Linear Regression Models
P8111

Lecture 18

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Columbia University
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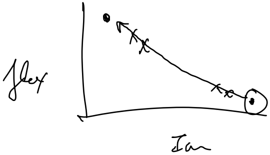
Today's Lecture

$$E(y|x) = f(x)$$

- Additive models
- Case study

Recall the goals of regression



- Estimation of $E(y|x) = f(x)$
- Prediction of future observations y given predictors x

Some methods we've seen

$E(y|x) = f(x)$

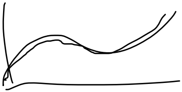
1 continuous x

Int, not flex

- Simple linear regression
- Polynomial regression
- Spline models
- Penalized spline regression
- Non-parametric models

flex not int

Piecewise linear



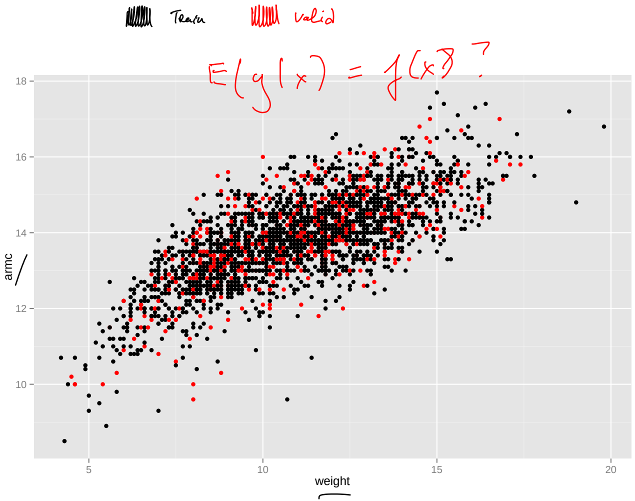
mult x; bin/categorical

- MLR
- Poly
- Interaction

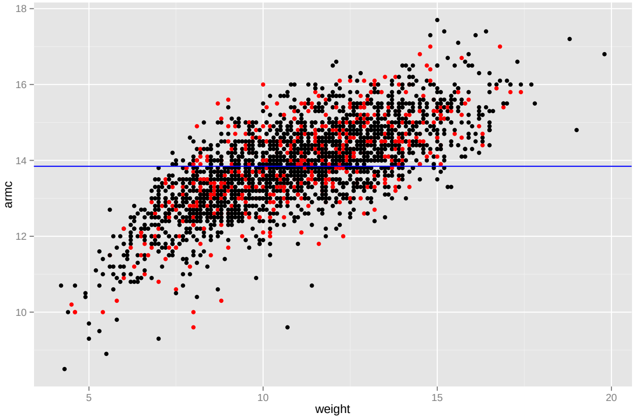
Example

- Arm circumference vs. weight
- How should we / can we estimate this?
  - Any of the above methods is possible
  - Which is “best” is a combination of inference, prediction, and model goals

Example

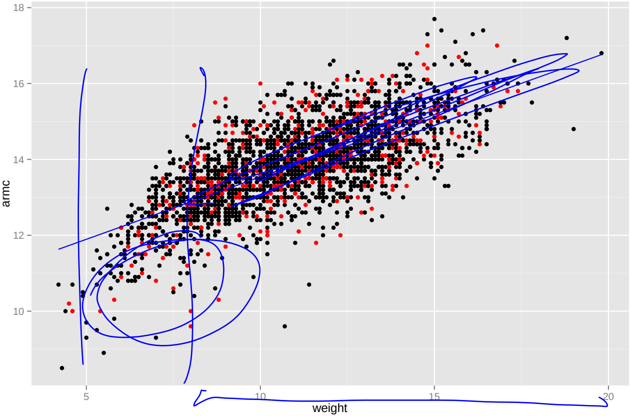


Example



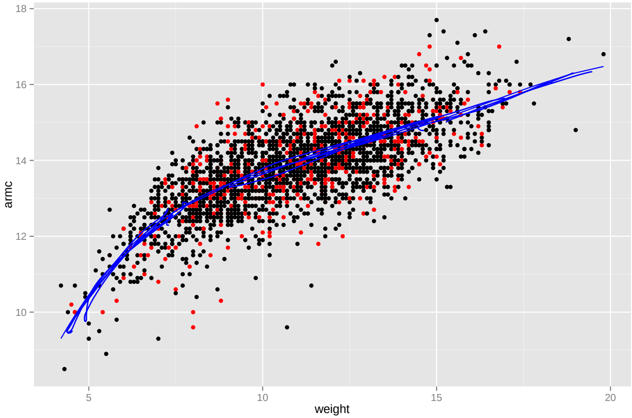
Example

SLR



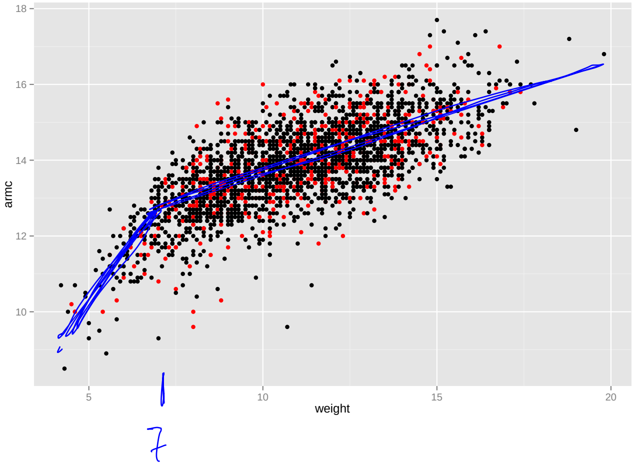
Example

Poly deg 4



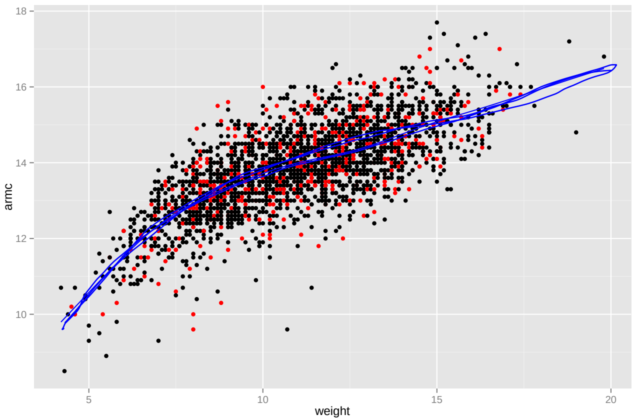
Example

PWL



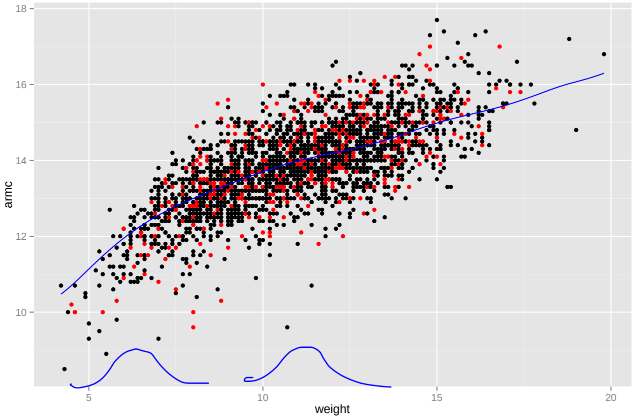
Example

Pen Splines (λ chos by CV)

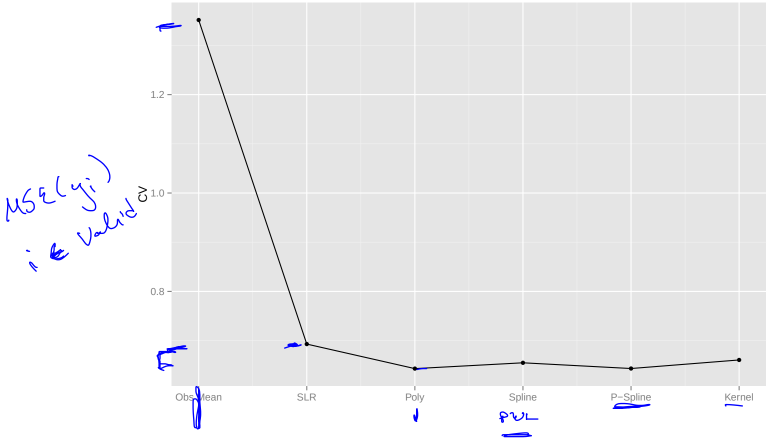


Example

Non-parametric (bw chosen by CV)



Example



cv
1.2
1.0
0.8
Obs Mean
SLR
Poly
Spline
P−Spline
Kernel
MSE(yi)
is valid
PWL

Example

So which one is best?

1 vote poly Flex / smooth

1 vote PWL Int

0 votes Pen Splines :(

~~SLR~~ Other fine

Additive models

- For scatterplot smoothing, we've focused on a single predictor
- Most real examples have multiple predictors
- Non-linearity can arise in any variable, or in multiple variables
- Previously we have addressed this using polynomials in MLRs

Additive models

Additive models are a very general framework for addressing non-linearity

- Given p predictors, the additive model is

$$\mathrm{E}[y|x_1, \ldots, x_p] = f(x_1, \ldots, x_p) = \beta_0 + \sum_{k=1}^{p} f(x_k) \tag{1}$$

- Each $f(\cdot)$ is a smooth function (can be a line)

Additive models

Additive models are a very general framework for addressing non-linearity

- In theory, each smooth function can be estimated in a variety of ways
  - Polynomials, splines, penalized splines, kernel smoothers, etc
- In practice, penalized splines is a pretty unified framework for fitting additive models
- Quick note – the intercept is not identifiable ...

$$(\beta_0 + c) + (g_1(x_1) - c)$$

How estimation might go ...

$$\min_{\underset{\sim}{\beta_1},\, \underset{\sim}{\beta_2}} RSS(\beta) + \underline{\lambda_1} Pen(\underset{\sim}{\beta_1}) + \underline{\lambda_2} Pen(\underset{\sim}{\beta_2})$$

$$\underset{\sim}{\beta_1} \to f_1(x_1) \qquad \underset{\sim}{\beta_2} \to f_2(x_2)$$

$$CV(\lambda_1, \lambda_2)$$

Backfitting

≃ Coordinate Descent

Backfitting is a more algorithmic method for estimating model parameters

- Start out by setting $f(x_k) = 0$ for all k
- Initialize $\hat{\beta}_0 = \bar{y}$
- Iterate the follow steps until convergence:
  - For each $f(x_k)$ in turn, estimate

$$f(x_k) = \text{smooth}\underbrace{(y - \hat{\beta}_0 - \sum_{k' \neq k} f(x_{k'}))}\tag{2}$$

  - Center each $f(x_k)$

Additive models vs MLR

- Additive models generalize the idea of including polynomial terms in an MLR
- Of course, there are tradeoffs ...
  - On the plus side:

    flexible

  - On the minus side:

    not easily interpretable

Additive models example

Continue with Nepalese children

- Looked at arm circumference vs weight
- Other variables include sex, age, height
- How can we include these other variables?

Some code notes

Fitting additive models in R:

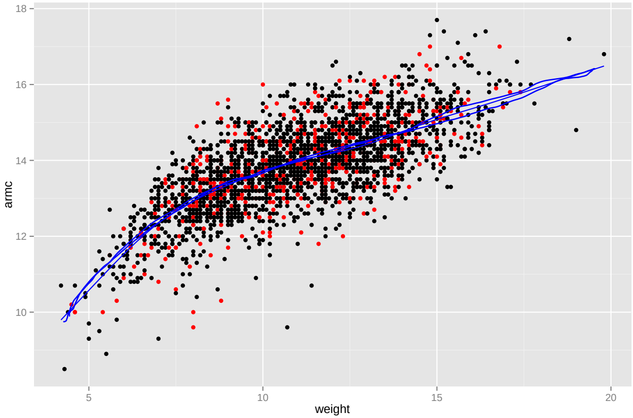
$y_i = \beta_0 + f(\text{weight}_i) + \epsilon_i$

```
library(mgcv)
fx = gam(armc ~ s(weight), data = data.train)
> summary(fx)

Family: gaussian
Link function: identity

Formula:
armc ~ s(weight)

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 13.82341    0.01472   939.3   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Approximate significance of smooth terms:
            edf Ref.df     F p-value
s(weight) 5.437  6.575 501.3  <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

R-sq.(adj) =  0.553   Deviance explained = 55.4%
GCV score = 0.57969  Scale est. = 0.57829   n = 2670
```

$S = X(X^TX + \lambda P)^{-1}X^T$

$\mathrm{tr}(S) = \mathrm{edf}$

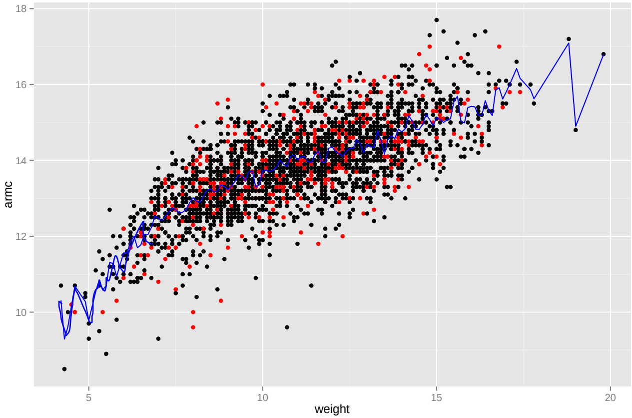
Plot



Some code notes

```
fx = gam(armc ~ s(weight, k = 100),
        data = data.train, sp = (.0001))
```

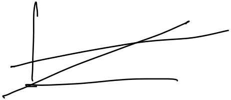
Plot



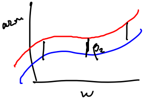
Separate boys and girls

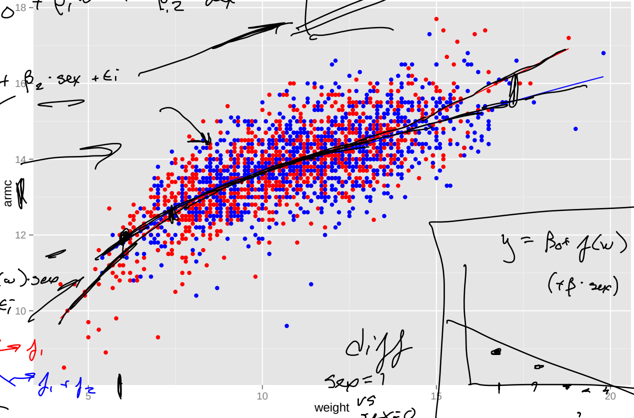
$$y = \beta_0 + \beta_1 w + \beta_2\, \text{sex} + \beta_3\, w \times \text{sex} + \epsilon_i$$

$$\beta_0 + \beta_1 w + \beta_2\, \text{sex}$$

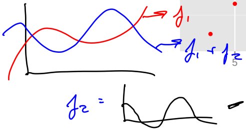


$$y = \beta_0 + f(w) + \beta_2 \cdot \text{sex} + \epsilon_i$$





$$y = \beta_0 + f_1(w) + f_2(w) \cdot \text{sex} + \epsilon_i$$



diff

sex = 1 vs sex = 0

$$y = \beta_0 + f(w) + \beta_w \cdot \text{sex} \quad (+\beta \cdot \text{sex}) \quad + \epsilon_i$$

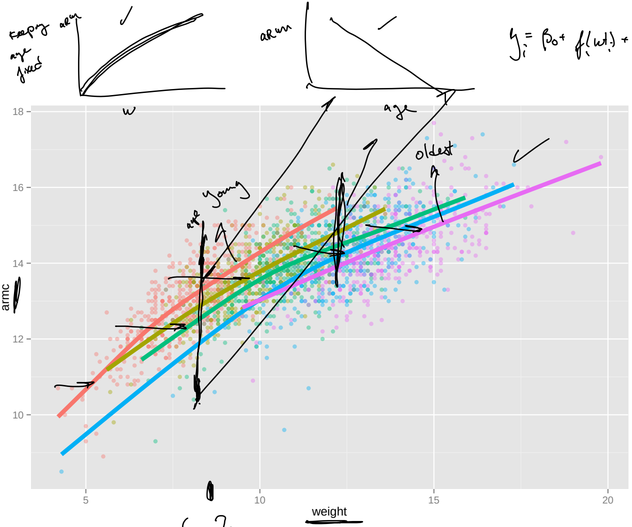
Separate boys and girls

```
> fx = gam(armc ~ sex + sex * weight + s(weight), data = data.train)
> summary(fx)

Family: gaussian
Link function: identity

Formula:
armc ~ sex + sex * weight + s(weight)

Parametric coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.497347   0.048504  10.254  < 2e-16 ***
sex         -0.374234   0.138216  -2.708  0.00682 **
weight       1.218742   0.005863 207.857  < 2e-16 ***
sex:weight   0.035782   0.012365   2.894  0.00384 **
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Approximate significance of smooth terms:
            edf Ref.df     F p-value
s(weight) 5.297  6.434 441.4  <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

R-sq.(adj) =  0.554   Deviance explained = 55.6%
GCV score = 0.57884  Scale est. = 0.57703   n = 2670
```

Separate by age

Keeping wt fix

$y_i = \beta_0 + f_1(wt_i) + f_2(age_i) + \epsilon_i$



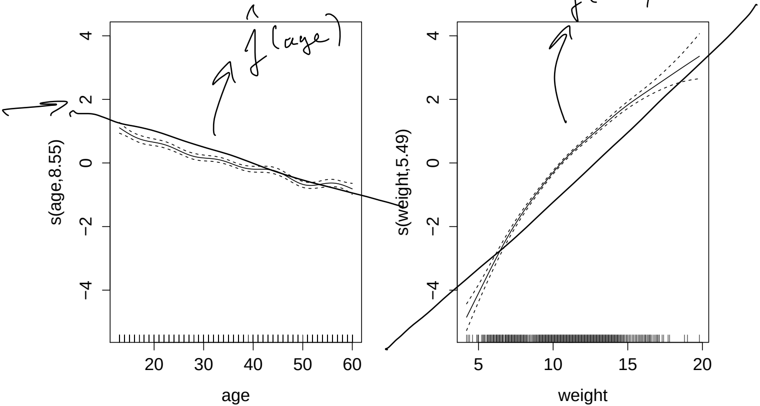
wt = 7

Separate by age

```
> fx = gam(armc ~ s(age) + s(weight), data = data.train)
> summary(fx)

Family: gaussian
Link function: identity

Formula:
armc ~ s(age) + s(weight)

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 13.82341    0.01352    1022   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Approximate significance of smooth terms:
            edf Ref.df      F p-value
s(age)    7.369  8.352  60.34  <2e-16 ***
s(weight) 4.916  6.054 487.88  <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

R-sq.(adj) =  0.623   Deviance explained = 62.5%
GCV score = 0.49054  Scale est. = 0.4881    n = 2670
```

Separate by age

plot(fx)



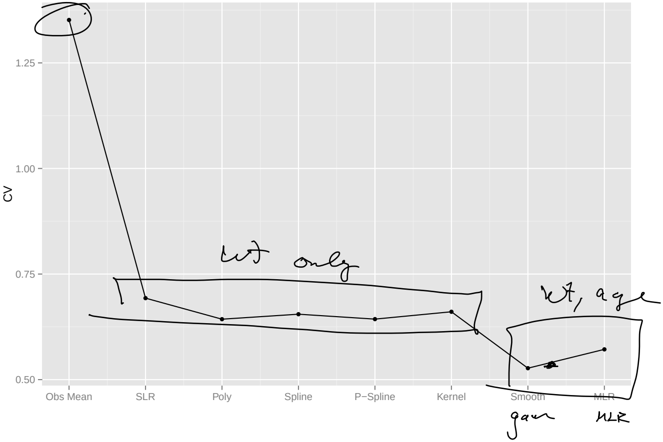
2 lines = MLR

$y_i = \beta_0 + \beta_1 wt_i + \beta_2 age_i + \epsilon_i$

For comparison

```
> fx = lm(armc ~ age + weight, data = data.train)
> summary(fx)

Call:
lm(formula = armc ~ age + weight, data = data.train)

Residuals:
    Min      1Q  Median      3Q     Max
-3.6662 -0.4746 -0.0039  0.4837  2.5447

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  9.711720   0.068146  142.51   <2e-16 ***
age         -0.037488   0.001770  -21.18   <2e-16 ***
weight       0.500365   0.009852   50.79   <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.7308 on 2667 degrees of freedom
Multiple R-squared: 0.5879, Adjusted R-squared: 0.5876
F-statistic:  1903 on 2 and 2667 DF,  p-value: < 2.2e-16
```

Final CV comparison



Today's big ideas

- Additive models
- Case study