Specifying GAMs & GAMMs with mgcv

David Lawrence Miller

CREEM, University of St Andrews

SPOILER ALERT

your model is probably some kind of (fancy) GLM

General setup of GAMs in `mgcv` (and my brain)

General setup

$$y = X\beta + \epsilon \qquad \text{with penalty } \beta^{\mathsf{T}} S \beta$$

I think of this as "linear", in the sense that $X\beta$ is linear

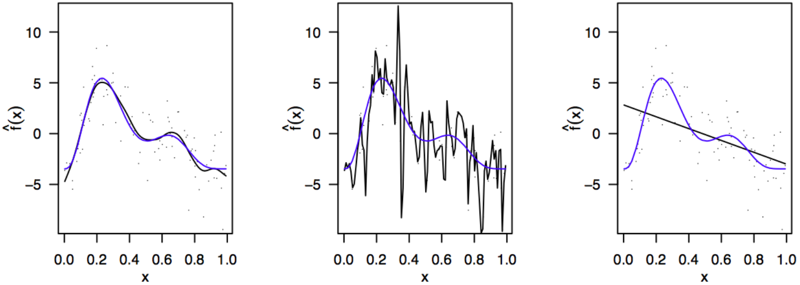
X includes a column for each parametric covariate, plus one for each basis evaluation (at knots or pseudo-knots).

what about this penalty thing?

$$\beta^{\mathsf{T}} S \beta = \int_{\Omega} \left(D^m f(\mathbf{x})\right)^2 d\mathbf{x}$$

where D^m is some differential operator, commonly for univariate:

$$D^m f(x) = \frac{\partial^2 f(x)}{\partial x^2}$$



A quick tour of spline bases

How many different bases?

Currently ~17 (some bases are v. similar or inter-related) in `mgcv`:

```
"ad", "sf", "cc", "so", "cp", "sos", "cr", "sw", "cs",
"t2", "ds", "tensor", "mrf", "tp", "ps", "ts", "re"
```

```
?smooth.terms
?smooth.construct.*.smooth.spec
?gam.models
```

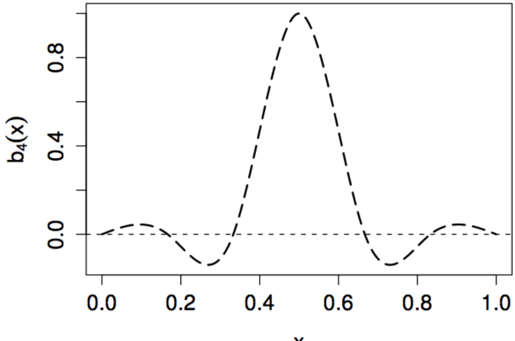
cubic splines

- simple basis construction
- orthogonal (Hermite) polynomials defined by their knots

```
s(x,bs="cr",k=10,knots=NULL)
```

without `knots`, knots are placed evenly over `x`

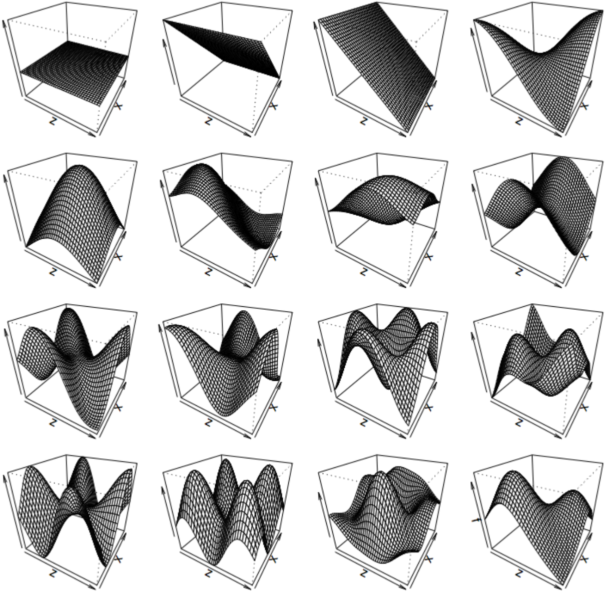
cp basis "more optimal" (see tprs)



thin plate splines

- multi-dimensional basis
- 2-part basis
  - global bits (orthogonal polynomial terms)
  - local bits (radial basis functions)
- requires 1 radial function per datum
- knots?

tprs basis



thin plate regression splines – Wood (2003)

- instead of knots, use all data *but*
- take eigendecomposition $X = UDU^{\mathsf{T}}$
- truncate to 1^{st} k columns (D is in "eigen-order")
- "more optimal" than knot-based approaches

```
s(x,y,..., bs="tp", k=M+k.def, knots=NULL)
```

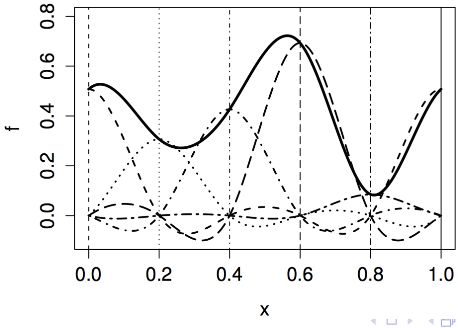
where `M` is nullspace size and `k.def` is 8 (1D), 27 (2D), 100 (3D+)

cyclic smoothers

- seasonality?
- temporal periodicity?
- angles?

```
s(x,bs="cc",k=10,knots=NULL)
```

wrap at `range(x)`, unless `knots` specified



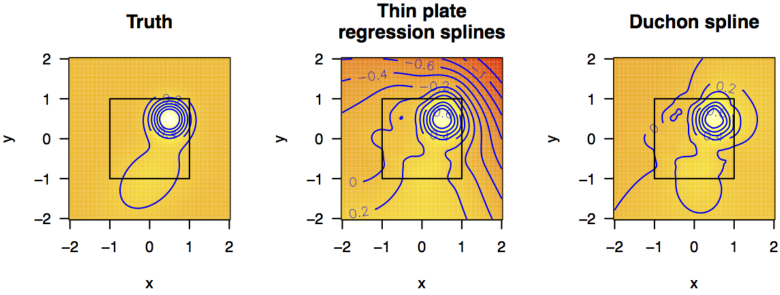
random effects

- IID normal random effects
- multivariate (`s(x,y,z,bs="re")` is `~x:y:z-1` interaction)
- exploits equivalence of random effects and splines
- useful when you just have a "few" random effects

```
s(x,bs="re")
?gam.vcomp
```

Duchon splines

- sometimes spatial smoothers curl up at the edges
- Duchon splines limit nullspace in 2D+

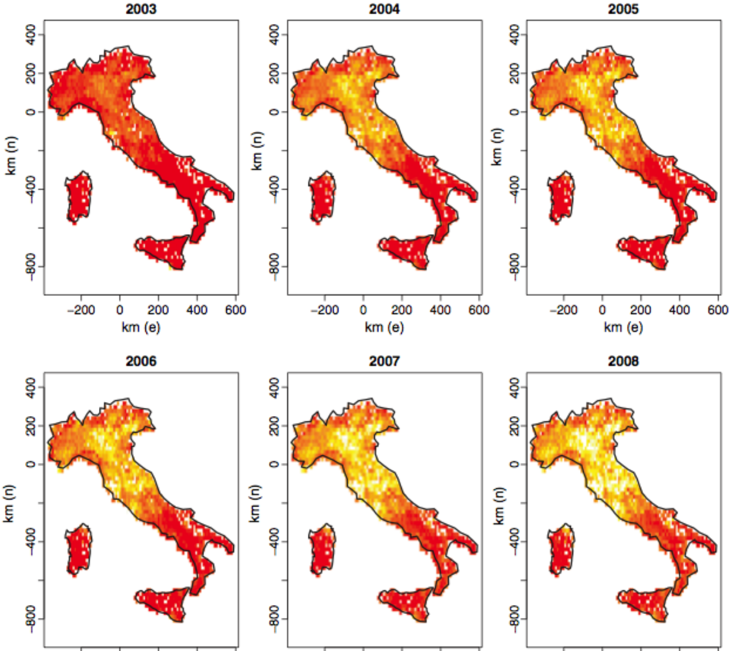


tensor products

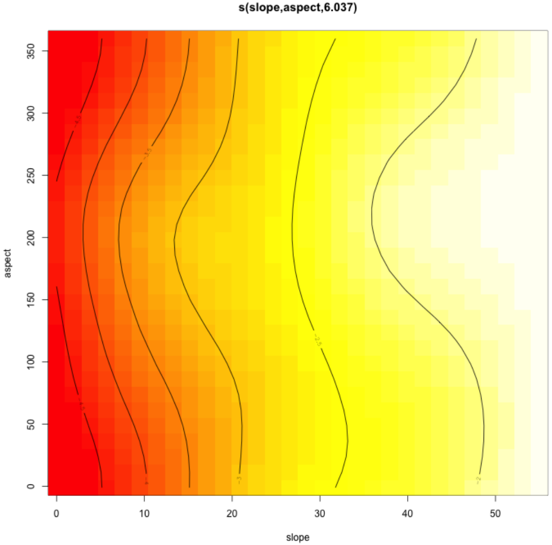
- tprs multivariate but assume isotropy
- are space and time the same? (hint: NO)
- "push" 2D spatial smoother through time

```
te(x,y,t, bs=c("tp","cr"), d=c(2,1), k=c(100,10))
```

tensor products (space-time)



tensor products (slope-aspect)



by=

- what if you only have a couple of years?
- for factors: multiple smooths
- for numerics: “parametric” tensor
- need to add parameteric term

```
s(x,y,bs="tp",by=as.factor(year)) + as.factor(year)
```

Model checking

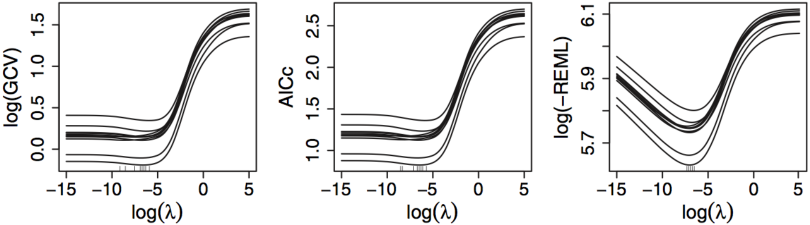
SECOND SPOILER

the default options are (almost definitely) wrong

(for you)

Quick note on fitting

- by default `gam` uses GCV for smoothing parameter selection
- GCV prone to overfitting (Wood, 2011)
- GCV also problematic w. correlated covariates (Wood, 2006; pers. obsn.)
- REML better – BUT can only compare nested models (ML?)



how do I best control flexibility?

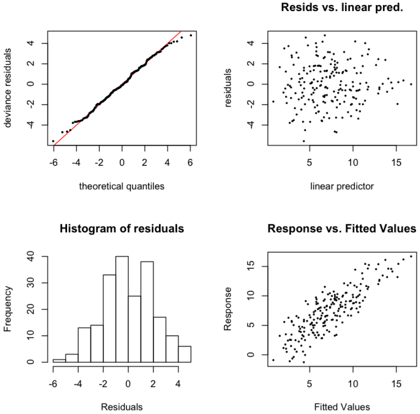
- `k` parameter controls "basis size"
- look at output of `summary` and `gam.check`
- `?choose.k`
- double `k`, see what happens?
- watch out, larger basis gives more, weirder functions

```
> gam.check(b)

Method: GCV   Optimizer: magic
Smoothing parameter selection converged after 8 iterations.
The RMS GCV score gradiant at convergence was 1.072609e-05 .
The Hessian was positive definite.
The estimated model rank was 37 (maximum possible: 37)
Model rank =  37 / 37

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

         k'   edf k-index p-value
s(x0) 9.000 2.318   0.996    0.45
s(x1) 9.000 2.306   0.969    0.35
s(x2) 9.000 7.655   0.961    0.25
s(x3) 9.000 1.233   1.037    0.68
```


DÉCHETS
MÉNAGERS
RÉSIDUELS
Je suis collecté le
Lun
Mar
Mer
Ven
Sam
Dim

how do I know when I've got it right?

- `plot` the `gam` object – over/under-fitting?
- looking at `gam.check` (brain scan example in Wood 2006)
  - left column – response distribution correct?
  - right column – non-constant variance?
- plot residuals vs. covariates



I've probably talked for too long already. . .

- randomised quantile residuals (Dunn and Smyth, 1996)
- `bam` for big additive models (Wood et al, 2014)
  - can do AR1 correlation structures (in order)
- `gamm` when you have "many" random effects or correlation
  - correlation specified as in `lme`
  - useful link: `http://glmm.wikidot.com/faq#modelspec`
  - e.g. `correlation=corAR1(form=~segment|tr.su)`
  - smooth $\leftrightarrow$ random effect relation
  - numerically unstable? (pers. opp.)
  - autocorrelogram can save you some stress :)

References (for later)

Almost all figures stolen from Wood (2006) or (2011)

Thanks!

Talk available at:

converged.yt/talks/creemcrackers-splines/talk.pdf