COMS 4721: Machine Learning for Data Science

Lecture 10, 2/21/2017

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FEATURE EXPANSIONS

FEATURE EXPANSIONS

Feature expansions (also called **basis expansions**) are names given to a technique we've already discussed and made use of.

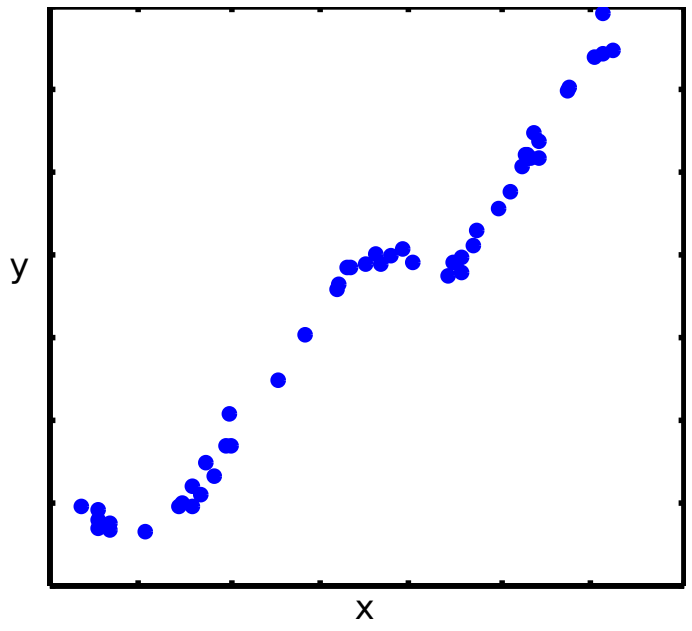
Problem: A linear model on the original feature space $x \in \mathbb{R}^d$ doesn't work.

Solution: Map the features to a higher dimensional space $\phi(x) \in \mathbb{R}^D$, where $D > d$, and do linear modeling there.

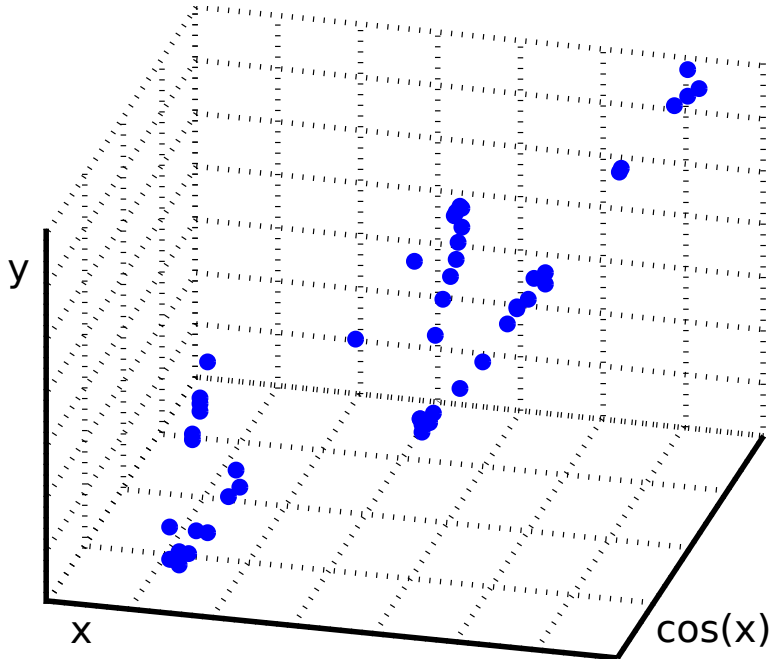
Examples

- For polynomial regression on $\mathbb{R}$, we let $\phi(x) = (x, x^2, \ldots, x^p)$.
- For jump discontinuities, $\phi(x) = (x, \mathbb{1}\{x < a\})$.

MAPPING EXAMPLE FOR REGRESSION



(a) Data for linear regression



(b) Same data mapped to higher dimension

High-dimensional maps can transform the data so output is linear in inputs.

Left: Original $x \in \mathbb{R}$ and response y.

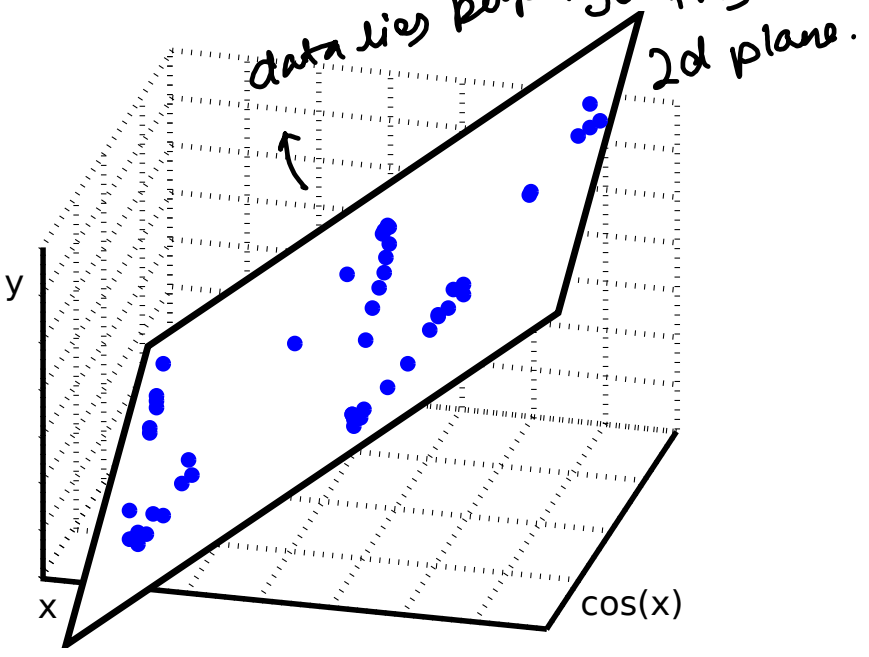
Right: x mapped to $\mathbb{R}^2$ using $\phi(x) = (x, \cos x)^T$.

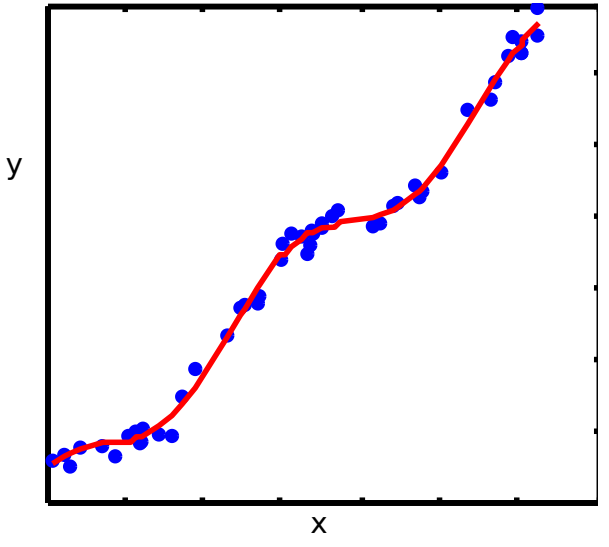
MAPPING EXAMPLE FOR REGRESSION

Using the mapping $\phi(x) = (x, \cos x)^T$, learn the linear regression model

$$\begin{aligned} y &\approx w_0 + \phi(x)^T w \\ &\approx w_0 + w_1 x + w_2 \cos x. \end{aligned}$$

learning 3 coefficients to do a linear regression in this space.

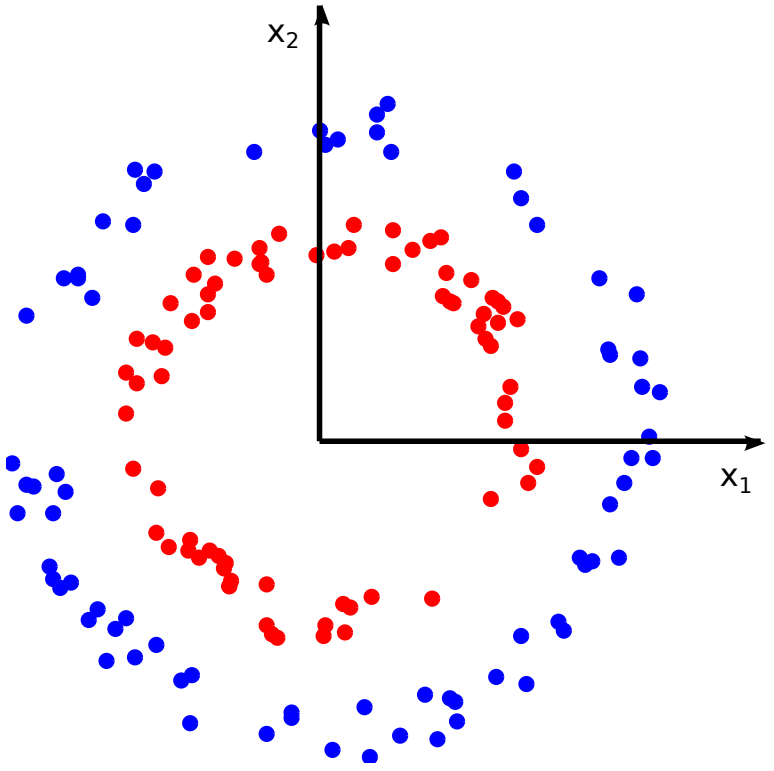




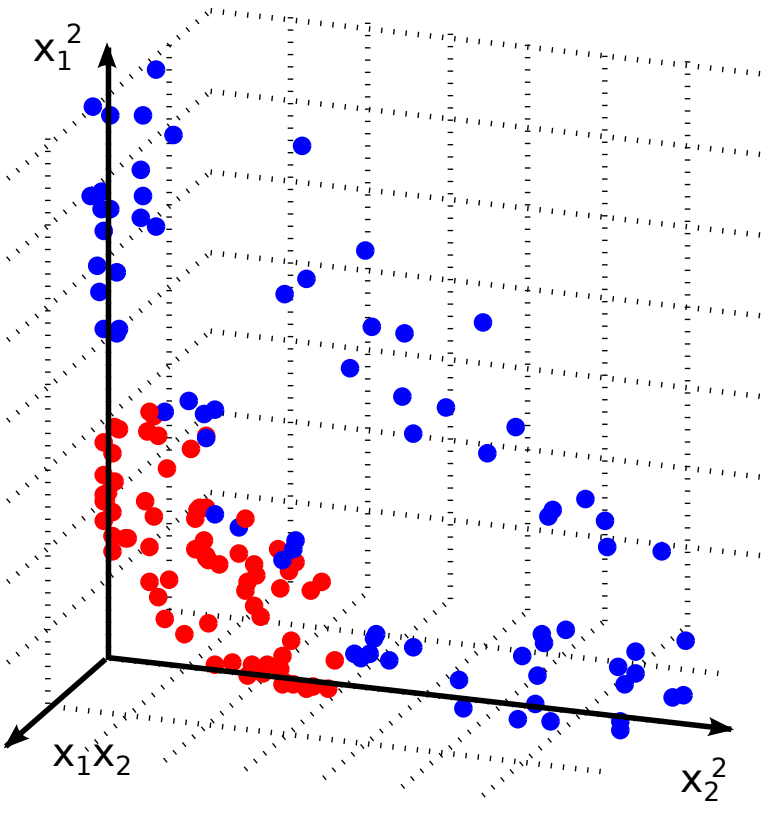
Left: Learn (w_0, w_1, w_2) to approximate data on the left with a plane.

Right: For each point x, map to $\phi(x)$ and predict y. Plot as a function of x.

MAPPING EXAMPLE FOR CLASSIFICATION



(e) Data for binary classification



(f) Same data mapped to higher dimension

High-dimensional maps can transform data so it becomes linearly separable.

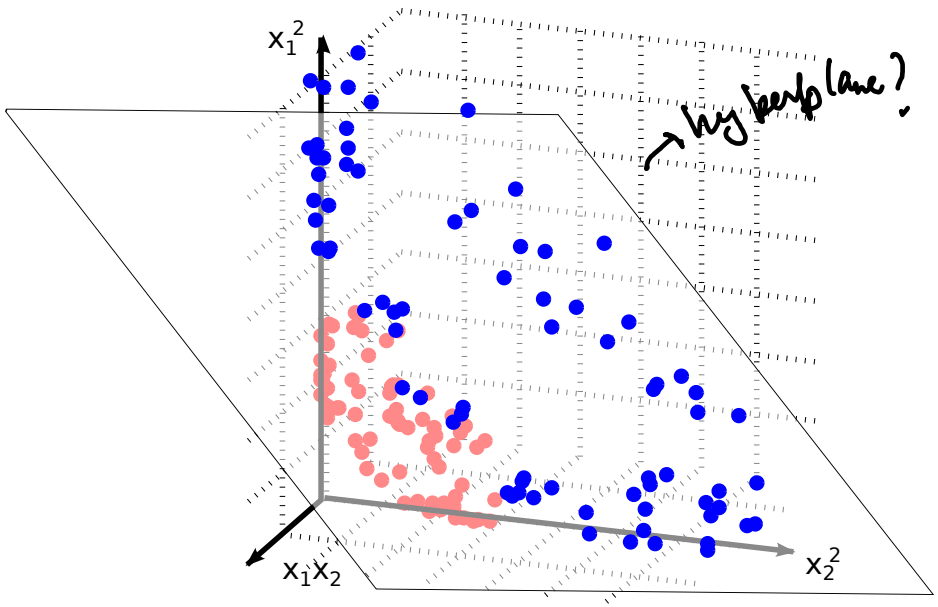
Left: Original data in $\mathbb{R}^2$.

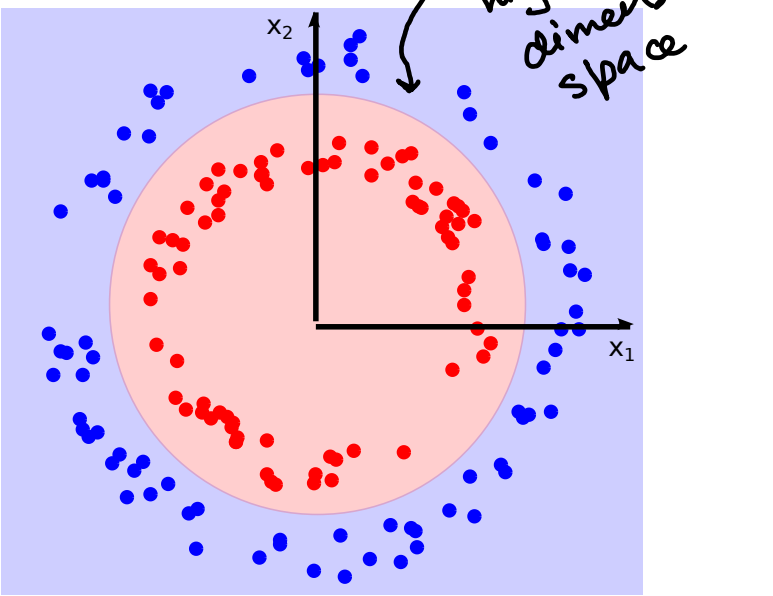
Right: Data mapped to $\mathbb{R}^3$ using $\phi(x) = (x_1^2, x_1x_2, x_2^2)^T$.

MAPPING EXAMPLE FOR CLASSIFICATION

Using the mapping $\phi(x) = (x_1^2,\ x_1x_2,\ x_2^2)^T$, learn a linear classifier

$$\begin{aligned} y &= \text{sign}(w_0 + \phi(x)^T w) \\ &= \text{sign}(w_0 + w_1x_1^2 + w_2x_1x_2 + w_3x_2^2). \end{aligned}$$





Left: Learn (w_0, w_1, w_2, w_3) to linearly separate classes with hyperplane.

Right: For each point x, map to $\phi(x)$ and classify. Color decision regions in $\mathbb{R}^2$.

What expansion should I use?

This is not obvious. The illustrations required knowledge about the data that we likely won't have (especially if it's in high dimensions).

One approach is to use the "kitchen sink": If you can think of it, then use it. Select the useful features with an ℓ_1 penalty

$$w_{\ell_1} = \arg\min_w \sum_{i=1}^{n} f(y_i, \phi(x_i), w) \; + \; \lambda \|w\|_1.$$

We know that this will find a sparse subset of the dimensions of $\phi(x)$ to use.

we define a dot product btw the feature expansion for 2 data points to be something called a kernel.

Often we only need to work with dot products $\phi(x_i)^T \phi(x_j) \equiv K(x_i, x_j)$. This is called a **kernel** and can produce some interesting results.

For many models, it actually can be shown that we don't need to work in the expansion space. That all we ever need to work with are what are these dot products between our feature expansions.

KERNELS

PERCEPTRON (SOME MOTIVATION)

1 dimension added for offset

Perceptron classifier

Let $x_i \in \mathbb{R}^{d+1}$ and $y_i \in \{-1, +1\}$ for $i = 1, \ldots, n$ observations. We saw that the Perceptron constructs the hyperplane from data,

$$w = \sum_{i \in \mathcal{M}} y_i x_i, \qquad w^{(t+1)} = w^{(t)} + y_i x_i$$

misclassified example

where $\mathcal{M}$ is the sequentially constructed set of misclassified examples.

Our final classifier is defined by a sum of sequences of misclassified examples times the label that is associated with that example.

Predicting new data

We also discussed how we can predict the label y_0 for a new observation x_0:

$$y_0 = \text{sign}(x_0^T w) = \text{sign}\left(\sum_{i \in \mathcal{M}} y_i x_0^T x_i\right)$$

We've taken feature expansions for granted, but we can explicitly write it as

feature map

$$y_0 = \text{sign}(\phi(x_0)^T w) = \text{sign}\left(\sum_{i \in \mathcal{M}} y_i \phi(x_0)^T \phi(x_i)\right)$$

We can represent the decision using dot products between data points.

Kernel between expanded vectors : $x_0 \& x_i$.

KERNELS

Kernel definition

A kernel $K(\cdot,\cdot) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a symmetric function defined as follows:

Definition: For any set of n data points $x_1, \ldots, x_n \in \mathbb{R}^d$, the $n \times n$ matrix K, where $K_{ij} = K(x_i, x_j)$, is *positive semidefinite*.

Intuitively, this means K satisfies the properties of a covariance matrix.

Mercer's theorem

If the function $K(\cdot,\cdot)$ satisfies the above properties, then there exists a mapping $\phi : \mathbb{R}^d \to \mathbb{R}^D$ such that

$$K(x_i, x_j) = \phi(x_i)^T \phi(x_j).$$

If we first define $\phi(\cdot)$ and then K, this is obvious. However, sometimes we first define $K(\cdot,\cdot)$ and avoid ever using $\phi(\cdot)$.

GAUSSIAN KERNEL (RADIAL BASIS FUNCTION)

By far the most popular kernel is the Gaussian kernel, also called the radial basis function (RBF),

$$K(x, x') = a \exp\left\{ -\frac{1}{b} \|x - x'\|^2 \right\}.$$

measure of proximity btw 2 pts that we i/p to it.

- This is a good, general-purpose kernel that usually works well. $0 \leq k(x,x') \leq a$
- It takes into account proximity in $\mathbb{R}^d$. Things close together in space have larger value (as defined by kernel width b).

In this case, the the mapping $\phi(x)$ that produces the RBF kernel is *infinite dimensional* (it's a continuous function instead of a vector). Therefore

we only ever need to calculate this, we never actually use the mapping itself.

$$K(x, x') = \int \phi_t(x)\phi_t(x')\, dt.$$

so a dot product in finite space becomes an integral over a product of 2 functions in infinite-dimensional space.

- $K(x, x')$ is like a Gaussian on x with x' as the mean (or vice versa).
- $\phi_t(x)$ can be thought of as a function of t with parameter x.

* as x & x' get closer, $k(x,x')$ becomes smaller. And the entire kernel converges to a in the limit, as they are equal.

As x & x' get farther & farther part this becomes bigger and bigger, And so this $\exp\{\cdot\}$ goes to 0. The kernels then converge to 0 as these two go infinitely far apart.

KERNELS

A higher dimensional mapping that looks like *, if we only took its dot product, would result in this kernel function.** So instead of mapping to this space and taking dot products, we can calculate this function.

Another kernel

Map : $\phi(x) = (1, \sqrt{2}x_1, \ldots, \sqrt{2}x_d, x_1^2, \ldots, x_d^2, \ldots, \sqrt{2}x_i x_j, \ldots)$ *

Kernel : $\phi(x)^T \phi(x') = K(x, x') = (1 + x^T x')^2$ **

In fact, we can show: $K(x, x') = (1 + x^T x')^b$, for $b > 0$ is a kernel as well.

Forex: for b=3, there's some mapping of x & x' to a higher dimensional space such that dot product in that space is equal to $(1+x^T x)^3$.

Kernel arithmetic

Certain functions of kernels can produce new kernels.

Let K_1 and K_2 be any two kernels, then constructing K in the following ways produces a new kernel (among many other ways):

$$
\begin{aligned}
K(x, x') &= K_1(x, x') K_2(x, x') \\
K(x, x') &= K_1(x, x') + K_2(x, x') \\
K(x, x') &= \exp\{K_1(x, x')\}
\end{aligned}
$$

we perform some functions of these kernels.

→ there is some high-dimensional mapping that would give that original function.

M → constructed by sequentially picking misclassified examples from the dataset.

Returning to the Perceptron

We write the feature-expanded decision as

project to higher dimensional space using ϕ.

$$\begin{aligned} y_0 &= \text{sign}\left(\sum_{i\in\mathcal{M}} y_i \phi(x_0)^T \phi(x_i)\right) \\ &= \text{sign}\left(\sum_{i\in\mathcal{M}} y_i K(x_0, x_i)\right) \end{aligned}$$

We can pick the kernel we want to use. Let's pick the RBF (set $a = 1$). Then

$$y_0 = \text{sign}\left(\sum_{i\in\mathcal{M}} y_i \, \mathrm{e}^{-\frac{1}{b}\|x_0 - x_i\|^2}\right)$$

the higher dimensional mapping is actually an infinite dimensional thing. So we could never write it out anyway. But we never have to write out that higher dimensional mapping because we only need the dot product.

Notice that we never actually need to calculate $\phi(x)$.

What is this doing?

- Notice $0 < K(x_0, x_i) \leq 1$, with bigger values when x_0 is closer to x_i.
- This is like a "soft voting" among the data picked by Perceptron.

(almost like soft nearest neighbour in a sense.)

* In a sense we're letting each point in the set vote for a label, for the x_0.

And if ① x_i is closer to x_0, then $e^{\frac{1}{2}}$ is closer to 1, label times and. closer to 1

② x_i far away from x_0, " " 0, label and weight it by 0.

So it's like saying if x_0 is very close to x_i, then I trust that label is likely to share that of x_i, whereas if x_0 is far away from x_i, then I can't say whether or not it's going to share the label with x_i.

Weigh things closer, more and more. And sum weighted labels.

KERNELIZED PERCEPTRON

Do we actually need to do the high dimension mapping to learn the perceptron to actually pick the sequence of misclassified points.

Ans: No, we never actually need to calculate this feature mapping, we only have to work with the kernel function between different points in our dataset.

Learning the kernelized Perceptron

Recall: Given a current vector $w^{(t)} = \sum_{i \in \mathcal{M}_t} y_i x_i$, we update it as follows,

1. Find a new x' such that $y' \neq \text{sign}(x'^T w^{(t)})$
2. Add the index of x' to $\mathcal{M}$ and set $w^{(t+1)} = \sum_{i \in \mathcal{M}_{t+1}} y_i x_i$

$w^{(t)}$ is the linear classifier at iteration t of the perceptron, by taking sum over classified points upto iteration t.

to check whether our current classifier misclassifies a pt. or doesn't misclassify a pt.

Again we only need dot products, meaning these steps are equivalent to

1. Find a new x' such that $y' \neq \text{sign}(\sum_{i \in \mathcal{M}_t} y_i K(x', x_i))$
2. Add the index of x' to $\mathcal{M}$ *but don't bother calculating* $w^{(t+1)}$

Making predictions on data we already have.

we only ever need dot products.

in order to find a misclassified point, we only need to calculate the kernel btw a proposed pt. & the points in our current misclassified set.

expand w_t to replace it with what it's a function of. And then we write the dot products out. And then we expand into a higher dimensional space. We see that all need to do is calculate the kernel function.

The trick is to realize that we never need to work with $\phi(x)$.

- We don't need $\phi(x)$ to do Step 1 above.
- We don't need $\phi(x)$ to classify new data (previous slide).
- We only ever need to calculate $K(x, x')$ between two points.

KERNEL k-NN

An extension

We can generalize kernelized Perceptron to *soft* k-NN with a simple change. Instead of summing over misclassified data $\mathcal{M}$, sum over *all* the data:

$$y_0 = \text{sign}\left(\sum_{i=1}^{n} y_i \, \mathrm{e}^{-\frac{1}{b}\|x_0 - x_i\|^2}\right).$$

Next, notice the *decision* doesn't change if we divide by a positive constant.

$$\text{Let :} \quad Z = \sum_{j=1}^{n} \mathrm{e}^{-\frac{1}{b}\|x_0 - x_j\|^2}$$

$$\text{Construct :} \quad \text{Vector } \; p(x_0), \text{ where } p_i(x_0) = \frac{1}{Z}\,\mathrm{e}^{-\frac{1}{b}\|x_0 - x_i\|^2}$$

$$\text{Declare :} \quad y_0 = \text{sign}\left(\sum_{i=1}^{n} y_i p_i(x_0)\right)$$

- We let all data vote for the label based on a "confidence score" $p(x_0)$.
- Set b so that most $p_i(x_0) \approx 0$ to only focus on neighborhood around x_0.

Nadaraya-Watson model

The developments are almost limitless.

Here's a regression example almost identical to the kernelized k-NN:

from previous slide.

Before: $y \in \{-1, +1\}$

Now: $y \in \mathbb{R}$ real valued no.

Using the RBF kernel, for a new (x_0, y_0) predict

$$y_0 = \sum_{i=1}^{n} y_i \frac{K(x_0, x_i)}{\sum_{j=1}^{n} K(x_0, x_j)}.$$

→ weighted acc. to proximity to x_0

What is this doing?

We're taking a locally weighted average of all y_i for which x_i is close to x_0 (as decided by the kernel width). *Gaussian processes* are another option...

GAUSSIAN PROCESSES

Think of Gaussian process as a Kernalized Bayesian regression model.
Before we can define it, we need to see where in Bayesian linear regression dot products between the data points come into play.

KERNELIZED BAYESIAN LINEAR REGRESSION

Regression setup: For n observations, with response vector $y \in \mathbb{R}^n$ and their feature matrix X, we define the likelihood and prior

$$y \sim N(Xw, \sigma^2 I), \quad w \sim N(0, \lambda^{-1} I).$$

Marginalizing: What if we integrate out w? We can solve this,

$$p(y|X) = \int p(y|X,w)p(w)dw = N(0, \sigma^2 I + \lambda^{-1} XX^T).$$

Kernelization: Notice that $(XX^T)_{ij} = x_i^T x_j$. Replace each x with $\phi(x)$ after which we can say $(\phi(X)\phi(X)^T)_{ij} = K(x_i, x_j)$. We can define K directly, so

$$p(y|X) = \int p(y|X,w)p(w)dw = N(0, \sigma^2 I + \lambda^{-1} K).$$

This is called a *Gaussian process*. We never use w or $\phi(x)$, but just $K(x_i, x_j)$.

Imagine that ϕ is extremely high dimensional, even infinite dimensional. Then this vector w is infinite dimensional as well.

No chance we can possibly learn this vector w, can't even store it in memory.

However, if we then use this marginalization fact, where we integrate out w, it doesn't actually matter that it's infinite dimensional Gaussian prior here, the result is something that we can easily calculate.

So we can just calculate the kernel function between all of our data points, and we get a nice n-dimensional multi-variate Gaussian distribution, where we have a way of actually calculating this portion of the covariance K.

Definition

- Let $f(x) \in \mathbb{R}$ and $x \in \mathbb{R}^d$.
- Define the *kernel* $K(x, x')$ between two points x and x'.
- Then $f(x)$ is a *Gaussian process* and $y(x)$ the noise-added process if for observed pairs $(x_1, y_1), \ldots, (x_n, y_n)$, where $x \in \mathcal{X}$ and $y \in \mathbb{R}$,

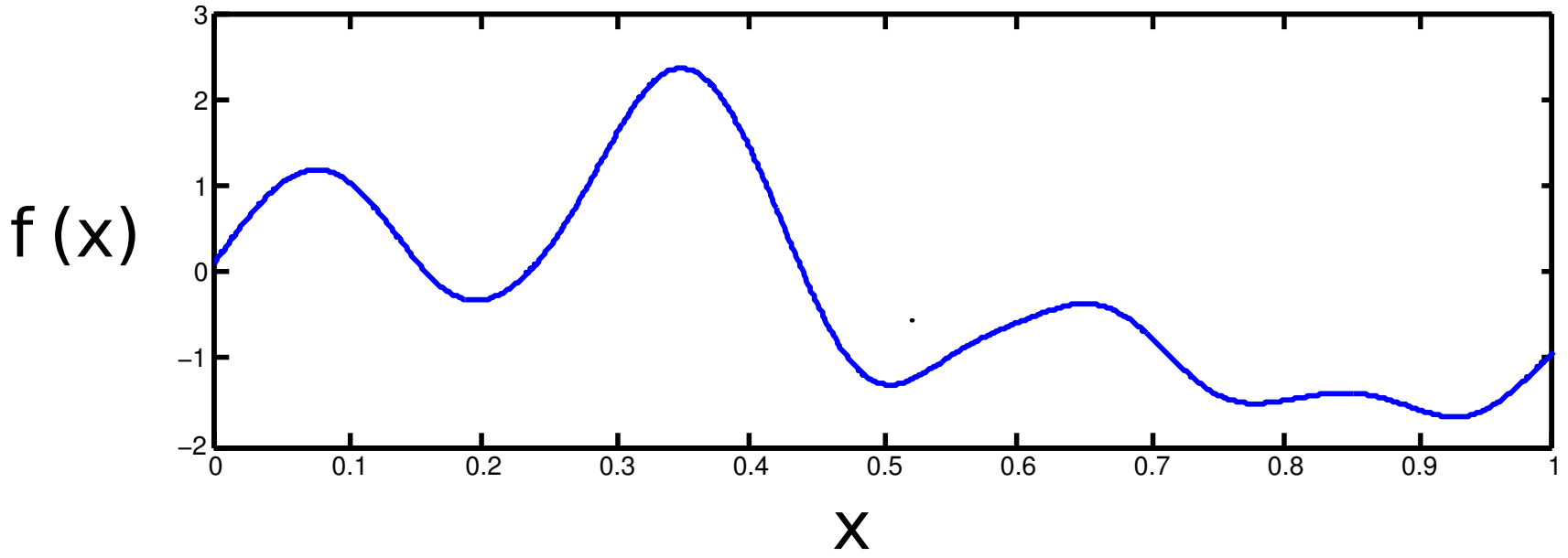
$$y \,|\, f \sim N(f, \sigma^2 I), \quad f \sim N(0, K) \quad \Leftrightarrow \quad y \sim N(0, \sigma^2 I + K)$$

where $y = (y_1, \ldots, y_n)^T$ and K is $n \times n$ with $K_{ij} = K(x_i, x_j)$.

Comments:

- We combined the previous λ^{-1} with K (for notation only).
- Typical breakdown: $f(x)$ is the GP and $y(x)$ equals $f(x)$ plus i.i.d. noise.
- The kernel is what keeps this from being "just a Gaussian."

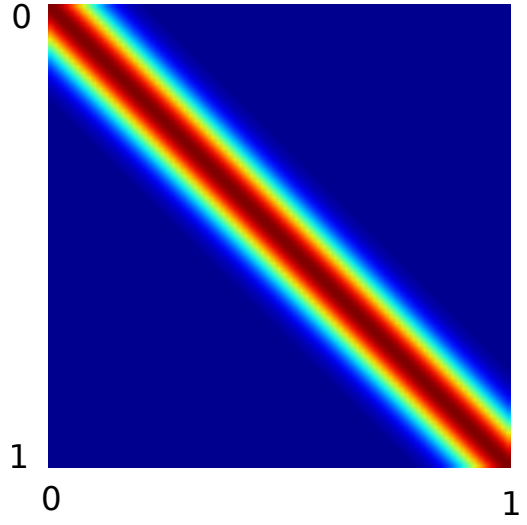
GAUSSIAN PROCESSES



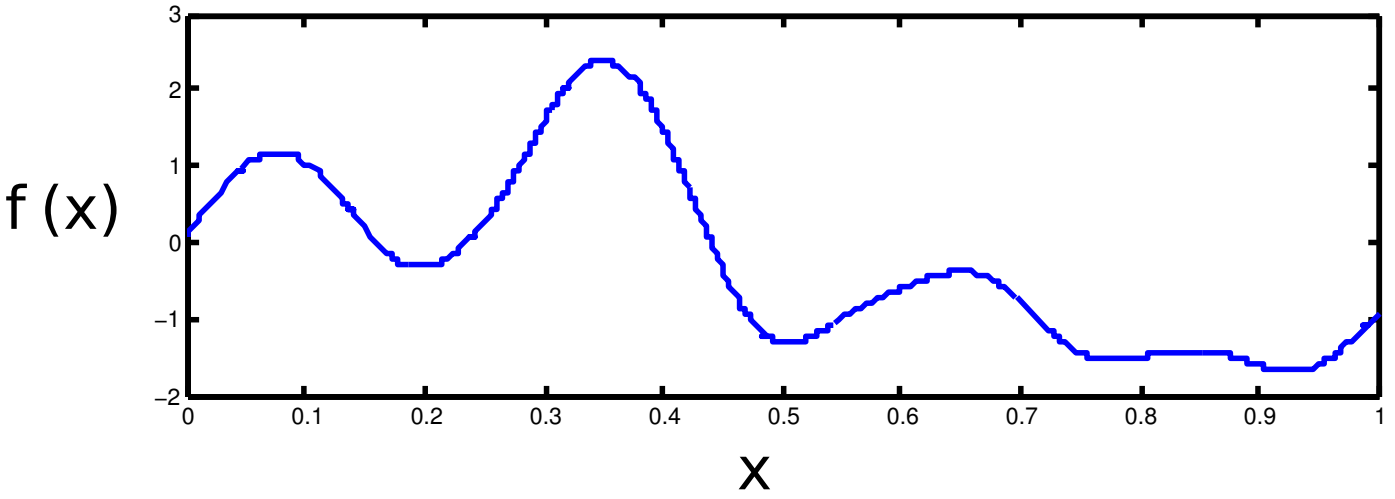
Above: A Gaussian process $f(x)$ generated using

$$K(x_i, x_j) = \exp\left\{-\frac{\|x_i - x_j\|^2}{b}\right\}.$$

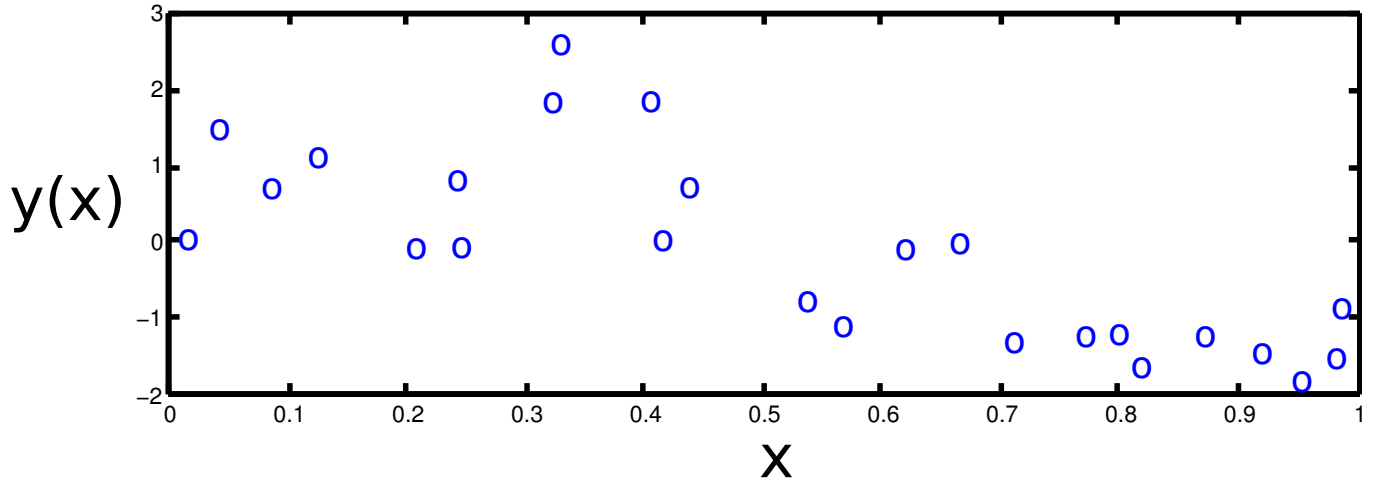
Right: The covariance of $f(x)$ defined by K.



GAUSSIAN PROCESSES



Top: Unobserved underlying function,
Bottom: Noisy observed data sampled from this function



Bayesian linear regression

Imagine we have n observation pairs $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ and want to predict y_0 given x_0. Integrating out w, the joint distribution is

$$\begin{bmatrix} y_0 \\ y \end{bmatrix} \sim \text{Normal}\left(\mathbf{0}\,,\ \sigma^2 I + \begin{bmatrix} x_0^T x_0 & (Xx_0)^T \\ Xx_0 & XX^T \end{bmatrix}\right)$$

We want to predict y_0 given $\mathcal{D}$ and x_0. Calculations can show that

$$\begin{aligned} y_0|\mathcal{D}, x_0 &\sim \text{Normal}(\mu_0, \sigma_0^2) \\ \mu_0 &= (Xx_0)^T (XX^T)^{-1} y \\ \sigma_0^2 &= \sigma^2 + x_0^T x_0 - (Xx_0)^T (XX^T)^{-1} (Xx_0) \end{aligned}$$

The since the infinite Gaussian process is only evaluated at a finite set of points, we can use this fact.

Predictive distribution of $y(x)$

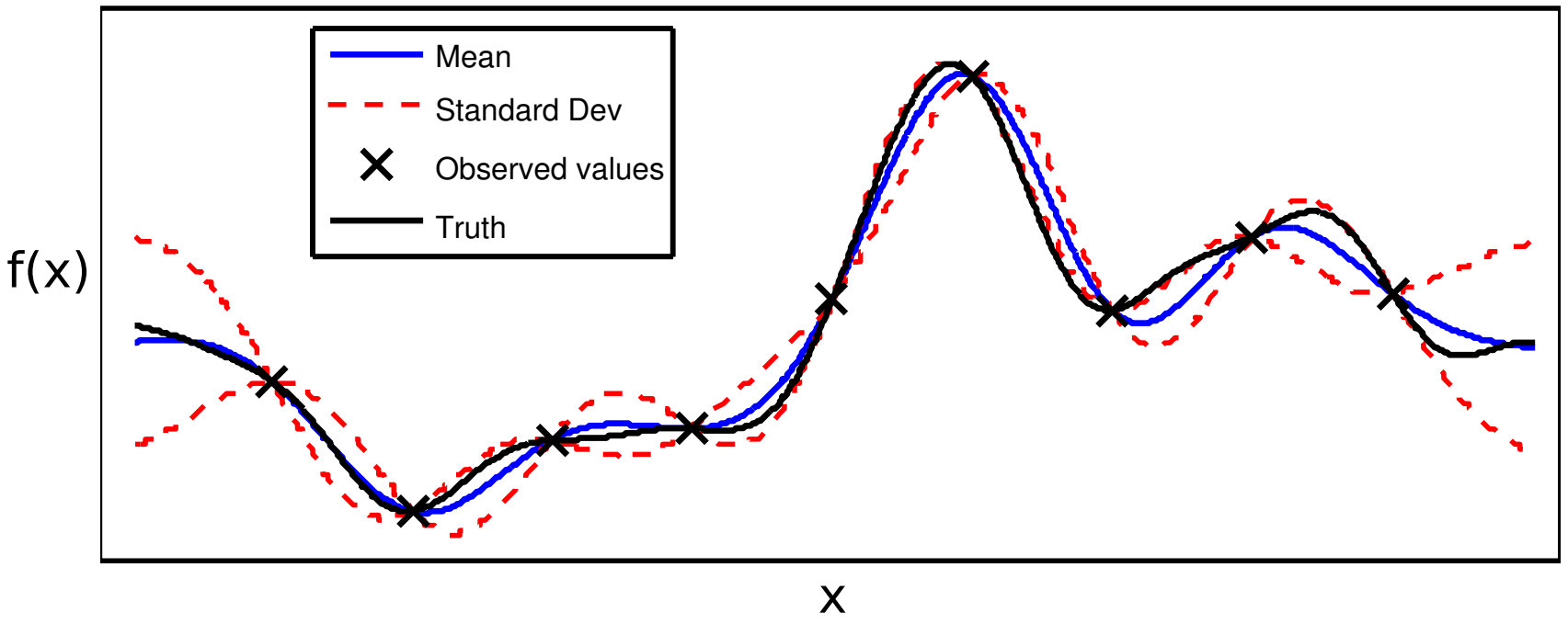
Given measured data $\mathcal{D}_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, the distribution of $y(x)$ can be calculated at any *new* x to make predictions.

Let $K(x, \mathcal{D}_n) = [K(x, x_1), \ldots, K(x, x_n)]$ and K_n be the $n \times n$ kernel matrix restricted points in $\mathcal{D}_n$. Then we can show

$$\begin{aligned} y(x)|\mathcal{D}_n &\sim N\left(\mu(x), \Sigma(x)\right), \\ \mu(x) &= K(x, \mathcal{D}_n) K_n^{-1} y, \\ \Sigma(x) &= \sigma^2 + K(x, x) - K(x, \mathcal{D}_n) K_n^{-1} K(x, \mathcal{D}_n)^T \end{aligned}$$

For the posterior of $f(x)$ instead of $y(x)$, just remove σ^2.

GAUSSIAN PROCESSES POSTERIOR



What does the posterior distribution of $f(x)$ look like?

- We have data marked by an $\times$.
- These values pin down the function $f(x)$ nearby
- We get a mean and variance for every possible x from a previous slide.
- The distribution on $y(x)$ adds variance σ^2 (*very* small above) point-wise.