Understanding the Stochastic Partial Differential Equation Approach to Smoothing

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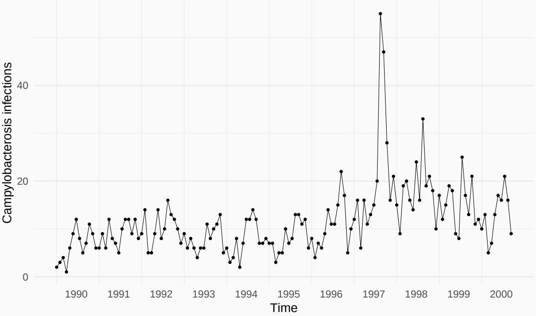
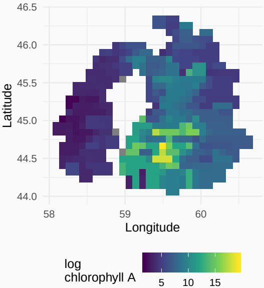
Andy and Richard

Introduction

The kinds of data we’ll talk about

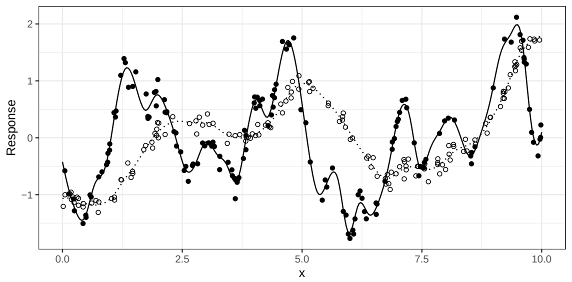




How to model dependence?

Tobler's law: "everything is related to everything else, but near things are more related than distant things."

Two ways to think about this: *Smoothness* and *Correlation*.



How to model dependence?

Two ways to think about this: Smoothness and Correlation.

Two popular approaches to modelling it: GAMs and SPDEs.

- GAMs ≈ "smoothing using spline-type things"
- SPDEs ≈ "Matérn covariance approximation using SPDEs/MRFs"

Jenny Bryan
@JennyBryan

All models are wrong, so why not start with one you actually understand?

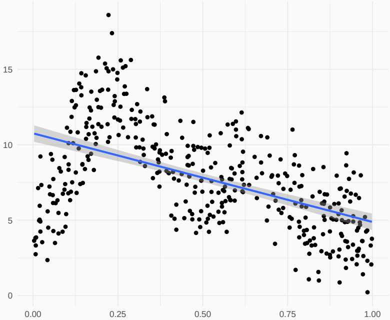
Refresh: what are GAMs made of?

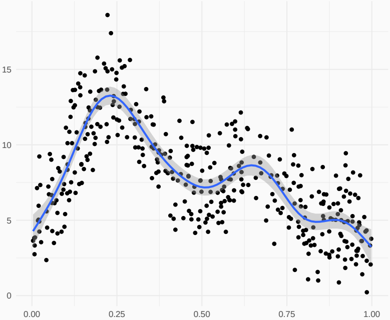
Explain: how does the SPDE method work?
Apply: how can we use these results in practice?

The GAM approach

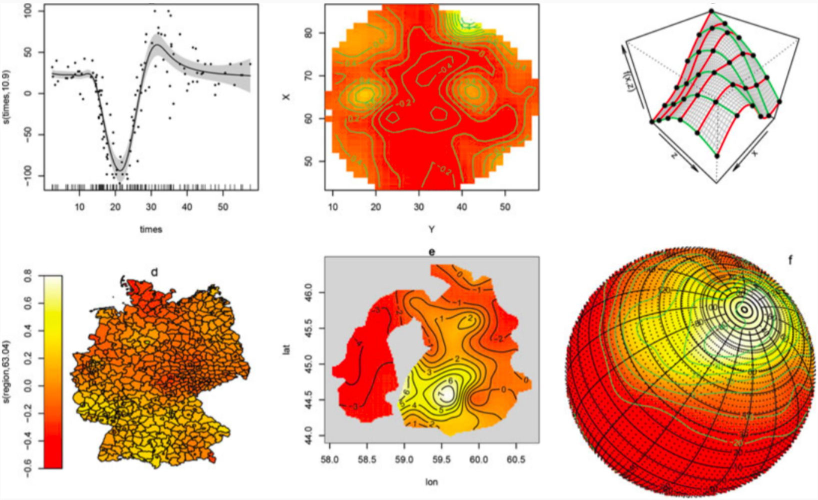
From GLMs to GAMs

- Want flexible, structured models
- GAM provides this via "smooths"
- $y \sim s(x)$, where s is a smooth function of x





Examples of smooths



Smooths come in 2 bits...

basis functions

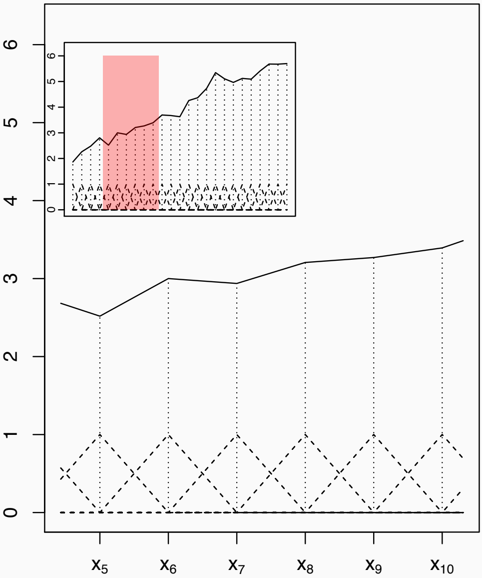
- join together to make up the overall curve, $s(x)$
- go in the design matrix, $\mathbf{X}$

penalties

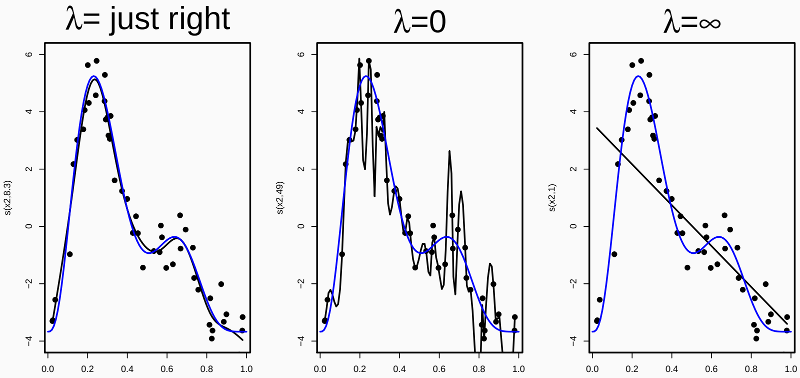
- controls how the line behaves
- penalty matrix $\mathbf{S}$ (structure)
- smoothing parameter λ (how wiggly)

"basis-penalty smoothers"

Basis functions



Penalty and smoothing parameter



SPDE approach

Lindgren et al, 2011

Journal of the
Royal Statistical Society

SERIES B
Statistical
Methodology

J. R. Statist. Soc. B (2011)
73, *Part* 4, *pp.* 423–498

An explicit link between Gaussian fields and Gaussian Markov random fields: the stochastic partial differential equation approach

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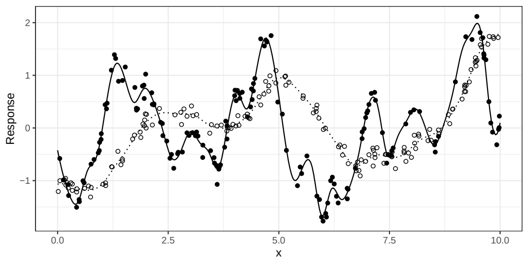
Norwegian University of Science and Technology, Trondheim, Norway

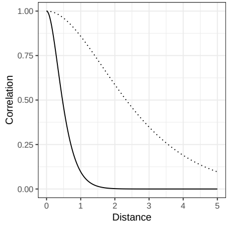
and Johan Lindström

Lund University, Sweden

Two Selling points of SPDE approach

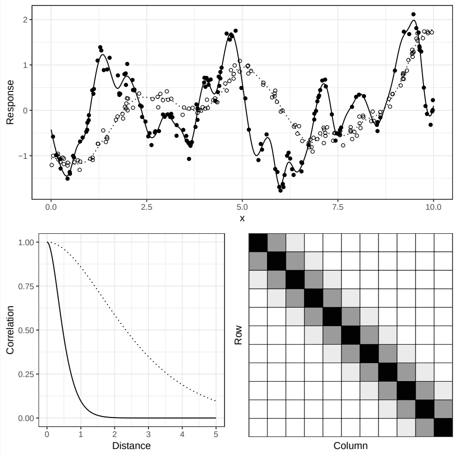
1. A certain kind of SPDE produces curves that have Matérn correlation functions, a popular choice of correlation function.





Two Selling points of SPDE approach

2. The precision matrix Q can be computed very efficiently, a bottleneck in many other correlation approaches.



SPDE method comes in 2 bits...

finite elements

- join together to make up the overall curve
- go in the predictor matrix, $\mathbf{A}$

precision

- controls how the curve behaves
- precision matrix $\mathbf{Q}$ (structure)
- correlation parameter κ (how wiggly)
- variance parameter τ

Wait a minute...

SPDE method comes in 2 bits...

~~finite elements~~

basis functions

- join together to make up the overall curve
- go in the predictor design matrix, $\mathbf{A} = \mathbf{X}$

~~precision~~

penalty

- controls how the curve behaves
- precision matrix $\mathbf{Q} = \mathbf{S}$ (structure)
- correlation parameter κ (how wiggly)
- variance parameter τ
- $\kappa, \tau \rightsquigarrow \lambda$

SPDE is a basis-penalty smoother

The SPDE has a corresponding smoothness penalty.

Pick same basis, then

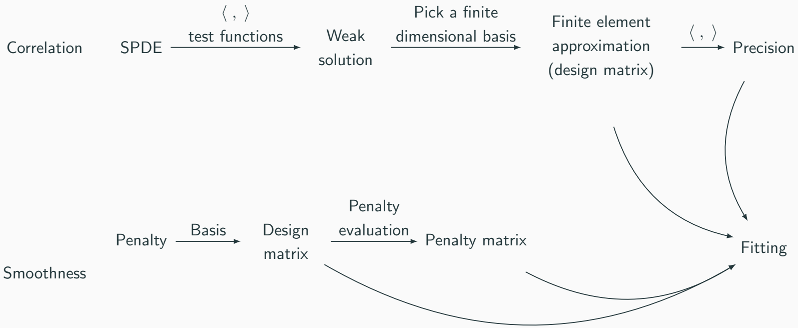
$$\mathbf{A} = \mathbf{X}$$

Use SPDE and corresponding penalty, then

$$\mathbf{Q} = \mathbf{S}$$

See our paper for more mathematical details.

The SPDE method is a basis-penalty smoother



Practical implications

What about R-INLA and mgcv?

- Both are ways to fit this same model.
- Both `R-INLA` and `mgcv` do approximations:
  - `R-INLA` does a Laplace approximation to get around MCMC.
  - `mgcv` does REML using Laplace approximation too.
- `mgcv` does empirical Bayes, so uses point estimates for hyperparameters (smoothing parameters, variance components).
- (`R-INLA` can do this too!)

What can we do with this?

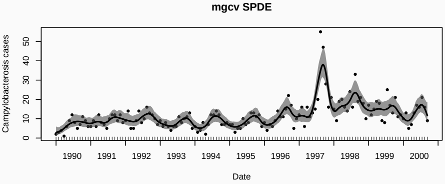
- Writing SPDE models as basis-penalty smoothers means we can use them elsewhere
- Anywhere structured random effects can be used!
- `mgcv`, `TMB`, Stan, etc
- We can combine them with other approaches!

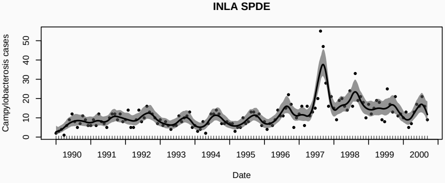
mgcv code

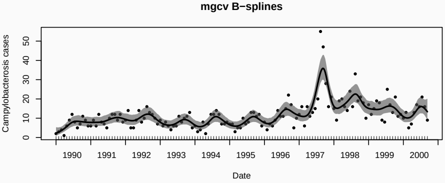
Setup using R-INLA, fit with mgcv

```r
## Simplified code-snippets
## Full code in supplementary materials

# get finite element matrices
inlamats <- inla.mesh.fem(mesh)
c1 <- as.matrix(inlamats$c1)
g1 <- as.matrix(inlamats$g1)
g2 <- as.matrix(inlamats$g2)

# construct the design matrix
X <- as.matrix(inla.spde.make.A(mesh, observed_locs))

# build the penalty / precision matrix
S <- kappa^4 * c1 + 2*kappa^2 * g1 + g2

# fit
b <- gam(y ~ X - 1,
         paraPen = list(X = list(S)),
         method = "REML")
```

1D comparison







Spatial smoothing comparison

Take-home

A modelling framework emerges

Use basis-penalty or basis-precision as a common currency.

1. **Choose a covariance model**: explicitly (as in kriging, etc), via smoothness penalty (e.g., splines), or with an SPDE;
2. **Approximate the precision matrix** Q: reduce dimension or induce sparsity in Q;
3. **Draw approximate inference using a software implementation**: e.g., with `mgcv`, MCMC (e.g., Stan; `JAGS`), `R-INLA`, `lme4` or `TMB`.

More info?

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Understanding the Stochastic Partial Differential Equation Approach to Smoothing

David L. Miller, Richard Glennie, and Andrew E. Seaton

Correlation and smoothness are terms used to describe a wide variety of random quantities. In time, space, and many other domains, they both imply the same idea: quantities that occur closer together are more similar than those further apart. Two popular statistical models that represent this idea are basis-penalty smoothers (Wood in Texts in statistical science, CRC Press, Boca Raton, 2017) and stochastic partial differential equations (SPDEs) (Lindgren et al. in J R Stat Soc Series B (Stat Methodol) 73(4):423–498, 2011). In this paper, we discuss how the SPDE can be interpreted as a smoothing penalty and can be fitted using the `R` package `mgcv`, allowing practitioners with existing knowledge of smoothing penalties to better understand the implementation and theory behind the SPDE approach.

Supplementary materials accompanying this paper appear online.

Key Words: Smoothing; Stochastic partial differential equations; Generalized additive model; Spatial modelling; Basis-penalty smoothing.

Slides: `https://github.com/dill/SPDE-talk-IBS`