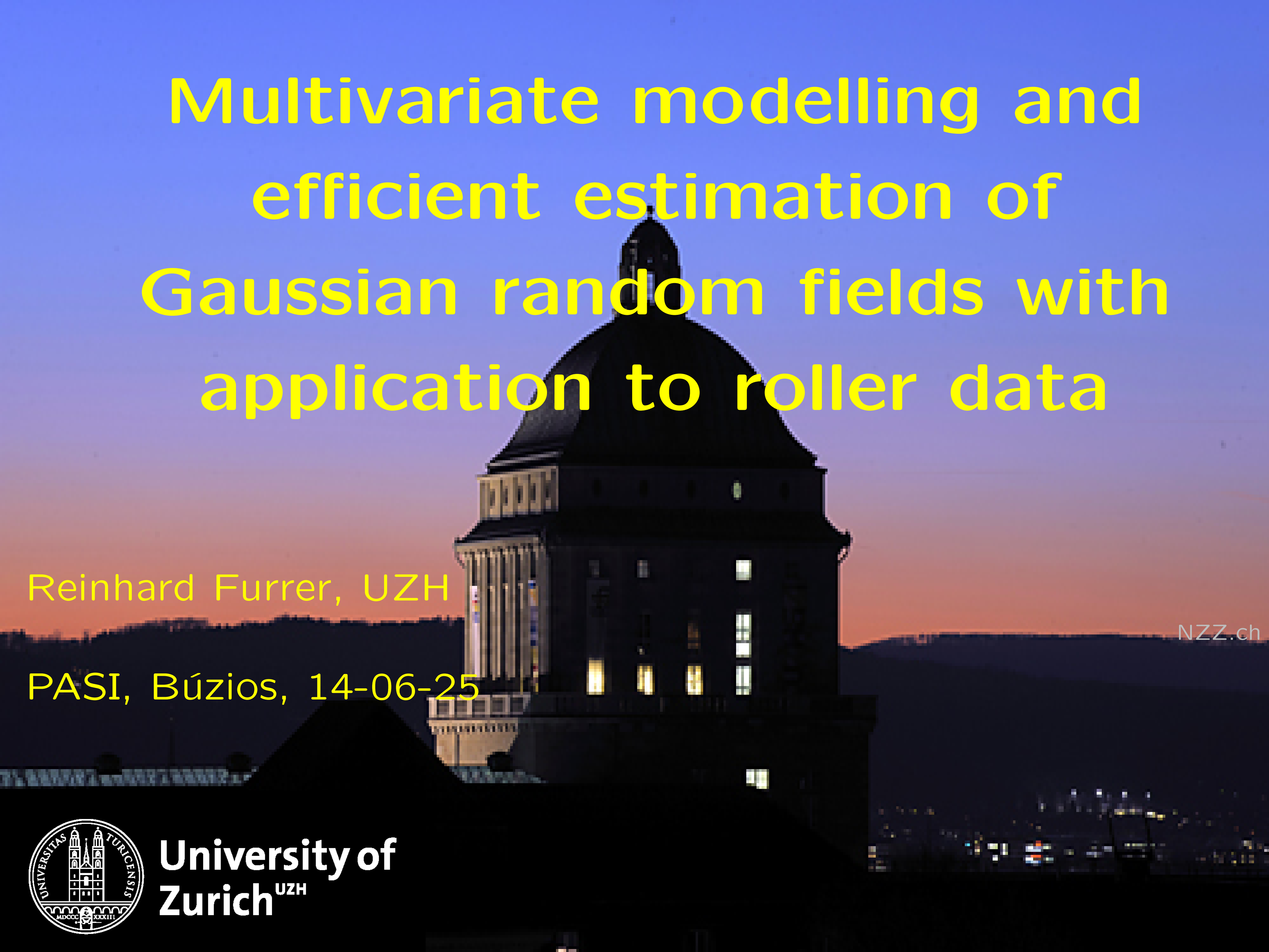
Multivariate modelling and efficient estimation of Gaussian random fields with application to roller data


NZZ.ch

Reinhard Furrer, UZH

PASI, Búzios, 14-06-25

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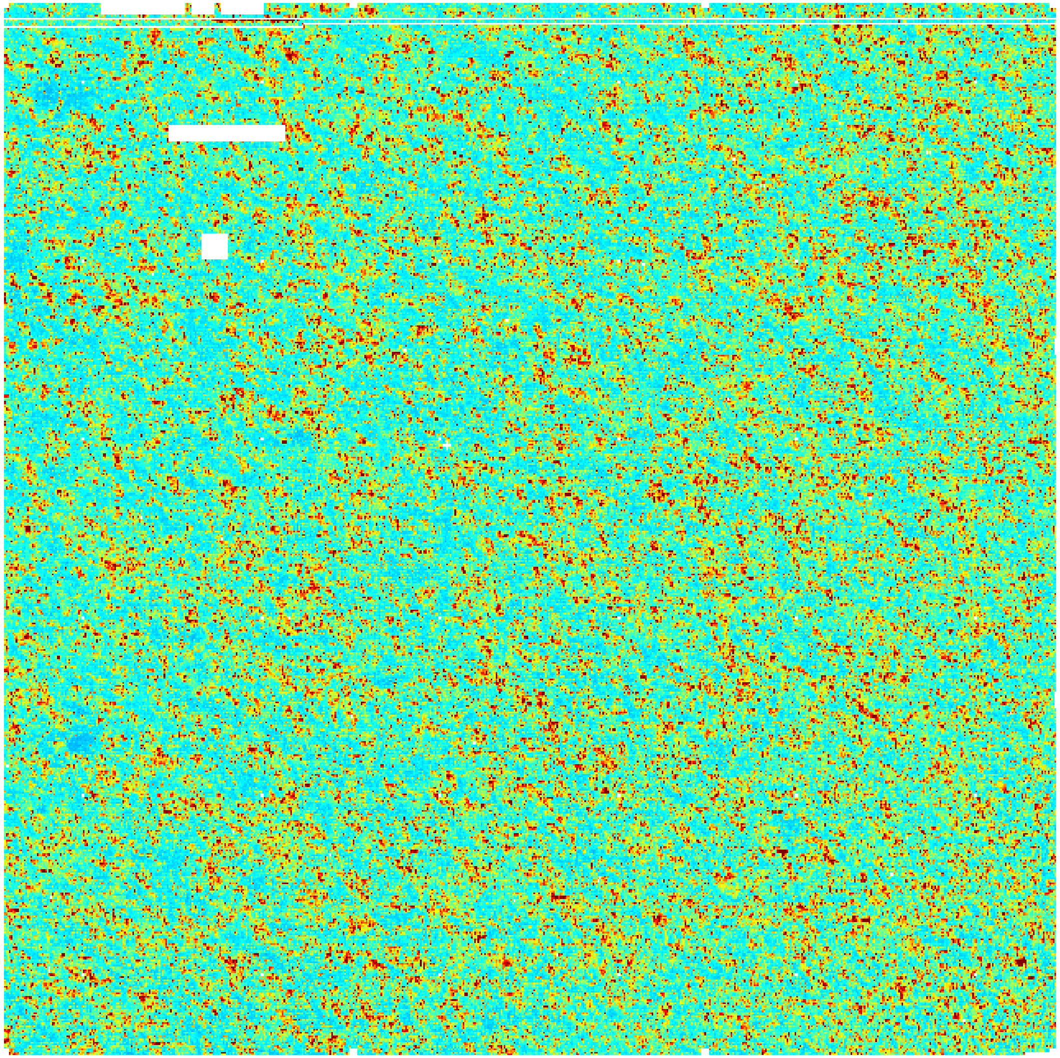
Motivation

- Microarray data:

  construct alternative "background" correction



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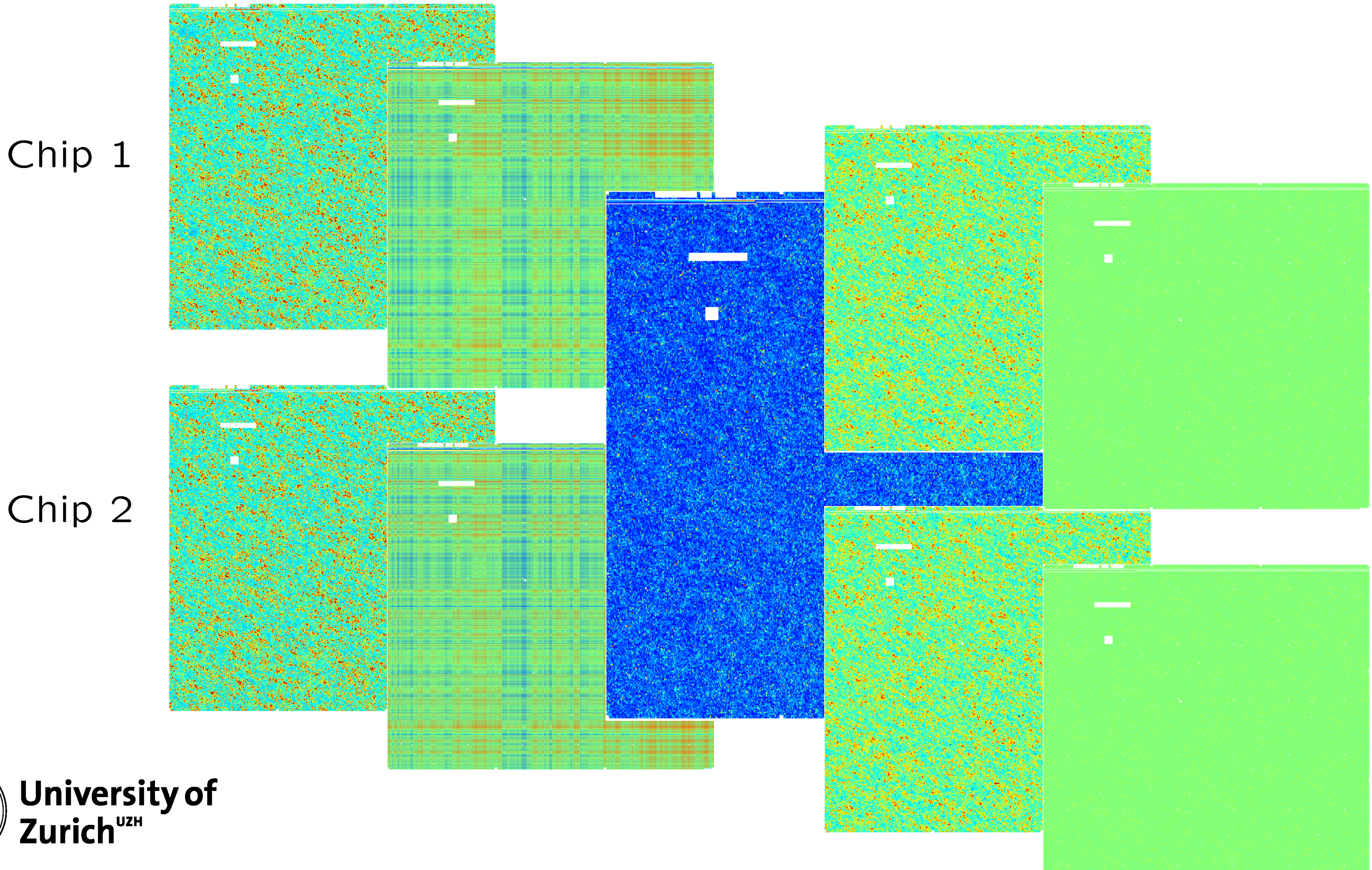
Motivation

observations = fixed effects + spatial term + “noise”



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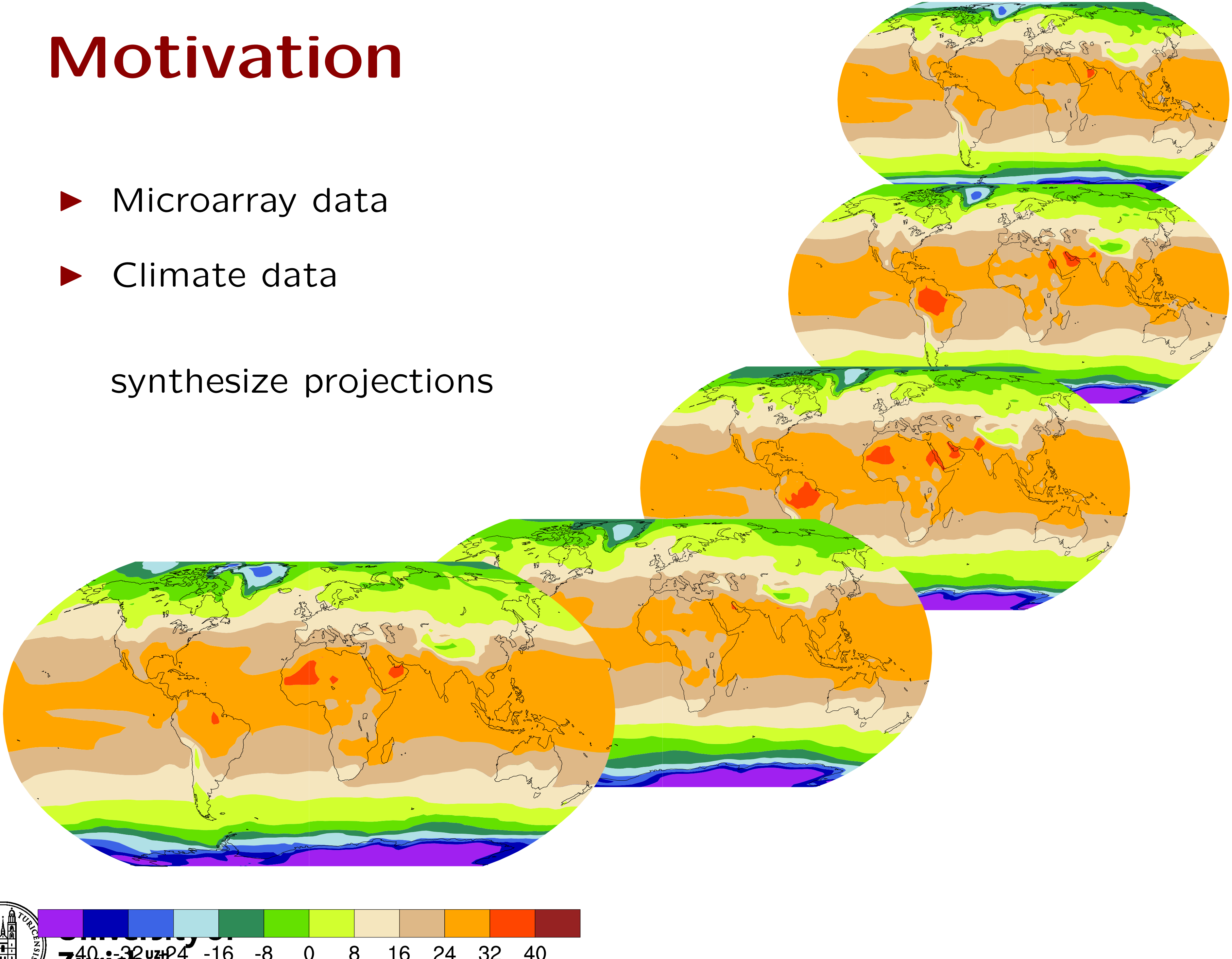
Motivation

- Microarray data
- Climate data

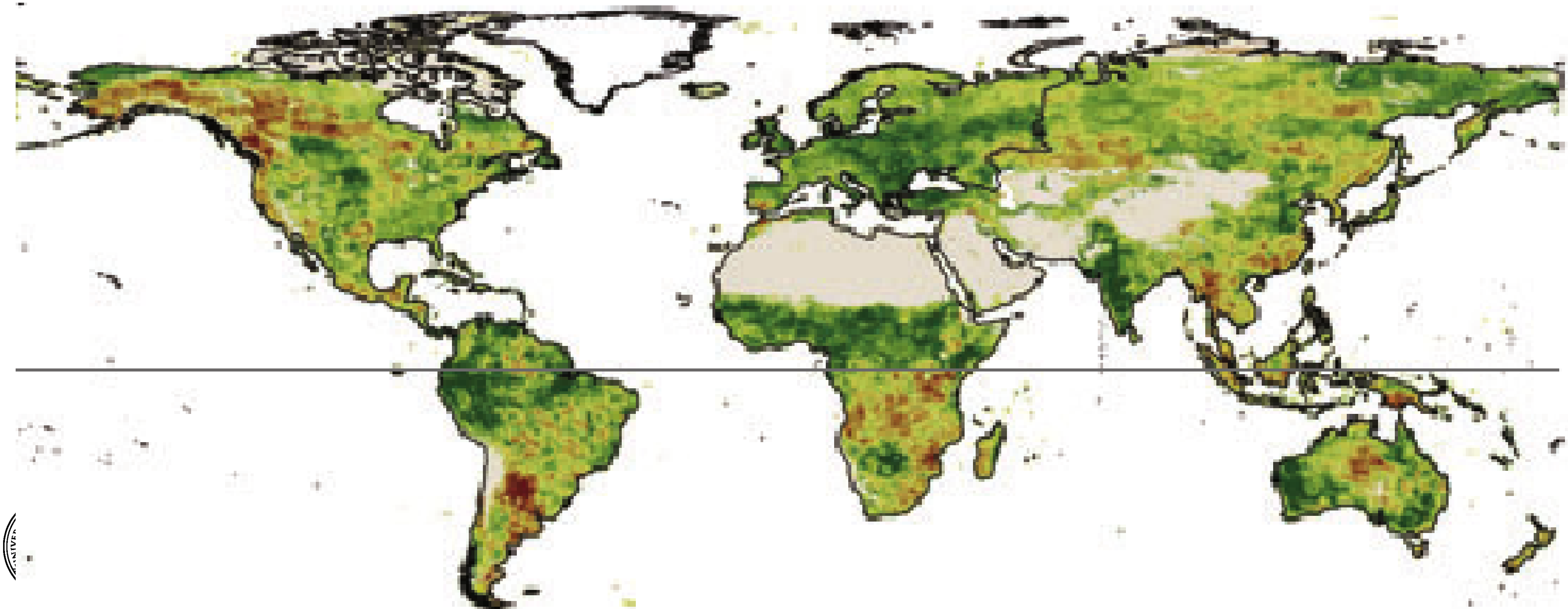
synthesize projections



Motivation

- Microarray data
- Climate data
- Satellite data

attribute spatial changes



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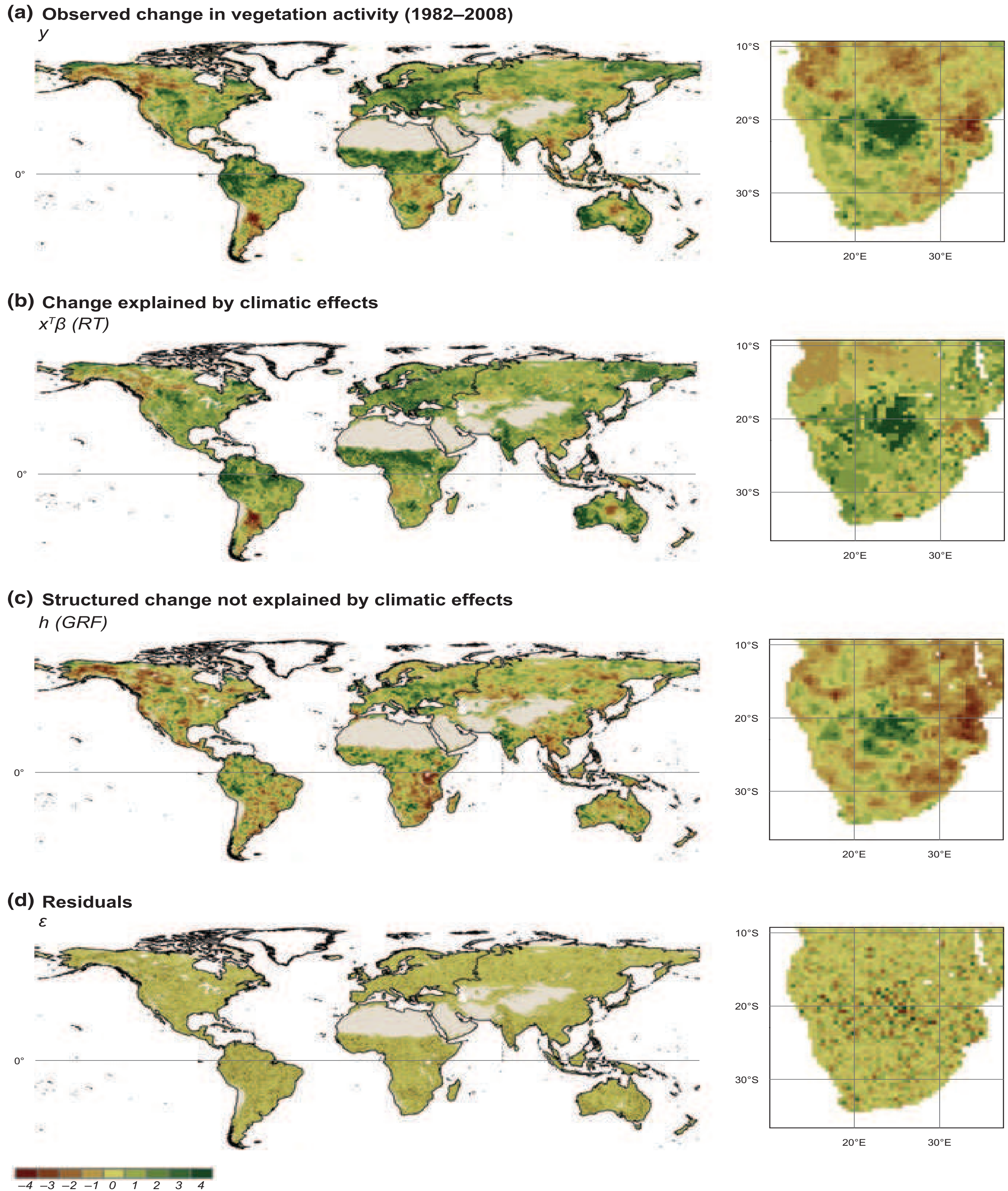

observations

trend

spatial term

“noise”

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Motivation for roller data analysis

Compaction for road construction:

- one vibrating drum
  (smooth drum or padfoot)
- rolling at 1m/s
- 20cm material per layer
- typical bed is 12–15m wide
  and 30–150m long
- sufficient compaction is
  'manually' tested after several
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Is an automatic quality assurance and intelligent compaction possible?

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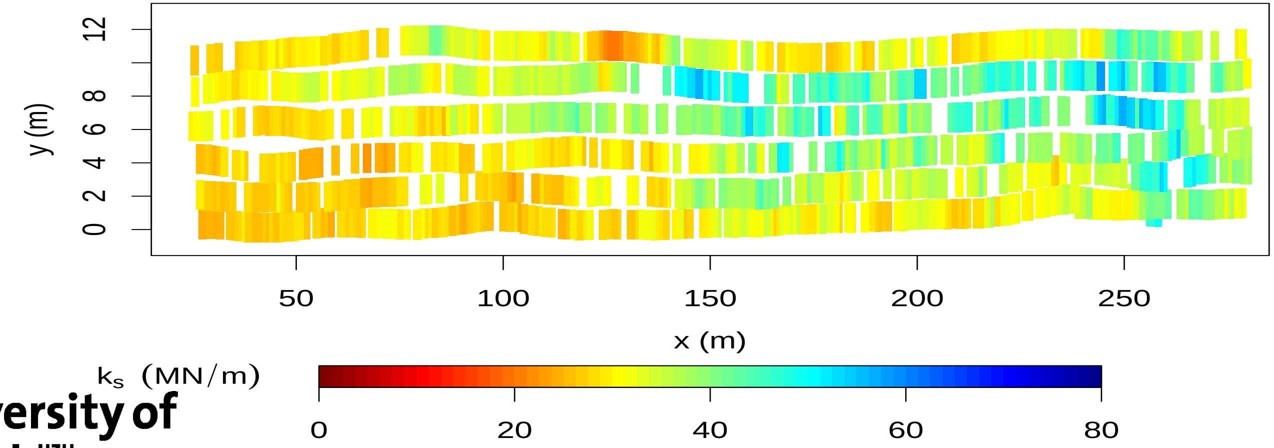
Motivation

Current "intelligent" compaction:

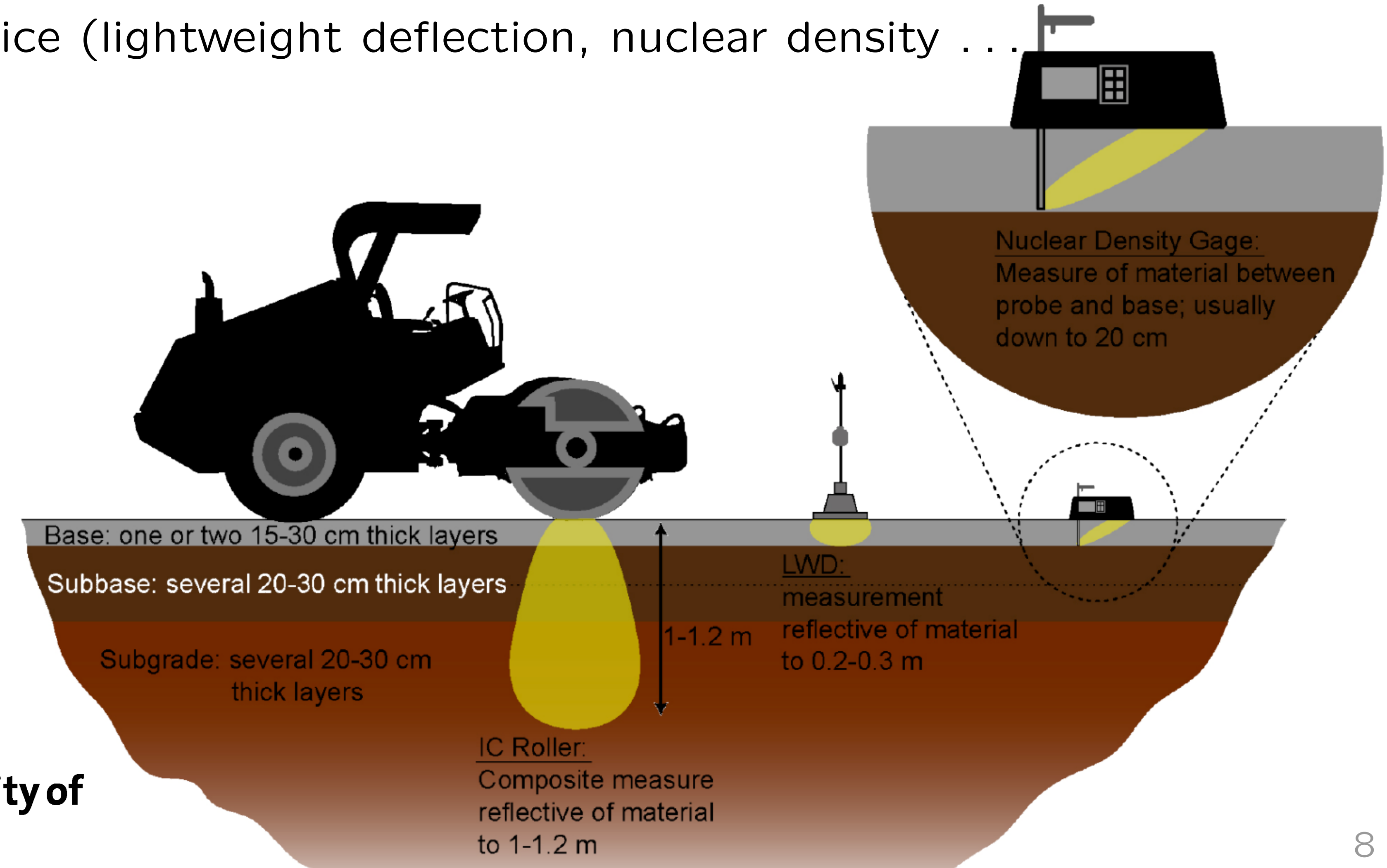
- precise GPS positioning
- on-board visualization
- off-board processing

Source: www.bomag.com



Motivation

- Relation between measurement and actual soil modulus is unknown.
- (Linear) relationship is determined with a second measurement device (lightweight deflection, nuclear density . . .



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Spatial model

Spatial, additive mixed effects model for roller measurement values:

$$\begin{aligned}\text{RMV} = \ & \text{amplitude} + \text{roller type} + \text{driving direction} + \ \ldots \\ & + \ \text{trend}(\mathbf{s}) + \text{spatial term}(\mathbf{s}) \ + \ \text{error}\end{aligned}$$

$$Y(\mathbf{s}) = \mathbf{X}\beta + \alpha(\mathbf{s}) + \gamma(\mathbf{s}) + \varepsilon(\mathbf{s}) \qquad \mathbf{s} \in \mathcal{D} \subset \mathbb{R}^d, \ d \geq 1$$

with

$\mathbf{X}\beta$: fixed effects and trend

$\alpha(\mathbf{s})$: spline component (trend)

$\gamma(\mathbf{s})$: zero mean spatial Gaussian process

$\varepsilon(\mathbf{s})$: iid noise, orthogonal to $\gamma(\mathbf{s})$

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with

$\mathbf{X}\boldsymbol{\beta}$: fixed effects and trend
coefficients $\boldsymbol{\beta}$

$\alpha(\mathbf{s})$: spline component (trend)
basis function coefficients $\boldsymbol{\theta}_\alpha$; smoothing parameter λ_α

$\gamma(\mathbf{s})$: zero mean spatial Gaussian process
parameters $\boldsymbol{\theta}_\gamma$ describing the covariance function

$\varepsilon(\mathbf{s})$: iid noise, orthogonal to $\gamma(\mathbf{s})$
variance σ^2

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Multivariate modeling: setting

Spatial, additive mixed effects model:

$$\begin{aligned} Y_1(\mathbf{s}) &= \mathbf{X}_1\boldsymbol{\beta}_1 + \alpha_1(\mathbf{s}) + \gamma_1(\mathbf{s}) + \varepsilon_1(\mathbf{s}) \\ &\vdots \\ Y_p(\mathbf{s}) &= \mathbf{X}_p\boldsymbol{\beta}_p + \alpha_p(\mathbf{s}) + \gamma_p(\mathbf{s}) + \varepsilon_p(\mathbf{s}) \qquad \mathbf{s} \in \mathcal{D} \subset \mathbb{R}^d,\ d \geq 1 \end{aligned}$$

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\end{aligned}
$$

Modeling the spatial processes themselves:

Random field:

Dependency:		GRF	GMRF
	cross-correlation model	①	③
	common process(es)	②	④

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Random field modeling

Dependency through a cross-correlation model ①:

$$\mathbf{X} \sim \mathcal{N}_n(\boldsymbol{\mu}_{\mathbf{X}}, \Sigma_{\mathbf{X}}) \qquad \mathrm{Cov}(\mathbf{X}, \mathbf{Y}) = \Sigma_{\mathbf{XY}}$$
$$\mathbf{Y} \sim \mathcal{N}_n(\boldsymbol{\mu}_{\mathbf{Y}}, \Sigma_{\mathbf{Y}})$$

$$\rightsquigarrow \quad \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix} \sim \mathcal{N}_{2n}\left(\begin{pmatrix} \boldsymbol{\mu}_{\mathbf{X}} \\ \boldsymbol{\mu}_{\mathbf{Y}} \end{pmatrix}, \begin{pmatrix} \Sigma_{\mathbf{X}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{XY}}{}^{\mathsf{T}} & \Sigma_{\mathbf{Y}} \end{pmatrix}\right)$$

(e.g., Gneiting, Kleiber, Schlather 2010, Apanasovich, Genton, Sun 2012, . . .)

Random field modeling

Dependency through a cross-correlation model ①:

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$$\mathbf{Y} \sim \mathcal{N}_n(\boldsymbol{\mu}_\mathbf{Y}, \Sigma_\mathbf{Y})$$

$$\rightsquigarrow \quad \begin{pmatrix}\mathbf{X}\\ \mathbf{Y}\end{pmatrix} \sim \mathcal{N}_{2n}\left(\begin{pmatrix}\boldsymbol{\mu}_\mathbf{X}\\ \boldsymbol{\mu}_\mathbf{Y}\end{pmatrix}, \begin{pmatrix}\Sigma_\mathbf{X} & \Sigma_{\mathbf{XY}}\\ {\Sigma_{\mathbf{XY}}}^\mathsf{T} & \Sigma_\mathbf{Y}\end{pmatrix}\right)$$

(e.g., Gneiting, Kleiber, Schlather 2010, Apanasovich, Genton, Sun 2012, . . .)

Dependency through common process(es) ②:

$$\mathbf{X} \sim \mathcal{N}_n(\boldsymbol{\mu}_\mathbf{X}, \Sigma_\mathbf{X}) \qquad \mathbf{Z} \sim \mathcal{N}_n(\mathbf{0}, \Sigma_\mathbf{Z})$$
$$\mathbf{Y} \sim \mathcal{N}_n(\boldsymbol{\mu}_\mathbf{Y}, \Sigma_\mathbf{Y})$$

$$\rightsquigarrow \quad \begin{pmatrix}\mathbf{X}+\mathbf{Z}\\ \mathbf{Y}+\mathbf{Z}\end{pmatrix} \sim \mathcal{N}_{2n}\left(\begin{pmatrix}\boldsymbol{\mu}_\mathbf{X}\\ \boldsymbol{\mu}_\mathbf{Y}\end{pmatrix}, \begin{pmatrix}\Sigma_\mathbf{X}+\Sigma_\mathbf{Z} & \Sigma_\mathbf{Z}\\ \Sigma_\mathbf{Z} & \Sigma_\mathbf{Y}+\Sigma_\mathbf{Z}\end{pmatrix}\right)$$

Backfitting

Recall:

$$\begin{aligned} Y_1(\mathbf{s}) &= \mathbf{X}_1\boldsymbol{\beta}_1 + \boldsymbol{\alpha}_1(\mathbf{s}) + \boldsymbol{\gamma}_1(\mathbf{s}) + \varepsilon_1(\mathbf{s}) \\ &\vdots \\ Y_p(\mathbf{s}) &= \mathbf{X}_p\boldsymbol{\beta}_p + \alpha_p(\mathbf{s}) + \gamma_p(\mathbf{s}) + \varepsilon_p(\mathbf{s}) \end{aligned}$$

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Backfitting

Recall:

$$
\begin{aligned}
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&\vdots \\
Y_p(\mathbf{s}) &= \mathbf{X}_p\boldsymbol{\beta}_p + \alpha_p(\mathbf{s}) + \gamma_p(\mathbf{s}) + \varepsilon_p(\mathbf{s})
\end{aligned}
$$

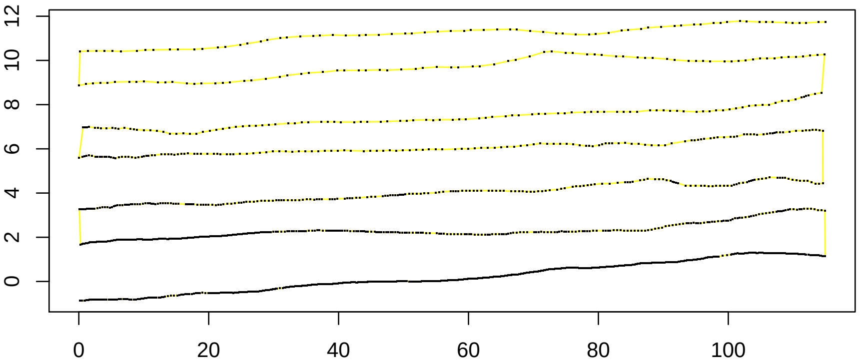
Extending the ‘classical’ backfitting approach to dependent data:

```
repeat until convergence
    repeat until convergence
        estimate fixed effects
    for all ‘stochastic’ effects
        estimate parameters
        predict smooth field
```

See Furrer, Sain (2009) Heersink, Furrer (2012|3)

Sparse covariance matrices

Calculate Σ:



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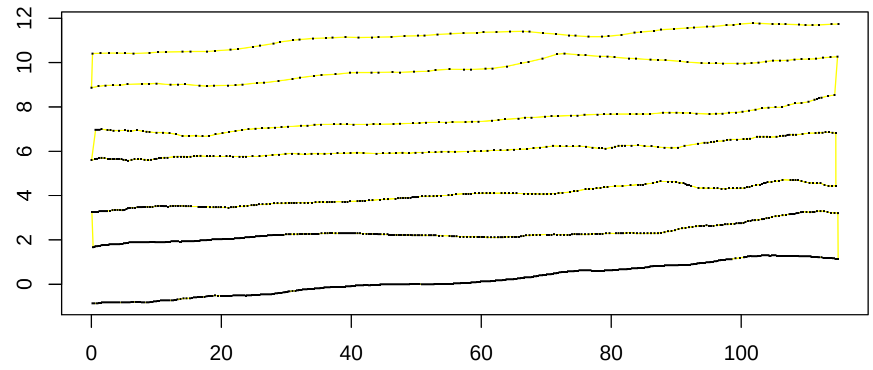

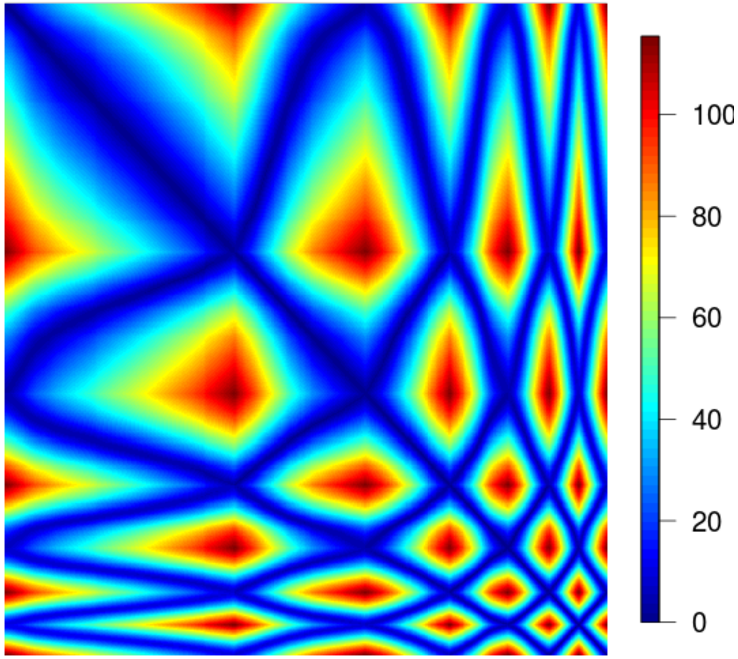

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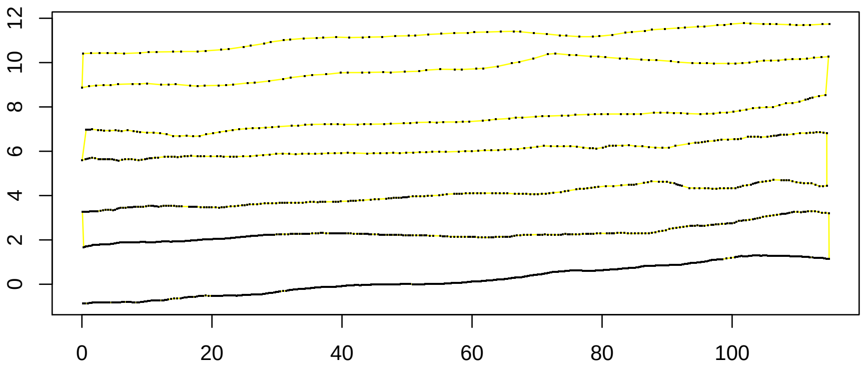
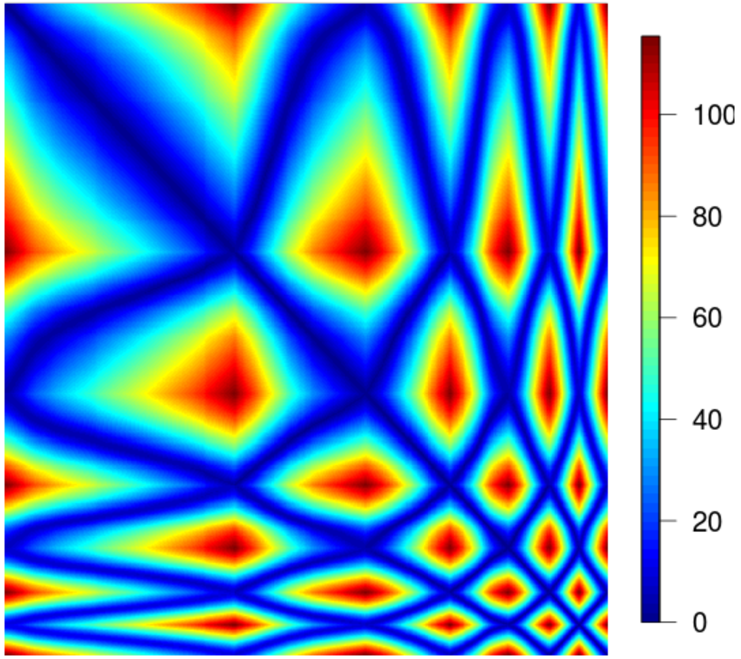
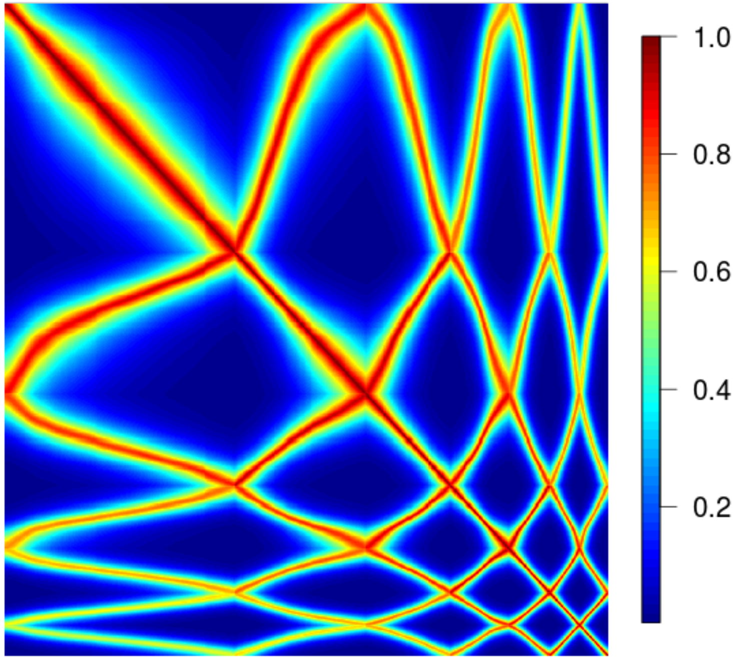


Distances :



Correlation(Distances) :



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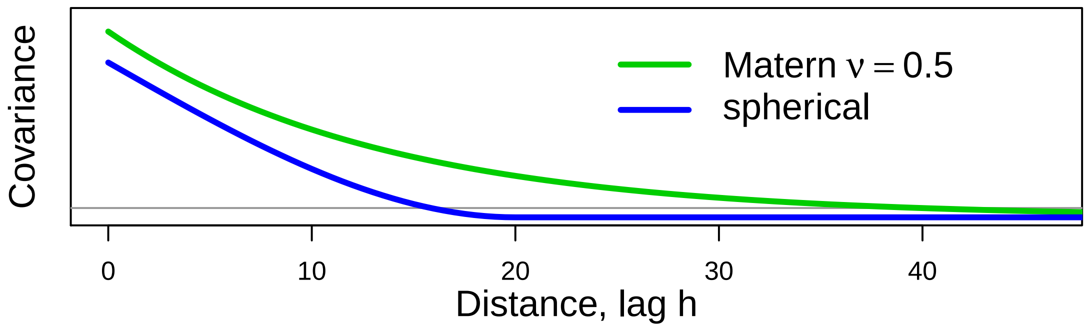
Sparse covariance matrices

Sparseness is guaranteed when

- the covariance function has a compact support
- a compact support is (artificially) imposed $\rightsquigarrow$ tapering



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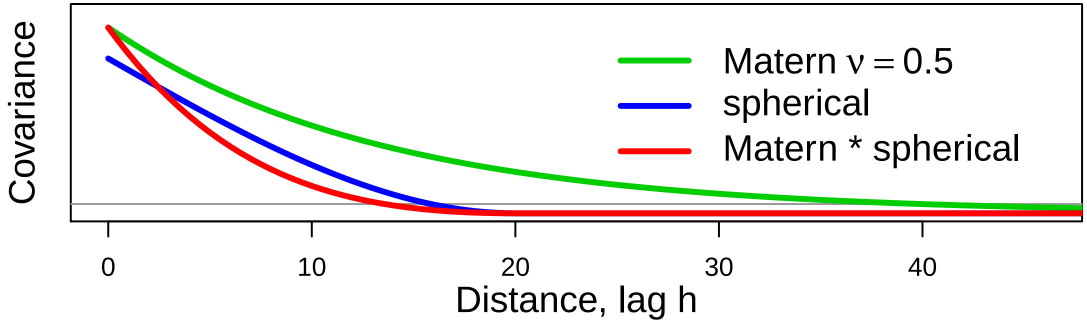

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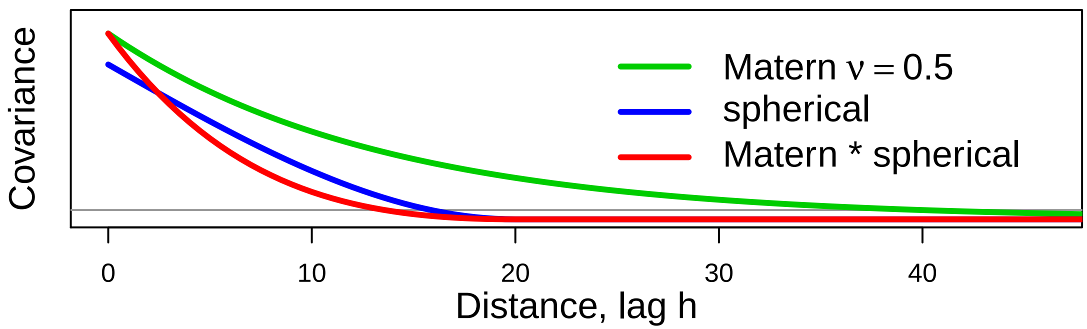

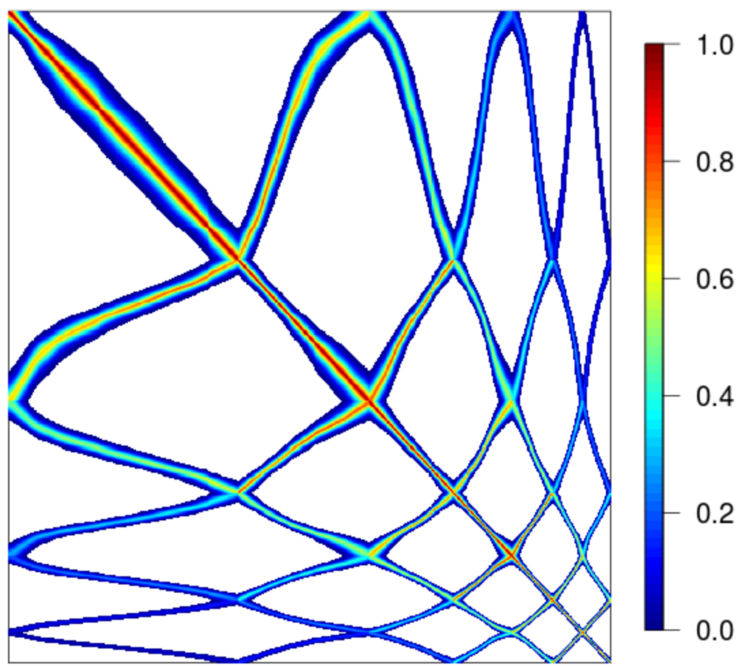

spam for R

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Multivariate tapering

- Concept of Gaussian equivalent measures does not exist
- Domain increasing framework
- $\|\mathbf{\Sigma} - \mathbf{\Sigma} \circ \mathbf{T}\| \to 0$ as $n \to \infty$

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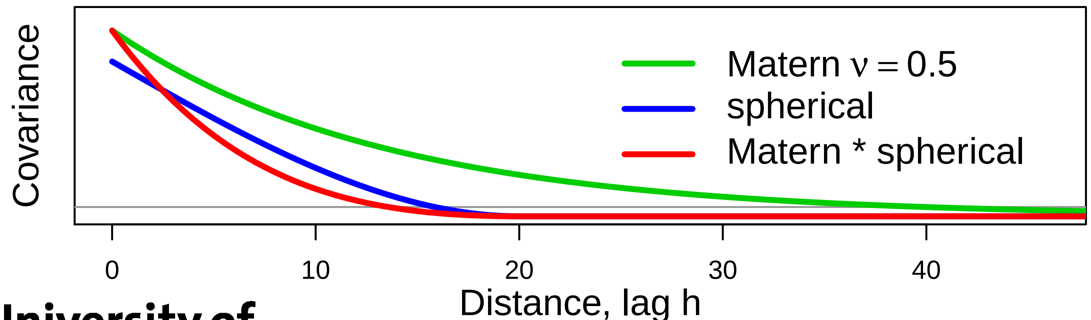

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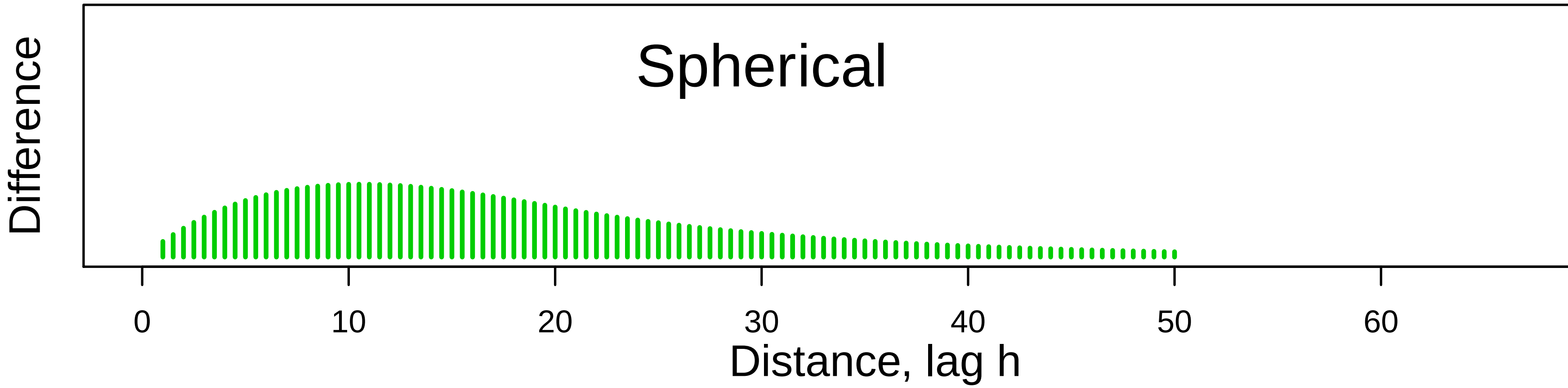

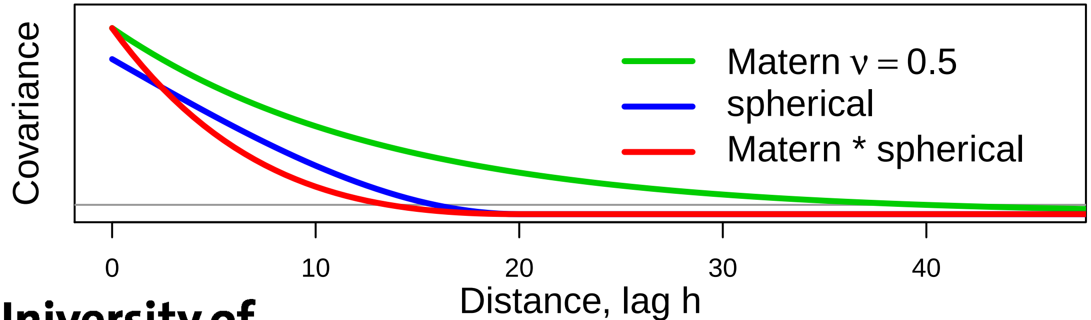

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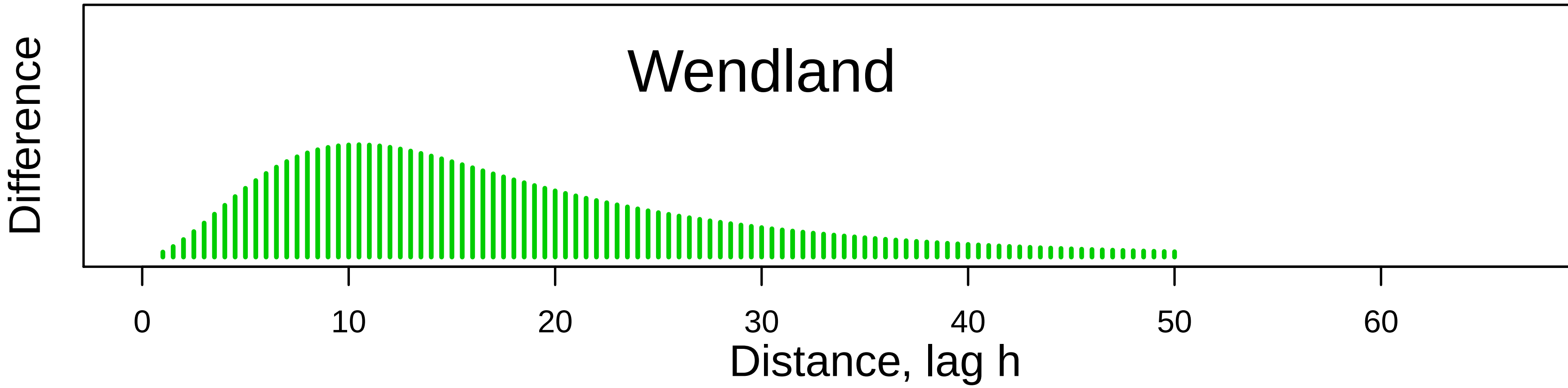

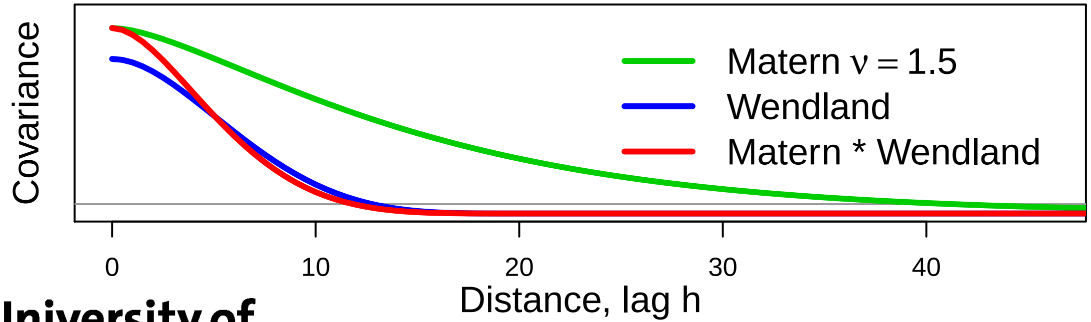

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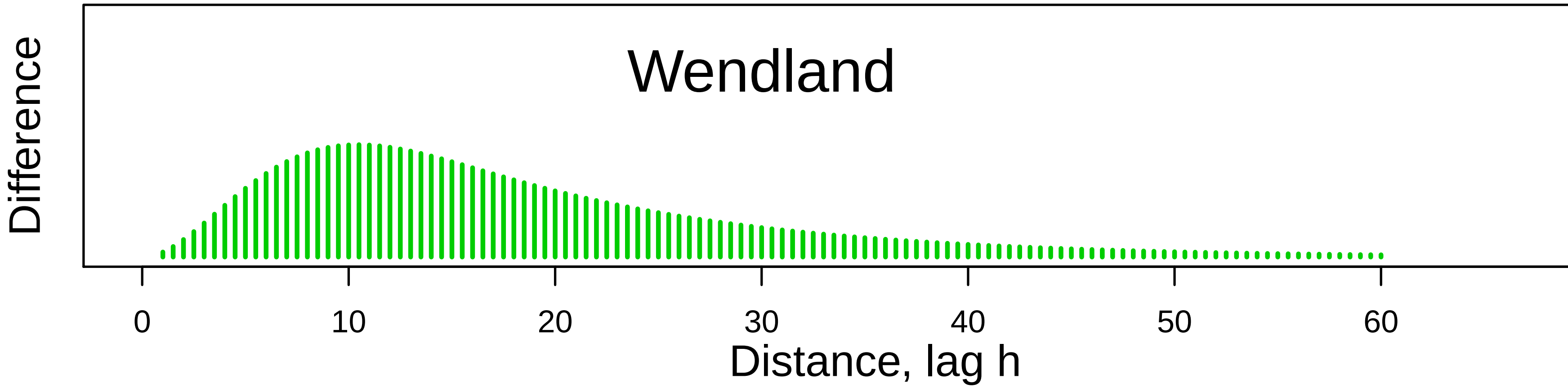

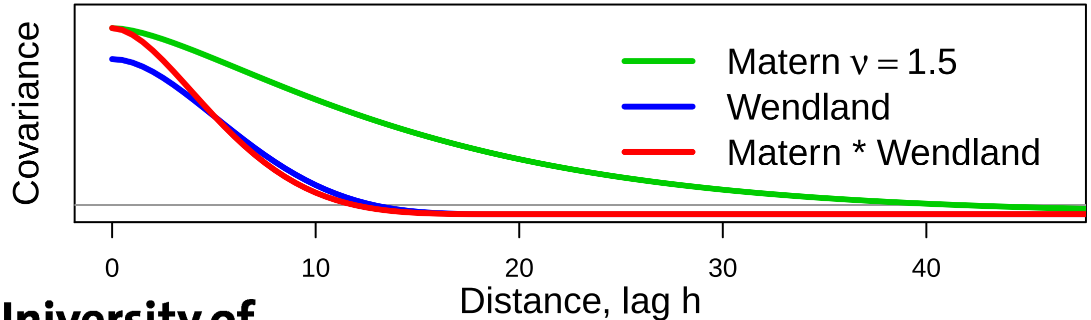

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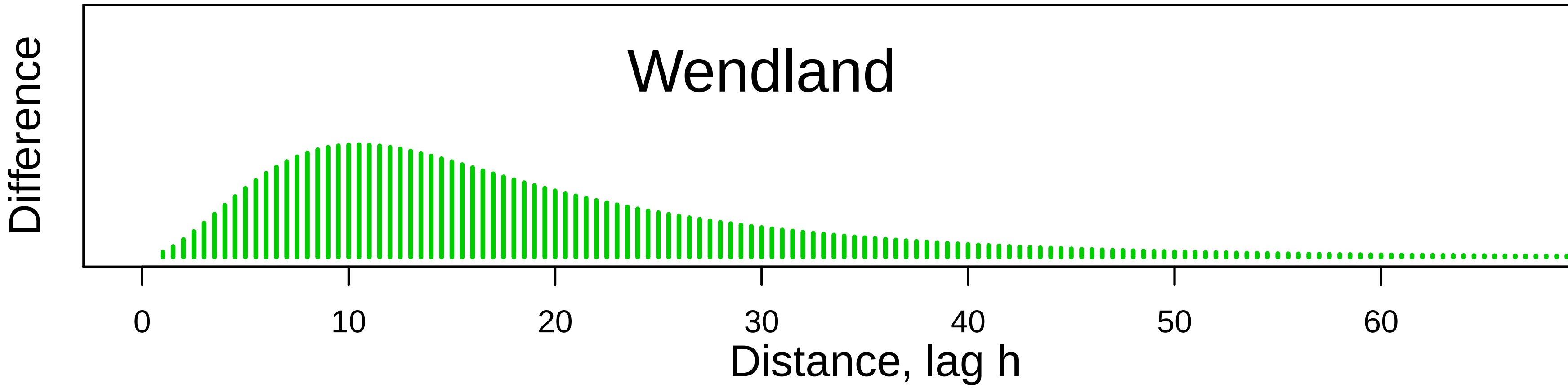

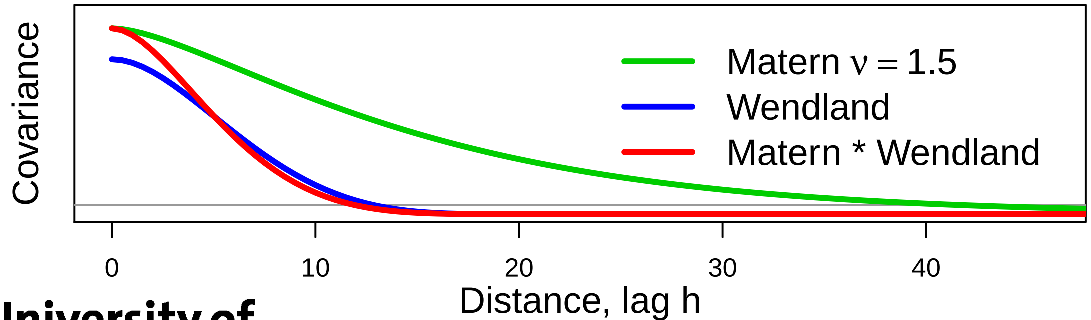

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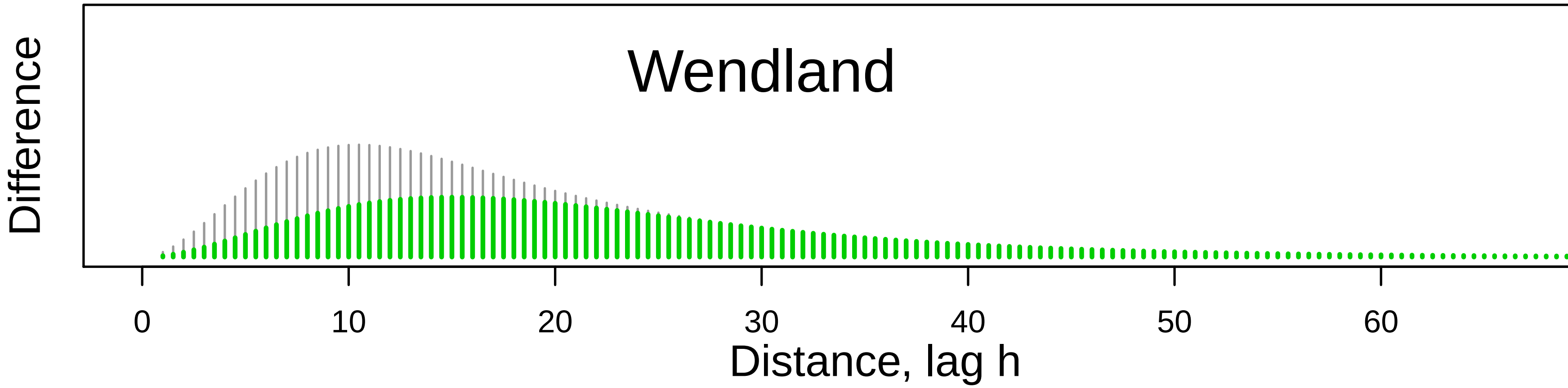

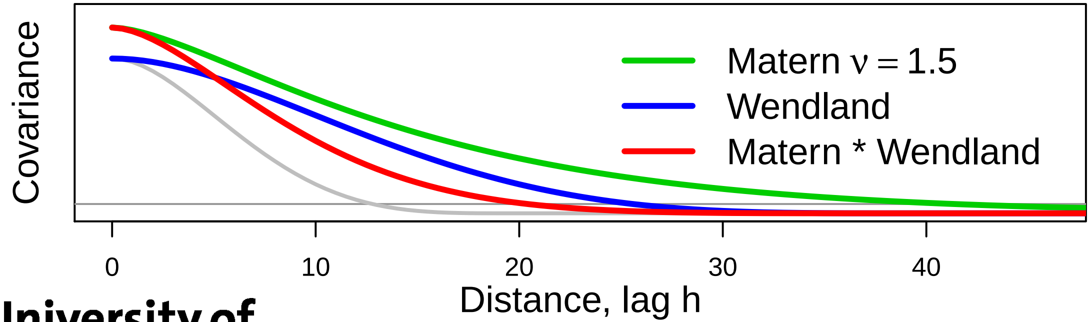

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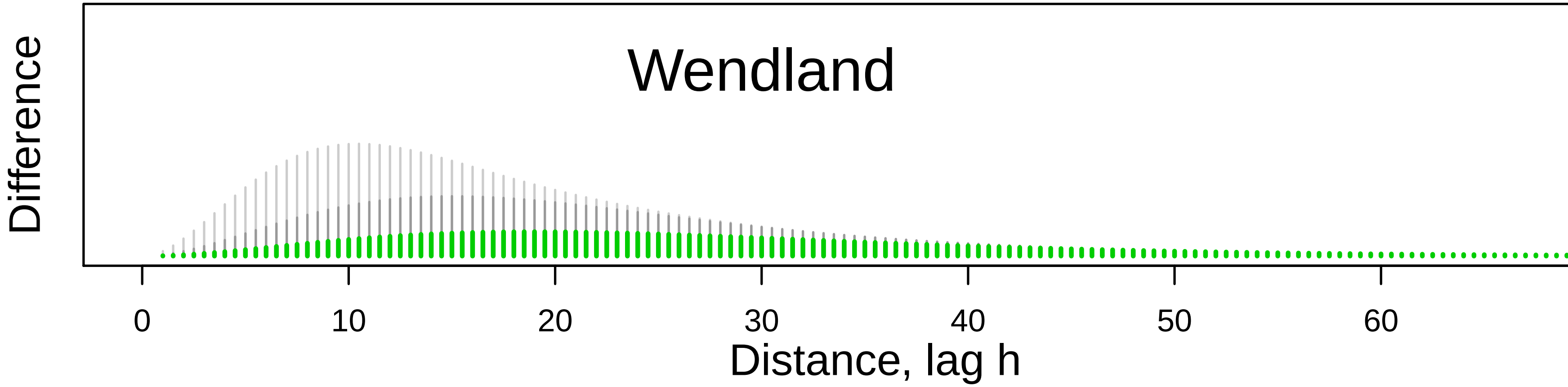

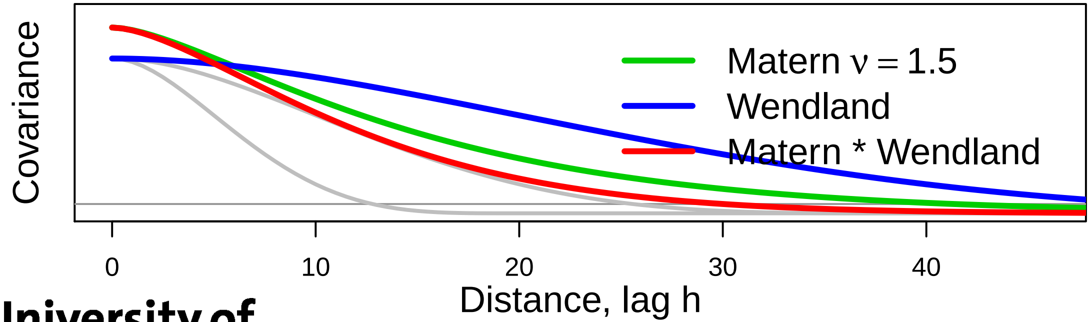

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Multivariate tapering

- Concept of Gaussian equivalent measures does not exist
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- Tapering is purely pragmatic
- $\mathbf{T} = \mathbf{Q} \otimes \mathbf{T}_i \qquad \mathbf{Q} = \epsilon\mathbf{I} + (1-\epsilon)\mathbf{J}$

“All models are wrong, but . . .”

- Iterative approaches
  - $+$ Flexible, numerically feasible
  - $-$ Uncertainties
- Maximum likelihood
  - $+$ Uncertainties, asymptotics
  - $-$ Numerical issues
- Bayesian hierarchical models
  - $+$ Flexible, uncertainties
  - $-$ MCMC
- SPDE models
  - $+$ flexible, scalable

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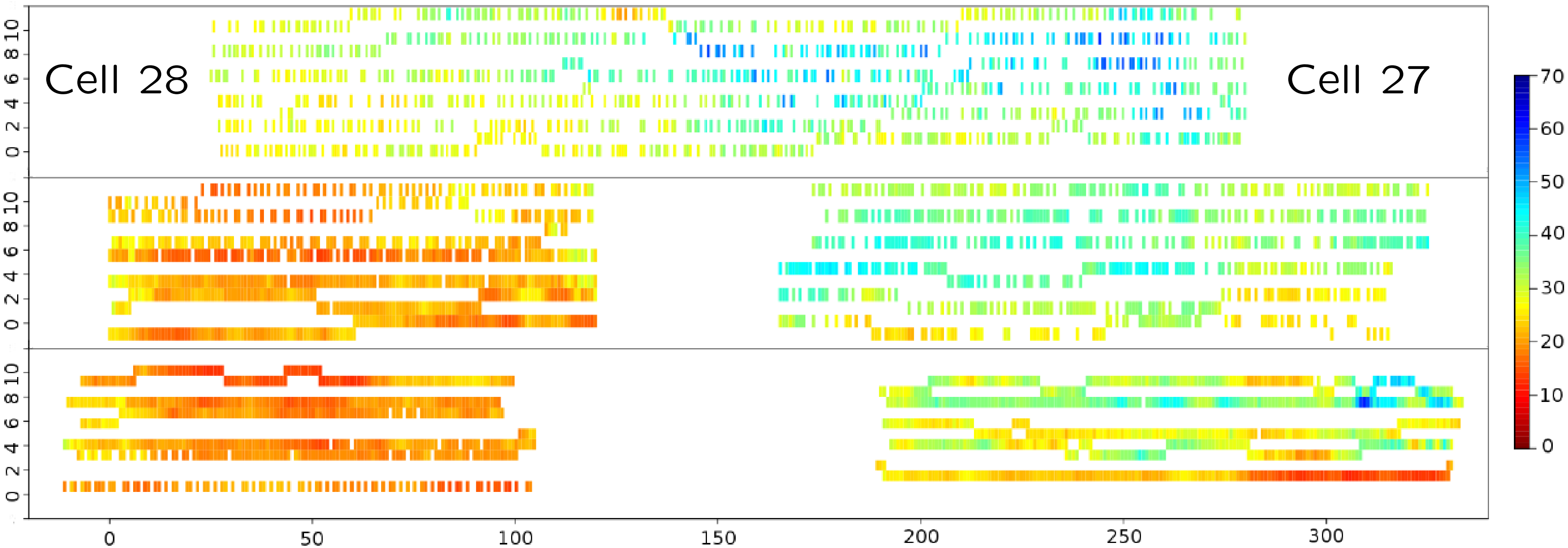
Example: Backfitting

Minnesota testbed:



Subgrade, subbase, base (top to bottom).

Example: Backfitting

Minnesota testbed:

Model:

$$
\begin{aligned}
Y_1(\mathbf{s}) &= \mathbf{X}_1\boldsymbol{\beta}_1 + \gamma_1(\mathbf{s}) + \varepsilon_1(\mathbf{s})\\
Y_2(\mathbf{s}) &= \mathbf{X}_2\boldsymbol{\beta}_2 + c_1\gamma_1(\mathbf{s}) + \gamma_2(\mathbf{s}) + \varepsilon_2(\mathbf{s})\\
Y_3(\mathbf{s}) &= \mathbf{X}_3\boldsymbol{\beta}_3 + c_2(c_1\gamma_1(\mathbf{s}) + \gamma_2(\mathbf{s})) + \gamma_3(\mathbf{s}) + \varepsilon_3(\mathbf{s})
\end{aligned}
$$

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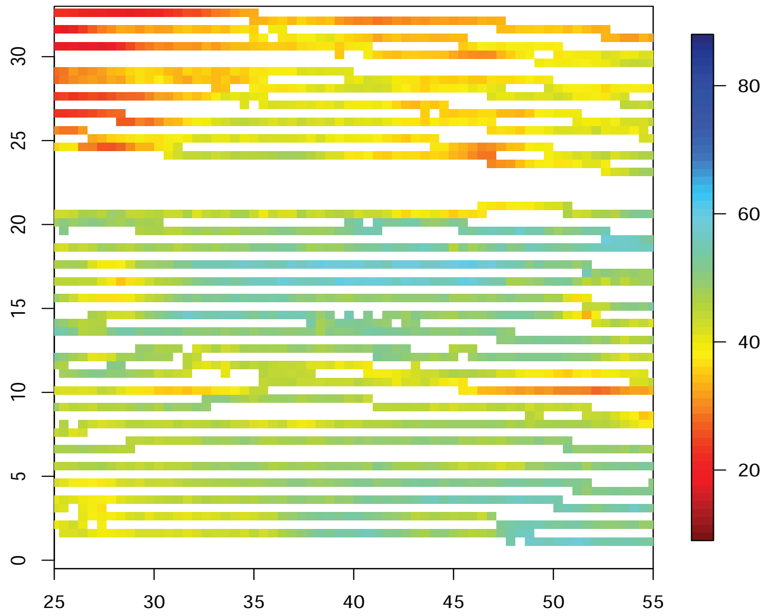
Inset: nonstationarity



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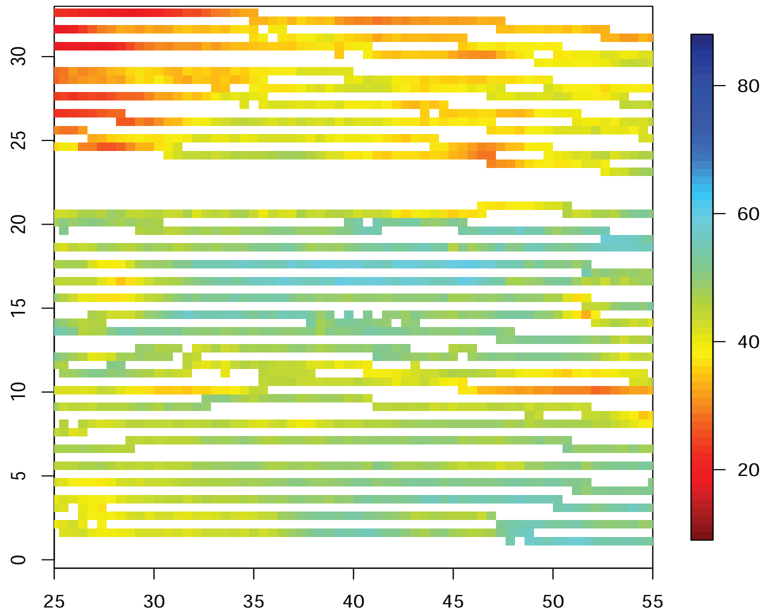

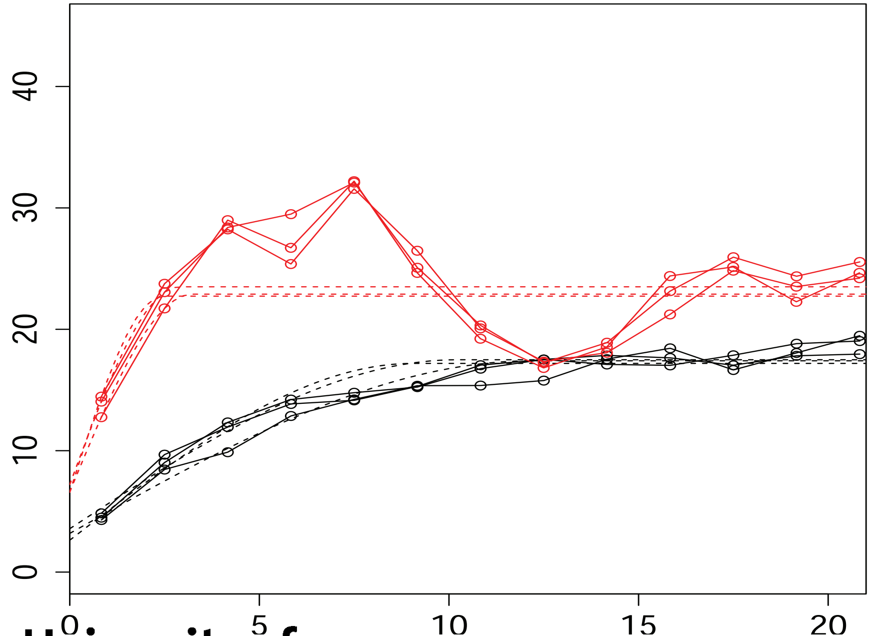

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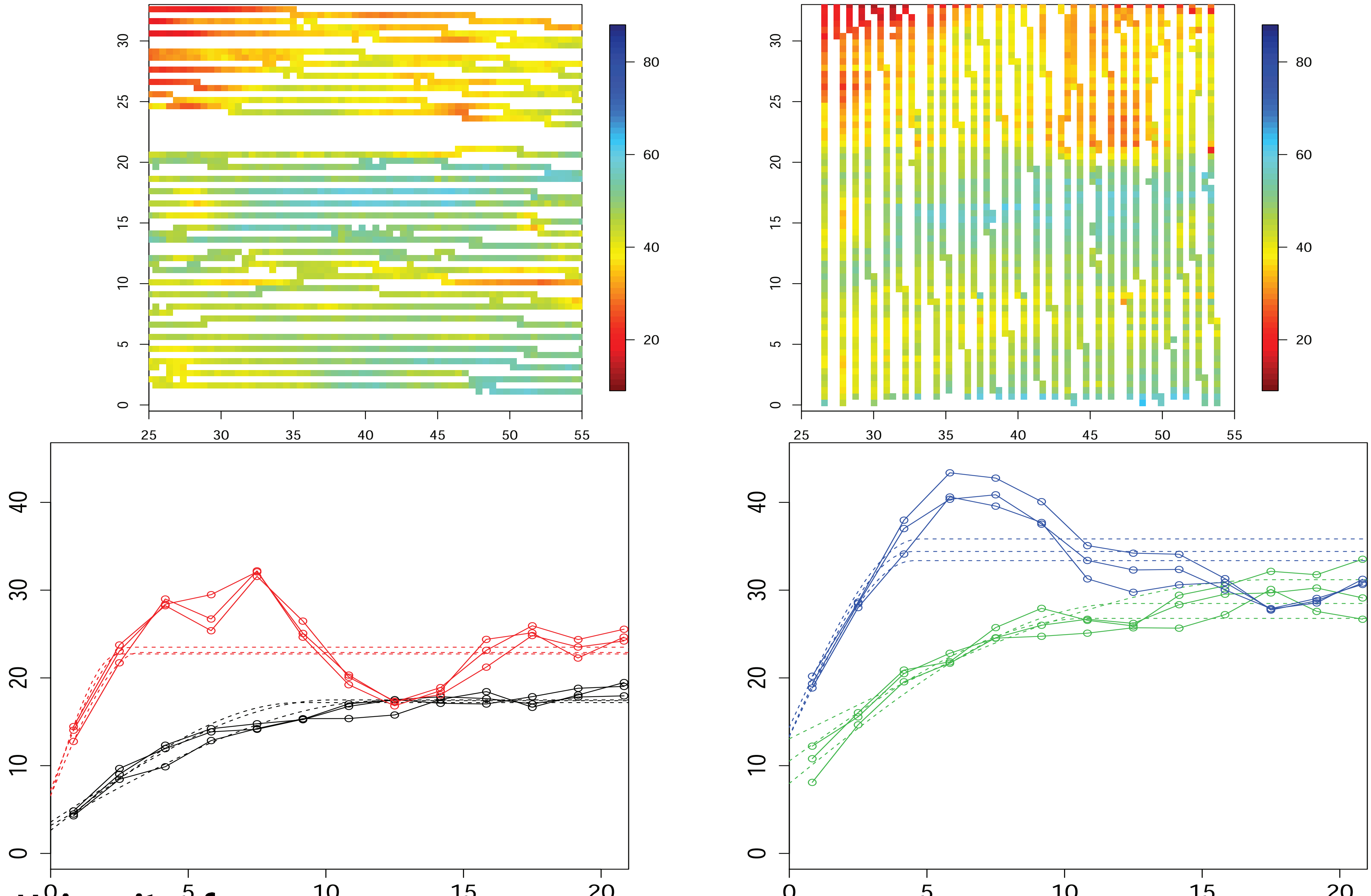

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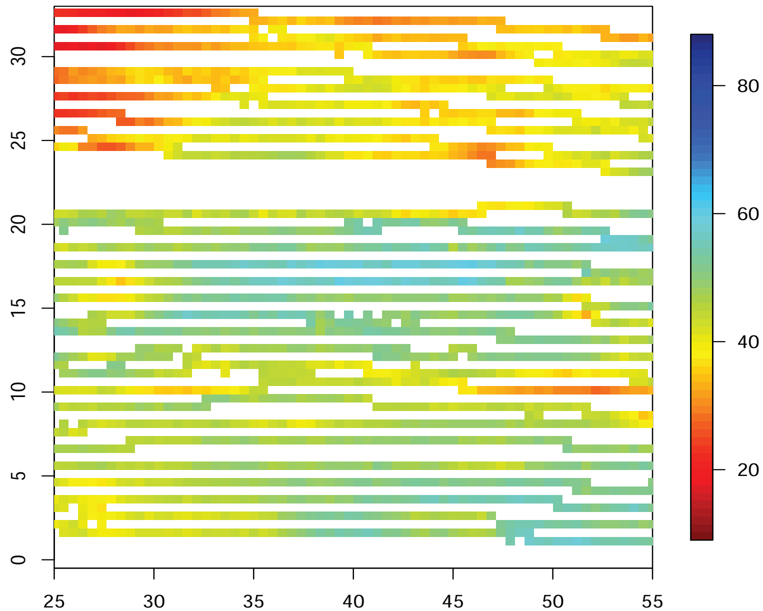

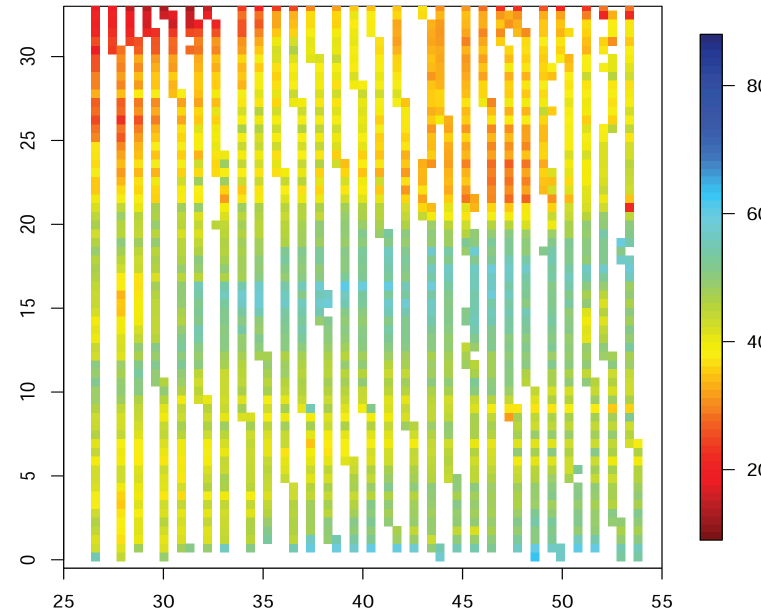

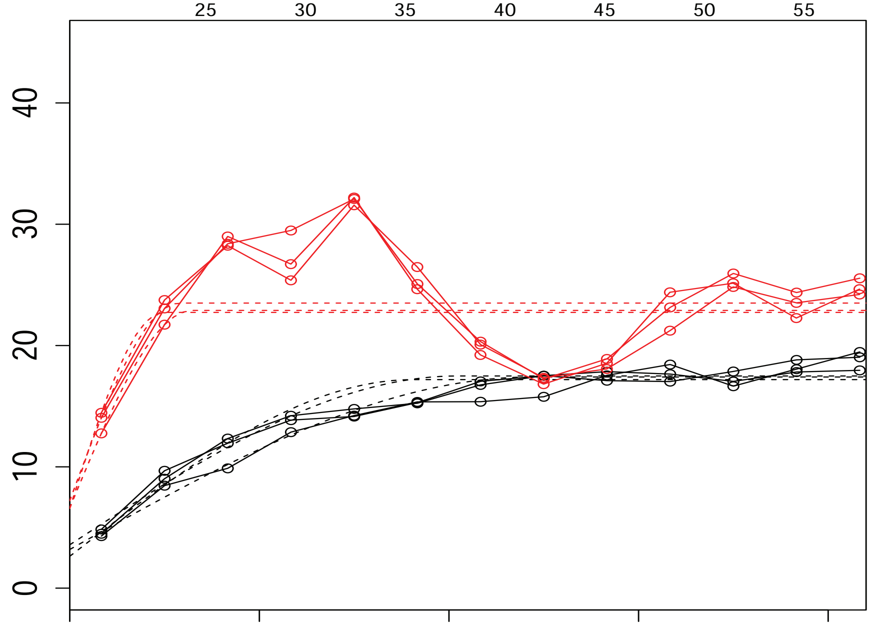

Geometric anisotropy
directionally colored noise

Example: Backfitting

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\end{aligned}
$$

(add measurement operator . . .)

Example: Backfitting

Minnesota testbed:

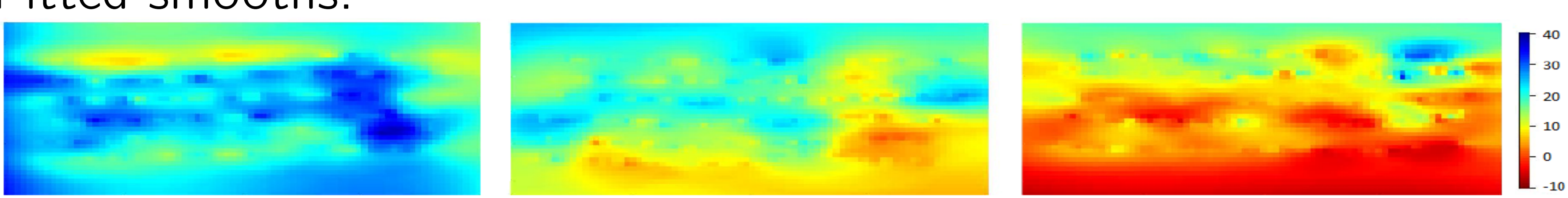
Model:

$$\begin{aligned}
Y_1(\mathbf{s}) &= \mathbf{X}_1\beta_1 + \gamma_1(\mathbf{s}) + \varepsilon_1(\mathbf{s}) \\
Y_2(\mathbf{s}) &= \mathbf{X}_2\beta_2 + c_1\gamma_1(\mathbf{s}) + \gamma_2(\mathbf{s}) + \varepsilon_2(\mathbf{s}) \\
Y_3(\mathbf{s}) &= \mathbf{X}_3\beta_3 + c_2(c_1\gamma_1(\mathbf{s}) + \gamma_2(\mathbf{s})) + \gamma_3(\mathbf{s}) + \varepsilon_3(\mathbf{s})
\end{aligned}$$

(add measurement operator . . .)

Cell 27:

Fitted smooths:



Multiresolution analysis

- Simultaneous inference for IC and QA
  $\rightsquigarrow$ "which features are 'really there'?"
- Using Holmström et al. (2010), extensions from original SiZER
  $\rightsquigarrow$ Ready to use software
- Decomposition into different scales:

$$0 = \lambda_1 < \lambda_2 < \cdots < \lambda_L = \infty$$

smoothing parameters

$$\gamma = \sum_{i=1}^{L-1} (\mathbf{S}_{\lambda_i} - \mathbf{S}_{\lambda_{i+1}})\gamma + \mathbf{S}_{\lambda_L}\gamma$$

$$\equiv \mathbf{z}_1 + \mathbf{z}_2 + \cdots + \mathbf{z}_L$$

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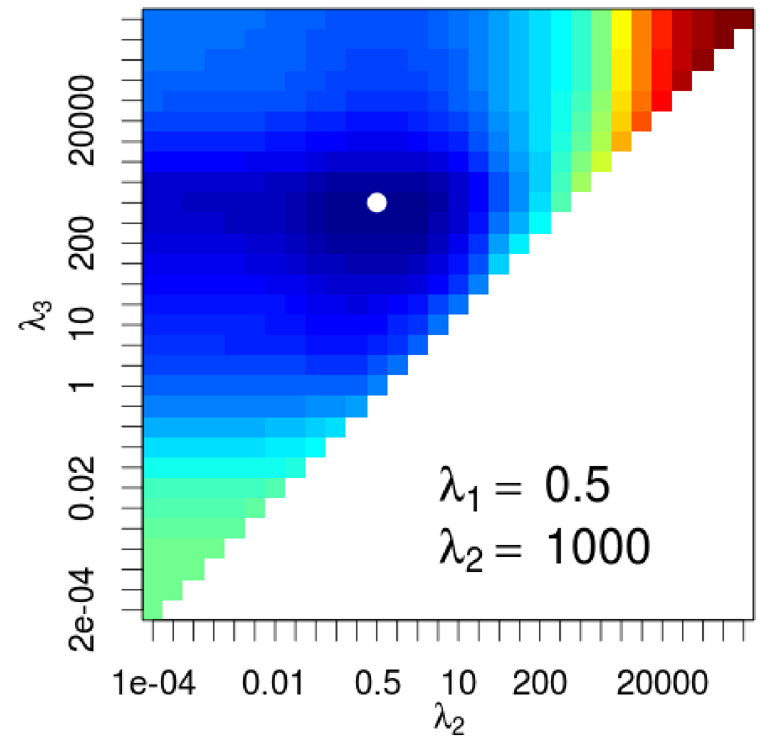
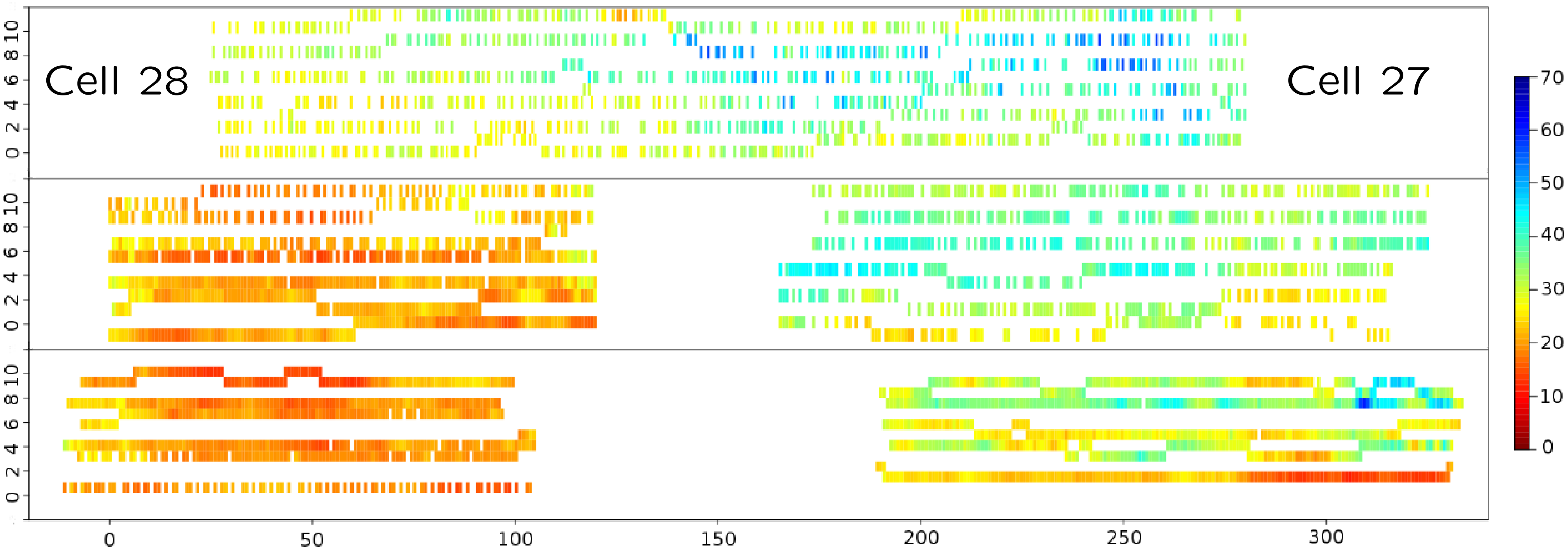


Example: multiresolution analysis

Minnesota testbed:

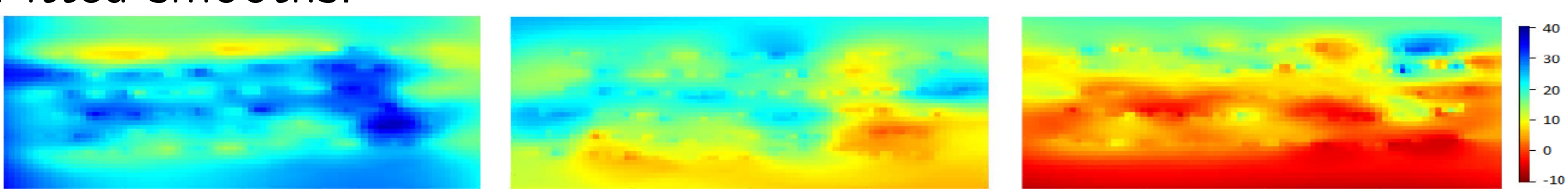


Subgrade, subbase, base (top to bottom).

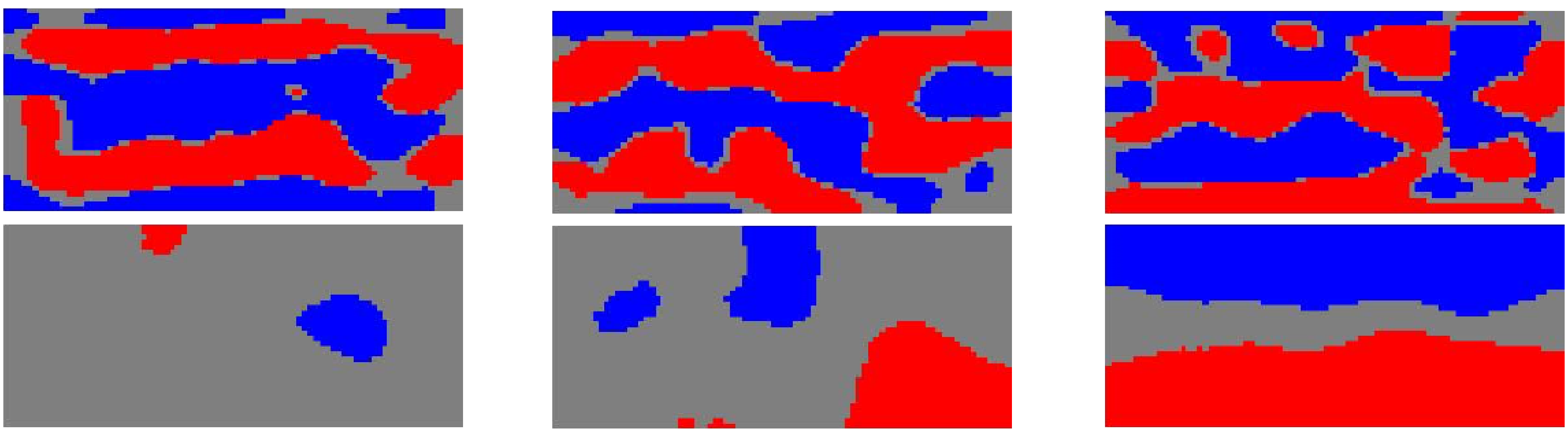
Example: Multiresolution analysis

Cell 27:

Fitted smooths:



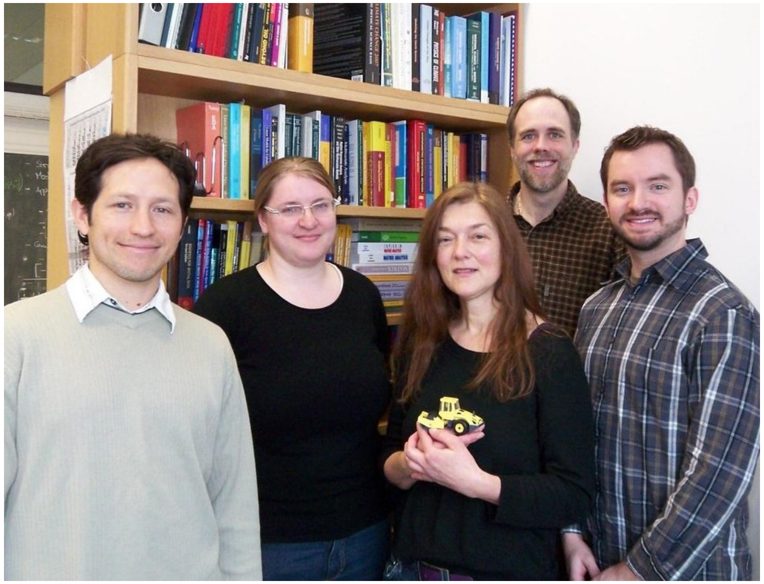
Multiresolution analysis:

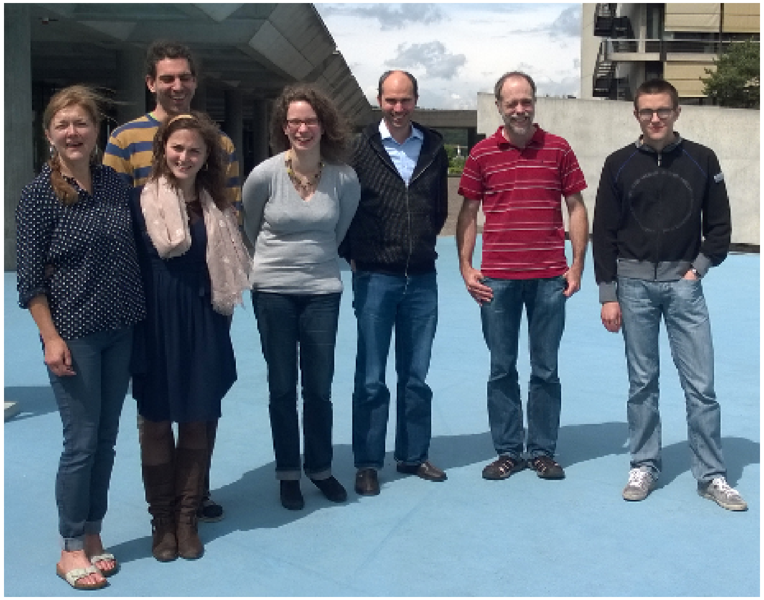


subgrade subbase base

Afterthoughts/outlook

- Flexible setting . . .   toolbox(es)
- Multivariate spatial (spatio-temporal) non-stationary data
- Bayesian framework
- Non-Gaussian data





Collaboration with:

— Daniel Heersink, now Research Scientist at CSIRO, Canberra
— Mike Mooney, CSM
— Roland Anderegg, FHNW . . .

URPP Systems Biology/Functional Genomics &
URPP Global Change and Biodiversity

FNSNF
Swiss National Science Foundation 129782, 143282, 144973

University of Zurich[UZH]

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