Lecture 16: High-dimensional regression, non-linear regression

Reading: Sections 6.4, 7.1

STATS 202: Data mining and analysis

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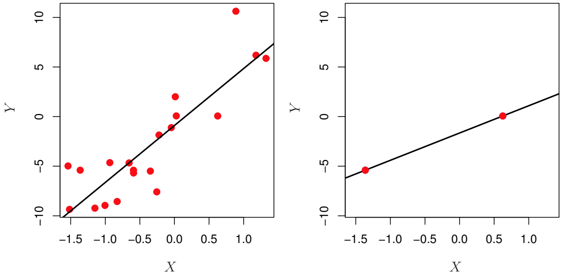
  1. **Medicine:** Instead of regressing heart disease onto just a few clinical observations (blood pressure, salt consumption, age), we use in addition 500,000 single nucleotide polymorphisms.
  2. **Marketing:** Using search terms to understand online shopping patterns. A *bag of words* model defines one feature for every possible search term, which counts the number of times the term appears in a person's search. There can be as many features as words in the dictionary.

Some problems we have talked about

- When $n = p$, we can find a fit that goes through every point.



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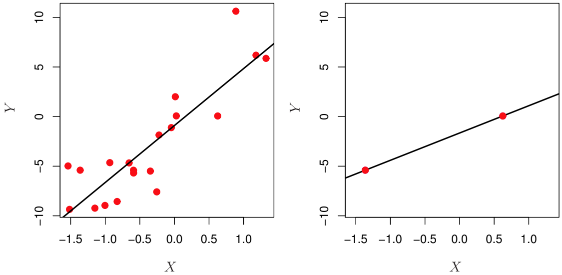

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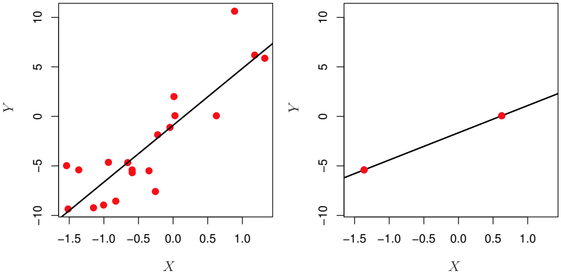

- Least-squares regression doesn't have a unique solution when $p > n$.
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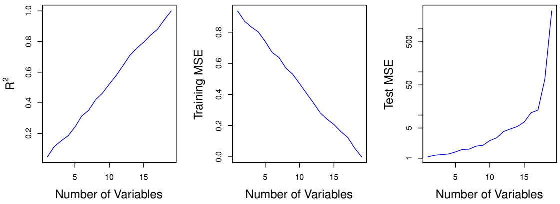
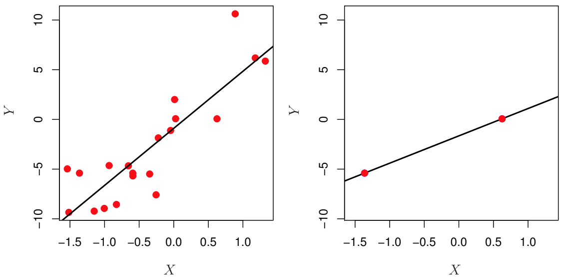
Some problems we have talked about

- We know that least-squares regression doesn't work when $p > n$.
- We can use regularization methods, such as variable selection, ridge regression and the lasso.
- When $n = p$, we can find a fit that goes through every point.
- Measures of training error are really bad.



Some new problems



- Furthermore, it becomes hard to estimate the noise $\hat{\sigma}^2$.
- Measures of model fit C_p, AIC, and BIC fail.

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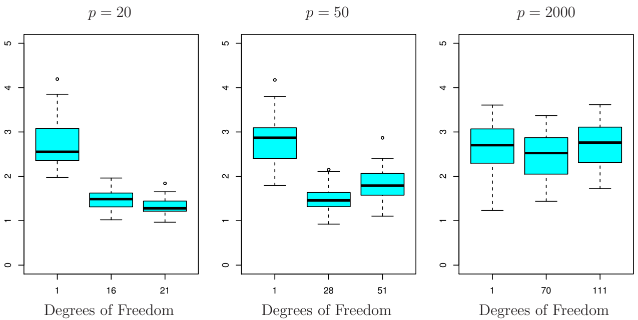

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- Plots show the test error of the Lasso.

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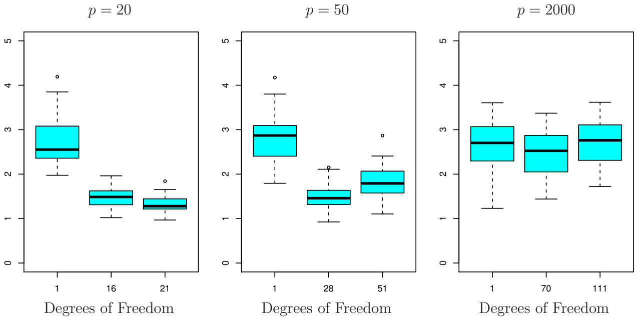

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- Plots show the test error of the Lasso.
- **Message:** Adding predictors that are uncorrelated with the response hurts the performance of the regression!

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- **Message:** Don't overstate the importance of the predictors selected.

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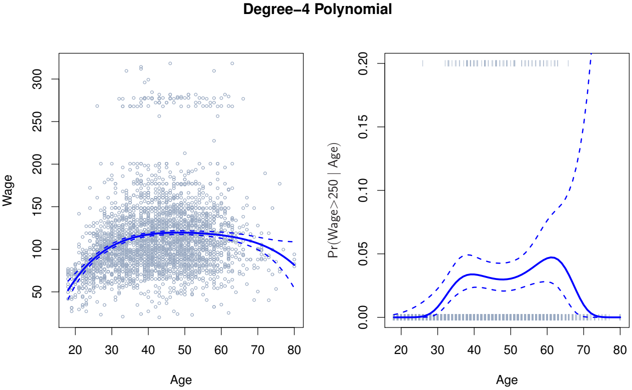
- **Message:** Don't use inferential methods developed for least squares regression for things like LASSO, forward stepwise, etc.
- Can we do better? Yes, but it's complicated.

Non-linear regression

Problem: How do we model a non-linear relationship?



Left: Regression of `wage` onto `age`.
Right: Logistic regression for classes `wage`> 250 and `wage`≤ 250

Basis functions

Strategy:

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$$Y = \beta_0 + \beta_1 f_1(X) + \beta_2 f_2(X) + \cdots + \beta_d f_d(X) + \epsilon.$$

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- Options for $f_1, \ldots, f_d$:
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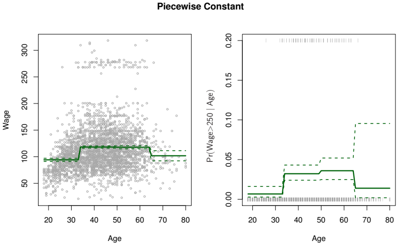
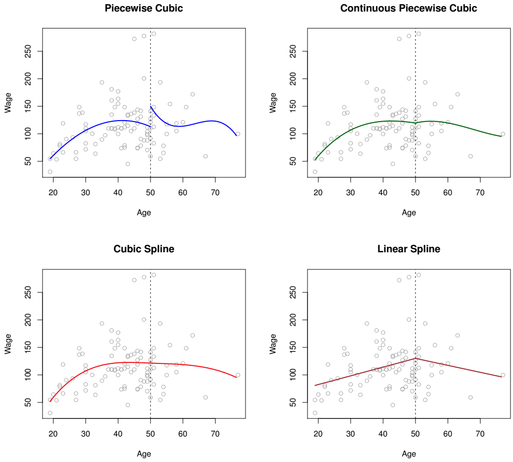
  2. Indicator functions, $f_i(x) = \mathbf{1}(c_i \leq x < c_{i+1})$.



Basis functions

- Options for $f_1, \ldots, f_d$:
  3. Piecewise polynomials:



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- It turns out, we can write f in terms of $K + 3$ basis functions:

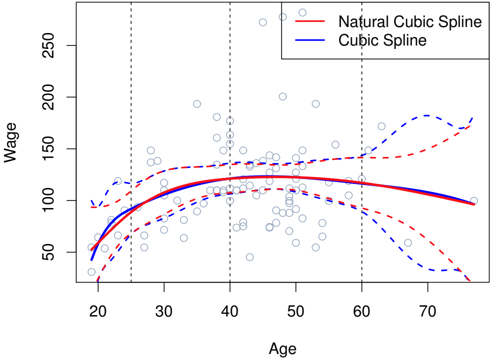
$$f(X) = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \beta_4 h(X, \xi_1) + \cdots + \beta_{K+3} h(X, \xi_K)$$

where,

$$h(x, \xi) = \begin{cases} (x - \xi)^3 & \text{if } x > \xi \\ 0 & \text{otherwise} \end{cases}$$

Natural cubic splines

Spline which is linear instead of cubic for $X < \xi_1$, $X > \xi_K$.



The predictions are more stable for extreme values of X.

Choosing the number and locations of knots

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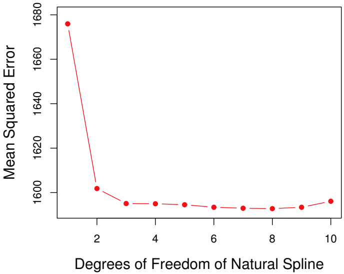
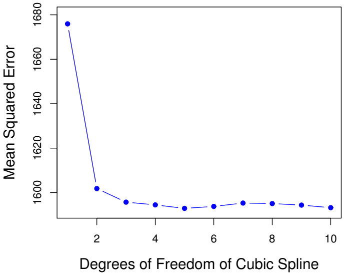
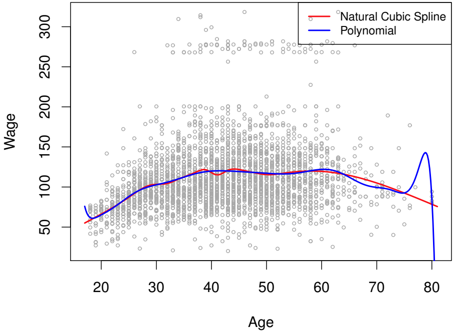
The number of knots, K, is chosen by cross validation:





Natural cubic splines vs. polynomial regression

- Splines can fit complex functions with few parameters.
- Polynomials require high degree terms to be flexible.
- High-degree polynomials can be unstable at the edges.



Smoothing splines

Find the function f which minimizes

$$\sum_{i=1}^{n}(y_i - f(x_i))^2 + \lambda \int f''(x)^2 dx$$

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Facts:

- The minimizer $\hat{f}$ is a natural cubic spline, with knots at each sample point $x_1, \ldots, x_n$.
- Obtaining $\hat{f}$ is similar to a Ridge regression.

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2. Deduce that the solution to the smoothing spline problem is a natural cubic spline, which can be written in terms of its basis functions.

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3. Letting $\mathbf{N}$ be a matrix with $\mathbf{N}(i,j) = f_j(x_i)$, we can write the objective function:

$$(y - \mathbf{N}\beta)^T (y - \mathbf{N}\beta) + \lambda \beta^T \Omega_{\mathbf{N}} \beta,$$

   where $\Omega_{\mathbf{N}}(i,j) = \int N_i''(t) N_j''(t) dt$.

Deriving a smoothing spline

4. By simple calculus, the coefficients $\hat{\beta}$ which minimize

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5. Note that the predicted values are a linear function of the observed values:

$$\hat{y} = \underbrace{\mathbf{N}(\mathbf{N}^T\mathbf{N} + \lambda\Omega_{\mathbf{N}})^{-1}\mathbf{N}^T}_{\mathbf{S}_\lambda} y$$