Boosting 1

-Introduction to Data Science-

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Preamble:

- Boosting looks superficially like bagging, but has an important difference
- To understand boosting, we need to discuss nonparametric regression
- Nonparametric regression provides a flexible fit, but can only be used in low dimensions
- Additive models are a relaxation of nonparametric models that can be fit in much higher dimensions
- Boosting is an algorithm for fitting a type of additive model

Boosting overview

Recall: Bagging is a procedure for taking a low bias, high variance procedure and (potentially) reducing its risk via averaging

Boosting has a similar philosophy: take a poor classifier and improve it

However, boosting is useful for the opposite situation: a classifier that has high bias but low variance!

Example: Linear regression. It would make sense to...

- ...use bagging with linear regression on all of the features
- ...use boosting with simple linear regression on only one feature at a time

Boosting overview

A direct contrast:

- Bagging: aggregates over many independent bootstrap draws

  (To be clear, the bootstrap sampling mechanism is independent, the bootstrap samples themselves are of course dependent)
- Boosting: finds the observations that are poorly classified, up weights these observations, and then trains a new classifier

  (Similar statement about regression)

Boosting for Regression

Boosting regression trees

Set $\hat{f} \equiv 0$ and $R = Y \in \mathbb{R}^n$

Fix the tree complexity M and learning rate λ

(ESL states that $M \in \{4, \ldots, 8\}$ works well. This controls how many interactions can be in the model. More on this later)

For $b = 1, \ldots, B$, do:

1. Fit $\hat{f}_b$ with M regions to $\tilde{\mathcal{D}} = \{(X_1, R_1), \ldots, (X_n, R_n)\}$
2. Update: $\hat{f} \leftarrow \hat{f} + \lambda \hat{f}_b$
3. Update: $R \leftarrow R - \lambda \hat{f}_b$

Output:

$$\hat{f} = \sum_{b=1}^{B} \lambda \hat{f}_b$$

This is a type of additive model, so called for obvious reasons

Boosting trees

In general

- A smaller λ means a larger required B
- Too large of λ means we take too long of steps, leading to poor solutions

  (Recall: gradient descent)

In practice,

- B is set via cross-validation

  (Though boosting is somewhat insensitive to choosing B too large, it is still an important part of the overall performance)
- λ is set at a small level, say $\lambda = 0.01$

As for the additive model part...

Curse of dimensionality and local averaging

From linear to nonlinear models

Goal: Develop a prediction function $\hat{f} : \mathbb{R}^p \to \mathbb{R}$ for predicting Y given an X

Commonly, $\hat{f}(X) = X^\top \beta$

(Constrained linear regression)

This greatly simplifies algorithms, while not sacrificing too much flexibility

However, sometimes directly modeling the nonlinearity is more natural

Prediction via local averaging

The fundamental quantities of interest we have been modeling are the Bayes' rules

$$\mathbb{E}[Y|X] \quad \text{or} \quad \arg\max_g \mathbb{P}(Y = g|X)$$

We know how to estimate expectations:

$\rightarrow$ If $Y_1, Y_2, \ldots, Y_n$ all have expectation μ, then

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} Y_i$$

is an intuitive estimator of μ

(and a reasonable prediction of a new Y)

Prediction via local averaging

Similarly, we can estimate $\mathbb{E}[Y|X_*]$ with $\mathcal{D}$:

$$\hat{f}(X_*) = \frac{1}{n_*} \sum_{i=1}^{n} Y_i \mathbf{1}(X_i = X_*)$$

where $n_* = \sum_{i=1}^{n} \mathbf{1}(X_i = X_*)$ is the number of training observations where $X_i = X_*$

In words: we are taking an average of all the observations Y_i such that $X_i = X_*$

(Of course, this is all conditional expectation really is)

There is a big problem: There generally aren't any X_i at X_*!

Prediction via local averaging

Suppose we relax the constraint $X_i = X_*$ a bit and include points that are close enough instead

Define a generic function $\mathrm{neighborhood}$ which takes in a value X_* and reports:

$$\mathrm{neighborhood}(X_*) = \text{all } X_i \text{ in the "neighborhood" of } X_*$$

To estimate $\mathbb{E}Y|X_*$, average the nearby training observations

$$\hat{f}(X_*) = \frac{1}{n_*} \sum_{i=1}^{n} Y_i \mathbf{1}(X_i \in \mathrm{neighborhood}(X_*))$$

where $n_* = |\mathrm{neighborhood}(X_*)|$ is the number of training observations where X_i is in the "neighborhood" of X_*

Prediction via local averaging

We need to define $\text{neighborhood}(X_*)$

(If it hasn't become clear, yet, this is a key aspect characterizing different methods)

Example: Let's define "neighborhood" in terms of having Euclidean norm less than or equal to some threshold t

$$\mathbf{1}(X_i \in \text{neighborhood}(X_*)) = \mathbf{1}(||X_i - X_*||_2 \leq t)$$

Here...

- ... the Euclidean norm quantifies distance
- ... t quantifies close

(In fact, it is a tuning parameter)

Prediction via local averaging: $X \in \mathbb{R}$

$$\hat{f}(X_*) = \frac{1}{n_*} \sum_{i=1}^{n} Y_i \mathbf{1}(||X_i - X_*||_2 \leq t), \qquad \text{and} \qquad X_* = 0.25$$

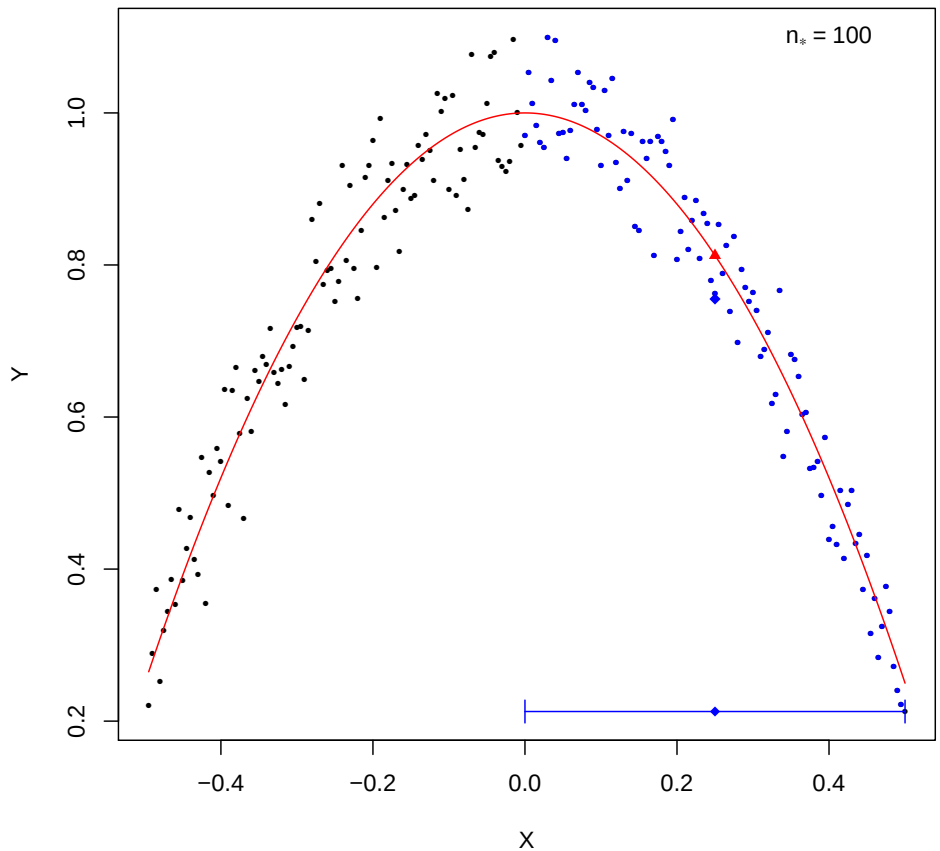


Figure: $t = 0.25$

Prediction via local averaging: $X \in \mathbb{R}$

$$\hat{f}(X_*) = \frac{1}{n_*} \sum_{i=1}^{n} Y_i \mathbf{1}(||X_i - X_*||_2 \leq t), \qquad \text{and} \qquad X_* = 0.25$$

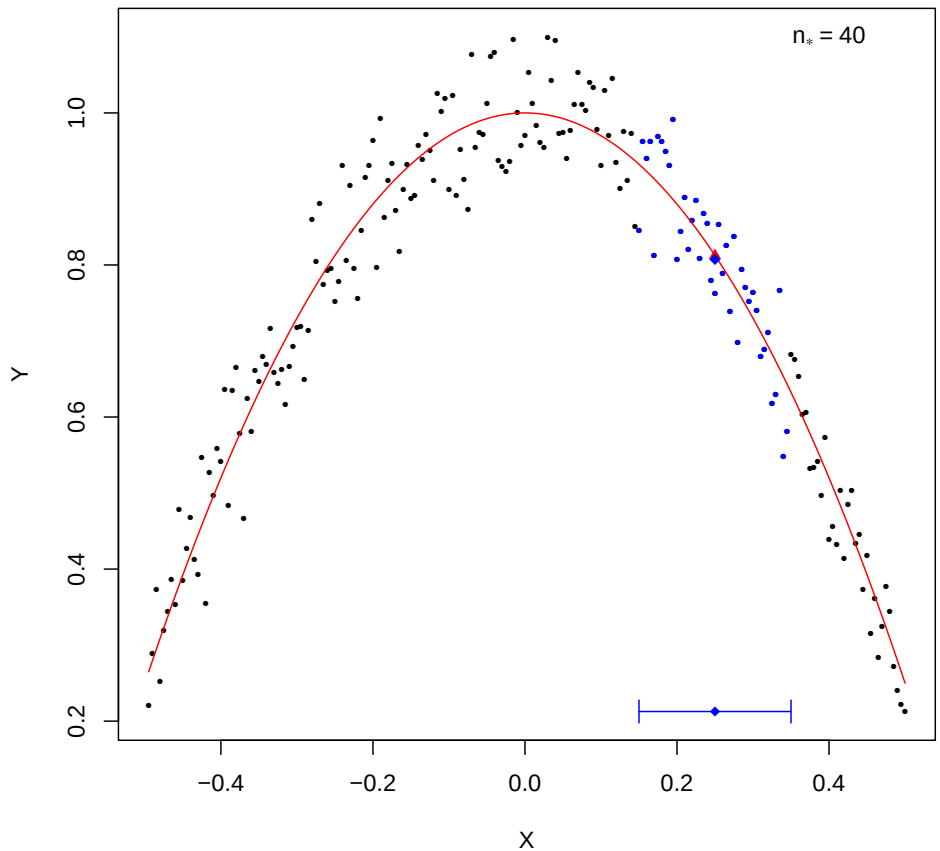


Figure: $t = 0.1$

Prediction via local averaging: $X \in \mathbb{R}$

$$\hat{f}(X_*) = \frac{1}{n_*} \sum_{i=1}^{n} Y_i \mathbf{1}(||X_i - X_*||_2 \leq t), \qquad \text{and} \qquad X_* = 0.25$$

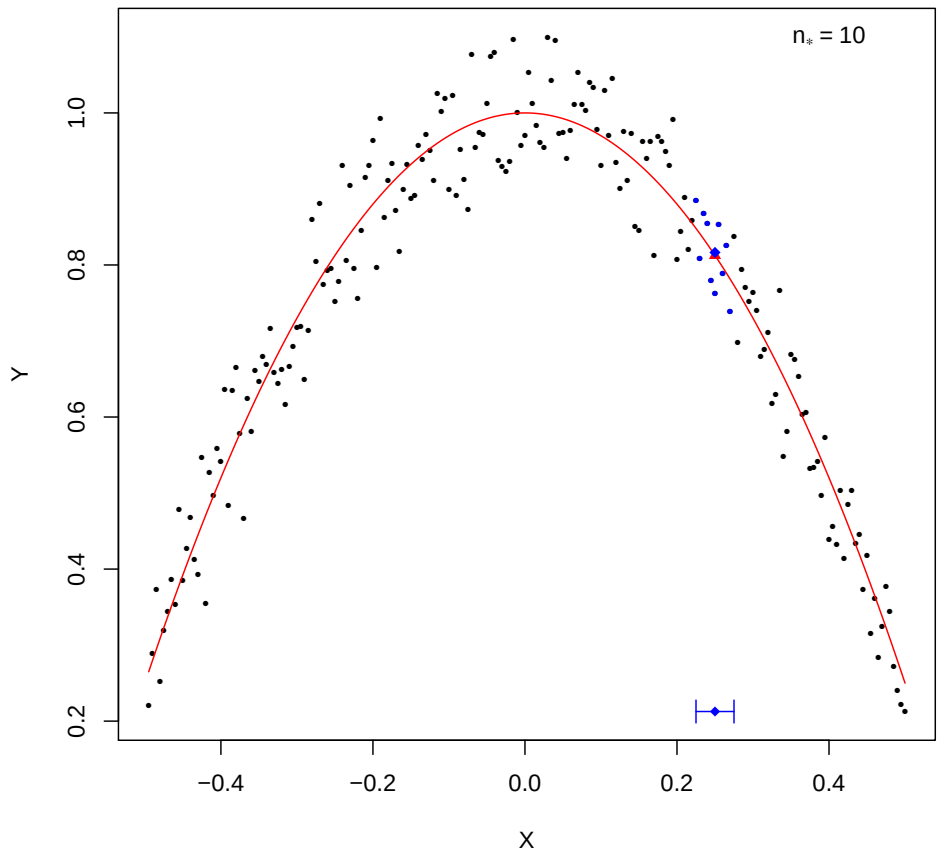


Figure: $t = 0.025$

Prediction via local averaging: $X \in \mathbb{R}$

$$\hat{f}(X_*) = \frac{1}{n_*} \sum_{i=1}^{n} Y_i \mathbf{1}(||X_i - X_*||_2 \leq t), \qquad \text{and} \qquad X_* = 0.25$$

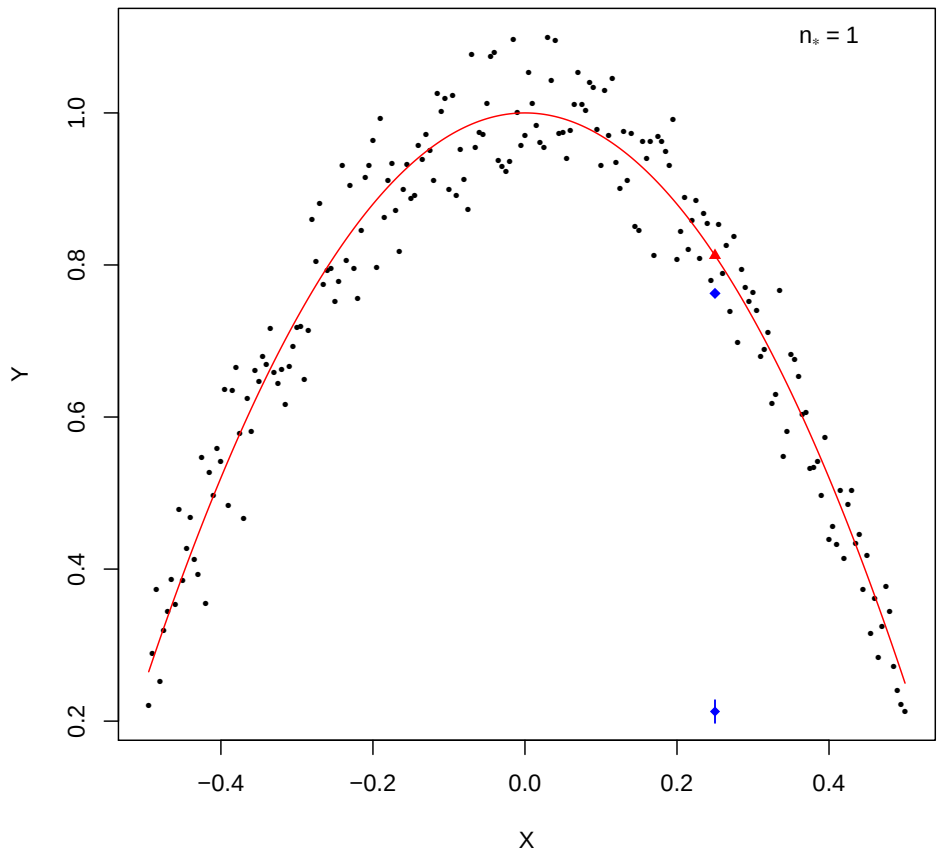


Figure: $t = 0.0001$

Prediction via local averaging: $X \in \mathbb{R}$

$$\hat{f}(X_*) = \frac{1}{n_*} \sum_{i=1}^{n} Y_i \mathbf{1}(||X_i - X_*||_2 \leq t)$$

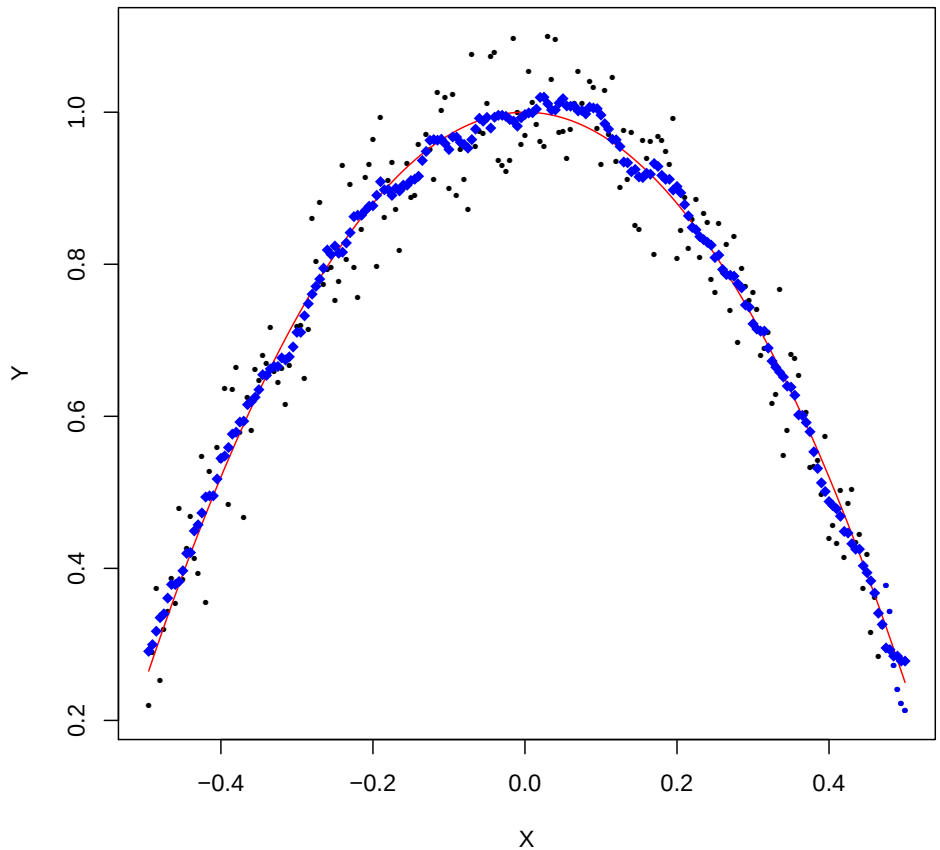


Figure: Over a grid of X_*'s, with $t = 0.025$

Prediction via local averaging

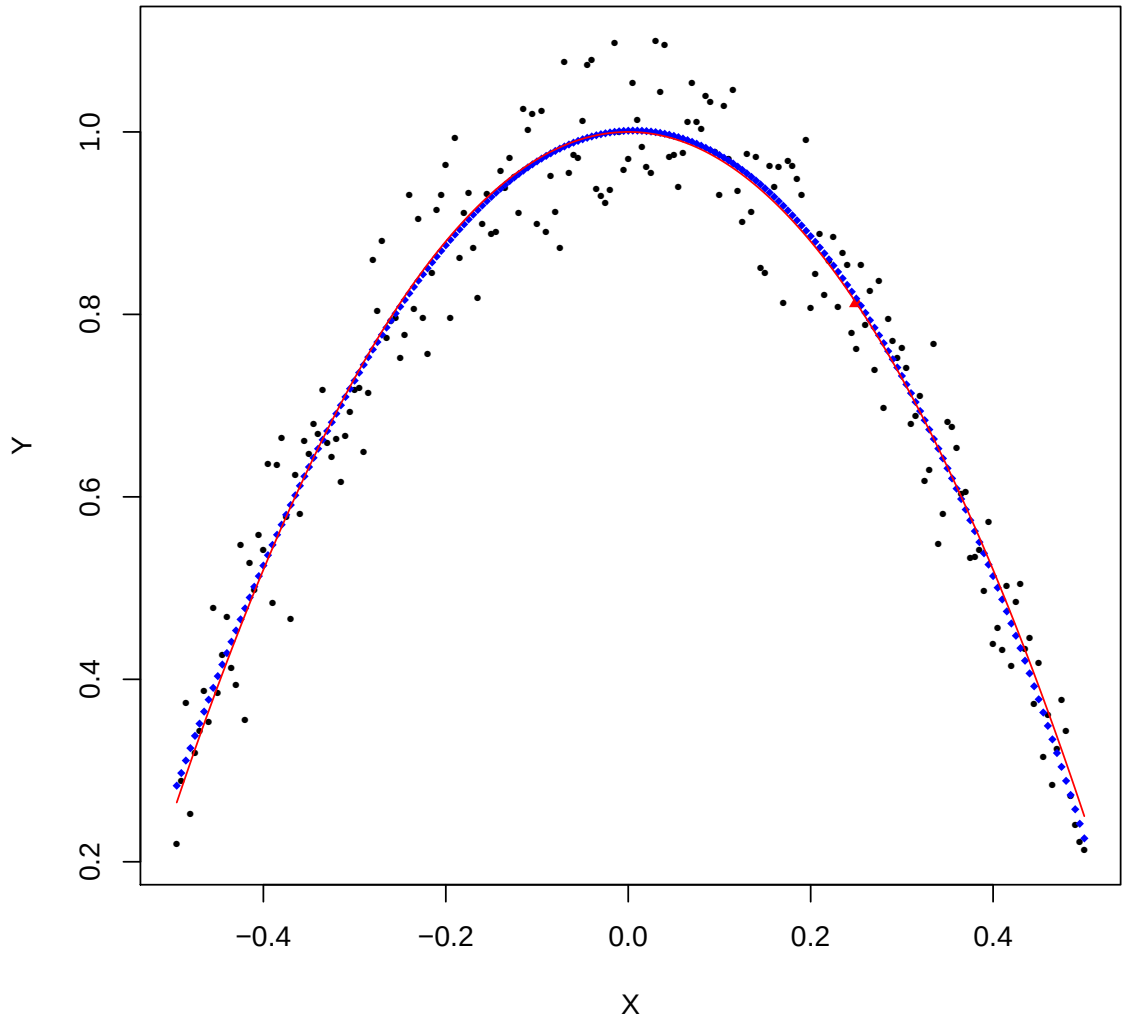


Figure: Using Regression Splines (ISL 7.4)

Nonparametric regression: Splines

Nonparametric regression

Example: Fitting polynomials

(See ISL 7.1 for details on fitting polynomials)

Suppose we want to consider the following 4-dimensional feature transformation of a original 2-dimensional feature vector $X = (x_1, x_2)^\top \in \mathbb{R}^2$:

$$\Phi(X) = (1, \phi_1(X), \phi_2(X), \phi_3(X)) = (1, x_1, x_2, x_2^2)$$

For regression, we can model

$$\begin{aligned} f_*(X) &= \beta^\top \Phi(X) \\ &= \beta_0 + \beta_1 \text{balance} + \beta_2 \text{income} + \beta_3 \text{income}^2 \end{aligned}$$

Nonparametric regression

In nonparametric regression, the functions ϕ_k are basis functions

(See ISL 7.3)

A general model would be

$$f_*(X) = \beta^\top \Phi(X)$$

Which we can fit via

$$\hat{\beta} = \underset{\beta}{\text{argmin}} \, ||Y - \Phi\beta||_2^2 ,$$

where $\Phi = [\phi_k(X_i)] \in \mathbb{R}^{n \times K}$,

- k indexes the columns of Φ: $k = 1, \ldots, K$
- i indexes the rows of Φ: $i = 1, \ldots, n$

Nonparametric regression: Splines

Choosing different ϕ_k, leads to different fits

A classic choice is splines

Splines are a basis that provides a very smooth representation of the regression function

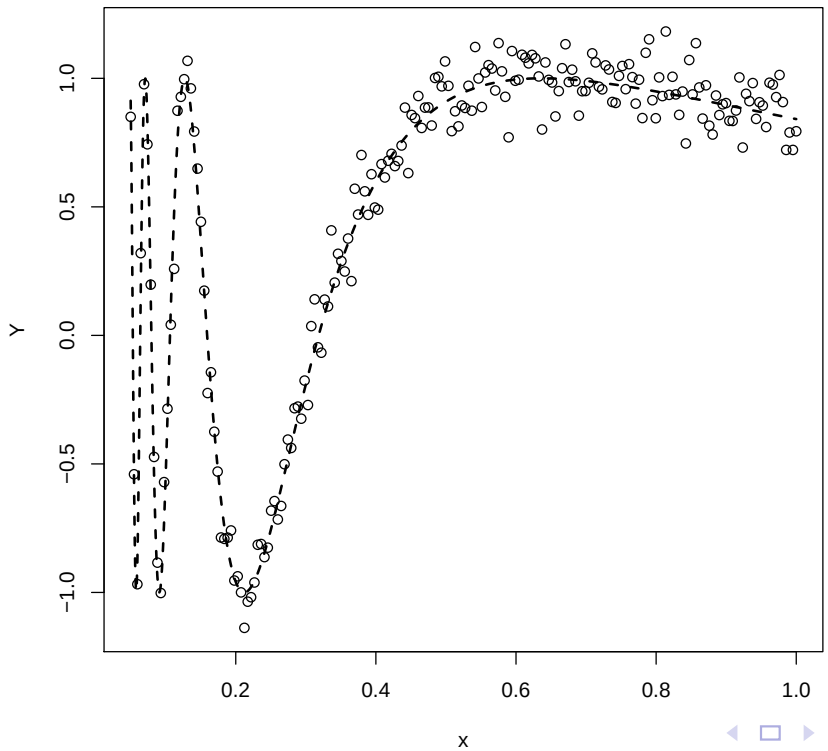
But, again, we can view them as a way of defining a distance and close

(See ISL or ESL for a more rigorous exposition)

Let's turn to the Doppler function for an example..

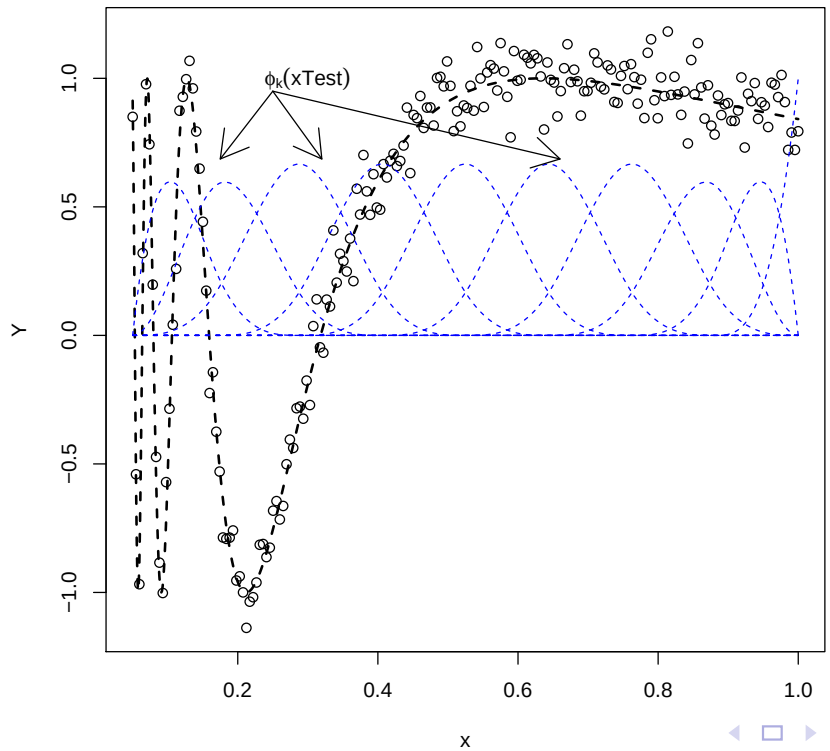
Nonparametric regression: Example

```
x = seq(.05,1,length=200)
Y = sin(1/x) + rnorm(100,0,.1)
plot(x,Y)
xTest = seq(.05,1,length=1000)
lines(xTest,sin(1/xTest),col='black',lwd=2,lty=2)
```



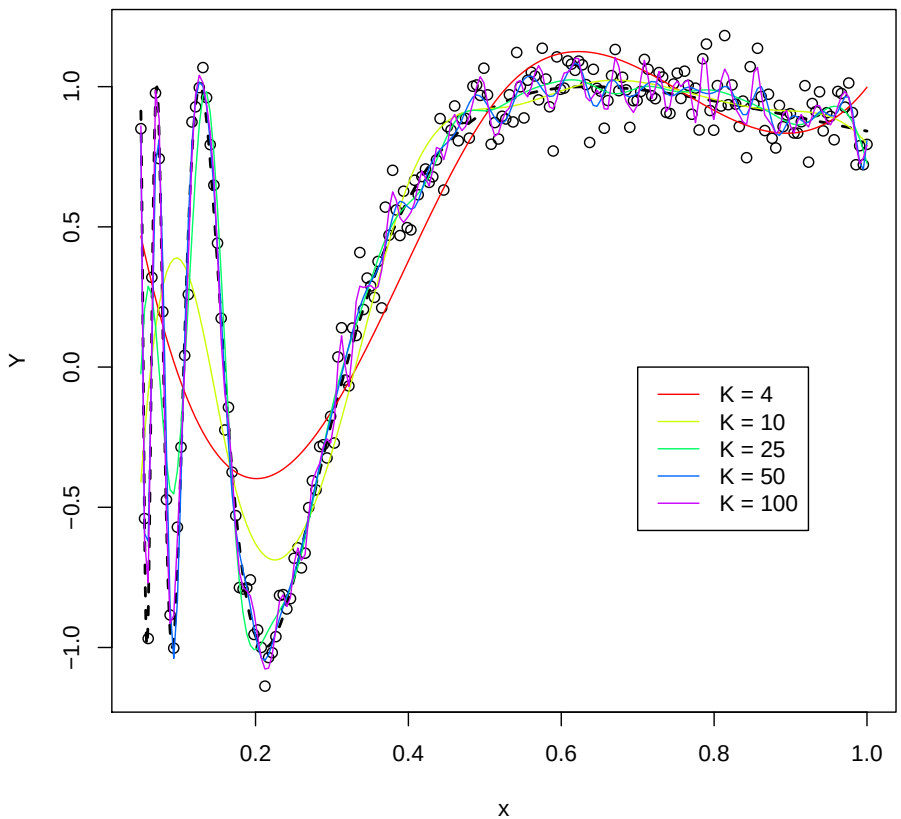
Nonparametric regression: Example

```
require(splines)
Phi = bs(x,df=10)
plot(x,Y)
lines(xTest,sin(1/xTest),col='black',lwd=2,lty=2)
matlines(x=x,Phi,lty=2,type='l',col='blue')
```



Nonparametric regression: Example

```
Phi  = bs(x,df=K)
Yhat = predict(lm(Y~.,data=Phi))
```



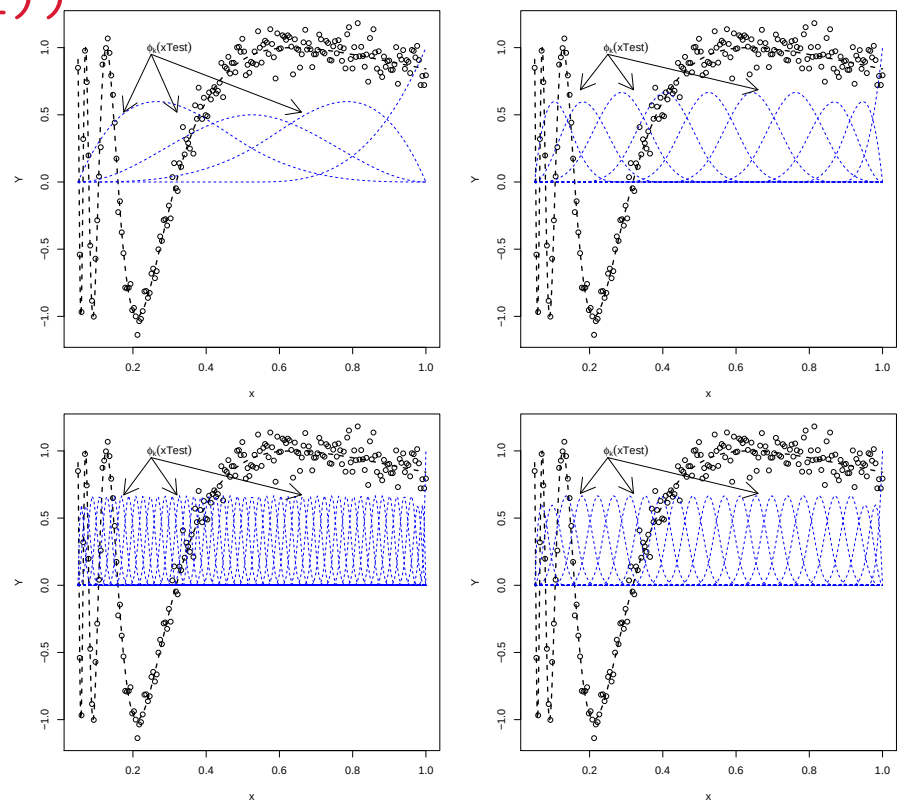


Figure: $K = 4, 10, 24, 50$, clockwise from top left

From linear to nonlinear models

Question: Why don't we always fit such a flexible model?

Answer: This works great if p is small (though it is easier to interpret linear regression output)

(and the specification of distance and close is good)

However, as p gets large

- nothing is nearby
- all points are on the boundary

  (Hence, predictions are generally extrapolations)

These aspects make up (part) of the curse of dimensionality

Curse of dimensionality

Fix the dimension p

(Assume p is even to ignore unimportant digressions)

Let S be a hypersphere with radius r

Let C be a hypercube with side length $2r$

Then, the volume of S and C are, respectively

$$V_S = \frac{r^p \pi^{p/2}}{(p/2)!} \text{ and } V_C = (2r)^p$$

(Interesting observation: this means for $r < 1/2$ the volume of the hypercube goes to 0, but the diagonal length is always $\propto \sqrt{p}$. Hence, the hypercube gets quite 'spiky' and is actually horribly jagged. Regardless of radius, the hypersphere's volume goes to zero quickly.)

Curse of dimensionality

Hence, the ratio of the volumes of a circumscribed hypersphere by a hypercube is

$$\frac{V_C}{V_S} = \frac{(2r)^p \cdot (p/2)!}{r^p \pi^{p/2}} = \frac{2^p \cdot (p/2)!}{\pi^{p/2}} = \left(\frac{4}{\pi}\right)^d d!$$

where $d = p/2$

Observation: This ratio of volumes is increasing really fast. This means that all of the volume of a hypercube is near the corners. Also, this is independent of the radius.

Additive models

(ISL 7.7, 7.8.3)

Additive models

The linear model looks like:

$$f(X) = \beta^\top X = \sum_{j=1}^{p} \beta_j x_j$$

The general nonparametric model looks like:

$$f(X) = \beta^\top \Phi(X) = \sum_{j=1}^{p} \beta_j \phi_j(X)$$

Combine them:

$$f(X) = f_1(x_1) + \cdots + f_p(x_p) = \sum_{j=1}^{p} f_j(x_j)$$

Estimation of such a procedure is not much more complicated than a fully linear model (as all inputs enter separately)

Additive models (for regression)

Additive models are usually phrased using the population level expectation

(These get replaced with empirical versions)

The update is a Gauss-Seidel-type update

(The Gauss-Seidel method is an iterative scheme for solving linear, square systems)

This is for $j = 1, \ldots, p, 1, \ldots, p, 1 \ldots$:

$$f_j(x_j) \leftarrow \mathbb{E}\left[Y - \sum_{k \neq j} f_k(x_k) | x_j \right]$$

Under fairly general conditions, this converges to $\mathbb{E}[Y|X]$

Additive models (for regression)

Backfitting for additive models is roughly as follows:

Choose a univariate nonparametric smoother $\mathcal{S}$ and form all univariate fits $\hat{f}_j$ on each x_j marginally

(Common choice: splines)

Iterate over j until convergence:

1. Define the residuals $R_i = Y_i - \sum_{k \neq j} \hat{f}_k(X_{ik})$
2. Smooth the residuals $\hat{f}_j = \mathcal{S}(R)$
3. Center $\hat{f}_j \leftarrow \hat{f}_j - n^{-1} \sum_{i=1}^{n} \hat{f}_j(X_{ij})$

Report

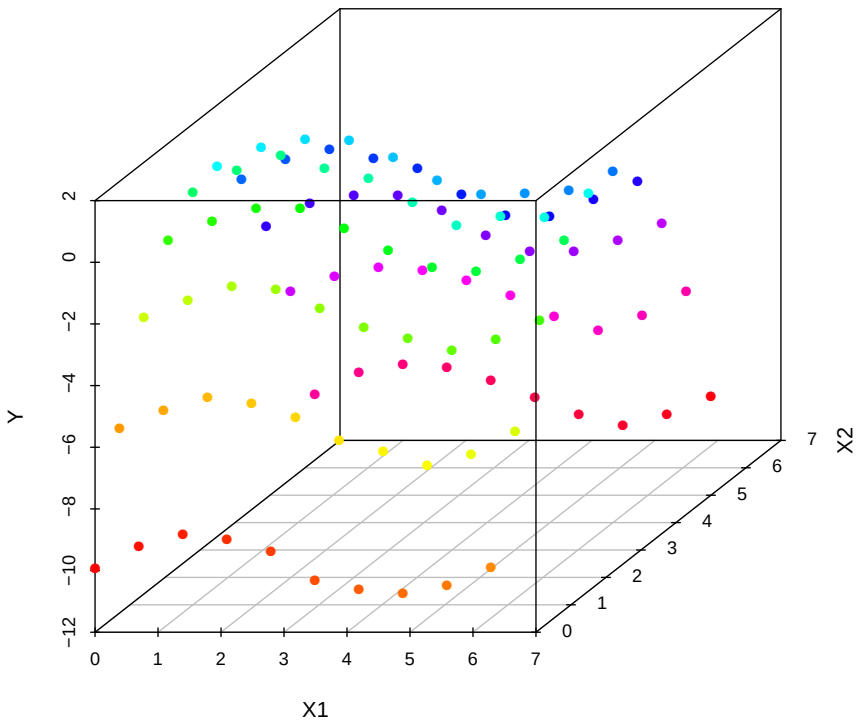
$$\hat{f}(X) = \overline{Y} + \hat{f}_1(x_1) + \cdot + \hat{f}_p(x_p)$$

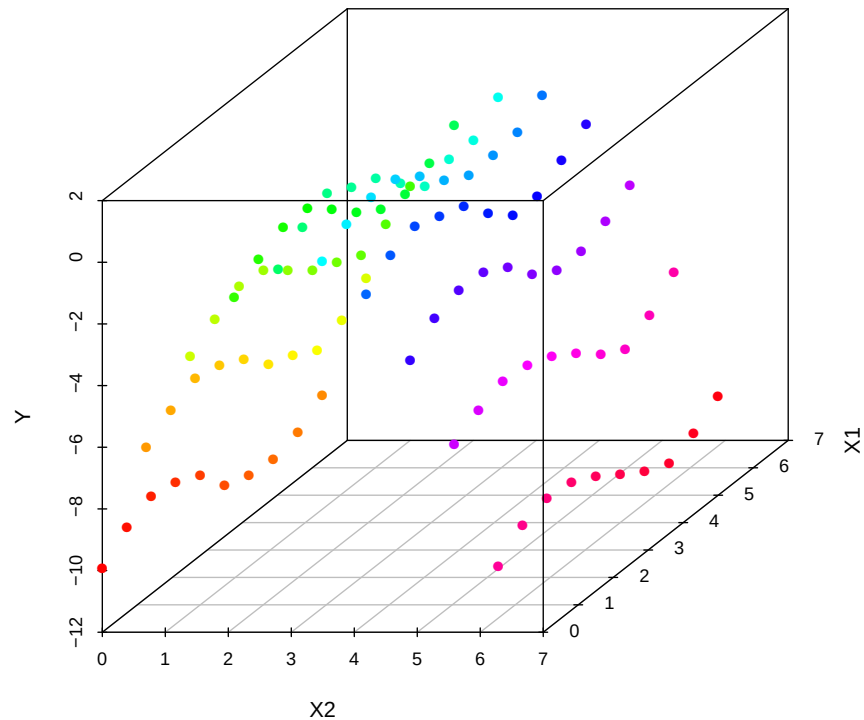
Fitting additive models R

```
library(gam)
x   = seq(0,2*pi,length=10)
xx = expand.grid(x,x)
x1 = xx[,1]
x2 = xx[,2]

Y =  sin(xx[,1]) - (xx[,2] - pi)^2 + rnorm(nrow(xx),0,.1)
sim = data.frame(x1=x1,x2=x2,Y=Y)

out = gam(Y~s(x1,3)+s(x2,3),data=sim)
```

Additive models: Simulation

Plotting the simulated data: Y as a function of x_1, x_2:





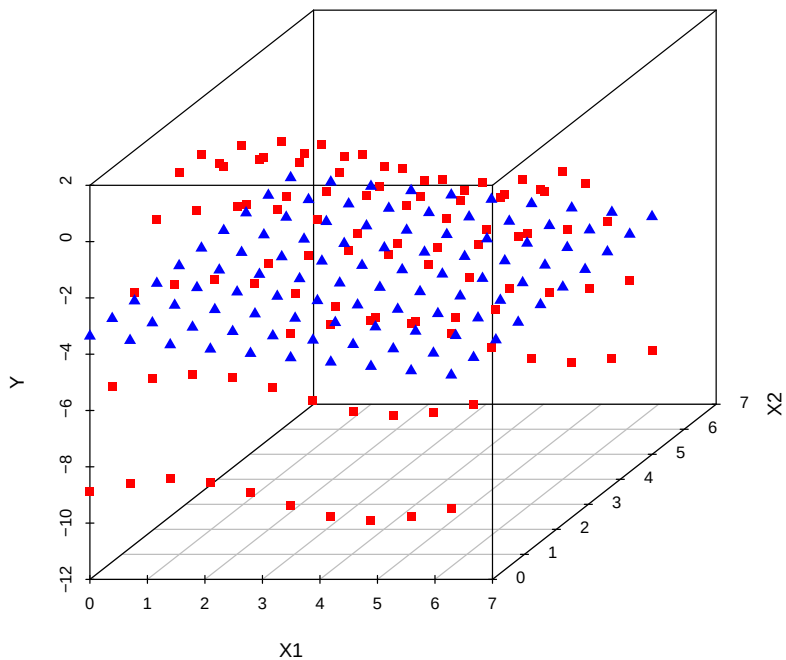
Additive models: Simulation results

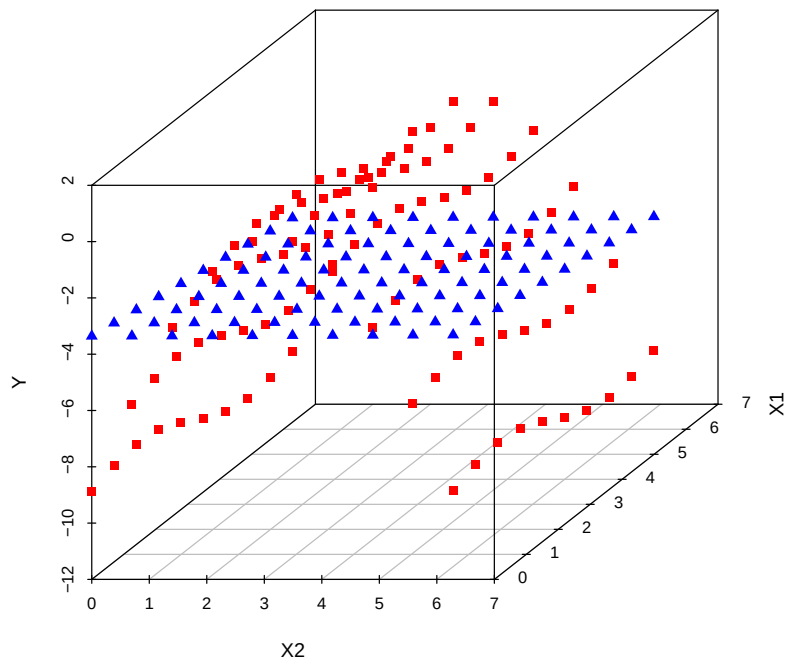
If we fit the (multiple) linear regression:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon,$$

we miss a lot of the structure (blue triangles)

The smoother GAM is able to capture it, however:





(These are the fitted values only. Red squares: GAM, Blue triangles: linear regression)

Detour: Plotting 3d in R

```
out = scatterplot3d(X1,X2,Y,pch=16,type='n')
xyz = out$xyz.convert(X1,X2,out.pred)
points(xyz,col='red',pch=15)
xyz = out$xyz.convert(X1,X2,out.pred.lm)
points(xyz,col='blue',pch=17)
```

Additive models (for classification)

As squared error loss isn't quite right for classification, additive logistic regression is a popular approach

Suppose $Y \in \{-1, 1\}$

$$\log\left(\frac{\mathbb{P}(Y=1|X)}{\mathbb{P}(Y=-1|X)}\right) = \sum_{j=1}^{p} f_j(x_j) = f(X)$$

This gets inverted in the usual way to acquire a probability estimate

$$\pi(X) = \mathbb{P}(Y=1|X) = \frac{e^{f(X)}}{1+e^{f(X)}}$$

($f_j(x_j) = \beta_j x_j$ and $f(X) = X^\top \beta$ gives us (linear) logistic regression)

These models are usually fit by numerically maximizing the binomial likelihood, and hence enjoy all the asymptotic optimality prospects of MLEs

Additive models (for classification)

Example: In R, this can be fit with the package gam

In the gam package there is a dataset kyphosis

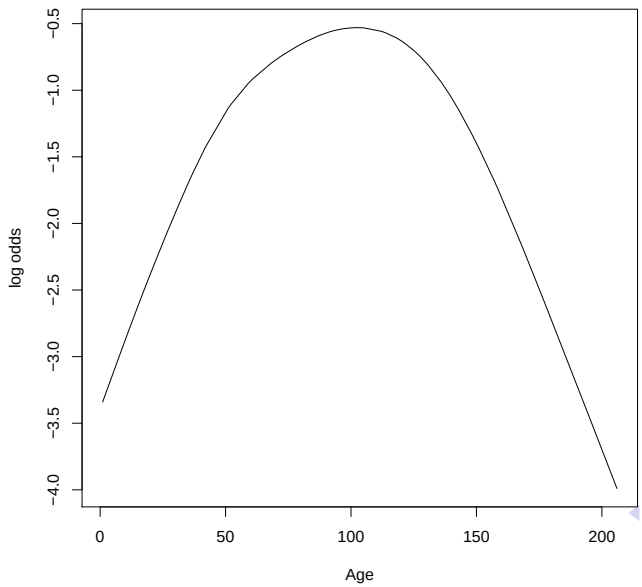
This dataset examines a disorder of the spine

Let's look at two possible features Age and Number

(Number refers to the number of vertebrae that were involved in a surgery)

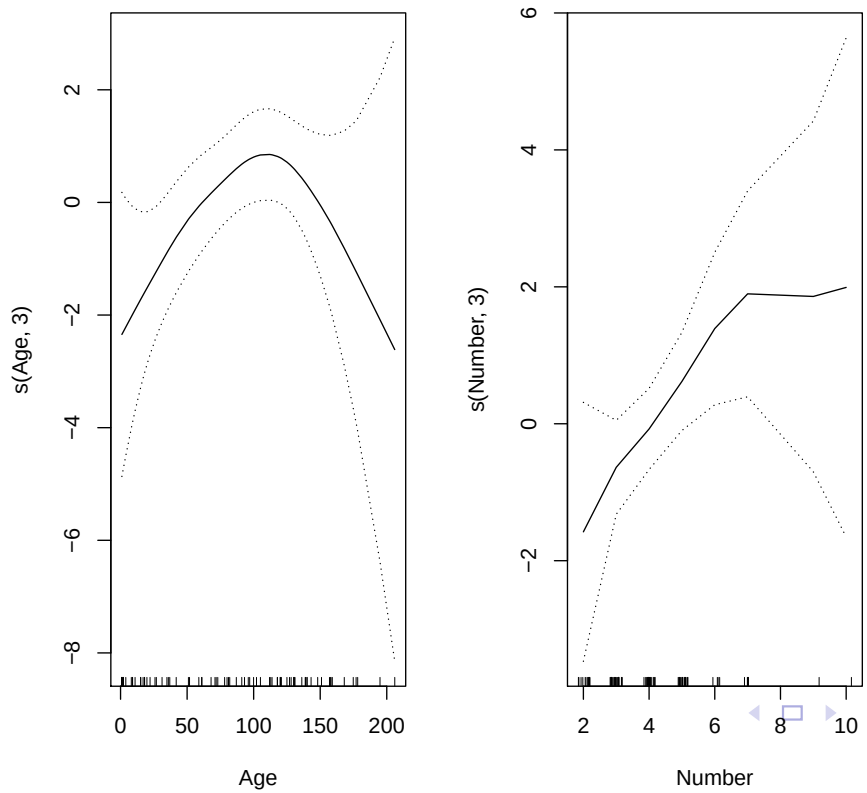
Additive models (for classification)

```
library(gam)
data(kyphosis)

out = gam(Kyphosis~s(Age,3),family=binomial,data=kyphosis)
out.pred = predict(out)
plot(sort(kyphosis$Age),out.pred[order(kyphosis$Age)],
       type='l',xlab='Age',ylab='log odds')
```



Additive models (for classification)

```
out = gam(Kyphosis ~ s(Age,3) + s(Number,3),
          family = binomial, data=kyphosis)
par(mfrow=c(1,2))
plot(out,se=T)
```



Postamble:

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  (Apply to high bias/low variance procedures)
- To understand boosting, we need to discuss nonparametric regression
- Nonparametric regression provides a flexible fit, but can only be used in low dimensions

  (Curse of dimensionality)
- Additive models are a relaxation of nonparametric models that can be fit in much higher dimensions
- Boosting is an algorithm for fitting a type of additive model

  (More on this in the next set of notes)