

Generalized Additive Models

David L Miller

Overview

- What is a GAM?
- What is smoothing?
- How do GAMs work?
- Fitting GAMs using `dsm`
- Model checking

What is a GAM?

”gam”

1. *Collective noun used to refer to a group of whales, or rarely also of porpoises; a pod.*
2. *(by extension) A social gathering of whalers (whaling ships).*

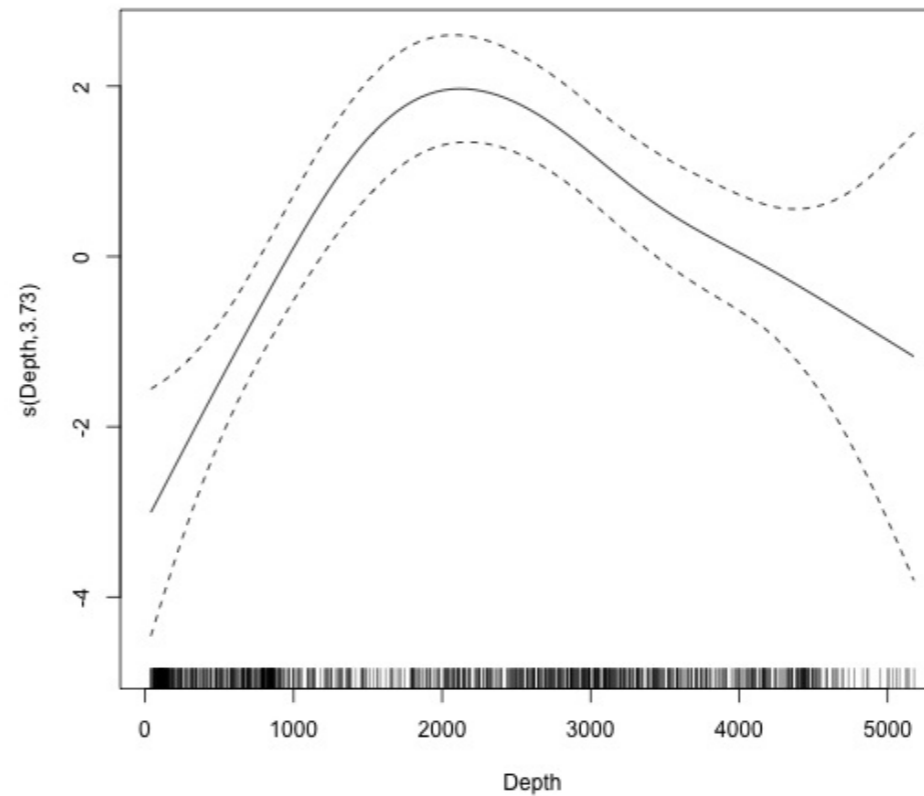
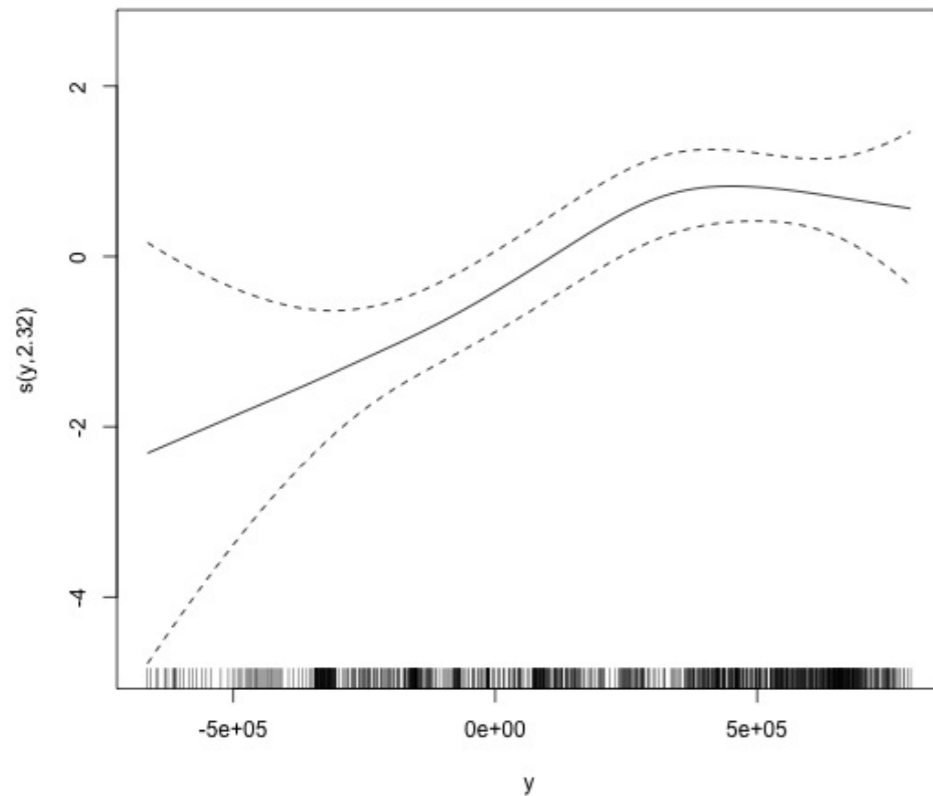
(via Natalie Kelly, CSIRO. Seen in Moby Dick.)

Generalized Additive Models

- Generalized: many response distributions
- Additive: terms **add** together
- Models: well, it's a model...

What does a model look like?

- Count n_j distributed according to some count distribution
- Model as sum of terms



Mathematically...

Taking the previous example...

$$n_j = A_j \hat{p}_j \exp \left[\beta_0 + s(y_j) + s(\text{Depth}_j) \right] + \epsilon_j$$

where $\epsilon_j \sim N(0, \sigma^2)$, $n_j \sim \text{count distribution}$

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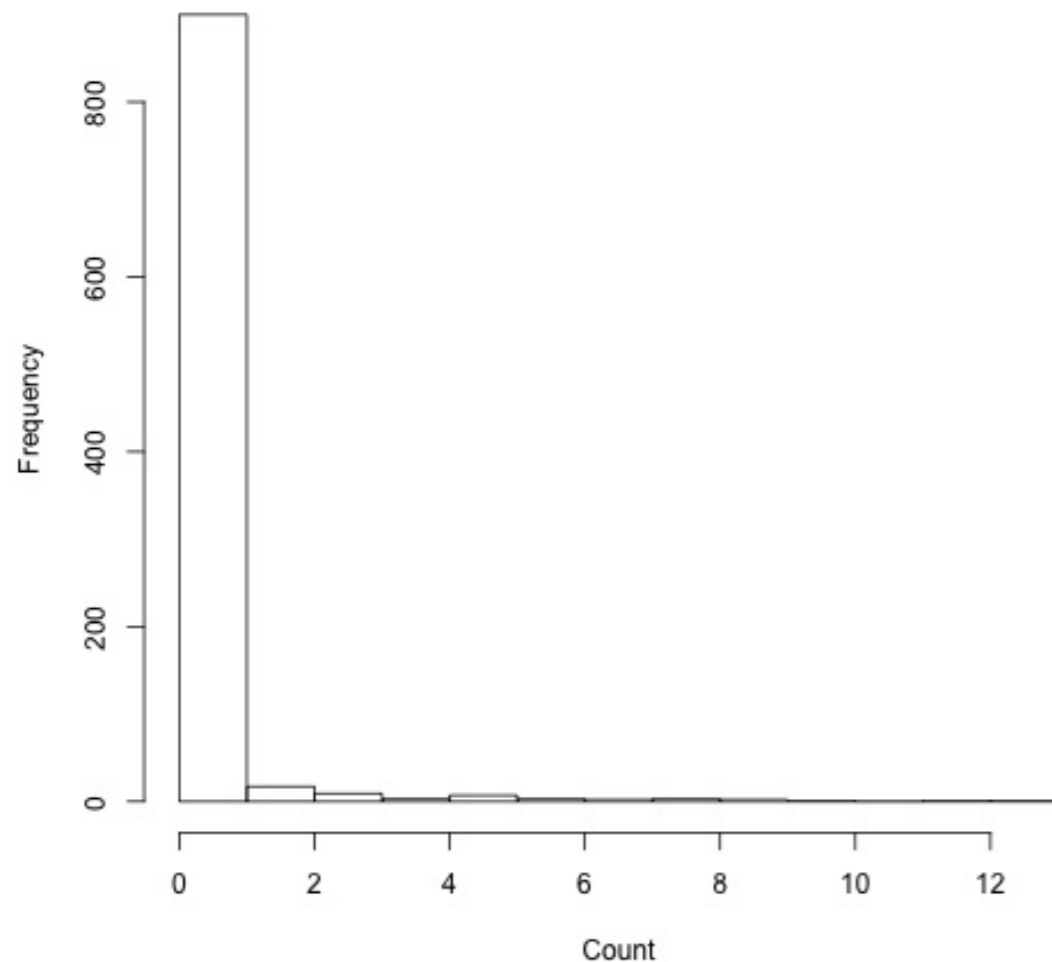
- area of segment - offset
- probability of detection in segment
- link function
- model terms

Response

$$\mathbf{n}_j = A_j \hat{p}_j \exp \left[\beta_0 + s(y_j) + s(\text{Depth}_j) \right] + \epsilon_j$$

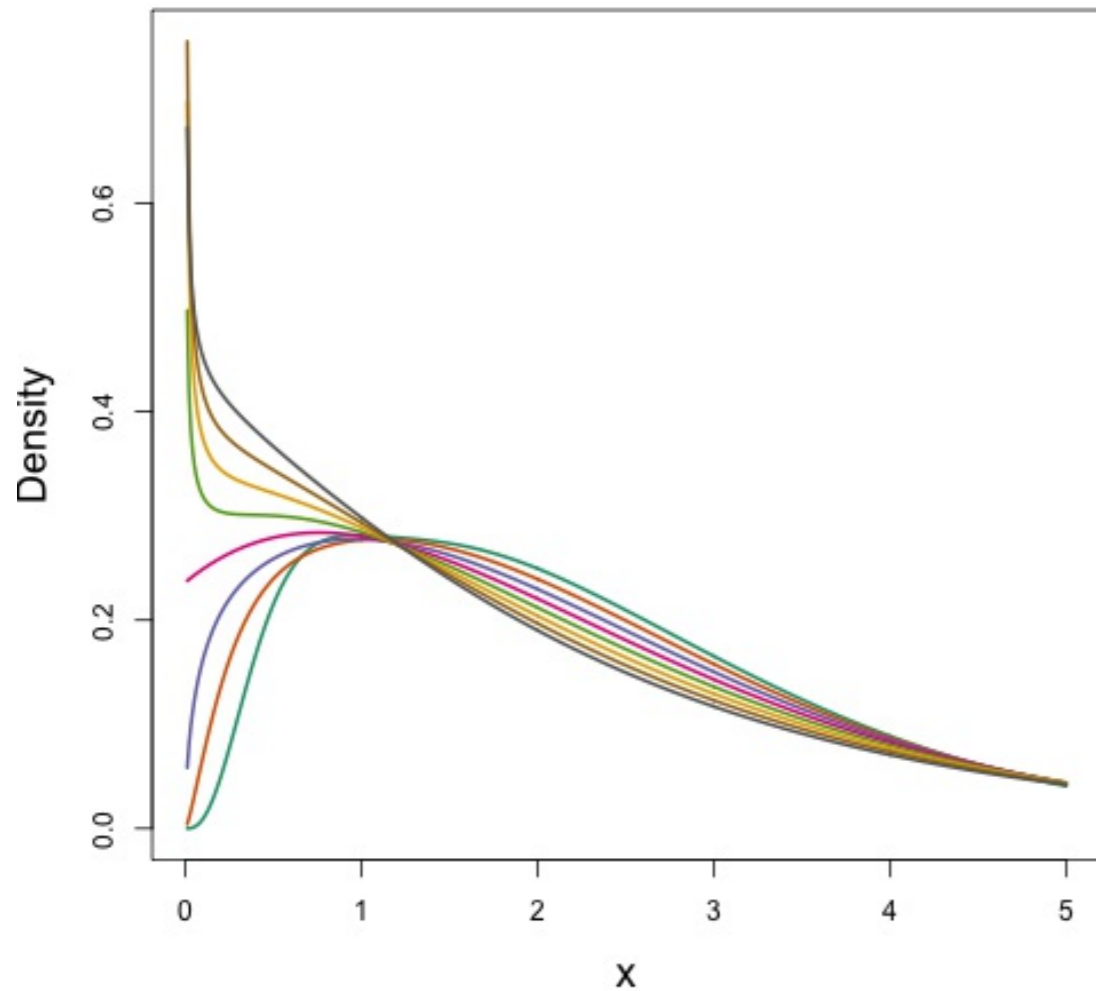
where $\epsilon_j \sim N(0, \sigma^2)$, $\mathbf{n}_j \sim$ count distribution

Count distributions



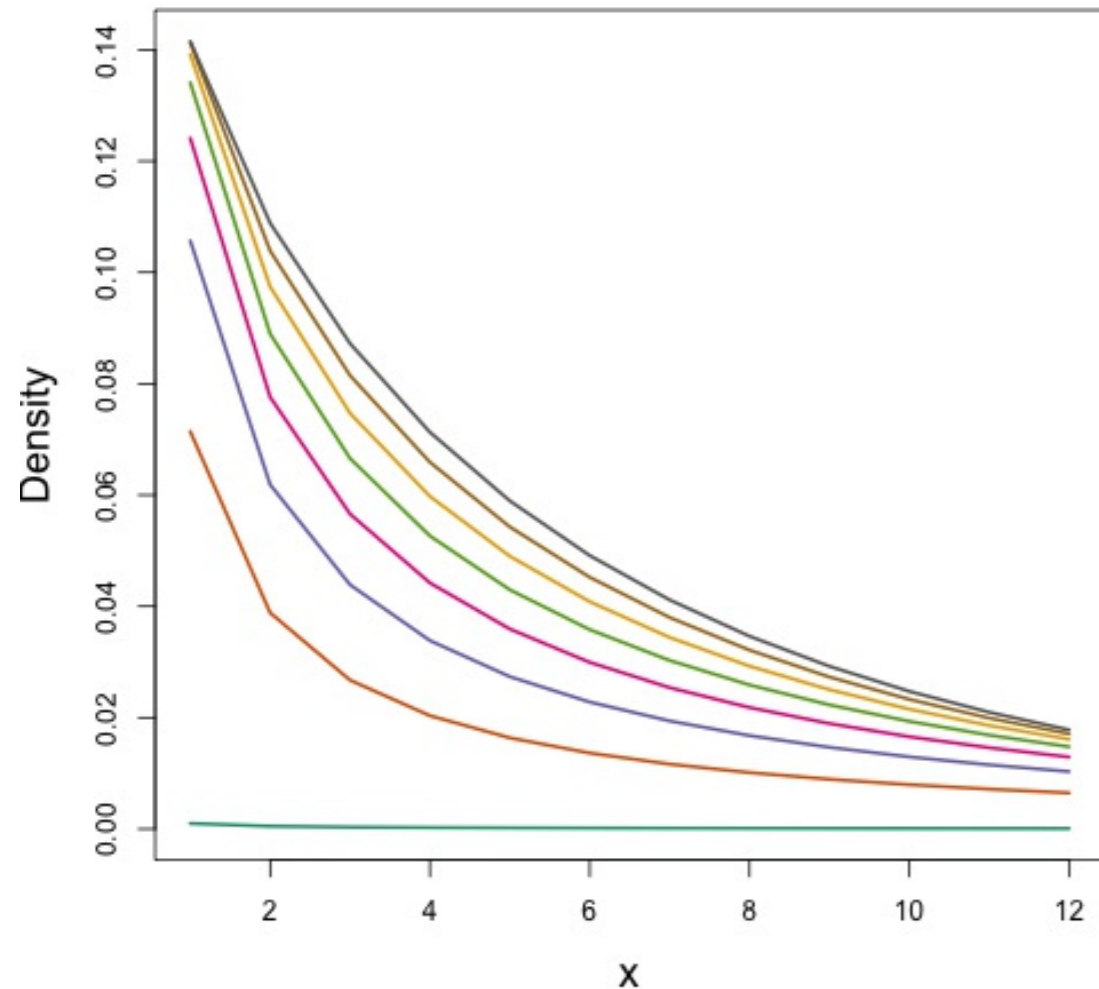
- Response is a count (not not always integer)
- Often, it's mostly zero (that's complicated)
- Want response distribution that deals with that
- Flexible mean-variance relationship

Tweedie distribution



- $\text{Var}(\text{count}) = \varphi(\text{count})^q$
- Common distributions are sub-cases:
 - $q = 1 \Rightarrow$ Poisson
 - $q = 2 \Rightarrow$ Gamma
 - $q = 3 \Rightarrow$ Normal
- We are interested in $1 < q < 2$
- (here $q = 1.2, 1.3, \dots, 1.9$)

Negative binomial



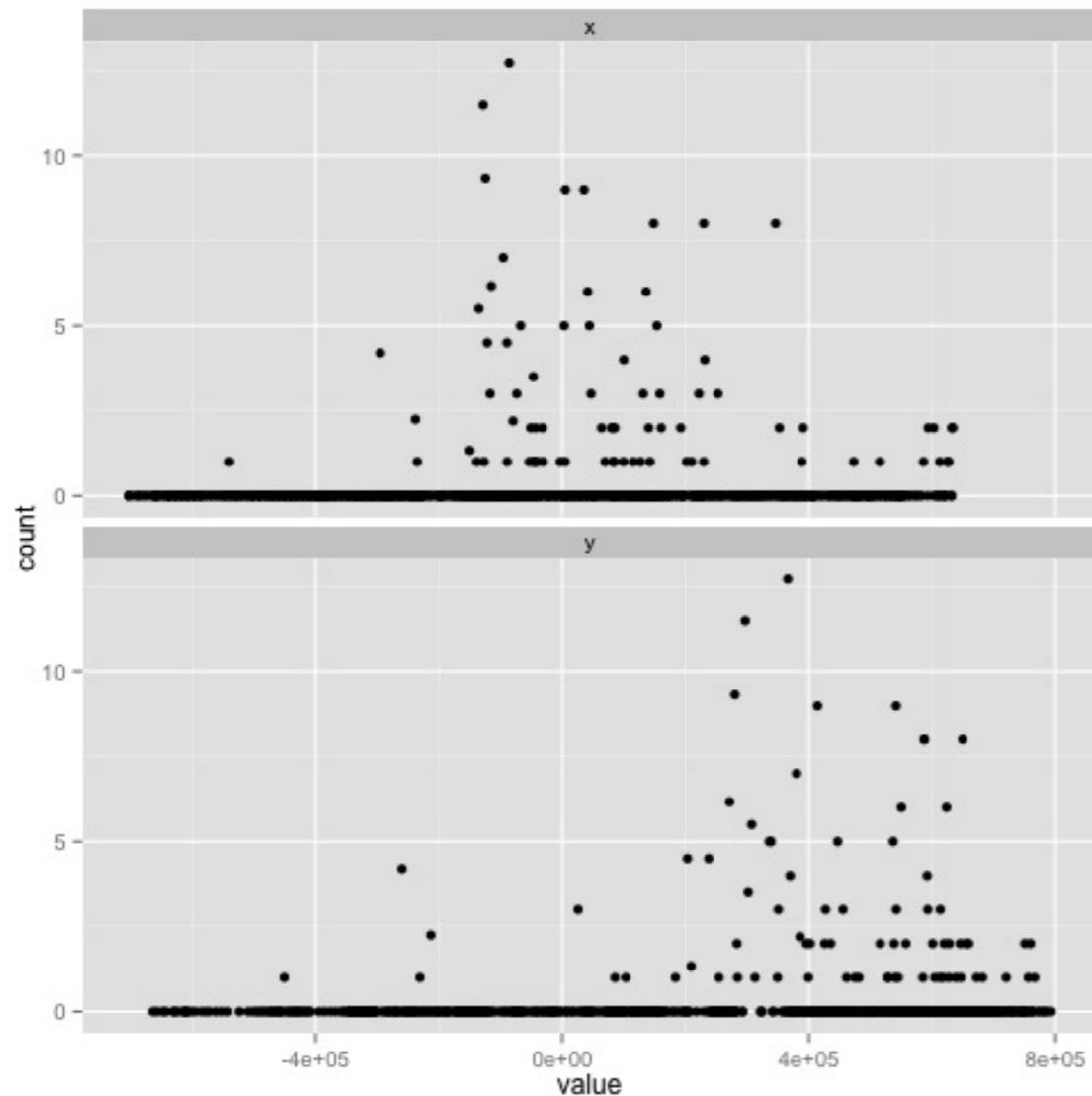
- $\text{Var}(\text{count}) = (\text{count}) + \kappa(\text{count})^2$
- Estimate κ
- Is quadratic relationship a “strong” assumption?
- Similar to Poisson:
 $\text{Var}(\text{count}) = (\text{count})$

Smooth terms

$$n_j = A_j \hat{p}_j \exp \left[\beta_0 + s(y_j) + s(\text{Depth}_j) \right] + \epsilon_j$$

where $\epsilon_j \sim N(0, \sigma^2)$, $n_j \sim$ count distribution

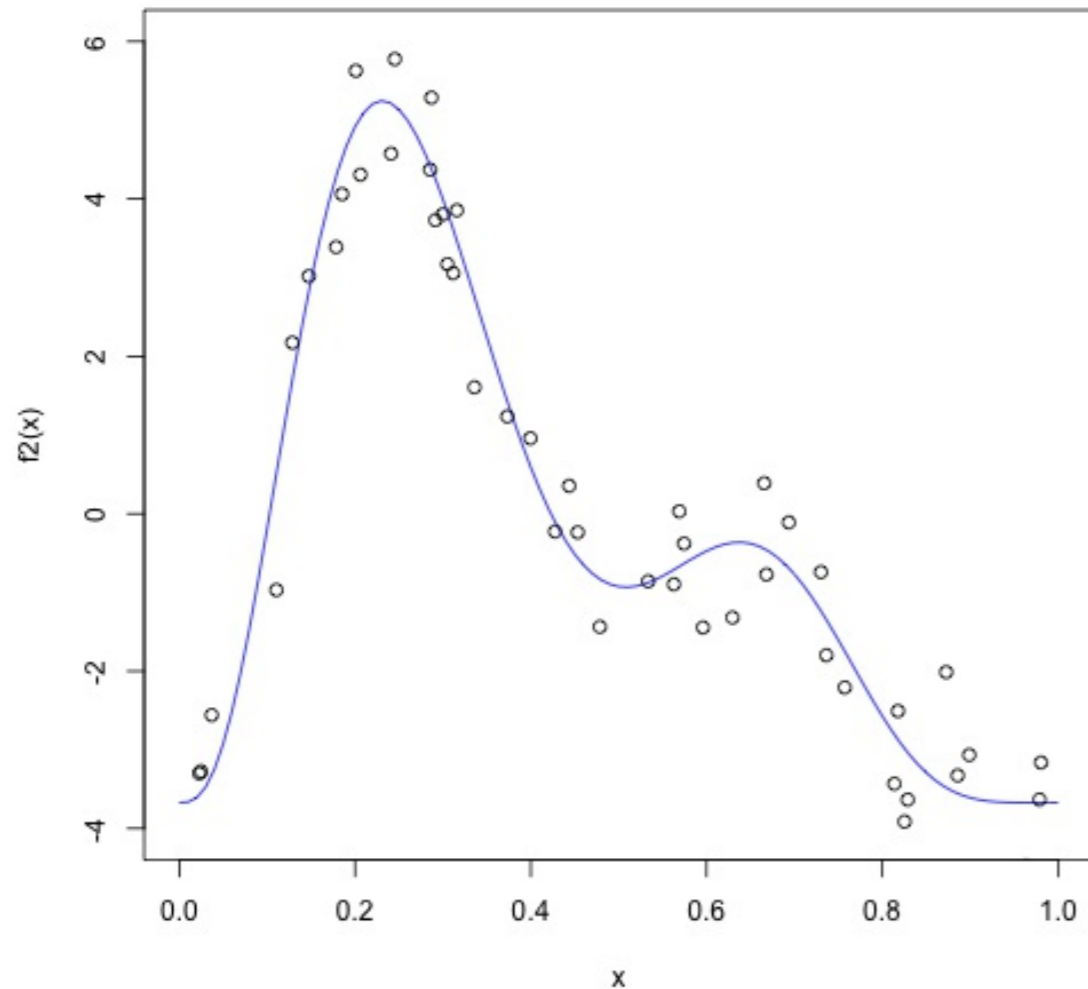
Okay, but what about these "s" things?



- Think s =**smooth**
- Want to model the covariates flexibly
- Covariates and response not necessarily linearly related!
- Want some wiggles

What is smoothing?

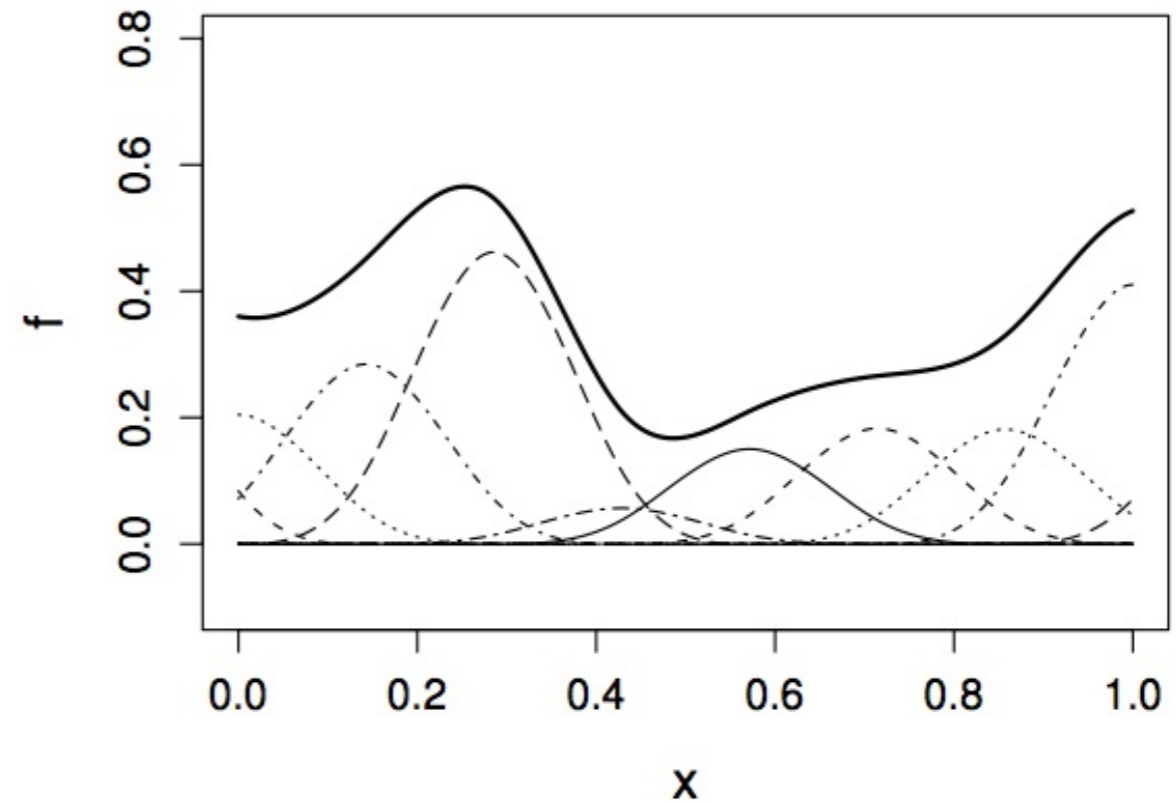
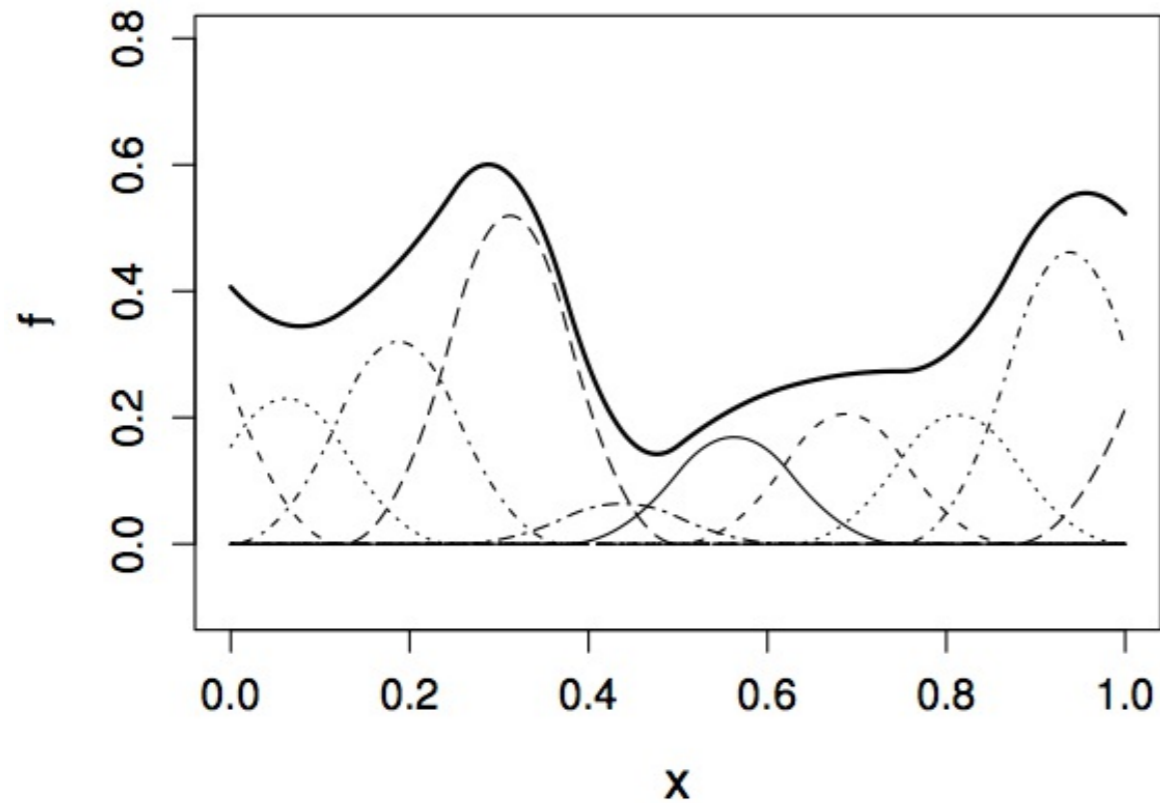
Straight lines vs. interpolation



- Want a line that is “close” to all the data
- Don't want interpolation – we know there is “error”
- Balance between interpolation and “fit”

Splines

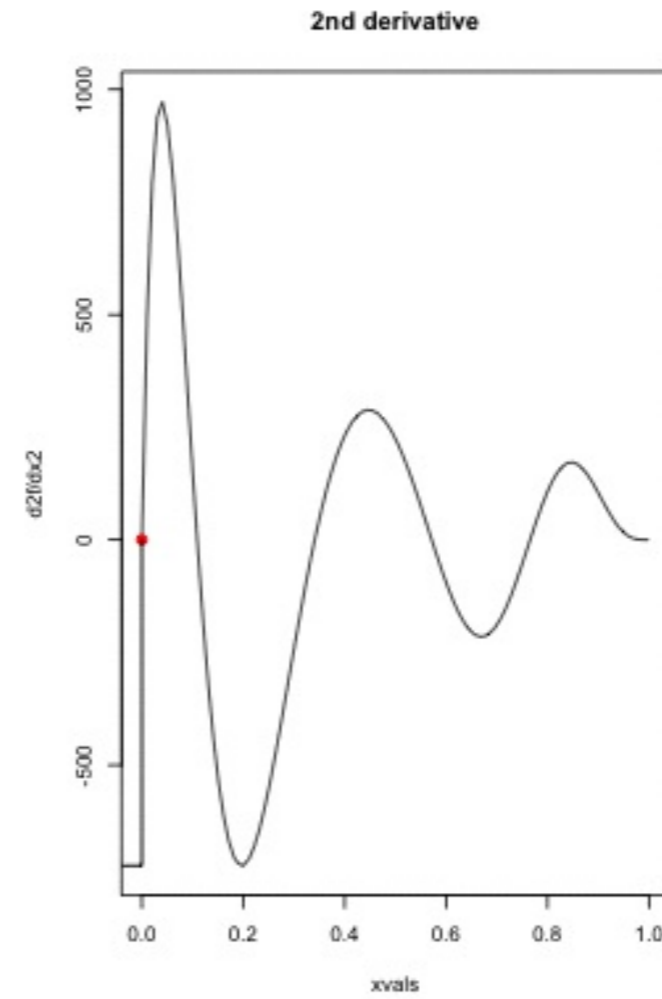
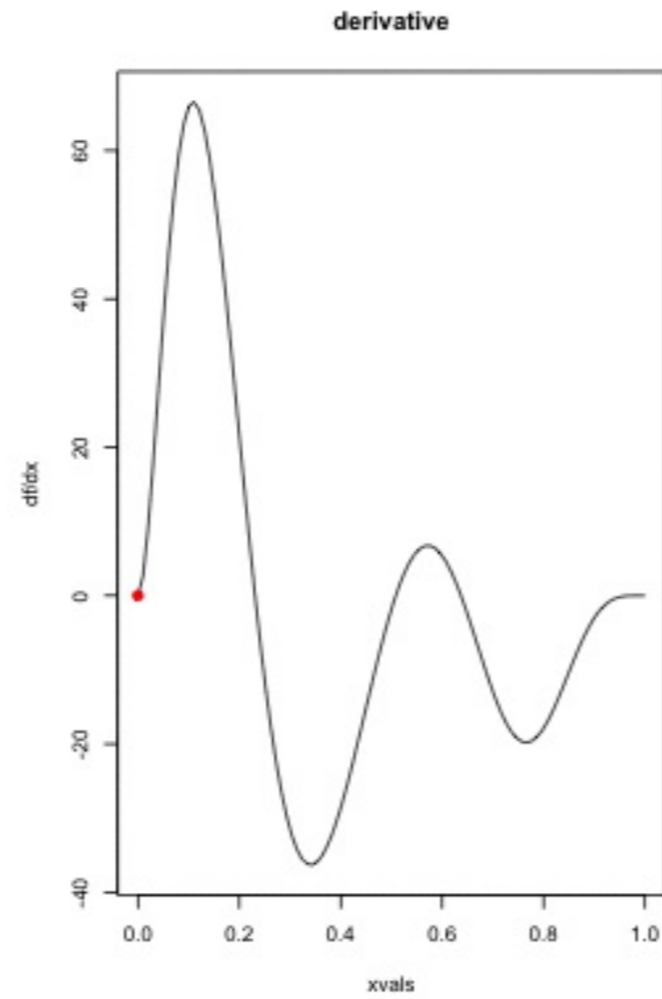
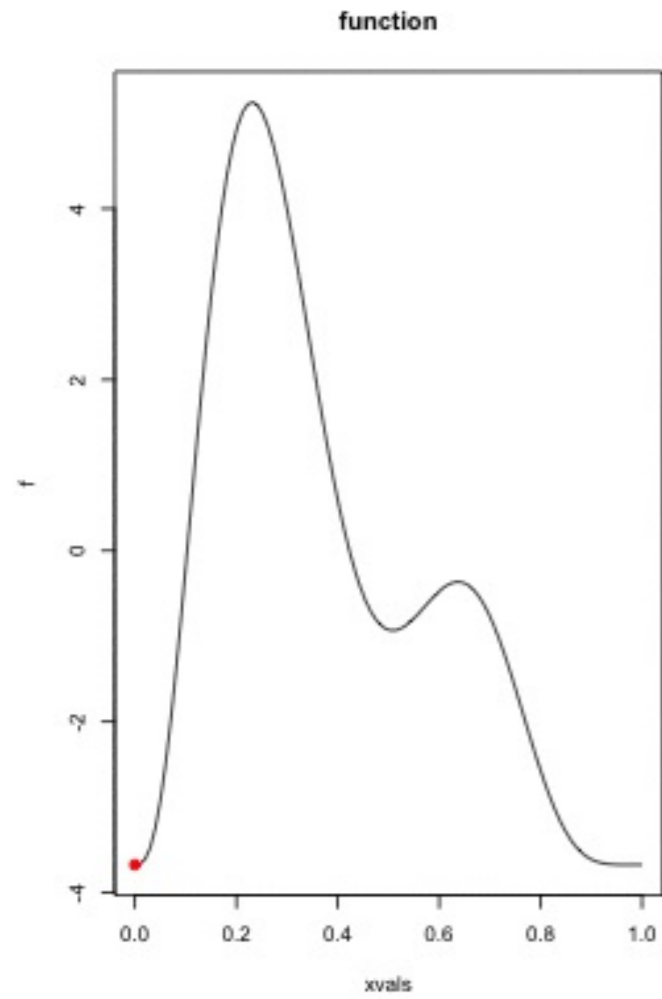
- Functions made of other, simpler functions
- **Basis functions** b_k , estimate β_k
- $s(x) = \sum_{k=1}^K \beta_k b_k(x)$
- Makes the math(s) much easier



Measuring wigglyness

- Visually:
 - Lots of wiggles == NOT SMOOTH
 - Straight line == VERY SMOOTH
- How do we do this mathematically?
 - Derivatives!
 - (Calculus *was* a useful class afterall)

Wigglyness by derivatives



Making wigglyness matter

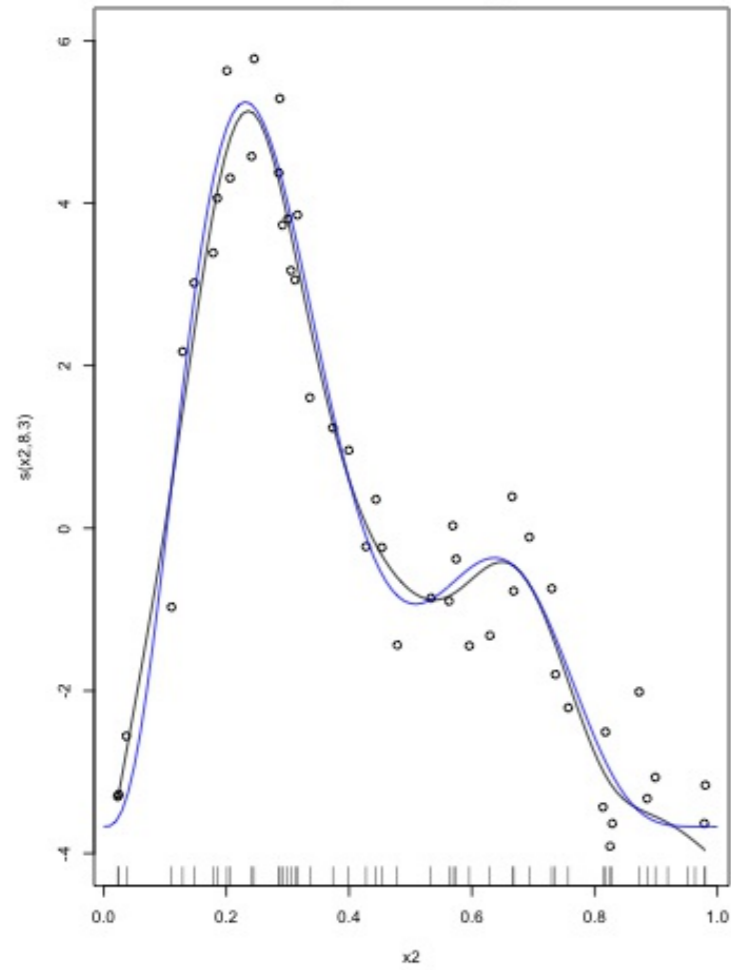
- Integration of derivative (squared) gives wigglyness
- Fit needs to be **penalised**
- **Penalty matrix** gives the wigglyness
- Estimate the β_k terms but penalise objective
 - “closeness to data” + penalty

Penalty matrix

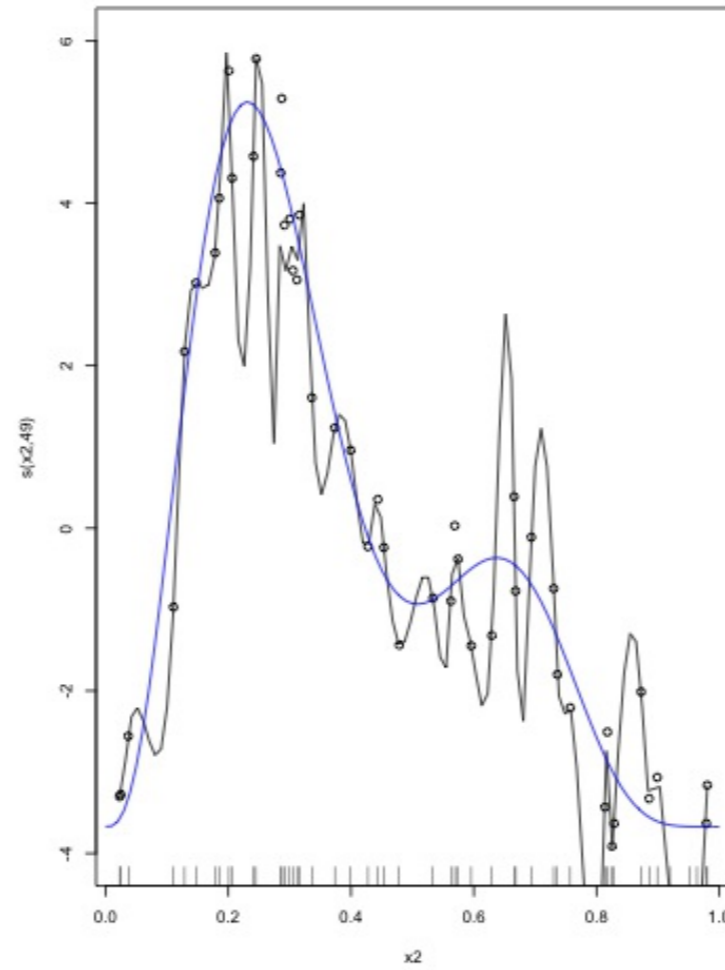
- For each b_k calculate the penalty
- Penalty is a function of β
 - $\lambda\beta^T S\beta$
- S calculated once
- smoothing parameter (λ) dictates influence

Smoothing parameter

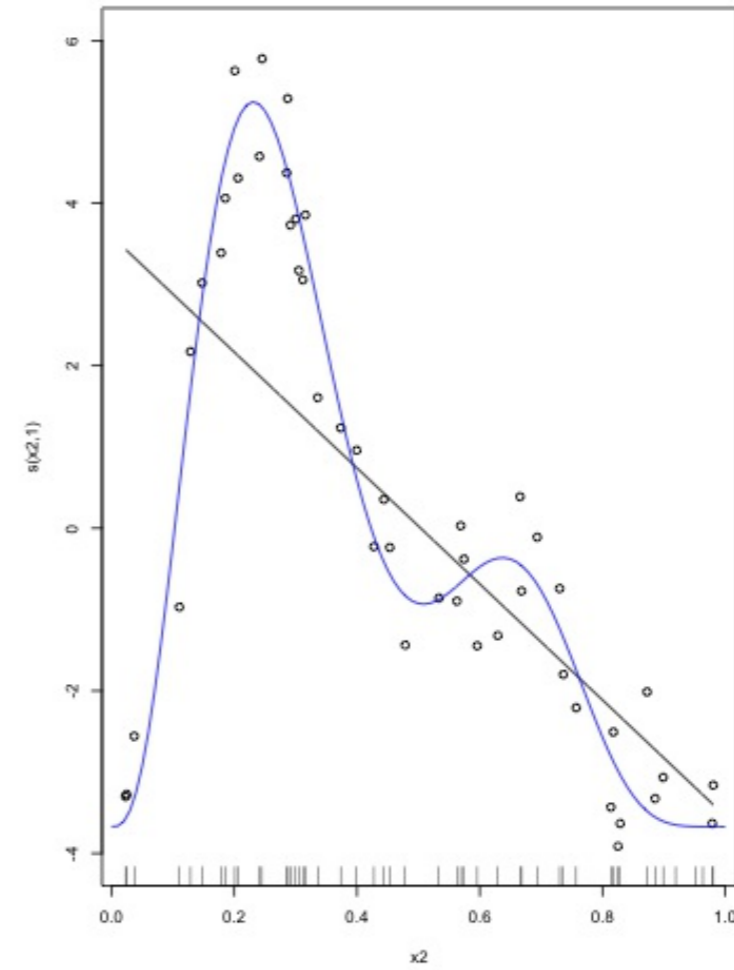
$\lambda = \text{just right}$



$\lambda = 0$



$\lambda = \infty$



How wiggly are things?

- We can set **basis complexity** or “size” (k)
 - Maximum wigglyness
- Smooths have **effective degrees of freedom** (EDF)
- $\text{EDF} < k$
- Set k “large enough”

Okay, that was a lot of theory...

Fitting GAMs using dsm

Translating maths into R

$$n_j = A_j \hat{p}_j \exp[\beta_0 + s(y_j)] + \epsilon_j$$

where $\epsilon_j \sim N(0, \sigma^2)$, $n_j \sim$ count distribution

- inside the link: `formula=count ~ s(y)`
- response distribution: `family=nb()` or `family=tw()`
- detectability: `ddf.obj=df_hr`
- offset, data: `segment.data=segs,`
`observation.data=obs`

Your first DSM

```
library(dsm)
dsm_x_tw <- dsm(count~s(x), ddf.obj=df_hr,
               segment.data=segs, observation.data=obs,
               family=tw(), method="REML")
```

(method="REML" uses REML to select the smoothing parameter)

dsm is based on mgcv by Simon Wood

What did that do?

```
summary(dsm_x_tw)
```

```
Family: Tweedie(p=1.326)  
Link function: log
```

```
Formula:  
count ~ s(x) + offset(off.set)
```

```
Parametric coefficients:
```

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	-19.7008	0.2277	-86.52	<2e-16	***

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

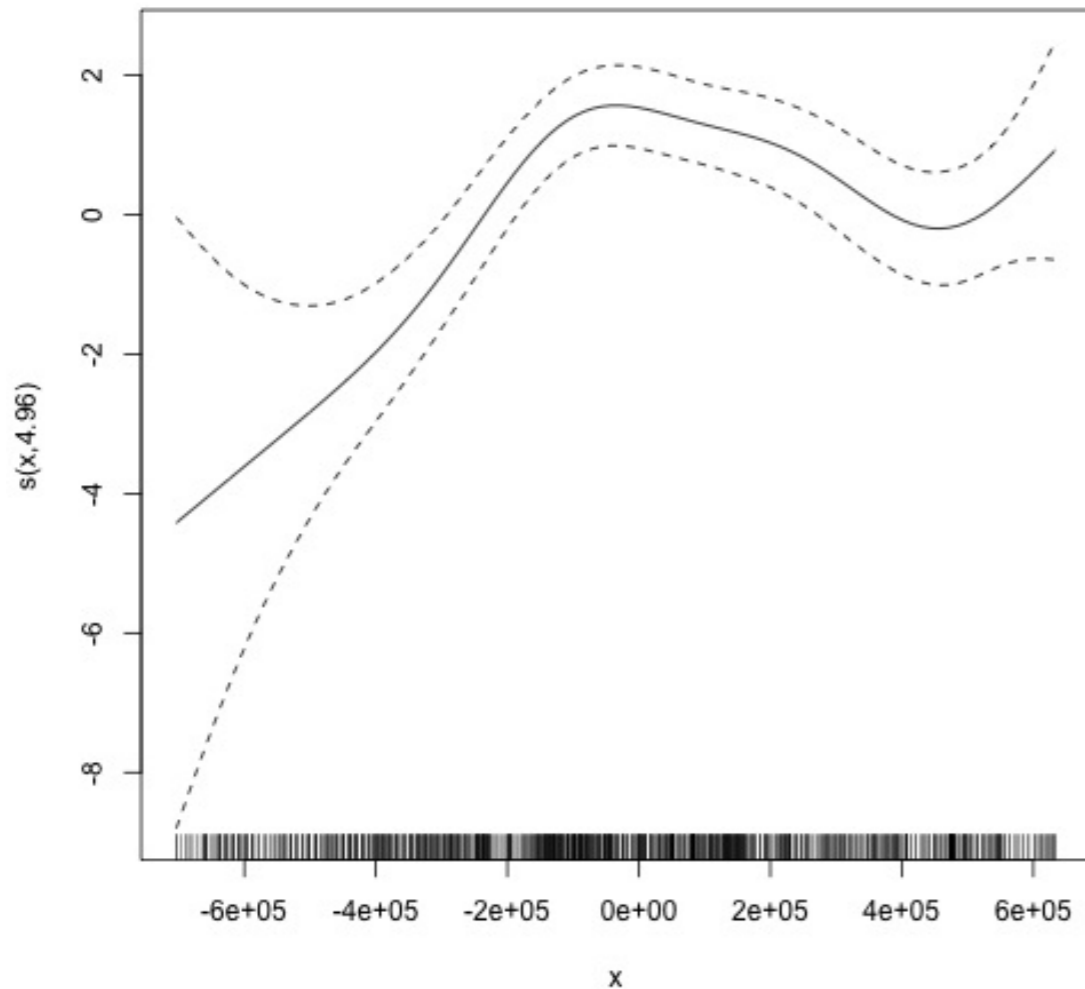
```
Approximate significance of smooth terms:
```

	edf	Ref.df	F	p-value	
s(x)	4.962	6.047	6.403	1.07e-06	***

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

```
R-sq.(adj) = 0.0283    Deviance explained = 17.7%  
-REML = 409.94    Scale est. = 6.0413    n = 949
```

Plotting



- `plot(dsm_x_tw)`
- Dashed lines indicate ± 2 standard errors
- Rug plot
- On the link scale
- EDF on y axis

Adding a term

- Just use +

```
dsm_xy_tw <- dsm(count ~ s(x) + s(y),  
                ddf.obj=df_hr,  
                segment.data=segs, observation.data=obs,  
                family=tw(), method="REML")
```

Summary

```
summary(dsm_xy_tw)
```

```
Family: Tweedie(p=1.306)  
Link function: log
```

```
Formula:  
count ~ s(x) + s(y) + offset(off.set)
```

```
Parametric coefficients:
```

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	-19.9801	0.2381	-83.93	<2e-16	***

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

```
Approximate significance of smooth terms:
```

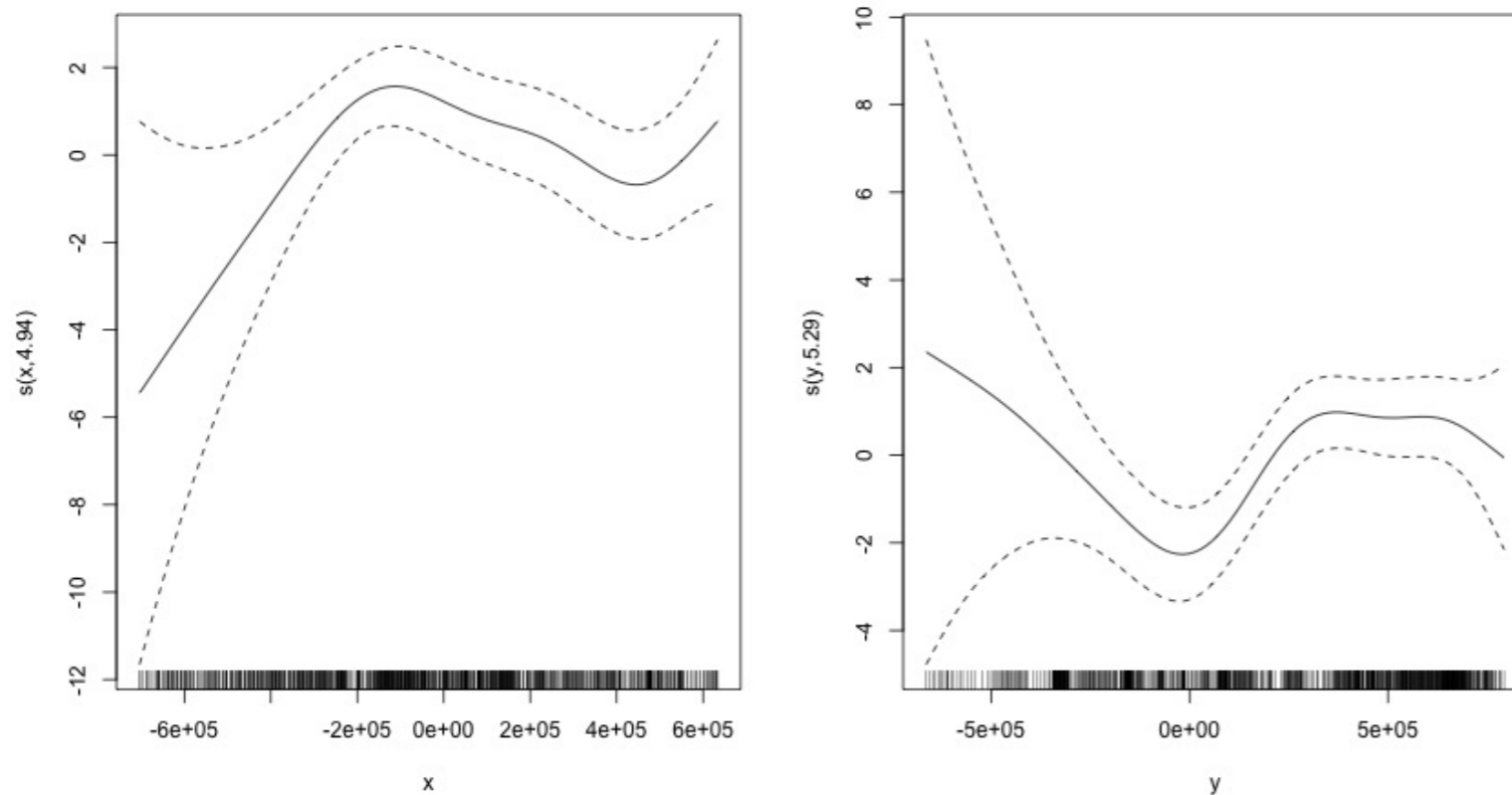
	edf	Ref.df	F	p-value	
s(x)	4.943	6.057	3.224	0.004239	**
s(y)	5.293	6.419	4.034	0.000322	***

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

```
R-sq.(adj) = 0.0678    Deviance explained = 27.3%  
-REML = 399.84    Scale est. = 5.3157    n = 949
```

Plotting

```
plot(dsm_xy_tw, scale=0, pages=1)
```



- `scale=0`: each plot on different scale
- `pages=1`: plot together

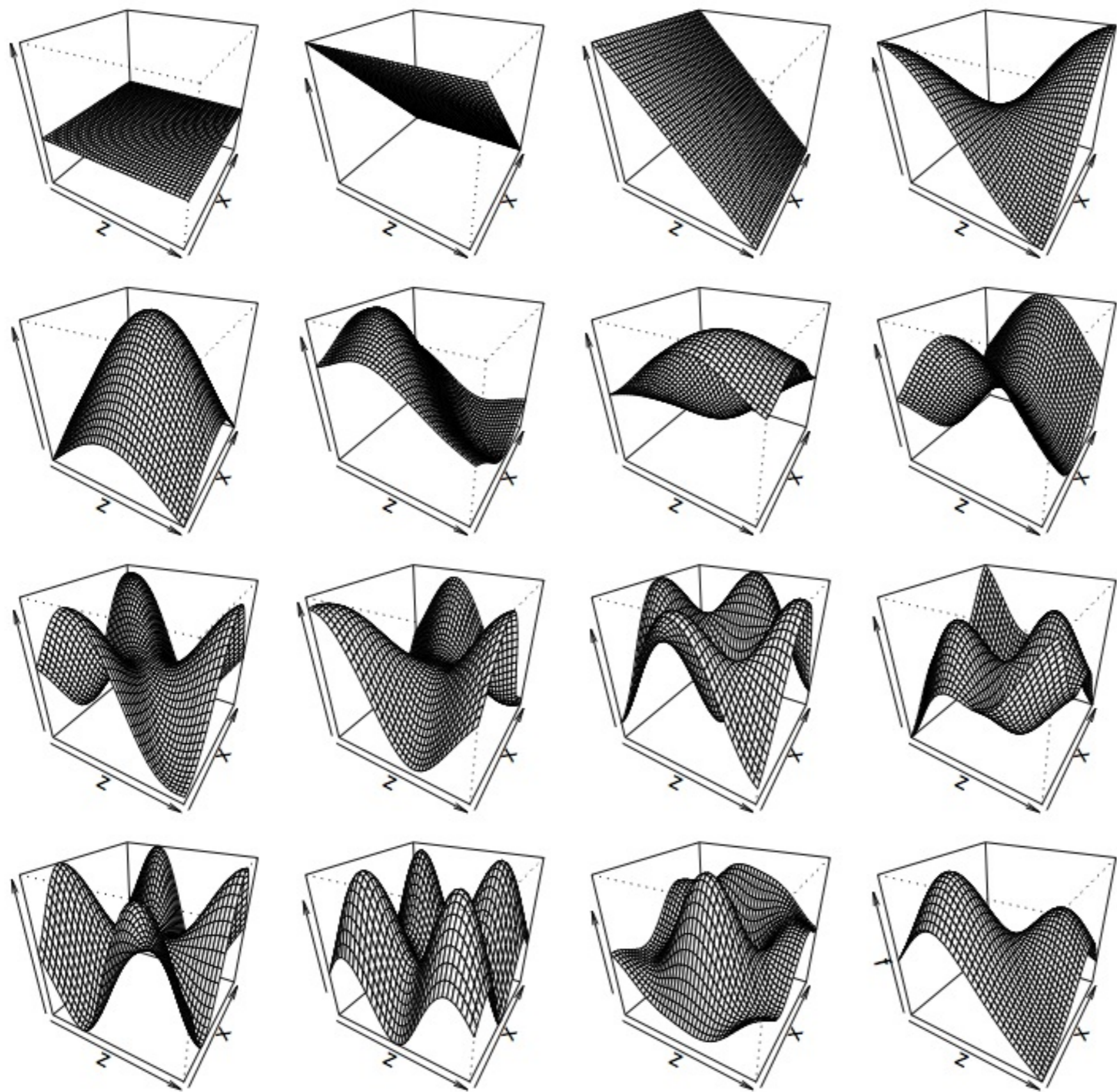
Bivariate terms

- Assumed an additive structure
- No interaction
- We can specify $s(x, y)$ (and $s(x, y, z, \dots)$)

Thin plate regression splines

- Default basis
- One basis function per data point
- Reduce # basis functions (eigendecomposition)
- Fitting on reduced problem
- Multidimensional

Thin plate splines (2-D)



Bivariate spatial term

```
dsm_xyb_tw <- dsm(count ~ s(x, y),  
                 ddf.obj=df_hr,  
                 segment.data=segs, observation.data=obs,  
                 family=tw(), method="REML")
```

Summary

```
summary(dsm_xyb_tw)
```

```
Family: Tweedie(p=1.29)  
Link function: log
```

```
Formula:  
count ~ s(x, y) + offset(off.set)
```

```
Parametric coefficients:
```

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	-20.1638	0.2477	-81.4	<2e-16	***

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

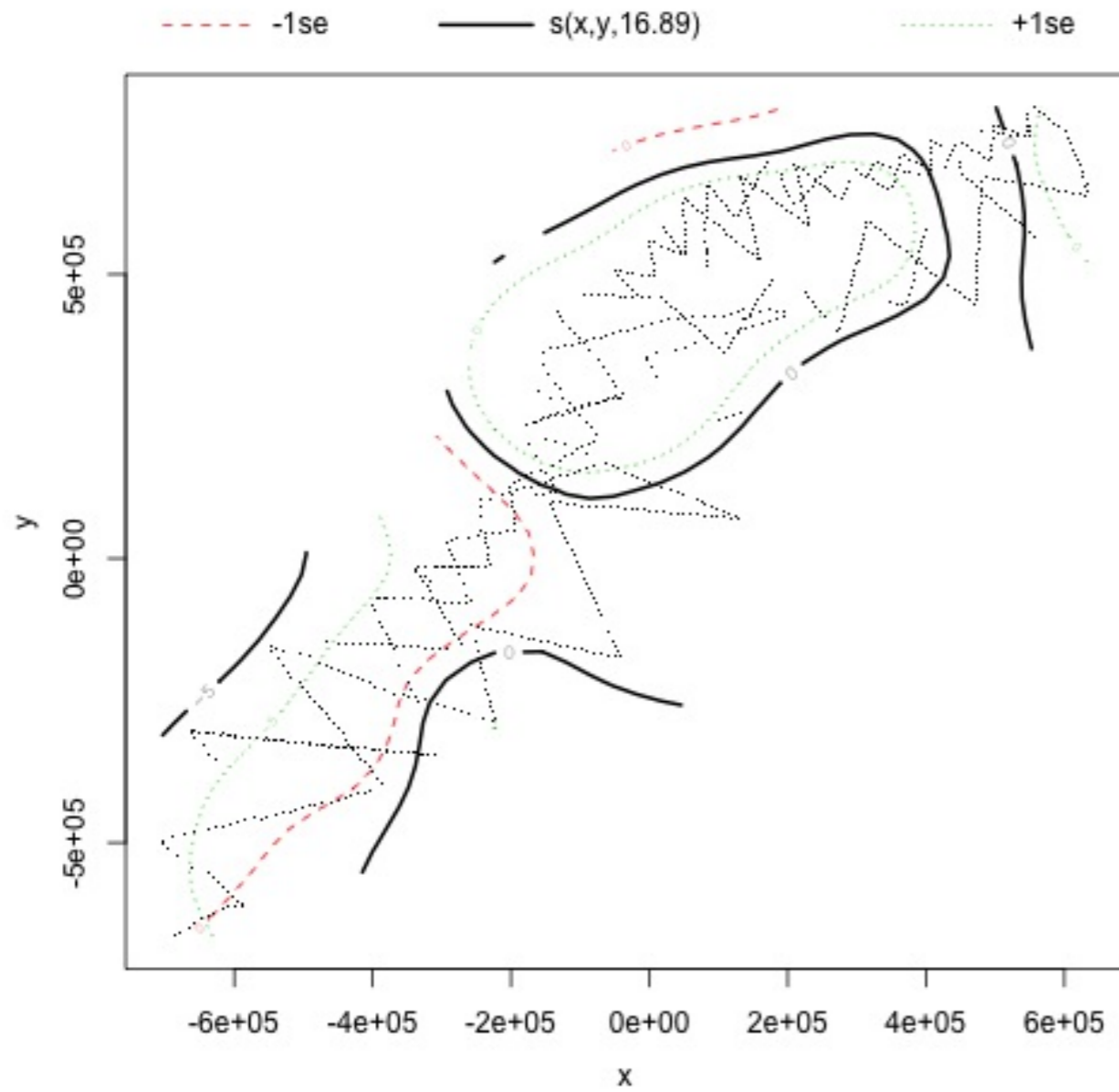
```
Approximate significance of smooth terms:
```

	edf	Ref.df	F	p-value	
s(x,y)	16.89	21.12	4.333	3.73e-10	***

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

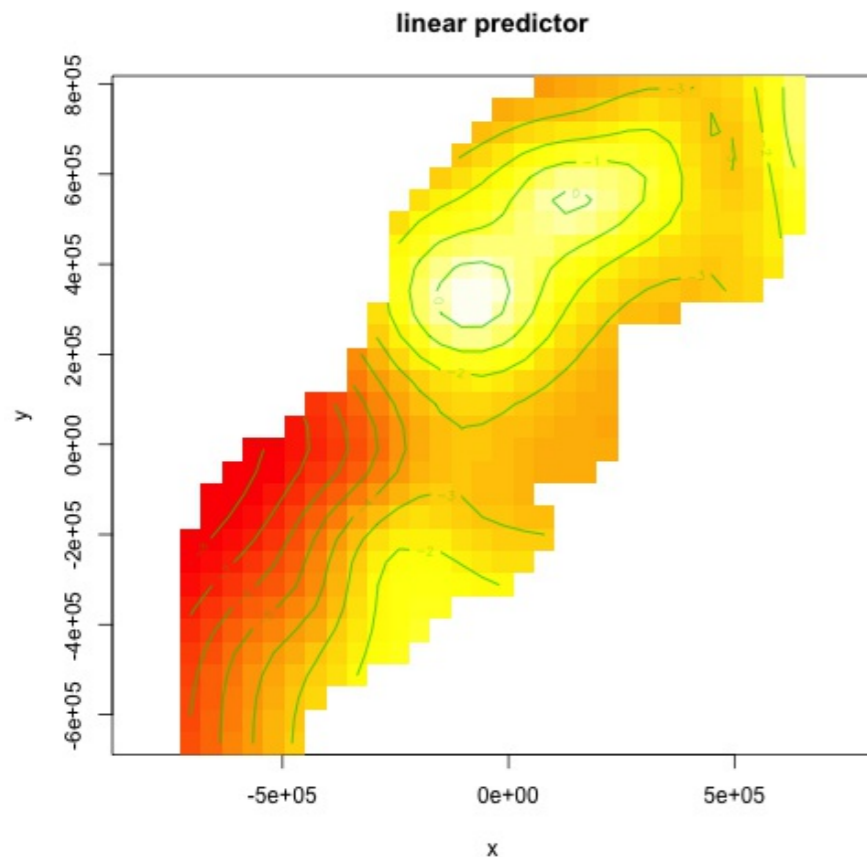
```
R-sq.(adj) = 0.102    Deviance explained = 34.5%  
-REML = 394.86    Scale est. = 4.8248    n = 949
```

Plotting... erm...



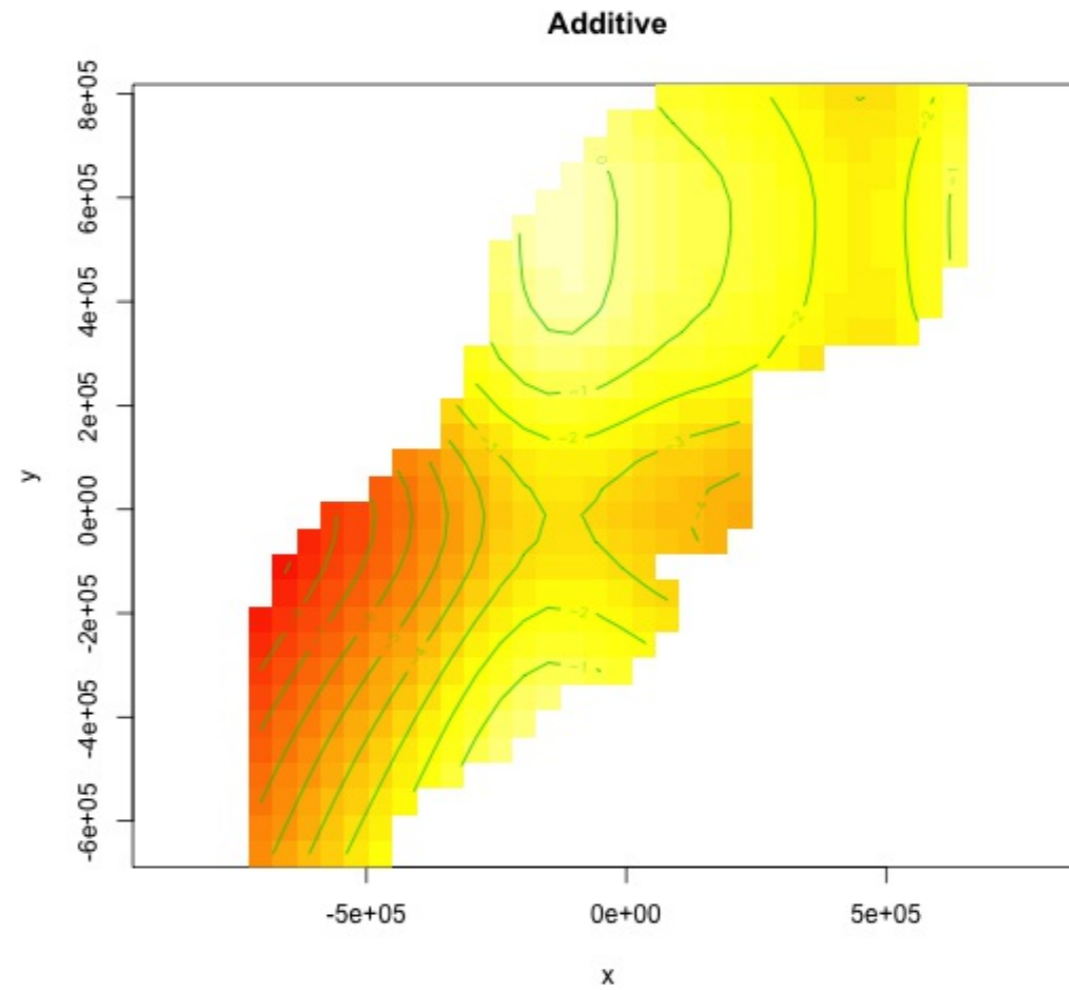
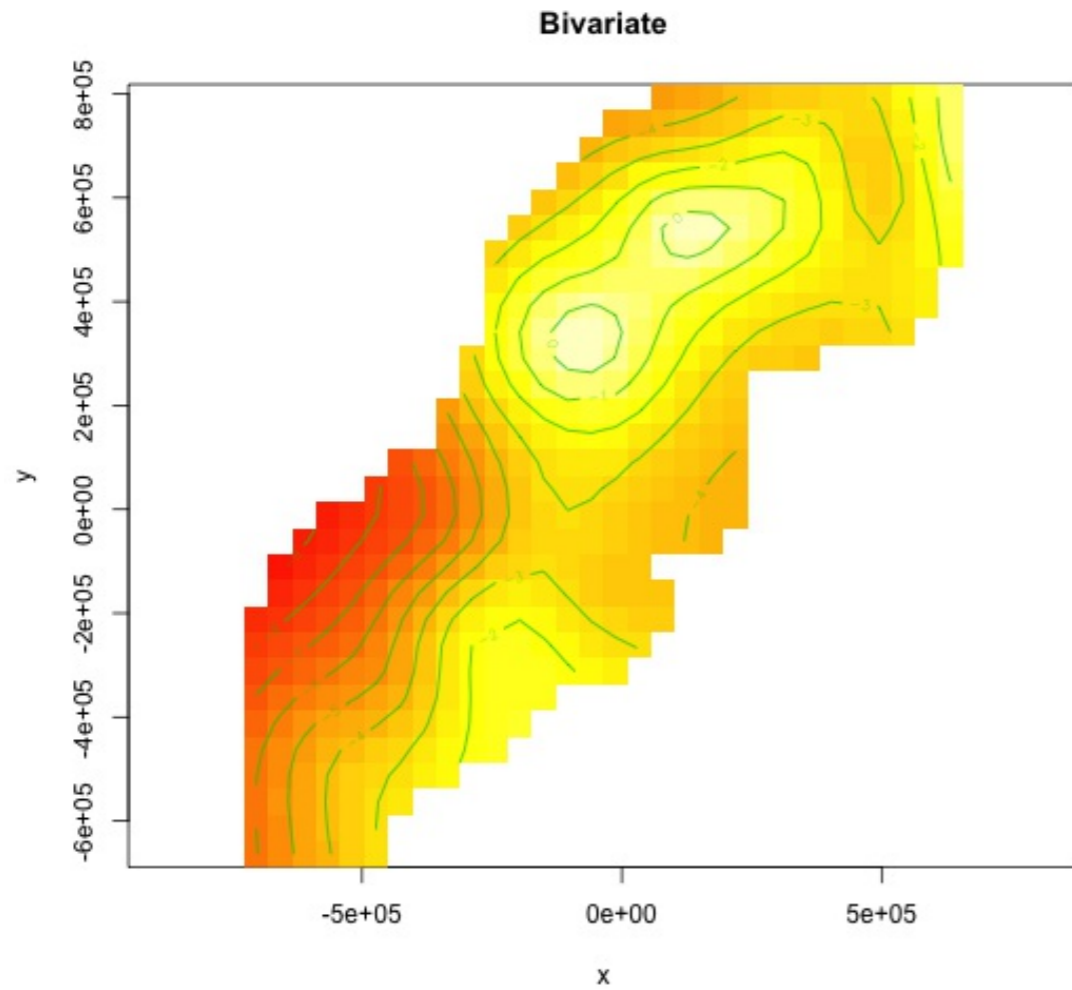
Let's try something different

```
vis.gam(dsm_xyb_tw, view=c("x", "y"), plot.type="contour",  
too.far=0.1, asp=1)
```



- Still on link scale
- `too.far` excludes points far from data

Comparing bivariate and additive models



Model checking

“perhaps the most important part of applied statistical modelling”

Simon Wood

Model checking

- As with detection function, checking is important
- Want to know the model conforms to assumptions
- What assumptions should we check?

What to check

- Convergence (not usually an issue)
- Basis size is big enough
- Residuals

Basis size

Basis size (k)

- Set k per term
- e.g. $s(x, k=10)$ or $s(x, y, k=100)$
- Penalty removes “extra” wigglyness
 - *up to a point!*
- (But computation is slower with bigger k)

Checking basis size

```
gam.check(dsm_x_tw)
```

```
Method: REML    Optimizer: outer newton  
full convergence after 7 iterations.  
Gradient range [-3.08755e-06,4.928062e-07]  
(score 409.936 & scale 6.041307).  
Hessian positive definite, eigenvalue range [0.7645492,302.127].  
Model rank = 10 / 10
```

Basis dimension (k) checking results. Low p-value (k-index<1) may indicate that k is too low, especially if edf is close to k'.

	k'	edf	k-index	p-value
s(x)	9.000	4.962	0.763	0.44

Increasing basis size

```
dsm_x_tw_k <- dsm(count~s(x, k=20), ddf.obj=df_hr,  
                 segment.data=segs, observation.data=obs,  
                 family=tw(), method="REML")  
gam.check(dsm_x_tw_k)
```

```
Method: REML   Optimizer: outer newton  
full convergence after 7 iterations.  
Gradient range [-2.301246e-08,3.930757e-09]  
(score 409.9245 & scale 6.033913).  
Hessian positive definite, eigenvalue range [0.7678456,302.0336].  
Model rank = 20 / 20
```

Basis dimension (k) checking results. Low p-value (k-index<1) may indicate that k is too low, especially if edf is close to k'.

	k'	edf	k-index	p-value
s(x)	19.000	5.246	0.763	0.36

Sometimes basis size isn't the issue...

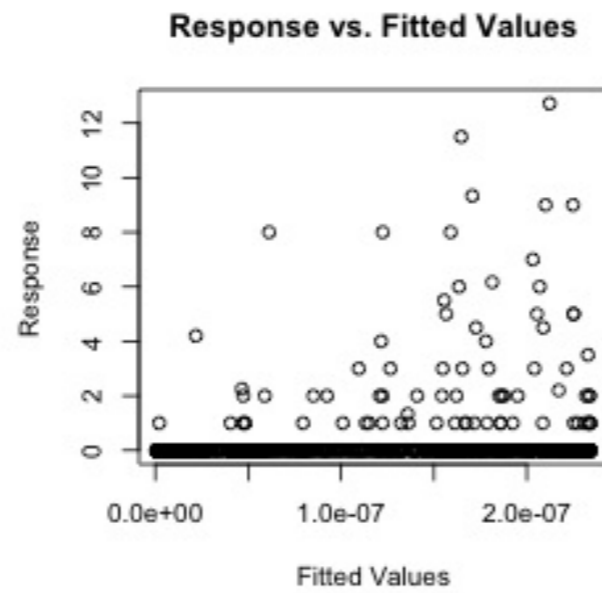
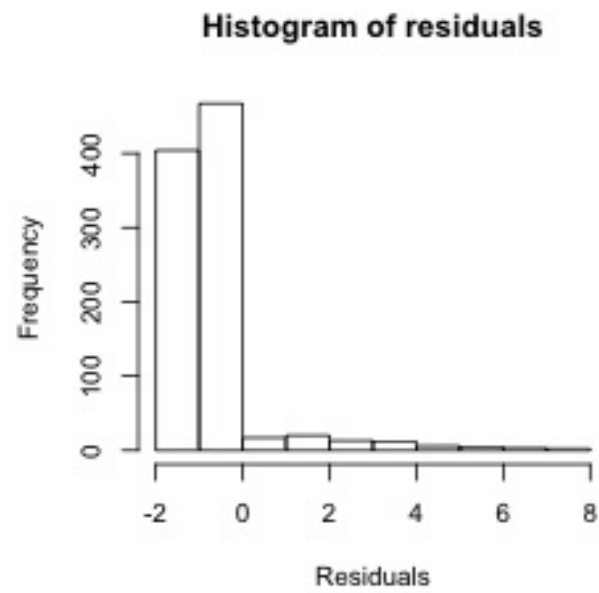
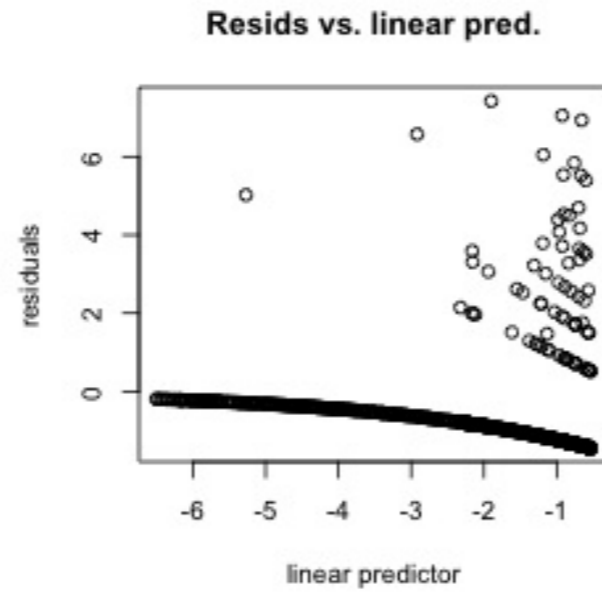
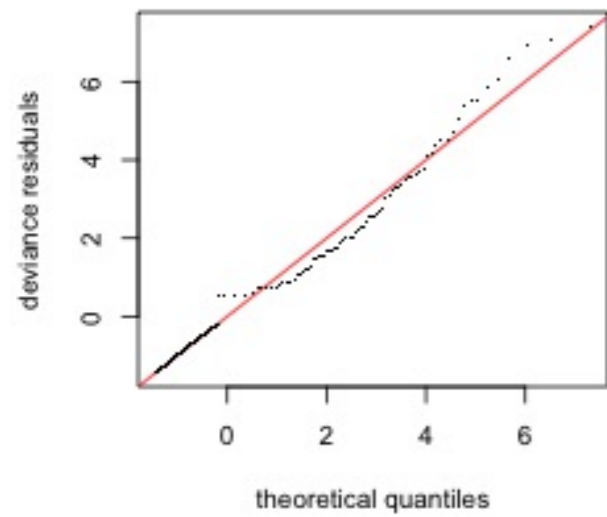
- Generally, double k and see what happens
- Didn't increase the EDF much here
- Other things can cause low “p-value” and “k-index”
- Increasing k can cause problems (nullspace)

Don't throw away your
residuals!

What are residuals?

- Generally residuals = observed value - fitted value
- BUT hard to see patterns in these “raw” residuals
- Need to standardise – **deviance residuals**
- Residual sum of squares \Rightarrow linear model
 - deviance \Rightarrow GAM
- Expect these residuals $\sim N(0, 1)$

Residual checking

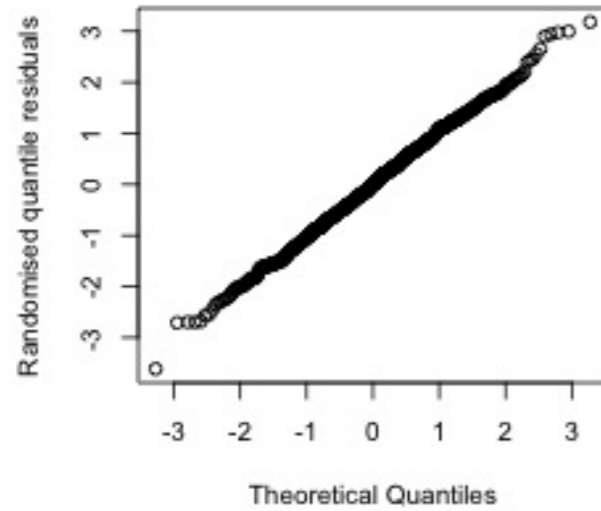


Shortcomings

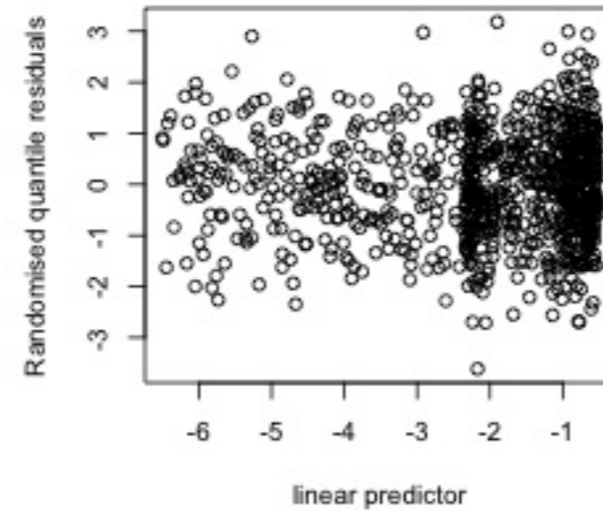
- `gam.check` left side can be helpful
- Right side is victim of artifacts
- Need an alternative
- “Randomised quantile residuals” (*experimental*)
 - `rqqam.check`
 - Exactly normal residuals (left side useless)

Randomised quantile residuals

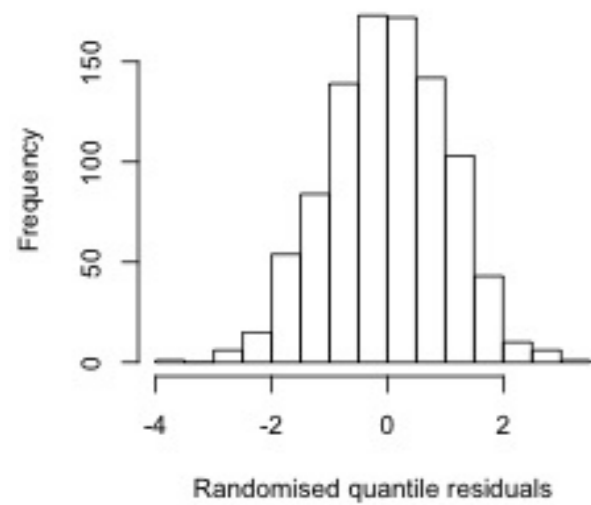
Normal Q-Q Plot



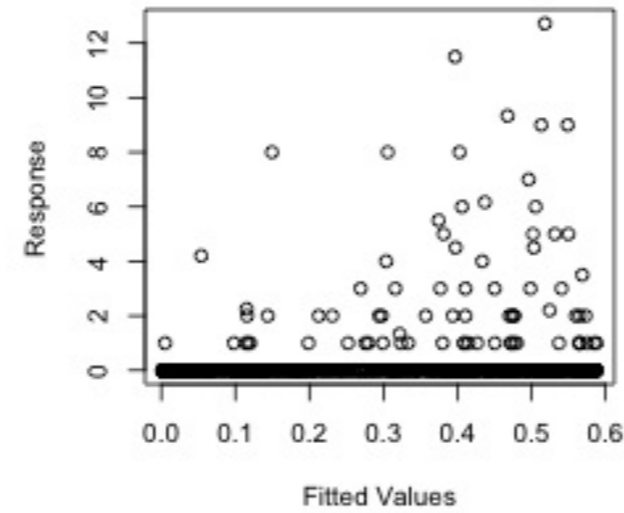
Resids vs. linear pred.



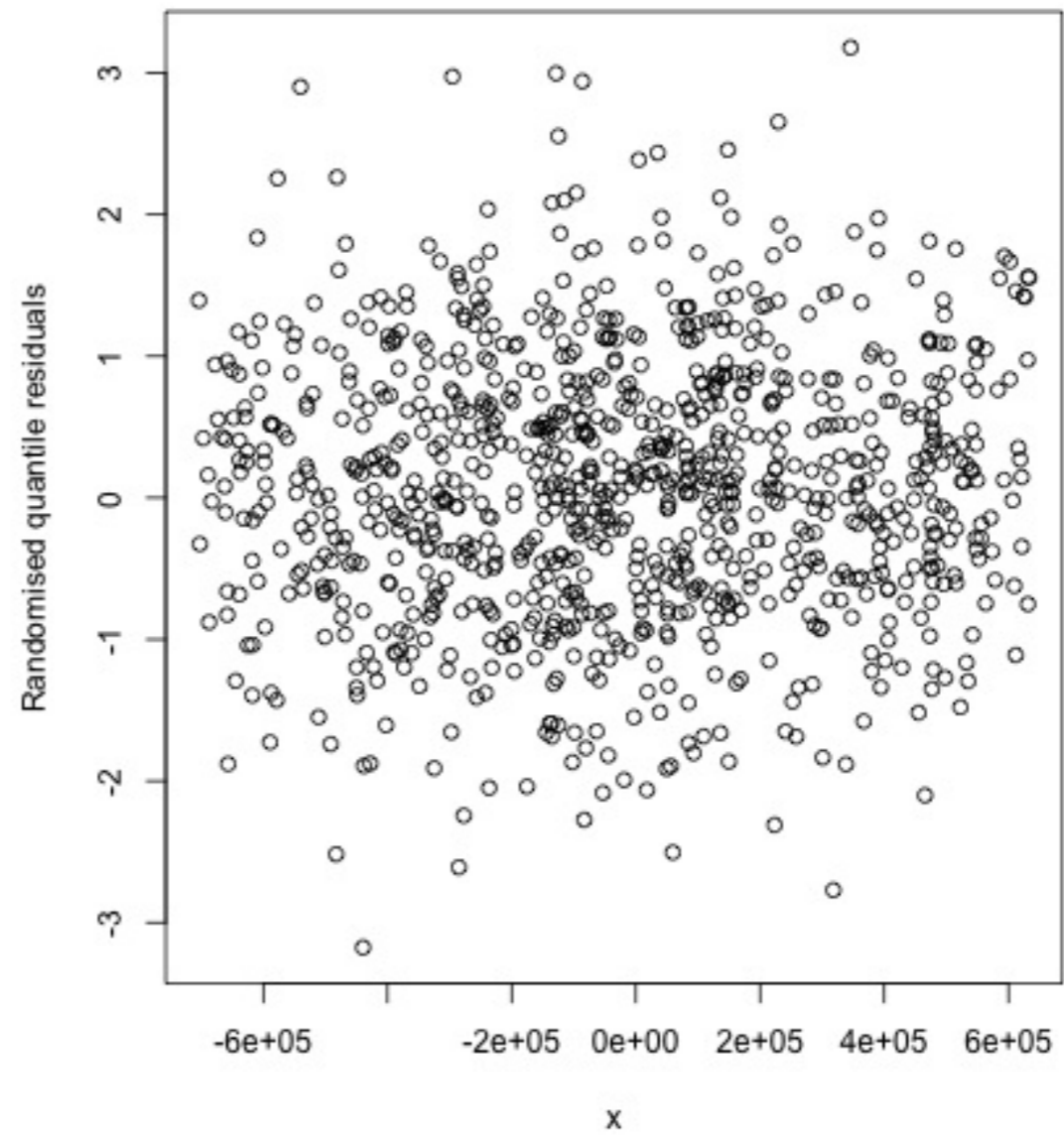
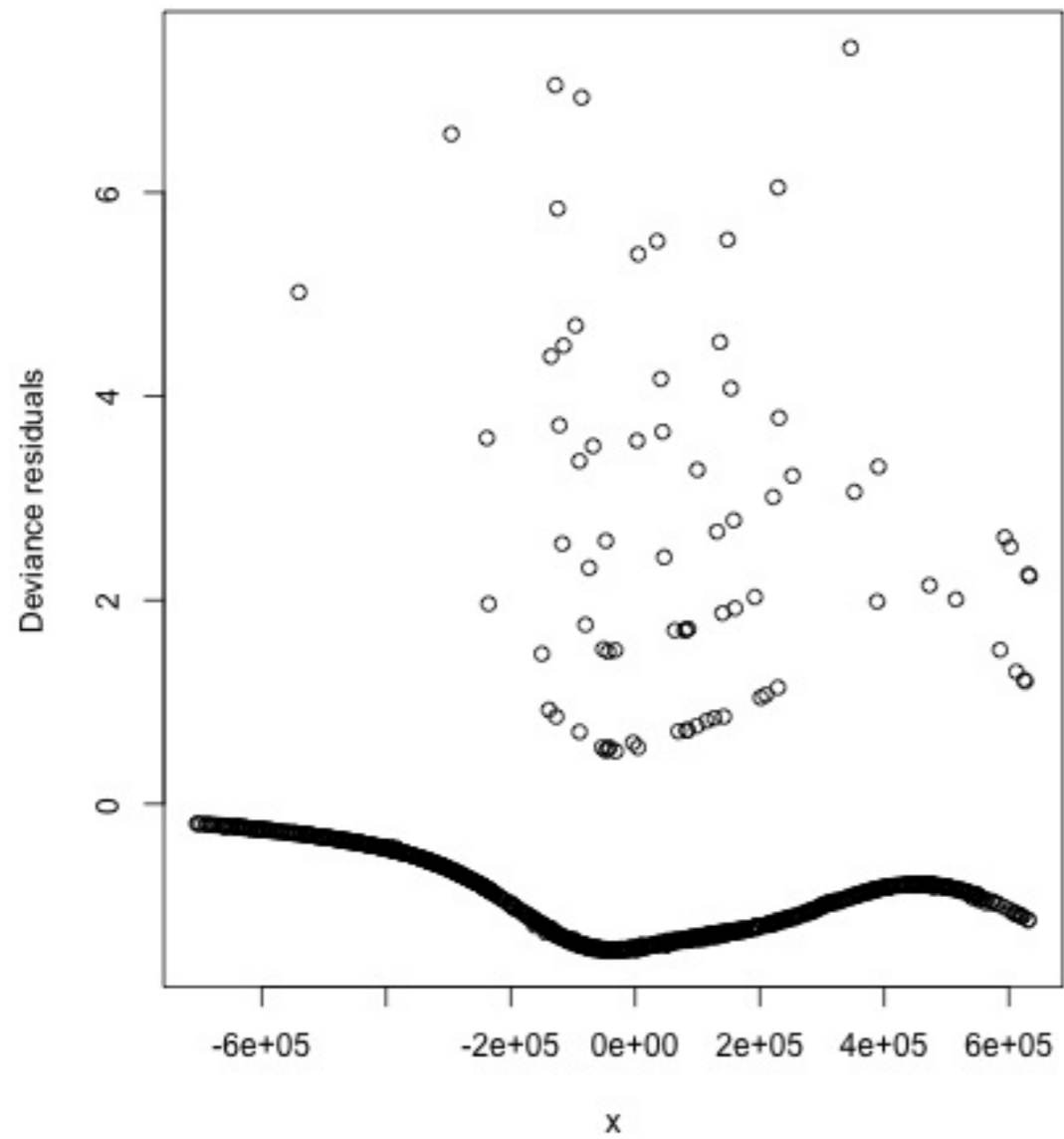
Histogram of residuals



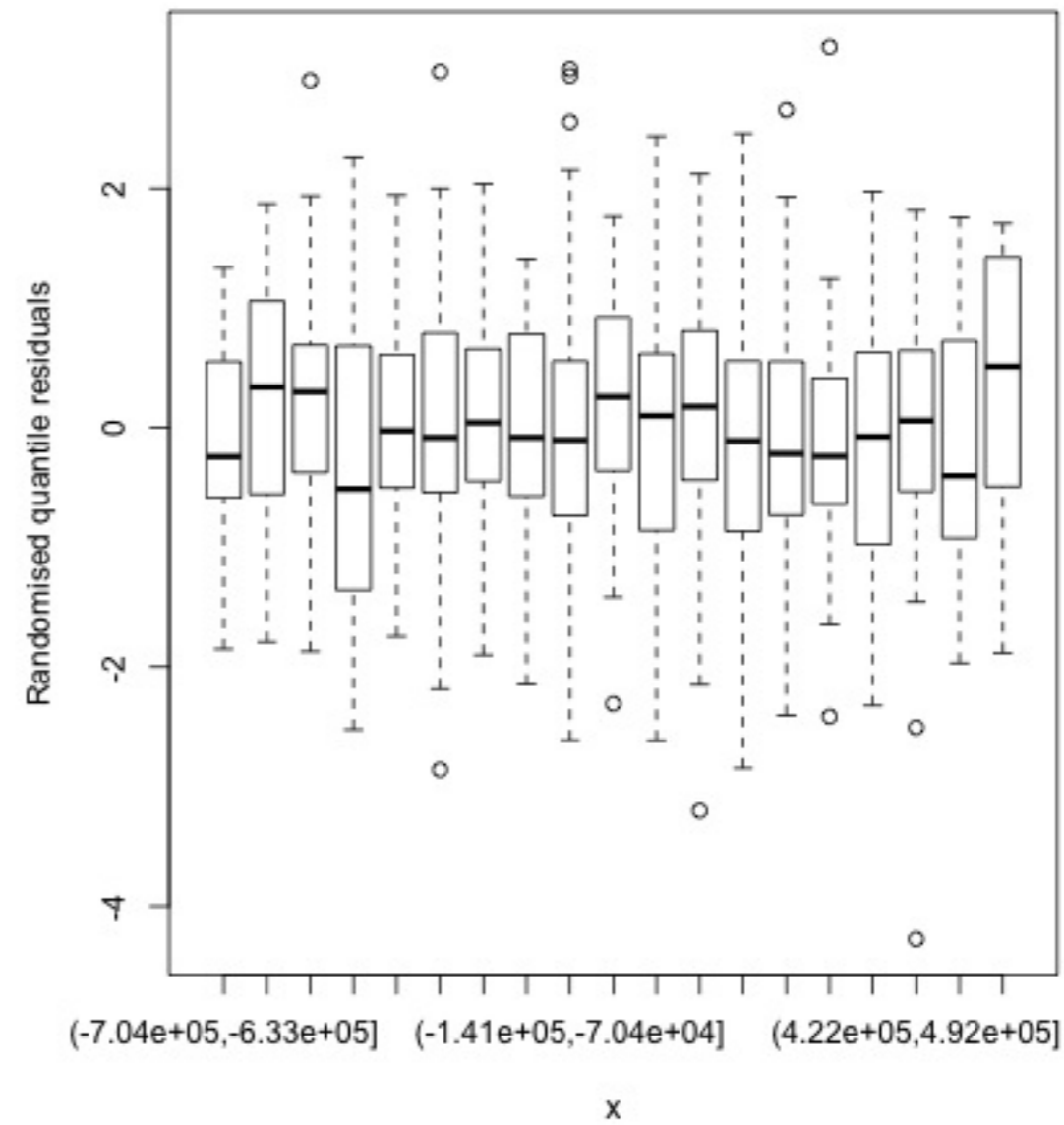
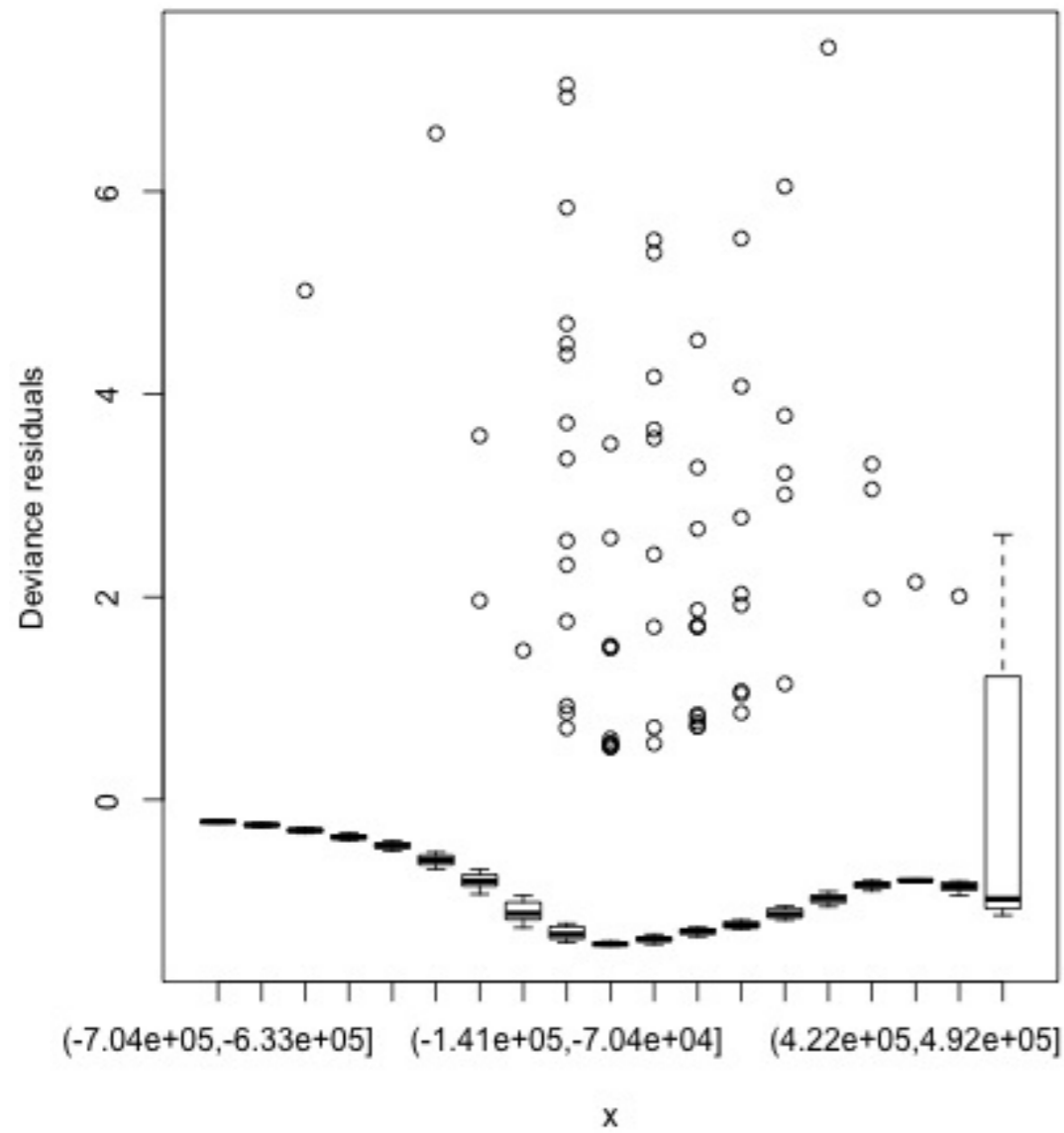
Response vs. Fitted Values



Residuals vs. covariates

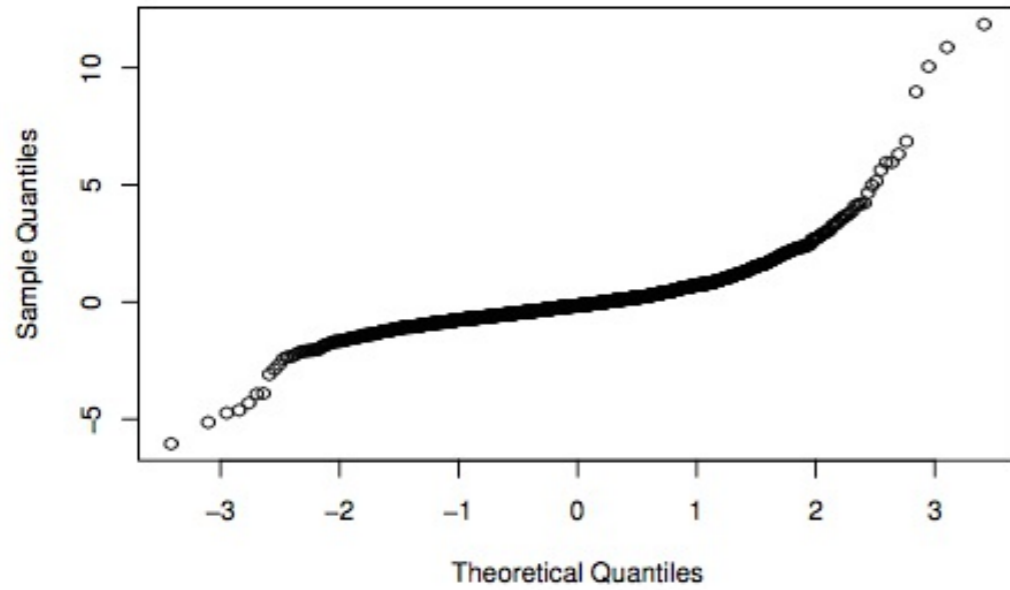


Residuals vs. covariates (boxplots)

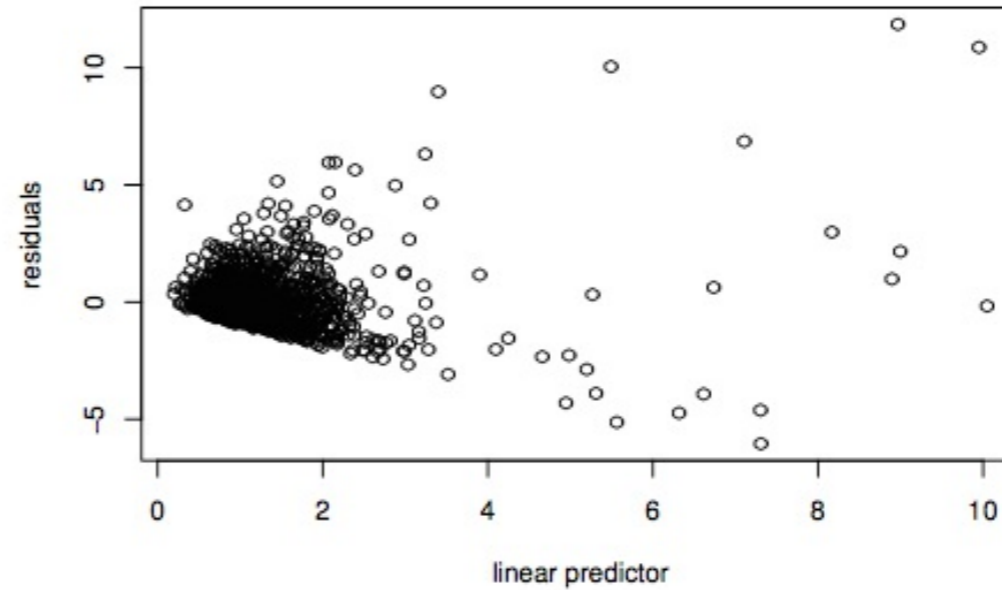


Example of "bad" plots

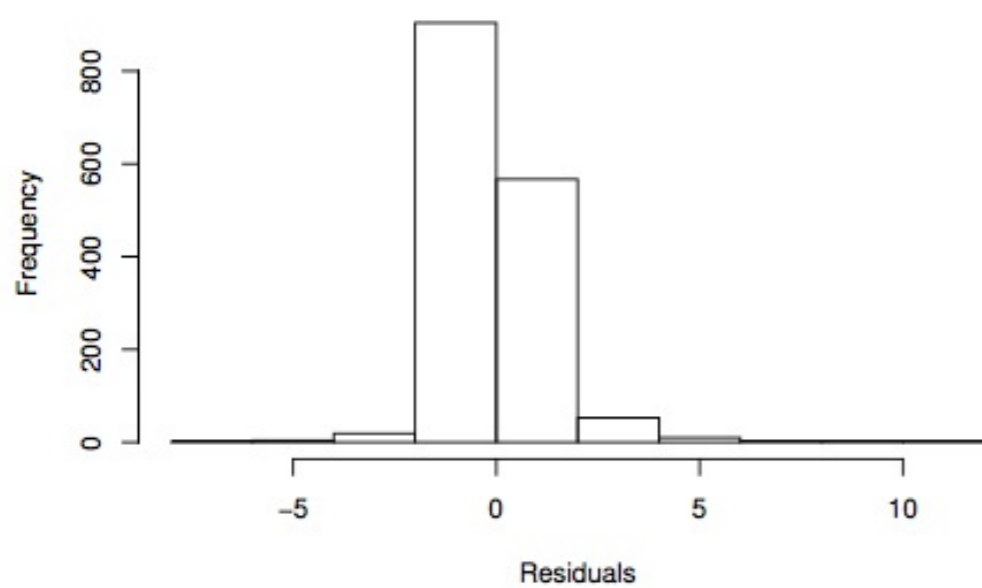
Normal Q-Q Plot



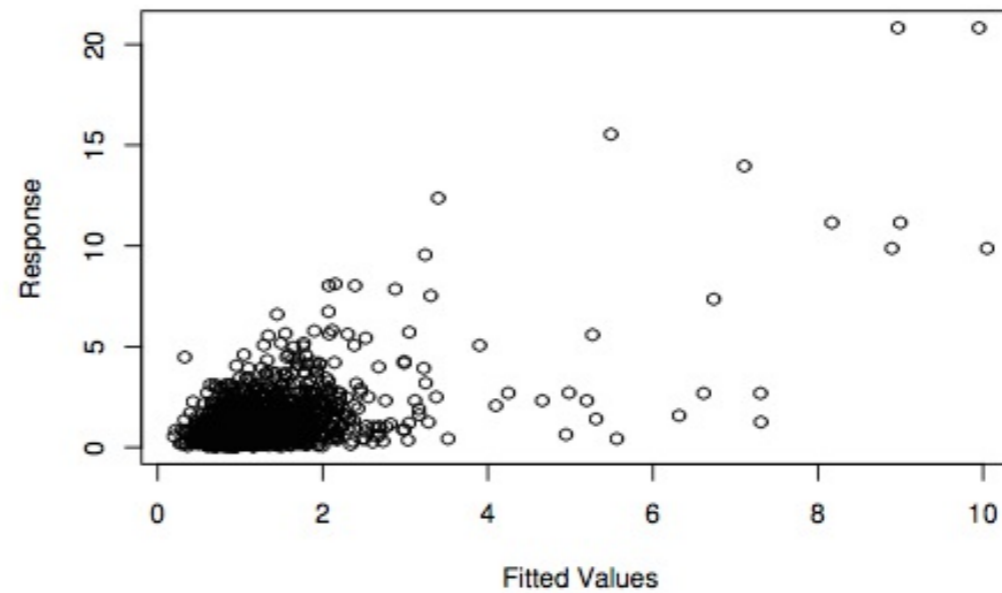
Resids vs. linear pred.



Histogram of residuals

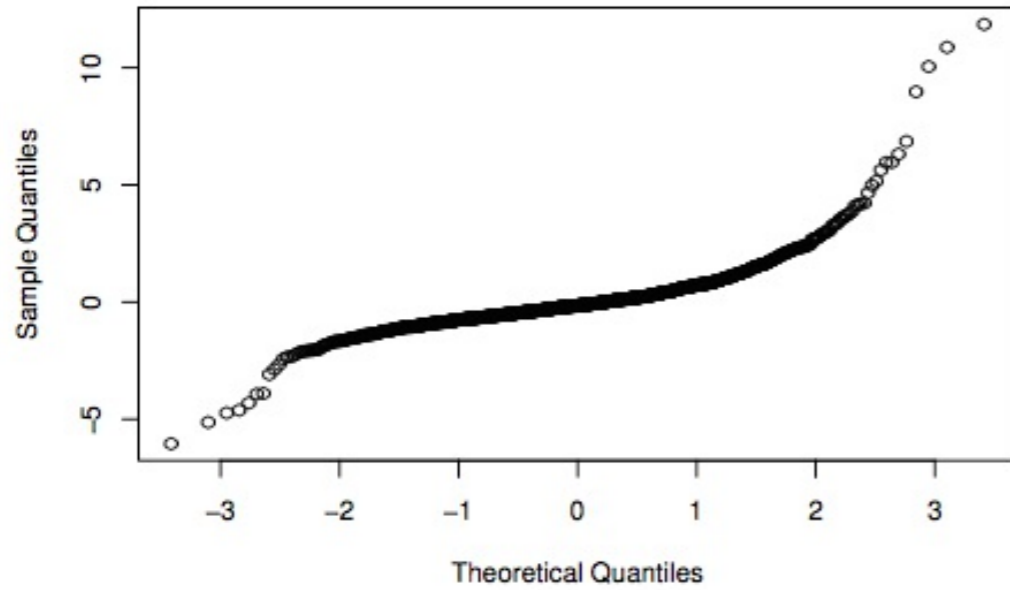


Response vs. Fitted Values

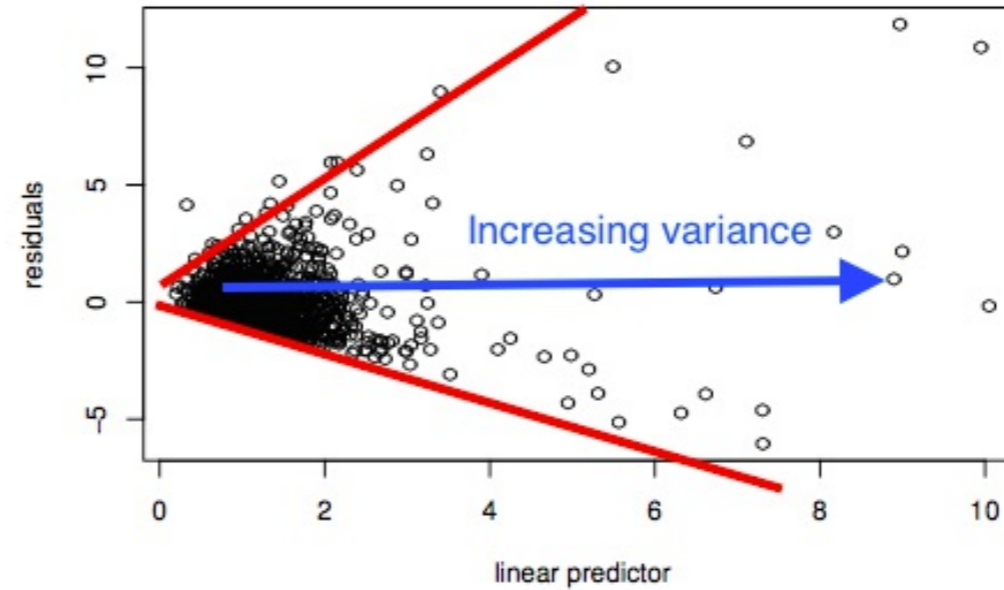


Example of "bad" plots

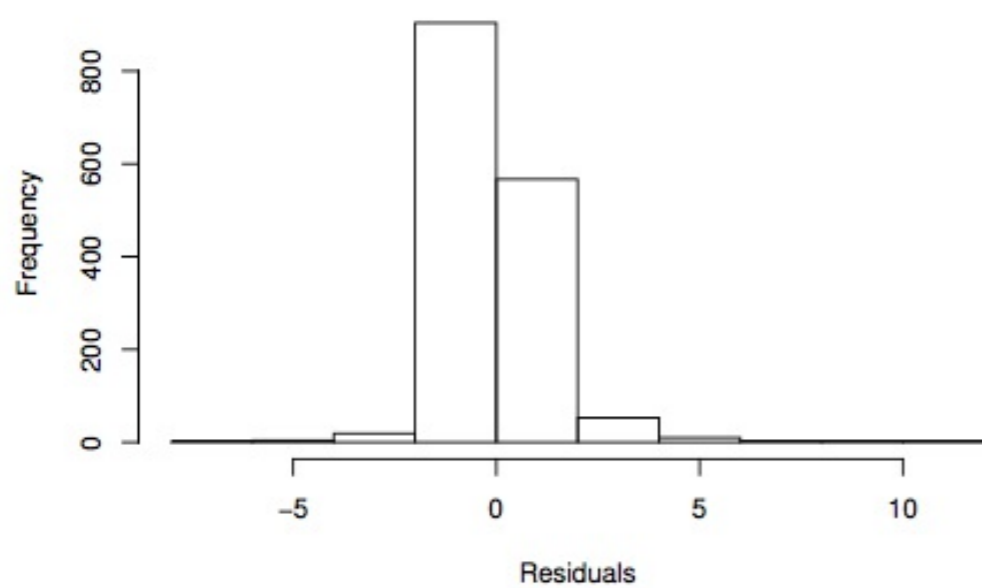
Normal Q-Q Plot



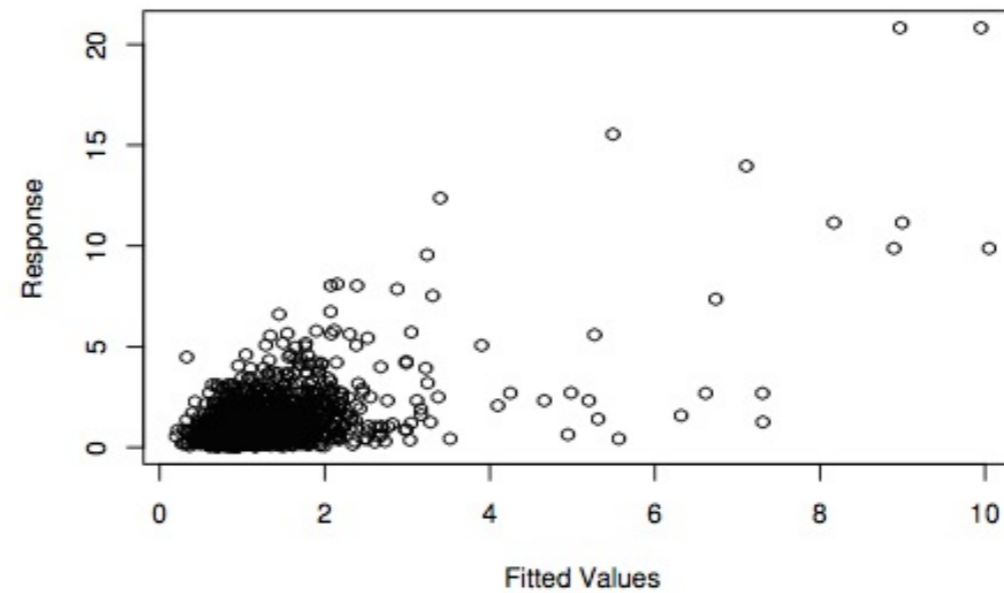
Resids vs. linear pred.



Histogram of residuals



Response vs. Fitted Values



Residual checks

- Looking for patterns (not artifacts)
- This can be tricky
- Need to use a mixture of techniques

Let's have a go...