COMP 680
Statistics for Computing and Data Science
Week 13: Beyong Linear Models

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Outline

The Truth is probably NOT Linear

- But often the linearity assumption is good enough
  - “all models are wrong, some are useful.”

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- But often the linearity assumption is good enough
  - "all models are wrong, some are useful."
- When linearity is clearly not enough:
  - polynomial regression
  - spline models
  - generalized additive models (GAM)
  - local regression
  - fully non-parametric models

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  - but OLS solution is **not available for** $p > n$
- Prediction accuracy:
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  - trade bias with variance to decrease MSE
- Model Interpretability:
  - penalize large models and large slopes
  - automatically perform variable selection

Shrinkage Estimate

- We fit a model involving all p covariates
- But the estimated slopes are shrunken towards 0 relative to OLS.
- This shrinkage is known as regularization
  - penalize “large” β by shrinking them - reduce variance
  - shrink some β to exactly 0 - variable selection

Ridge Regression

- Recall that OLS estimates $\hat{\beta}^{OLS}$ using the values that minimize

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- In contrast, the ridge regression coefficient estimates $\hat{\beta}^{\boldsymbol{R}}$ are the values that minimize

$$\sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 = \text{RSS} + \lambda \|\boldsymbol{\beta}\|_{L2}^2,$$

where $\lambda \geq 0$ is a tuning parameter , to be determined separately

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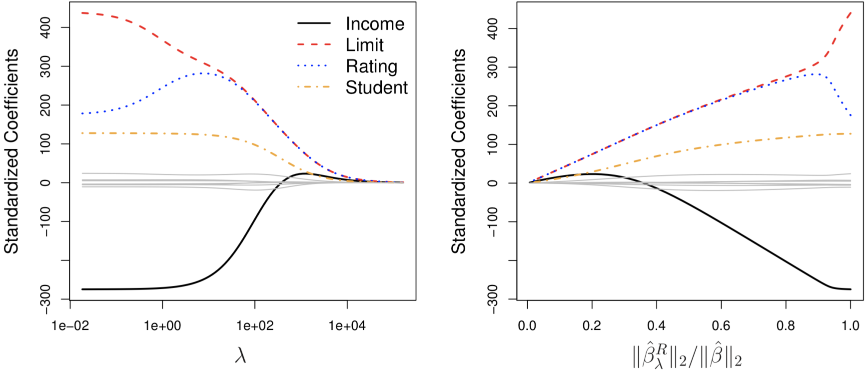
- The tuning parameter λ serves to control the relative impact of these two terms on the regression coefficient estimates.
- Selecting a good value for λ is critical!

Ridge Solution Path



Example from ISLR

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- In the left-hand panel, each curve corresponds to the ridge regression coefficient estimate for one of the ten variables, plotted as a function of λ.

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- The notation $\|\beta\|_2$ denotes the L^2 norm of a vector, and is defined as $\|\beta\|_2 = \sqrt{\sum_{j=1}^p \beta_j^2}$.

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- **Lasso uses an L1 penalty while Ridge uses an L2 penalty.**

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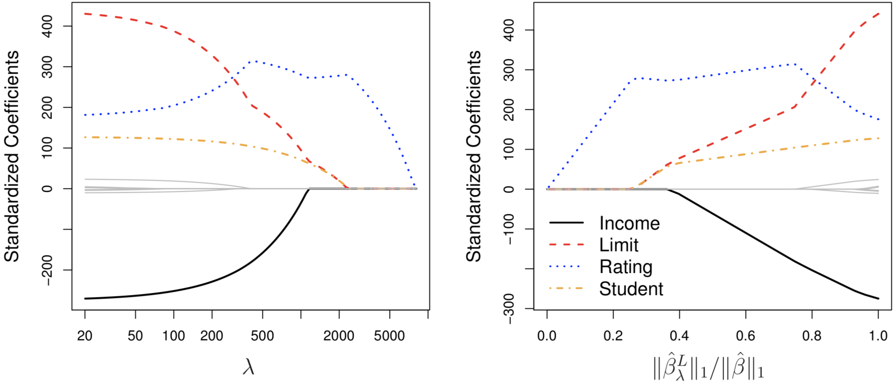
- Therefore, Lasso performs variable selection automatically when estimating the model
    - yields sparse models — that is, models that involve only a subset of the variables
- Same as in ridge regression, selecting a good value of λ for the lasso is critical!

Lasso Solution Path



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Why is it that the lasso, unlike ridge regression, results in coefficient estimates that are exactly equal to zero?

$$\hat{\beta}^{\boldsymbol{R}} = \arg\min \left[\sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right]$$

this is equivalent to an optimization with constrain:

$$\text{minimize}_{\beta} \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \qquad \text{subject to } \sum_{j=1}^{p} \beta_j^2 \leq s$$

i.e. there is a 1-1 correspondence of λ and s that produce the same solution!

The Variable Selection Property of the Lasso

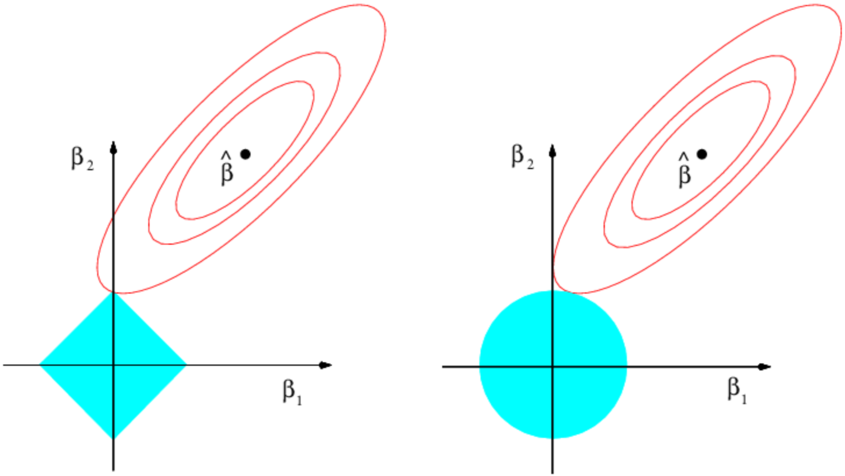
Use two covariates as example for visualization purpose:

$$\text{minimize}_\beta \sum_{i=1}^{n} (y_i - \beta_1 x_{i1} - \beta_2 x_{i2})^2$$

Ridge penalty: $\lambda(\beta_1^2 + \beta_2^2) \implies$ min RSS subject to $\beta_1^2 + \beta_2^2 \leq s$

Lasso penalty: $\lambda(|\beta_1| + |\beta_2|) \implies$ min RSS subject to $|\beta_1| + |\beta_2| \leq s$

The Intuition



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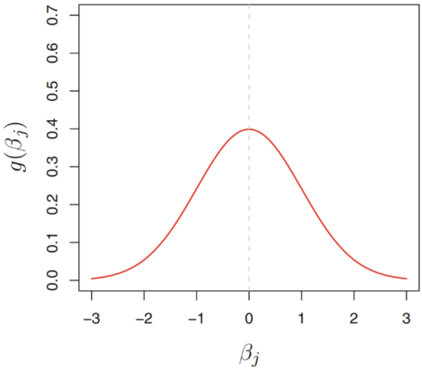
  - cares more about prediction than what is the "true" model
- Post selection inference is an active area of research:
  - can we recover true signals if we have infinity amount of data
  - what if number of variables increases with sample size

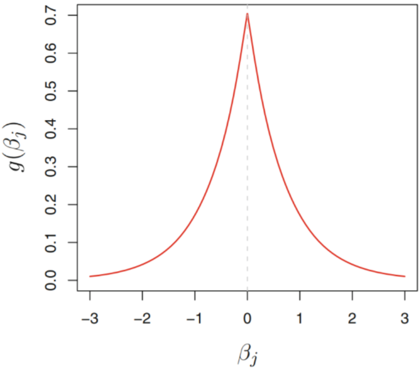
Connection to Bayesian Methods

Solutions are posterior mode with corresponding prior on β:

- Ridge prior: Gaussian
  $$g(\beta_j) = \frac{1}{\sqrt{2\pi\tau}} \exp\left(\frac{\beta_j^2}{2\tau^2}\right)$$

- Lasso prior: Laplace
  $$g(\beta_j) = \frac{1}{2b} \exp\left(\frac{|\beta_j|}{b}\right)$$





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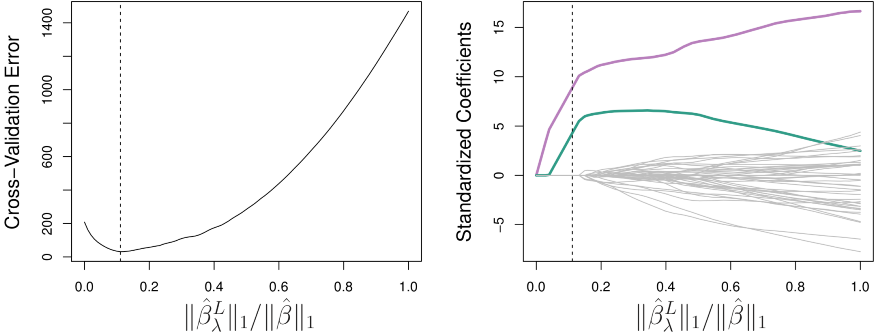
- Ridge or Lasso?
  - neither will universally dominate the other
  - Lasso wins when true regression function is sparse!
- Can be applied to any model fitting using optimization:
  - GLM, spline models, GAM...
  - all parametric ML models...

Lasso with CV



Example from ISLR

Outline

Polynomial Regression

- Introduce nonlinearity by adding polynomial terms

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \cdots + \epsilon_i$$

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  - degree of freedom $\approx$ number of parameters
- How to select the degree of polynomial?
  - Stat approach - ANOVA test to compare nested models
  - ML approach - treat as a tuning parameter

Piecewise Polynomials

- Instead of a single polynomial in X over its whole domain, we can rather use different polynomials in regions defined by knots

$$y_i = \begin{cases} \beta_{01} + \beta_{11}x_i + \beta_{21}x_i^2 + \beta_{31}x_i^3 + \epsilon_i, & \text{if } x_i < c \\ \beta_{02} + \beta_{12}x_i + \beta_{22}x_i^2 + \beta_{32}x_i^3 + \epsilon_i, & \text{if } x_i \geq c \end{cases}$$

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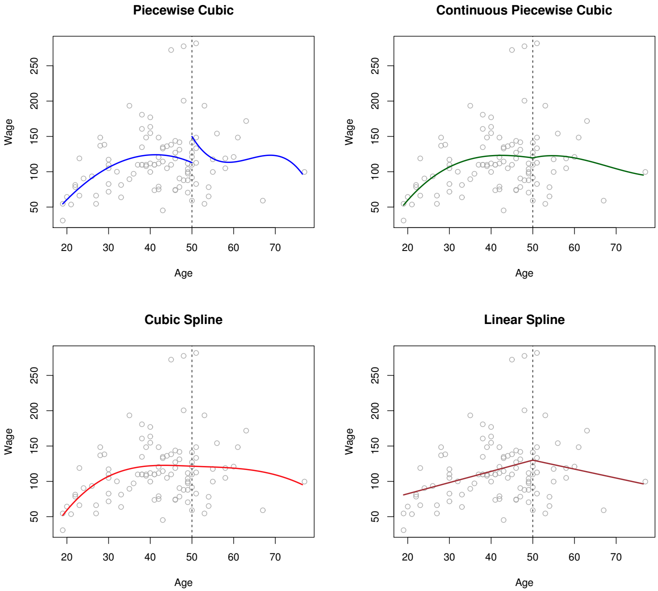
- Splines have the “maximum” amount of continuity
  - piece together local polynomials smoothly


Piecewise Cubic
Continuous Piecewise Cubic
Cubic Spline
Linear Spline
Wage
Age
50
100
150
200
250
20
30
40
50
60
70

Cubic Splines

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- We can represent this model with truncated power basis functions:

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \cdots + \beta_{K+3} b_{K+3}(x_i) + \epsilon_i$$

where the b_k are basis functions

Cubic Spline Basis

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\begin{aligned}
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- where

$$
(x_i - \xi_k)_+^3 = \begin{cases} (x_i - \xi_k)^3 & \text{if } x_i > \xi_k \\ 0 & \text{otherwise} \end{cases}
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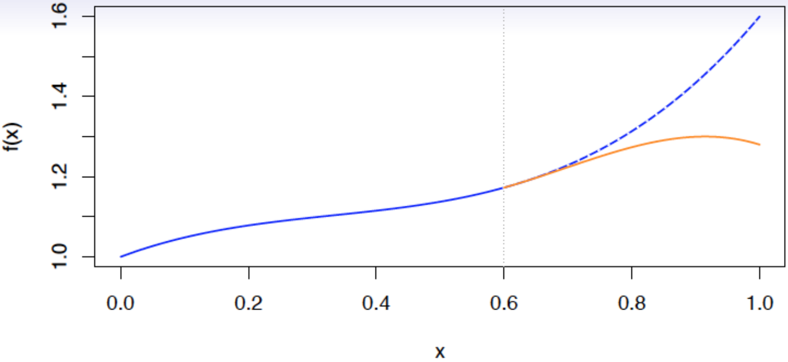
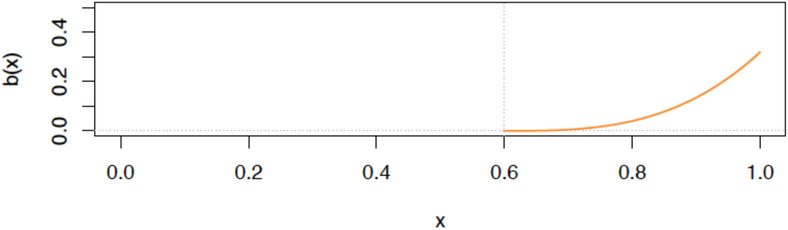


f(x)
1.0
1.2
1.4
1.6
0.0
0.2
0.4
0.6
0.8
1.0
x



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  - extrapolates linearly beyond the boundary knots
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- Smoothing splines
  - choose knot at each data point x_i
  - add smoothing penalty to control df

Smoothing Splines

- Consider a regression model $y_i = g(x_i) + \epsilon_i$ where we solve for:

$$\hat{g} = \arg\min_{g \in \mathbb{S}} \left(\sum_{i=1}^{n} (y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt \right)$$

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  - $\lambda \to 0$?
  - $\lambda \to \infty$?

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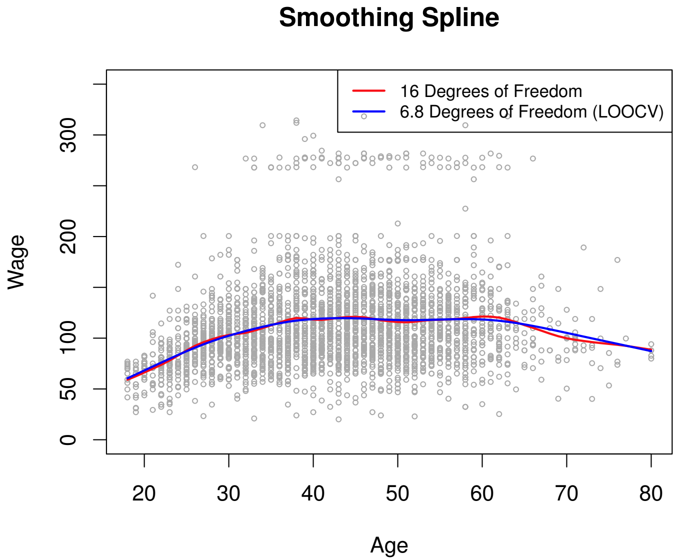
- Most software can specify df rather than λ
  - ML approach: treat λ as a tuning parameter
  - same regularization idea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16 Degrees of Freedom
6.8 Degrees of Freedom (LOOCV)
Wage
Age
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Generalized Additive Models (GAM)

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  - fitted function values are (partial plot)
- Relax additive assumption?
  - bivariate smoothers
  - low-order interactions

Outline

1. Beyond Linearity
2. Regularization
3. Splines and GAM
4. Nonparametric Models
5. Code Demo

Kernel Density Estimate

- Nonparametric method to estimate a density function:

$$\hat{f}(x) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{h} K\left(\frac{x - X_i}{h}\right)$$

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  - h is the bandwidth

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- "Smoothed out" histogram
  - converges faster
- In practice, need to choose a kernel and a bandwidth
  - some asymptotic guideline
  - software default choice

Kernel Regression

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with observed data (x_i, y_i) for $i = 1, 2, \cdots n$.

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- Kernel regression with kernel K and bandwidth h:

$$\hat{f}(x) = \sum_{i=1}^{n} \omega_i(x) y_i, \quad \text{where} \quad \omega_i(x) = \frac{K(\frac{x-x_i}{h})}{\sum_{k=1}^{n} K(\frac{x-x_k}{h})}$$

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with observed data (x_i, y_i) for $i = 1, 2, \cdots n$.

- Kernel regression with kernel K and bandwidth h:

$$\hat{f}(x) = \sum_{i=1}^{n} \omega_i(x) y_i, \quad \text{where} \quad \omega_i(x) = \frac{K(\frac{x-x_i}{h})}{\sum_{k=1}^{n} K(\frac{x-x_k}{h})}$$

- K and h play the similar role in KDE

Local Regression

- Locally Weighted Scatterplot Smoothing
  - fit linear regression locally by weighted least squares
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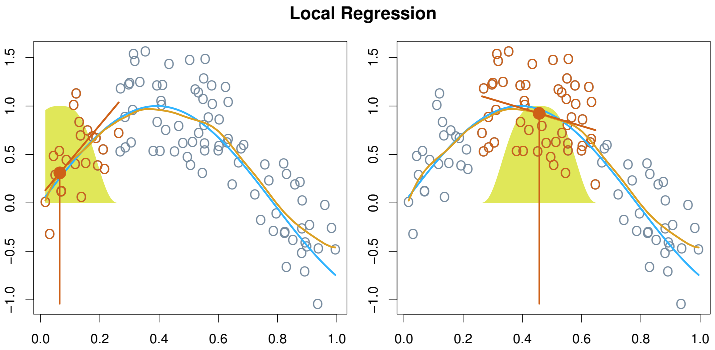


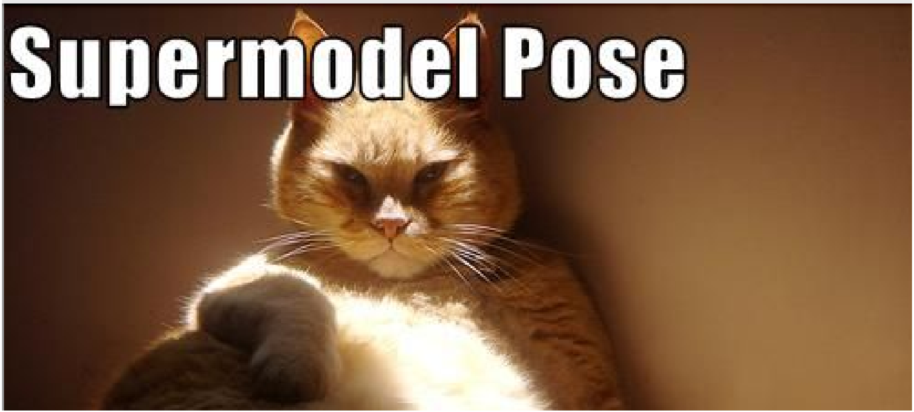
Example from ISLR

Summary

- With GAM in your statistics toolbox, you are able to:
  - model any type of **response variable** in the GLM family:
    - continuous: Gaussian, Gamma, Beta
    - counts: Poisson, Negative Binomial
    - binary: Binomial
    - categorical: Multinomial
  - include both numerical and categorical **predictors**
  - include a **mix of linear and nonlinear** effects
    - how do you decide?
  - include interaction terms to relax additive assumption
    - interpretation is key
  - apply regularization with Ridge or Lasso penalty

Which means...

You are now officially a supermodeler. Bravo!!!



Outline