Predicting a Continuous Outcome

Data Mining
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The Regression Task

- So far we have considered the classification task
- In this task the goal is to predict the value of a categorical outcome
- In order to do this we have training data that includes the value of both predictors and outcome
- Another type of supervised learning is prediction of the value of a continuous outcome; this is called the regression task
- We will still have training data that includes the value of both predictors and outcome

Multiple Linear Regression

Let Y_i be the outcome variable, and x_{ij} be the jth predictor value, for the ith observation. Multiple linear regression does prediction of Y_i as a linear function of the predictors:

Multiple linear regression model with p predictors:

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip} + \epsilon_i$$

$$\epsilon_i \overset{\text{iid}}{\sim} N(0, \sigma^2)$$

$$i = 1, \ldots, n$$

Multiple Linear Regression

The assumptions of multiple linear regression are:

Multiple Linear Regression

The training step for multiple linear regression consists of:

The prediction step consists of:

Example: Cheese Data

Example: 30 samples of cheese; for each we know:

Taste: Subjective taste test score, obtained by combining the scores of several tasters

Acetic: Log of concentration of acetic acid

H2S: Log of concentration of hydrogen sulfide

Lactic: Concentration of lactic acid

Cheese Data

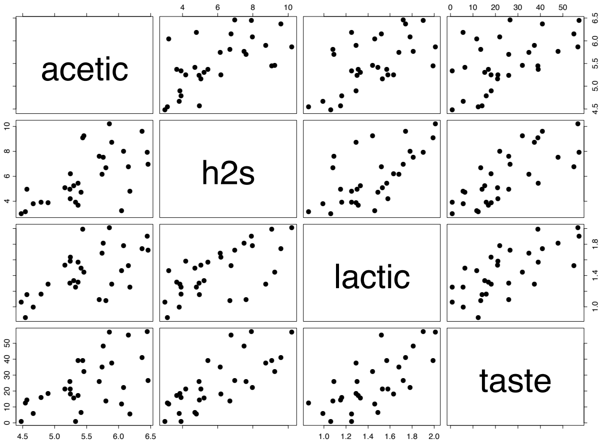
Case	taste	Acetic	H2S	Lactic
1	12.3	4.543	3.135	0.86
2	20.9	5.159	5.043	1.53
3	39	5.366	5.438	1.57
4	47.9	5.759	7.496	1.81
5	5.6	4.663	3.807	0.99
6	25.9	5.697	7.601	1.09
7	37.3	5.892	8.726	1.29
8	21.9	6.078	7.966	1.78
9	18.1	4.898	3.85	1.29
10	21	5.242	4.174	1.58
11	34.9	5.74	6.142	1.68

Cheese Data

- Goal: to predict taste based on the chemical composition. Why?

Cheese Data

Pairwise scatterplots (interpretation?):



Cheese Data

How would you characterize the relationships?

So fit the linear regression model with Y_i equal to the taste score, and the predictors x_{i1}, x_{i2}, and x_{i3} equal to the values of Acetic, H2S, and Lactic.

Multiple Linear Regression

- R code for TRAINING step on cheese data (estimation of $\beta_0, \beta_1, \beta_2, \beta_3, \sigma^2$ using the 30 cheese samples):

  ```
  cheeseLM = lm(formula = taste ~ acetic + h2s + lactic,
     data = cheese)

  summary( cheeseLM )
  ```

R Syntax

Side note about R:

- In R, functions like lm have arguments, like formula and data
- When you call the function you can write:
  myFunction(myArgument1 = “hello”, myArgument2 = 5)
- It also works if you leave out the argument names, but only if all the arguments are in the correct order:
  myFunction(“hello”, 5)

Cheese Linear Model

Results for cheese data:

```
Call: lm(formula = taste ~ acetic + h2s + lactic, data = cheese)
Residuals:
    Min      1Q Median     3Q    Max
 -17.39 -6.612 -1.009 4.908 25.45

Coefficients:
               Value Std. Error  t value Pr(>|t|)
(Intercept) -28.8768  19.7354    -1.4632   0.1554
     acetic   0.3277   4.4598     0.0735   0.9420
        h2s   3.9118   1.2484     3.1334   0.0042
     lactic  19.6705   8.6291     2.2796   0.0311

Residual standard error: 10.13 on 26 degrees of freedom
Multiple R-Squared: 0.6518
F-statistic: 16.22 on 3 and 26 degrees of freedom, the p-value is
   3.81e-006
```

Cheese Linear Model

Mark the estimate of β_0
Mark the estimate of β_2, the regression coefficient for H2S
Mark the estimate of σ

```
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Multiple Linear Regression

- Recall that in naive Bayes we calculated $Pr(Y|X_1, \ldots, X_p)$ from our model in order to predict the value of Y.

- In linear regression we are also calculating $Pr(Y|X_1, \ldots, X_p)$, the distribution of Y given $X_1, \ldots, X_p$, from our model, to predict the value of Y

Multiple Linear Regression

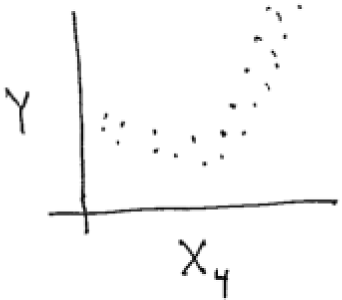
- For the cheese example, what do we predict the taste rating to be if Acetic = 5.1, H2S = 9, and Lactic = 1.2?

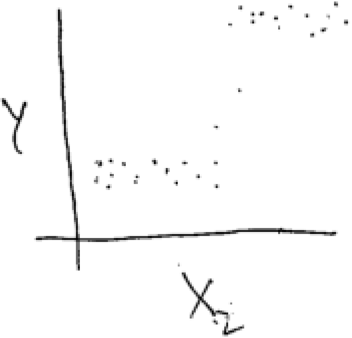
Multiple Linear Regression

When should we transform the (outcome or predictor) variables?

Nonlinearities in a continuous outcome

- What do we do when we're predicting a continuous outcome and the relationship between the predictors and outcome is nonlinear?



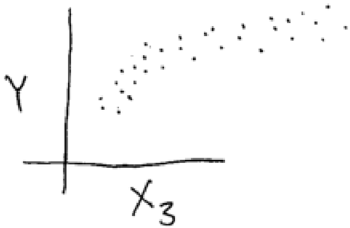


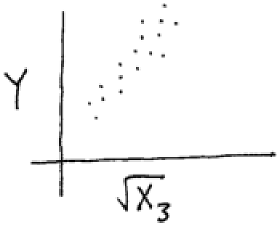
Nonlinearities in a continuous outcome

Option 1:

- **Transform the predictor so that the relationship is linear**
  Note: This works sometimes but not always.

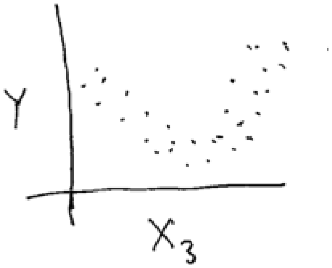
example of when this works:





Nonlinearities in a continuous outcome

Example of when this doesn't work:



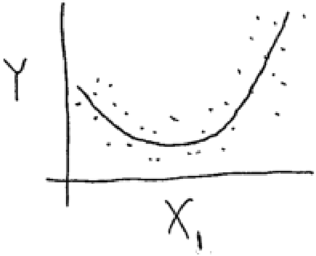
Reason:

Nonlinearities in a continuous outcome

Option 2:

- **Include polynomial terms in the regression:**

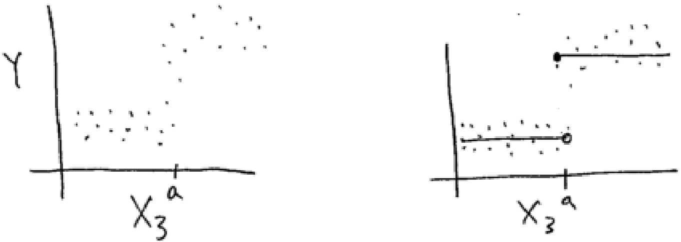
$$Y_i = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 + \epsilon_i$$



Nonlinearities in a continuous outcome

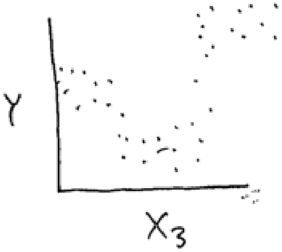
Option 3:

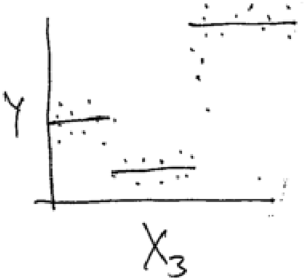
- **Discretize the predictor:**
  e.g.: cut into $X_3 < a$, $X_3 \geq a$; then the linear regression for this new binary predictor looks like:



Nonlinearities in a continuous outcome

- If you instead discretize into more categories you can get a more flexible model





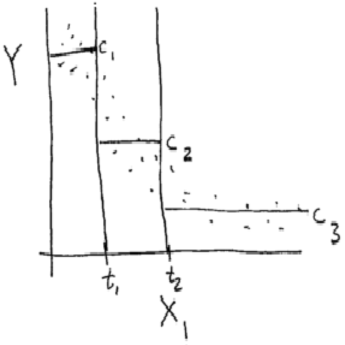
Nonlinearities in a continuous outcome

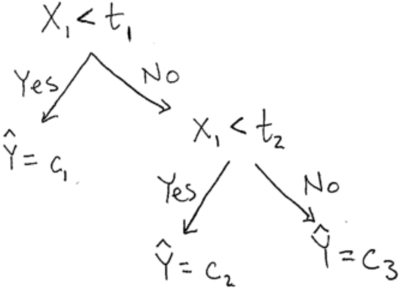
- A method based on this discretization idea is regression trees.

- The corresponding method for categorical outcomes is called classification trees; we saw an informal version of these in the first week of class.

Nonlinearities in a continuous outcome

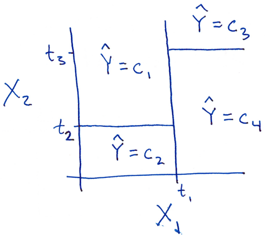
Ex 1: One predictor X_1

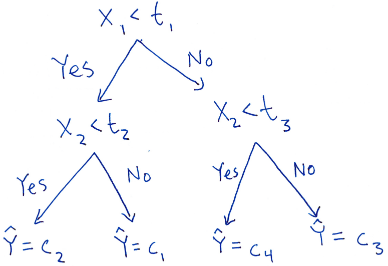




Nonlinearities in a continuous outcome

<u>Ex 2:</u> 2 continuous predictors X_1, X_2





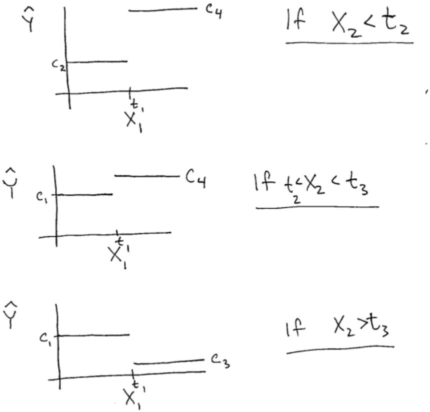
Regression Trees

Regression tree benefits:

-
-

Regression Trees

<u>Back to Ex 2:</u>



Notice the **interaction:** the effect of X_1 on $\hat{Y}$ depends on the value of X_2.