

Introduction to Generalized Additive Models

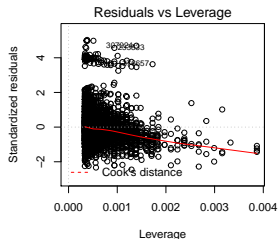
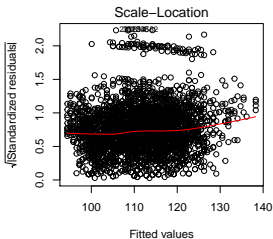
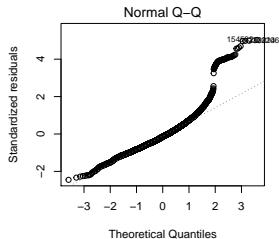
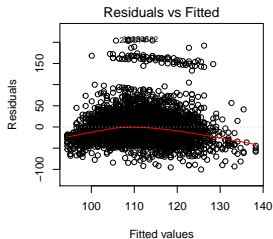
ISLR Chapter 7

April 3, 2017

Moving Beyond Linearity

Wage data from ISLR data(Wage)

Residual plots from Simple Linear Regression of Wage on Age:



Polynomial Regression

```
> summary(lm(wage ~ age + I(age^2) + I(age^3) + I(age^4),  
             data=Wage))
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	-1.842e+02	6.004e+01	-3.067	0.002180	**
age	2.125e+01	5.887e+00	3.609	0.000312	***
I(age^2)	-5.639e-01	2.061e-01	-2.736	0.006261	**
I(age^3)	6.811e-03	3.066e-03	2.221	0.026398	*
I(age^4)	-3.204e-05	1.641e-05	-1.952	0.051039	.

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 39.91 on 2995 degrees of freedom
Multiple R-squared: 0.08626, Adjusted R-squared: 0.0850
F-statistic: 70.69 on 4 and 2995 DF, p-value: < 2.2e-16

Orthogonal Polynomial

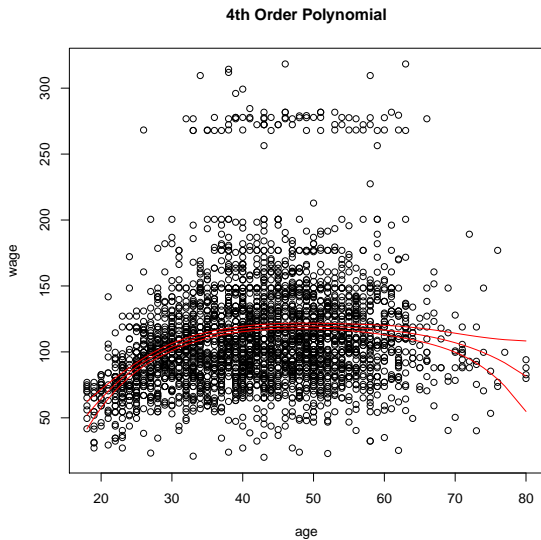
```
> summary(lm(wage ~ poly(age,4),data=Wage))
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	111.7036	0.7287	153.283	< 2e-16	***
poly(age, 4)1	447.0679	39.9148	11.201	< 2e-16	***
poly(age, 4)2	-478.3158	39.9148	-11.983	< 2e-16	***
poly(age, 4)3	125.5217	39.9148	3.145	0.00168	**
poly(age, 4)4	-77.9112	39.9148	-1.952	0.05104	.

Residual standard error: 39.91 on 2995 degrees of freedom
Multiple R-squared: 0.08626, Adjusted R-squared: 0.0850
F-statistic: 70.69 on 4 and 2995 DF, p-value: < 2.2e-16

Fitted Values



Problems

- ▶ Higher order terms may be needed to fit data globally

Problems

- ▶ Higher order terms may be needed to fit data globally
- ▶ generally do not go above 3rd order or 4th order polynomial - may be too flexible

Problems

- ▶ Higher order terms may be needed to fit data globally
- ▶ generally do not go above 3rd order or 4th order polynomial - may be too flexible
- ▶ fit piece-wise polynomials over different ranges

Problems

- ▶ Higher order terms may be needed to fit data globally
- ▶ generally do not go above 3rd order or 4th order polynomial - may be too flexible
- ▶ fit piece-wise polynomials over different ranges
- ▶ is function continuous where they join?

Problems

- ▶ Higher order terms may be needed to fit data globally
- ▶ generally do not go above 3rd order or 4th order polynomial - may be too flexible
- ▶ fit piece-wise polynomials over different ranges
- ▶ is function continuous where they join?
- ▶ is function differentiable where they join?

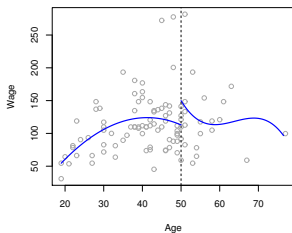
Problems

- ▶ Higher order terms may be needed to fit data globally
- ▶ generally do not go above 3rd order or 4th order polynomial - may be too flexible
- ▶ fit piece-wise polynomials over different ranges
- ▶ is function continuous where they join?
- ▶ is function differentiable where they join?

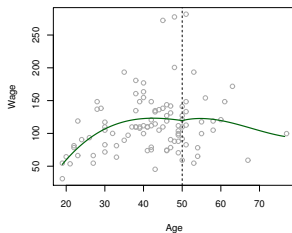
Add constraints - lose degrees of freedom

Piecewise Polynomials

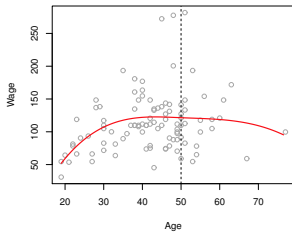
Piecewise Cubic



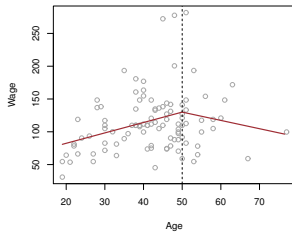
Continuous Piecewise Cubic



Cubic Spline



Linear Spline



Spline Basis

Alternative way to represent the model so that we have continuity, continuous first and second derivatives is

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + h(x_i, \xi) \beta_4 + \epsilon_i$$

where ξ is a “knot” in a truncated cubic basis function

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

Spline Basis

Alternative way to represent the model so that we have continuity, continuous first and second derivatives is

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + h(x_i, \xi) \beta_4 + \epsilon_i$$

where ξ is a “knot” in a truncated cubic basis function

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

We can add additional terms that each with 1 degree of freedom

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \sum_k^K h(x_i, \xi_k) \beta_4 + \epsilon_i$$

Spline Basis

Alternative way to represent the model so that we have continuity, continuous first and second derivatives is

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + h(x_i, \xi) \beta_4 + \epsilon_i$$

where ξ is a “knot” in a truncated cubic basis function

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

We can add additional terms that each with 1 degree of freedom

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \sum_k^K h(x_i, \xi_k) \beta_4 + \epsilon_i$$

Splines

- ▶ B-splines (reduces multicollinearity between terms from truncated basis) `splines` package in R to use `bs(x)` to construct basis

Splines

- ▶ B-splines (reduces multicollinearity between terms from truncated basis) `splines` package in R to use `bs(x)` to construct basis
- ▶ natural splines (add more constraints so that function is linear outside range of data)

Splines

- ▶ B-splines (reduces multicollinearity between terms from truncated basis) `splines` package in R to use `bs(x)` to construct basis
- ▶ natural splines (add more constraints so that function is linear outside range of data)
- ▶ smoothing splines

Splines

- ▶ B-splines (reduces multicollinearity between terms from truncated basis) `splines` package in R to use `bs(x)` to construct basis
- ▶ natural splines (add more constraints so that function is linear outside range of data)
- ▶ smoothing splines

Choice of knots and/or degrees of freedom?

Splines

- ▶ B-splines (reduces multicollinearity between terms from truncated basis) `splines` package in R to use `bs(x)` to construct basis
- ▶ natural splines (add more constraints so that function is linear outside range of data)
- ▶ smoothing splines

Choice of knots and/or degrees of freedom? Smoothing splines place a knot at each data point, but adds a penalty to prevent over-fitting:

$$\sum (Y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

Splines

- ▶ B-splines (reduces multicollinearity between terms from truncated basis) `splines` package in R to use `bs(x)` to construct basis
- ▶ natural splines (add more constraints so that function is linear outside range of data)
- ▶ smoothing splines

Choice of knots and/or degrees of freedom? Smoothing splines place a knot at each data point, but adds a penalty to prevent over-fitting:

$$\sum (Y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

This can be reformulated as a Bayesian model with a Gaussian g-prior. packages use LOOCV or GCV to choose λ

Fitting GAMs in R

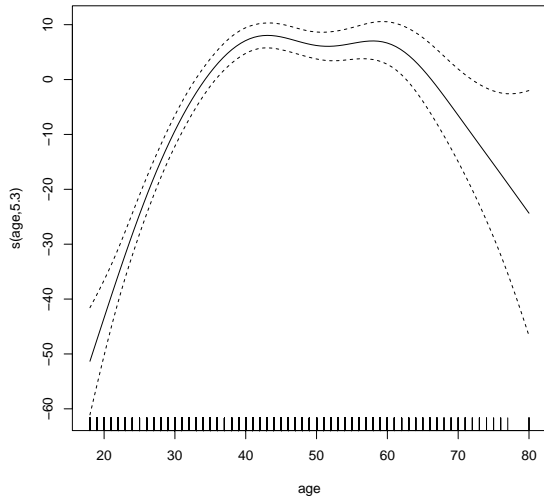
```
> wage.gam = gam(wage ~ s(age), data=Wage)
> summary(wage.gam)
Parametric coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) 111.7036      0.7282   153.4   <2e-16 ***

Approximate significance of smooth terms:
              edf Ref.df      F p-value
s(age) 5.298   6.399 44.34   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1 1

R-sq.(adj) = 0.0864   Deviance explained = 8.8%
GCV = 1594.2   Scale est. = 1590.9      n = 3000
```

Fitted Curve

```
plot(wage.gam, rug=T)
```



More terms

```
> wage.gam2 = gam(wage ~ s(year,k=7) + s(age), data=Wage)
> summary(wage.gam2)
```

Parametric coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	111.7036	0.7266	153.7	<2e-16 ***

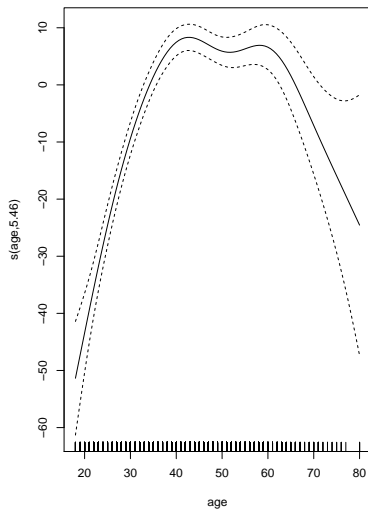
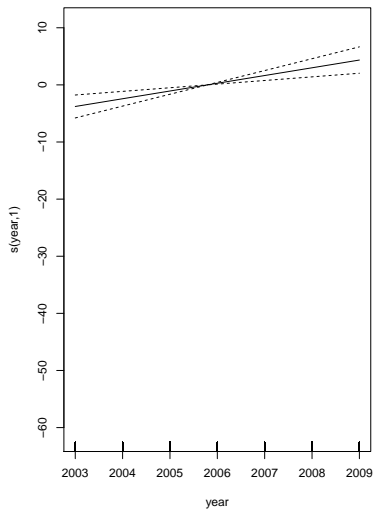
Approximate significance of smooth terms:

	edf	Ref.df	F	p-value
s(year)	1.000	1.000	14.18	0.000169 ***
s(age)	5.462	6.568	43.37	< 2e-16 ***

R-sq.(adj) = 0.0905 Deviance explained = 9.24%

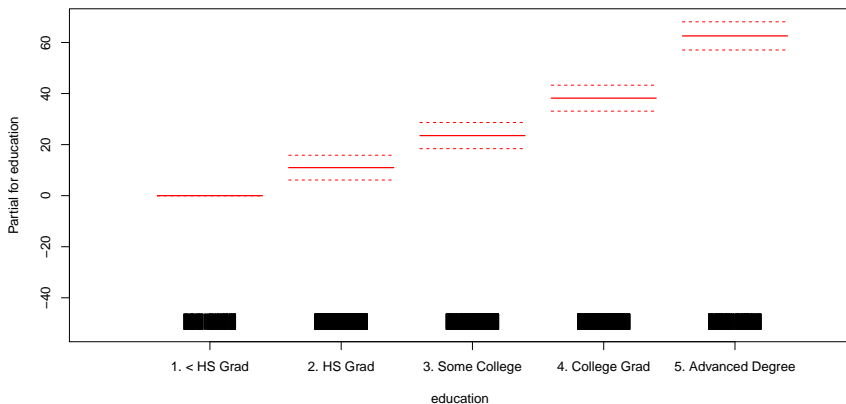
GCV = 1587.7 Scale est. = 1583.7 n = 3000

Year and Age Smooth fits



Showing Factors

```
wage.gam3 = gam(wage ~ s(year,k=7) + s(age) + education,  
                 data=Wage)  
termplot(wage.gam3, se=T, rug=T, ask=F, col.se=2)
```



Summary

GAMS:

- ▶ Allow flexible non-linear functions of predictors. Do not need to try various transformations or polynomials to capture relationships

Summary

GAMS:

- ▶ Allow flexible non-linear functions of predictors. Do not need to try various transformations or polynomials to capture relationships
- ▶ May be used to suggest parametric models (i.e linear or quadratic may be fine)

Summary

GAMS:

- ▶ Allow flexible non-linear functions of predictors. Do not need to try various transformations or polynomials to capture relationships
- ▶ May be used to suggest parametric models (i.e linear or quadratic may be fine)
- ▶ nonlinear functions can extend to multiple predictors for interactions, but soon run into curse of dimensionality

Summary

GAMS:

- ▶ Allow flexible non-linear functions of predictors. Do not need to try various transformations or polynomials to capture relationships
- ▶ May be used to suggest parametric models (i.e linear or quadratic may be fine)
- ▶ nonlinear functions can extend to multiple predictors for interactions, but soon run into curse of dimensionality
- ▶ Nonlinear fits can lead to improved prediction

Summary

GAMS:

- ▶ Allow flexible non-linear functions of predictors. Do not need to try various transformations or polynomials to capture relationships
- ▶ May be used to suggest parametric models (i.e linear or quadratic may be fine)
- ▶ nonlinear functions can extend to multiple predictors for interactions, but soon run into curse of dimensionality
- ▶ Nonlinear fits can lead to improved prediction
- ▶ Additive functions may be more interpretable