Smooth additive models for large datasets

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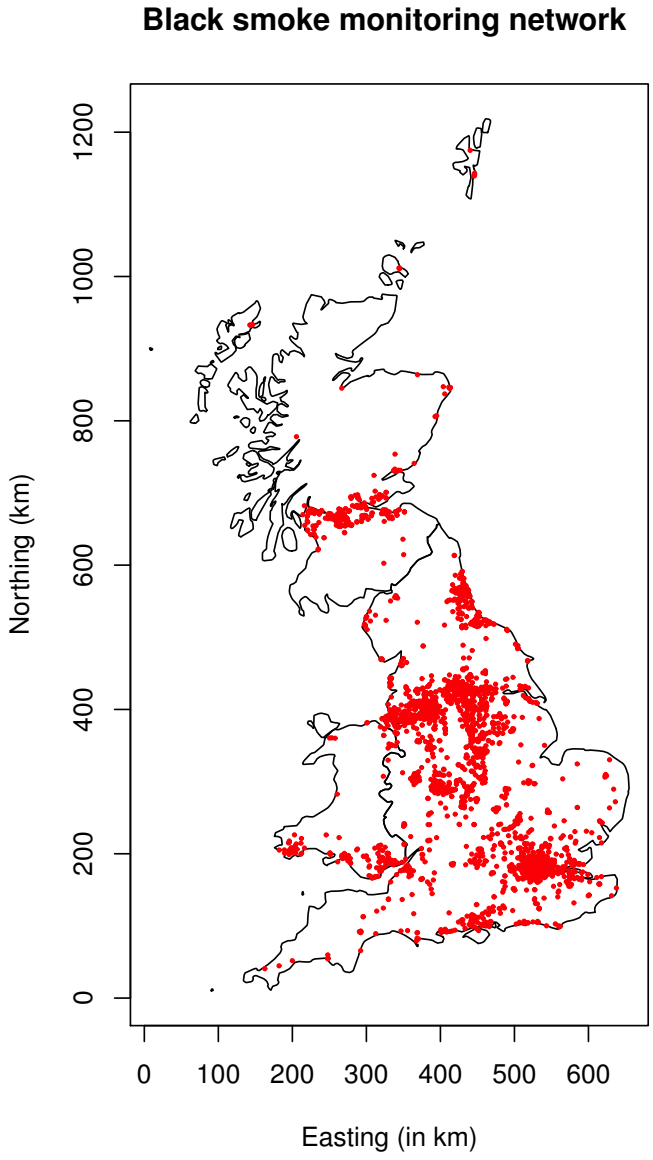
Example motivation: London smog 1952

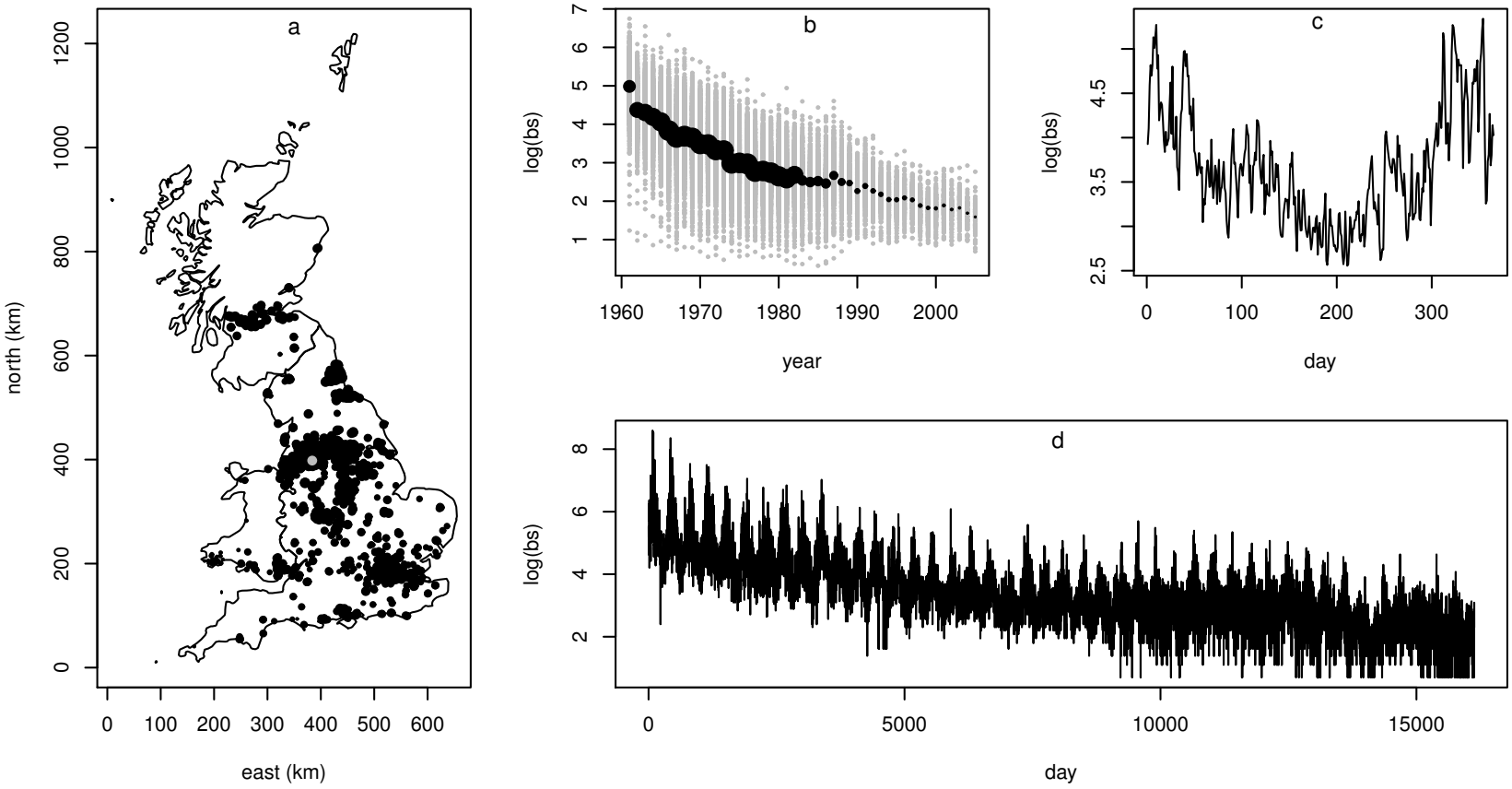
- 5-9 Dec 1952.
- 4-12 thousand premature deaths.
- Black smoke (particulates) and sulphur from domestic coal fires.
- Clean air act 1956.
- Monitoring from 1961.

Black smoke monitoring…



- 4 decades of daily 'black smoke' monitoring at a variable subset of the 2400+ stations shown.
- Started in 1961 to monitor air pollution (then mostly from coal), in wake of 1950s smog deaths.
- Epidemiological studies need estimates of *daily* exposure away from stations.
- $O(10^7)$ measurements and suitable smooth latent Gaussian models have $O(10^4)$ coefficients with 10-30 variance parameters.

Daily BS data



Black smoke modelling

- A reasonable daily black smoke model is

$$\begin{aligned}\log(\mathtt{bs}_i) = {} & f_1(\mathtt{y}_i) + f_2(\mathtt{doy}_i) + f_3(\mathtt{dow}_i) \\ & + f_4(\mathtt{y}_i, \mathtt{doy}_i) + f_5(\mathtt{y}_i, \mathtt{dow}_i) + f_6(\mathtt{doy}_i, \mathtt{dow}_i) \\ & + f_7(\mathtt{n}_i, \mathtt{e}_i) + f_8(\mathtt{n}_i, \mathtt{e}_i, \mathtt{y}_i) + f_9(\mathtt{n}_i, \mathtt{e}_i, \mathtt{doy}_i) + f_{10}(\mathtt{n}_i, \mathtt{e}_i, \mathtt{dow}_i) \\ & + f_{11}(\mathtt{h}_i) + f_{12}(\mathtt{T}_i^0, \mathtt{T}_i^1) + f_{13}(\bar{\mathtt{T}}\mathtt{1}_i, \bar{\mathtt{T}}\mathtt{2}_i) + f_{14}(\mathtt{r}_i) + \alpha_{k(i)} + b_{\mathrm{id}(i)} + e_i\end{aligned}$$

  The model has around 10^4 coefficients, and was well beyond previous model fitting technology (weeks of computing time).
- Even without worrying about computing time, *storing* a $10^7 \times 10^4$ model matrix requires nearly a terabyte of memory.
- We need to reduce memory footprint and speed up computation.

Memory bandwidth, Cache, block algorithms

- Most numerical computation is limited by the rate of data transfer to the CPU, not the CPU speed.
- Cache is small fast access memory between CPU and main memory (RAM).
- Big speed up if most flops involve data already in Cache.
- Consider two 10^6 flop computations
  1. $\mathbf{C}$ is a 1000×1000 matrix, and $\mathbf{y}$ a 1000-vector. Compute $\mathbf{Cy}$. Each of 10^6 elements of $\mathbf{C}$ read once, no re-use.
  2. $\mathbf{A}$ and $\mathbf{B}$ are both 100×100 matrices. Form $\mathbf{AB}$. Repeatedly revisits the 2×10^4 elements of $\mathbf{A}$ and $\mathbf{B}$.

  ...provided $\mathbf{A}$ and $\mathbf{B}$ fit in Cache, 2 is *much* faster.
- Structure algorithms around Cache friendly blocks! e.g.

$$\begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{11}\mathbf{B}_{11} + \mathbf{A}_{12}\mathbf{B}_{21} & \mathbf{A}_{11}\mathbf{B}_{12} + \mathbf{A}_{12}\mathbf{B}_{22} \\ \mathbf{A}_{21}\mathbf{B}_{11} + \mathbf{A}_{22}\mathbf{B}_{21} & \mathbf{A}_{21}\mathbf{B}_{12} + \mathbf{A}_{22}\mathbf{B}_{22} \end{bmatrix}$$

Scalable GAM methods

- Model fitting requires the second derivative matrix of the log likelihood. Need ways to compute this, or its Cholesky factor, without ever forming the whole model matrix.
- Computations need to be block oriented. This means finding algorithms that are rich in matrix crossproducts and pivoted Cholesky decompositions, but avoid QR, SVD, and eigen methods, which have high matrix-vector operations counts.
- Can then leverage optimized BLAS or openMP parallelization.
- Speed is facilitated by casting Newton estimation of model as iterative weighted penalized linear model estimation, and estimating smoothing parameters via REML applied to each working model.

Cheaper $\mathbf{X}^{\mathrm{T}}\mathbf{W}\mathbf{X}$: discrete covariate methods

- The required Hessian involves terms $\mathbf{X}^{\mathrm{T}}\mathbf{W}\mathbf{X}$ where $\mathbf{W}$ is diagonal.
- Formation of $\mathbf{X}^{\mathrm{T}}\mathbf{W}\mathbf{X}$ is the leading order cost: $O(np^2)$.
- Lang et al.[1] point out that for a single 1D smooth, $f(x)$, the product $\mathbf{X}^{\mathrm{T}}\mathbf{W}\mathbf{X}$ is very efficiently computable if x has only $m \ll n$ discrete values, so $\mathbf{X}$ has only m unique rows.
- As statisticians we should be prepared to discretise x to $m = O(\sqrt{n})$ bins.
- It is possible to find (novel) efficient computational methods for the multiple discretised covariate case, both for multiple 1D smooths and for 'tensor product' smooths of multiple covariates (which also have to be parallelized).

[1] Lang, Umlauf, Wechselberger, Harttgen & Kneib, 2014, Statistics & Computing.

Simple discrete method example

- For a single smooth, its $n \times p_j$ model matrix becomes

$$X_j(i,l) = \bar{X}_j(k_j(i),l)$$

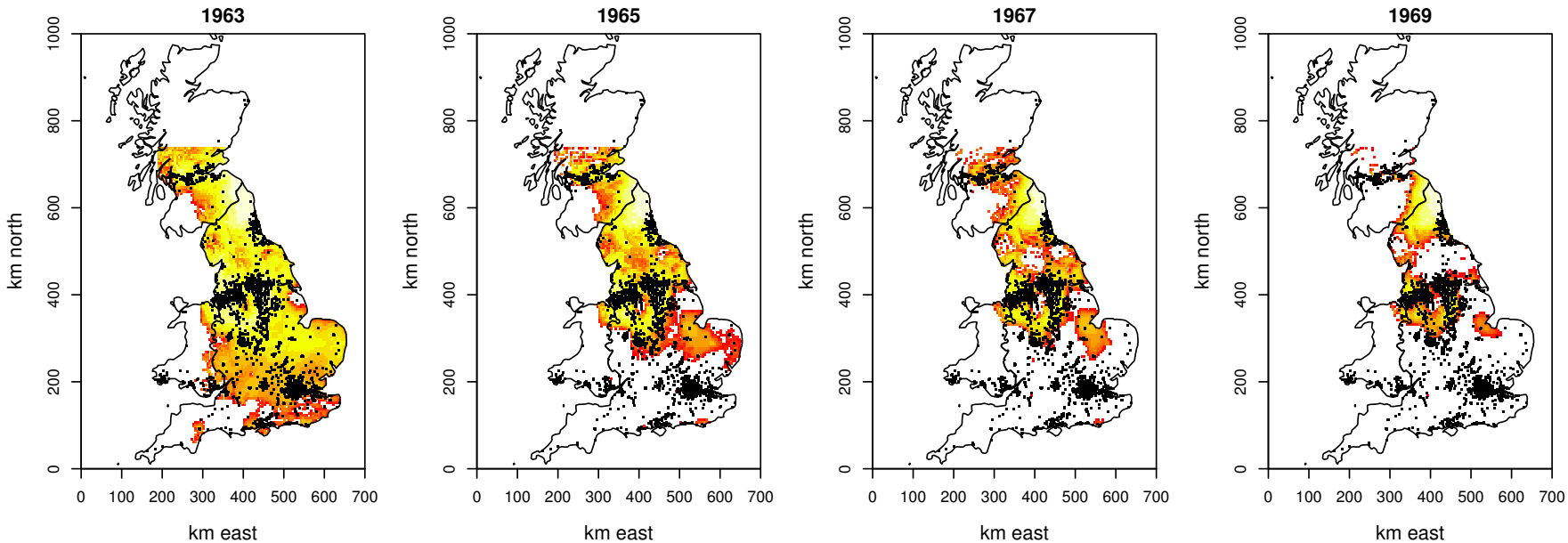
  where $\bar{\mathbf{X}}_j$ is an $m_j \times p_j$ matrix evaluating the smooth at the corresponding gridded values.
- Then, for example

$$X_j^{\mathrm{T}} y = \bar{X}_j^{\mathrm{T}} \bar{y} \text{ where } \bar{y}_l = \sum_{k_j(i)=l} y_i$$

  Cost: $O(n) + O(m_j p_j)$ – for $m_j \ll n$ this a factor of p_j saving.
- In general all required (cross)products are a factor of p_j more efficient, where p_j is the largest (marginal) basis dimension involved in the term.

`bam(...,discrete=TRUE)`

- In the end the black smoke model could be estimated in just under 5 minutes on a 10 core workstation using the methods built in to `mgcv:bam(...,discrete=TRUE)`.[2]
- So far the methods only apply to single linear predictor models.
- Map shows average daily probability of exceeding current EU daily limit, for 4 years in the 1960s.



[2] Wood et al. (2017) JASA