

Linear Regression Models

P8111

Lecture 17

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THE DEPARTMENT OF
BIostatISTICS



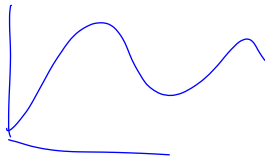
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Today's Lecture

Scatter plot smoothing

y, x

- Spline models
- Penalized spline regression



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

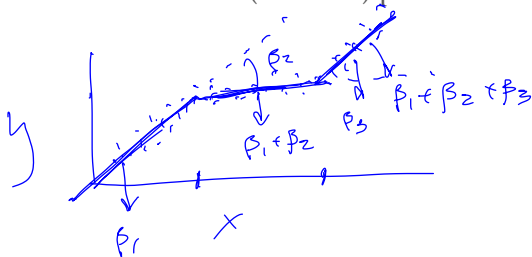
Spline models

- Last class – talked about penalized ~~splines~~ as an example of penalization, especially for bias/variance tradeoff
- Today we'll talk about spline regression more particularly

Piecewise linear models

A piecewise linear model (also called a change point model or broken stick model) contains a few linear components

- Outcome is linear over full domain, but with a different slope at different points
- Points where relationship changes are referred to as “change points” or “knots”
- Often there’s one (or a few) potential change points



Piecewise linear models

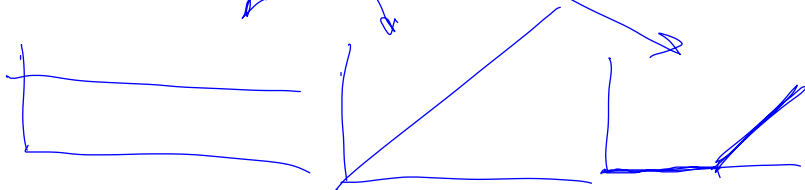
Suppose we want to estimate $E(y|x) = f(x)$ using a piecewise linear model.

- For one knot we can write this as

$$E(y|x) = \beta_0 + \beta_1 x + \beta_2 (x - \kappa)_+$$

$$\begin{cases} x - \kappa & \text{if } x > \kappa \\ 0 & \text{otherwise} \end{cases}$$

where κ is the location of the change point



Interpretation of regression coefficients

Estimation

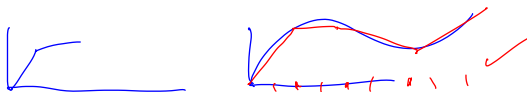
- Piecewise linear models are low-dimensional (no need for penalization)
- Parameters are estimated via OLS
- The design matrix is ...

$$\begin{bmatrix} \cdot & x_1 & 0 \\ \cdot & x_2 & 0 \\ \cdot & \vdots & 0 \\ \cdot & \vdots & x_{10} - k \\ \cdot & \vdots & \vdots \\ \cdot & x_n & x_n - k \end{bmatrix}$$

↓

$$(X^T X)^{-1} X^T y$$

Multiple knots



Suppose we want to estimate $E(y|x) = f(x)$ using a piecewise linear model.

- For multiple knots we can write this as

$$E(y|x) = \beta_0 + \beta_1 x + \sum_{k=1}^K \beta_{k+1} (x - \kappa_k)_+$$

where $\{\kappa_k\}_{k=1}^K$ are the locations of the change points

- Note that knot locations are defined before estimating regression coefficients
- Also, regression coefficients are interpreted conditional on the knots.

Piecewise quadratic and cubic models

Suppose we want to estimate $E(y|x) = f(x)$ using a piecewise quadratic model.

- For multiple knots we can write this as

$$E(y|x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \sum_{k=1}^K \beta_{k+2} (x - \kappa_k)_+^2$$

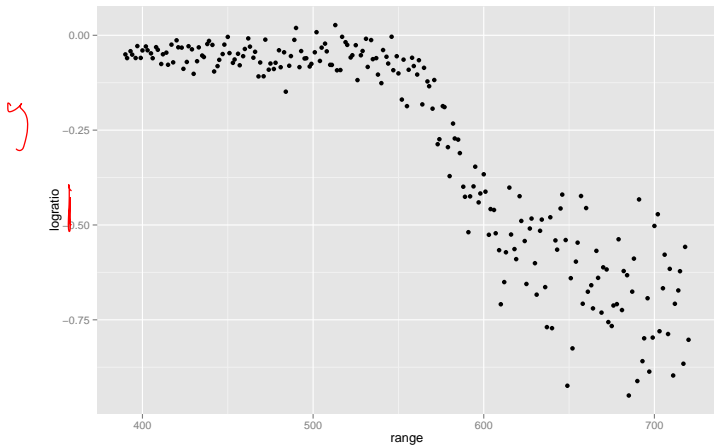
where $\{\kappa_k\}_{k=1}^K$ are the locations of the change points

- Similar extension for cubics
- Piecewise quadratic models are smooth and have continuous first derivatives

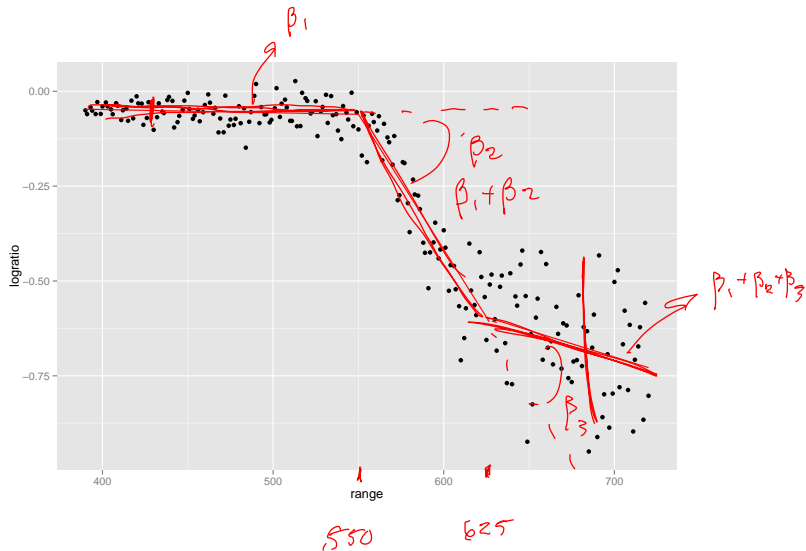
Several ways to choose the location of knots ...

Example

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



Example: piecewise linear

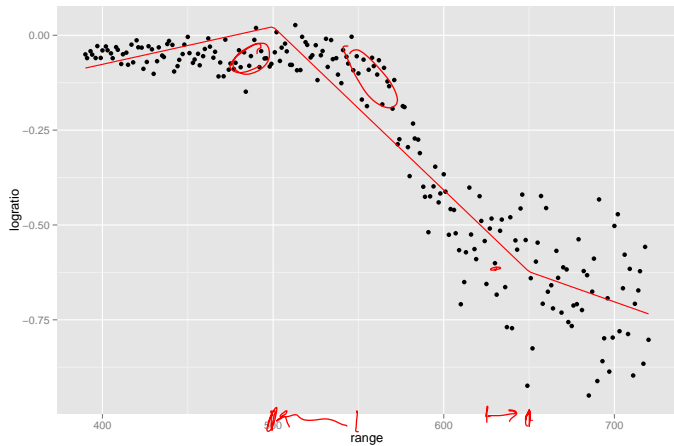


Example: piecewise linear

```
> knots <- c(550, 625)
> X.des = cbind(1, range, sapply(knots, function(k)
+               ((range - k > 0) * (range - k))))
>
> lm.lin = lm(y ~ X.des - 1)
>
> summary(lm.lin)
Coefficients:
```

	Estimate	Std. Error	t value	Pr(> t)	
β_0 X.des	-1.444e-02	6.874e-02	-0.210	0.834	
β_1 X.desrange	-8.407e-05	1.427e-04	-0.589	<u>0.556</u>	
β_2 X.des	-7.043e-03	3.834e-04	-18.368	<2e-16 ***	✓
β_3 X.des	5.723e-03	5.154e-04	11.105	<2e-16 ***	✓

Example: piecewise linear



Example: piecewise linear

```
> knots <- c(500, 650)
> X.des = cbind(1, range, sapply(knots, function(k)
+   ((range - k > 0) * (range - k))))
>
> lm.lin = lm(y ~ X.des - 1)
>
> summary(lm.lin)
Coefficients:
```

	Estimate	Std. Error	t value	Pr(> t)	
X.des	-0.4732124	0.1167565	-4.053	7.05e-05	***
X.desrange	0.0009918	0.0002533	3.915	0.000121	***
X.des	-0.0052984	0.0003695	-14.340	< 2e-16	***
X.des	0.0027191	0.0005668	4.798	2.98e-06	***

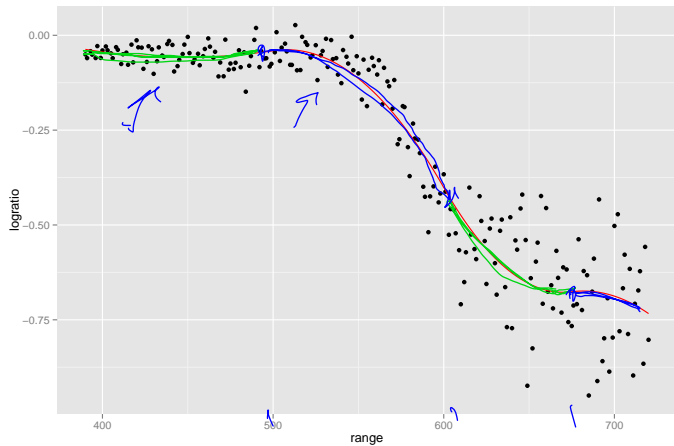
F test

LRT

- AIC }
- BIC } ✓
CV }

} Adj R²

Example: piecewise quadratic



Example: piecewise quadratic

```
> knots <- c(500, 600, 675)
> X.des = cbind(1, range, range^2, sapply(knots, function(k)
+           ((range - k > 0) * (range - k)^2)))
>
> lm.lin = lm(y ~ X.des - 1)
>
> summary(lm.lin)
```

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
X.des	1.228e+00	1.058e+00	1.160	0.2472
X.desrange	-5.749e-03	4.574e-03	-1.257	0.2101
X.des	6.424e-06	4.905e-06	1.310	0.1917
X.des	-4.923e-05	8.055e-06	-6.111	4.59e-09 ***
X.des	9.910e-05	1.012e-05	9.798	< 2e-16 ***
X.des	-9.708e-05	3.841e-05	-2.527	0.0122 *

AIC

BIC

CV

Advantages of piecewise models

Piecewise (linear, quadratic, etc) models have several advantages

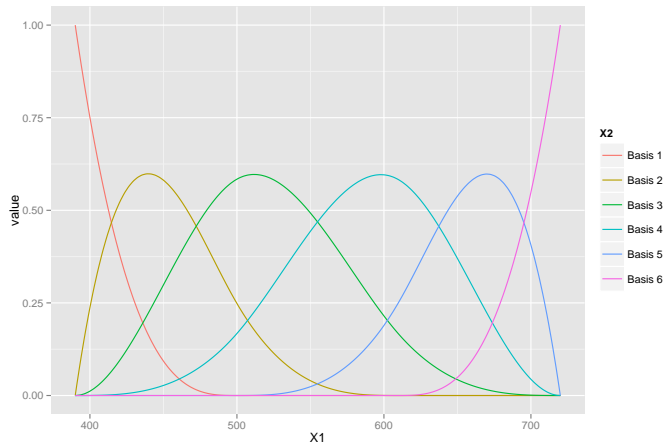
- Easy construction of basis functions
- Flexible, and don't rely on determining an appropriate form for $f(x)$ using standard functions
- Allow for significance testing on change point slopes
- Fairly direct interpretations

Other common spline models

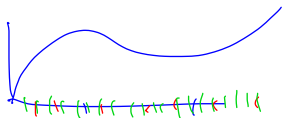
- B-splines and natural splines similarly define a basis over the domain of x
- They are made up of piecewise polynomials of a given degree, and have defined derivatives similarly to the piecewise defined functions

B-splines

Cubic B-splines



Penalized splines



- Often deciding the number and placement of knots is not straightforward
- If particular knots or associated tests are not of interest, penalization can help a lot
- It's been shown that, if one penalizes, the number and location of knots is not particularly important provided there are enough

Penalized splines

$$\text{Ridge Reg} : \min_{\beta} \left[\text{RSS}(\beta) + \lambda \text{Pen}(\beta) \right]$$

- Penalized splines are fairly common
- Recall we minimize RSS subject to a penalty; for smoothing, this penalty is often related to the second derivative of $f(x)$
- In the end, whatever penalty we use has an associated penalty matrix, and our estimates are of the form

$$\hat{\beta}_{\lambda} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{P})^{-1} \mathbf{X}^T \mathbf{y}$$

- Penalty matrix is known; λ is not

Penalized spline fits

Given $\hat{\beta}_\lambda$:

- Fitted values are given by

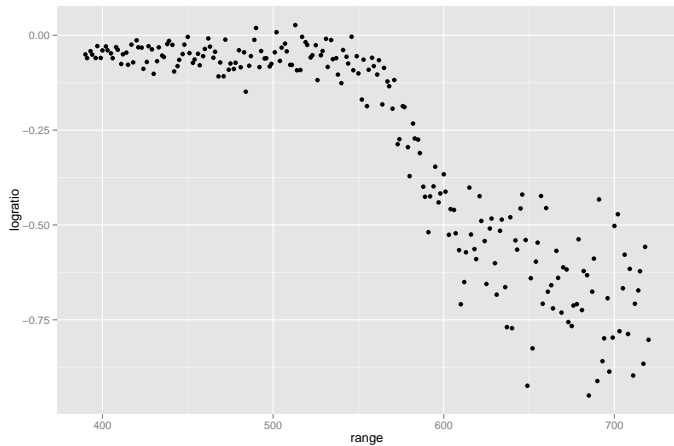
$$\begin{aligned}\hat{\mathbf{y}} &= \mathbf{X}\hat{\beta}_\lambda \\ &= \mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda P)^{-1}\mathbf{X}^T\mathbf{y}\end{aligned}$$

- The matrix $S = \mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda P)^{-1}\mathbf{X}^T$ is called the smoother matrix

Smoother matrix

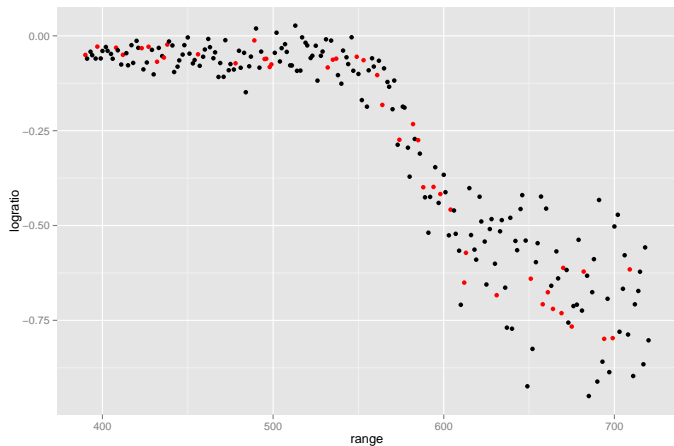
- The smoother matrix is like a hat matrix, but not quite:
 - ▶ For instance $SS \neq S$, unlike hat matrices
 - ▶ However, it gives fitted values and smooths the y 's
- Recall that $tr(\mathbf{H}) = df$ for ordinary least squares
- For smoothing, $tr(S)$ is often called the effective degrees of freedom

Example: LIDAR data



Partition data

We'll random set aside about 20% of the data as "test" data and fit our model on the remaining points



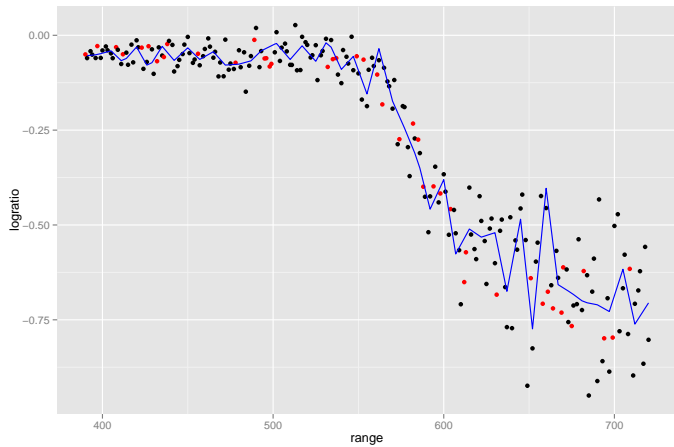
Proposed model

- Use a piecewise linear model
- Allow a lot of “break points” or knots
- (For precision, we’re using a spline model and will talk more about this when we get to scatterplot smoothing)
- Tons of flexibility in the model ... maybe even too much

Proposed model

```
> beta.lm = solve(t(X.train) %*% X.train)%*% t(X.train) %*% y.train
> as.vector(beta.lm)
 [1] -0.7072990330  0.0016678905 -0.0010621060 -0.0038462296  0.0063795230
 [6] -0.0070019621  0.0064736762 -0.0066731019  0.0084198391 -0.0068898605
[11]  0.0025832865 -0.0019203044 -0.0001653192  0.0070482441 -0.0059000564
[16]  0.0040792516 -0.0062804686  0.0166425081 -0.0272267085  0.0175451642
[21] -0.0058689652  0.0015588681 -0.0103188499  0.0250757111 -0.0299488973
[26]  0.0043359248  0.0057320047 -0.0194584632  0.0370714034 -0.0438342911
[31]  0.0321158653  0.0129884439 -0.0215919386 -0.0010528402  0.0381845809
[36] -0.0740150394  0.0675670684 -0.0380309741  0.0052680924  0.0277772008
[41] -0.0304799103  0.0155170138  0.0042768975 -0.0340085357  0.0436823108
```

Full model

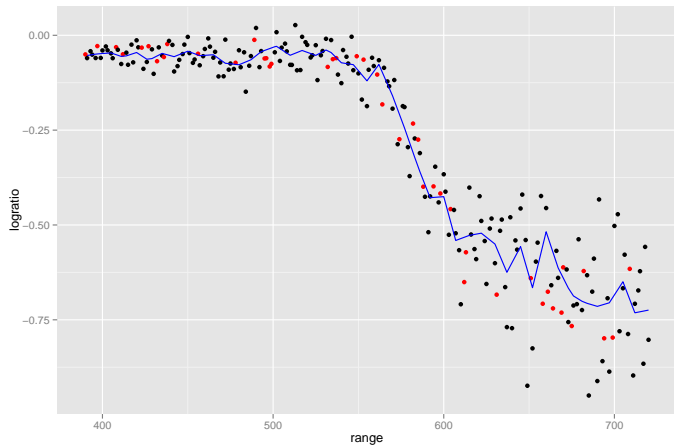


Penalized model

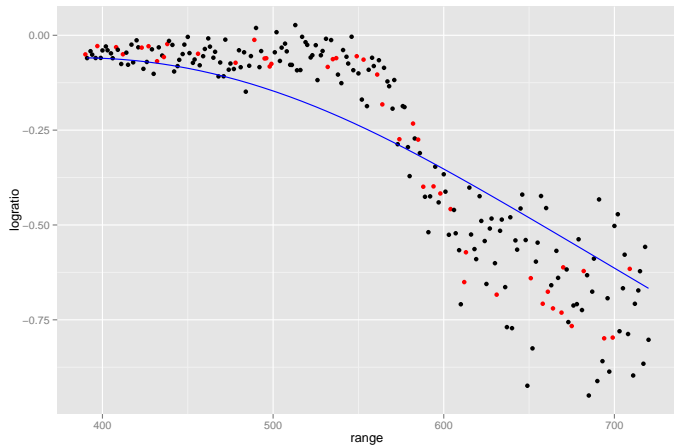
Penalization in this case can help

- Without penalization we're over-fitting, and estimates would change dramatically if we were given a different data set
- Penalization can induce “shrinkage” toward zero for the piecewise linear components
- Too much penalization will result in under-fitting ...

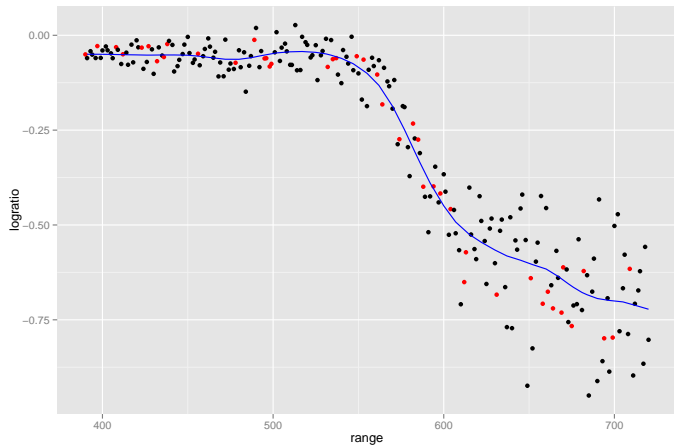
Penalized model



Penalized model



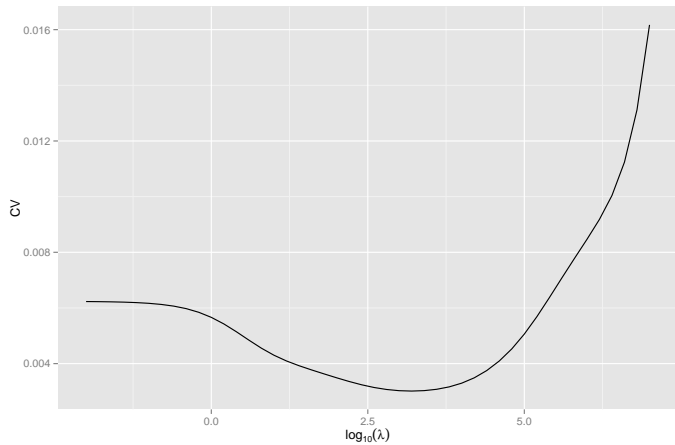
Penalized model



Comparing fits

- Visual inspection of data is useful, but maybe we should look at the validation data as a way to compare model fits
- In effect, we're asking for the impact of λ on our predictions, and trying to identify the "best" tuning parameter
- Our criterion for λ is to minimize $E(\hat{y}_{i,\lambda} - y_i)^2$

CV plot



Connection with other models

- The effects of over- and under-fitting are easiest to understand when you can see them, as in scatterplot smoothing
- These problems exist for other models, though, especially when the number of parameters is high
- In general penalization is a reasonable tool to balance variance and bias to make predictions
- Cross validation is a standard method for selecting tuning parameters

Tradeoffs for spline approaches

Penalization has some advantages and disadvantages

- Less reliant on user input for knot placement
- Overall fit is data-driven
- More complex overall model and estimation
- No interpretable change point

Non-parametric smoothing

- Spline models are parametric smoothing techniques, since

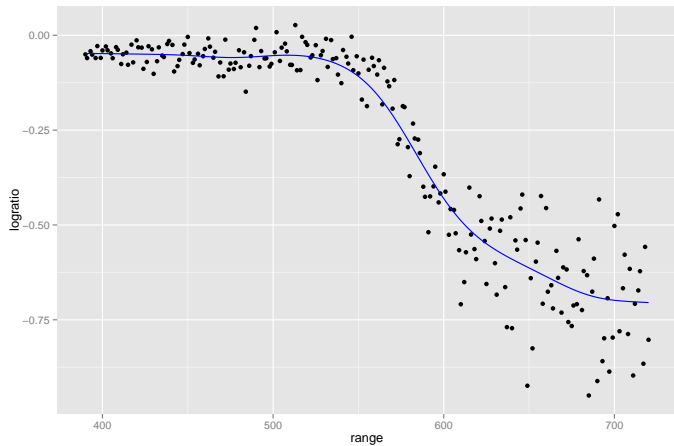
$$E(y|x) = f(x) = f(x; \beta)$$

- (Penalized regression is often called “semi-parametric” since it is an unspecified smooth function)
- There are also non-parametric smoothing approaches

Non-parametric smoothing

- A moving average is the most direct and intuitive non-parametric smoother
- To estimate $f(x_0)$, one looks at all points in a pre-defined range of x_0 and takes the average
- This is repeated for many points in the domain of x
- Can fix this up using weighted averages, where weights often depend on a “kernel” (for example, a Gaussian kernel smoother)

Example: non-parametric smoothing



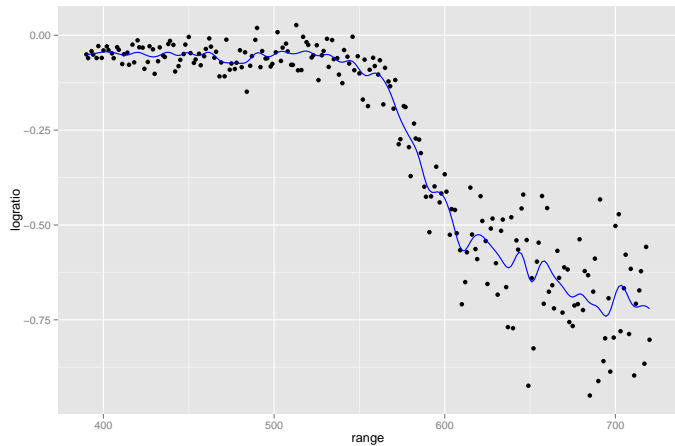
Example: Gaussian kernel smoother

```
> kern.smooth1 = ksmooth(range, y, kernel = "normal", bandwidth = 50)
```

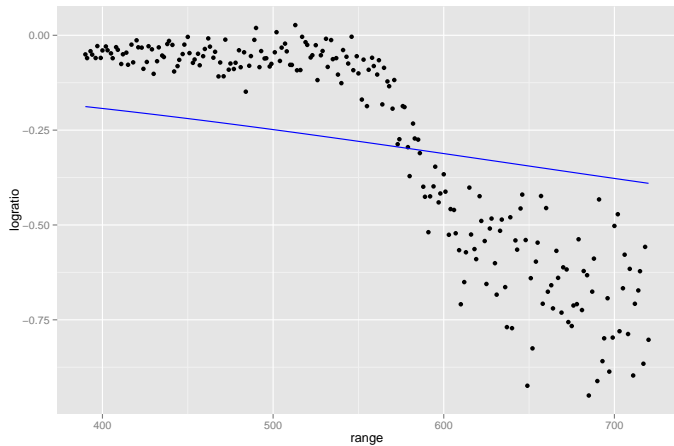

Points on non-parametric smoothing

- Non-parametric approaches are flexible and don't need model assumptions
- They also lack any interpretable distributions or parameters
- Don't avoid tuning parameters – bandwidth still has to be chosen (often via CV)

Spline models



Spline models



Today's big ideas

- Spline models
 - Penalized spline regression
 - Kernel smoothers
-