Spatio-Temporal Smoothing for Very Large Datasets

Satellite Based Vegetation Measurements

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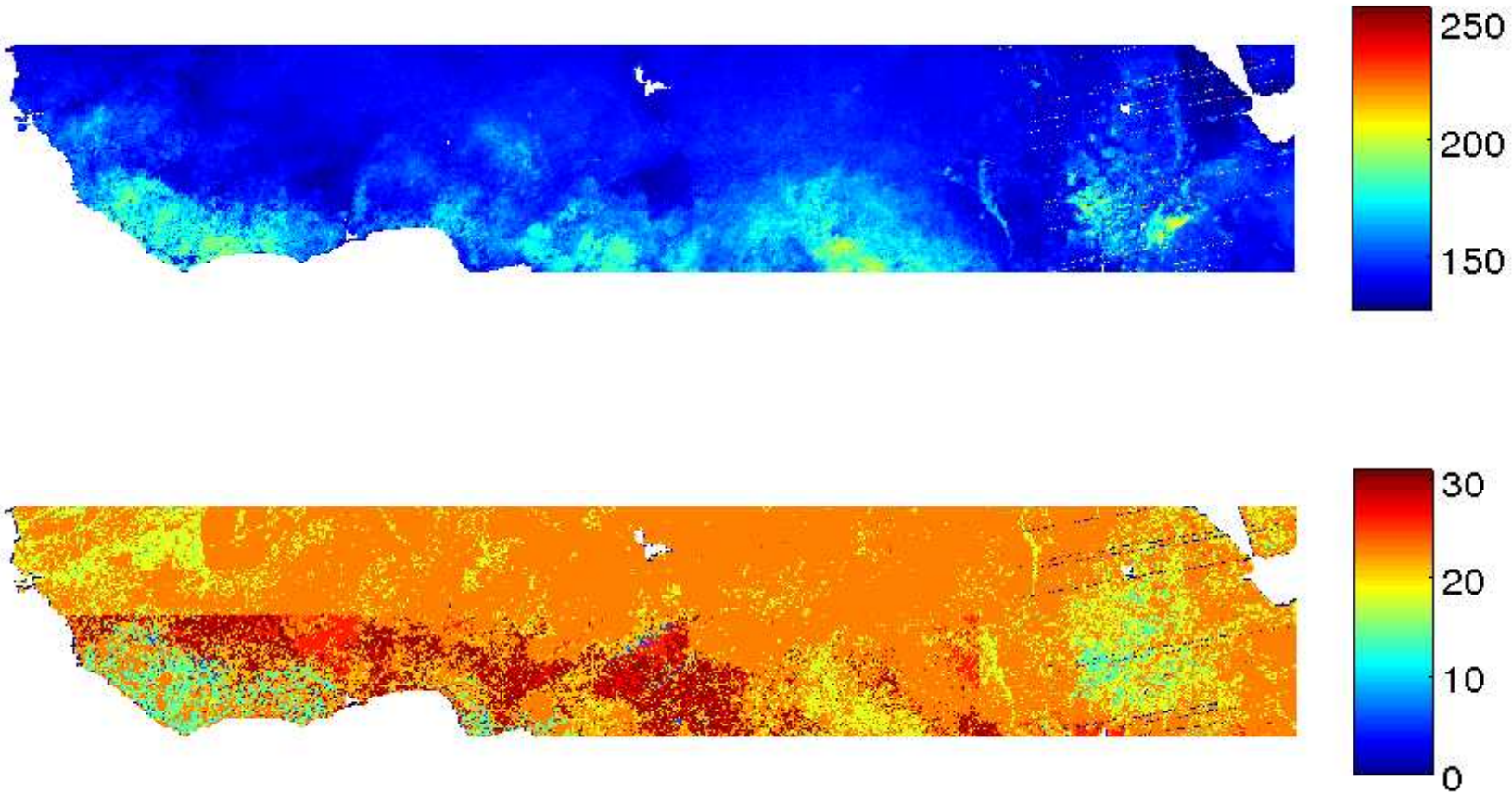
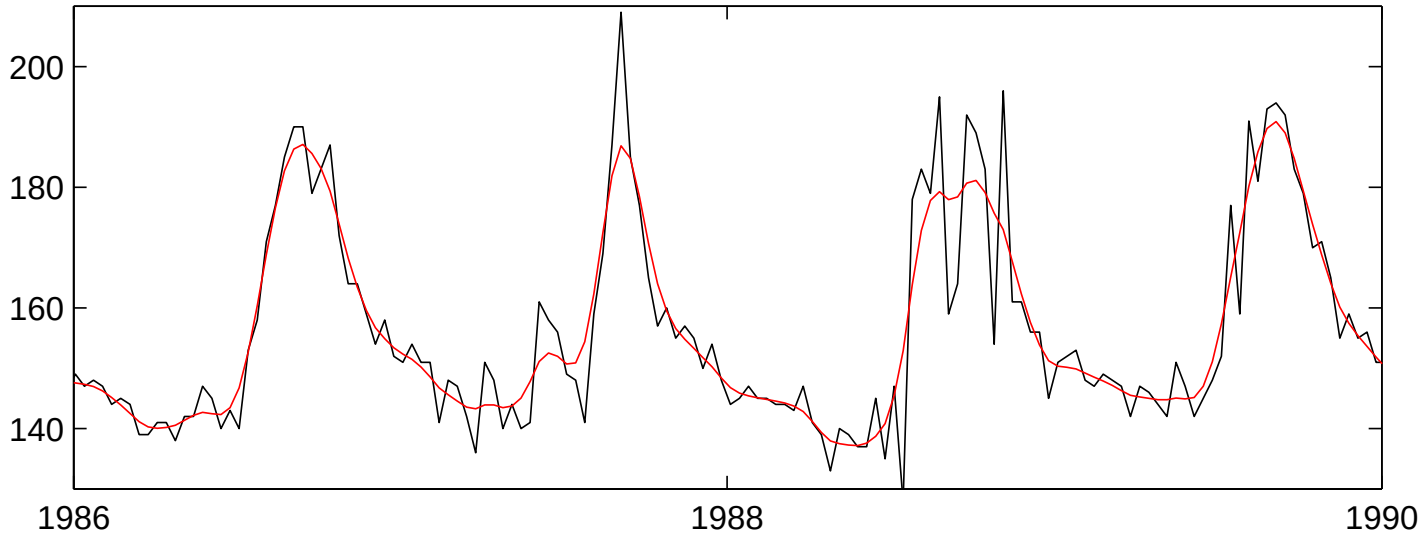
Satellite measured vegetation — The African Sahel



NDVI $[0, 255]$ and cloud $[0, 31]$ data from February 1985.

Smoothed version of the NDVI Data

Smooth the data to fill in missing values and remove noise due to cloud cover, etc.



Important ecological questions:

- Plant phenology (start and end of season)
- Plant productivity (integral)

What can the methods handle?

Assuming a standard desktop computer.

	N
Standard Kriging	$\sim 10^3$
Big N-methods	$\sim 10^5$
Satellite data	$\sim 10^8$

Big N-methods: process convolution (Higdon, 2001), tapering (Furrer et al., 2006), predictive processes (Banerjee et al., 2008), block composite (Eidsvik et al., 2014), SPDE/GMRF (Lindgren et al., 2011).

Space-time is often **worse**. For the SPDE-methods:

Dimension	Time for $R = \text{chol}(Q)$	$\text{nnz}(Q)$	$\text{nnz}(R)$
$\mathbb{R}^1$	$\mathcal{O}\left(N^1\right)$	$c^1 N$	$\sim N^1$
$\mathbb{R}^2$	$\mathcal{O}\left(N^{1.5}\right)$	$c^2 N$	$\sim N^{1+1/2}$
$\mathbb{R}^3$	$\mathcal{O}\left(N^2\right)$	$c^3 N$	$\sim N^{1+2/3}$
$\mathbb{R}^d$	???	$c^d N$	$\sim N^{1+(d-1)/d}$

Can't we just wait for better computers?

Current Satellite data (1982–)

$10\ \text{day}$ temporal resolution

$\sim 8\ \text{km}$ spatial resolution

New EU earth observation platform (launch 2015–)

$3 - 5\ \text{day}$ temporal resolution

$\leq 1\ \text{km}$ spatial resolution

Available data grows faster than processing power!

The standard likelihood

Log-likelihood

$$l(\theta|\boldsymbol{y}) = -\frac{1}{2}\log|\Sigma(\theta)| - \frac{1}{2}\Big(\boldsymbol{y} - \mu(\theta)\Big)^\top \Sigma(\theta)^{-1}\Big(\boldsymbol{y} - \mu(\theta)\Big),$$

with derivatives

$$\begin{aligned}\frac{\partial l(\theta|\boldsymbol{y})}{\partial \theta} = &-\frac{1}{2}\operatorname{tr}\left(\Sigma^{-1}\frac{\partial \Sigma}{\partial \boldsymbol{\theta}}\right) + (\boldsymbol{y} - \mu)^\top \Sigma^{-1}\frac{\partial \mu}{\partial \boldsymbol{\theta}} \\ &+ \frac{1}{2}(\boldsymbol{y} - \mu)^\top \Sigma^{-1}\frac{\partial \Sigma}{\partial \boldsymbol{\theta}}\Sigma^{-1}(\boldsymbol{y} - \mu).\end{aligned}$$

Spline smoothing (Wahba, 1981)

$$\mathrm{GCV}(\theta) = \frac{\|\boldsymbol{y} - \boldsymbol{S}(\theta)\boldsymbol{y}\|_2^2}{\Big(n - \operatorname{tr}(\boldsymbol{S}(\theta))\Big)^2}, \qquad \boldsymbol{S}(\theta) \propto \Big(\boldsymbol{A}^\top \boldsymbol{A} + \boldsymbol{Q}(\theta)\Big)^{-1}$$

Parameter estimates

Parameters are estimated by one of:

1. $\text{argmax}_\theta \, l(\theta|\boldsymbol{y})$.
2. Solving: $\nabla l(\theta|\boldsymbol{y}) = 0$.
3. $\text{argmin}_\theta \, \text{GCV}(\theta)$.

and we need to compute:

$\log \lvert\Sigma\rvert$	For case 1.
$\Sigma^{-1}\boldsymbol{y}$	For all cases.
$\text{tr}\left(\Sigma^{-1}\right)$	For cases 2, 3.

These can be approximated to high accuracy (Aune et al., 2014; Anitescu et al., 2012; Stein et al., 2013)

The Hutchinson (1990) trace estimator

The trace of a matrix Σ^{-1} is given by

$$\operatorname{tr}\left(\Sigma^{-1}\right) \approx \frac{1}{K}\sum_{k=1}^{K} \boldsymbol{e}_k^\top \Sigma^{-1} \boldsymbol{e}_k$$

where the elements of $\boldsymbol{e}_k$ are iid $\{-1, 1\}$ with probability $1/2$.

$$\mathsf{E}\left(\boldsymbol{e}^\top \Sigma^{-1} \boldsymbol{e}\right) = \operatorname{tr}\left(\Sigma^{-1}\mathsf{E}(\boldsymbol{e}\boldsymbol{e}^\top)\right) = \operatorname{tr}\left(\Sigma^{-1}\boldsymbol{I}\right)$$

$$\mathsf{V}\left(\boldsymbol{e}^\top \Sigma^{-1} \boldsymbol{e}\right) = 2\left(\left\|\Sigma^{-1}\right\|_F^2 - \sum_i \left(\Sigma_{ii}^{-1}\right)^2\right) = 2\sum_{i\neq j}\left(\Sigma_{ij}^{-1}\right)^2$$

Usefull matrix algebra Harville (1997); Petersen and Pedersen (2012)

Probing vectors

A time series example ($K = 5$):

$$\mathcal{V} = \begin{bmatrix} \pm 1 & 0 & 0 & 0 & 0 \\ 0 & \pm 1 & 0 & 0 & 0 \\ 0 & 0 & \pm 1 & 0 & 0 \\ 0 & 0 & 0 & \pm 1 & 0 \\ 0 & 0 & 0 & 0 & \pm 1 \\ \pm 1 & 0 & 0 & 0 & 0 \\ 0 & \pm 1 & 0 & 0 & 0 \\ & & \vdots & & \end{bmatrix} \quad \mathsf{V}(\mathcal{V}\mathcal{V}^\top) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 1 & 0 & \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & \\ & & \vdots & & & & & \ddots \end{bmatrix}$$

$\boldsymbol{v}_k$ columns of $\mathcal{V}$.

Similar argument in $\mathbb{R}^2$.

In general a **NP-complete graph-colouring** problem, but **near optimal gready algorithms** exist.

Probing vectors II

Variance for the original estimator:

$$\mathrm{V}\left(\frac{1}{K}\sum_{k=1}^{K} \boldsymbol{e}_k^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{e}_k\right) = \frac{2}{K}\sum_{i\neq j}\left(\boldsymbol{\Sigma}^{-1}_{ij}\right)^2$$

Variance for the new estimator:

$$\mathrm{V}\left(\sum_{k=1}^{K} \boldsymbol{v}_k{}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{v}_k\right) = 2\left(\left\|\boldsymbol{\Sigma}^{-1}\circ \mathrm{V}(\boldsymbol{\nu}\boldsymbol{\nu}^\top)\right\|_F^2 - \sum_{i=1}^{n}\left(\boldsymbol{\Sigma}^{-1}_{ii}\right)^2\right)$$

$$= 2\sum_{\substack{i=j+mK \\ m\in\mathbb{Z}^+}}\left(\boldsymbol{\Sigma}^{-1}_{ij}\right)^2$$

This is better if elements in $\boldsymbol{\Sigma}^{-1}$ **decrease away from the diagonal**

Parameter estimates (again)

Parameters are estimated by one of:

1. $\text{argmax}_\theta \, l(\theta|\boldsymbol{y})$.
2. Solving: $\nabla l(\theta|\boldsymbol{y}) = 0$.
3. $\text{argmin}_\theta \, \text{GCV}(\theta)$.

and we need to compute:

$\log \lvert\Sigma\rvert$	For case 1.
$\Sigma^{-1}\boldsymbol{y}$	For all cases.
$\text{tr}\left(\Sigma^{-1}\right)$	For cases 2, 3.

We can reduce $\text{tr}\left(\Sigma^{-1}\right)$ to computations of $\Sigma^{-1}\boldsymbol{b}$.

Aune et al. (2014) uses $\log \lvert\Sigma\rvert = \text{tr} \log \Sigma$, and a series expansion of $\log \Sigma$.

Using the trace estimator the problem reduces to computing

$$x = A^{-1}b \qquad \text{for different } b$$

Preconditioned Conjugate Gradient

Iterative method for solving

$$Ax = b$$

using a **preconditioner**, M, and computing only Ax and $M^{-1}x$.

A suitable preconditioner M has

- $M^{-1}x$ easy to compute
- $M^{-1}A \approx I$.

Classical solutions

- Use $\text{diag}(A)^{-1}$.
- For sparse matrices use the (modified) incomplete Cholesky.

Comments

The Good

- No need to store the full matrices.
- $\mathcal{O}\left(N^1\right)$ for sparse matrices.
- Anitescu et al. can be seen as GEE $\rightarrow$ parameter uncertainties

The Bad

- Still $\mathcal{O}\left(N^2\right)$ for covariances matrices.
- Only Aune et al. evaluates the likelihood.

The Ugly

- Numerical linear solvers in MATLAB and R are reasonable, but not outstanding.
- Sparse matrix support is "lacking" in MATLAB and bad in R.
- Optimal preconditioner depends on the problem.

Smoothing splines (Wahba, 1981)

Find $\hat{\mu}(\boldsymbol{s})$ such that

$$\hat{\mu} = \underset{\mu}{\operatorname{argmin}} \frac{1}{n} \sum_i \|y_i - \mu_i\|_2^2 + \lambda \int \left(\frac{\partial^\alpha \mu(\boldsymbol{s})}{\partial \boldsymbol{s}^\alpha} \right)^2 \mathrm{d}\boldsymbol{s}$$

$\hat{\mu}$ is given as the solutions to an SPDE (Wahba, 1981):

$$\Delta^{\alpha/2} \boldsymbol{x}(\boldsymbol{s}) = \mathcal{W}$$

This corresponds to a Matérn (1960) covariance with range $\to \infty$, and the spline can be seen as a hierarchical model

$$\boldsymbol{y}|\boldsymbol{x} \in \mathrm{N}\left(\boldsymbol{A}\boldsymbol{x}, \sigma^2 \boldsymbol{I}\right) \qquad \boldsymbol{x} \in \mathrm{N}\left(0, \left(\tau^2 \boldsymbol{Q}\right)^{-1}\right).$$

Smoothing splines ≈ Gaussian processes

The spline smoothing of $\boldsymbol{y}$ can be seen as a conditional expectation

$$\begin{aligned}\widehat{\mu} = \mathsf{E}\left(\boldsymbol{x}|\boldsymbol{y};\tau^2,\sigma^2\right) &= \left(\tau^2\boldsymbol{Q} + \boldsymbol{A}^\top(\sigma^2\boldsymbol{I})^{-1}\boldsymbol{A}\right)^{-1}\left(\boldsymbol{A}^\top(\sigma^2\boldsymbol{I})^{-1}\boldsymbol{y}\right) \\ &= \left(\lambda\boldsymbol{Q} + \boldsymbol{A}^\top\boldsymbol{A}\right)^{-1}\boldsymbol{A}^\top\boldsymbol{y},\end{aligned}$$

where $\lambda = \tau^2\sigma^2$.

λ found by minimizing the GCV-error

$$GCV(\lambda) = \frac{\sum_i \|y_i - \widehat{\mu}_i\|_2^2}{(n - \mathsf{tr}(\boldsymbol{S}(\lambda)))^2}$$

with $\boldsymbol{S}(\lambda) = \boldsymbol{A}\left(\lambda\boldsymbol{Q} + \boldsymbol{A}^\top\boldsymbol{A}\right)^{-1}\boldsymbol{A}^\top$

Smoothing splines on a regular grid

For our splines ($\alpha = 2$) we have

$$\widehat{\mu} = \left(\lambda \boldsymbol{Q} + \boldsymbol{A}^\top \boldsymbol{A}\right)^{-1} \boldsymbol{A}^\top \boldsymbol{y}$$
$$\boldsymbol{Q} = \boldsymbol{G}^\top \boldsymbol{G}$$

where $\boldsymbol{G} \approx \Delta$.

For a regular grid in $1D$:

$$\boldsymbol{G} = \begin{bmatrix} 1 & -1 & 0 & \cdots & \\ -1 & 2 & -1 & 0 & \cdots \\ 0 & -1 & 2 & -1 & \cdots \end{bmatrix}$$

Neumann boundary condition

Smoothing splines on a regular grid

For our splines ($\alpha = 2$) we have

$$\widehat{\mu} = \left(\lambda \boldsymbol{Q} + \boldsymbol{A}^\top \boldsymbol{A}\right)^{-1} \boldsymbol{A}^\top \boldsymbol{y}$$
$$\boldsymbol{Q} = \boldsymbol{G}^\top \boldsymbol{G}$$

where $\boldsymbol{G} \approx \Delta$.

For a regular grid in $1D$:

$$\boldsymbol{G} = \begin{bmatrix} 2 & -1 & 0 & \cdots & 1 \\ -1 & 2 & -1 & 0 & \cdots \\ 0 & -1 & 2 & -1 & \cdots \end{bmatrix}$$

Cyclic boundary condition (Thon et al., 2012)

Preconditioner on the grid

Assume complete observations, $\boldsymbol{A} = \boldsymbol{I}$, and take $\boldsymbol{M} = \lambda \boldsymbol{Q} + \boldsymbol{I}$.

$$\boldsymbol{M} = \lambda \underbrace{\boldsymbol{G}^\top \boldsymbol{G}}_{=\boldsymbol{U}\boldsymbol{\Gamma}\boldsymbol{U}^\top} + \underbrace{\boldsymbol{I}}_{=\boldsymbol{U}\boldsymbol{U}^\top} = \boldsymbol{U} \underbrace{\left(\lambda \boldsymbol{\Gamma}^2 + \boldsymbol{I}\right)}_{=\boldsymbol{\Xi}} \boldsymbol{U}^\top,$$

where

$$\boldsymbol{U} = \begin{cases} \text{DCT}, & \text{Neumann} \\ \text{FFT}, & \text{Cyclic} \end{cases}$$

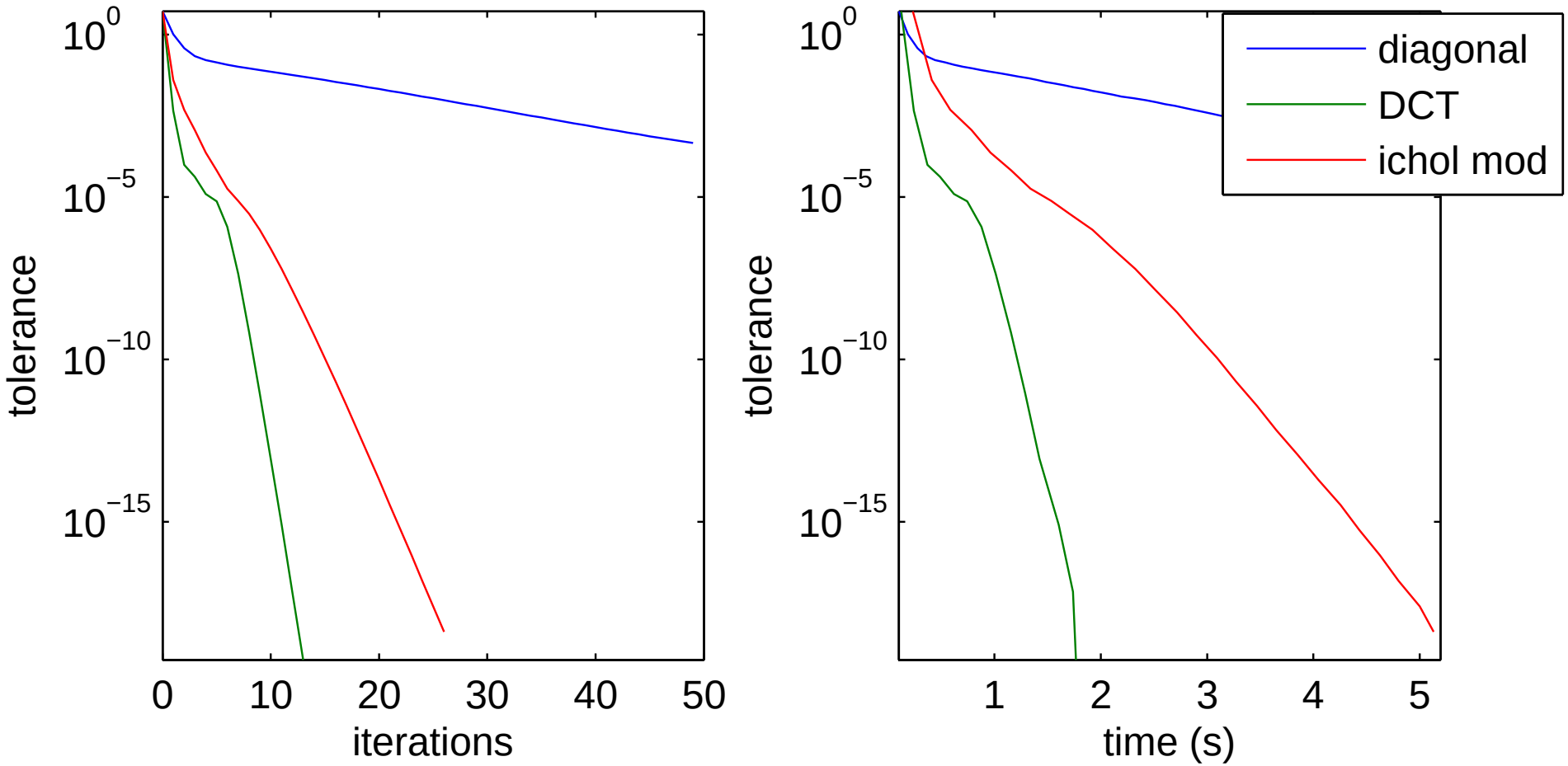
$$\boldsymbol{\Gamma}_{ii} = \begin{cases} 2 - 2\cos\left((i-1)\frac{\pi}{n}\right), & \text{Neumann} \\ 2 - 2\cos\left((i-1)\frac{2\pi}{n}\right), & \text{Cyclic} \end{cases}$$

For Neumann boundary conditions

$$\boldsymbol{M}^{-1}\boldsymbol{b} = \text{iDCT}\left(\boldsymbol{\Xi}^{-1}\,\text{DCT}(\boldsymbol{b})\right), \qquad \boldsymbol{\Xi}_{ii} = \lambda \boldsymbol{\Gamma}_{ii}^2 + 1$$

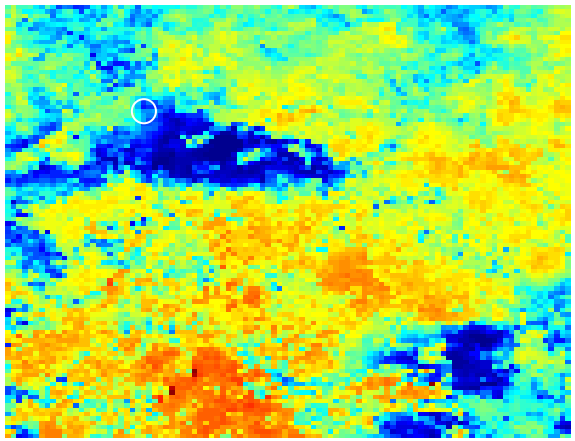
Convergence speed for PCG

Test run on a $2D$ 256×256 grid

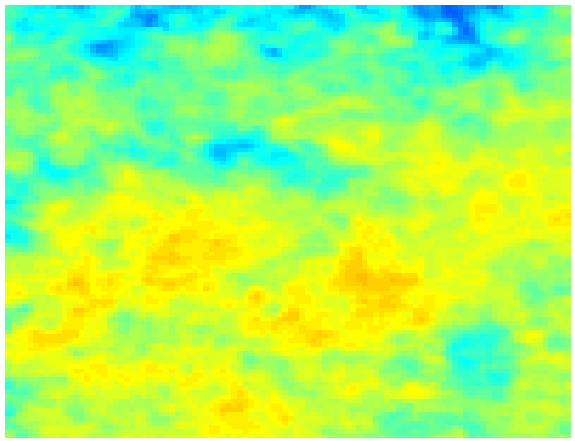


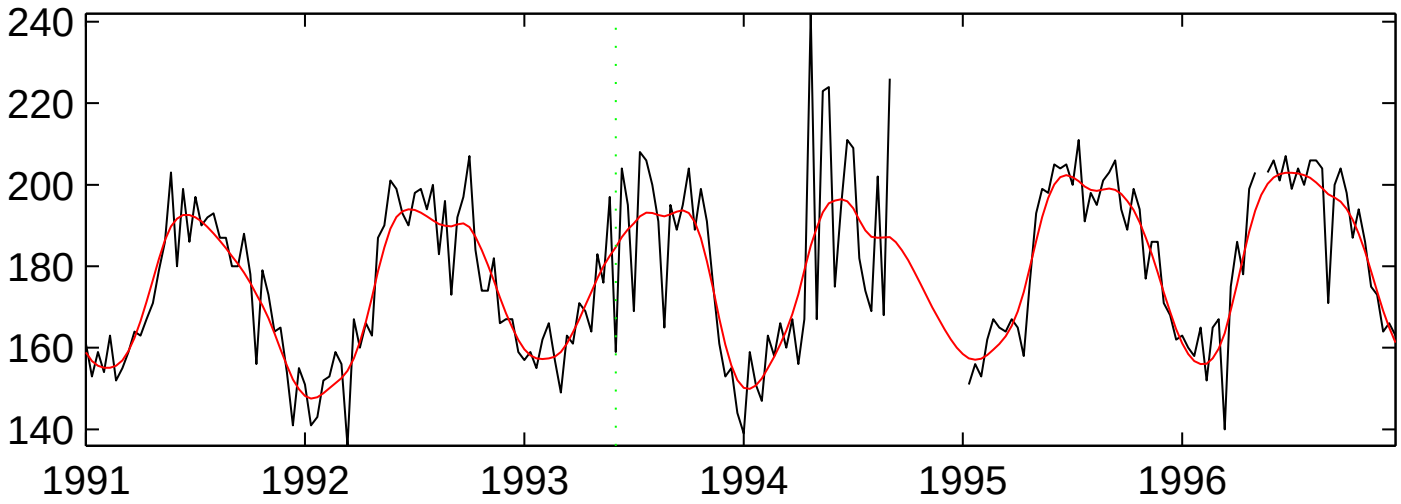
Preliminary results

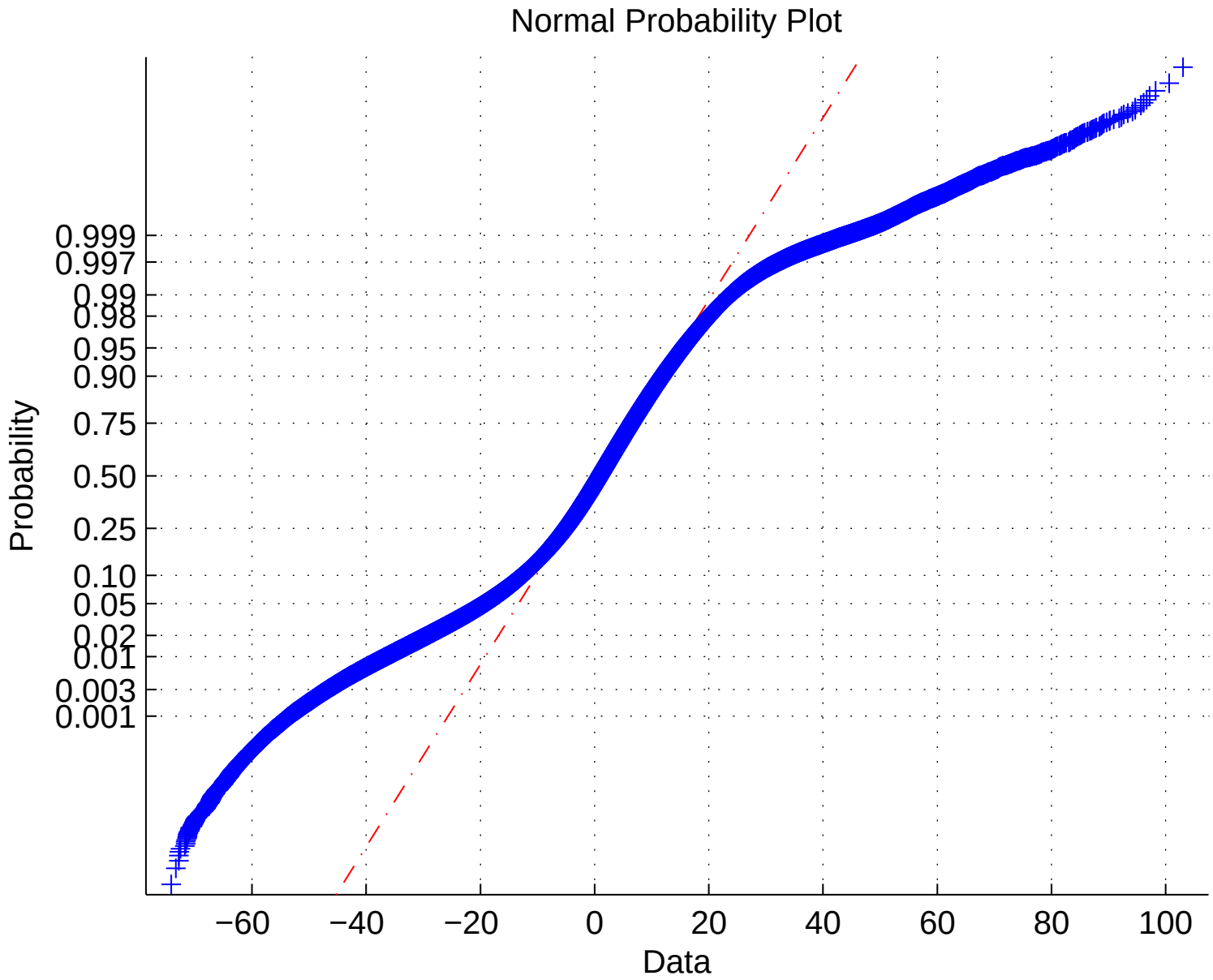
NDVI May 1993



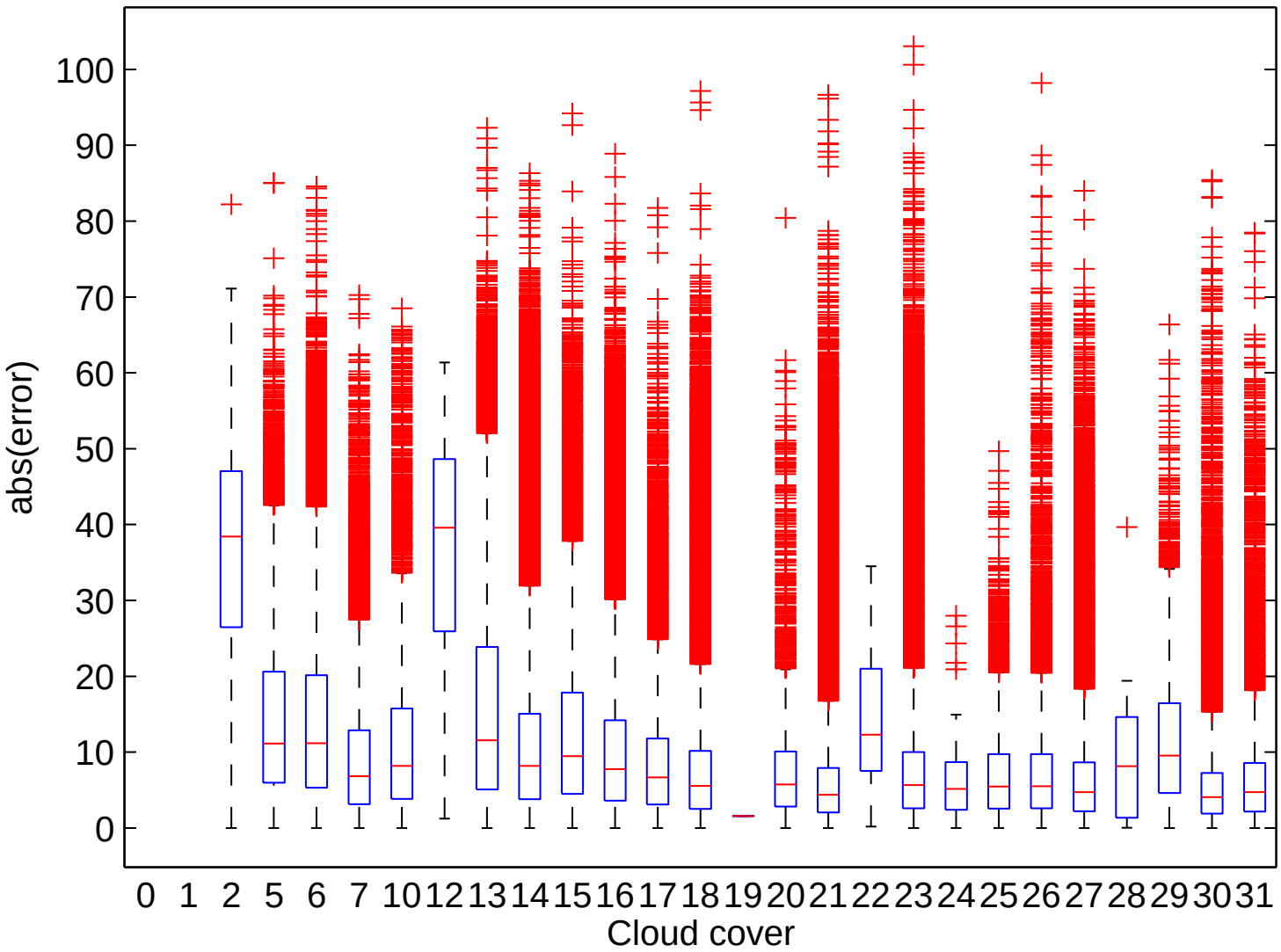
Smooth





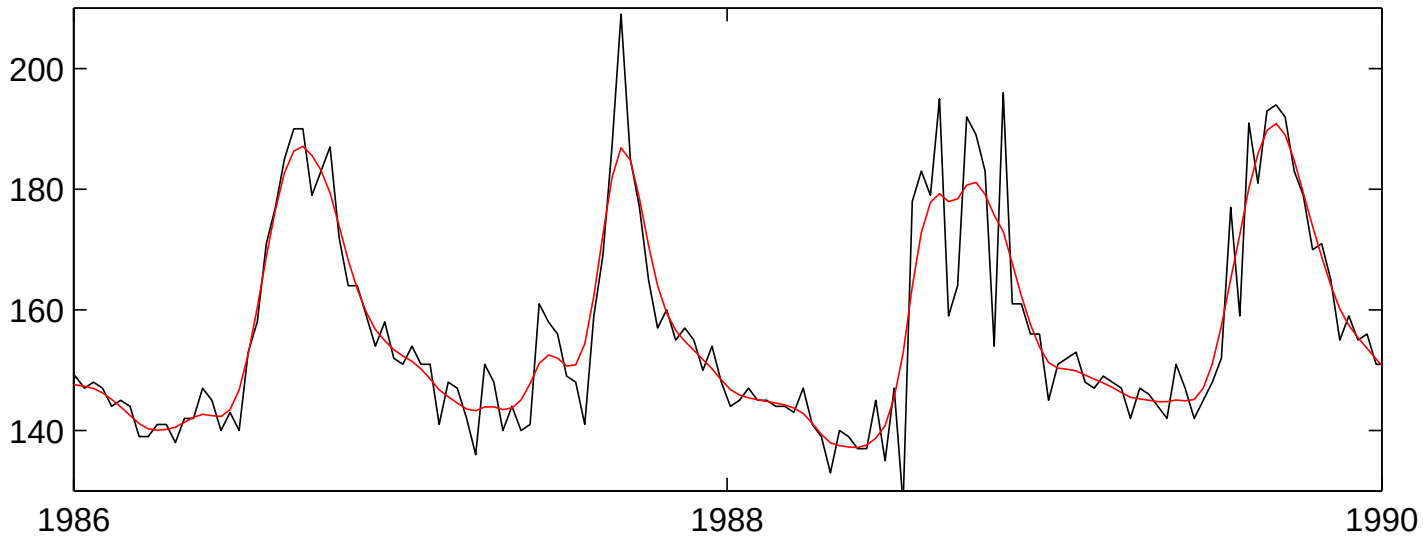

Normal Probability Plot
Probability
0.999
0.997
0.99
0.98
0.95
0.90
0.75
0.50
0.25
0.10
0.05
0.02
0.01
0.003
0.001
−60
−40
−20
0
20
40
60
80
100
Data

Can we use the cloud cover?



Further problems

- Non-Gaussian errors
- Axis anisotropy
- Non-stationarity in time
- Spatially correlated errors (due to clouds)
- Non-stationarity in space?



"When optimising function that involve high-dimensional determinant approximations, it is important to **use whatever structure is available** *in order to speed up computations."*

— Aune et al. (2014, pp. 256)

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