Statistical models for large spatial datasets

Lecture 3

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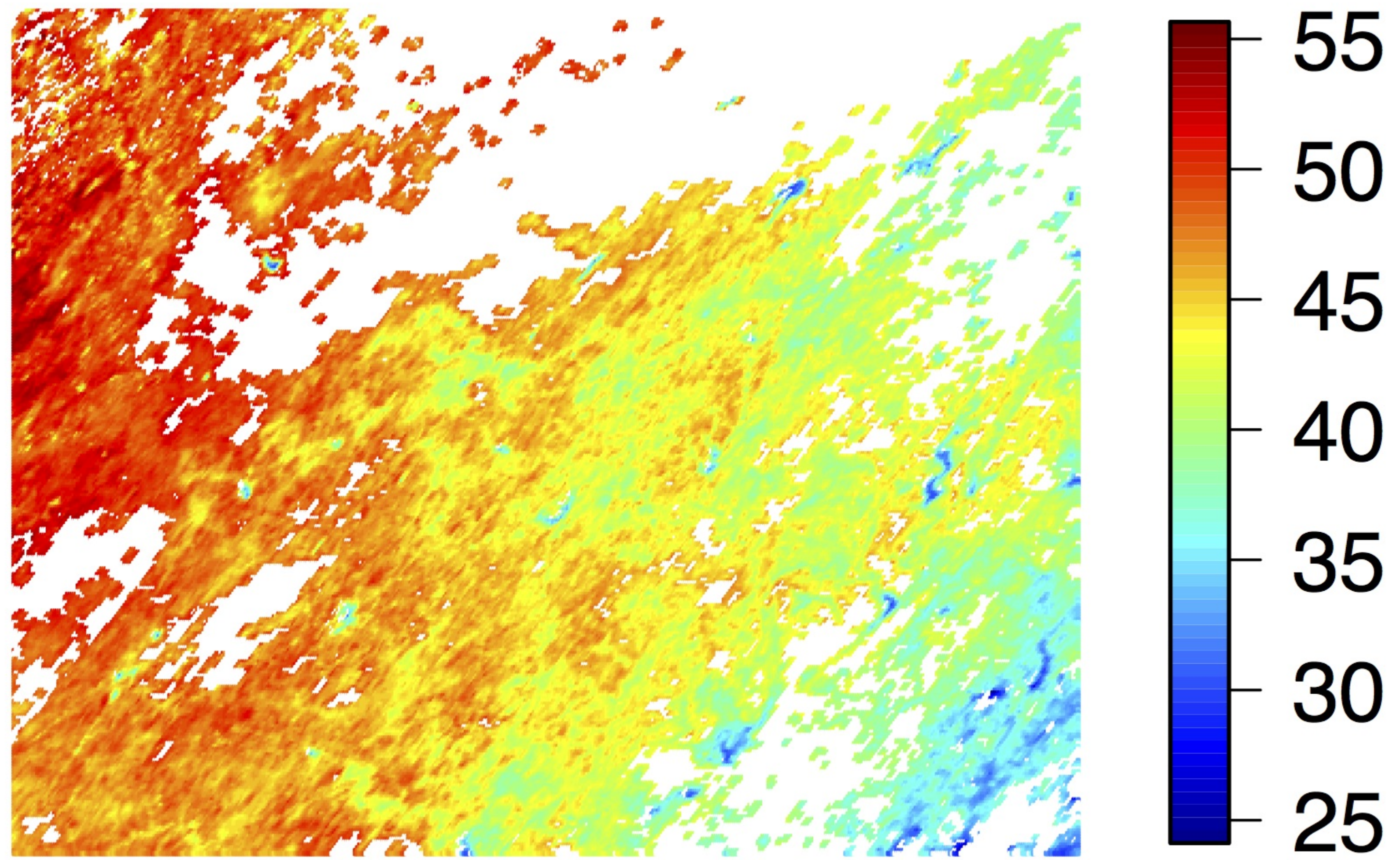
Introduction

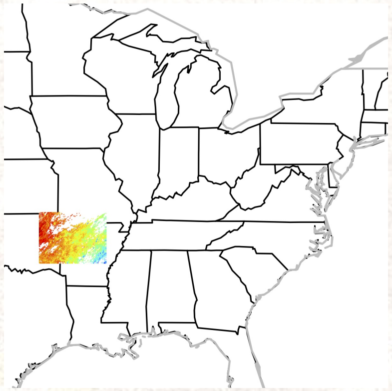
- Examples of large spatial data and the problems
- Some cartoons and a spatial model
- Multi-resolution model
- LatticeKrig – properties
- LatticeKrig in action.

Credits:

- Dorit Hammerling, SAMSI/STATMOS/NCAR
- Soutir Bandyopadhyay, Lehigh U
- Steve Sain, Climate Corp
- Nathan Lenssen, Columbia
- Finn Lindgren, U Bath
- John Paige, NCAR

Remotely sensed temperatures



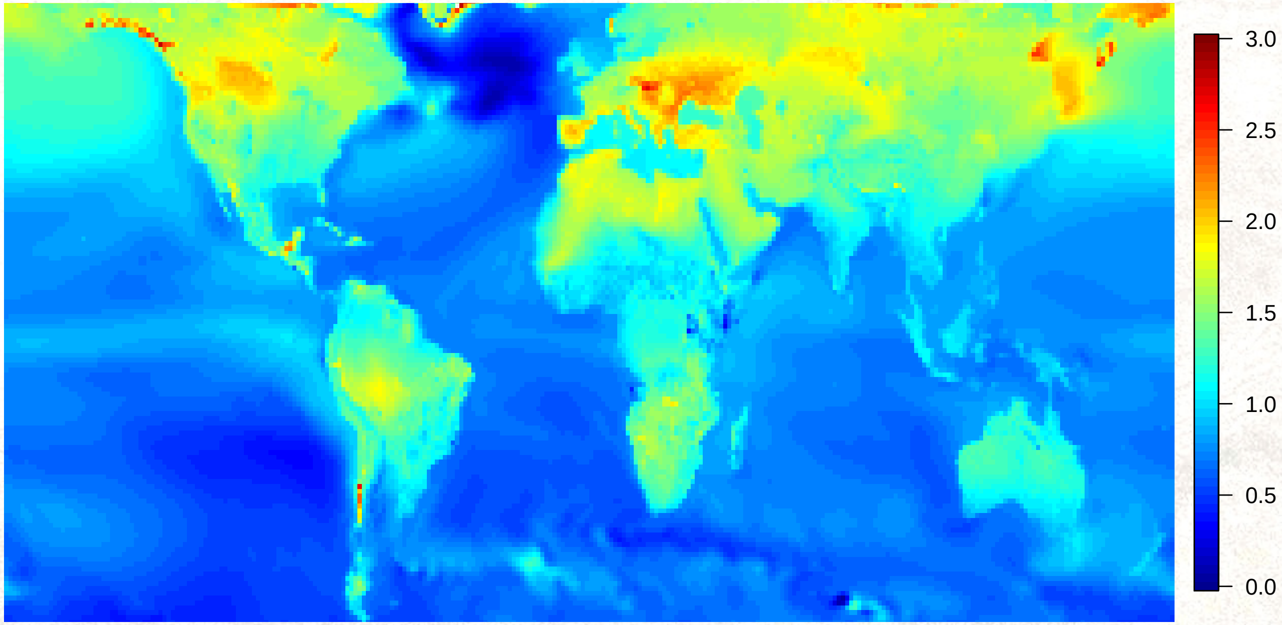


About 100K observations

Climate model output

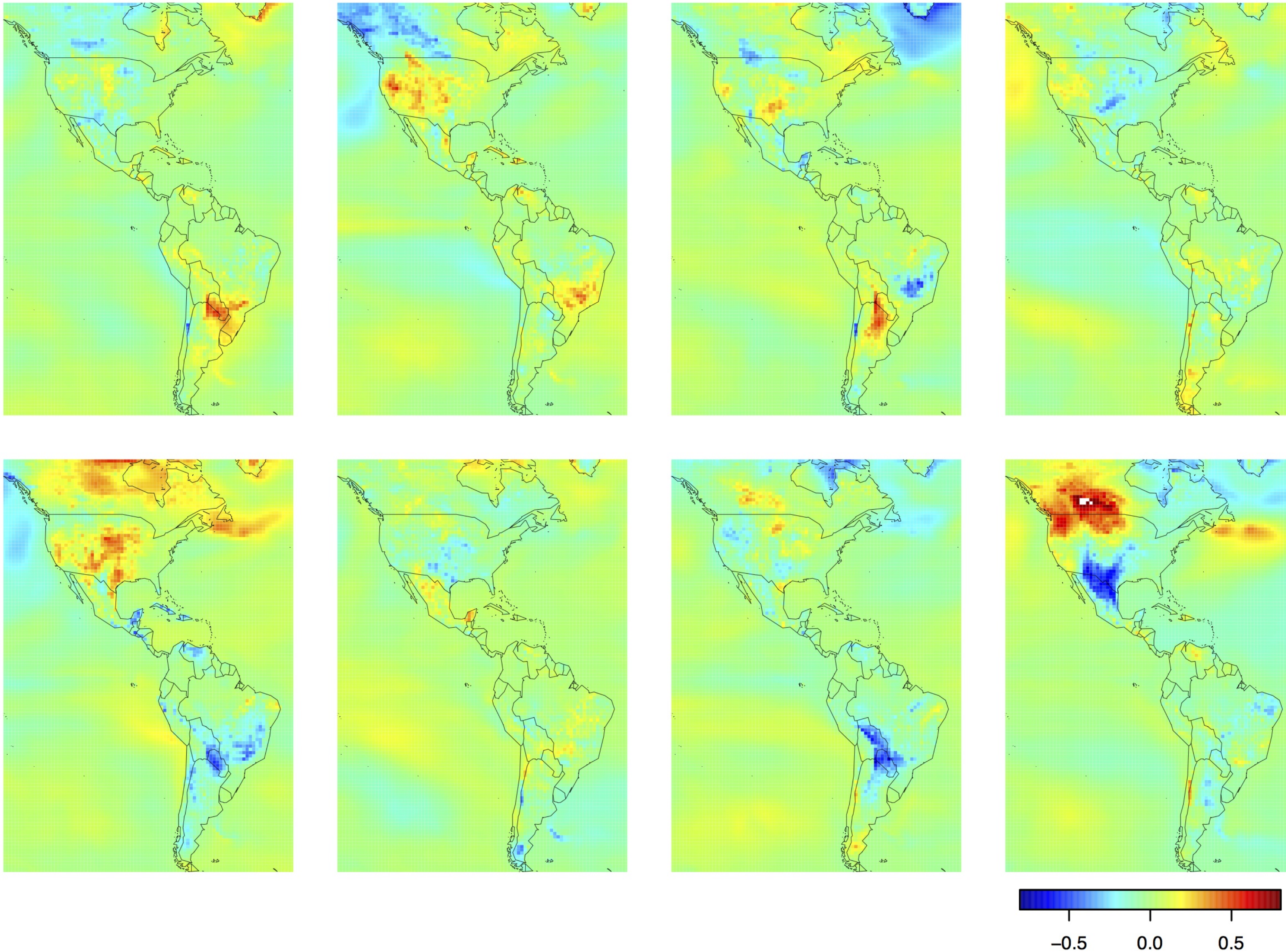
Local sensitivity to changes in global temperature for JJA.

Mean field



about 50K spatial locations (1 degree resolution), 30 member ensemble

First 8 centered ensemble members . . . there are 22 more of these!



Problems with large spatial data sets

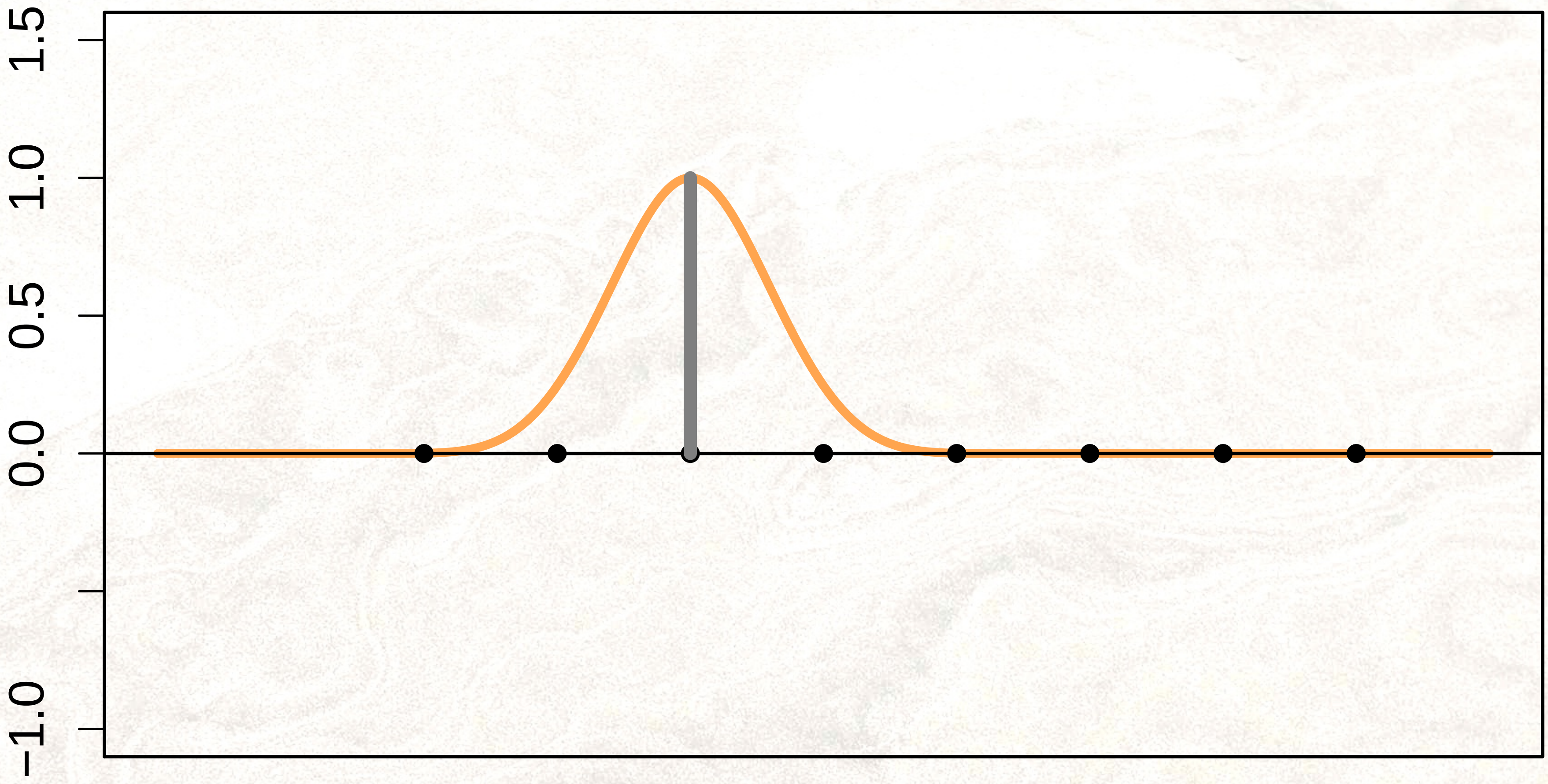
- Storage: Covariance matrices are large – size of the number of observations

- Computation: Linear algebra for the usual Kriging estimator grows as the cube of the number of observations.

- Inference: Exact prediction standard errors are not computationally feaisible.

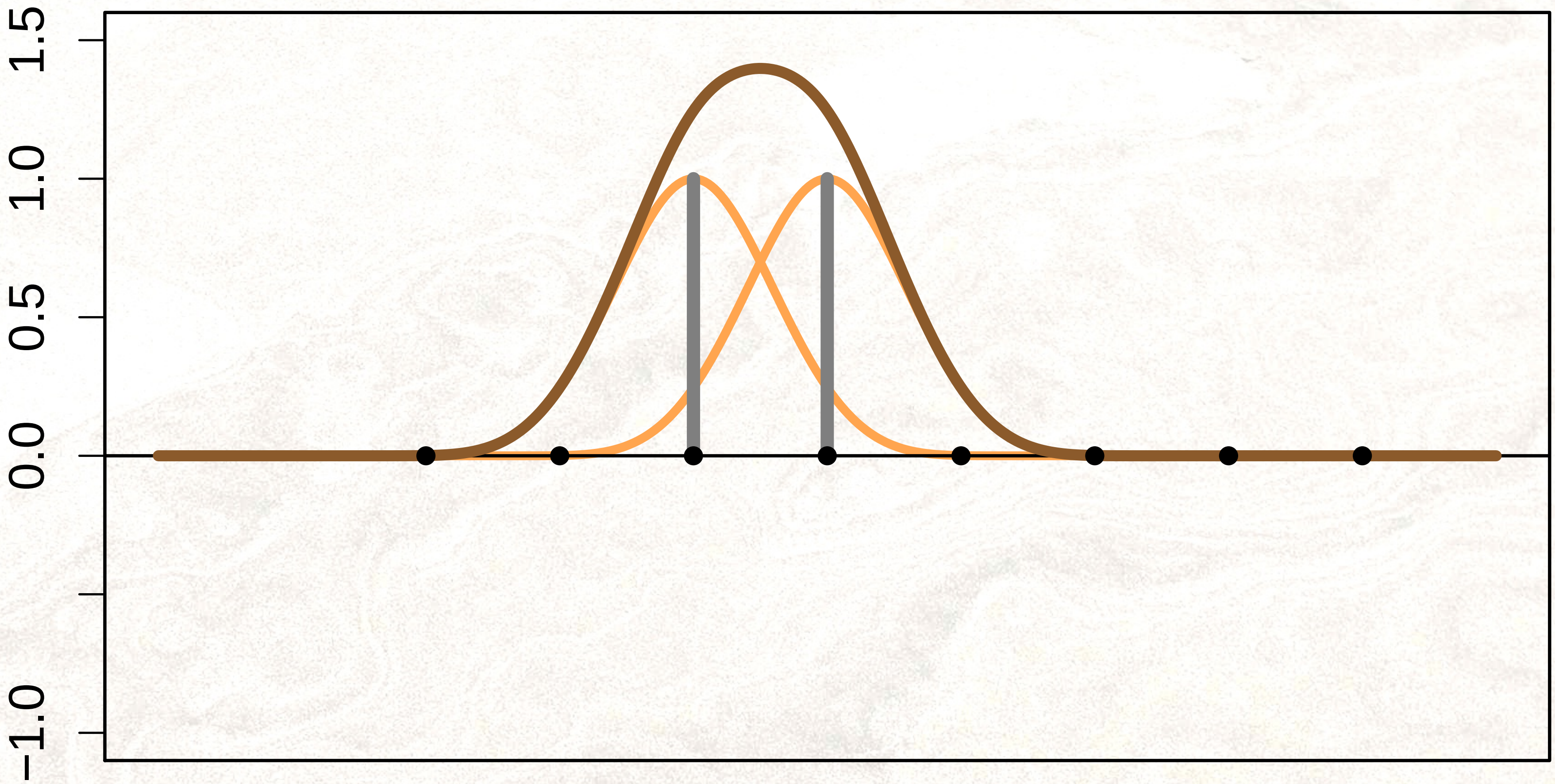
Cartoons

Building a curve from bumps



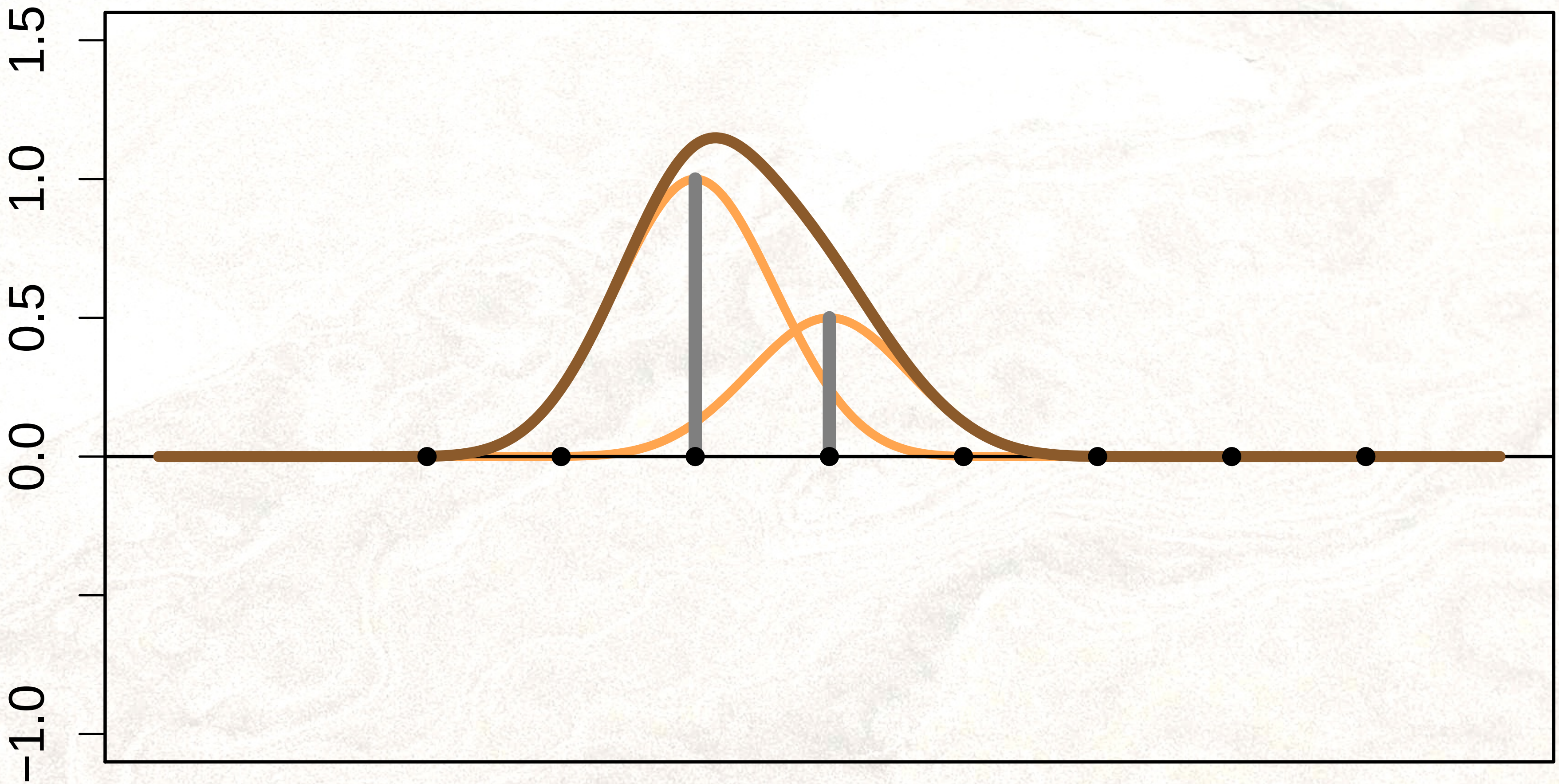
Single bump

Building a curve from bumps



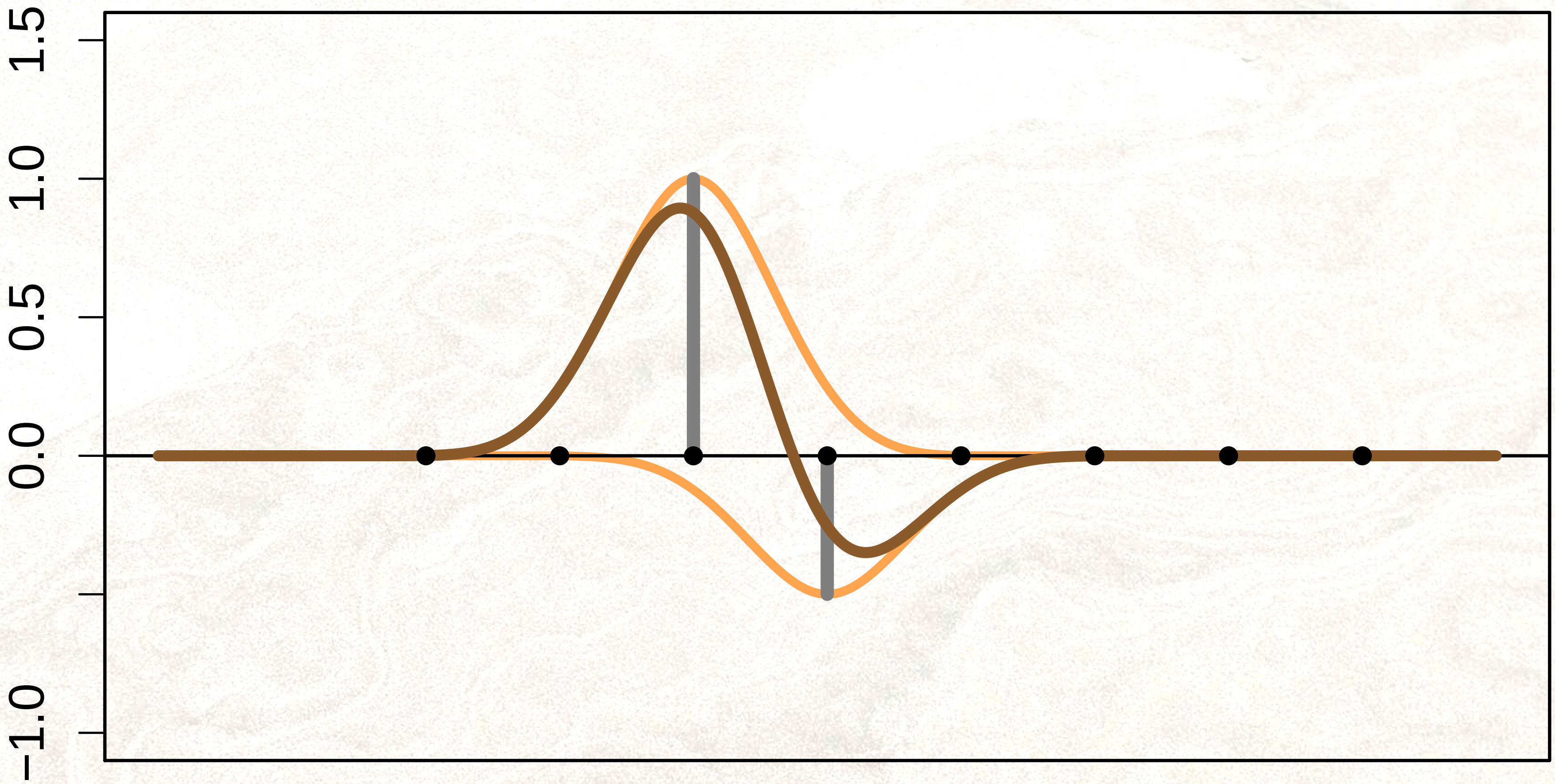
Two bumps same height

Building a curve from bumps



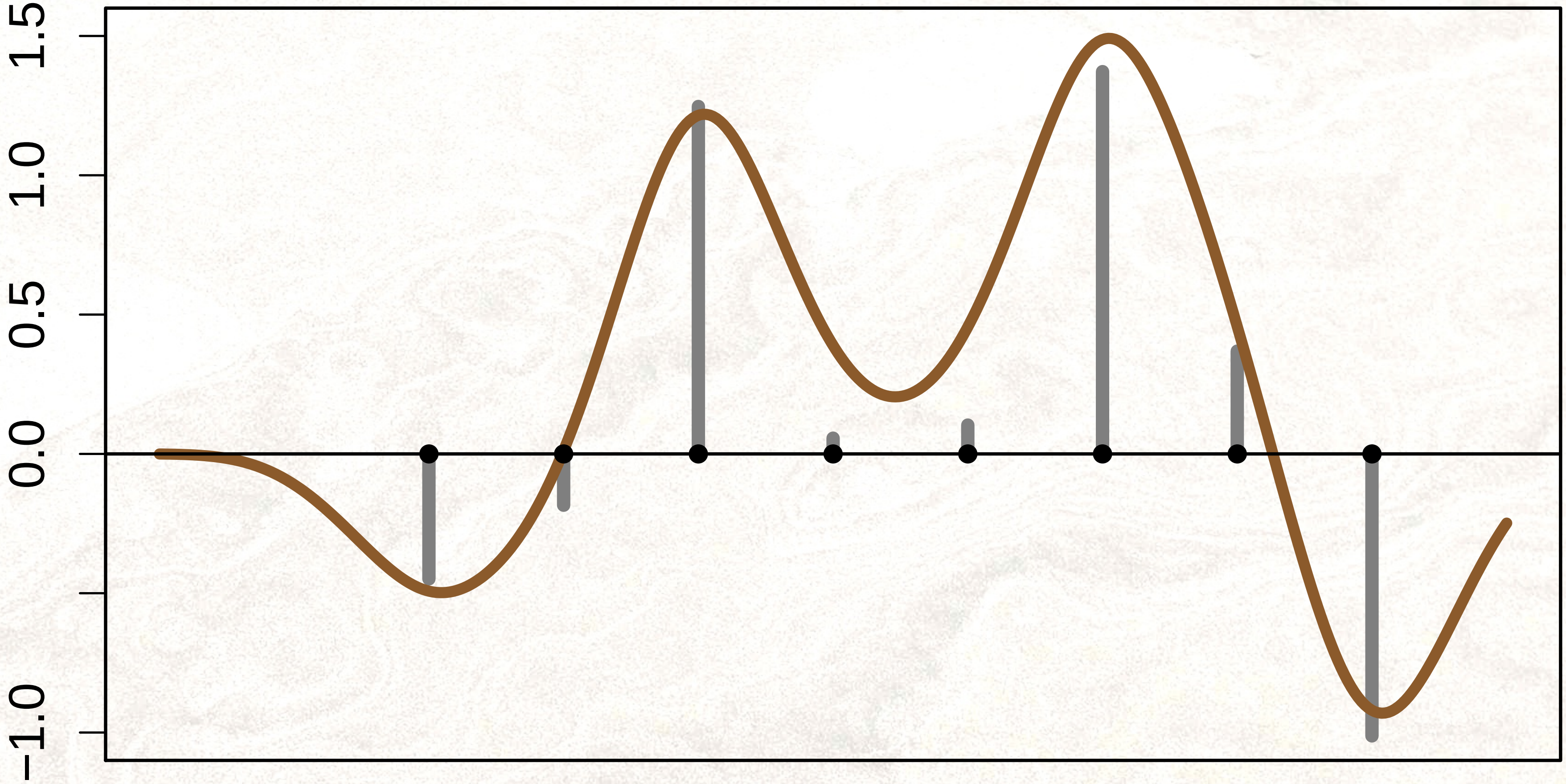
Two bumps different heights

Building a curve from bumps



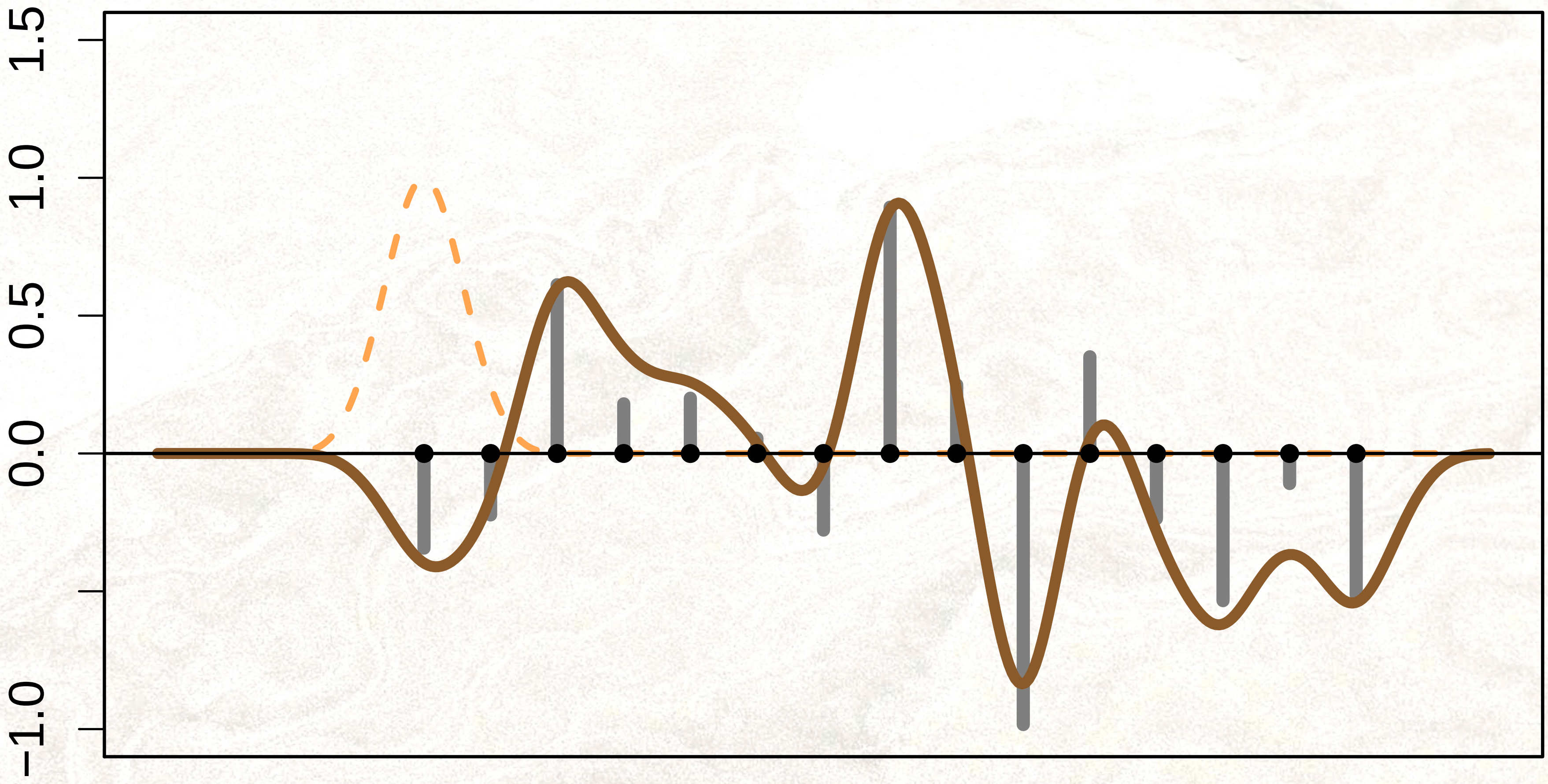
Two bumps different heights

Building a curve from bumps



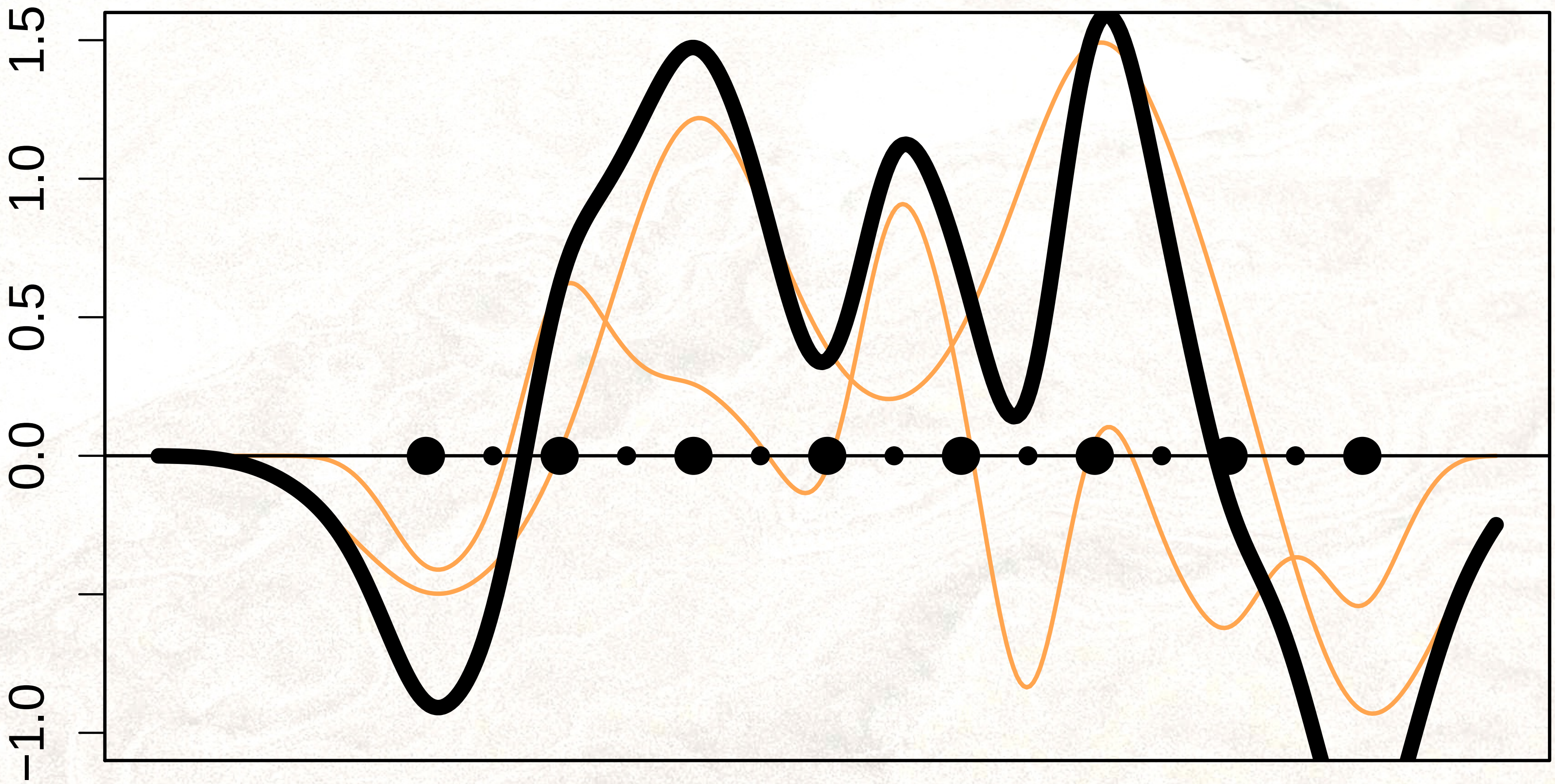
Eight bumps – all different heights

Building a curve from bumps



16 bumps – all different heights

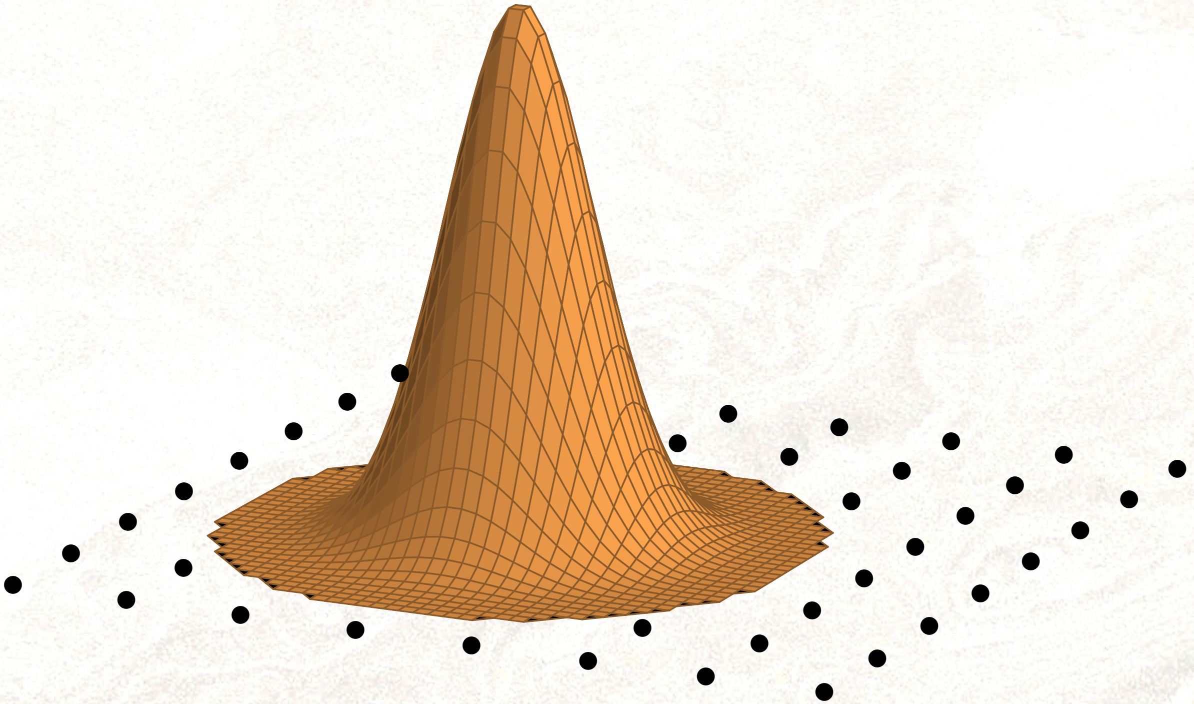
Building a curve from bumps



Adding them together

bumps = basis functions, bump heights = coefficients

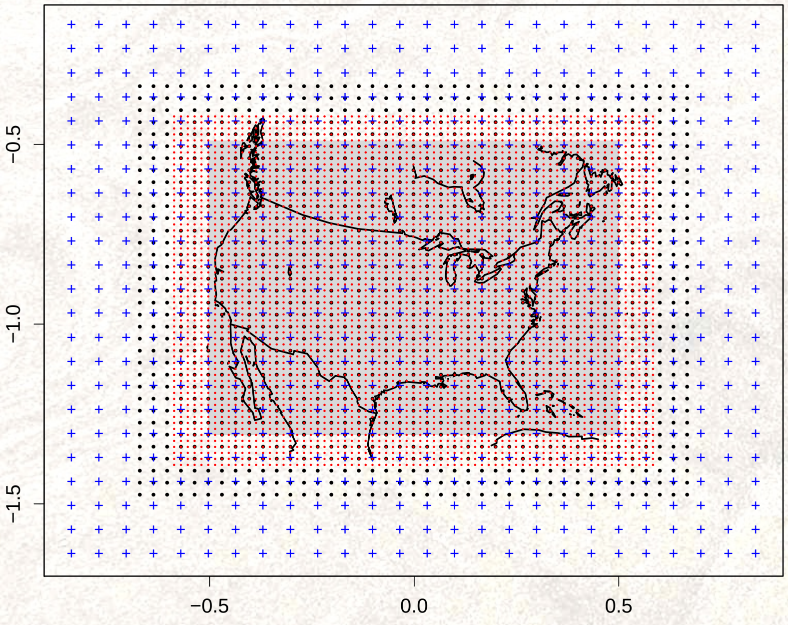
A (Wendland Basis function

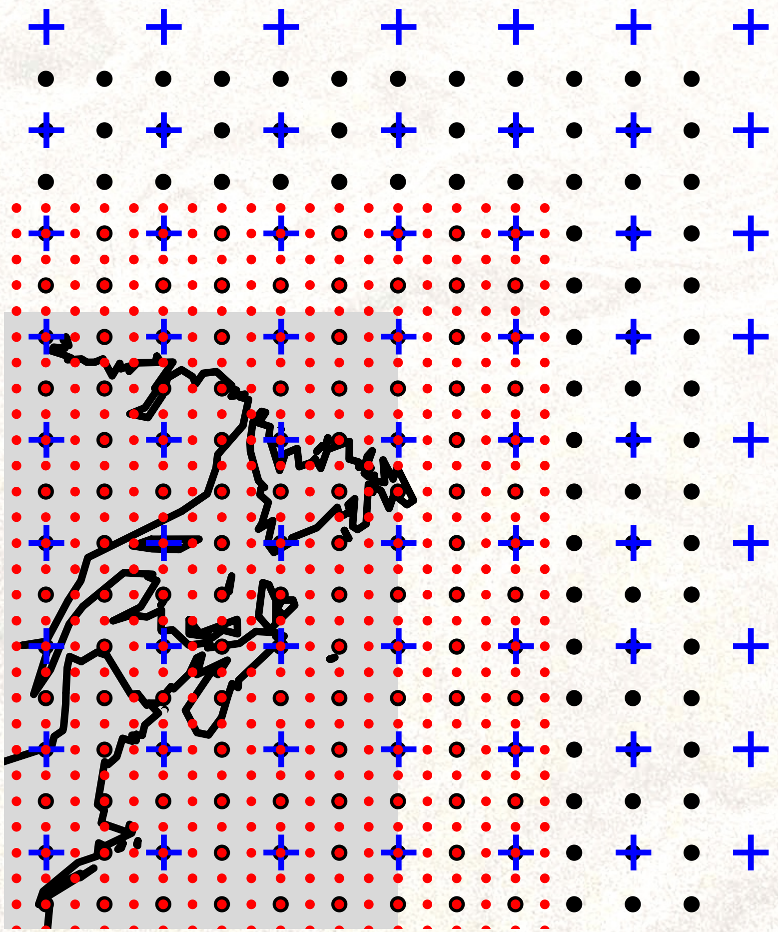


Example of a 2-d bump

A lattice example

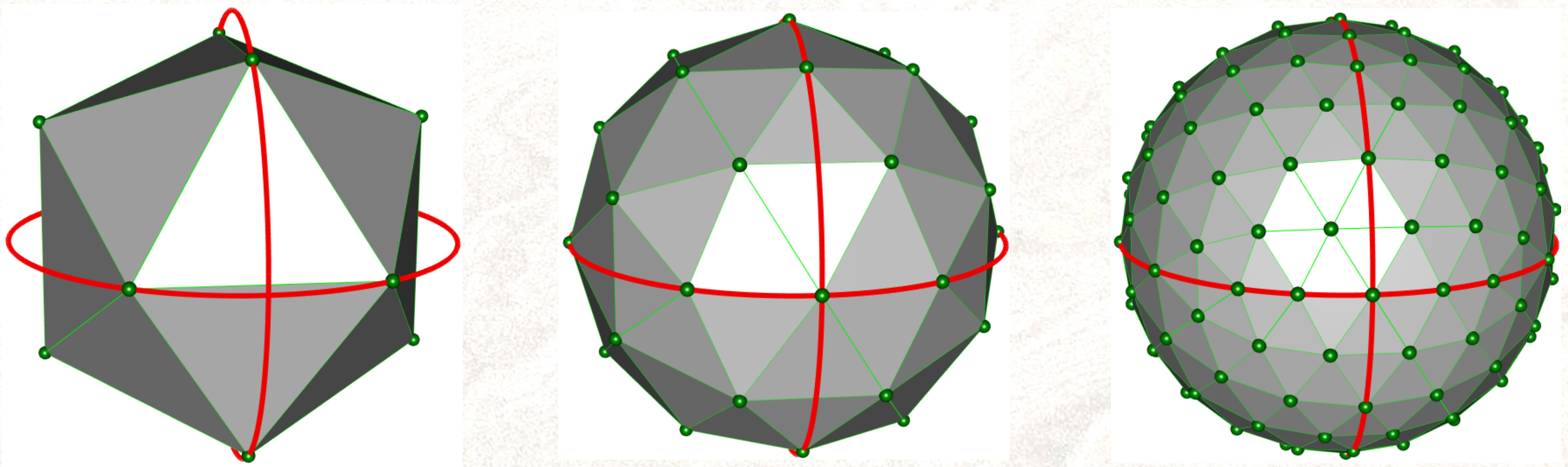
- Three levels
- Extra points on margins to minimize edges effects
- About 4000 total lattice points





Another lattice

Icosohedra grids for the sphere.



Spatial model

A linear (random effects) model

- X a regression matrix with $X_{i,j} = \phi_j(\boldsymbol{x}_i)$

Observations:

$$\boldsymbol{y} = X\boldsymbol{c} + \boldsymbol{e} \quad \boldsymbol{e} \sim MN(0, \sigma^2 I)$$

Process:

$$g(x) = \sum_j \phi_j(x) c_j, \quad \boldsymbol{c} \sim MN(0, \rho Q^{-1})$$

Potential Priors:

$$[\rho, \sigma^2, Q]$$

Derived Covariance

$$Cov(g(\boldsymbol{x}), g(\boldsymbol{x}')) = \rho \sum_{j,k} \phi_j(\boldsymbol{x}) \left[Q^{-1}\right]_{j,k} \phi_k(\boldsymbol{x}')$$

- The model is written so that the covariance never needs to be explicitly found.

Computing the estimate

Integrating out $\boldsymbol{c}$:
$[\boldsymbol{y}|\rho, \sigma^2, Q] \sim MN(0, (\rho \boldsymbol{X}^T Q^{-1} \boldsymbol{X} + \sigma^2 I)$

Likelihood/posterior computation for ρ, σ^2, Q

dominated by

$$|\rho \boldsymbol{X}^T Q^{-1} \boldsymbol{X} + \sigma^2 I| \text{ or equivalently } |(\sigma^2 \boldsymbol{X}^T \boldsymbol{X} + (1/\rho) Q|$$

Kriging estimate of $\boldsymbol{c}$:

$$\hat{c} = (\boldsymbol{X}^T \boldsymbol{X} + (\sigma^2/\rho) Q)^{-1} \boldsymbol{X}^T \boldsymbol{y}$$

This is also the penalized least squares solution from Lecture 1.

Conditional simulation

Based on *unconditional* simulation of $\boldsymbol{c}$ and Kriging estimate.

- Fast computation hinges on sparsity of Q and X.

Details and engineering

More about Q

At a single level

Some coefficients:

.	.	.	.	.
.	.	c_1	.	.
.	c_2	c_*	c_3	.
.	.	c_4	.	.
.	.	.	.	.

Some weights:

.	.	.	.	.
.	.	-1	.	.
.	-1	a	-1	.
.	.	-1	.	.
.	.	.	.	.

The filter:

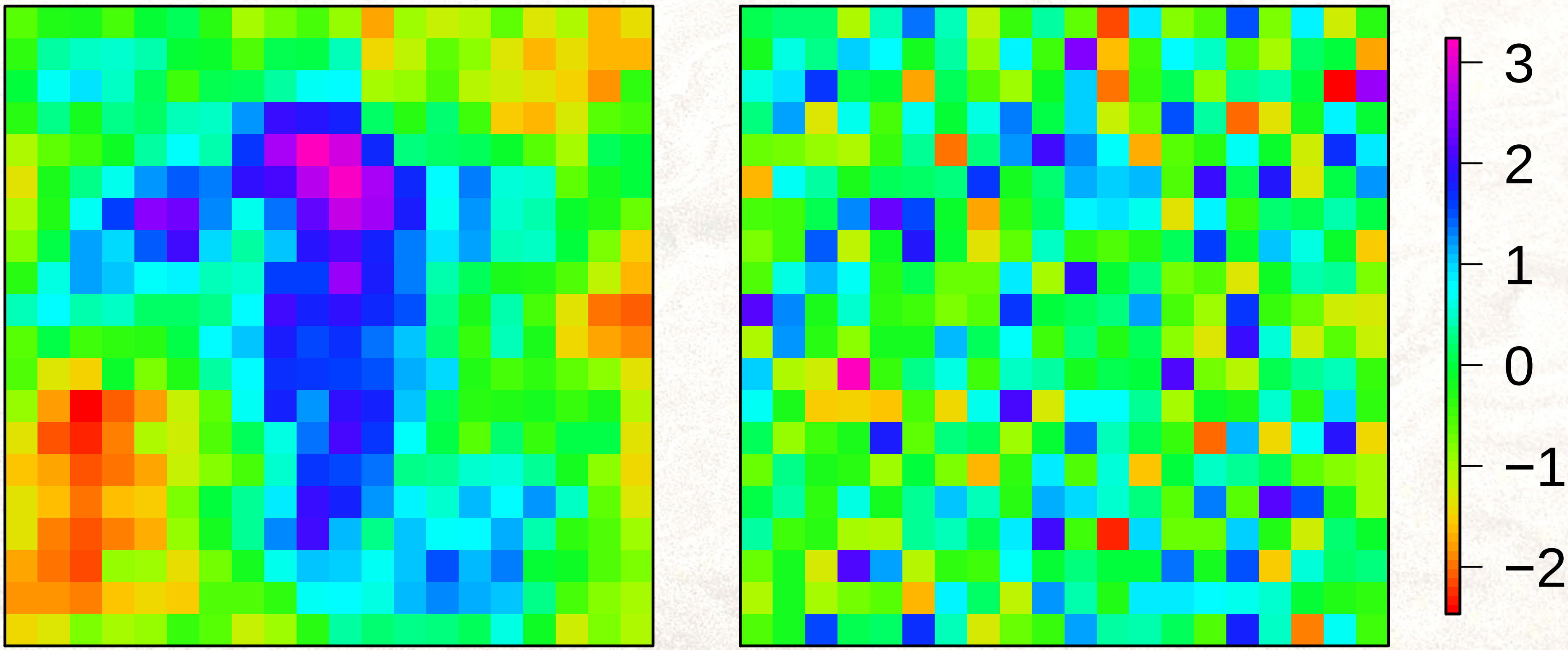
$ac_* - (c_1 + c_2 + c_3 + c_4) =$ white noise

If $Bc =$ iid $N(0,1)$, $\qquad Q = BB^T$

- a needs to be greater than 4.
- A simple discretization of the Laplacian. $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$

Filtering coefficients

Coefficients on the lattice *Applying the filter*

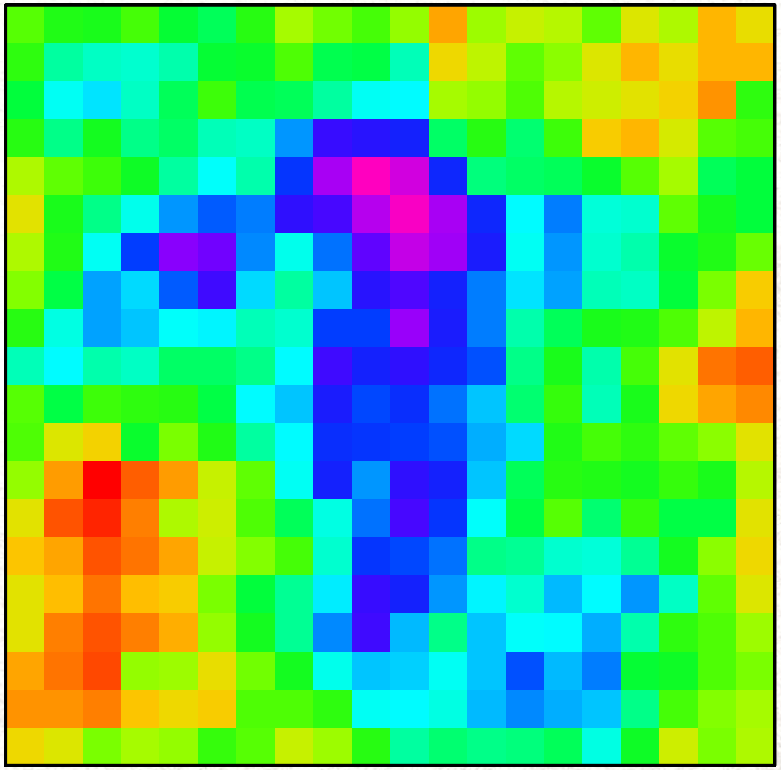


$$c_* \to ac_* - (c_1 + c_2 + c_3 + c_4)$$

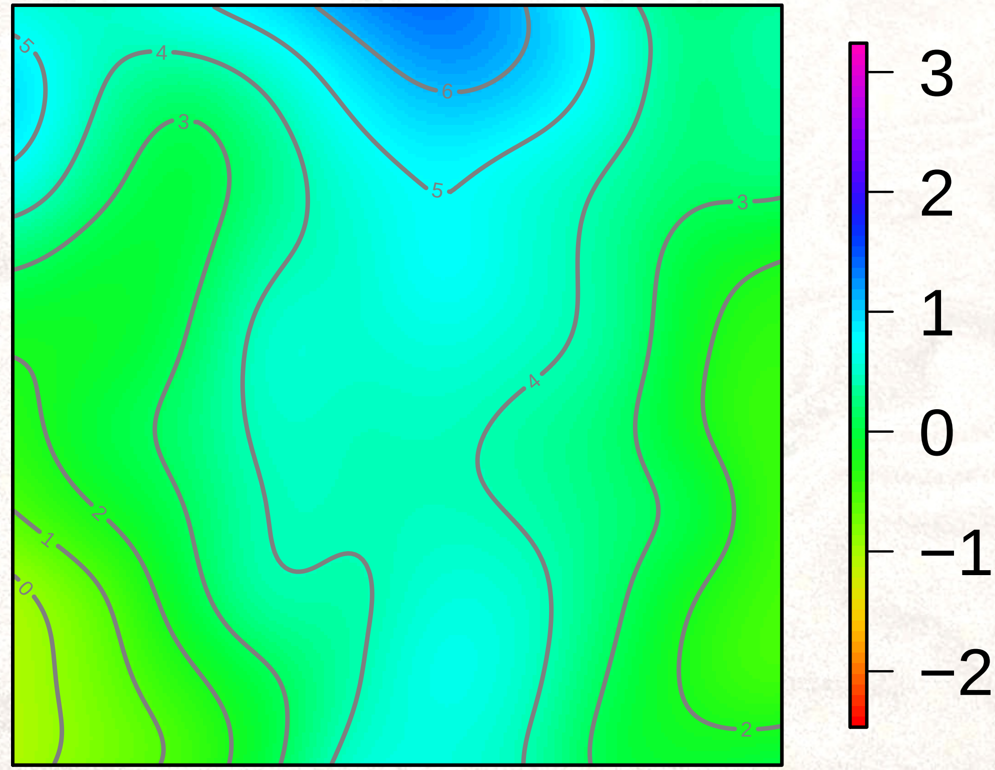
$a = 4.01$

Applying the basis functions

Coefficients on the lattice



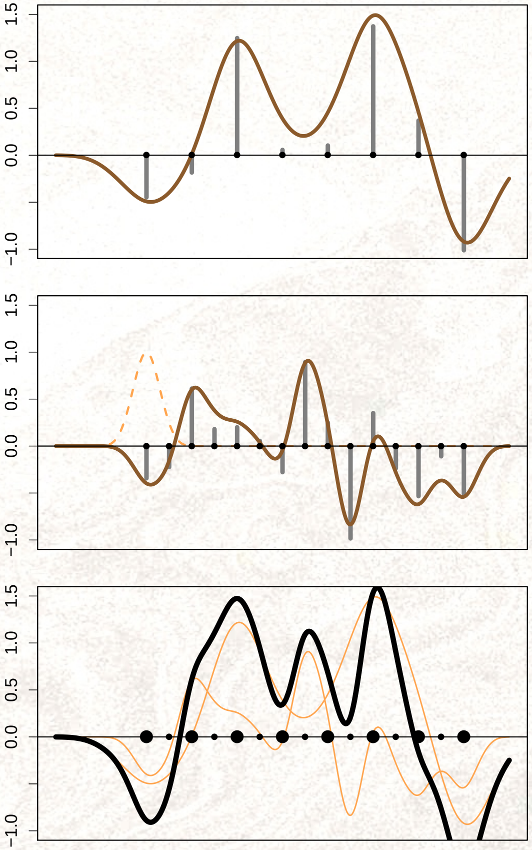
Expanding with basis functions



$$c_k \to \sum \phi_k(x) c_k = g(\boldsymbol{x})$$

More than one level:

Adding different resolutions together:



$$g(\boldsymbol{x}) = \rho(\alpha_1 g_1(\boldsymbol{x}) + \alpha_2 g_2(\boldsymbol{x}) + \alpha_3 g_3(\boldsymbol{x}) + \ldots)$$

$$Q = (1/\rho)\begin{bmatrix} \alpha_1 B_1^T B_1 & 0 & 0 \\ 0 & \alpha_2 B_2^T B_2 & 0 \\ 0 & 0 & \alpha_3 B_3^T B_3 \end{bmatrix}$$

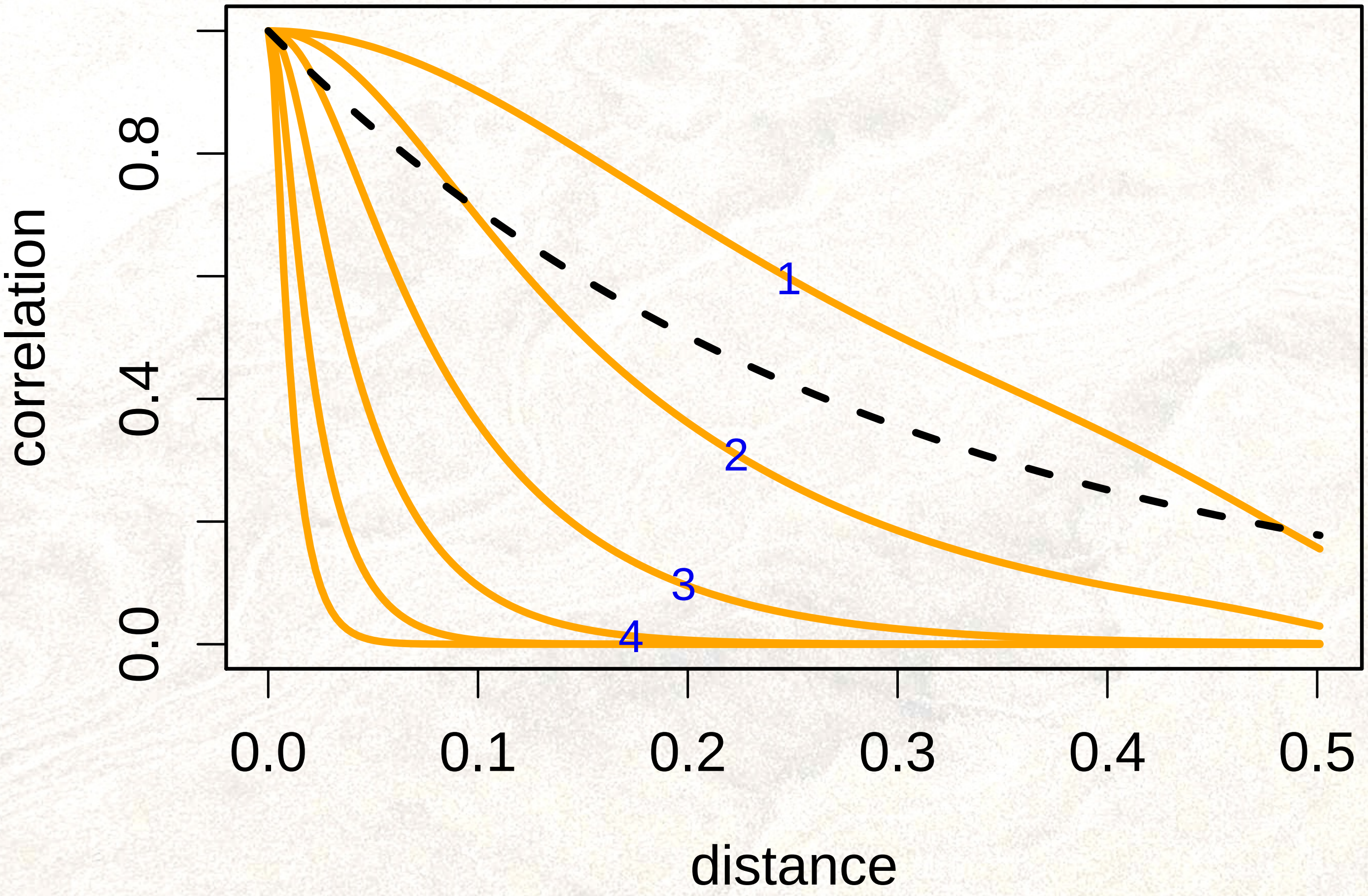
- ρ marginal variance of the process
- $\alpha_1, \alpha_2, \alpha_3$ relative weight for each level – all nonnegative and add to 1.

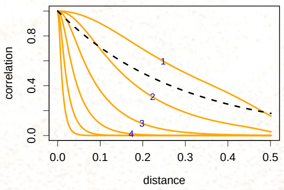
Benefits of a multi-resolution

Approximating standard covariances

Approximating an exponential covariance

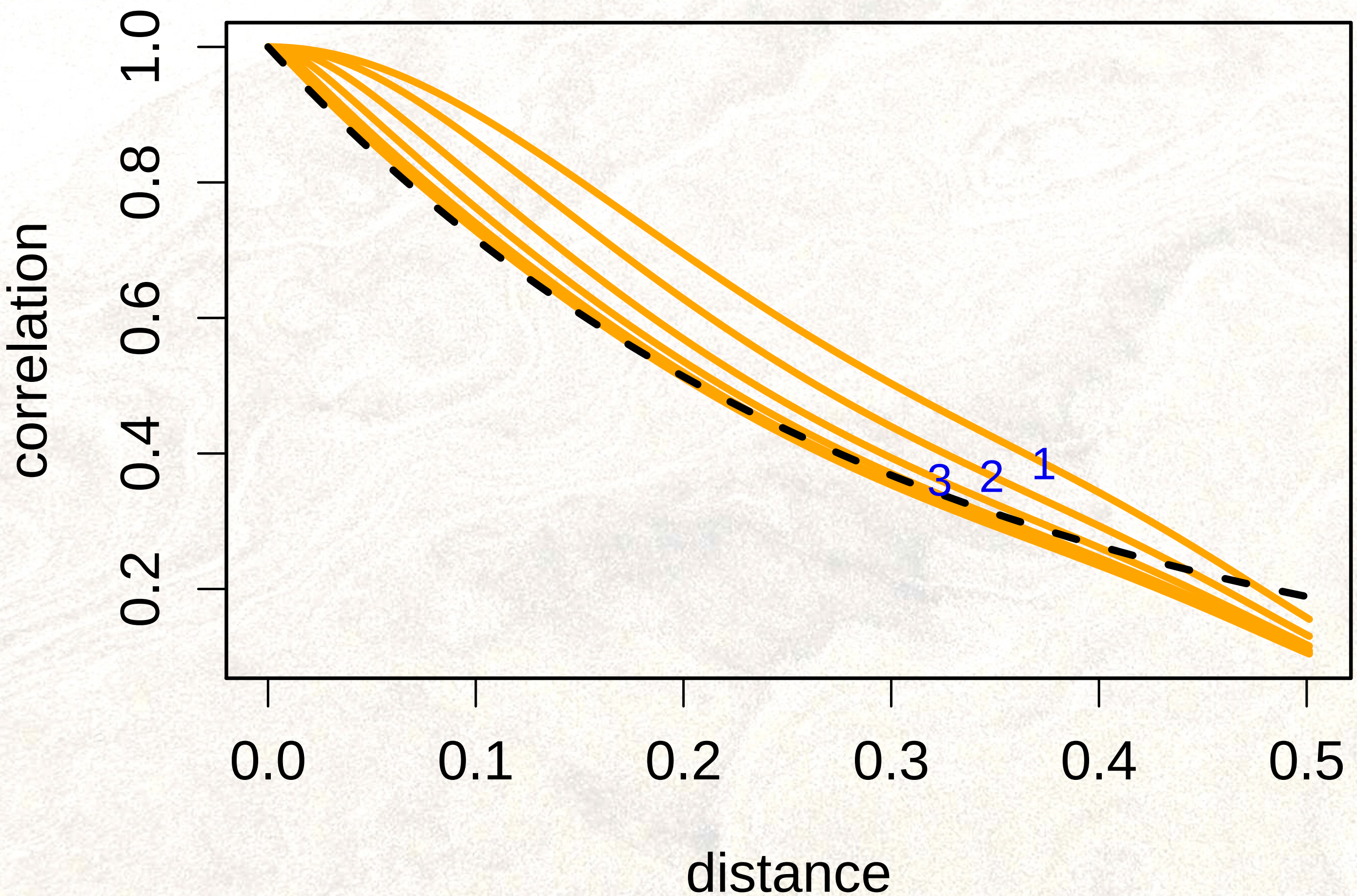
Correlation functions for 6 levels and a target exponential





Weighting by $2^{-level/2}$

Correlation functions adding levels and the target exponential



Timing

On my mac laptop and in R

— i.e. a single core and `LatticeKrig` pacakge

Computation may be dominated by :

- matrix setup
- normalization to stationarity
- *Cholesky decomposition*

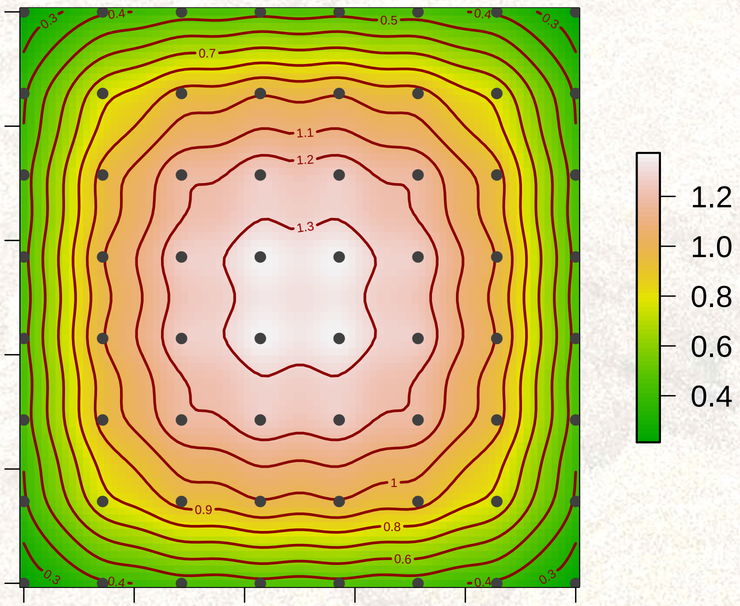
For 20,000 observations, single likelihood evaluation:

- standard Kriging (dense Cholesky) is $\approx$ 20 minutes
- `LatticeKrig` (sparse Cholesky) is $\approx$ 10 seconds.

Stationarity?

Recall $Cov(g(\boldsymbol{x}), g(\boldsymbol{x}')) = \rho \sum_{j,k} \phi_j(\boldsymbol{x}) \left[Q^{-1}\right]_{j,k} \phi_k(\boldsymbol{x}')$

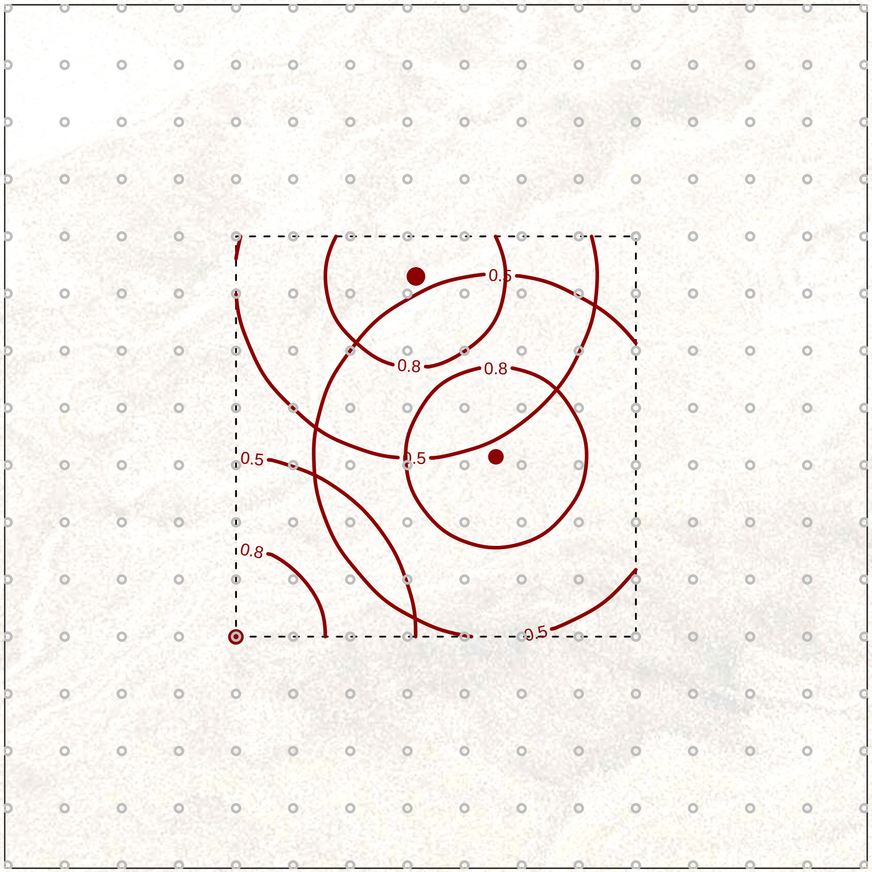
Correlation function for a single level $a = 4.2$
Marginal variance $VAR(g(x)$ from a 8$\times$ 8 grid



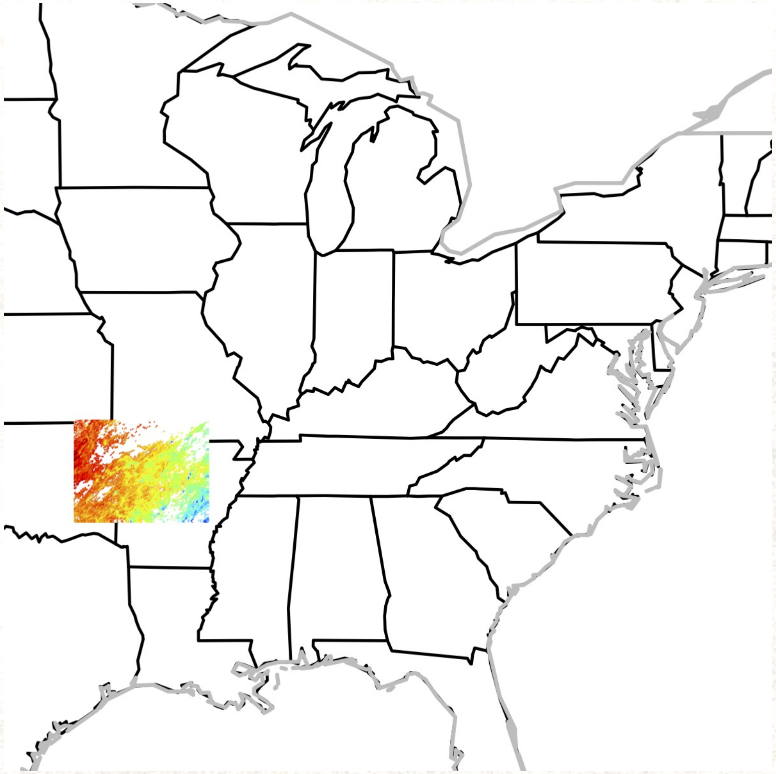
Adding buffer and normalizing

8× 8 grid with 4 grid points of buffer and normalized

Correlation function for a single level, $a = 4.2$

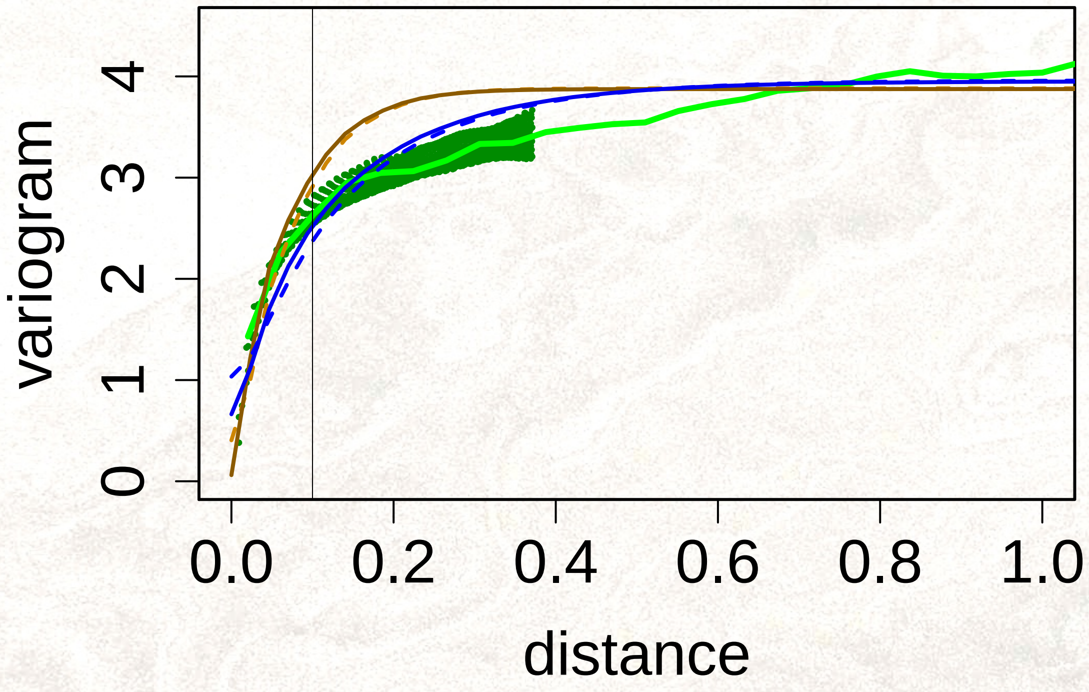


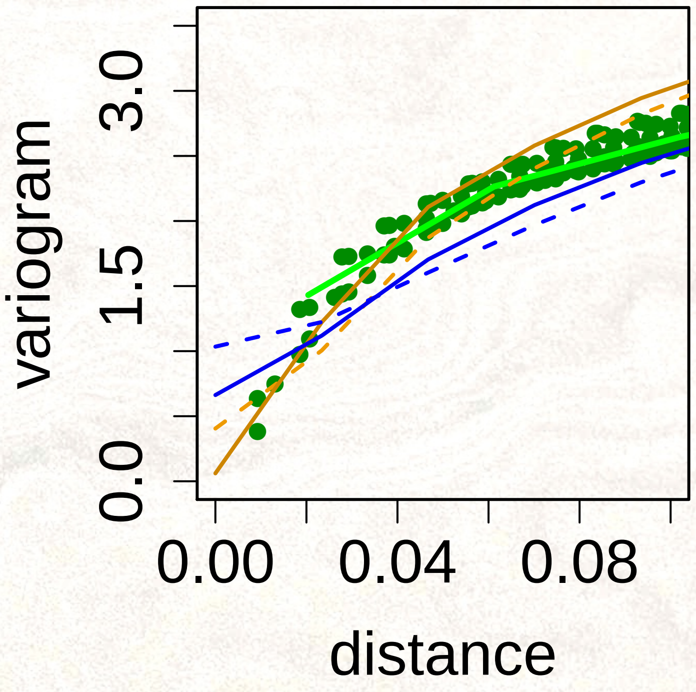
Surface temperatures



Variogram fitting

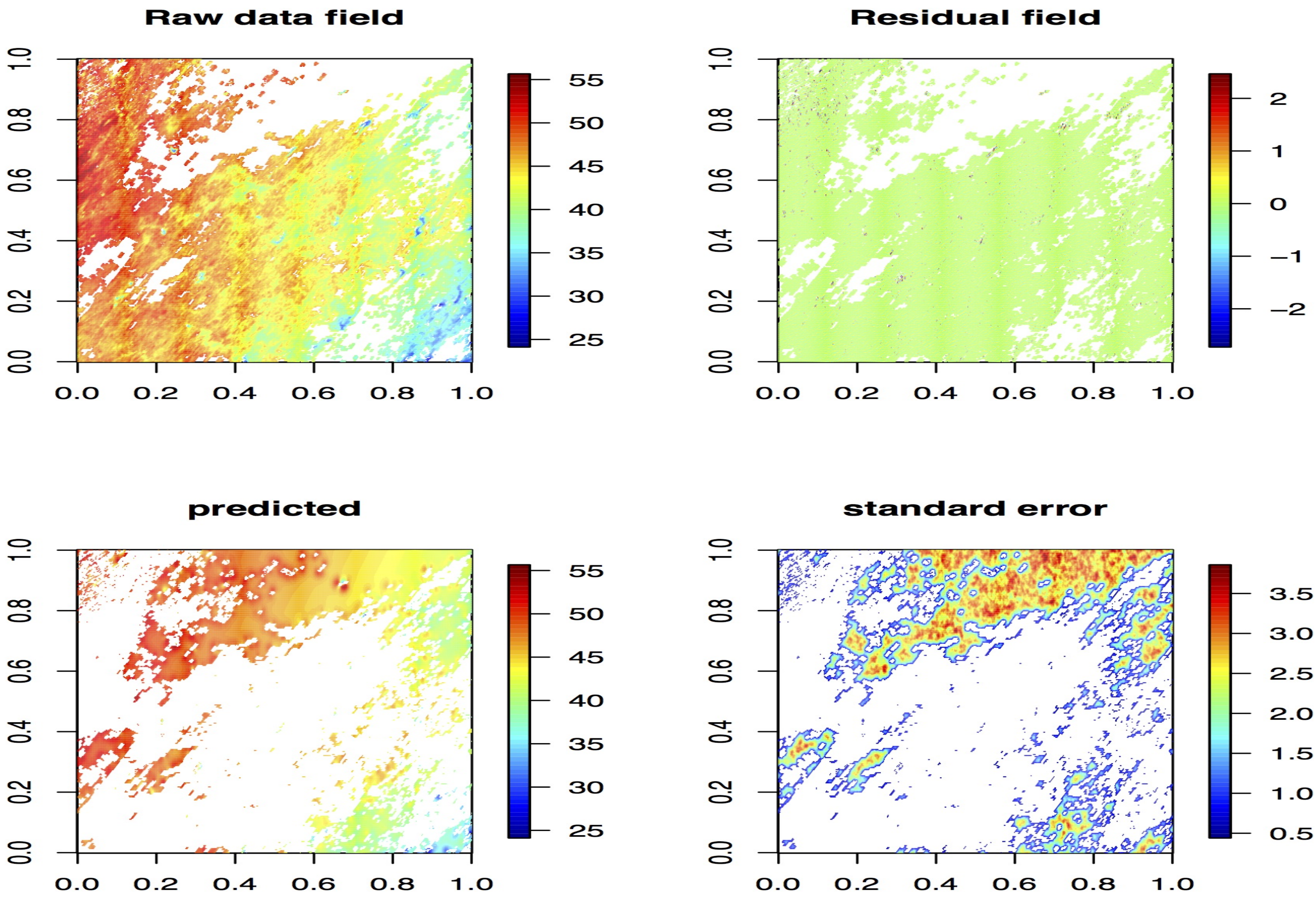
Sample Variogram with some different LatticeKrig models





- First level - 50 basis functions in longer dimension,
- a = 10, a = 4.5
- dashed - 3 levels, solid – 4 levels

Some results



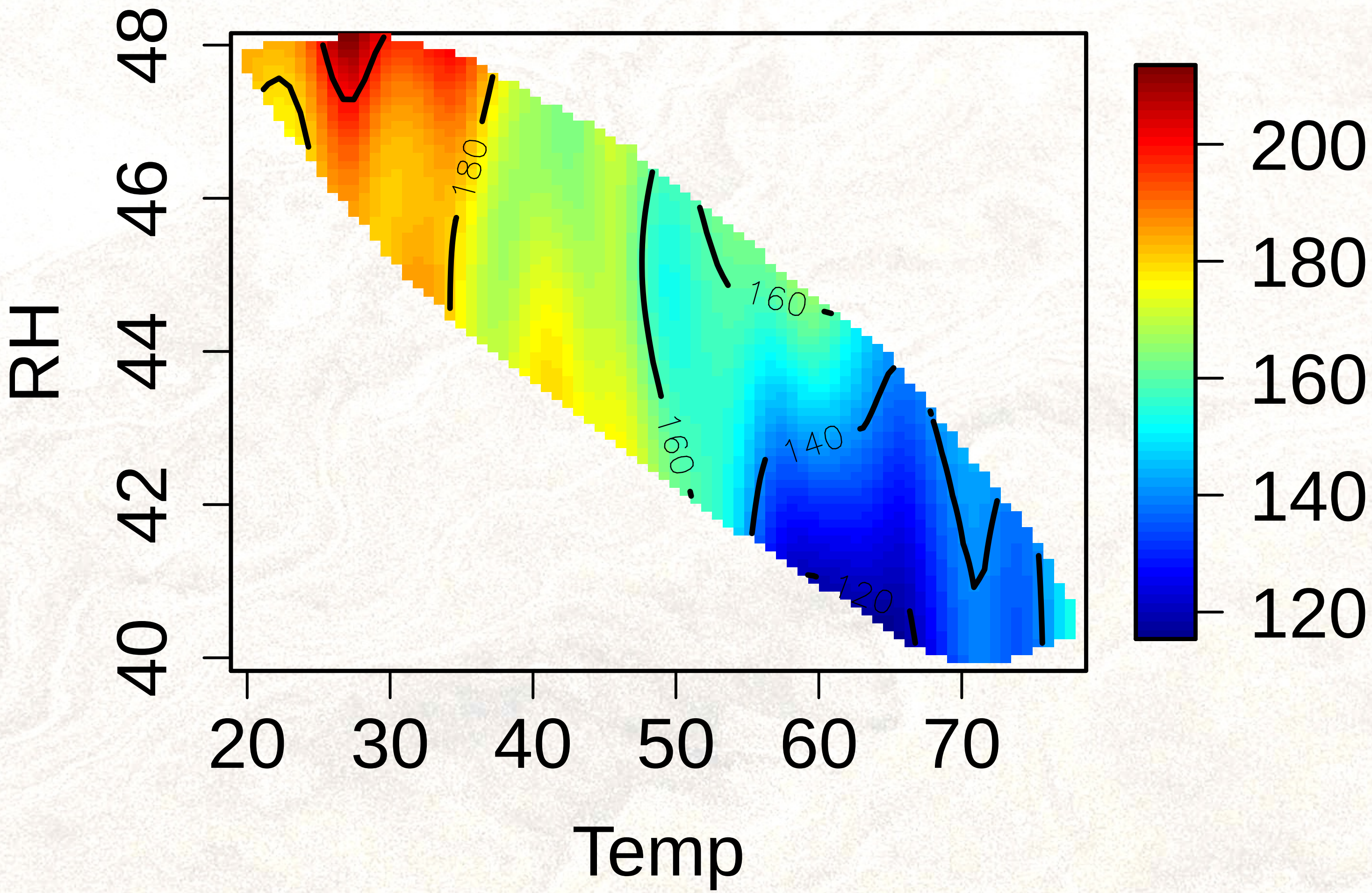
LatticeKrig package

```
# x and y are the power use data for the NCAR/WY  Supercomputing center

  fit<- LatticeKrig( x,y, NC=10, nlevel=4) # takes about 10 seconds
  print( fit)

  quilt.plot( x, fit$residuals)

  surface( fit, xlab="Temp", ylab="RH")

# Conditional simulation with fixed covariance parameters
#  50 draws 80X80 grid takes about 40 seconds

  simFit<- LKrig.sim.conditional( fit,  M=50)
```

print(fit)

```
 Call:
LatticeKrig(x = x, y = y, nlevel = 4, NC = 10)

 Number of Observations:                        1677
 Number of parameters in the fixed component 3
 Effective degrees of freedom (EDF)             32.2
    Standard Error of EDF estimate:             1.595
 MLE sigma                                      30.7
 MLE rho                                        21270
 MLE lambda = sigma^2/rho                       0.04432

Fixed part of model is a polynomial of degree 1 (m-1)
Basis function :  Radial
Basis function used:  WendlandFunction
Distance metric:  Euclidean

Lattice summary:
4  Level(s) 3112 basis functions with overlap of  2.5  (lattice units)

 Level Lattice points   Spacing
     1            240 6.5664444
     2            377 3.2832222
     3            752 1.6416111
     4           1743 0.8208056

Nonzero entries in Ridge regression matrix 357579
```

```
surface(fit, xlab="Temp", ylab="RH")
```



Final thoughts on the next steps

- Estimate parameters using score equations to avoid determinant

- Estimate parameters using cross validation.

Randomized trace Generalized Cross-Validation is amenable to iterative methods

- Parameter searching can be easily parallelized using `Rmpi`

Summary

- **Computational efficiency gained by compact basis functions and sparse roughness (precision) matrix.**

- **Multi-resolution can approximate standard covariance families (e.g. Matern)**

- **Easy to generate uncertainty measures.**

See `LatticeKrig` contributed package in R

Thank you!