Generalized Additive Models

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Overview

- What is a GAM?
- What is smoothing?
- How do GAMs work? (*Roughly*)
- Fitting and plotting simple models

What is a GAM?

Generalized Additive Models

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

To GAMs from GLMs and LMs

(Generalized) Linear Models

Models that look like:

$$y_i = \beta_0 + x_{1i}\beta_1 + x_{2i}\beta_2 + \ldots + \epsilon_i$$

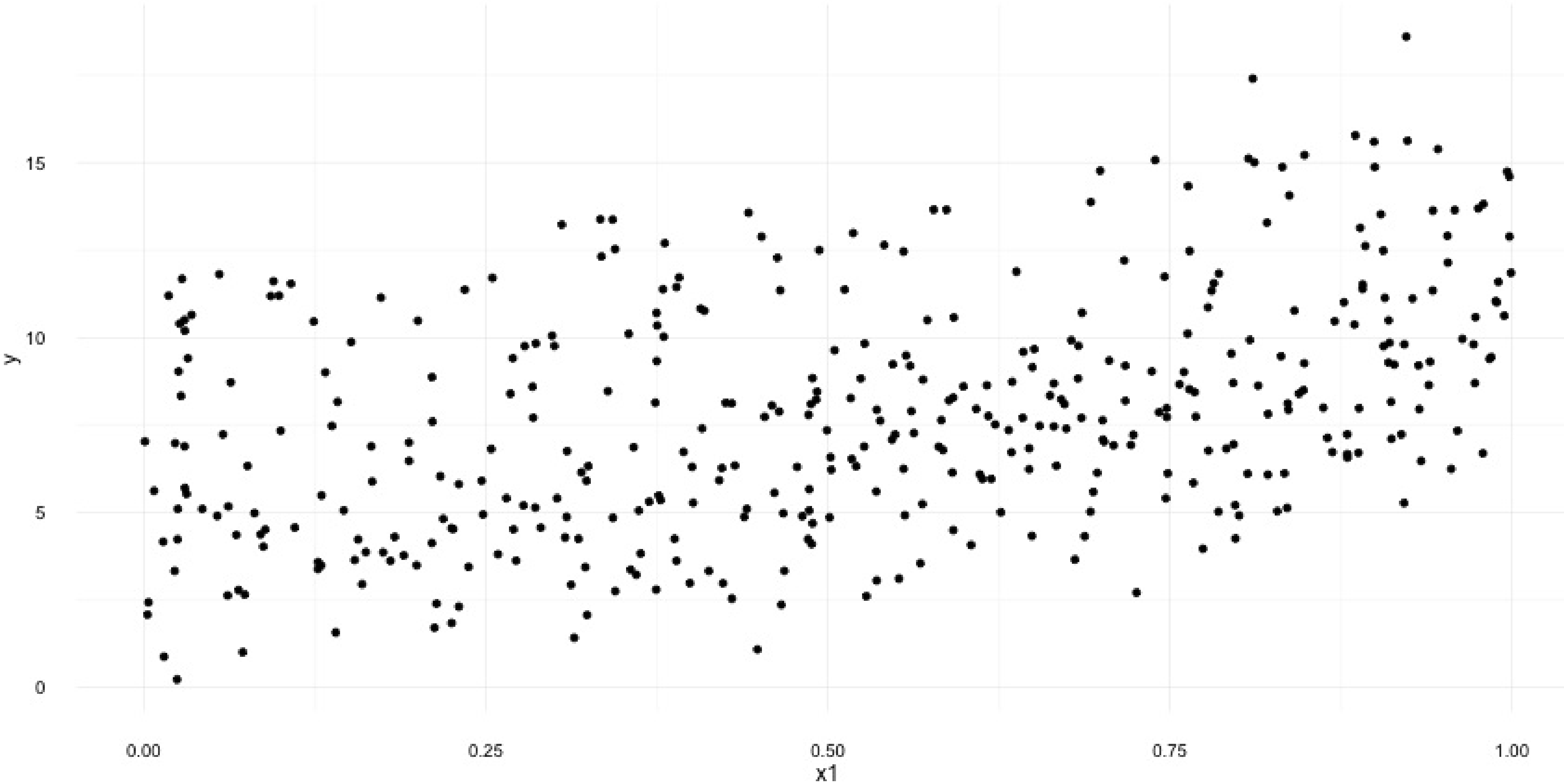
(describe the response, y_i, as linear combination of the covariates, x_{ji}, with an offset)

We can make $y_i \sim$ any exponential family distribution (Normal, Poisson, etc).

Error term ϵ_i is normally distributed (usually).

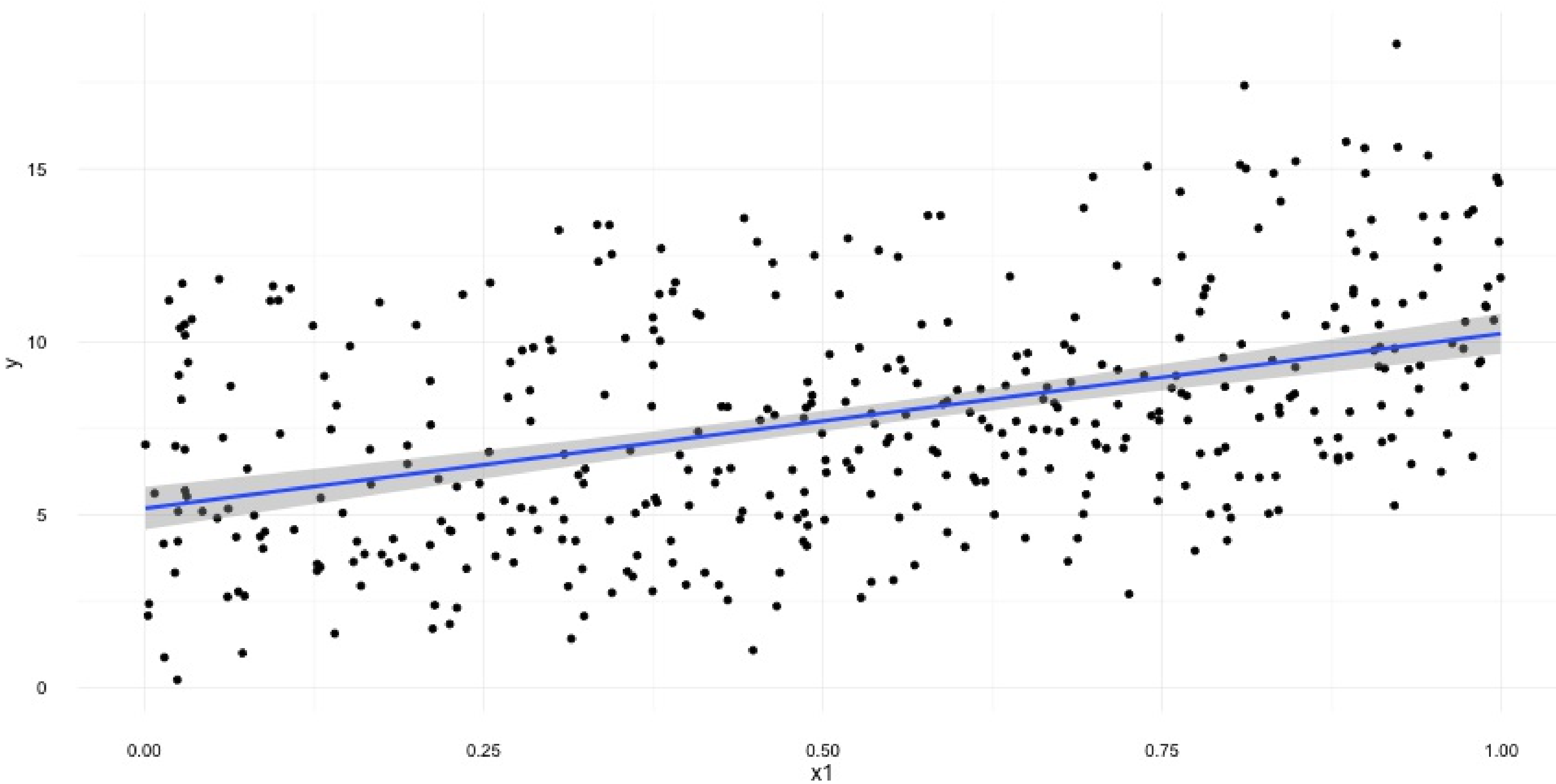
Why bother with anything more complicated?!

Is this linear?



Is this linear? Maybe?

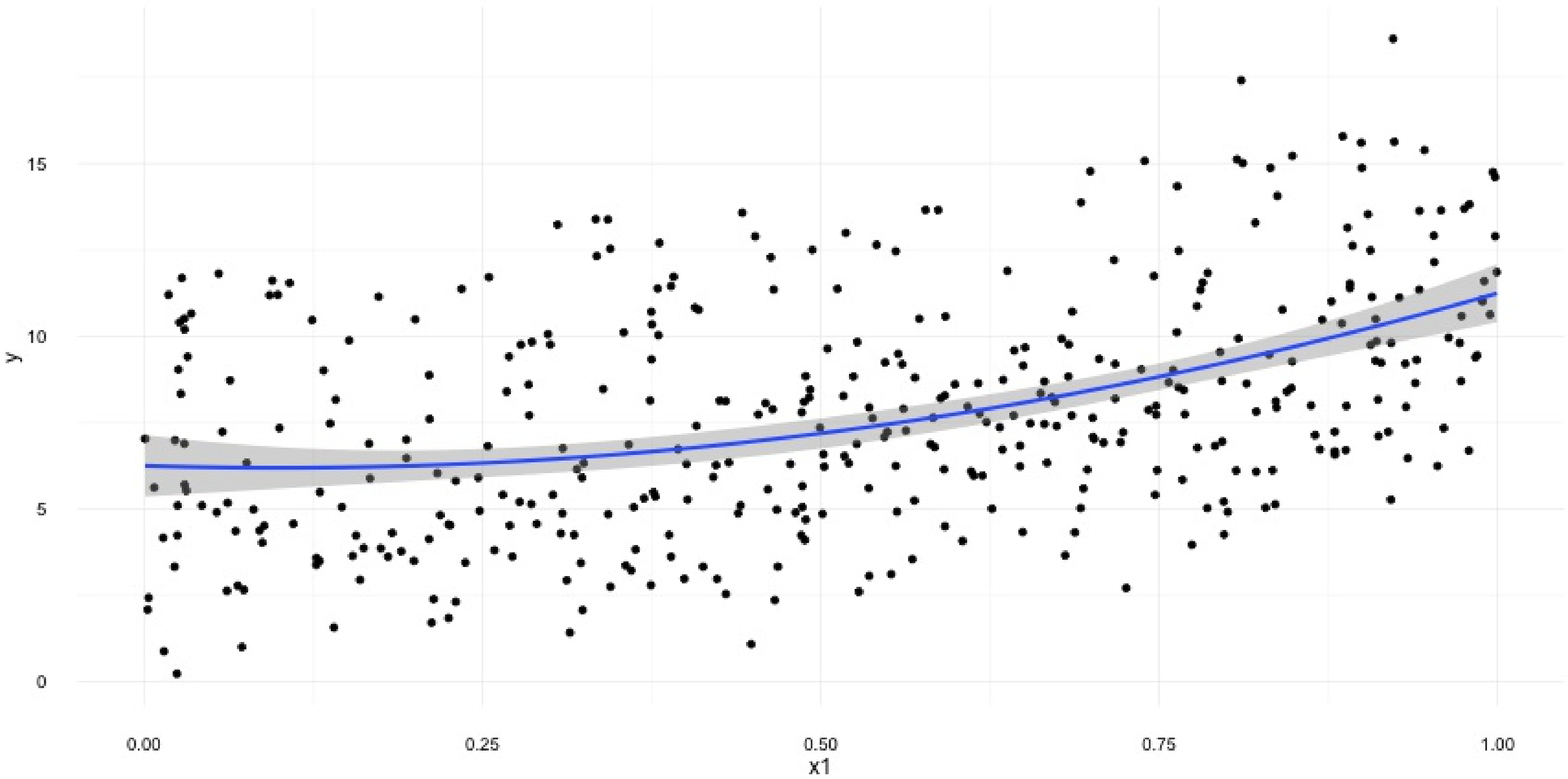
```
lm(y ~ x1, data=dat)
```



What can we do?

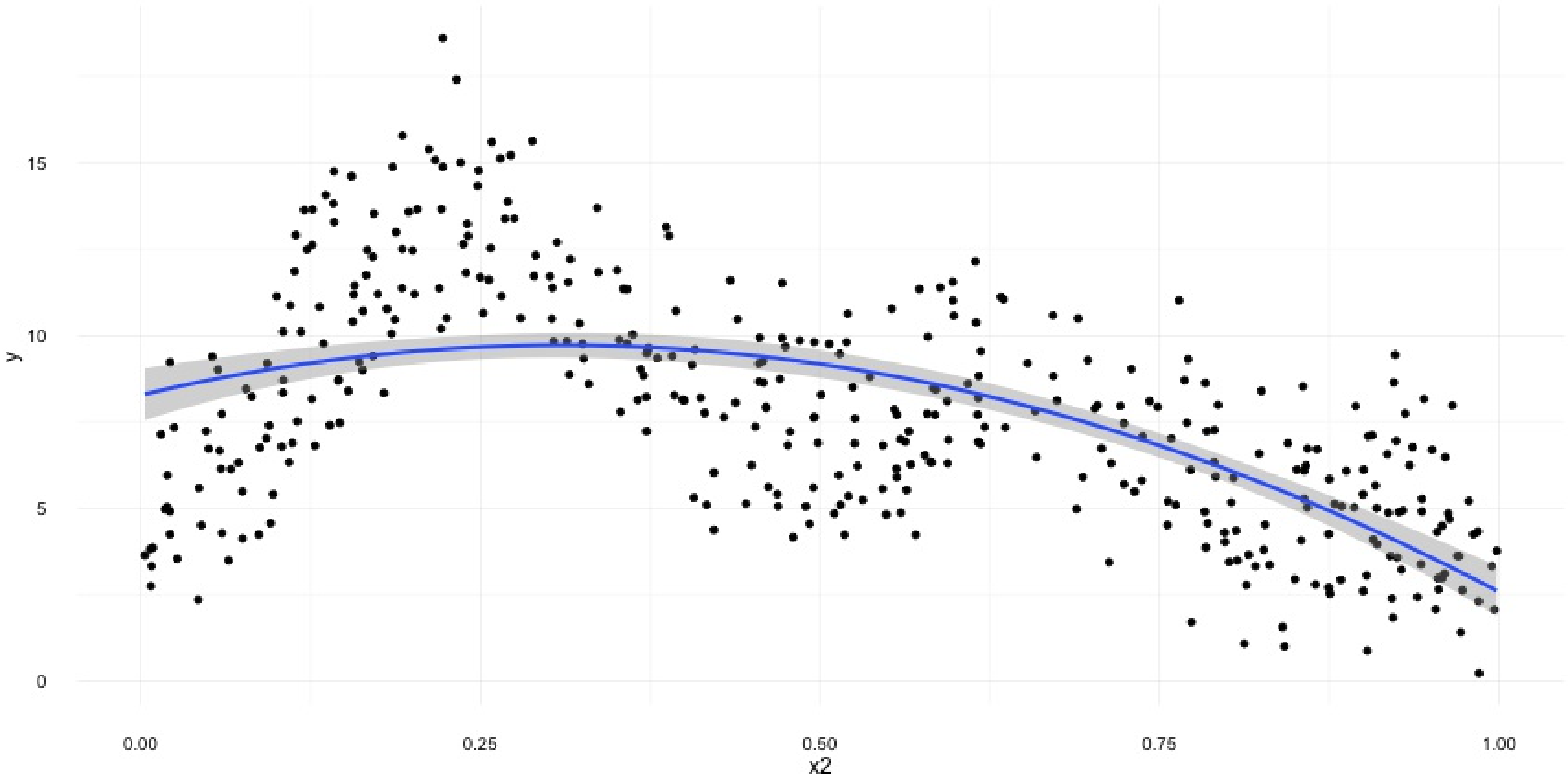
Adding a quadratic term?

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



Is this sustainable?

- Adding in quadratic (and higher terms) *can* make sense
- This feels a bit *ad hoc*
- Better if we had a **framework** to deal with these issues?



[drumroll]

What does a model look like?

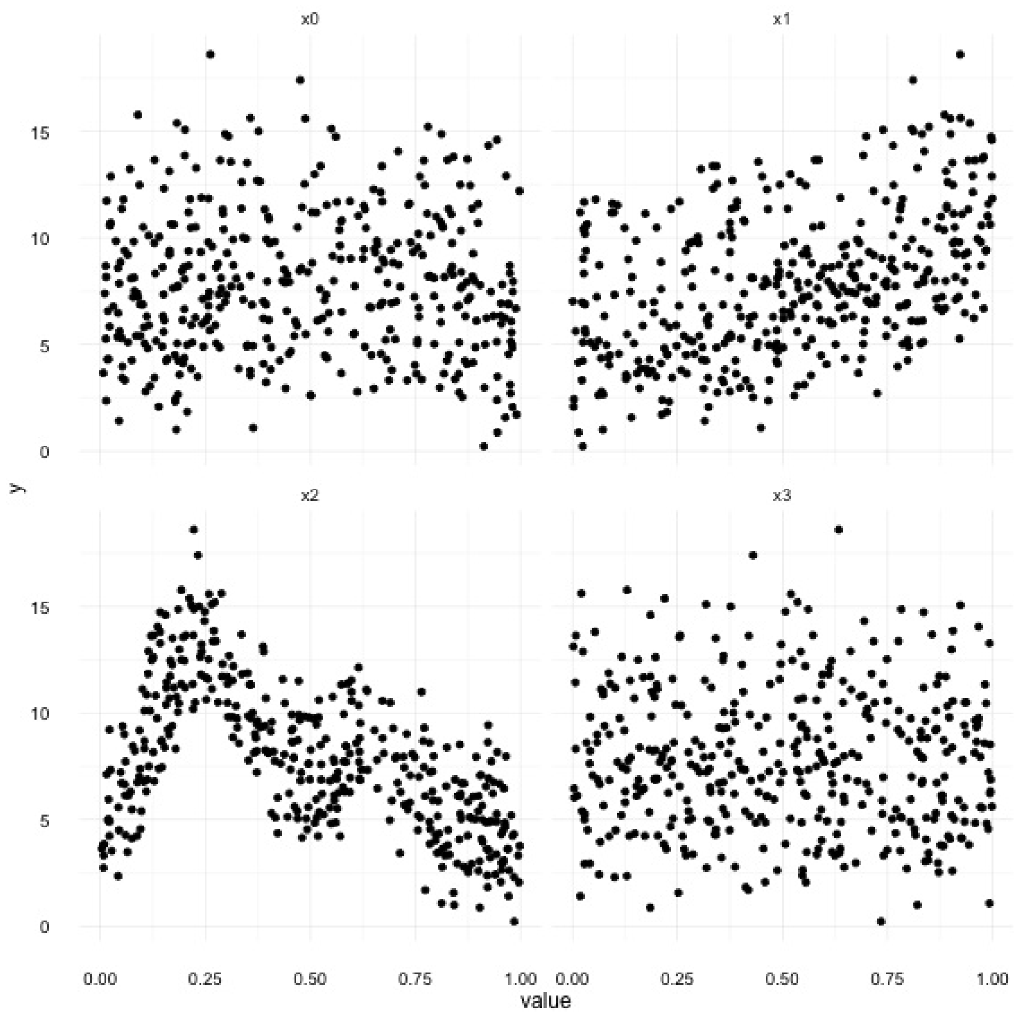
$$y_i = \beta_0 + \sum_j s_j(x_{ji}) + \epsilon_i$$

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

Remember that we're modelling the mean of this distribution!

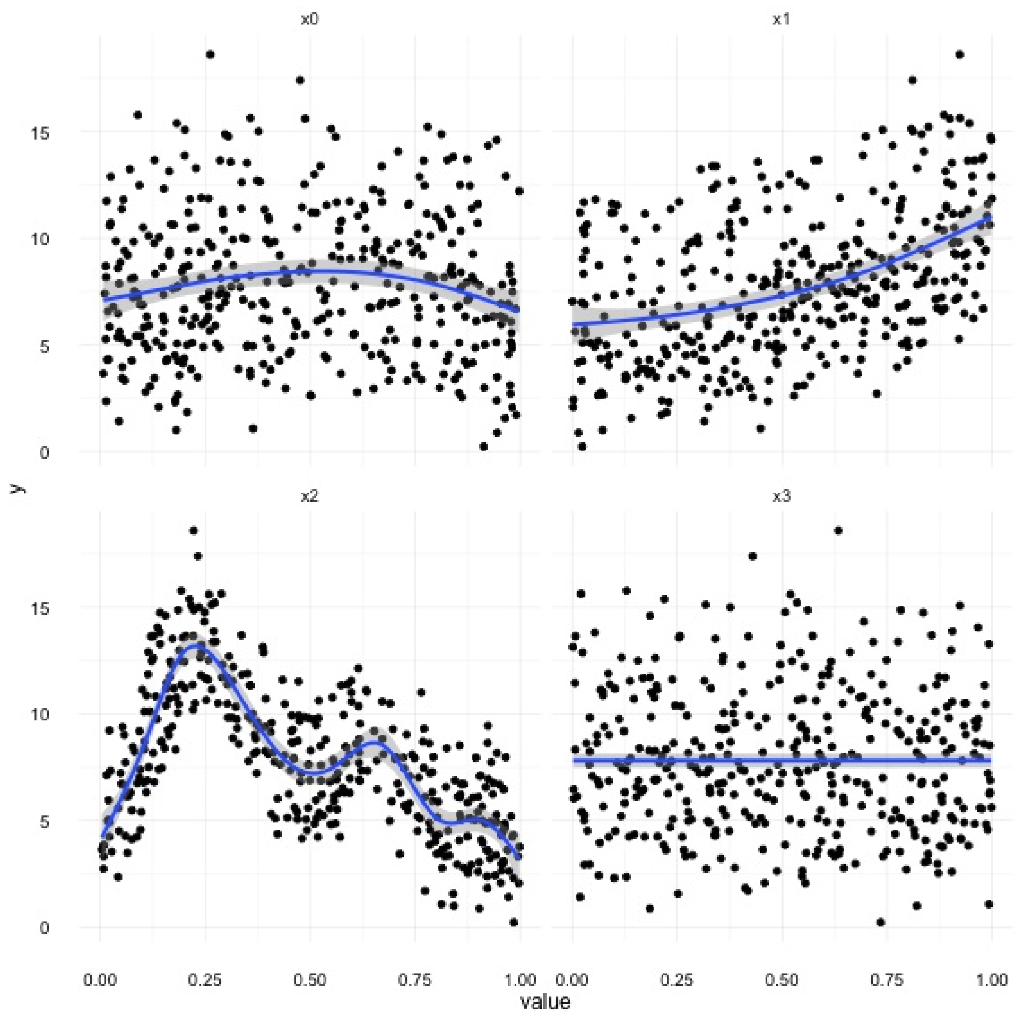
Call the above equation the **linear predictor**

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”

Okay, but what about these ”s” things?



- Think s=**smooth**
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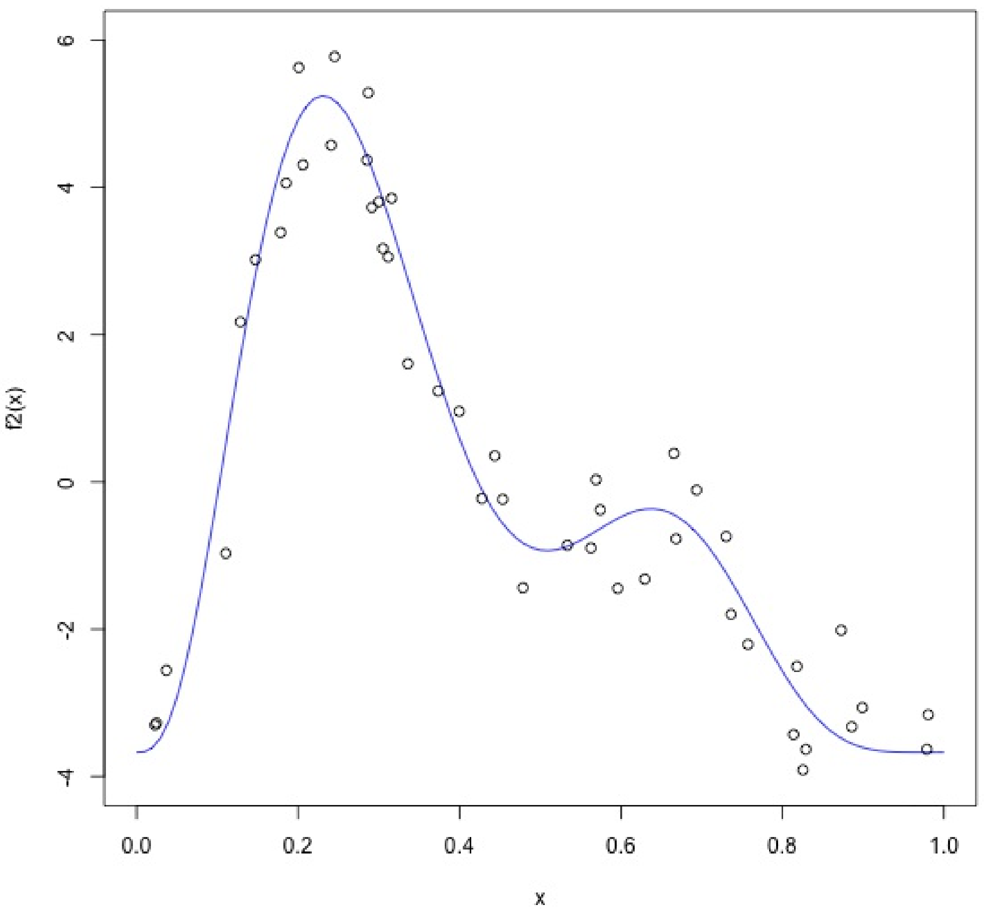
What is smoothing?

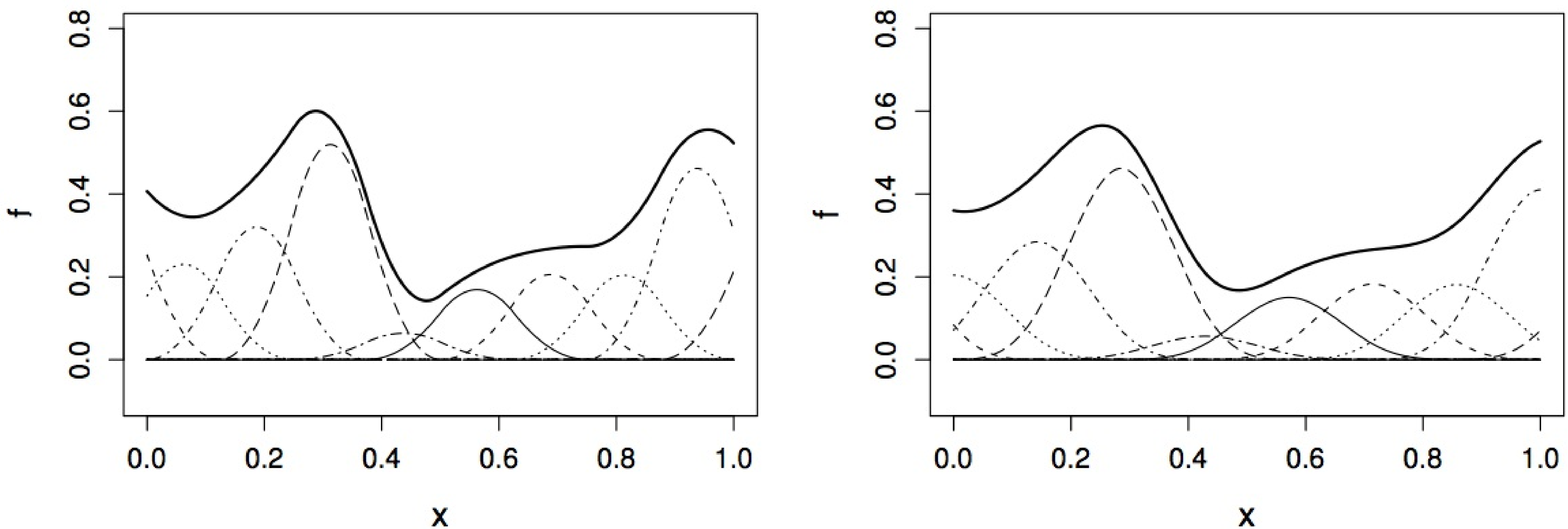
Straight lines vs. interpolation



- 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



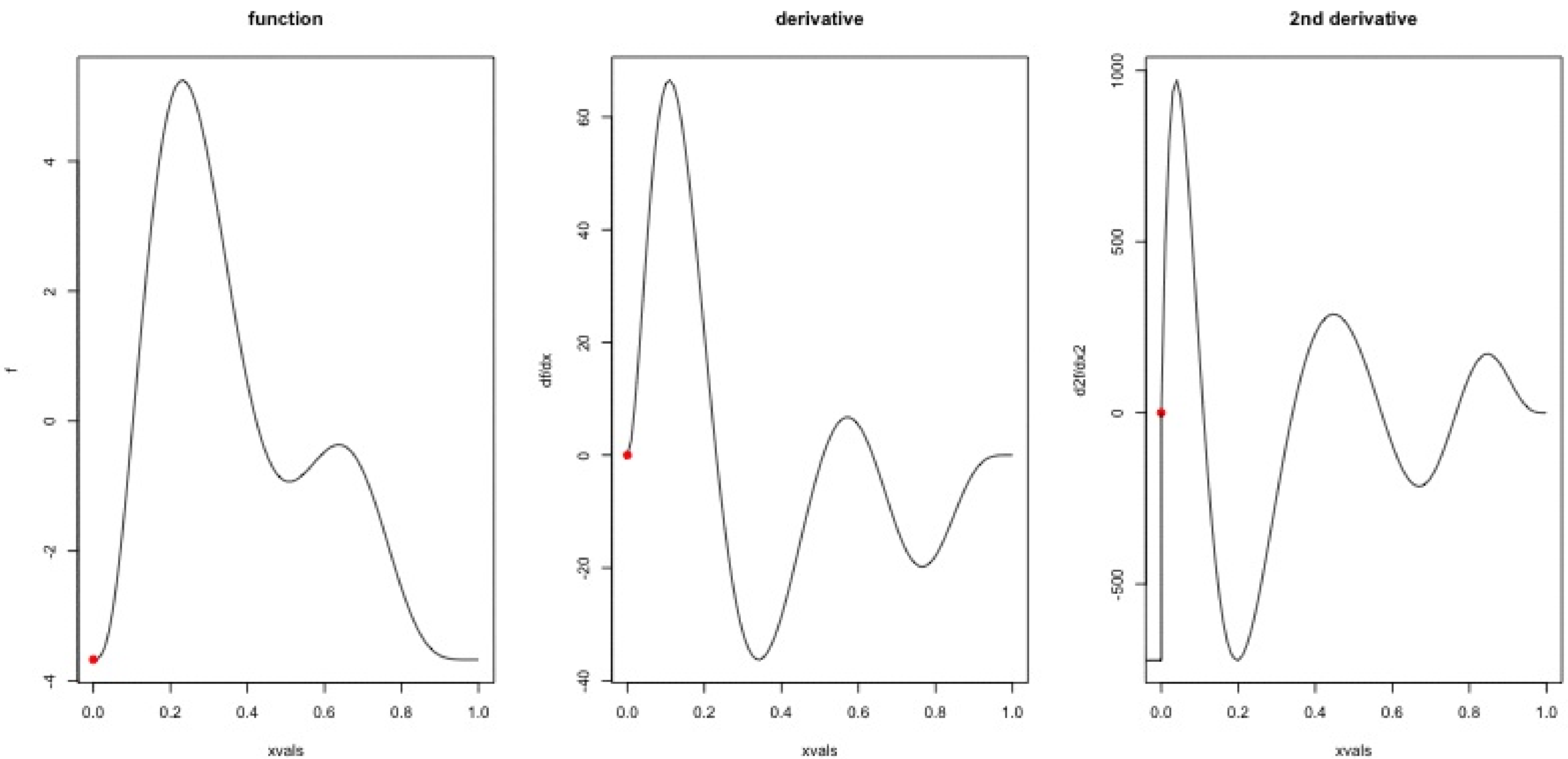
Design matrices

- We often write models as $X\boldsymbol{\beta}$
  - X is our data
  - $\boldsymbol{\beta}$ are parameters we need to estimate
- For a GAM it's the same
  - X has columns for each basis, evaluated at each observation
  - again, this is the linear predictor

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



What was that grey bit?

$$\int_{\mathbb{R}} \left(\frac{\partial^2 f(x)}{\partial^2 x} \right)^2 dx$$

(Take some derivatives of the smooth and integrate them over x)

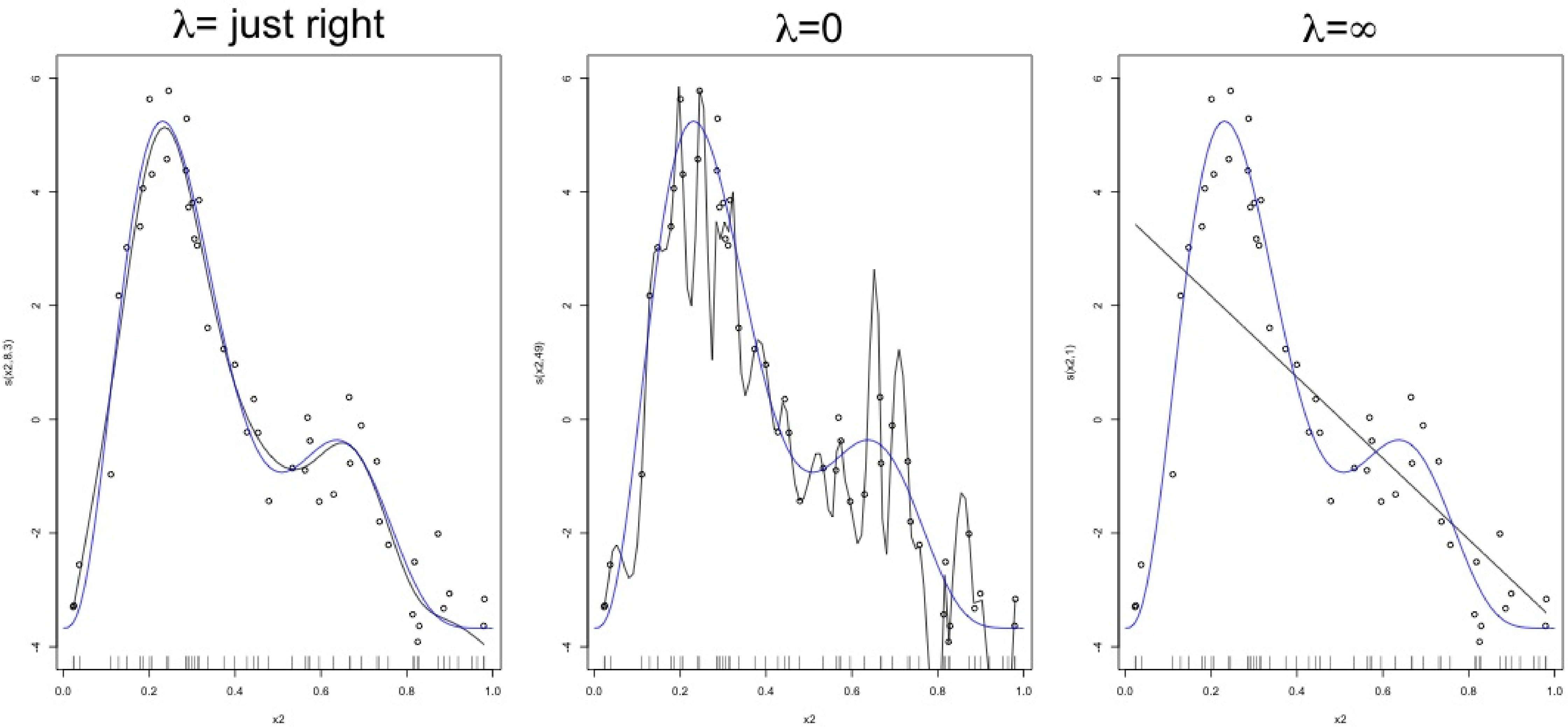
(*Turns out* we can always write this as $\boldsymbol{\beta}^{\mathrm{T}} \mathrm{S} \boldsymbol{\beta}$, so the $\boldsymbol{\beta}$ is separate from the derivatives)

(Call S the **penalty matrix**)

Making wigglyness matter

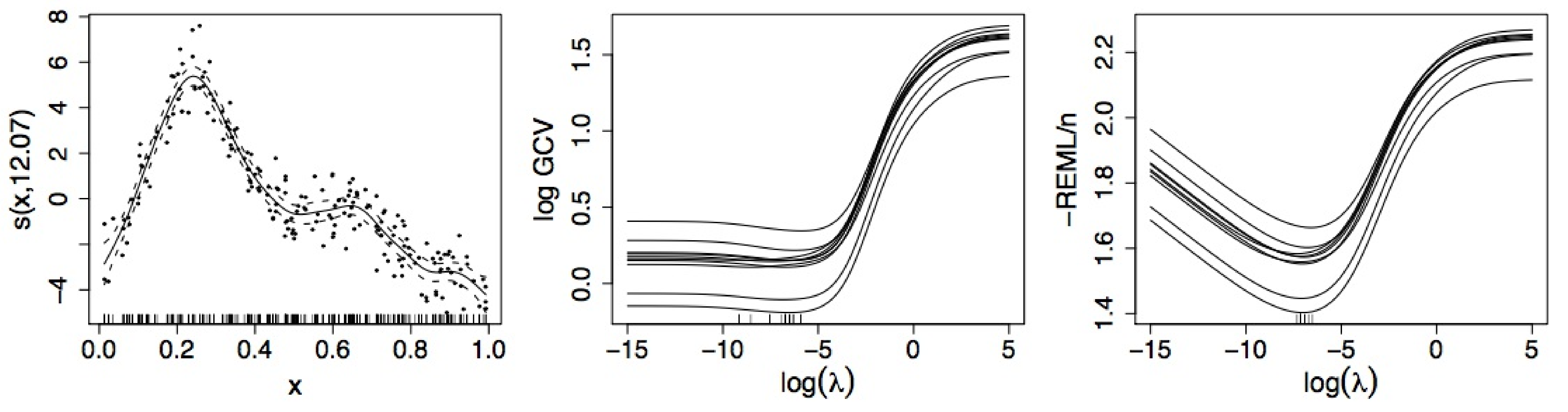
- $\boldsymbol{\beta}^{\mathrm{T}}\mathrm{S}\boldsymbol{\beta}$ measures wigglyness
- "Likelihood" measures closeness to the data
- Penalise closeness to the data…
- Use a **smoothing parameter** to decide on that trade-off…
  - $\lambda\beta^{\mathrm{T}}\mathrm{S}\beta$
- Estimate the β_{k} terms but penalise objective
  - "closeness to data" + penalty

Smoothing parameter



Smoothing parameter selection

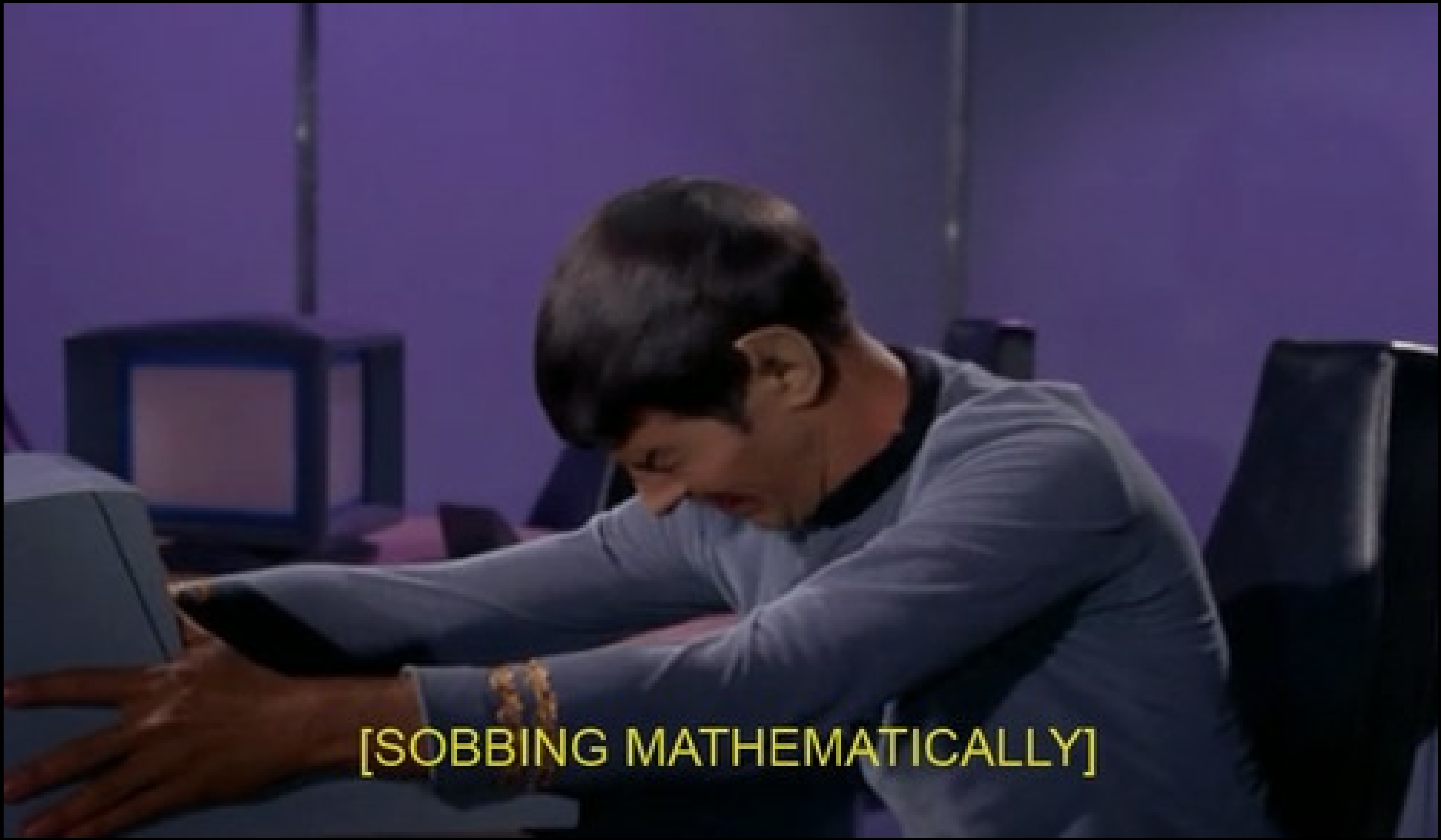
- Many methods: AIC, Mallow's C_p, GCV, ML, REML
- Recommendation, based on simulation and practice:
  - Use REML or ML
  - Reiss & Ogden (2009), Wood (2011)



Maximum wiggliness

- We can set **basis complexity** or “size” (k)
  - Maximum wigglyness
- Smooths have **effective degrees of freedom** (EDF)
- EDF < k
- Set k “large enough”
  - Penalty does the rest

More on this in a bit…


[SOBBING MATHEMATICALLY]

GAM summary

- Straight lines suck — we want **wiggles**
- Use little functions (**basis functions**) to make big functions (**smooths**)
- Need to make sure your smooths are **wiggly enough**
- Use a **penalty** to trade off wiggliness/generality

Fitting GAMs in practice

Translating maths into R

A simple example:

$$y_i = \beta_0 + s(x) + s(w) + \epsilon_i$$

where $\epsilon_i \sim N(0, \sigma^2)$

Let's pretend that $y_i \sim \text{Normal}$

- linear predictor: `formula = y ~ s(x) + s(w)`
- response distribution: `family=gaussian()`
- data: `data=some_data_frame`

Putting that together

```
my_model <- gam(y ~ s(x) + s(w),
                family = gaussian(),
                data = some_data_frame,
                method = "REML")
```

- `method="REML"` uses REML for smoothness selection (default is `"GCV.Cp"`)

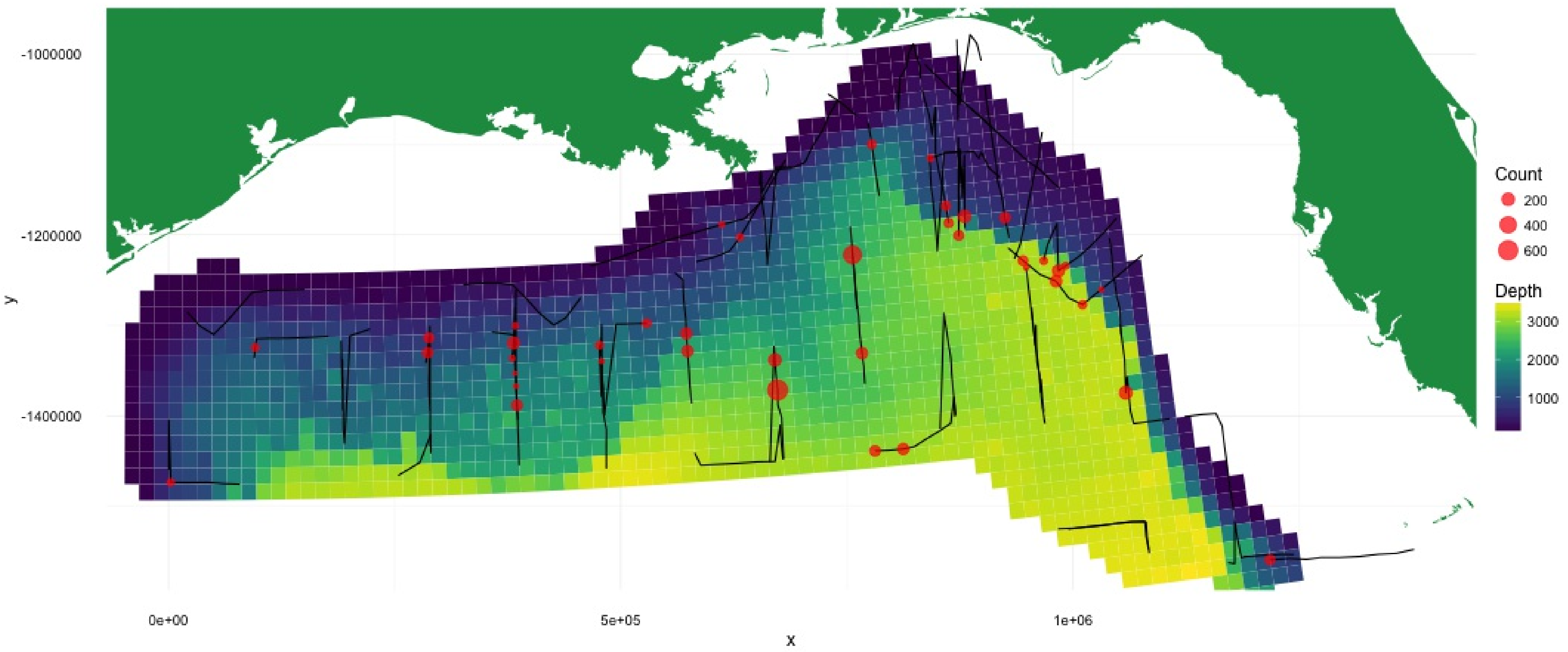
What about a practical example?

Pantropical spotted dolphins

- Example taken from Miller et al (2013)
- Paper appendix has a better analysis
- Simple example here, ignoring all kinds of important stuff!

Inferential aims

- How many dolphins are there?
- Where are the dolphins?
- What are they interested in?



A simple dolphin model

```
library(mgcv)
dolphins_depth <- gam(count ~ s(depth) + offset(off.set),
                      data = mexdolphins,
                      family = quasipoisson(),
                      method = "REML")
```

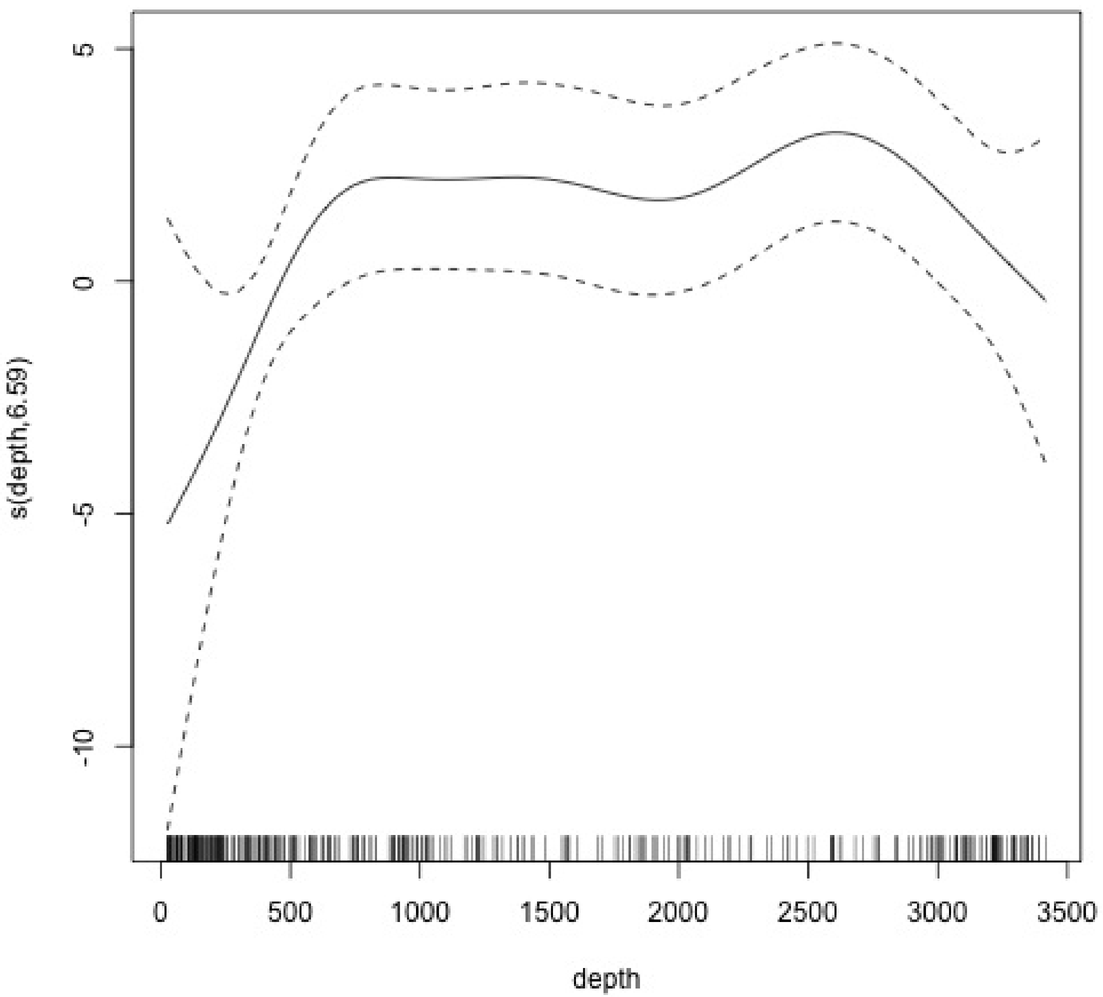
- count is a function of depth
- `off.set` is the effort expended
- we have count data, try quasi-Poisson distribution

What did that do?

```r
summary(dolphins_depth)
```

```
Family: quasipoisson
Link function: log

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

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -18.2344     0.8949  -20.38   <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(depth) 6.592  7.534 2.329  0.0224 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

R-sq.(adj) =  0.0545   Deviance explained = 26.4%
-REML = 948.28  Scale est. = 145.34    n = 387
```

Plotting



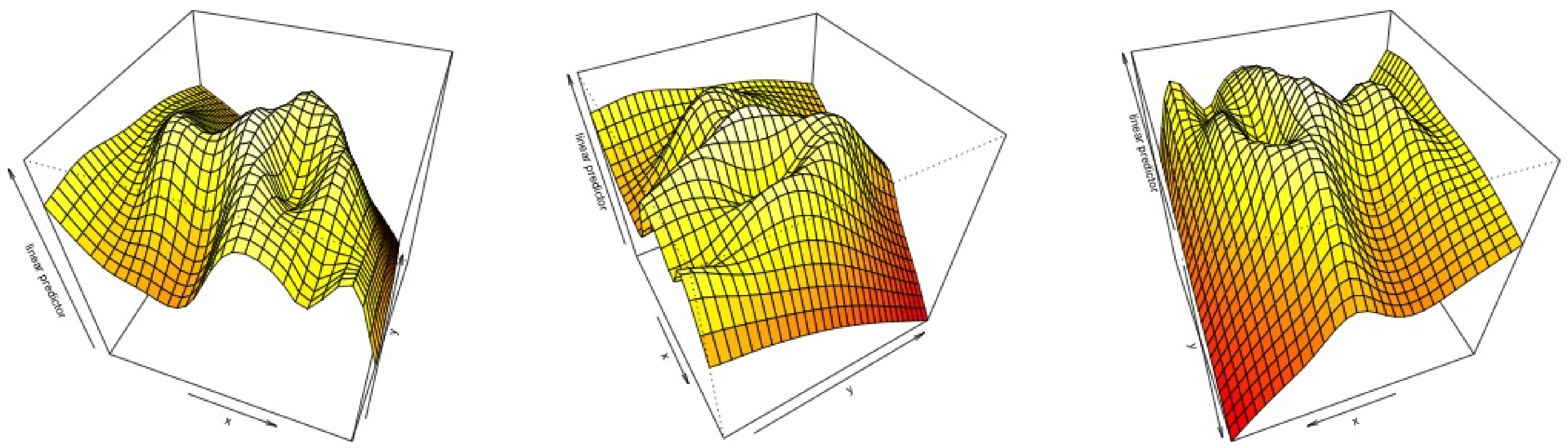
- `plot(dolphins_depth)`
- Dashed lines indicate +/- 2 standard errors
- Rug plot
- On the link scale
- EDF on y axis

Thin plate regression splines

- Default basis
- One basis function per data point
- Reduce # basis functions (eigendecomposition)
- Fitting on reduced problem
- Multidimensional
- Wood (2003)

Bivariate terms

- Assumed an additive structure
- No interaction
- We can specify `s(x,y)` (and `s(x,y,z,...)`)
- (Assuming *isotropy* here...)



Adding a term

- Add a **surface** for location (x and y)
- Just use + for an extra term

```
dolphins_depth_xy <- gam(count ~ s(depth) + s(x, y) +
offset(off.set),
                 data = mexdolphins,
                 family=quasipoisson(), method="REML")
```

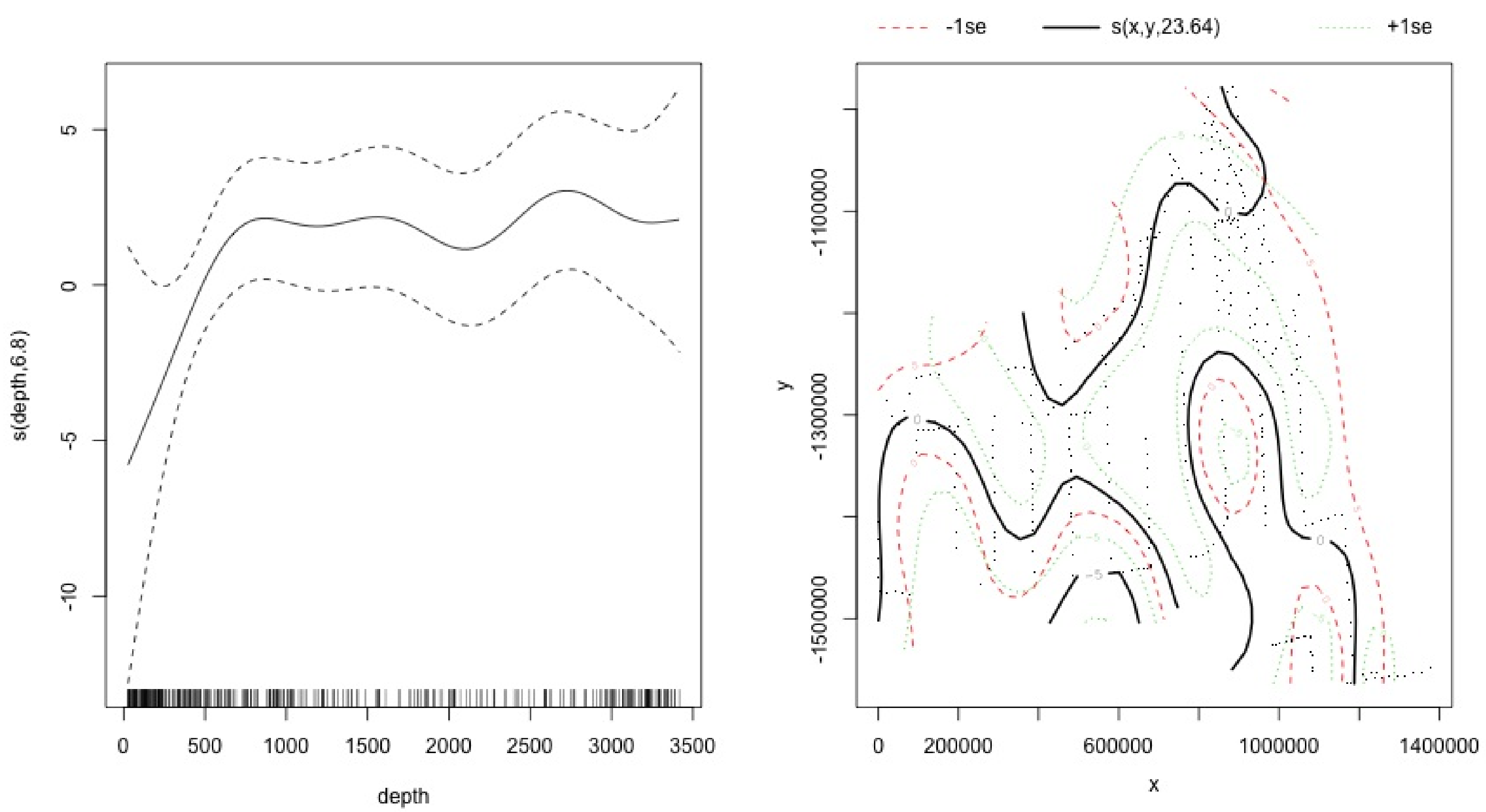
Summary

```r
summary(dolphins_depth_xy)
```

```

Family: quasipoisson
Link function: log

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

Parametric coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -19.1933     0.9468  -20.27   <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(depth)  6.804  7.669 1.461   0.191
s(x,y)   23.639 26.544 1.358   0.114

R-sq.(adj) =   0.22   Deviance explained = 49.9%
-REML =  923.9  Scale est. = 79.474    n = 387
```

Plotting

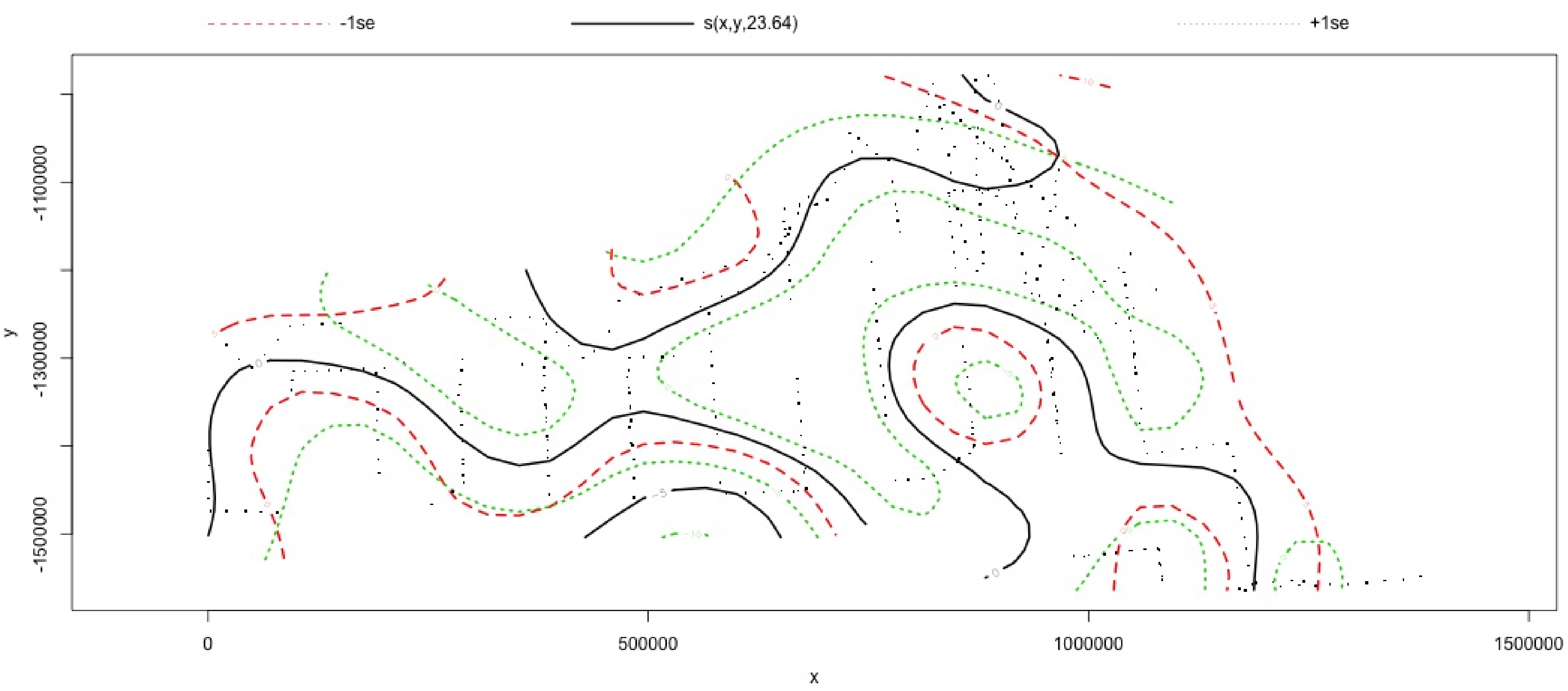
```
plot(dolphins_depth_xy, scale=0, pages=1)
```



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

Plotting 2d terms... erm...

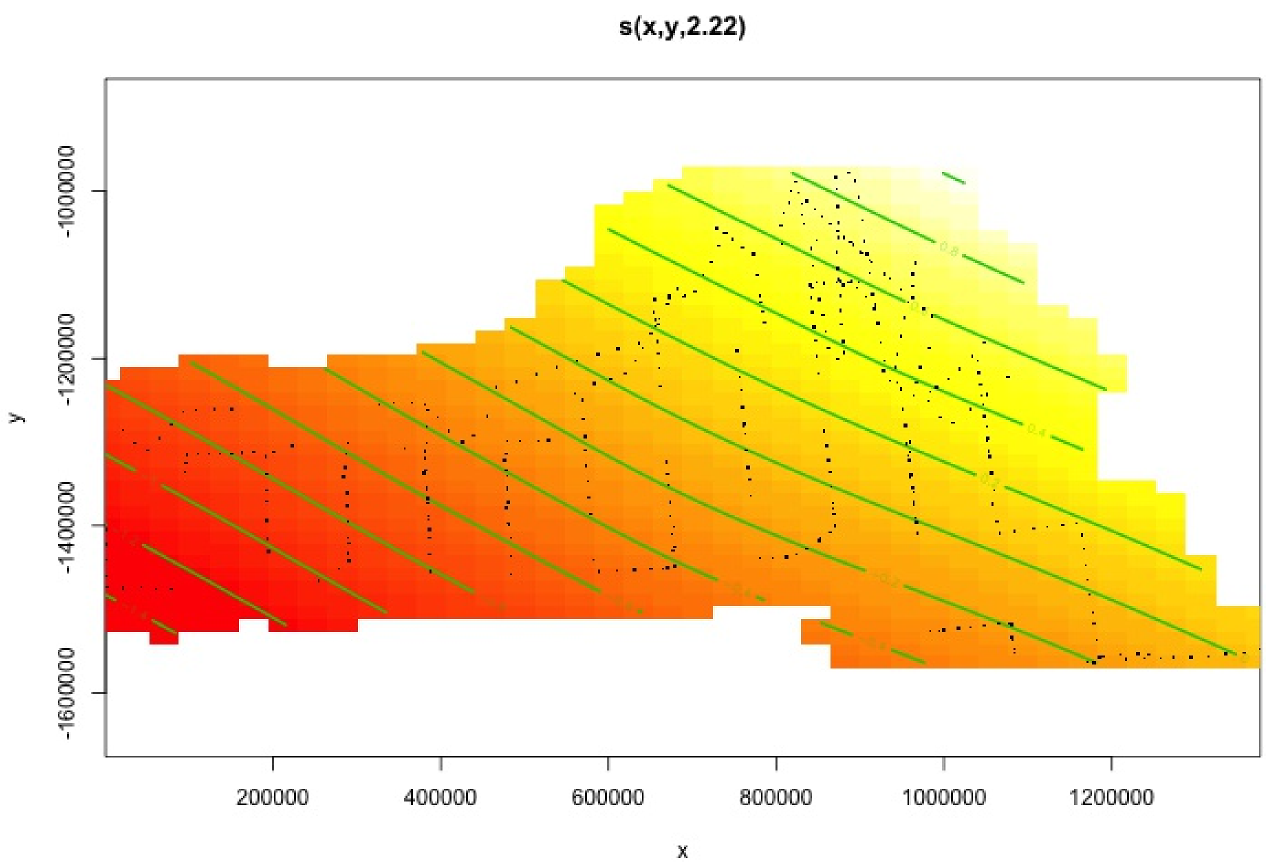
```
plot(dolphins_depth_xy, select=2, cex=2, asp=1, lwd=2)
```



- `select=` picks which smooth to plot

Let's try something different

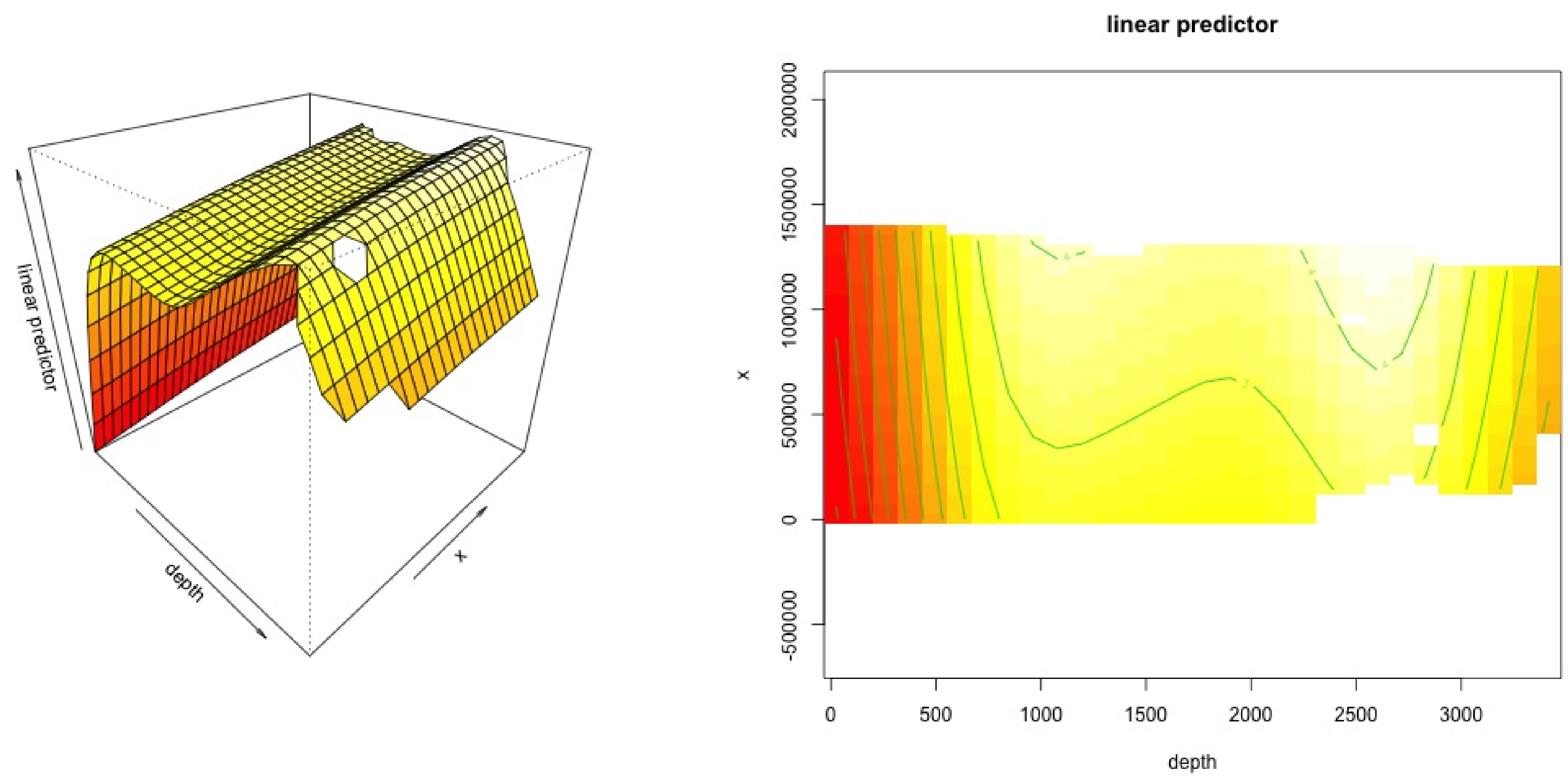
```
plot(dolphins_depth_xy, select=2, cex=2, asp=1, lwd=2, scheme=2)
```



- `scheme=2` much better for bivariate terms
- `vis.gam()` is much more general

More complex plots

```
par(mfrow=c(1,2))
vis.gam(dolphins_depth_xy, view=c("depth","x"), too.far=0.1,
phi=30, theta=45)
vis.gam(dolphins_depth_xy, view=c("depth","x"),
plot.type="contour", too.far=0.1,asp=1/1000)
```



Fitting/plotting GAMs summary

- `gam` does all the work
- very similar to `glm`
- `s` indicates a smooth term
- `plot` can give simple plots
- `vis.gam` for more advanced stuff

Prediction

What is a prediction?

- Evaluate the model, at a particular covariate combination
- Answering (e.g.) the question "at a given depth, how many dolphins?"
- Steps:

1. evaluate the $\text{s}(\ldots)$ terms
2. move to the response scale (exponentiate? Do nothing?)
3. (multiply any offset etc)

Example of prediction

- in maths:
  - Model: $\text{count}_i = A_i \exp\left(\beta_0 + s(x_i, y_i) + s(\text{Depth}_i)\right)$
  - Drop in the values of x, y, Depth (and A)
- in R:
  - build a `data.frame` with x, y, Depth, A
  - use `predict()`

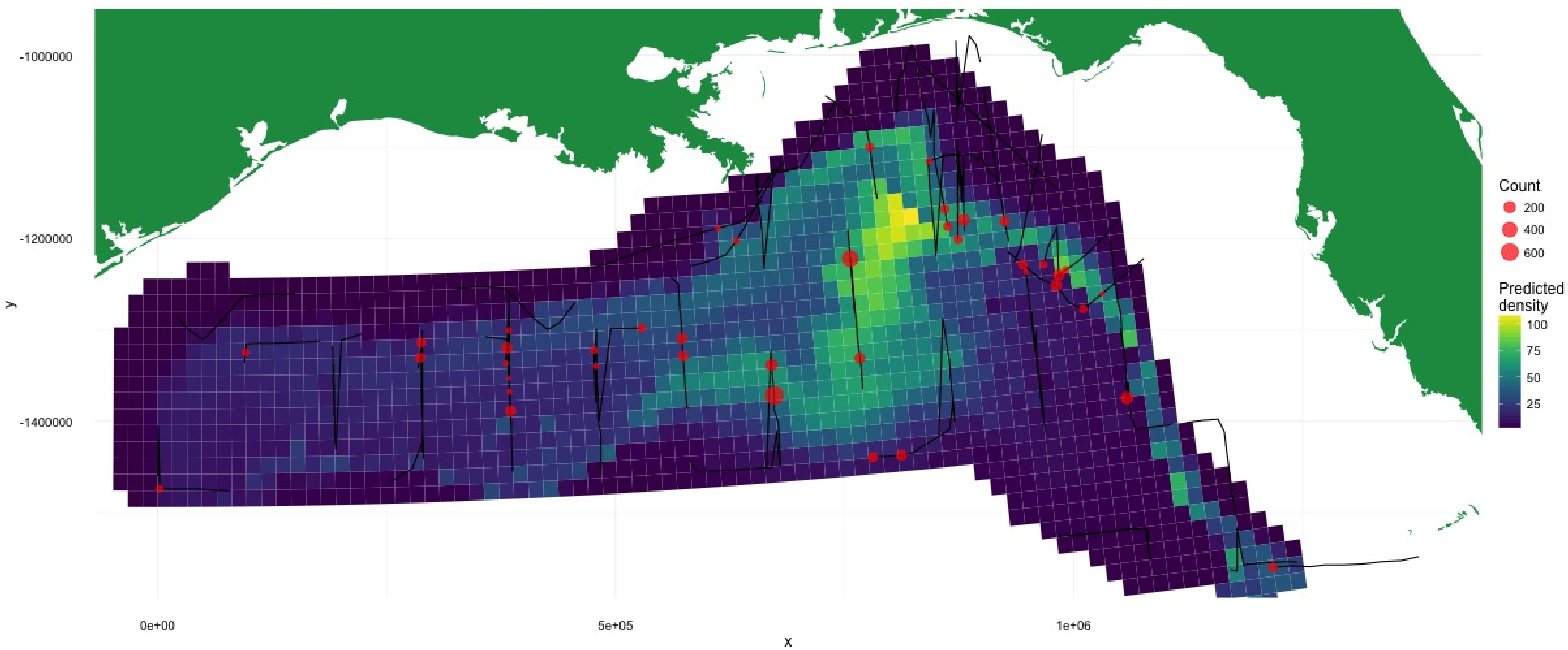
```
preds <- predict(my_model, newdat=my_data, type="response")
```

(`se.fit=TRUE` gives a standard error for each prediction)

Back to the dolphins...

Where are the dolphins?

```
dolphin_preds <- predict(dolphins_depth_xy, newdata=preddata,
                         type="response")
```



(`ggplot2` code included in the slide source)

Prediction summary

- Evaluate the fitted model at a given point
- Can evaluate many at once (`data.frame`)
- Don't forget the `type=...` argument!
- Obtain per-prediction standard error with `se.fit`

What about uncertainty?

Without uncertainty, we’re not doing statistics

Where does uncertainty come from?

- $\boldsymbol{\beta}$: uncertainty in the spline parameters
- $\boldsymbol{\lambda}$: uncertainty in the smoothing parameter

- (Traditionally we've only addressed the former)

- (New tools let us address the latter…)

Parameter uncertainty

From theory:

$$\boldsymbol{\beta} \sim \mathrm{N}(\hat{\boldsymbol{\beta}}, \mathbf{V}_{\boldsymbol{\beta}})$$

(*caveat: the normality is only* **approximate** *for non-normal response*)

What does this mean? Variance for each parameter.

In `mgcv`: `vcov(model)` returns $\mathbf{V}_{\boldsymbol{\beta}}$.

What can we do this this?

- confidence intervals in `plot`
- standard errors using `se.fit`
- derived quantities? (see bibliography)


Huh. Well, there's only
one way to solve this.
Well, there's probably,
like, a lot of different ways.

The lpmatrix, magic, etc

For regular predictions:

$$\hat{\boldsymbol{\eta}}_{\mathrm{p}} = \mathrm{L}_{\mathrm{p}}\hat{\boldsymbol{\beta}}$$

form L_{p} using the prediction data, evaluating basis functions as we go.

(Need to apply the link function to $\hat{\boldsymbol{\eta}}_{\mathrm{p}}$)

But the L_{p} fun doesn't stop there...

[[mathematics intensifies]]

Variance and lpmatrix

To get variance on the scale of the linear predictor:

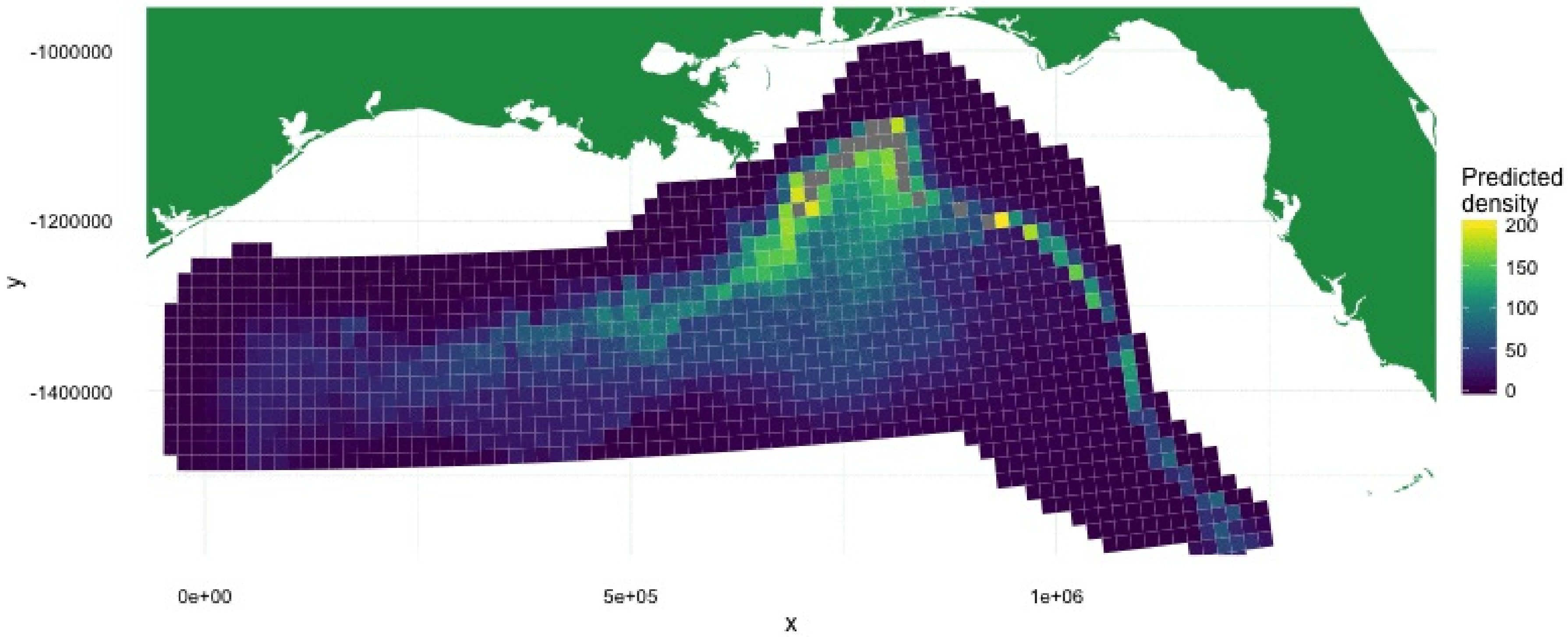
$$\mathrm{V}_{\hat{\boldsymbol{\eta}}} = \mathrm{L}_\mathrm{p}^\mathrm{T} \mathrm{V}_{\hat{\boldsymbol{\beta}}} \mathrm{L}_\mathrm{p}$$

pre-/post-multiplication shifts the variance matrix from parameter space to linear predictor-space.

(Can then pre-/post-multiply by derivatives of the link to put variance on response scale)

Simulating parameters

- $\boldsymbol{\beta}$ has a distribution, we can simulate



Uncertainty in smoothing parameter

- Recent work by Simon Wood
- "smoothing parameter uncertainty corrected" version of $V_{\hat{\boldsymbol{\beta}}}$
- In a fitted model, we have:
  - `$Vp` what we got with `vcov`
  - `$Vc` the corrected version
- Still experimental

Variance summary

- Everything comes from variance of parameters
- Need to re-project/scale them to get the quantities we need
- `mgcv` does most of the hard work for us
- Fancy stuff possible with a little maths
- Can include uncertainty in the smoothing parameter too

Okay, that was a lot of information

Summary

- GAMs are GLMs plus some extra wiggles
- Need to make sure things are *just wiggly enough*
  - Basis + penalty is the way to do this
- Fitting looks like `glm` with extra `s()` terms
- Most stuff comes down to matrix algebra, that `mgcv` sheilds you from
  - To do fancy stuff, get inside the matrices

COFFEE