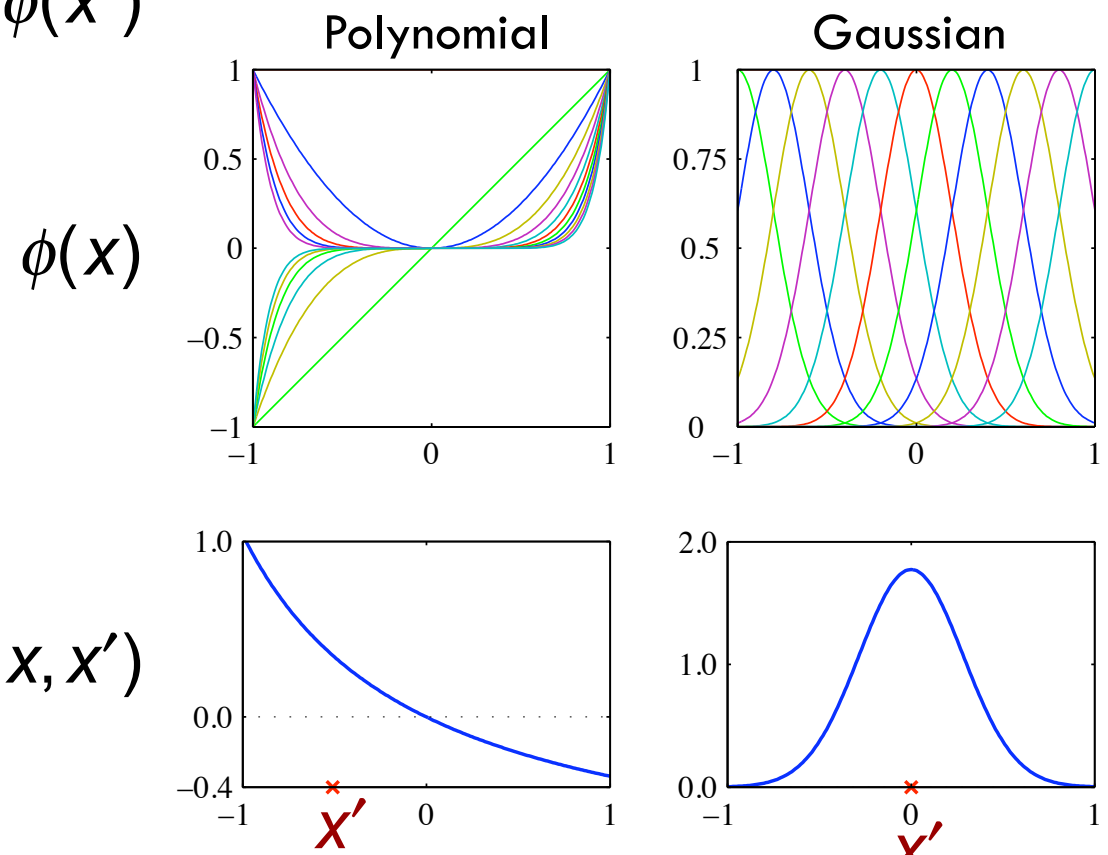
and $k\left(\mathbf{x}_n, \mathbf{x}_m\right) = \phi\left(\mathbf{x}_n\right)^t \phi\left(\mathbf{x}_m\right)$

- Thus predictions are expressed entirely in terms of kernel functions on input vector pairs.

Constructing Kernels

- One can construct a kernel by selecting a feature space mapping $\phi(x)$ and then defining

$$k(x, x') = \phi(x)^t \phi(x')$$



Constructing Kernels

- We can construct a kernel by selecting a feature space mapping $\phi(x)$ and then defining

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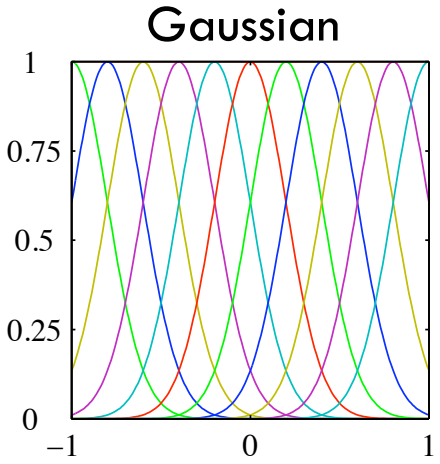
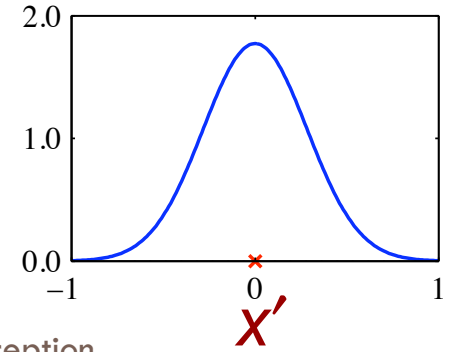
$\phi(x')$



$k(x, x')$



Constructing Kernels

- Alternatively, we can construct the kernel function directly, ensuring that it corresponds to an inner product in some (possibly infinite-dimensional) feature space.

Constructing Kernels

$$k(x) = \phi(x)^t \phi(x')$$

Example 1: $k(x,z) = x^t z$

Example 2: $k(x,z) = x^t z + c, \; c > 0$

Example 3: $k(x,z) = \left(x^t z\right)^2$

Constructing Kernels

More generally, $k(\mathbf{x}, \mathbf{x}')$ is a valid kernel if the Gram matrix $\mathbf{K}$ whose elements are given by $k(\mathbf{x}_n, \mathbf{x}_m)$ is positive semidefinite for all possible choices of $\{\mathbf{x}_n\}$.

Kernel Properties

- Kernels obey certain properties that make it easy to construct complex kernels from simpler ones.

Kernel Properties

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

$$
\begin{aligned}
k(\boldsymbol{x}, \boldsymbol{x}') &= c k_1(\boldsymbol{x}, \boldsymbol{x}') && (6.13)\\
k(\boldsymbol{x}, \boldsymbol{x}') &= f(\boldsymbol{x}) k_1(\boldsymbol{x}, \boldsymbol{x}') f(\boldsymbol{x}') && (6.14)\\
k(\boldsymbol{x}, \boldsymbol{x}') &= q(k_1(\boldsymbol{x}, \boldsymbol{x}')) && (6.15)\\
k(\boldsymbol{x}, \boldsymbol{x}') &= exp(k_1(\boldsymbol{x}, \boldsymbol{x}')) && (6.16)\\
k(\boldsymbol{x}, \boldsymbol{x}') &= k_1(\boldsymbol{x}, \boldsymbol{x}') + k_2(\boldsymbol{x}, \boldsymbol{x}') && (6.17)\\
k(\boldsymbol{x}, \boldsymbol{x}') &= k_1(\boldsymbol{x}, \boldsymbol{x}') k_2(\boldsymbol{x}, \boldsymbol{x}') && (6.18)\\
k(\boldsymbol{x}, \boldsymbol{x}') &= k_3(\boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}')) && (6.19)\\
k(\boldsymbol{x}, \boldsymbol{x}') &= \boldsymbol{x}^T \mathbf{A} \boldsymbol{x}' && (6.20)\\
k(\boldsymbol{x}, \boldsymbol{x}') &= k_a(\boldsymbol{x}_a, \boldsymbol{x}'_a) + k_b(\boldsymbol{x}_b, \boldsymbol{x}'_b) && (6.21)\\
k(\boldsymbol{x}, \boldsymbol{x}') &= k_a(\boldsymbol{x}_a, \boldsymbol{x}'_a) k_b(\boldsymbol{x}_b, \boldsymbol{x}'_b) && (6.22)
\end{aligned}
$$

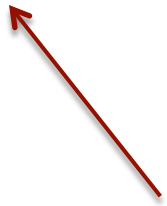
where $c > 0$, $f(\cdot)$ is any function, $q(\cdot)$ is a polynomial with nonnegative coefficients, $\phi(\mathbf{x})$ is a mapping from $\mathbf{x} \rightarrow \mathbb{R}^M$, A is a symmetric positive semidefinite matrix, $\mathbf{x}_a$ and $\mathbf{x}_b$ are variables such that $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$ and k_a, k_b are valid kernels over their respective spaces.

Constructing Kernels

- Examples:

$$k(x^t, x') = \left(x^t x' + c\right)^M, c > 0 \qquad \text{(Use 6.18)}$$

$$k(x, x') = \exp\left(-\left\|x - x'\right\|^2 / 2\sigma^2\right) \qquad \text{(Use 6.14 and 6.16.)}$$



Corresponds to infinite-dimensional feature vector

Radial Basis Functions

- Widely used choice of basis function for linear regression.

For example, given training input vectors $\{x_1,\ldots,x_N\}$ and corresponding target values $\{t_1,\ldots t_N\}$, we can define an interpolation function $f(x)$ as:

$$f(x)=\sum_{n=1}^{N} w_n h\left(\|x-x_n\|\right)$$

Since **w** and **t** have the same dimensionality, we can fit the training data exactly, while providing predictions for input vectors we haven't yet seen.

END OF LECTURE
NOV 3, 2010

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Kernel Regression

- Can also be used for prediction when there is noise in **x**, as well as **t** (the **Nadaraya-Watson** model):

Let ξ be the noise in **x**, drawn from distribution $\nu(\xi)$. Then

$$E = \frac{1}{2}\sum_{n=1}^{N}\int\left\{y\left(\mathbf{x}_n + \xi\right) - t_n\right\}^2 \nu(\xi)\, d\xi$$

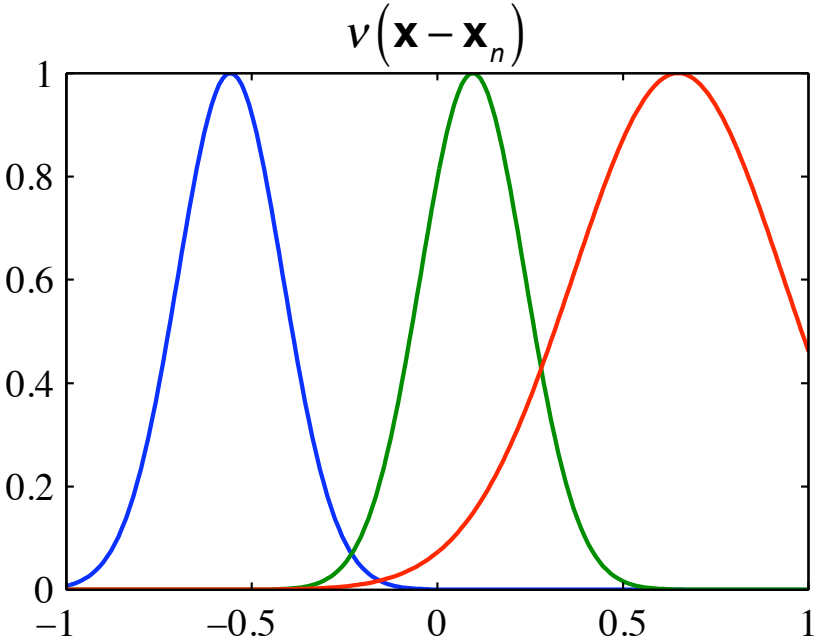
Using the calculus of variations (Appendix D),
we can find the optimal interpolation function $y(\mathbf{x})$:

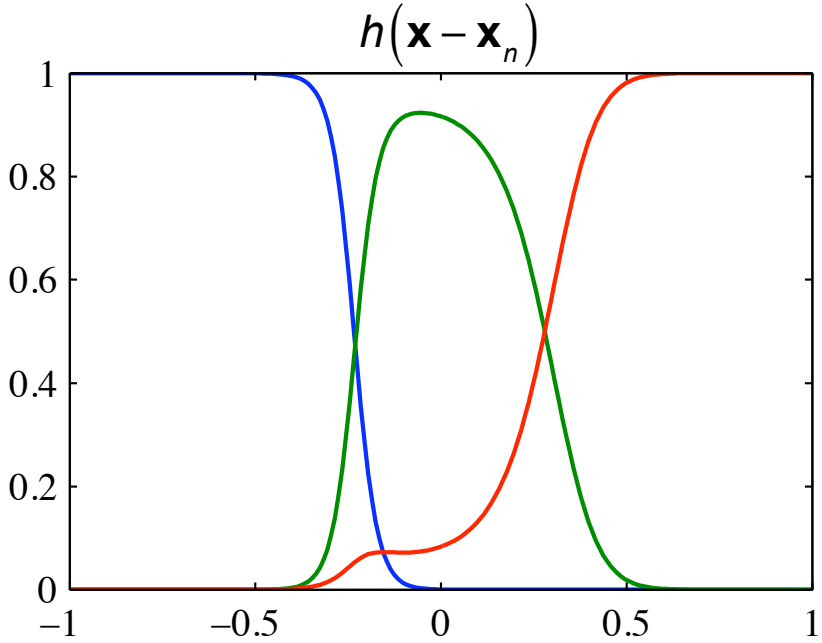
$$y(\mathbf{x}) = \sum_{n=1}^{N} t_n h\left(\mathbf{x} - \mathbf{x}_n\right)$$

where

$$h\left(\mathbf{x} - \mathbf{x}_n\right) = \frac{\nu\left(\mathbf{x} - \mathbf{x}_n\right)}{\sum_{n=1}^{N}\nu\left(\mathbf{x} - \mathbf{x}_n\right)}$$

Kernel Regression





$$y(\mathbf{x}) = \sum_{n=1}^{N} t_n h(\mathbf{x}-\mathbf{x}_n), \quad \text{where} \quad h(\mathbf{x}-\mathbf{x}_n) = \frac{v(\mathbf{x}-\mathbf{x}_n)}{\sum_{n=1}^{N} v(\mathbf{x}-\mathbf{x}_n)}$$

Nadaraya-Watson Model

- The Nadaraya-Watson model can also be understood as a form of kernel density estimation:

Given a training set $\{\mathbf{x}_n, t_n\}$, we model the joint distribution $p(\mathbf{x}, t)$ using a Parzen density estimator

$$p(\mathbf{x}, t) = \frac{1}{N}\sum_{n=1}^{N} f(\mathbf{x} - \mathbf{x}_n, t - t_n)$$

Then the regression fuction $y(\mathbf{x})$ is given by

$$y(\mathbf{x}) = E[t \mid \mathbf{x}] = \sum_n k(\mathbf{x}, \mathbf{x}_n) t_n$$

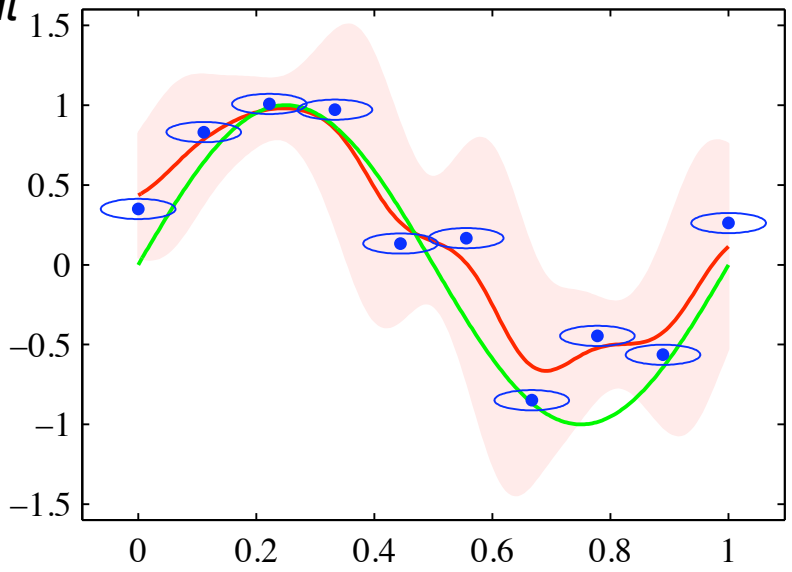
where $k(\mathbf{x}, \mathbf{x}_n) = \frac{g(\mathbf{x} - \mathbf{x}_n)}{\sum_m g(\mathbf{x} - \mathbf{x}_m)}$ and $g(\mathbf{x}) = \int_{-\infty}^{\infty} f(\mathbf{x}, t)\, dt$

Nadaraya-Watson Model

- The model provides not only the expected target value, but the entire posterior:

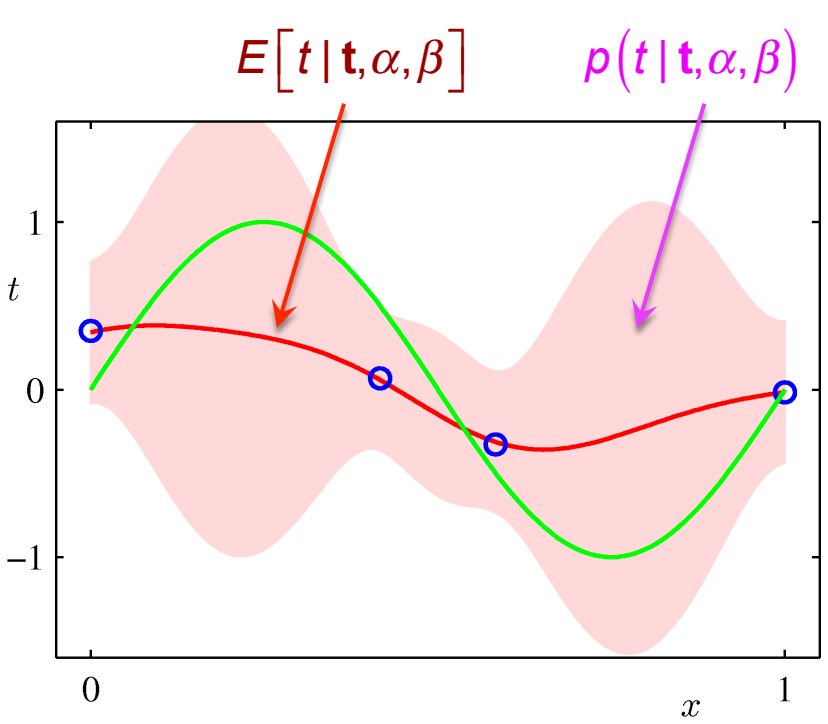
Given a training set $\{\mathbf{x}_n, t_n\}$, we model the joint distribution $p(\mathbf{x}, t)$ using a Parzen density estimator

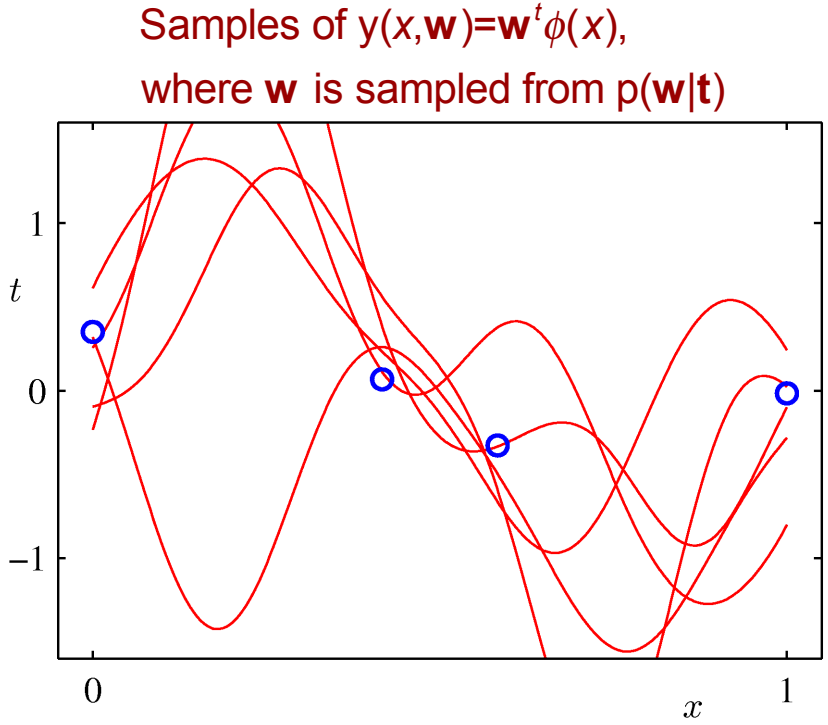
$$p(t \mid \mathbf{x}) = \frac{p(t,\mathbf{x})}{\int p(t,\mathbf{x})\,dt} = \frac{\sum_n f(\mathbf{x}-\mathbf{x}_n, t-t_n)}{\sum_m \int f(\mathbf{x}-\mathbf{x}_m, t-t_m)\,dt}$$



Gaussian Processes

- In linear regression, we estimate a posterior distribution over parameters **w**.
- This determines a prior distribution p(y) over the function y.





Gaussian Processes

- In the Gaussian process approach, we dispense with the parameters **w** and define the prior over y directly.

More precisely, a Gaussian process defines a probability distribution over functions $y(\mathbf{x})$ such that the set of values of $y(\mathbf{x})$ evaluated at an arbitrary set of points $\mathbf{x}_1,\ldots\mathbf{x}_N$ are jointly Gaussian.

Equivalence with Classical Regression

$$y(\mathbf{x}) = \mathbf{w}^t \phi(\mathbf{x})$$

Assume a Gaussian prior over the weight vector: $p(\mathbf{w}) = N\left(\mathbf{w} \mid \mathbf{0}, \alpha^{-1}\mathbf{I}\right)$.

We have training data $\mathbf{x}_1, \ldots \mathbf{x}_N$

For given $\mathbf{w}$, this determines a vector of function values $\mathbf{y} = \left(y\left(\mathbf{x}_1\right), \ldots y\left(\mathbf{x}_N\right)\right)^t$:

$$\mathbf{y} = \Phi\mathbf{w}, \quad \text{where } \Phi_{nk} = \phi_k\left(\mathbf{x}_n\right)$$

Since y is a linear function of $\mathbf{w}$, it is also Gaussian, with:

$$E\left[y\right] = 0$$

$$\text{cov}\left[y\right] = \frac{1}{\alpha}\Phi\Phi^t = \mathbf{K},$$

$$\text{where } K_{nm} = k\left(\mathbf{x}_n, \mathbf{x}_m\right) = \frac{1}{\alpha}\phi\left(\mathbf{x}_n\right)\phi\left(\mathbf{x}_m\right)$$

Gaussian Processes

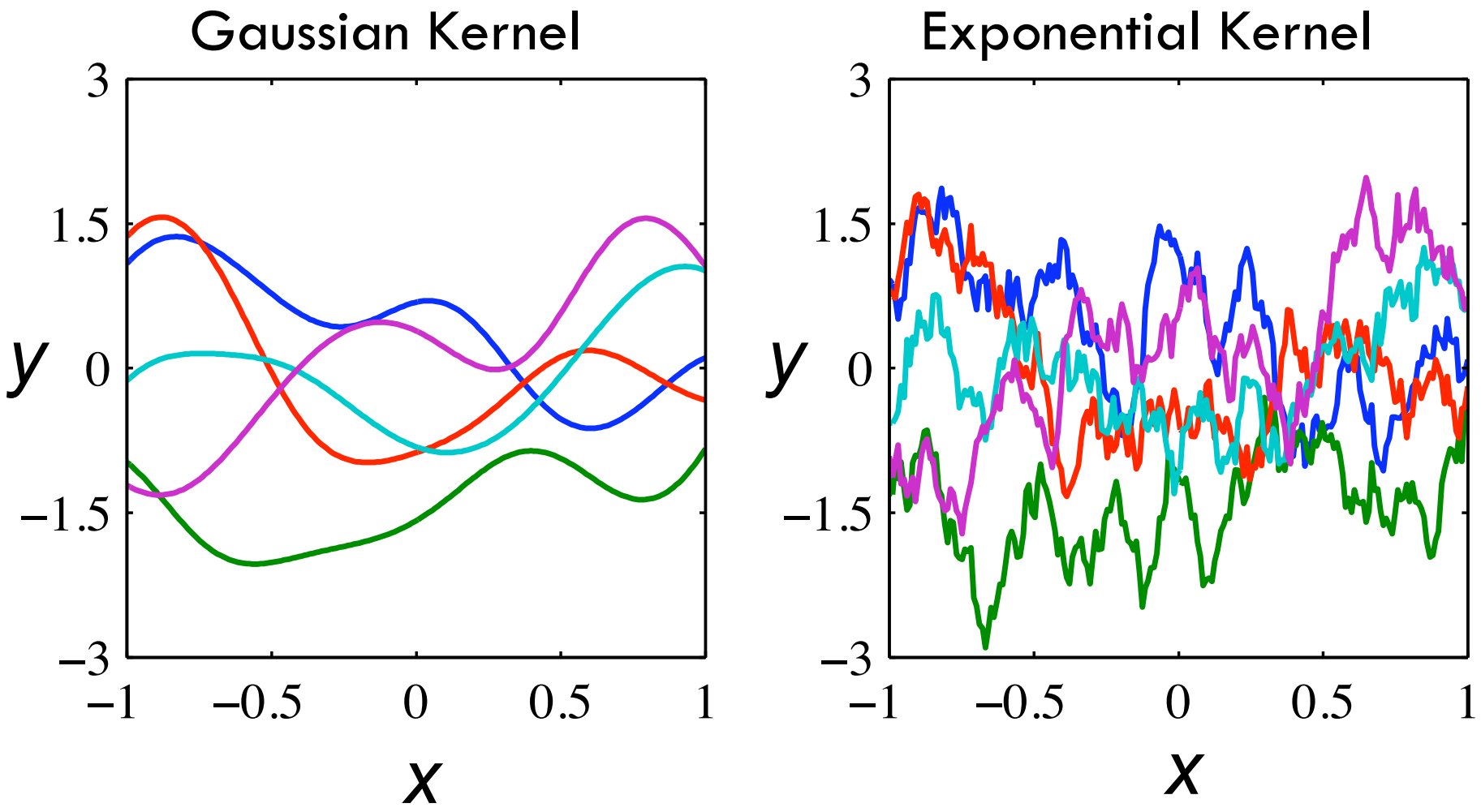
- Thus we have a direct probabilistic model for $y(\mathbf{x}_n)$:

$$p(y) = N(y \mid 0, \mathbf{K})$$

$$\text{where } K_{nm} = k(\mathbf{x}_n, \mathbf{x}_m) = \frac{1}{\alpha}\phi(\mathbf{x}_n)\phi(\mathbf{x}_m)$$

- Notes
  - All we need to specify this model is the kernel function evaluated over all pairs of training input vectors.
  - The kernel function can be defined in terms of feature vectors, as above, or directly.
  - Normally, the kernel function is defined so that $y(\mathbf{x}_n)$ and $y(\mathbf{x}_m)$ are strongly correlated if $\mathbf{x}_n$ and $\mathbf{x}_m$ are close to each other.

Gaussian Processes: Examples



Using Gaussian Processes for Prediction

- To use Gaussian processes for prediction, we need to account for the noise in the observed target values:

$$t_n = y_n + \varepsilon_n$$

where ε_n is Gaussian iid, so that:

$$p(\mathbf{t} \mid \mathbf{y}) = N(\mathbf{t} \mid \mathbf{y}, \beta^{-1}\mathbf{I})$$

Using Gaussian Processes for Prediction

Knowing $p(\mathbf{y})$ and $p(\mathbf{t}|\mathbf{y})$, we can use the results from Chapter 2 to determine $p(\mathbf{t})$:

$$p(\mathbf{t}) = N(\mathbf{t}|\mathbf{0},\mathbf{C})$$

where $C_{nm} = k(\mathbf{x}_n,\mathbf{x}_m) + \beta^{-1}\delta_{nm}$

Predictions can now be made using the partitioned Gaussian equations from Chapter 2.3.2:

$$p(t_{N+1}|\mathbf{t}) = N(t_{N+1}|m(\mathbf{x}_{N+1}),\sigma^2(\mathbf{x}_{N+1}))$$

where

$$m(\mathbf{x}_{N+1}) = \mathbf{k}^t\mathbf{C}_N^{-1}\mathbf{t} \qquad k_n = k(\mathbf{x}_n,\mathbf{x}_{N+1})$$

$$\sigma^2(\mathbf{x}_{N+1}) = c - \mathbf{k}^t\mathbf{C}_N^{-1}\mathbf{k} \qquad c = k(\mathbf{x}_{N+1},\mathbf{x}_{N+1}) + \beta^{-1}$$

Learning the Hyperparameters

We have assumed that the kernel functions $k(\mathbf{x}_n, \mathbf{x}_m)$ are fixed.

This corresponds to a fixed feature space mapping $\phi(\mathbf{x})$.

In practice, we may instead wish to define the covariance function through a parameterized family of kernels, and then infer the parameters θ from the data.

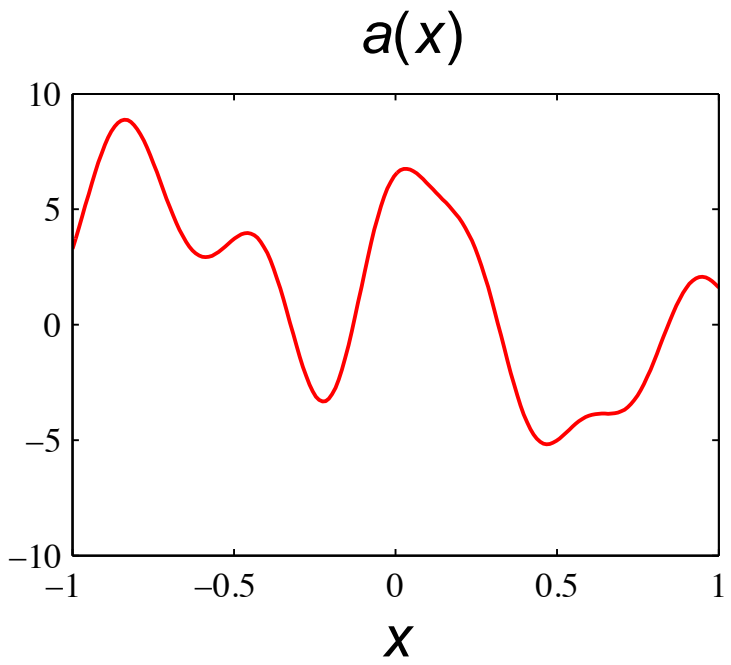
In general, this will require iterative optimization and approximation methods.

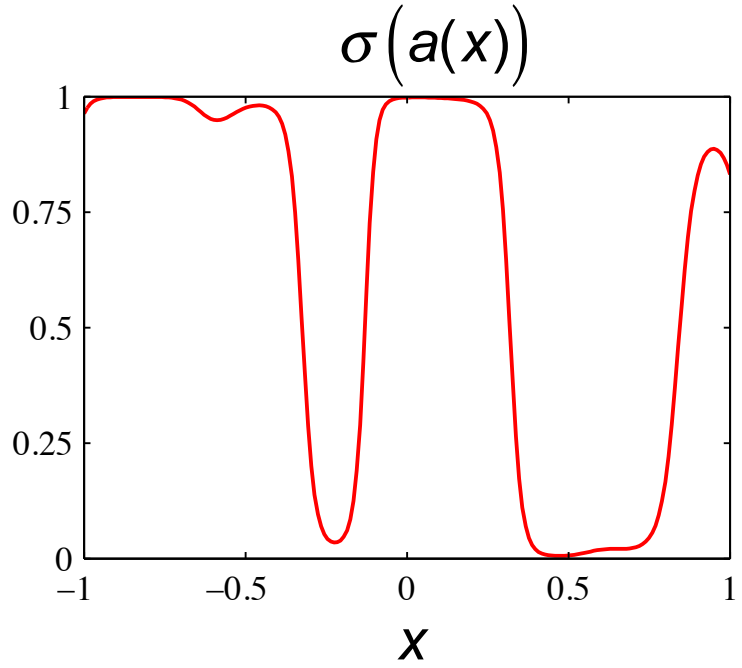
Gaussian Processes for Classification

For Gaussian process regression, y is Gaussian, and assumes values on $\mathbb{R}$.

For binary classification, where $t \in \{0,1\}$, we let a(**x**) be a Gaussian process,

and define $y(\mathbf{x}) = \sigma(a)$, where $\sigma(a)$ is the sigmoid function $\dfrac{1}{1+\exp(-a)}$





Gaussian Processes for Classification

Now $p(t \mid a) = \sigma(a)^t \left(1 - \sigma(a)\right)^{1-t}$

Given training data $\mathbf{x}_1, \ldots \mathbf{x}_N$, define

$\mathbf{t}_N = (t_1, \ldots t_N)^t$

$\mathbf{a}_{N+1} = \left(a(\mathbf{x}_1), \ldots, a(\mathbf{x}_{N+1})\right)^t$

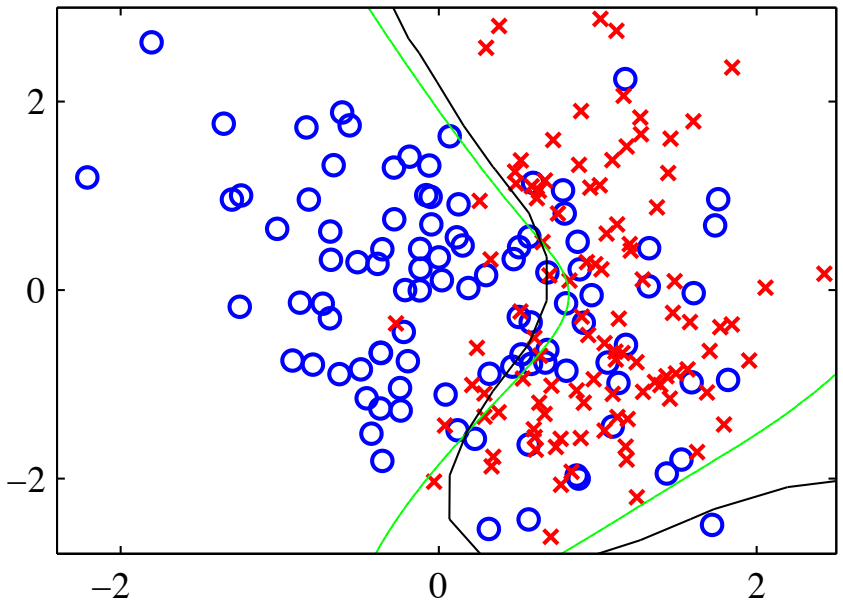
where $p(\mathbf{a}_{N+1}) = N(\mathbf{a}_{N+1} \mid \mathbf{0}, \mathbf{C}_{N+1})$

and $\mathbf{C}_{nm} = k(\mathbf{x}_n, \mathbf{x}_m) + \nu\delta_{nm}$

Then $p(t_{N+1} = 1 \mid \mathbf{t}_N) = \int p(t_{N+1} = 1 \mid a_{N+1}) p(a_{N+1} \mid \mathbf{t}_N) da_{N+1} = \int \sigma(a_{N+1}) p(a_{N+1} \mid \mathbf{t}_N) da_{N+1}$

This integrable is intractable - must approximate. See text for details.

Example



$p\left(t_{N+1}=1\,|\,\mathbf{t}_N\right)$