Generalised additive models

An introduction with R

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2017-10-17

Preamble

What are GAMs?

Generalized **A**dditive **M**odel

- Generalized because they can handle response distibutions beyond the normal or Gaussian
  - **mgcv** can handle many types of data that lie even beyond traditional GLMs
- Additive — terms simply **add** together
- Model — a GAM has lots of theory for doing inference

Linear Models

$$y_i \, \mathcal{N}(\mu_i, \sigma^2)$$

$$\mu_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \cdots + \beta_j x_{ji}$$

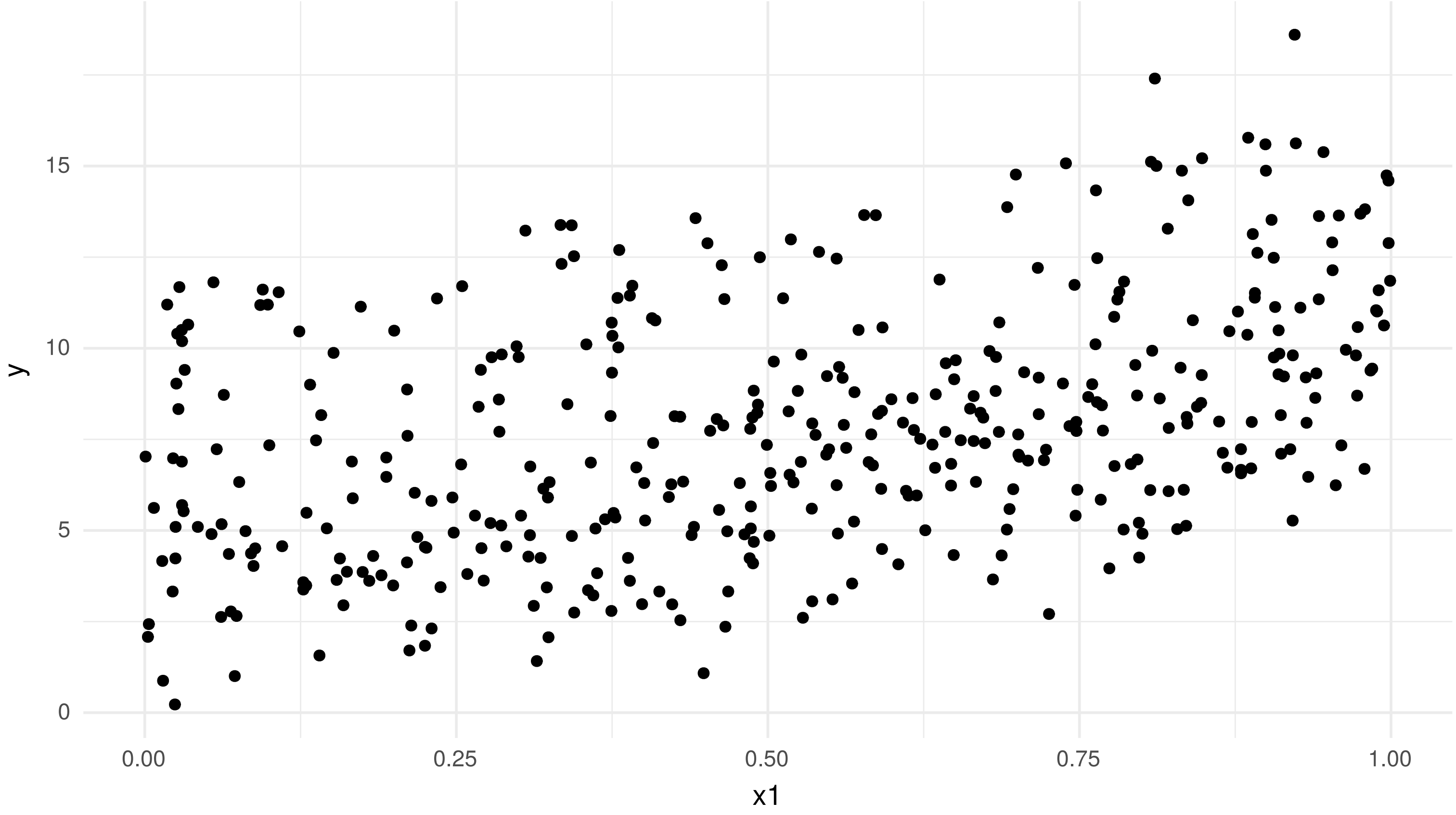
Assumptions

- linear effects of covariates are good approximation of the true effects
- conditional on the values of covariates, $y_i | \mathbf{X} \sim \mathcal{N}(0, \sigma^2)$
- this implies all observations have the same *variance*
- $y_i | \mathbf{X}$ are *independent*

An **additive** model address the first of these

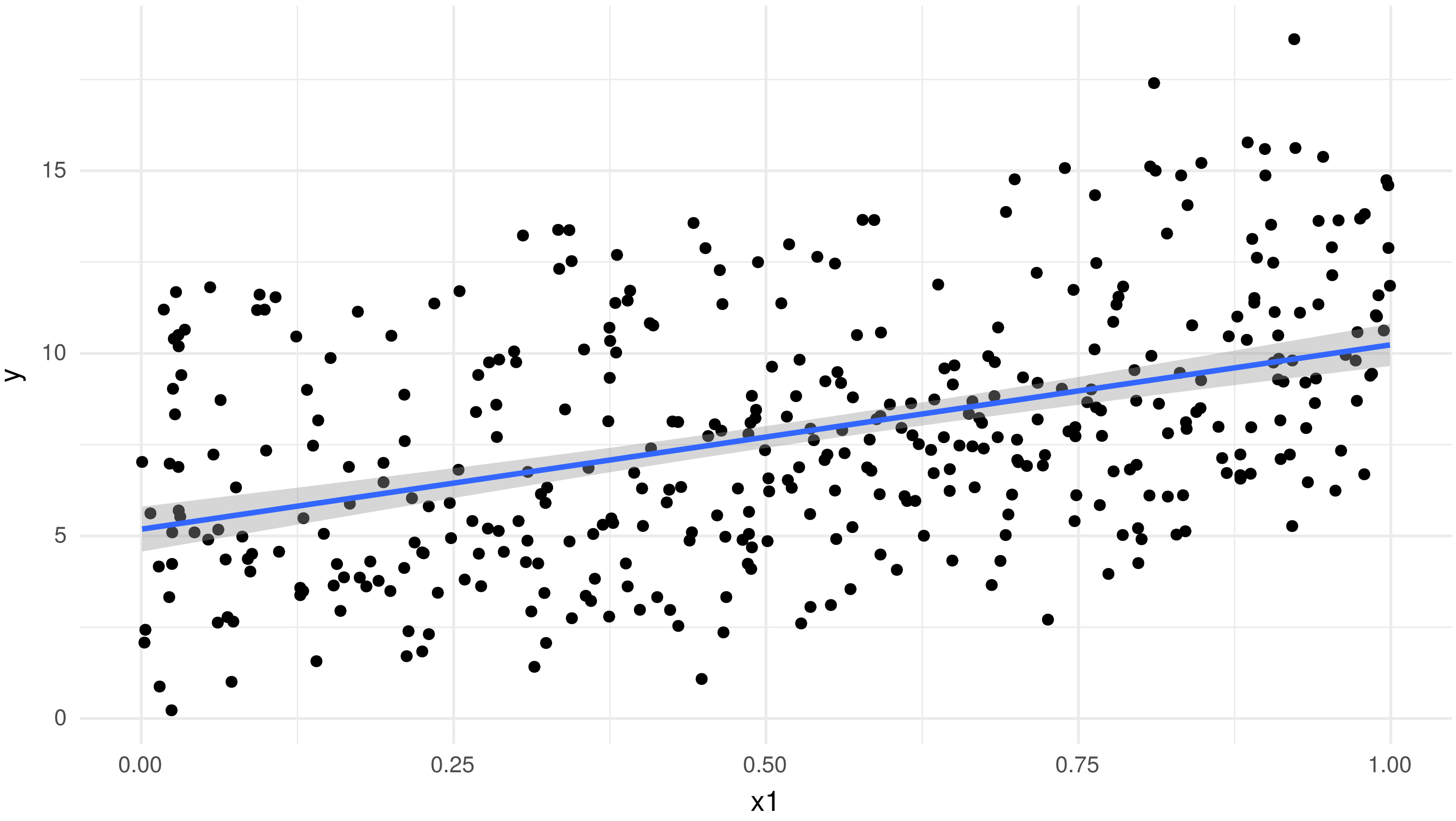
Why bother with anything more complex?

Is this linear?



Is this linear? Maybe?

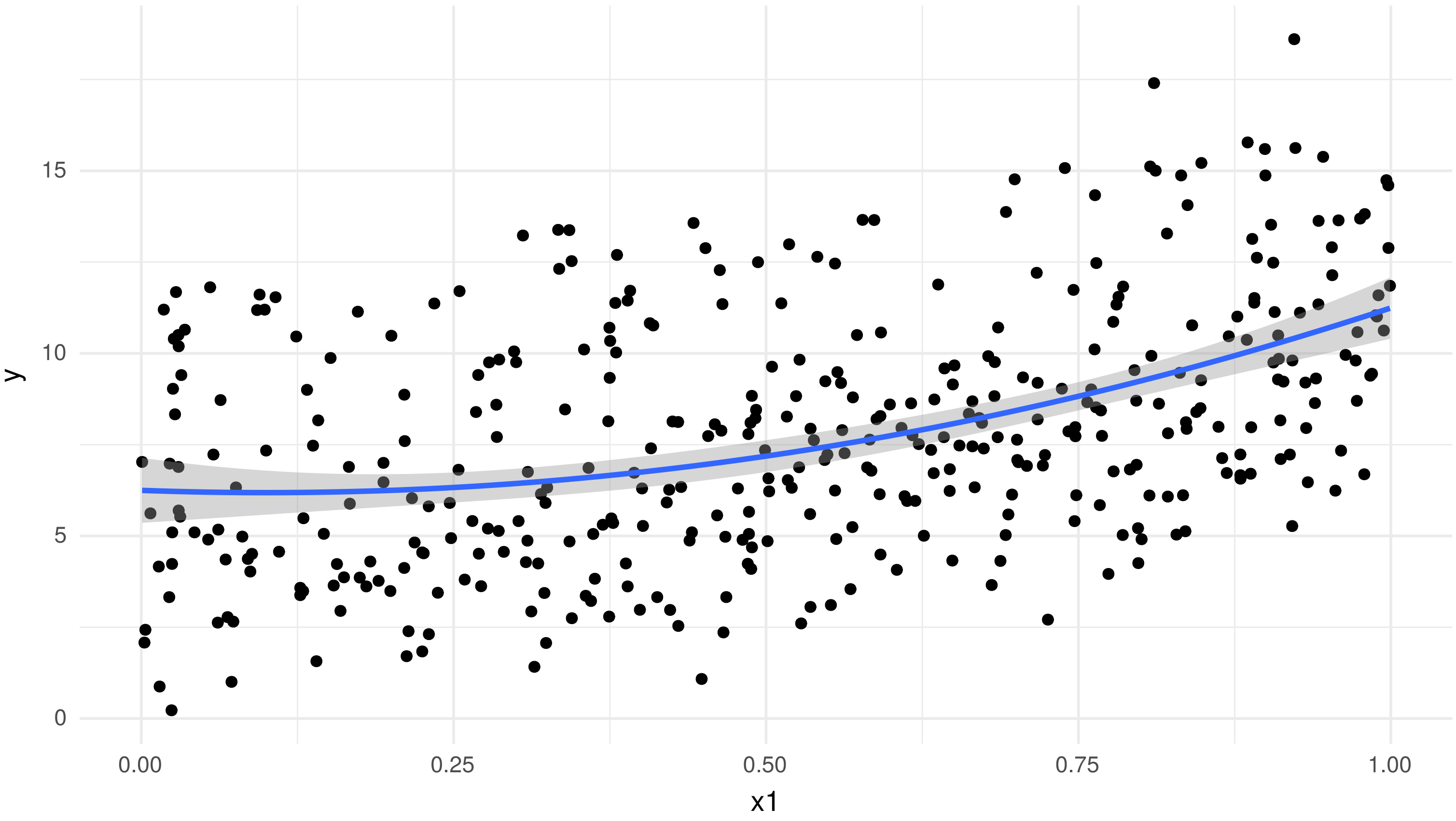
```
lm(y ~ x1, data=dat)
```



What can we do about it?

Adding a quadratic term?

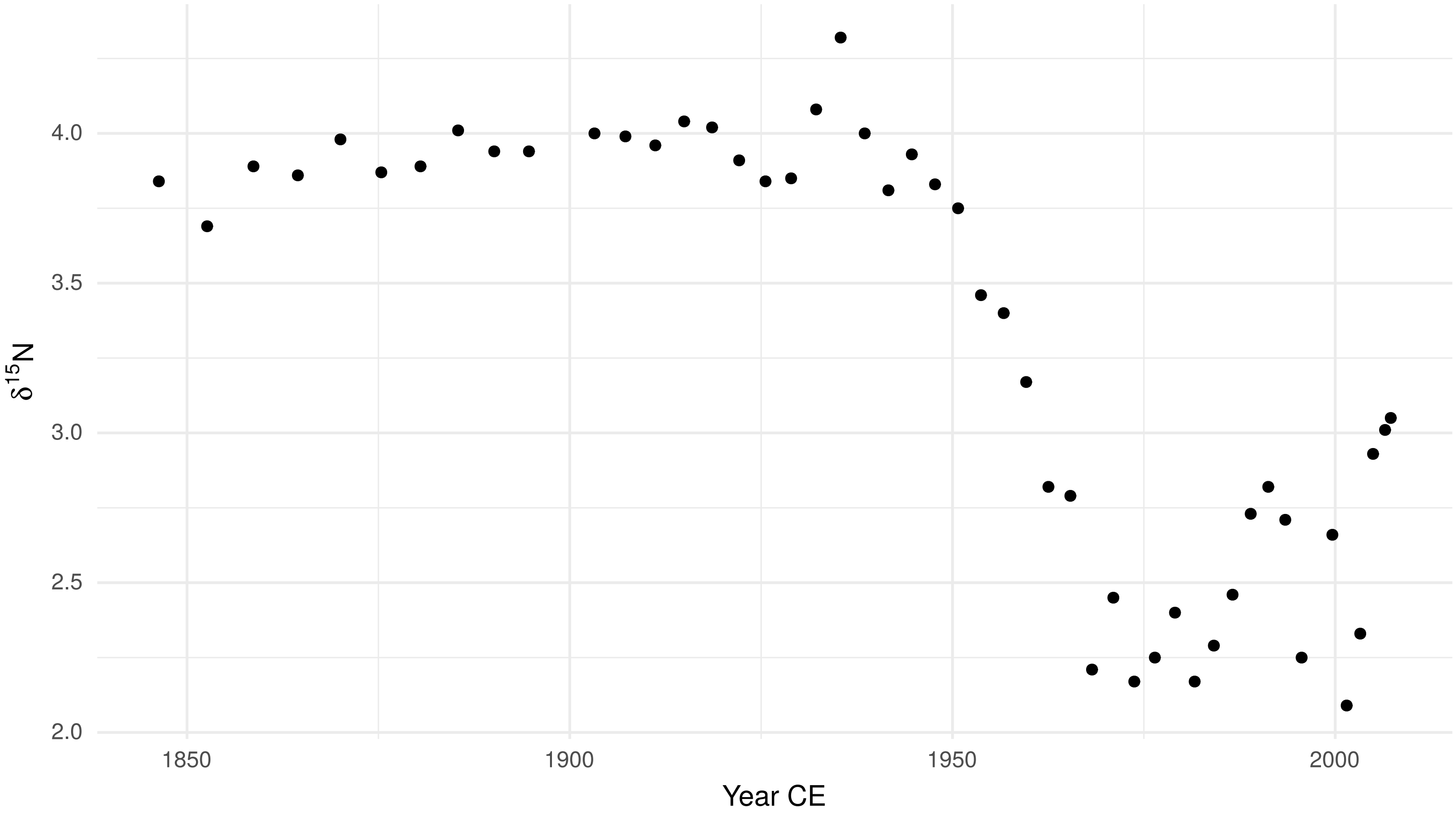
```
lm(y ~ poly(x1, 2), data = dat)
```



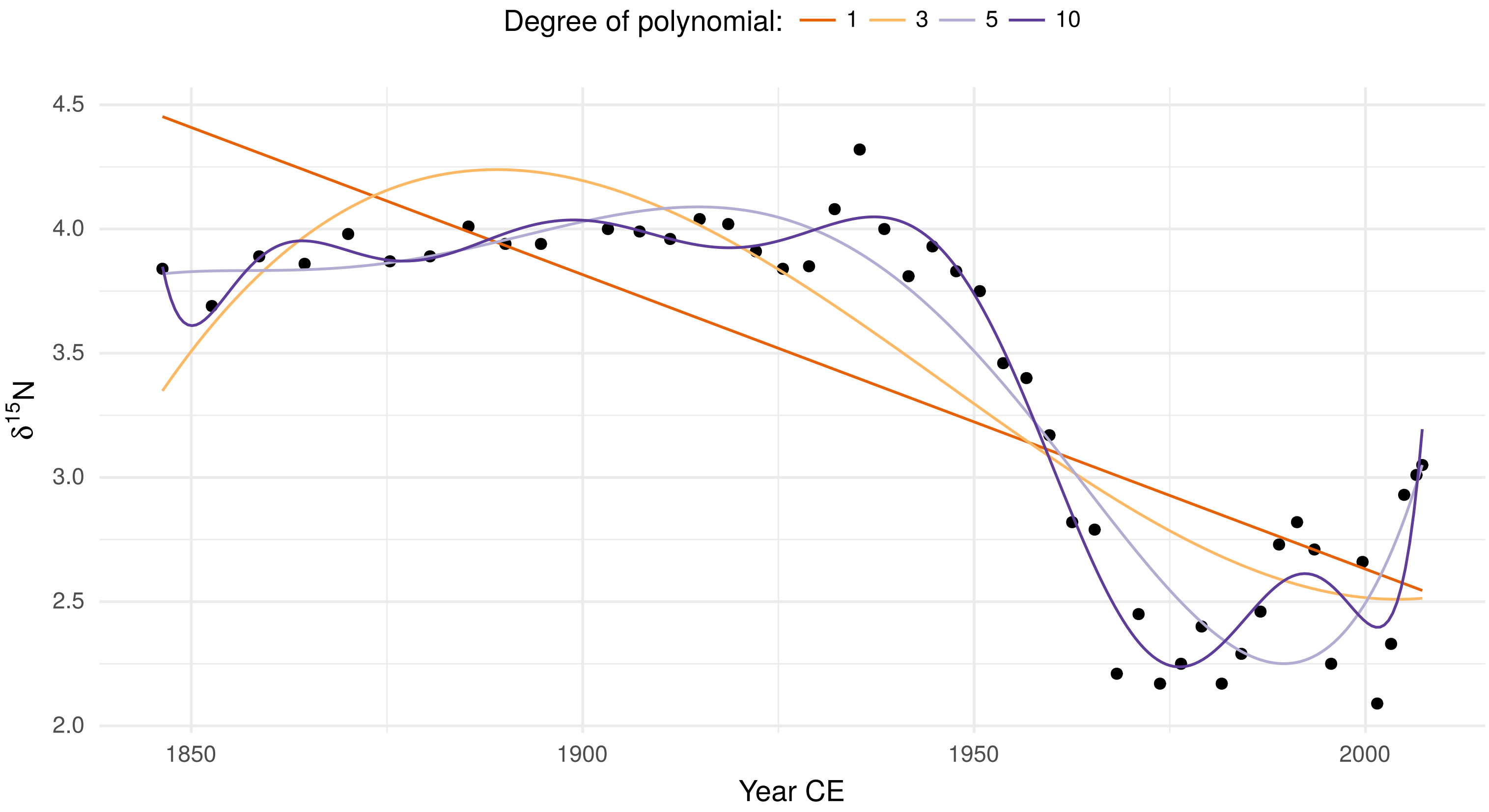
What about real data?

Small Water

What degree polynomial should we use here?



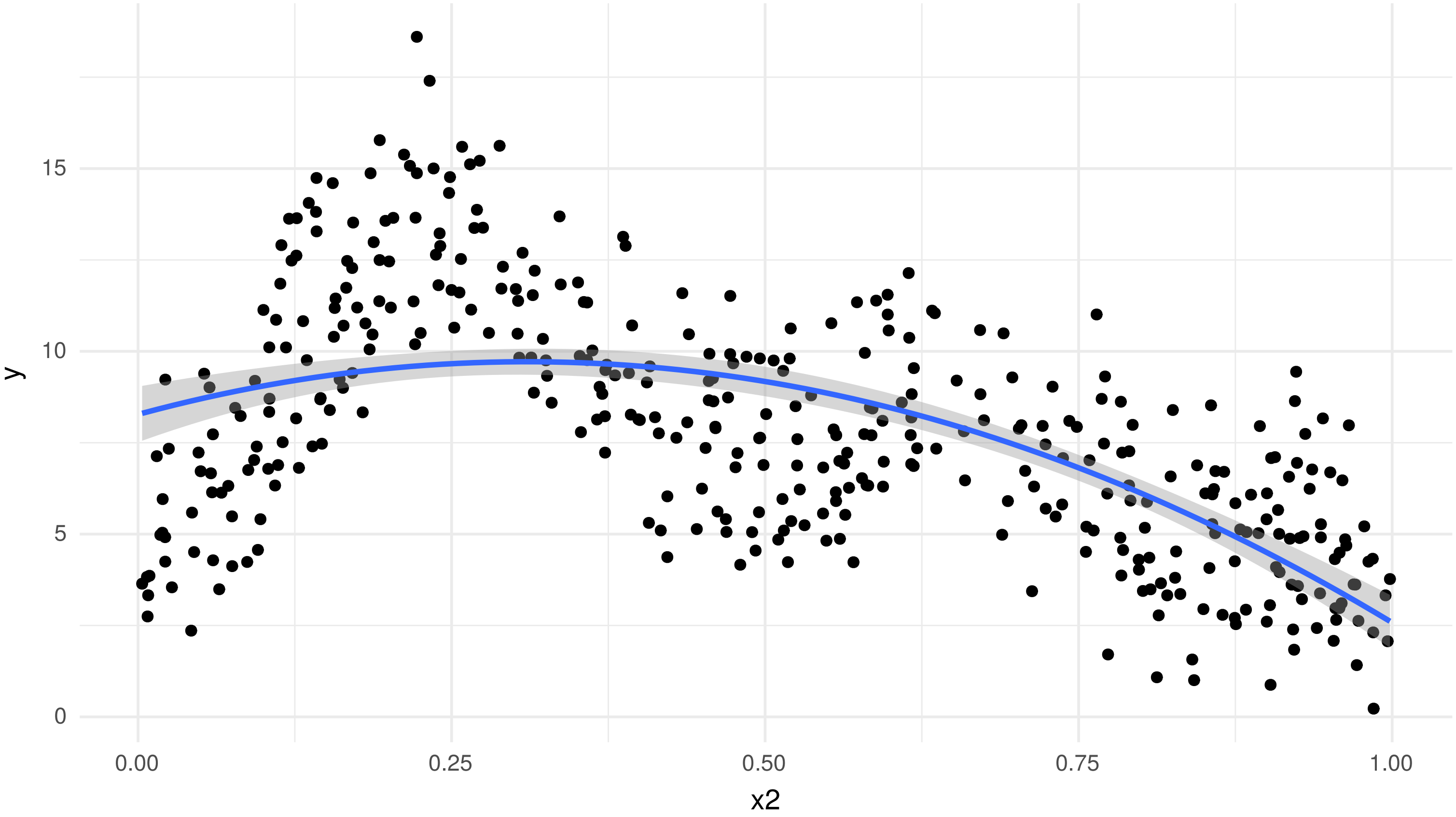
Polynomials



Is this sustainable?

Adding in quadratic (and higher terms) *can* make sense — feels a bit *ad hoc*

Better if we had a **framework** to deal with these issues?



This is where GAMs are useful

How is a GAM different?

In GLM we model the mean of data as a sum of linear terms:

$$y_i = \beta_0 + \sum_j \beta_j x_{ji} + \epsilon_i$$

A GAM is a sum of *smooth functions* or *smooths*

$$y_i = \beta_0 + \sum_j s_j(x_{ji}) + \epsilon_i$$

where $\epsilon_i \sim N(0, \sigma^2)$, $y_i \sim \text{Normal}$ (for now)

Call the above equation the **linear predictor** in both cases.

Fitting a GAM in R

```r
model <- gam(y ~ s(x1) + s(x2) + te(x3, x4), # formuala describing model
             data = my_data_frame,           # your data
             method = 'REML',                # or 'ML'
             family = gaussian)              # or something more exotic
```

`s()` terms are smooths of one or more variables

`te()` terms are the smooth equivalent of *main effects + interactions*

Your turn

Load the Small Water data

```
small <- readRDS('./data/small-water-isotope-data.rds')
head(small)
```

```
  Depth   d13C  TotalC d15N TotalN DryWeight     Year
1   0.2 -27.57  806.49 3.05  64.21       8.2 2007.254
2   0.4 -27.67  949.33 3.01  73.26       7.6 2006.510
3   0.8 -27.63 1305.52 2.93  93.25      11.6 2004.941
4   1.2 -27.62 1136.04 2.33  86.09       9.6 2003.269
5   1.6 -27.48 1028.27 2.09  93.80      10.9 2001.496
6   2.0 -27.39  809.91 2.66  79.98       9.9 1999.626
```

Fit the GAM

```r
sw <- gam(d15N ~ s(Year), data = small, method = 'REML')
```

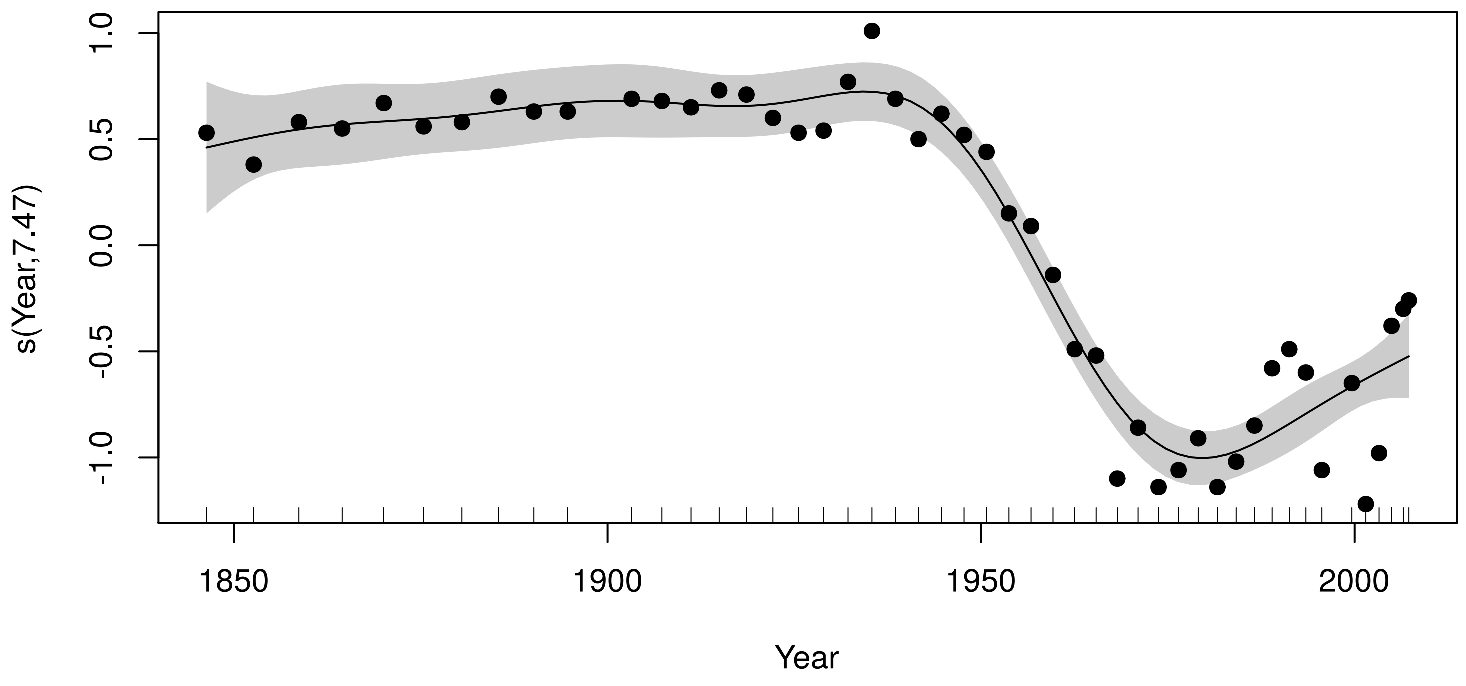
Look at the model summary

```
summary(sw)
```

```
Family: gaussian
Link function: identity

Formula:
d15N ~ s(Year)

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  3.30958    0.02805     118   <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(Year) 7.466  8.416 70.13  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.926   Deviance explained = 93.8%
-REML = 4.8282  Scale est. = 0.037771  n = 48
```

Plot the fitted smooth

```
plot(sw, shade = TRUE, residuals = TRUE, pch = 19)
```



What magic is this?

Rob Potter

Splines

Splines are *functions* composed of simpler functions

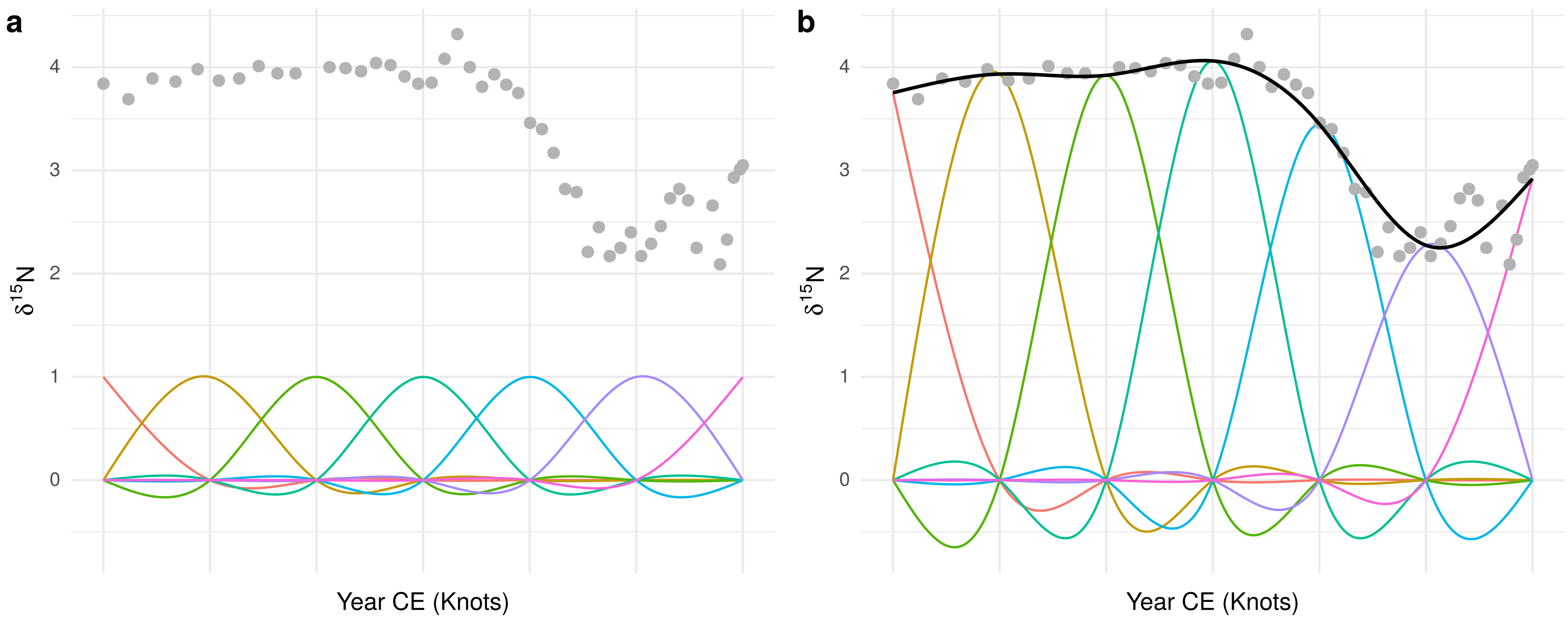
Simpler functions are *basis functions* & the set of basis functions is a *basis*

When we model using splines, each basis function b_k has a coefficient β_k

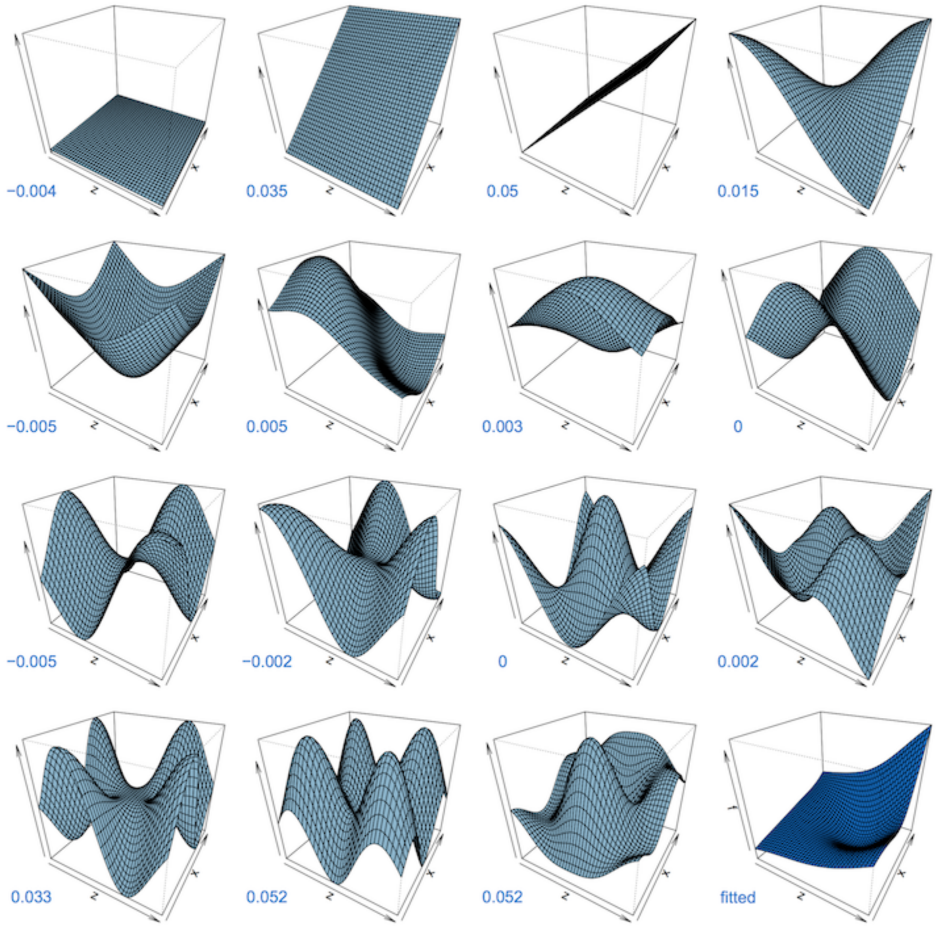
Resultant spline is a the sum of these weighted basis functions, evaluated at the values of x

$$s(x) = \sum_{k=1}^{K} \beta_k b_k(x)$$

Basis functions

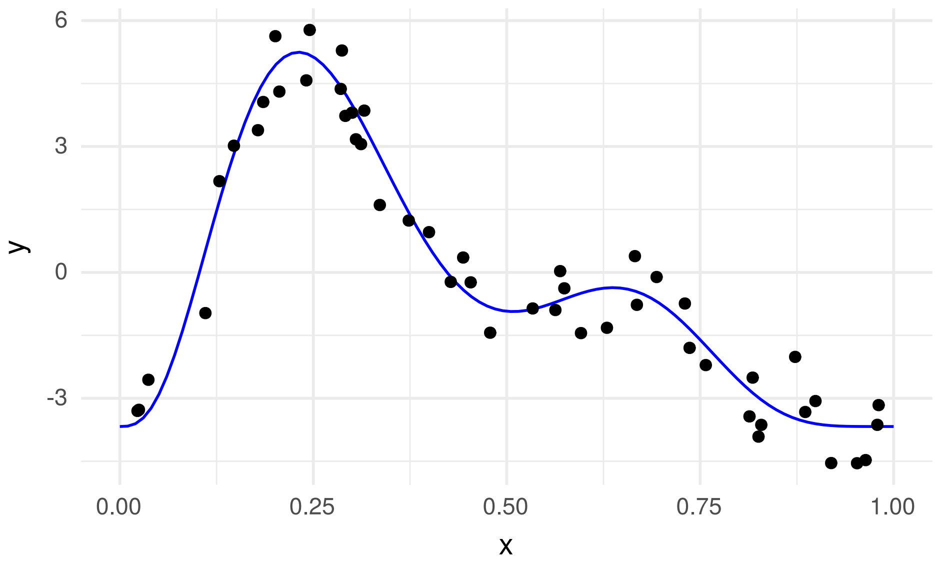


Basis functions



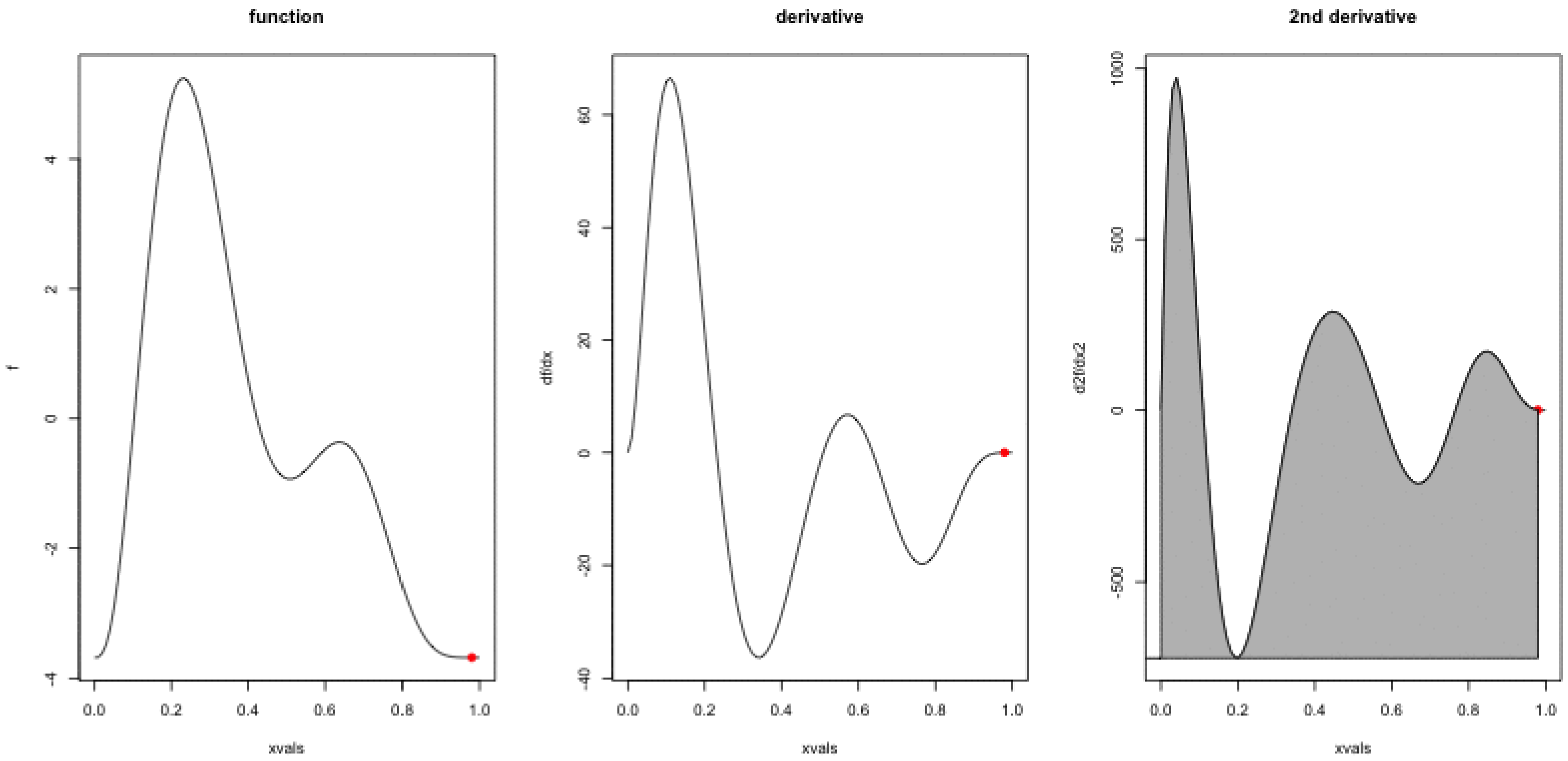
How do we avoid overfitting?

Avoiding overfitting



- Want a line that is *close* to all the data (high likelihood)
- Splines *could* just fit every data point, but this would be overfitting. We know there is *error*
- Easy to overfit — *smooth* curve.
- How do we measure smoothness? Calculus!

Measuring wiggliness



What was that grey bit? Wigglyness

$$\int_{\mathbb{R}} \left(\frac{\partial^2 f(x)}{\partial^2 x} \right)^2 \mathrm{d}x = \boldsymbol{\beta}^{\mathrm{T}} S \boldsymbol{\beta} = W$$

(Wigglyness is 100% the right mathy word)

We penalize wiggliness to avoid overfitting

Making wigglyness matter

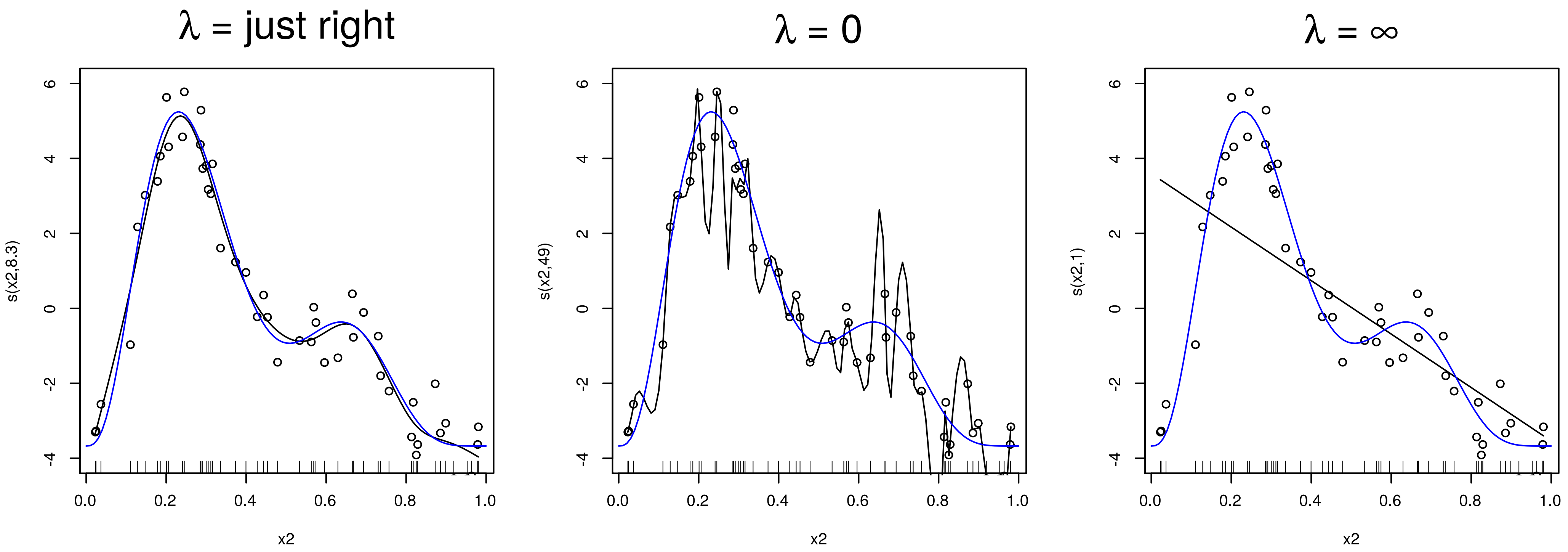
W measures **wigglyness**

(log) likelihood measures closeness to the data

We use a **smoothing parameter** λ to define the trade-off, to find the spline coefficients B_k that maximize the **penalized** log-likelihood

$$\mathcal{L}_p = \log(\text{Likelihood}) - \lambda W$$

Picking the right wiggliness



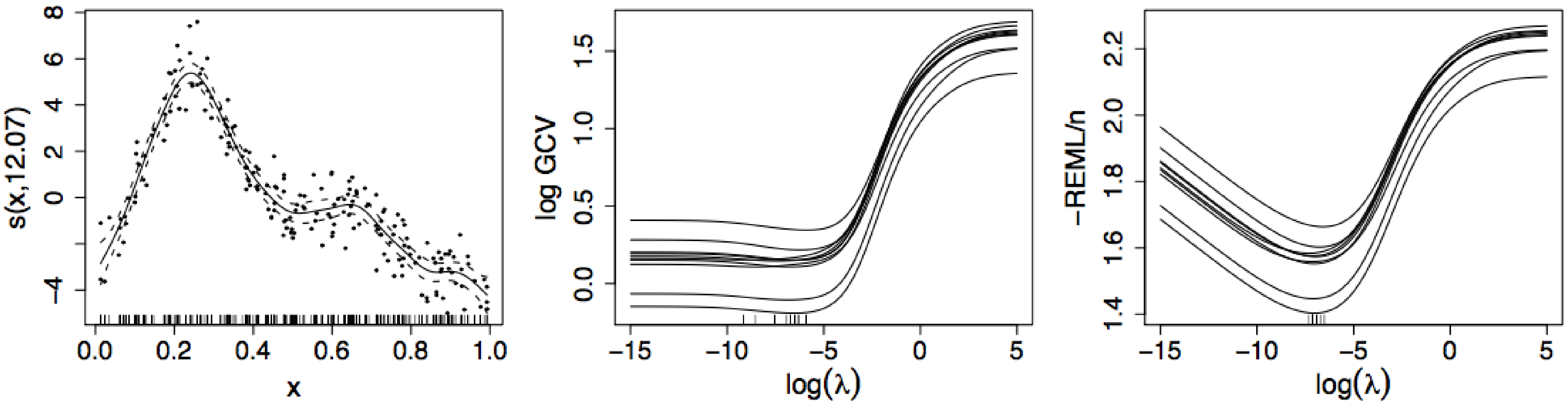
Picking the right wiggliness

Two ways to think about how to optimize λ:

- Predictive: Minimize out-of-sample error
- Bayesian: Put priors on our basis coefficients

Many methods: AIC, Mallow's C_p, GCV, ML, REML

- **Practically**, use **REML**, because of numerical stability
- Hence `gam(..., method="REML")`



Maximum wiggliness

We set **basis complexity** or "size" k

This is *maximum wigglyness*, can be thought of as number of small functions that make up a curve

Once smoothing is applied, curves have fewer **effective degrees of freedom (EDF)**

EDF < k

k must be *large enough*, the λ penalty does the rest

Large enough — space of functions representable by the basis includes the true function or a close approximation to the tru function

Bigger k increases computational cost

In **mgcv**, default k values are arbitrary — after choosing the model terms, this is the key user choice

Must be checked! — `gam.check()`

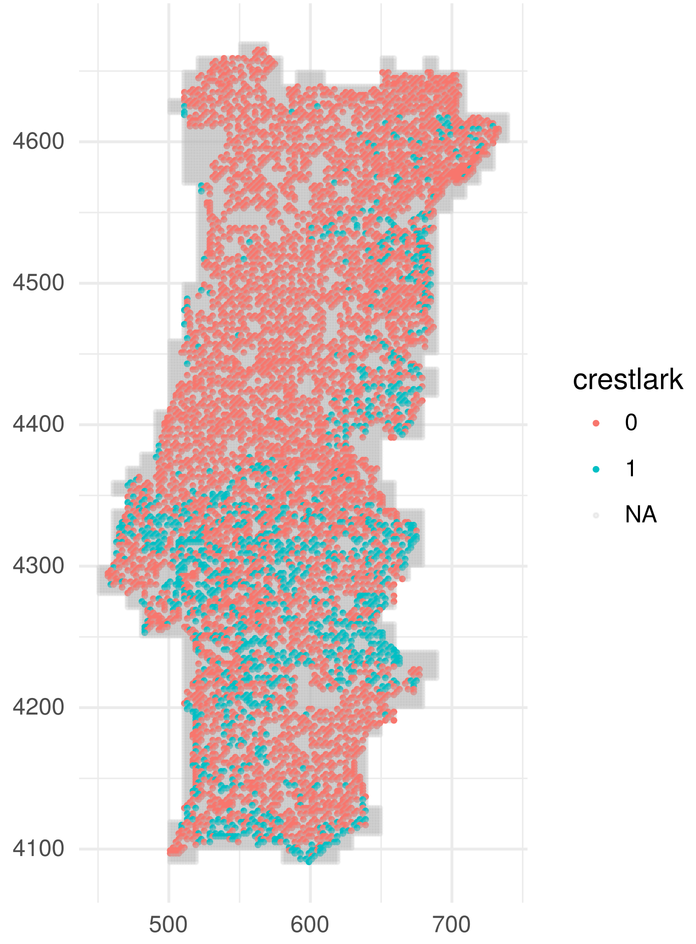
GAM summary so far

1. GAMs give us a framework to model flexible nonlinear relationships
2. Use little functions (**basis functions**) to make big functions (**smooths**)
3. Use a **penalty** to trade off wiggliness/generality
4. Need to make sure your smooths are **wiggly enough**

Portugese larks

```r
library('gamair')
data(bird)

bird <- transform(bird,
            crestlark = factor(crestlark),
            linnet = factor(linnet),
            e = x / 1000,
            n = y / 1000)
head(bird)
```

```
      QUADRICULA TET crestlark linnet      x       y   e
13705       NG56   E      <NA>   <NA> 551000 4669000 551
13710       NG56   J      <NA>   <NA> 553000 4669000 553
13715       NG56   P      <NA>   <NA> 555000 4669000 555
13720       NG56   U      <NA>   <NA> 557000 4669000 557
13725       NG56   Z      <NA>   <NA> 559000 4669000 559
13880       NG66   E      <NA>   <NA> 561000 4669000 561
```



Portugese larks — binomial GAM

```r
crest <- gam(crestlark ~ s(e, n, k = 100),
             data = bird,
             family = binomial,
             method = 'REML')
```

$s(e, n)$ indicated by `s(e, n)` in the formula

Isotropic thin plate spline

`k` sets size of basis dimension; upper limit on EDF

Smoothness parameters estimated via REML

```r
summary(crest)
```

```

Family: binomial
Link function: logit

Formula:
crestlark ~ s(x, y, k = 100)

Parametric coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -2.24192    0.07743  -28.95   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
         edf Ref.df Chi.sq p-value
s(x,y) 74.05  86.62  859.3  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.234   Deviance explained = 25.8%
-REML = 2501.6  Scale est. = 1         n = 6457
```

Portugese larks — binomial GAM

Model checking with binary data is a pain — residuals look weird

Alternatively we can aggregate data at the `QUADRICULA` level & fit a binomial count model

```r
## convert back to numeric
bird <- transform(bird,
                  crestlark = as.numeric(as.character(crestlark)),
                  linnet = as.numeric(as.character(linnet)))
## some variables to help aggregation
bird <- transform(bird, tet.n = rep(1, nrow(bird)),
                  N = rep(1, nrow(bird)), stringsAsFactors = FALSE)
## set to NA if not surveyed
bird$N[is.na(as.vector(bird$crestlark))] <- NA
## aggregate
bird2 <- aggregate(data.matrix(bird), by = list(bird$QUADRICULA),
                   FUN = sum, na.rm = TRUE)
## scale by Quads aggregated
bird2 <- transform(bird2, e = e / tet.n, n = n / tet.n)

## fit binomial GAM
crest2 <- gam(cbind(crestlark, N - crestlark) ~ s(e, n, k = 100),
              data = bird2, family = binomial, method = 'REML')
```

Model checking

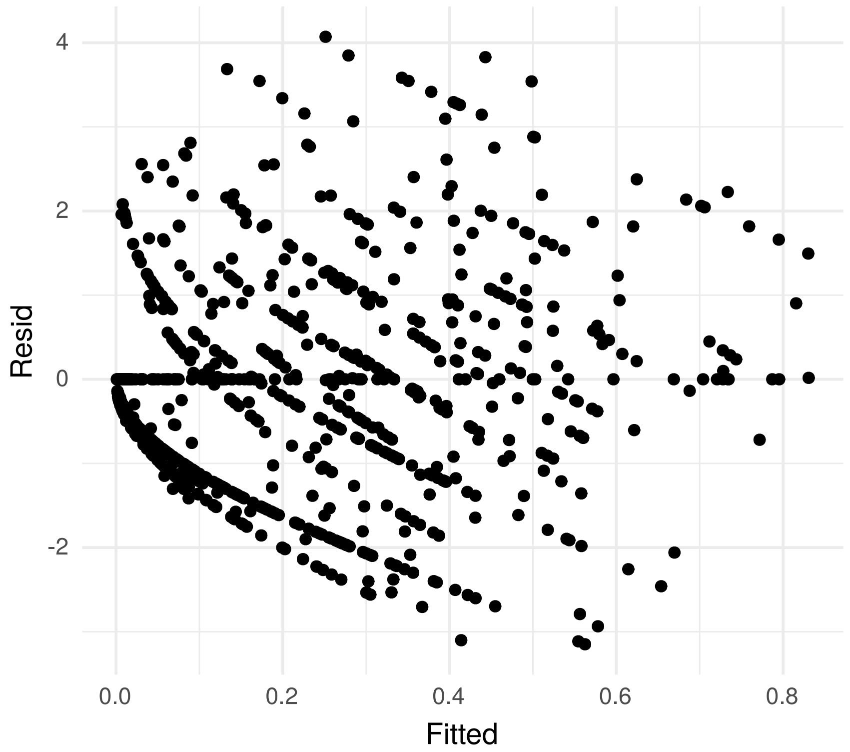
Model residuals don't look too bad

Bands of points due to integers

```
crest3 <- gam(cbind(crestlark, N - crestlark) ~
                  s(e, n, k = 100),
              data = bird2, family = quasibinomial,
              method = 'REML')
```

Some overdispersion — φ = 2.32

```
ggplot(data.frame(Fitted = fitted(crest2),
                  Resid = resid(crest2)),
       aes(Fitted, Resid)) + geom_point()
```



Model checking

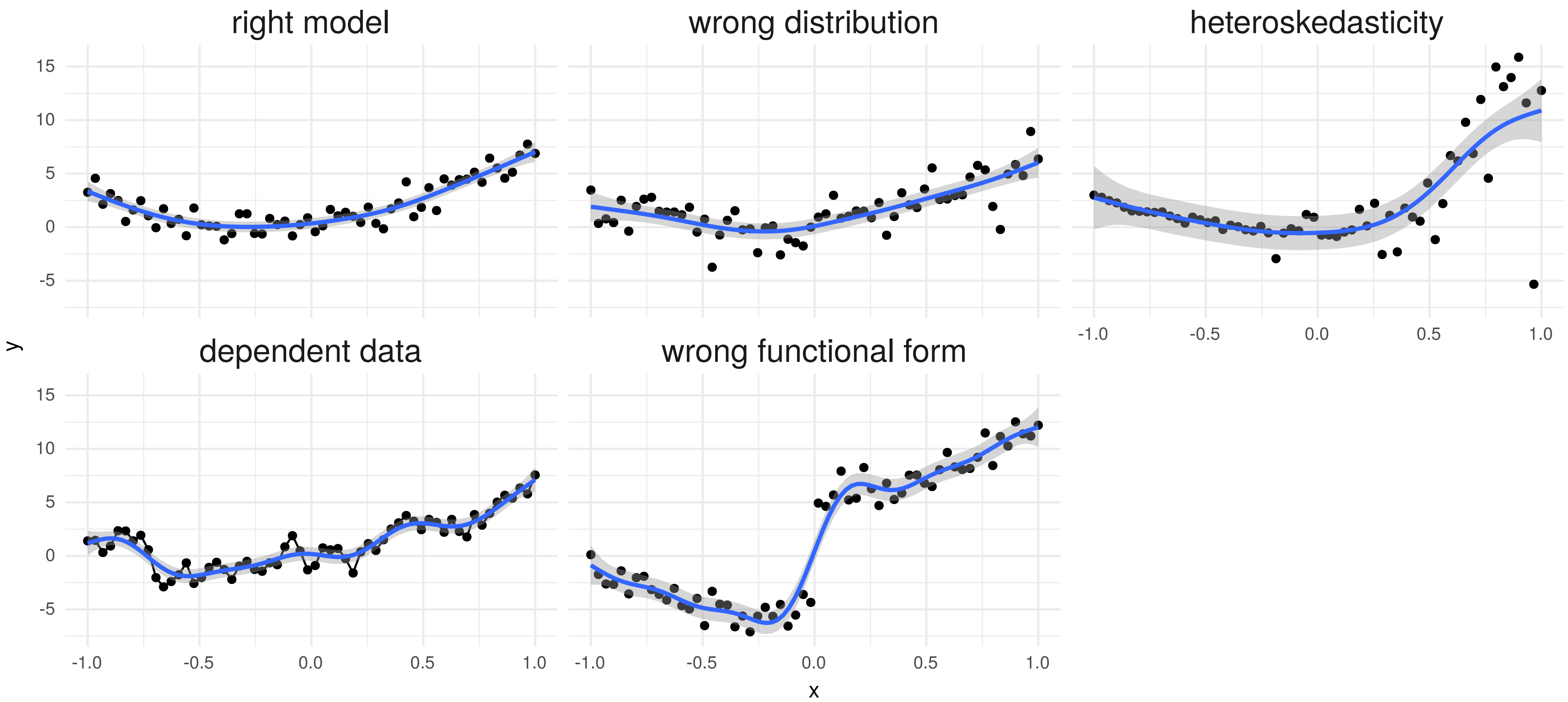
Model checking

So you have a GAM:

- How do you know you have the right degrees of freedom? `gam.check()`
- Diagnosing model issues: `gam.check()` part 2

GAMs are models too

With all models, how accurate your predictions will be depends on how good the model is

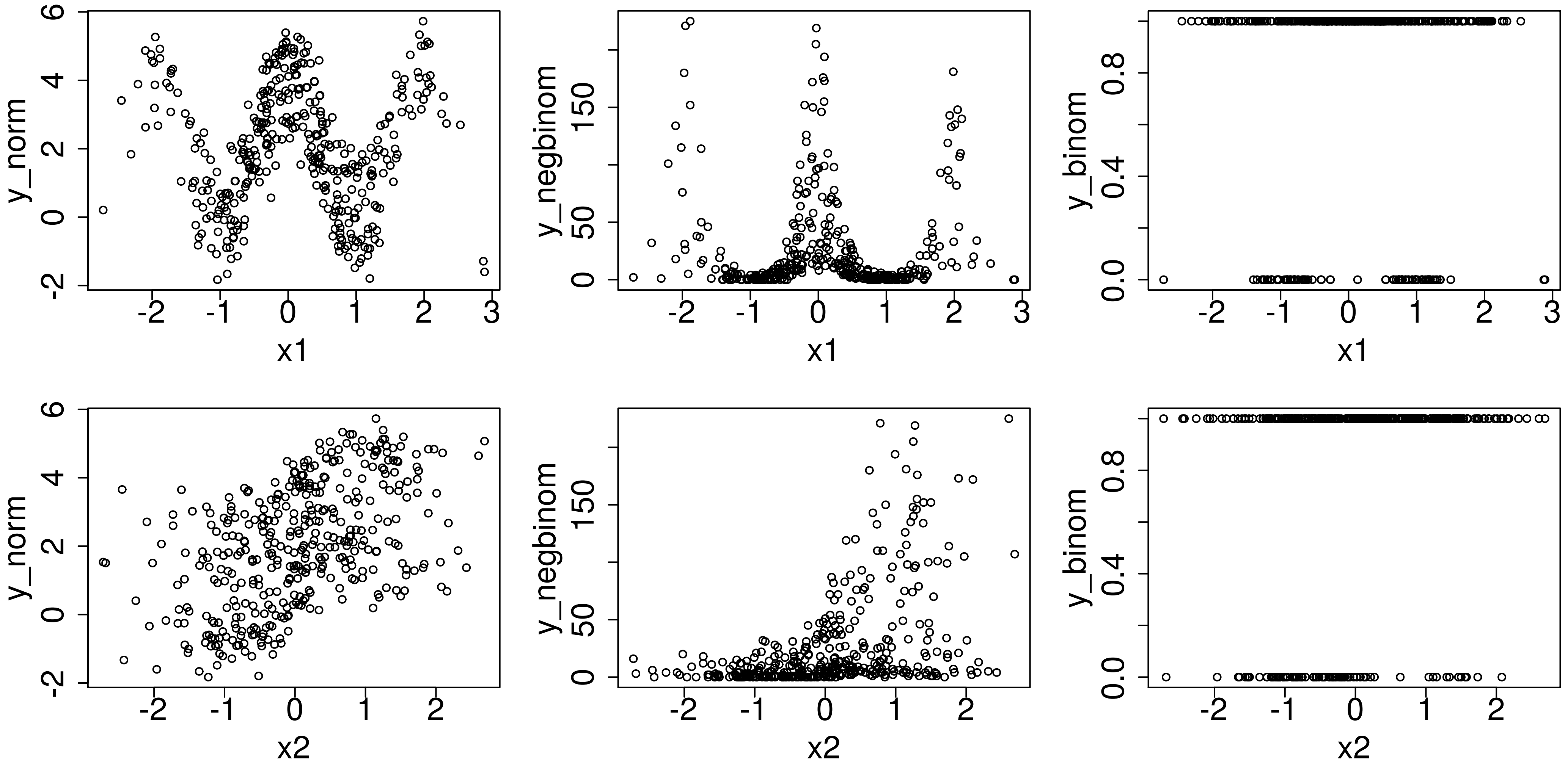


How do we test how well our model fits?

Examples

```r
set.seed(2)
n <- 400
x1 <- rnorm(n)
x2 <- rnorm(n)
y_val <- 1 + 2*cos(pi*x1) + 2/(1+exp(-5*(x2)))
y_norm <- y_val + rnorm(n, 0, 0.5)
y_negbinom <- rnbinom(n, mu = exp(y_val),size=10)
y_binom <- rbinom(n,1,prob = exp(y_val)/(1+exp(y_val)))
```

Examples


y_norm
x1
y_negbinom
x1
y_binom
x1
y_norm
x2
y_negbinom
x2
y_binom
x2

gam.check() part 1: do you have the right functional form?

How well does the model fit?

- Many choices: k, family, type of smoother, …
- How do we assess how well our model fits?

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

```r
norm_model_1 = gam(y_norm~s(x1,k=4)+s(x2,k=4),method= "REML")
gam.check(norm_model_1)
```

```
Method: REML   Optimizer: outer newton
full convergence after 8 iterations.
Gradient range [-0.0003467788,0.0005154578]
(score 736.9402 & scale 2.252304).
Hessian positive definite, eigenvalue range [0.000346021,198.5041].
Model rank =  7 / 7 

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(x1) 3.00 1.00    0.13  <2e-16 ***
s(x2) 3.00 2.91    1.04    0.79    
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Checking basis size

```
norm_model_2 = gam(y_norm~s(x1,k=12)+s(x2,k=4),method= "REML")
gam.check(norm_model_2)
```

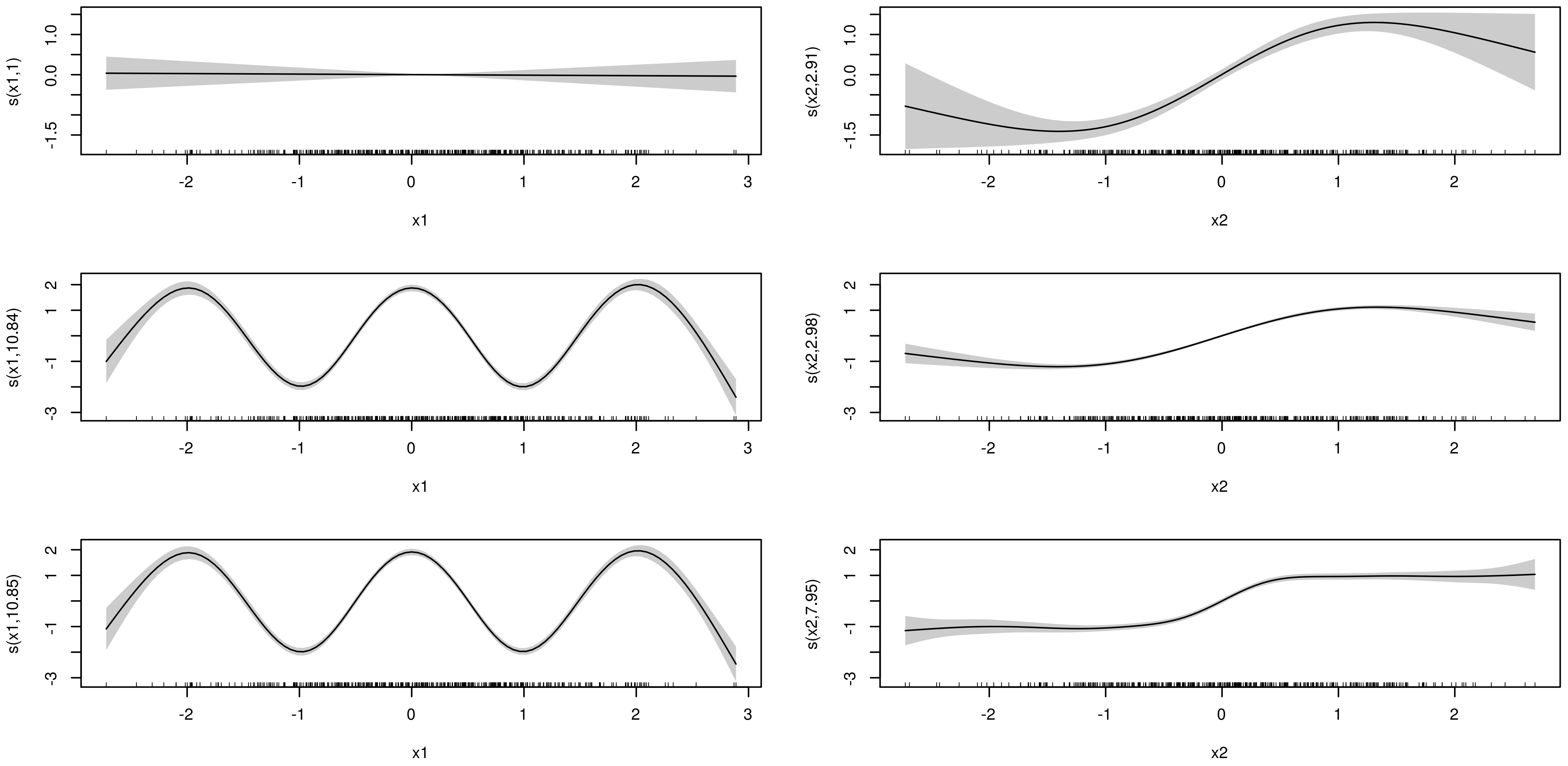
```
Method: REML   Optimizer: outer newton
full convergence after 11 iterations.
Gradient range [-5.658609e-06,5.392657e-06]
(score 345.3111 & scale 0.2706205).
Hessian positive definite, eigenvalue range [0.967727,198.6299].
Model rank =  15 / 15

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(x1) 11.00 10.84    0.99    0.41
s(x2)  3.00  2.98    0.86  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Checking basis size

```
norm_model_3 = gam(y_norm~s(x1,k=12)+s(x2,k=12),method= "REML")
gam.check(norm_model_3)
```

```
Method: REML   Optimizer: outer newton
full convergence after 8 iterations.
Gradient range [-5.103686e-05,-1.089481e-08]
(score 334.2084 & scale 0.2485446).
Hessian positive definite, eigenvalue range [2.812257,198.6868].
Model rank =  23 / 23 

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(x1) 11.00 10.85    0.98    0.28
s(x2) 11.00  7.95    0.95    0.12
```

Checking basis size



Using gam.check() part 2: visual checks

gam.check() plots

`gam.check()` creates 4 plots:

1. Quantile-quantile plots of residuals. If the model is right, should follow 1-1 line
2. Histogram of residuals
3. Residuals vs. linear predictor
4. Observed vs. fitted values

`gam.check()` uses deviance residuals by default

gam.check() plots: Gaussian data, Gaussian model

```r
norm_model <- gam(y_norm ~ s(x1, k=12) + s(x2, k=12), method = 'REML')
gam.check(norm_model)
```

gam.check() plots: negative binomial data, Poisson model

```
pois_model <- gam(y_negbinom ~ s(x1, k=12) + s(x2, k=12), family=poisson, method= 'REML')
gam.check(pois_model)
```

gam.check() plots: neg binomial data, neg binomial model

```
negbin_model <- gam(y_negbinom ~ s(x1, k=12) + s(x2, k=12), family = nb, method = 'REML')
gam.check(negbin_model)
```

Model selection

Model selection

Model (or variable) selection — an important area of theoretical and applied interest

- In statistics we aim for a balance between *fit* and *parsimony*
- In applied research we seek the set of covariates with strongest effects on $\boldsymbol{y}$

We seek a subset of covariates that improves *interpretability* and *prediction accuracy*

Shrinkage & additional penalties

Shrinkage & additional penalties

Smoothing parameter estimation allows selection of a wide range of potentially complex functions for smooths...

But, cannot remove a term entirely from the model because the penalties used act only on the *range space* of a spline basis. The *null space* of the basis is unpenalised.

- **Null space** — the basis functions that are smooth (constant, linear)
- **Range space** — the basis functions that are wiggly

Shrinkage & additional penalties

mgcv has two ways to penalize the null space, i.e. to do selection

- *double penalty approach* via `select = TRUE`
- *shrinkage approach* via special bases for
    - thin plate spline (default, `s(..., bs = 'ts')`),
    - cubic splines (`s(..., bs = 'cs')`)

double penalty tends to works best, but applies to all smooths *and* doubles the number of smoothness parameters to estimate

Other shrinkage/selection approaches *are available* in other software

Empirical Bayes...?

$\mathbf{S}_j$ can be viewed as prior precision matrices and λ_j as improper Gaussian priors on the spline coefficients.

The impropriety derives from $\mathbf{S}_j$ not being of full rank (zeroes in $\mathbf{\Lambda}_j$).

Both the double penalty and shrinkage smooths remove the impropriety from the Gaussian prior

Empirical Bayes...?

- **Double penalty** — makes no assumption as to how much to shrink the null space. This is determined from the data via estimation of λ_j^*

- **Shrinkage smooths** — assumes null space should be shrunk less than the wiggly part

Marra & Wood (2011) show that the double penalty and the shrinkage smooth approaches

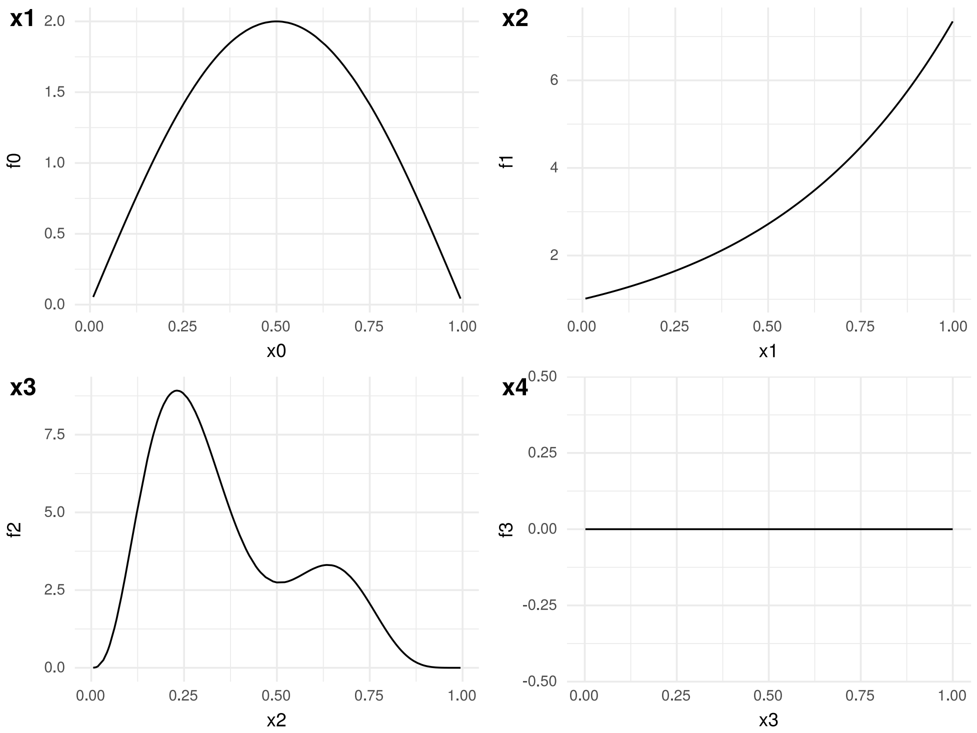
- performed significantly better than alternatives in terms of *predictive ability*, and

- performed as well as alternatives in terms of variable selection

Example

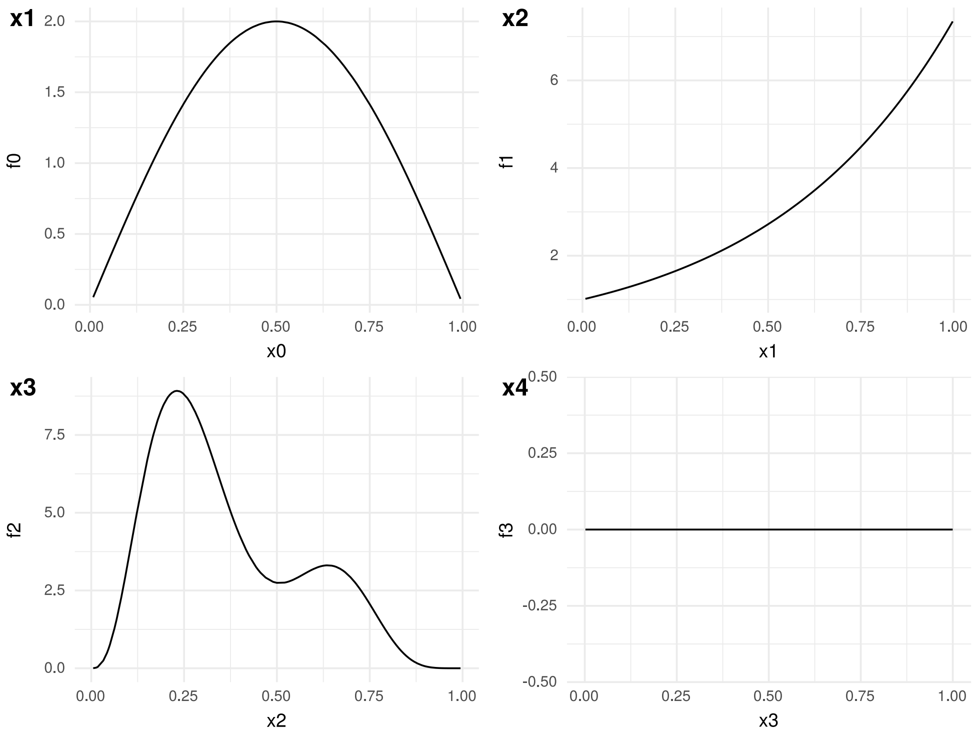
- Simulate Poisson counts
- 4 known functions (left)
- 2 spurious covariates (`runif()` & not shown)

```r
b <- gam(y ~ s(x0) + s(x1) + s(x2) + s(x3) +
               s(x4) + s(x5),
         data = dat,
         family = poisson,
         select = TRUE, method = 'REML')
```

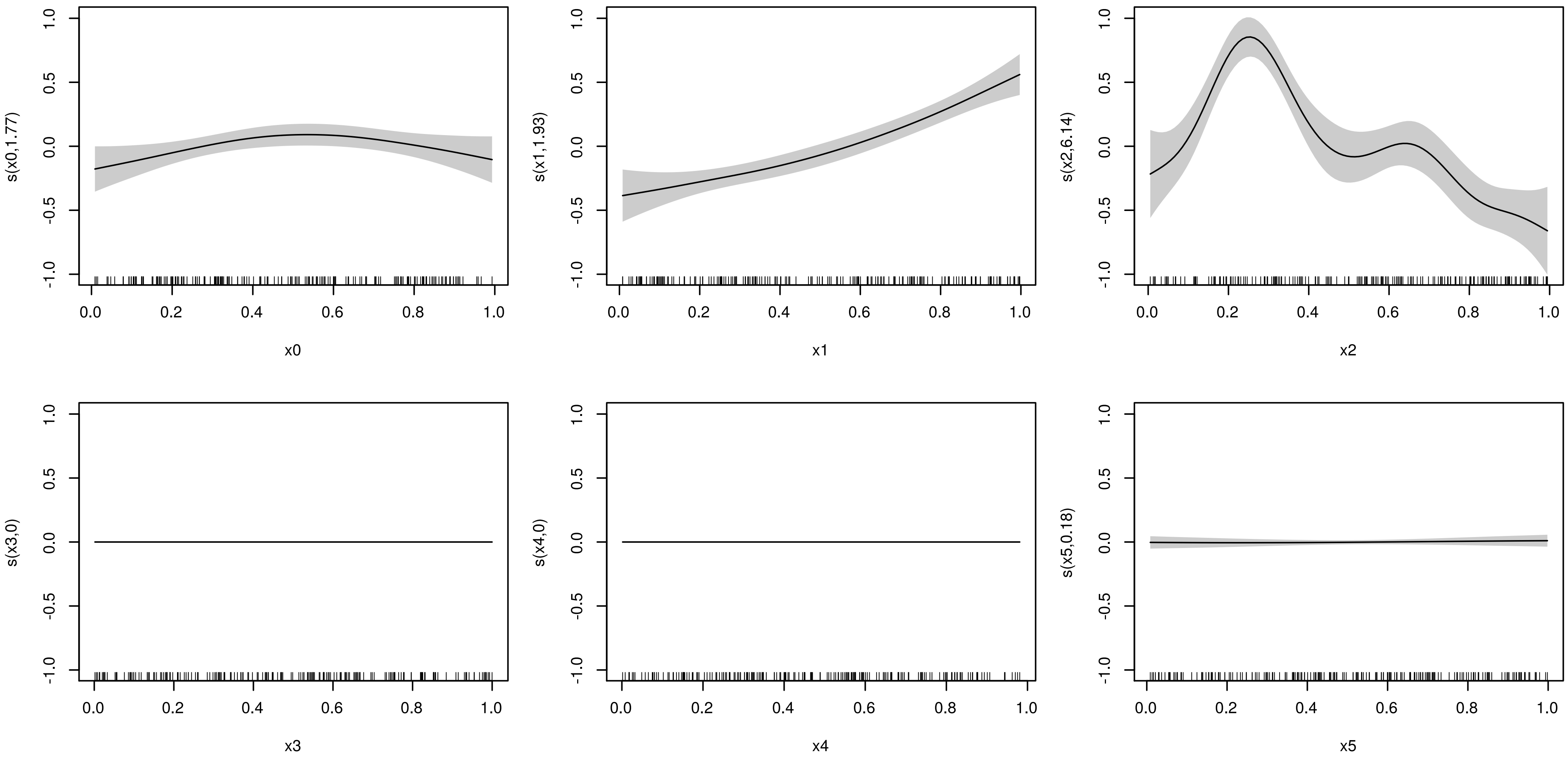


Example

```
Family: poisson
Link function: log

Formula:
y ~ s(x0) + s(x1) + s(x2) + s(x3) + s(x4) + s(x5)

Parametric coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)  1.21758    0.04082   29.83   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Approximate significance of smooth terms:
            edf Ref.df  Chi.sq p-value
s(x0) 1.7655082      9   5.264  0.0397 *
s(x1) 1.9271042      9  65.356  <2e-16 ***
s(x2) 6.1351238      9 156.204  <2e-16 ***
s(x3) 0.0003538      9   0.000  0.3836
s(x4) 0.0001553      9   0.000  1.0000
s(x5) 0.1756882      9   0.195  0.2963
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.545   Deviance explained = 51.6%
-REML = 430.78  Scale est. = 1         n = 200
```



Example



s(x0,1.77)
s(x1,1.93)
s(x2,6.14)
s(x3,0)
s(x4,0)
s(x5,0.18)
x0
x1
x2
x3
x4
x5
-1.0
-0.5
0.0
0.5
1.0
0.0
0.2
0.4
0.6
0.8
1.0

Confidence intervals for smooths

Confidence intervals for smooths

`plot.gam()` produces approximate 95% intervals (at +/- 2 SEs)

What do these intervals represent?

Nychka (1988) showed that standard Wahba/Silverman type Bayesian confidence intervals on smooths had good **across-the-function** frequentist coverage properties

When *averaged* over the range of covariate, $1 - \alpha$ coverage is approximately $1 - \alpha$

Confidence intervals for smooths

Marra & Wood (2012) extended this theory to the generalised case and explain where the coverage properties failed:

Musn't over-smooth too much, which happens when λ_j *are over-estimated*

Two situations where this might occur

1. where true effect is almost in the penalty null space, $\hat{\lambda}_j \rightarrow \infty$
    - ie. close to a linear function
2. where $\hat{\lambda}_j$ difficult to estimate due to highly correlated covariates
    - if 2 correlated covariates have different amounts of wiggliness, estimated effects can have degree of smoothness *reversed*

Don't over-smooth

> In summary, we have shown that Bayesian componentwise variable width intervals... for the smooth components of an additive model **should achieve close to nominal *across-the-function* coverage probability**, provided only that we do not over-smooth so heavily... Beyond this requirement not to oversmooth too heavily, the results appear to have rather weak dependence on smoothing parameter values, suggesting that the neglect of smoothing parameter variability should not significantly degrade interval performance.

Basically

1. Don't over smooth, and

2. Effect of uncertainty due to estimating smoothness parameter is small

Confidence intervals for smooths

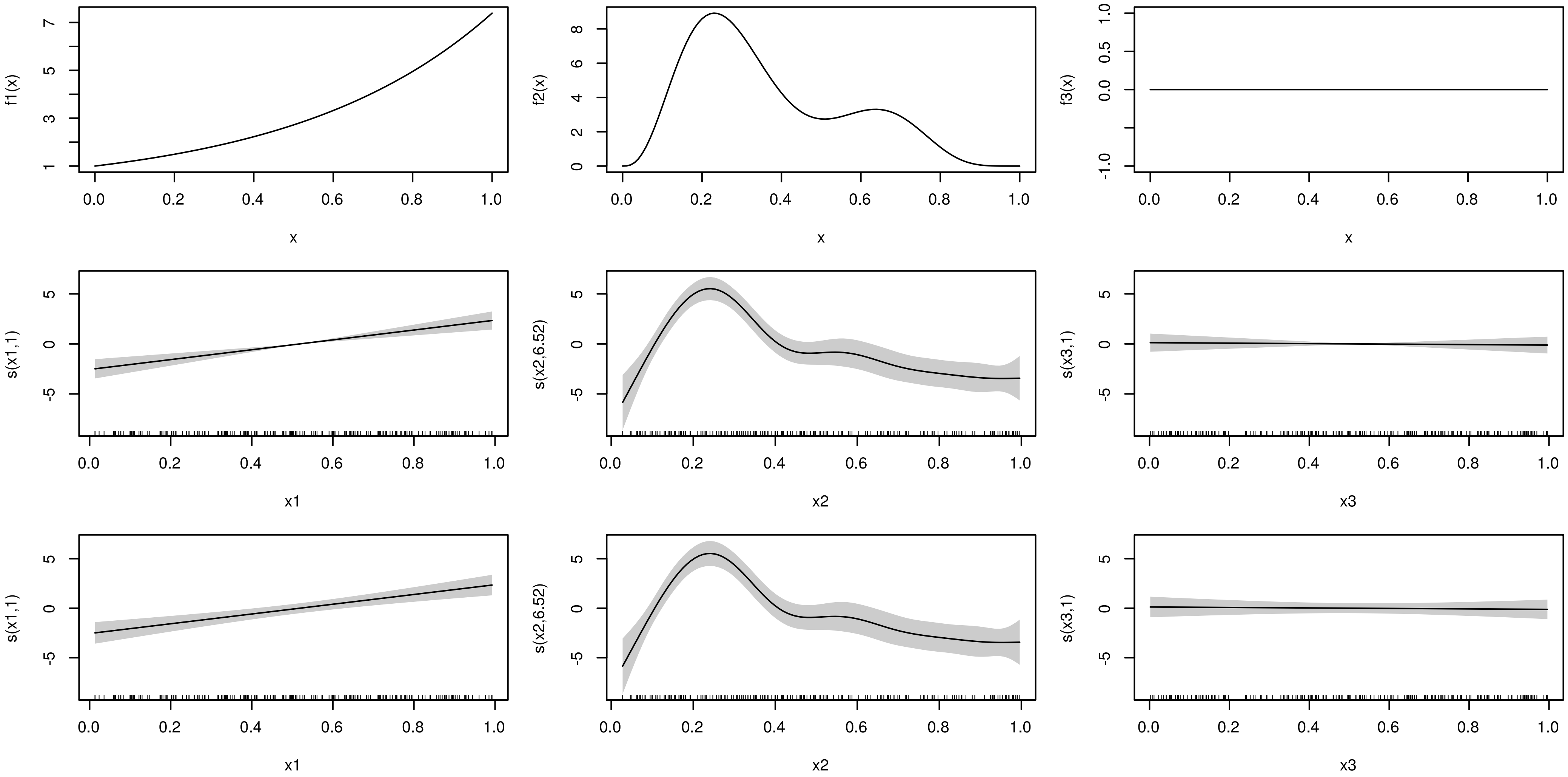
Marra & Wood (2012) suggested a solution to situation 1., namely true functions close to the penalty null space.

Smooths are normally subject to *identifiability* constraints (centred), which leads to zero variance where the estimated function crosses the zero line.

Instead, compute intervals for j th smooth as if it alone had the intercept; identifiability constraints go on the other smooth terms.

Use `seWithMean = TRUE` in call to `plot.gam()`

Example



p values for smooths

p values for smooths

p values for smooths are approximate:

1. they don't account for the estimation of λ_j — treated as known, hence *p* values are biased low

2. rely on asymptotic behaviour — they tend towards being right as sample size tends to ∞

The approach described in Wood (2006) is "*no longer recommended*"!

p values for smooths

...are a test of **zero-effect** of a smooth term

Default *p* values rely on theory of Nychka (1988) and Marra & Wood (2012) for confidence interval coverage

If the Bayesian CI have good across-the-function properties, Wood (2013a) showed that the *p* values have

- almost the correct null distribution
- reasonable power

Test statistic is a form of χ^2 statistic, but with complicated degrees of freedom

p values for unpenalized smooths

The results of Nychka (1988) and Marra & Wood (2012) break down if smooth terms are unpenalized

This include i.i.d. Gaussian random effects, (e.g. `bs = "re"`)

Wood (2013b) proposed instead a test based on a likelihood ratio statistic:

- the reference distribution used is appropriate for testing a H_0 on the boundary of the allowed parameter space...
- ...in other words, it corrects for a H_0 that a variance term is zero

p values for smooths

Have the best behaviour when smoothness selection is done using ML, then REML.

Neither of these are the default, so remember to use `method = "ML"` or `method = "REML"` as appropriate

p values for parametric terms

p values are based on Wald statistics using the Bayesian covariance matrix for the coefficients.

This is the *right thing to do* when there are random effects terms present and doesn't really affect performance if there aren't.

Hence in most instances you won't need to change the default `freq = FALSE` in `summary.gam()`

anova()

mgcv provides an `anova()` method for `"gam"` objects:

1. Single model form: `anova(m1)`

2. Multi model form: `anova(m1, m2, m3)`

anova() — single model form

This differs from `anova()` methods for `"lm"` or `"glm"` objects:

- the tests are Wald-like tests as described for `summary.gam()` of a H_0 of zero-effect of a smooth term
- these are not *sequential* tests!

```
b1 <- gam(y ~ x0 + s(x1) + s(x2) + s(x3),
          method = "REML")
anova(b1)
```

```
Family: gaussian
Link function: identity

Formula:
y ~ x0 + s(x1) + s(x2) + s(x3)

Parametric Terms:
   df     F  p-value
x0  3 26.94 1.57e-14

Approximate significance of smooth terms:
        edf Ref.df      F  p-value
s(x1) 1.000  1.001 26.682 5.83e-07
s(x2) 6.694  7.807 18.755  < 2e-16
s(x3) 1.000  1.000  0.068    0.795
```

anova() — multi model form

The multi-model form should really be used with care — the *p* values are really *approximate*

```r
b1 <- gam(y ~ s(x0) + s(x1) + s(x2) + s(x3) + s(x4) + s(x5),
          data = dat, family=poisson, method = "ML")
b2 <- update(b1, . ~ . - s(x3) - s(x4) - s(x5))
anova(b2, b1, test = "Chisq")
```

```
Analysis of Deviance Table

Model 1: y ~ s(x0) + s(x1) + s(x2)
Model 2: y ~ s(x0) + s(x1) + s(x2) + s(x3) + s(x4) + s(x5)
  Resid. Df Resid. Dev     Df Deviance Pr(>Chi)
1    186.23     248.97
2    183.34     248.01 2.8959  0.96184    0.795
```

Don't used for testing random effect splines!

For *general smooths* deviance is replaced by $-2\mathcal{L}(\hat{\beta})$

AIC for GAMs

- Comparison of GAMs by a form of AIC is an alternative frequentist approach to model selection
- Rather than using the marginal likelihood, the likelihood of the β_j *conditional* upon λ_j is used, with the EDF replacing k, the number of model parameters
- This *conditional* AIC tends to select complex models, especially those with random effects, as the EDF ignores that λ_j are estimated
- Wood et al (2016) suggests a correction that accounts for uncertainty in λ_j

$$AIC = -2\mathcal{L}(\hat{\beta}) + 2\mathrm{tr}(\widehat{\mathcal{I}}V^{'}_{\beta})$$

AIC

In this example, x_3, x_4, and x_5 have no effects on y

```
AIC(b1, b2)
```

```
         df      AIC
b1 15.03493 847.7961
b2 12.12435 842.9368
```

When there is *no difference* in compared models, accepts larger model ~16% of the time: consistent with probability AIC chooses a model with 1 extra spurious parameter $Pr(\chi^2_1 > 2)$

```
pchisq(2, 1, lower.tail = FALSE)
```

```
[1] 0.1572992
```

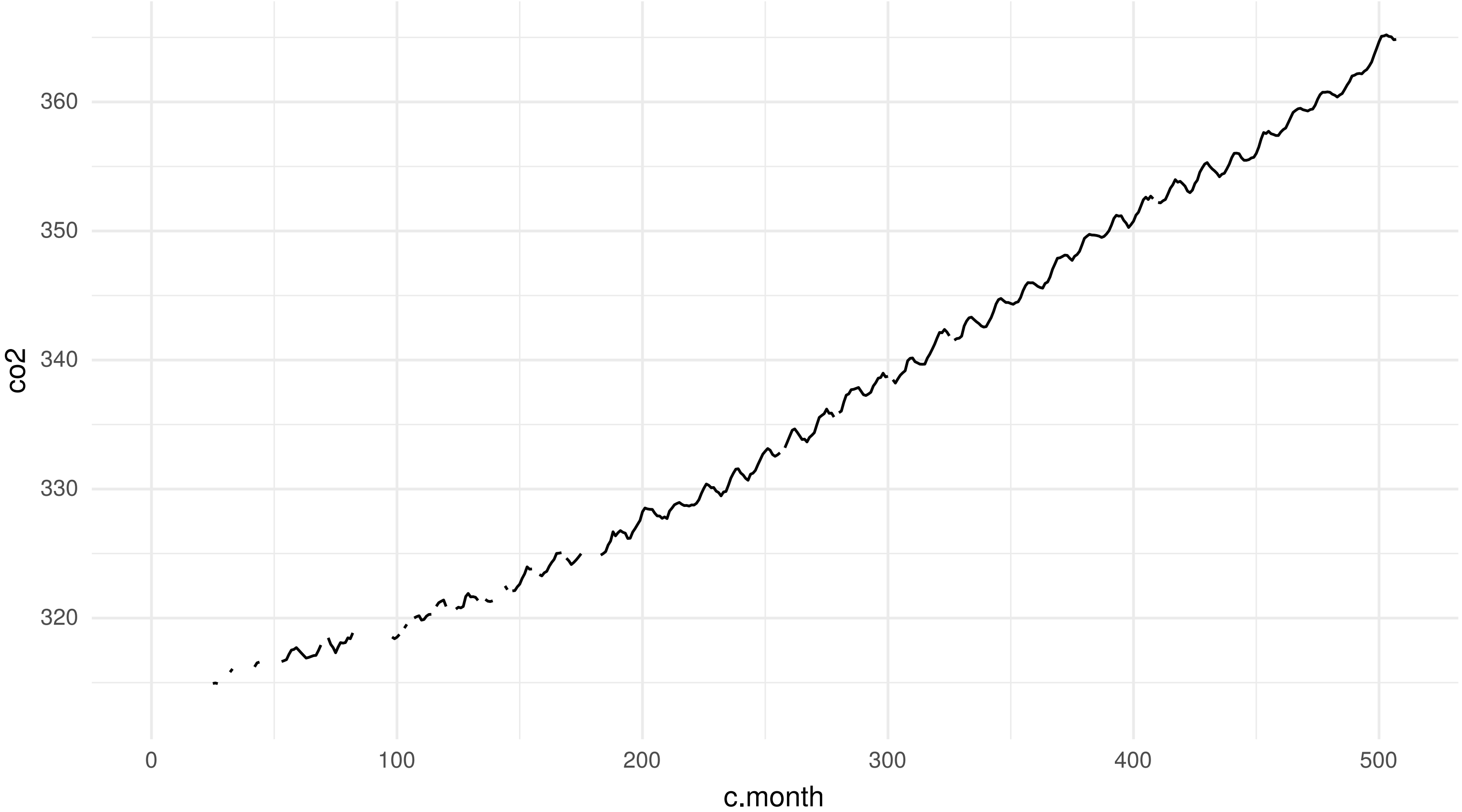
Atmospheric CO_2

```
data(co2s)
head(co2s)
```

```
     co2 c.month month
1     NA       1     1
2     NA       2     2
3     NA       3     3
4     NA       4     4
5     NA       5     5
6 313.21       6     6
```

Atmospheric CO_2

```
ggplot(co2s, aes(x = c.month, y = co2)) +
    geom_line()
```



Atmospheric CO_2 — fit naive GAM

```r
b <- gam(co2 ~ s(c.month, k=300, bs="cr"), data = co2s, method = 'REML')
summary(b)
```

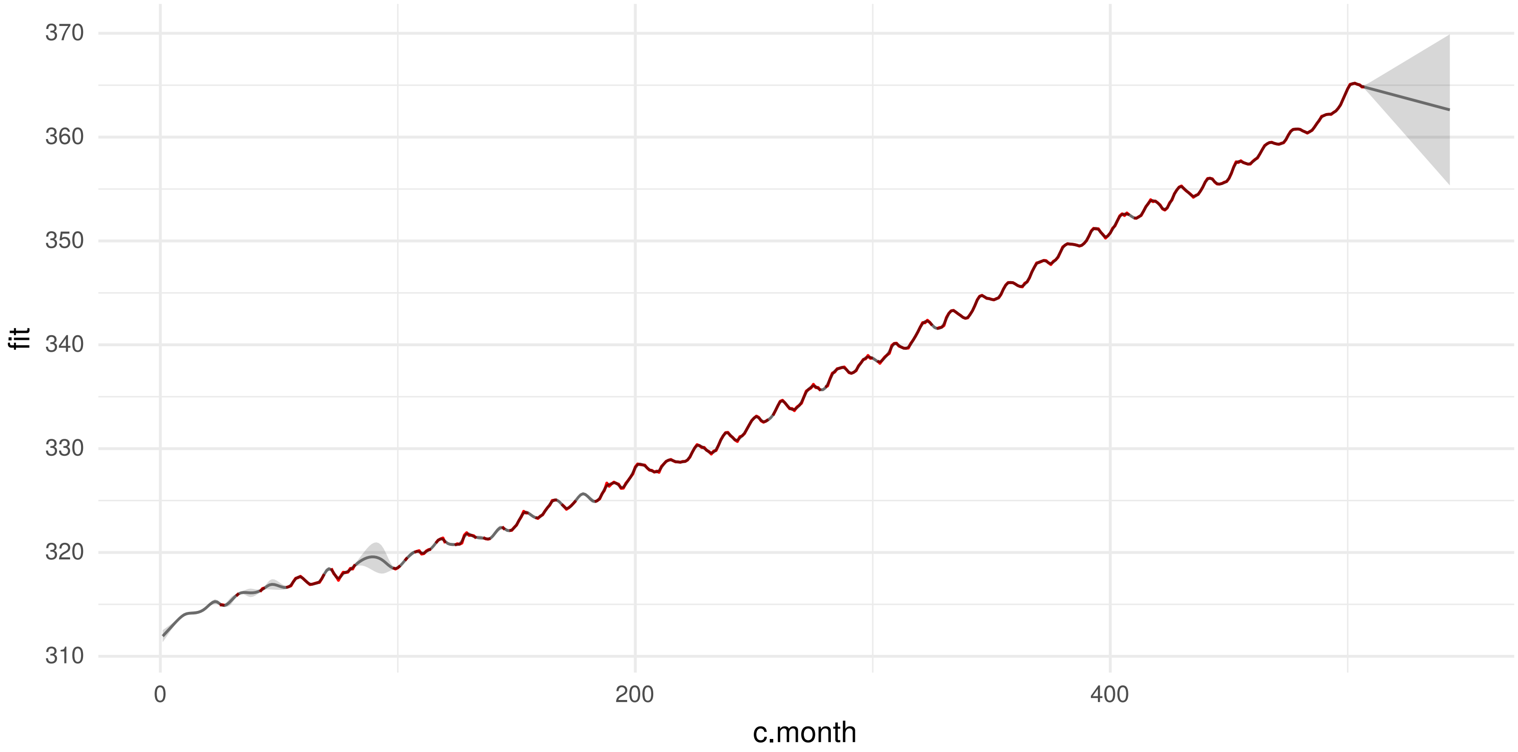
```
Family: gaussian
Link function: identity

Formula:
co2 ~ s(c.month, k = 300, bs = "cr")

Parametric coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 3.382e+02  4.444e-03   76111   <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(c.month) 205.3  241.4 44646  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =      1   Deviance explained =  100%
-REML = 36.492  Scale est. = 0.0084334  n = 427
```

Atmospheric CO_2 — predict

```
pd <- with(co2s, data.frame(c.month = 1:(nrow(co2s)+36)))
pd <- cbind(pd, predict(b, pd, se = TRUE))
pd <- transform(pd, upr = fit + (2*se.fit), lwr = fit - (2 * se.fit))
```

Atmospheric CO_2 — predict

```
ggplot(pd, aes(x = c.month, y = fit)) +
    geom_ribbon(aes(ymin = lwr, ymax = upr), alpha = 0.2) +
    geom_line(data = co2s, aes(c.month, co2), col = 'red') +
    geom_line(alpha = 0.5)
```



Atmospheric CO_2 — better model

```r
b2 <- gam(co2 ~ s(month, bs="cc") + s(c.month, bs ="cr", k = 300),
          data = co2s, method = 'REML',
          knots = list(month=seq(1,13,length=10)))
```

Atmospheric CO_2 — better model

```
summary(b2)
```

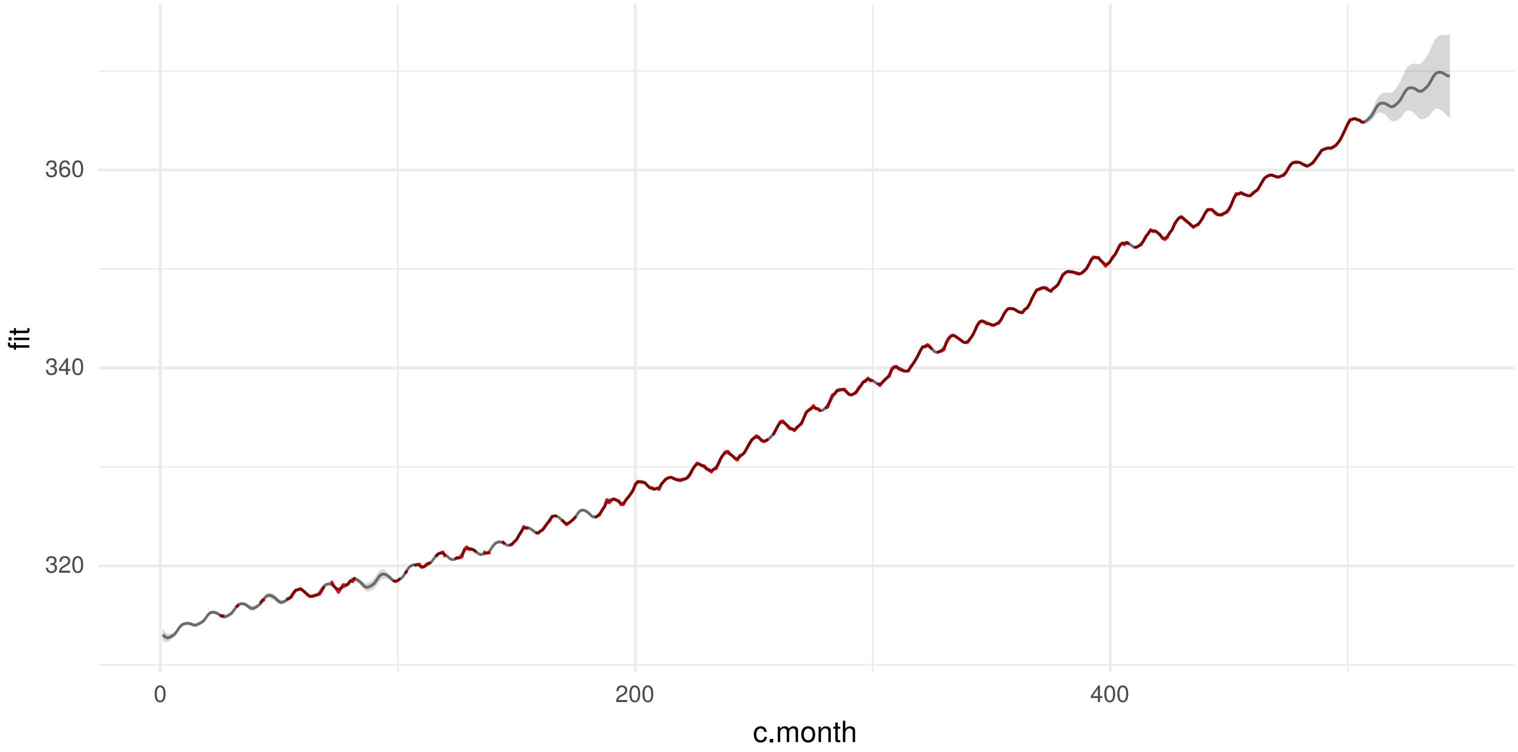
```
Family: gaussian
Link function: identity

Formula:
co2 ~ s(month, bs = "cc") + s(c.month, bs = "cr", k = 300)

Parametric coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 3.382e+02  5.435e-03   62229   <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(month)     7.251    8.0   169.9  <2e-16 ***
s(c.month) 104.823  128.8 55572.6  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =      1   Deviance explained =  100%
-REML = -101.49  Scale est. = 0.012615  n = 427
```

Atmospheric CO_2 — predict

```
nr <- nrow(co2s)
pd2 <- with(co2s, data.frame(c.month = 1:(nr+36),
                             month = rep(1:12, length.out=nr+36)))
pd2 <- cbind(pd2, predict(b2, pd2, se = TRUE))
pd2 <- transform(pd2, upr = fit + (2*se.fit), lwr = fit - (2 * se.fit))
```

Atmospheric CO_2 — predict

```
ggplot(pd2, aes(x = c.month, y = fit)) +
    geom_ribbon(aes(ymin = lwr, ymax = upr), alpha = 0.2) +
    geom_line(data = co2s, aes(c.month, co2), col = 'red') +
    geom_line(alpha = 0.5)
```



Next steps

Read Simon Wood's book

Tonnes more material on our ESA GAM Workshop site

https://noamross.github.io/mgcv-esa-workshop/

Also see my blog: www.fromthebottomoftheheap.net

References

- Marra & Wood (2011) *Computational Statistics and Data Analysis* **55** 2372--2387.
- Marra & Wood (2012) *Scandinavian Journal of Statistics, Theory and Applications* **39**(1), 53--74.
- Nychka (1988) *Journal of the American Statistical Association* **83**(404) 1134--1143.
- Wood (2006, 2017) *Generalized Additive Models: An Introduction with R*. Chapman and Hall/CRC. (New 2nd Edition)
- Wood (2013a) *Biometrika* **100**(1) 221--228.
- Wood (2013b) *Biometrika* **100**(4) 1005--1010.
- Wood et al (2016) *JASA* **111** 1548--1563