Application: French Precipitation Data, and a few Miscellaneous Comments/Directions

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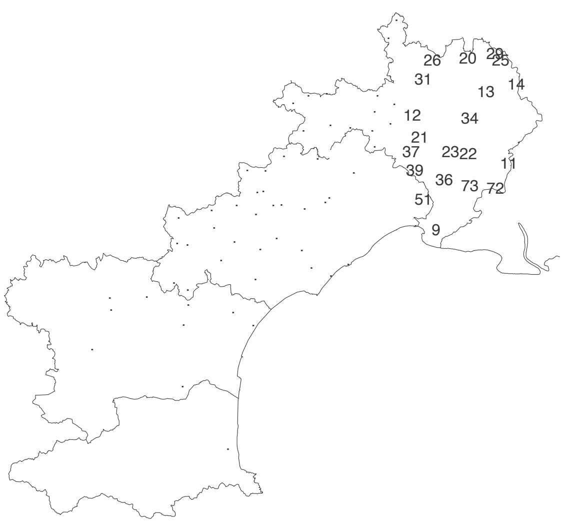
(Joint work with Peter Guttorp, Paul Sampson, Pascal Monestiez)



Environmental and ecological data usually exhibit dependence in space and time

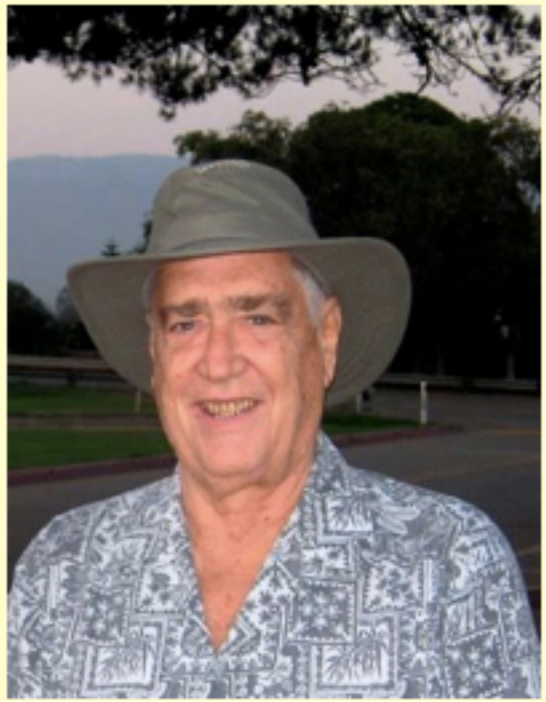
Aim: use this dependence to estimate/predict process of interest in space and time,

taking into account both small-scale space-time dependence, and large-scale space-time trends

Tobler's First Law of Geography

"Everything is related to everything else, but near things are more related than distant things."

Professor Waldo Tobler, UCSB Geography Dept

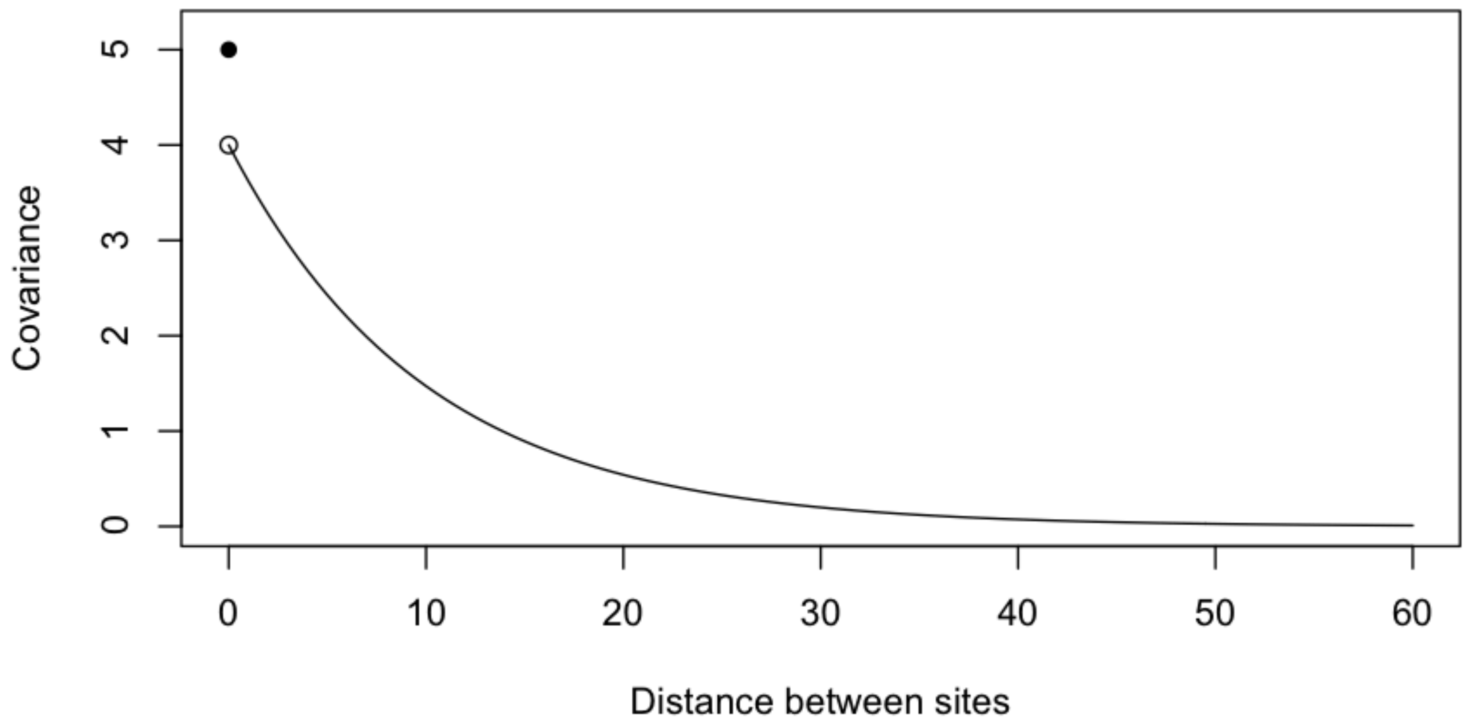


Source: ESRI online GIS dictionary
http://support.esri.com/es/knowledgebase/GISDictionary/term/Tobler's%20First%20Law%20of%20Geography

How can we model associations between observations at two spatial locations?

Frequently use spatial Covariance and Correlation (assuming finite variance field)

An example of an “isotropic” spatial covariance function: an exponential spatial covariance function with nugget



More generally - spatial variogram/structure function/spatial dispersion

Consider data $Z(x_i)$, N monitoring sites
Spatial dispersion between sites x_i and x_j

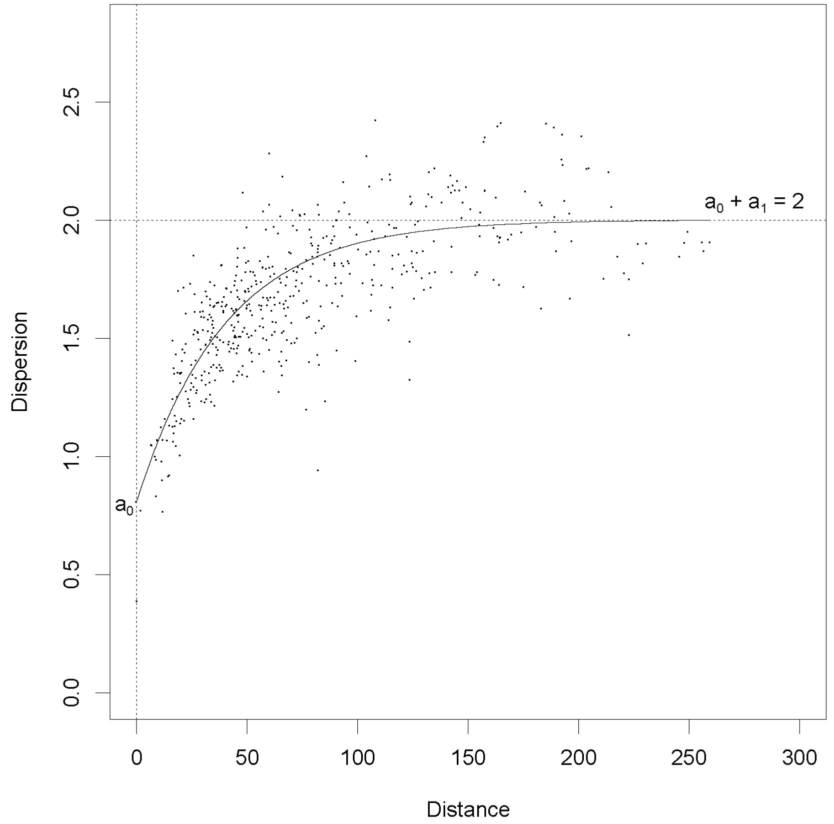
$$D(x_i, x_j) = \text{var}[Z(x_i) - Z(x_j)]$$

(Spatial variogram or structure function)

If spatial covariances exist, then standardizing by variance field gives

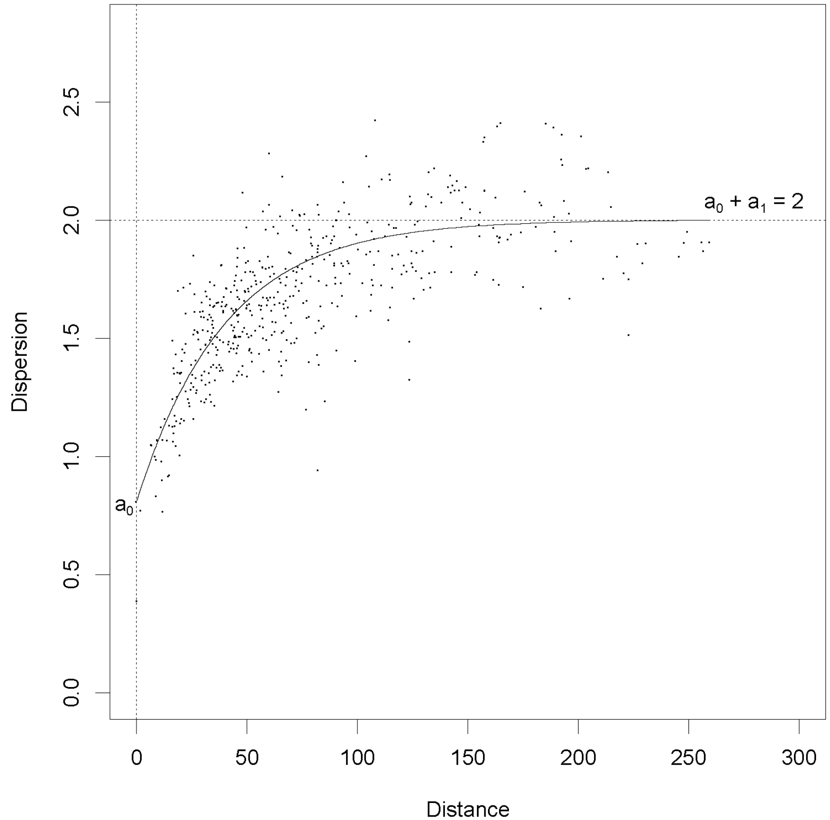
$$D(x_i, x_j) = 2(1 - \text{Corr}[Z(x_i), Z(x_j)])$$

An Exponential variogram (on a standardized scale) - an example of an isotropic model for spatial association



$$D(x_i, x_j) = \begin{cases} 0 & \text{if } h_{ij} = 0 \\ a_0 + a_1\{1 - \exp(-t_0\, h_{ij})\} & \text{if } h_{ij} > 0 \end{cases}$$

An Exponential variogram (on a standardized scale) - an example of an isotropic model for spatial association



Here spatial dependence only depends on the Euclidean distance between geographic locations.

$$D(x_i, x_j) = \begin{cases} 0 & \text{if } h_{ij} = 0 \\ a_0 + a_1 \{1 - \exp(-t_0 \, h_{ij})\} & \text{if } h_{ij} > 0 \end{cases}$$

Non-isotropic spatial covariance modeling

- A deformation approach. **Sampson-Guttorp approach**
- There are many other approaches – active development area. **Non-stationary covariance workshop**

My collaborations on deformation approach:

- Work with Peter Guttorp and Paul Sampson at U. Washington, Pascal Monestiez and Olivier Perrin in France.

Terminology and definitions

1. Consider data $Z(x_i, t)$

   N monitoring sites

   T time points. Independent in time.

(For simplicity in this talk, assume independence in time. Replications.)

2. Spatial dispersion between sites x_i and x_j

$$D\left(x_i, x_j\right) = \text{var}\left[Z(x_i, t) - Z(x_j, t)\right]$$

3. Sample estimates d^*_{ij}.

$$d^*_{ij} = s_{ii} + s_{jj} - 2s_{ij}$$

   where s_{ij} = sample covariance.

   Standardize to correlations.

$$d_{ij} = 2\left(1 - r_{ij}\right)$$

s_{ii} may vary in space. r_{ij} is the sample correlation.

- Consider

$$Z(x,t) \;=\; \mu(x,t) + E_{\tau}(x) + E_{\epsilon}(x,t)$$

- Model

$$d_{ij} \;=\; \gamma_{\theta}\left(\left\| x_i^* \;-\; x_j^* \right\| \right) + e_{ij}$$

Variogram is modeled as isotropic as a function of distance in the deformed space (in D-space)

γ_{θ} isotropic variogram.

$$w:\; \underbrace{\mathbf{R}^p}_{\text{G-space}} \;\rightarrow\; \underbrace{\mathbf{R}^d}_{\text{D-space}}, \qquad x_i^* = w(x_i).$$

- Spatial dispersions are stationary and isotropic in D-space.

- Consider

$$Z(x,t) \; = \; \mu(x,t) + E_{\tau}(x) + E_{\epsilon}(x,t)$$

- Model

$$d_{ij} \; = \; \gamma_{\theta}\left(\left\| x_i^* \; - \; x_j^* \right\| \right) + e_{ij}$$

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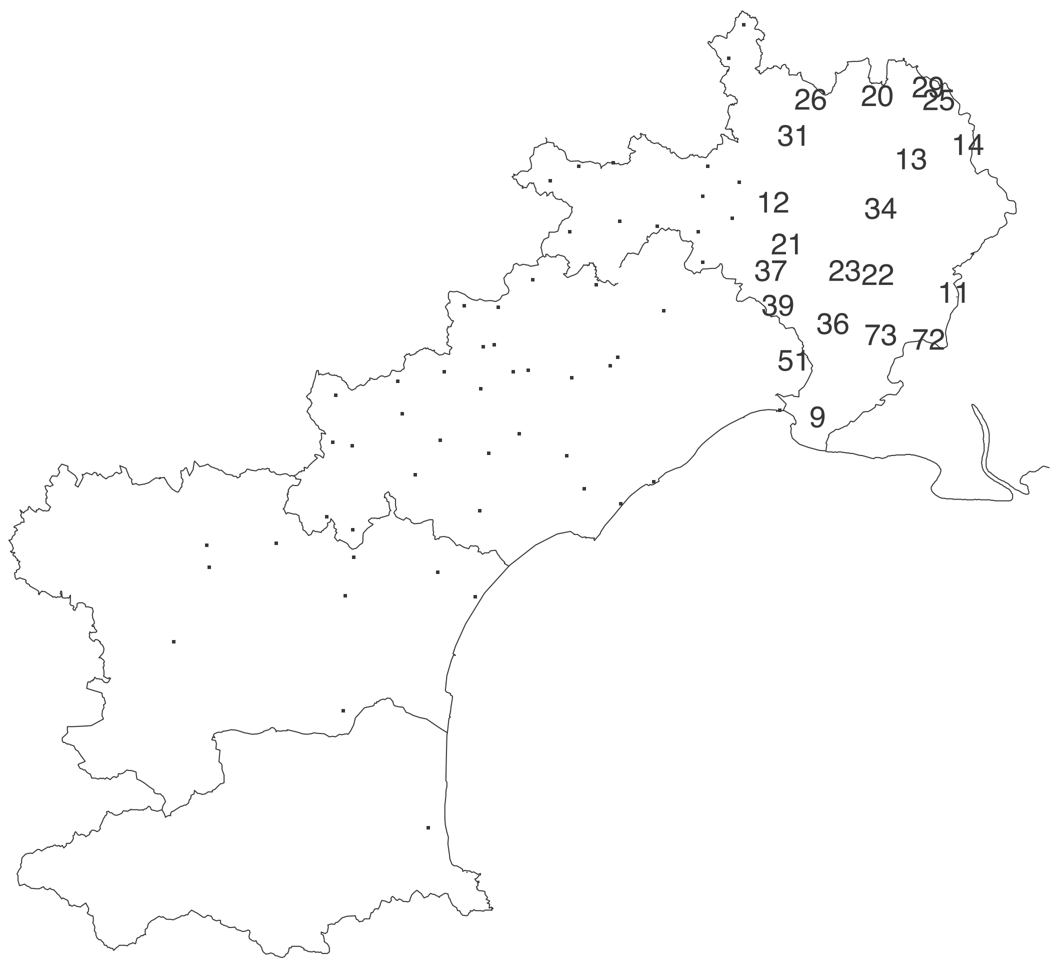
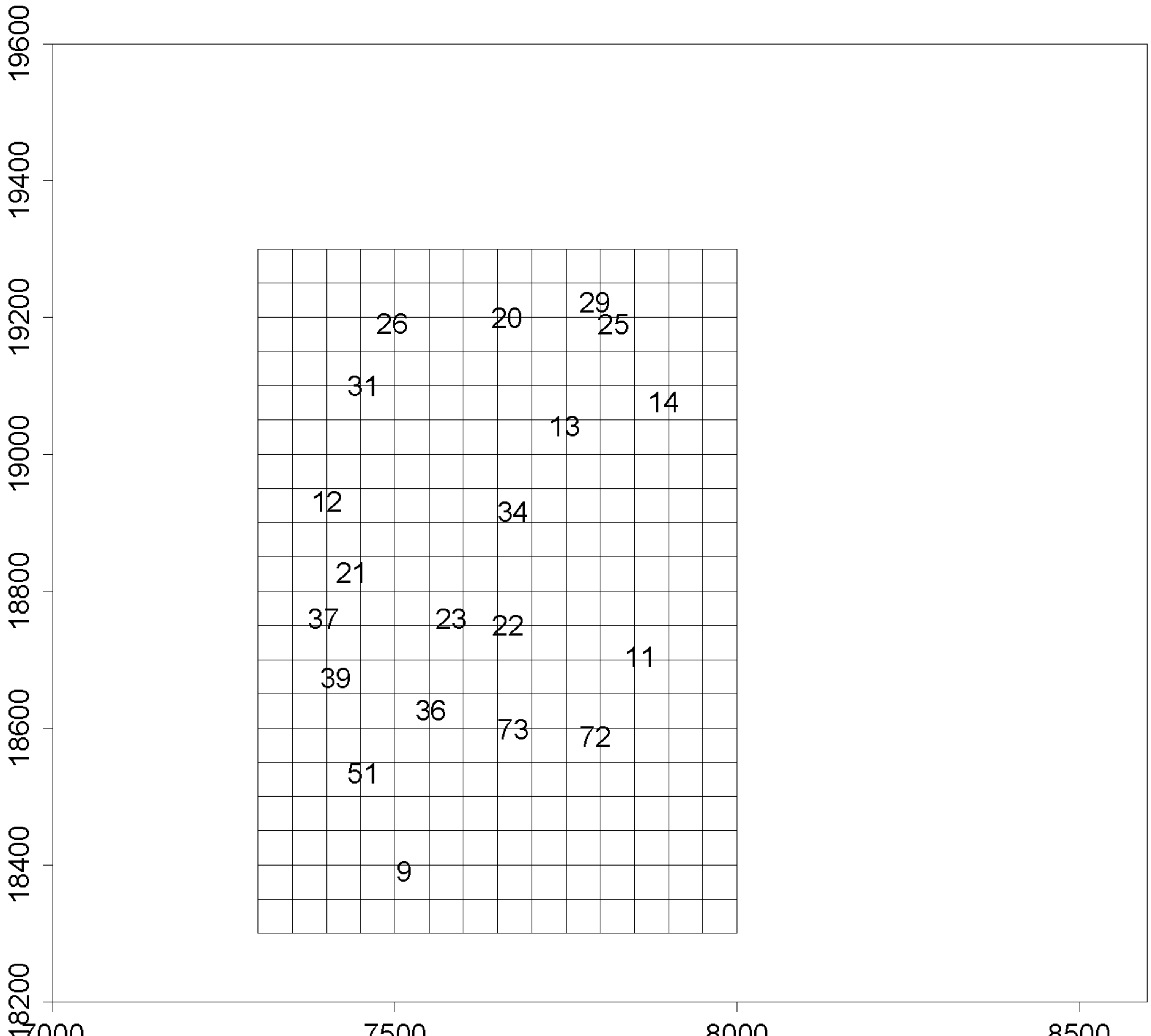
$$w: \underbrace{\mathbf{R}^p}_{\text{G-space}} \to \underbrace{\mathbf{R}^d}_{\text{D-space}}, \qquad x_i^* = w(x_i).$$

In this talk p=d=2

- Spatial dispersions are stationary and isotropic in D-space.

Network of Precipitation Monitoring Sites in France





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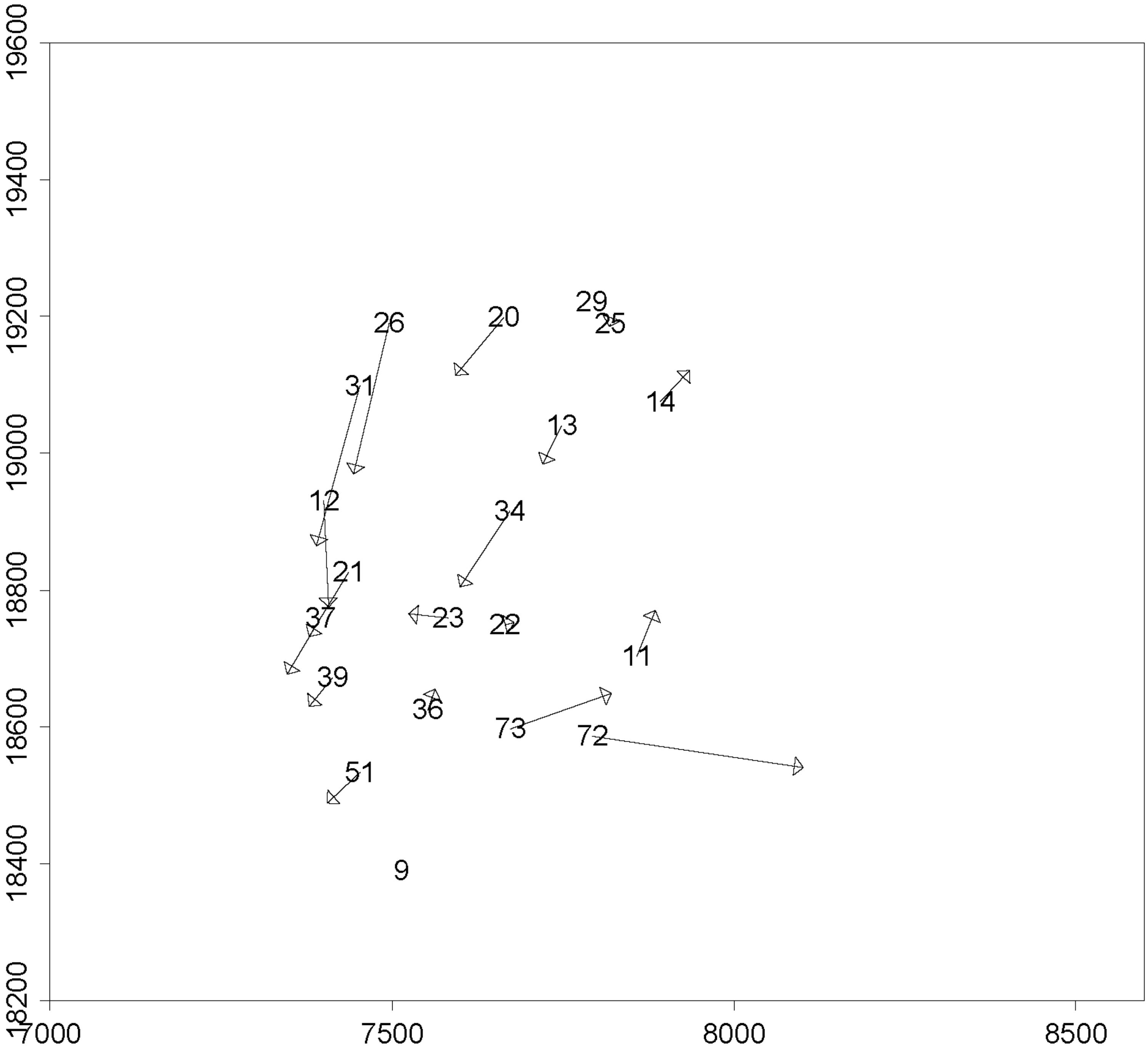

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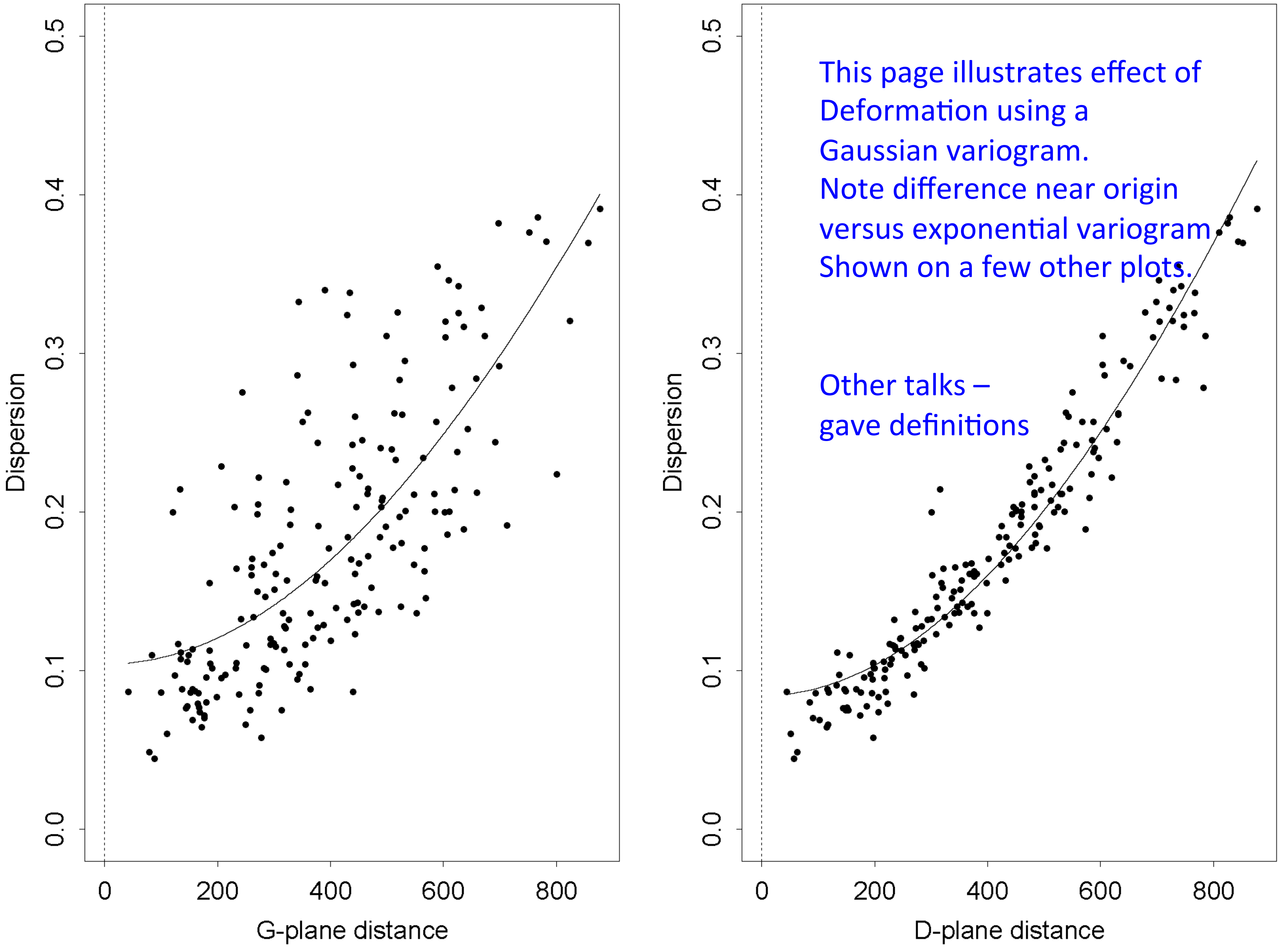
This page illustrates effect of Deformation using a Gaussian variogram.
Note difference near origin versus exponential variogram Shown on a few other plots.

Other talks – gave definitions



- Consider

$$Z(x,t) = \mu(x,t) + E_\tau(x) + E_\epsilon(x,t)$$

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$$d_{ij} = \gamma_\theta\left(\left\| x_i^* - x_j^* \right\| \right) + e_{ij}$$

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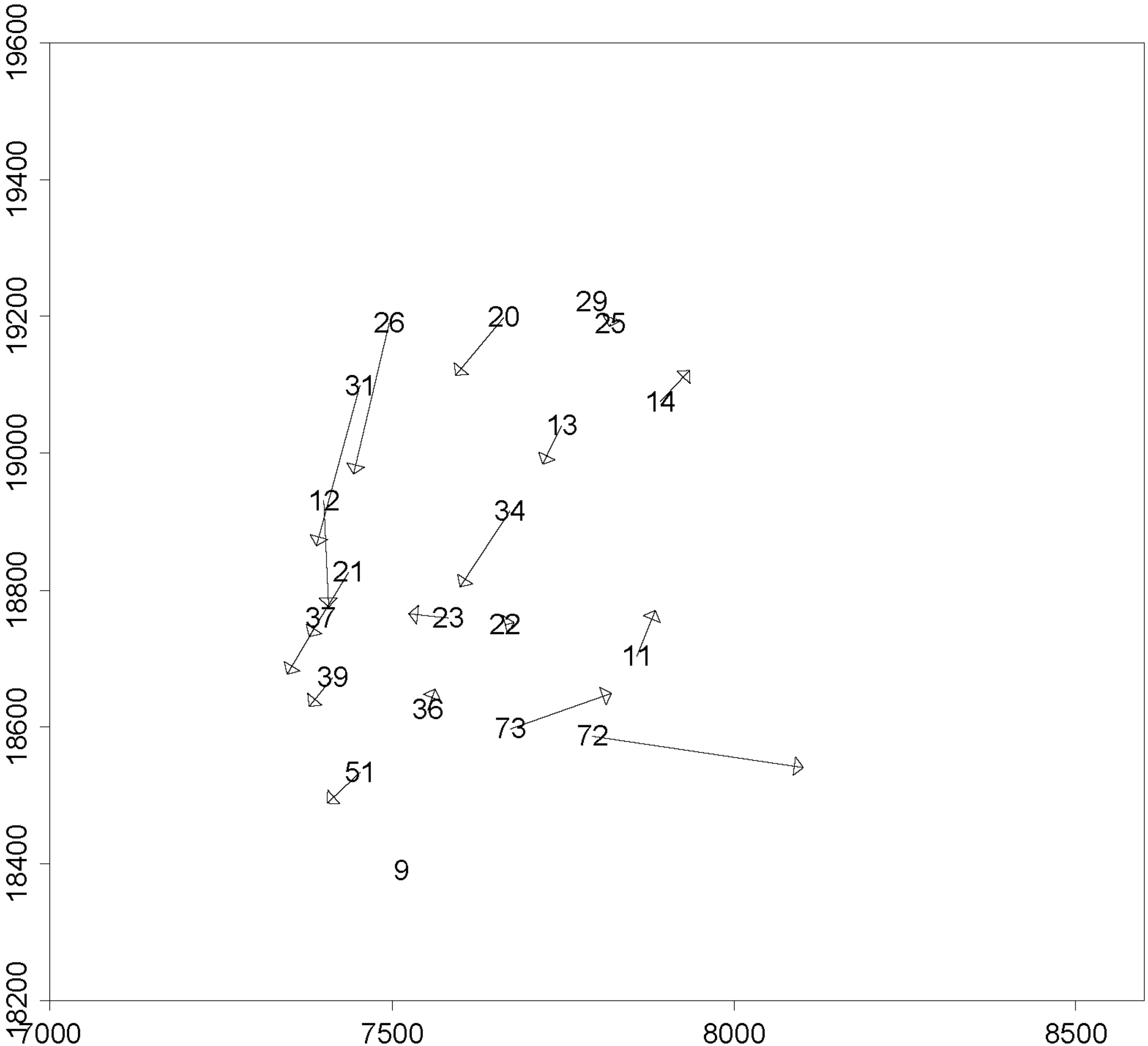
- Spatial dispersions are stationary and isotropic in D-space.



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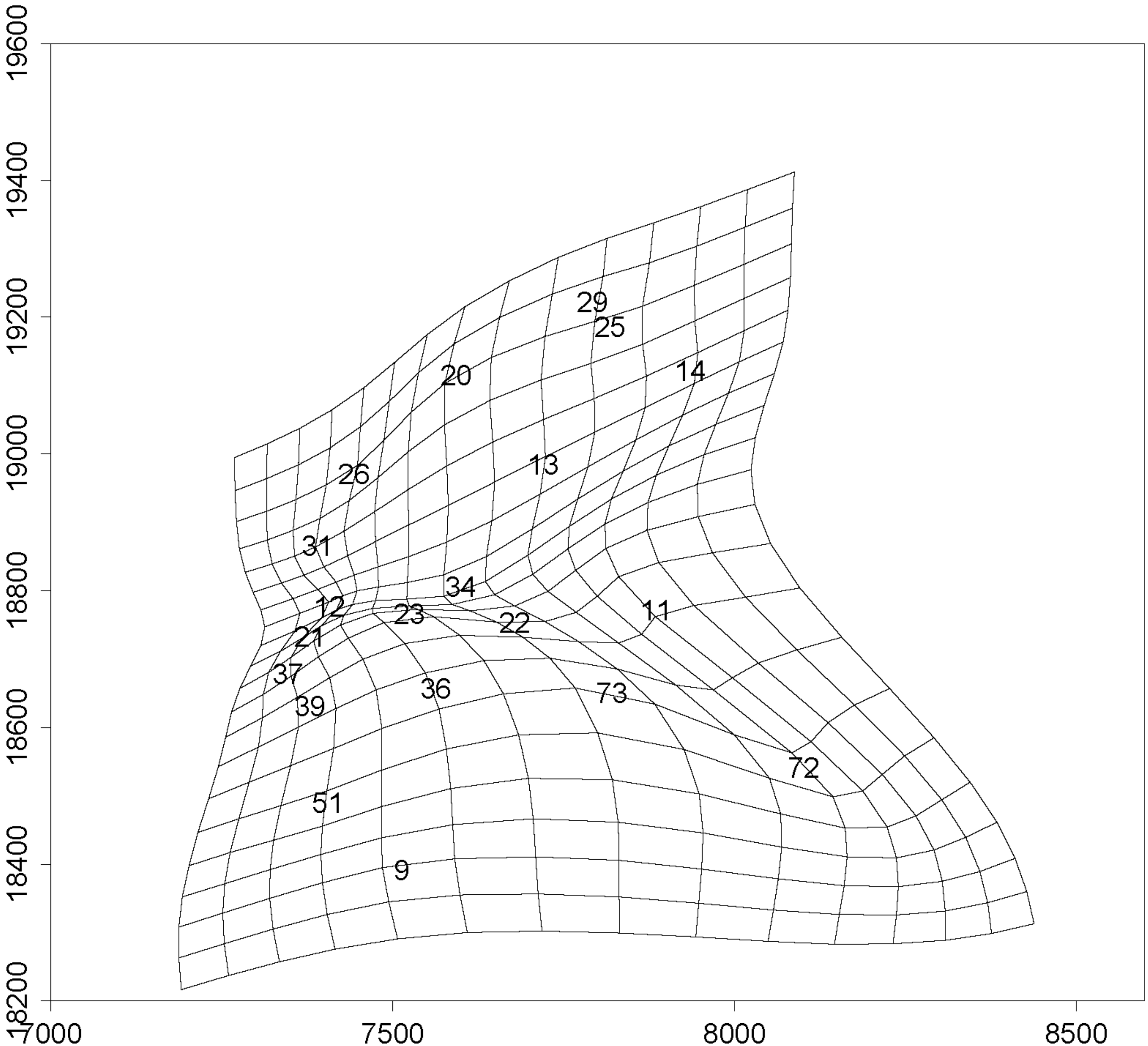
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$\mathbf{R}^2 \to \mathbf{R}^2$ deformations.

$$w(x,y) = (f_1(x,y), f_2(x,y))$$

f_1: $\mathbf{R}^2 \to \mathbf{R}$ thin-plate spline mapping.
f_2: $\mathbf{R}^2 \to \mathbf{R}$ thin-plate spline mapping.

$$f_i(x,y) \;=\; a + bx + cy + \sum_{j=1}^{N} \eta_j\, h_j^2 \log\left(h_j^2\right)$$

where

$$h_j \;=\; \left\|\left(x_j, y_j\right) - (x\ , y)\right\|$$

Wahba (1991).
Spline models for observational data.

Estimation decisions, Including penalized weighted least squares optimization Criterion.

Other approaches: variants on Penalized likelihood (Paul Sampson's talk)

- Choose form of variogram γ_θ.
- Transformation map and variogram parameters chosen to minimize

$$\sum_{j=2}^{N} \sum_{i=1}^{j-1} \left[\frac{d_{ij} - \widehat{d_{ij}}}{\widehat{d_{ij}}} \right]^2 + \lambda \, \mathrm{BEP},$$

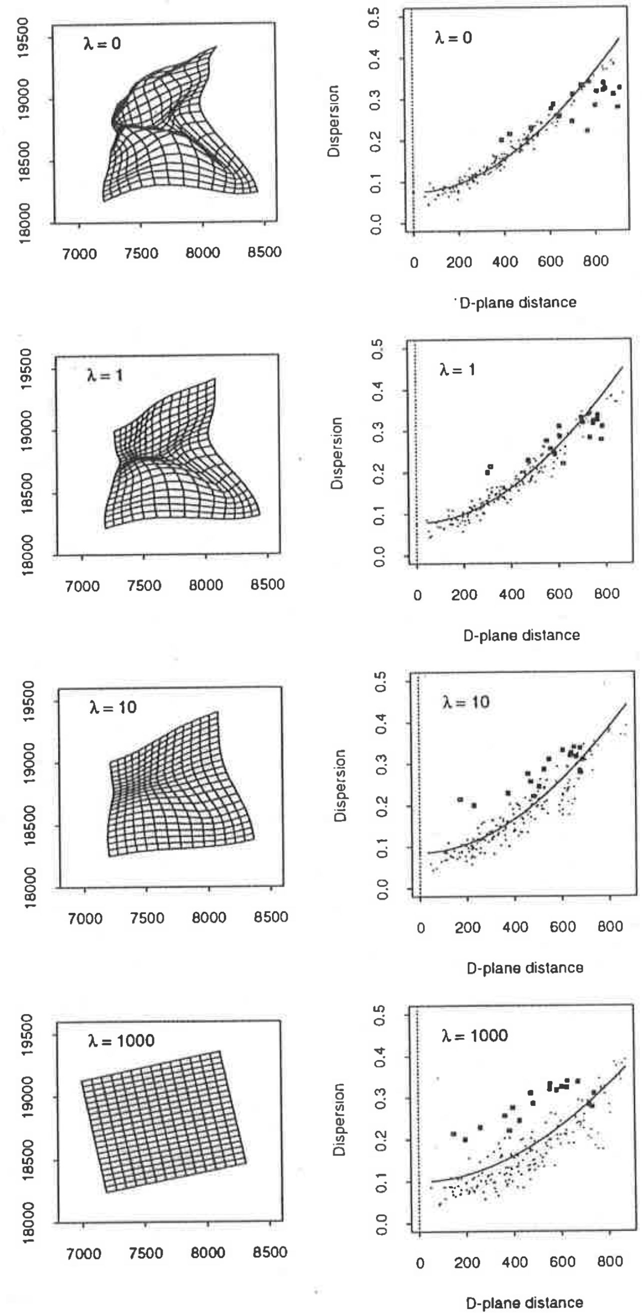
where $\widehat{d_{ij}} = \gamma_{\hat{\theta}}\left(\left\| x_i^* - x_j^* \right\| \right)$, and BEP is the sum of the bending energies for the two thin-plate spline mappings.

- Choice of λ.

  For $\lambda = 0$, overfitting, folding.

  As $\lambda \to \infty$, homogeneous model.

  Cross-validation (Monestiez et al. 1993).


λ = 0
λ = 1
λ = 10
λ = 1000
7000 7500 8000 8500
18000 18500 19000 19500
Dispersion
0.0 0.1 0.2 0.3 0.4 0.5
0 200 400 600 800
D-plane distance

$\mathbf{R}^2 \to \mathbf{R}^2$ deformations.

$$w(x,y) = (f_1(x,y), f_2(x,y))$$

f_i: $\mathbf{R}^2 \to \mathbf{R}$ thin-plate spline mapping,
$i = 1, 2.$

$$\mathbf{u} = (f_1(x_1), \ldots, f_1(x_N)),$$

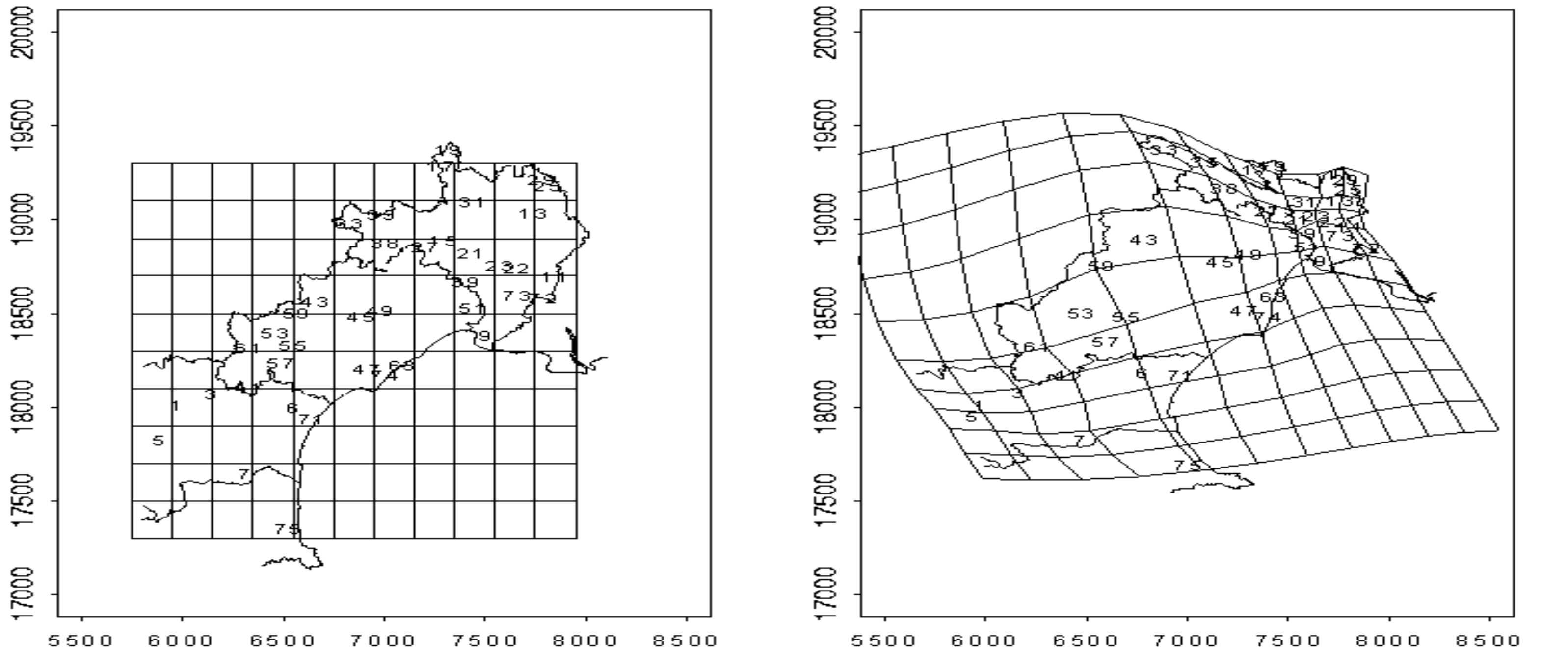
$$\mathbf{v} = (f_2(x_1), \ldots, f_2(x_N))$$

$$\text{BEP} = \mathbf{u}'\mathbf{B}\mathbf{u} + \mathbf{v}'\mathbf{B}\mathbf{v}$$

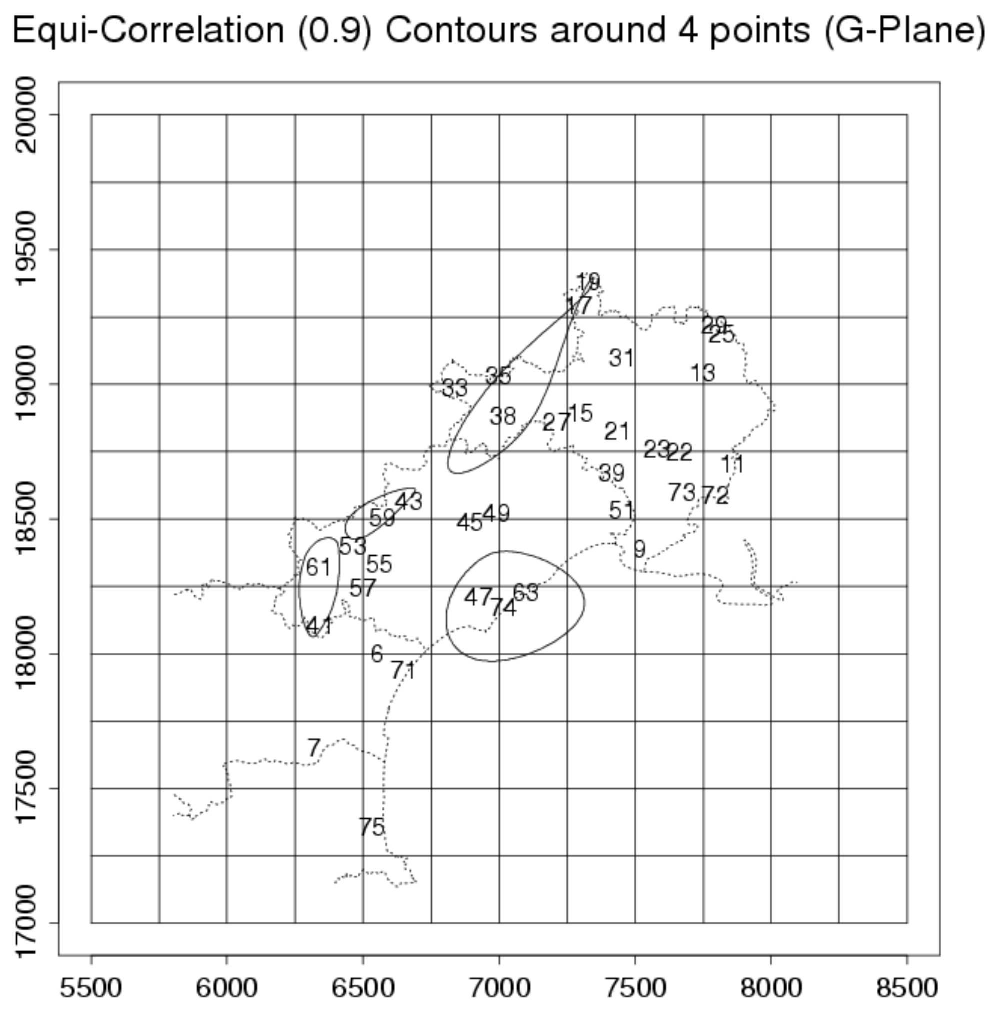
B depends only on geographic locations of monitoring sites.

$$\mathbf{u}'\mathbf{B}\mathbf{u} \propto \int_{\Re^2} \left[\left(\frac{\partial^2 f_1}{\partial x^2} \right) + 2 \left(\frac{\partial^2 f_1}{\partial x \partial y} \right)^2 + \left(\frac{\partial^2 f_1}{\partial y^2} \right) \right] dx\, dy$$

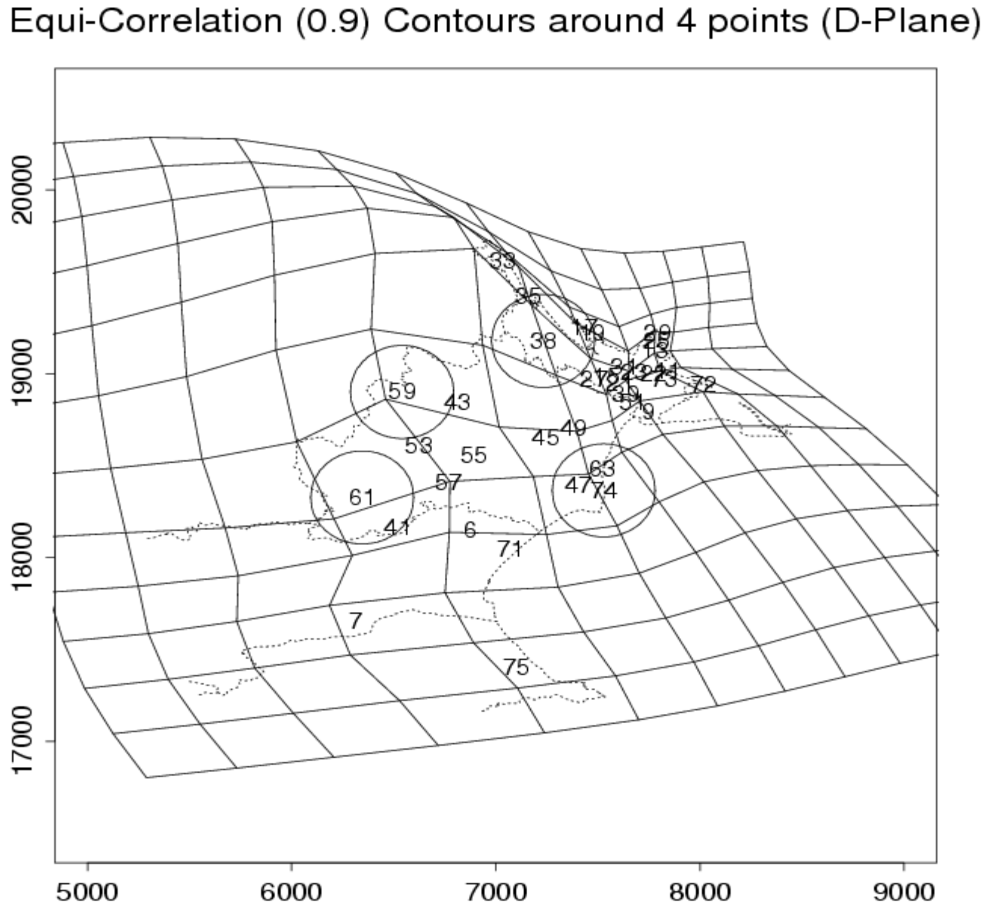
Fig. 7: Precipitation in Southern France -
an example of a non-linear deformation



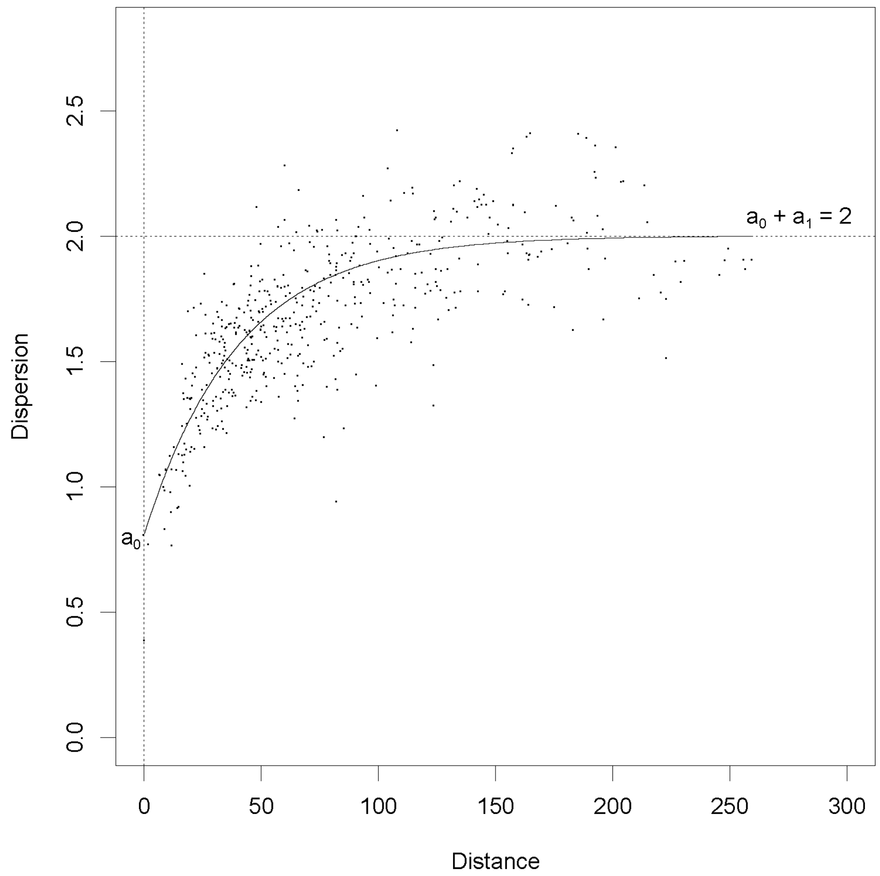
G-plane Equicorrelation Contours



D-plane Equicorrelation Contours



Exponential variogram - an example of an isotropic model for spatial association



$$D(x_i, x_j) = \begin{cases} 0 & \text{if } h_{ij} = 0 \\ a_0 + a_1 \{1 - \exp(-t_0\ h_{ij})\} & \text{if } h_{ij} > 0 \end{cases}$$

Cross-validation choice of λ

Omit each monitoring site x_i in turn.

For each λ, $\hat{w}_{i\lambda}$ and $\gamma_{\hat{\theta}_{i\lambda}}$ found.

λ chosen to minimize

$$\sum_{i\in\mathcal{N}}\sum_{j\in\mathcal{N}-\{i\}}\left(\frac{d_{ij}-\gamma_{\hat{\theta}_{i\lambda}}\left(\left\|\hat{w}_{i\lambda}(x_i)-\hat{w}_{i\lambda}(x_j)\right\|\right)}{\gamma_{\hat{\theta}_{i\lambda}}\left(\left\|\hat{w}_{i\lambda}(x_i)-\hat{w}_{i\lambda}(x_j)\right\|\right)}\right)^2$$

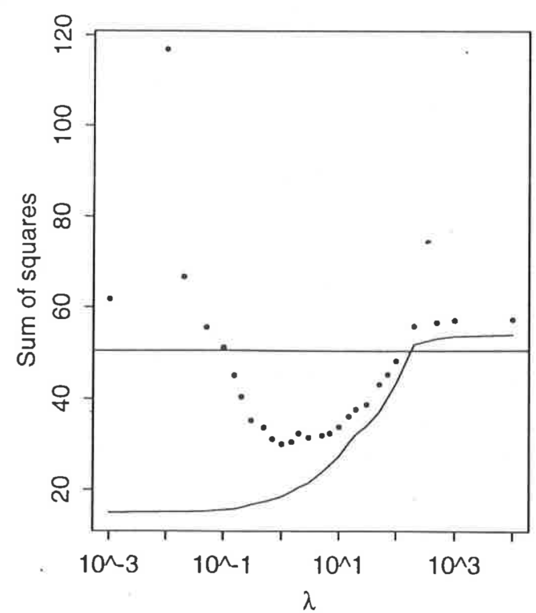


Figure based on a Simulation study.

Estimation decisions, Including penalized weighted least squares optimization Criterion.

Other approaches: variants on Penalized likelihood (Paul Sampson's talk)

EnviroStat – currently Uses penalized least squares

- Choose form of variogram γ_θ.
- Transformation map and variogram parameters chosen to minimize

$$\sum_{j=2}^{N} \sum_{i=1}^{j-1} \left[\frac{d_{ij} - \widehat{d_{ij}}}{\widehat{d_{ij}}} \right]^2 + \lambda \text{ BEP},$$

where $\widehat{d_{ij}} = \gamma_{\hat{\theta}}\left(\left\| x_i^* - x_j^* \right\| \right)$, and BEP is the sum of the bending energies for the two thin-plate spline mappings.

- Choice of λ.

For $\lambda = 0$, overfitting, folding.

As $\lambda \to \infty$, homogeneous model.

Cross-validation (Monestiez et al. 1993).

Optimization

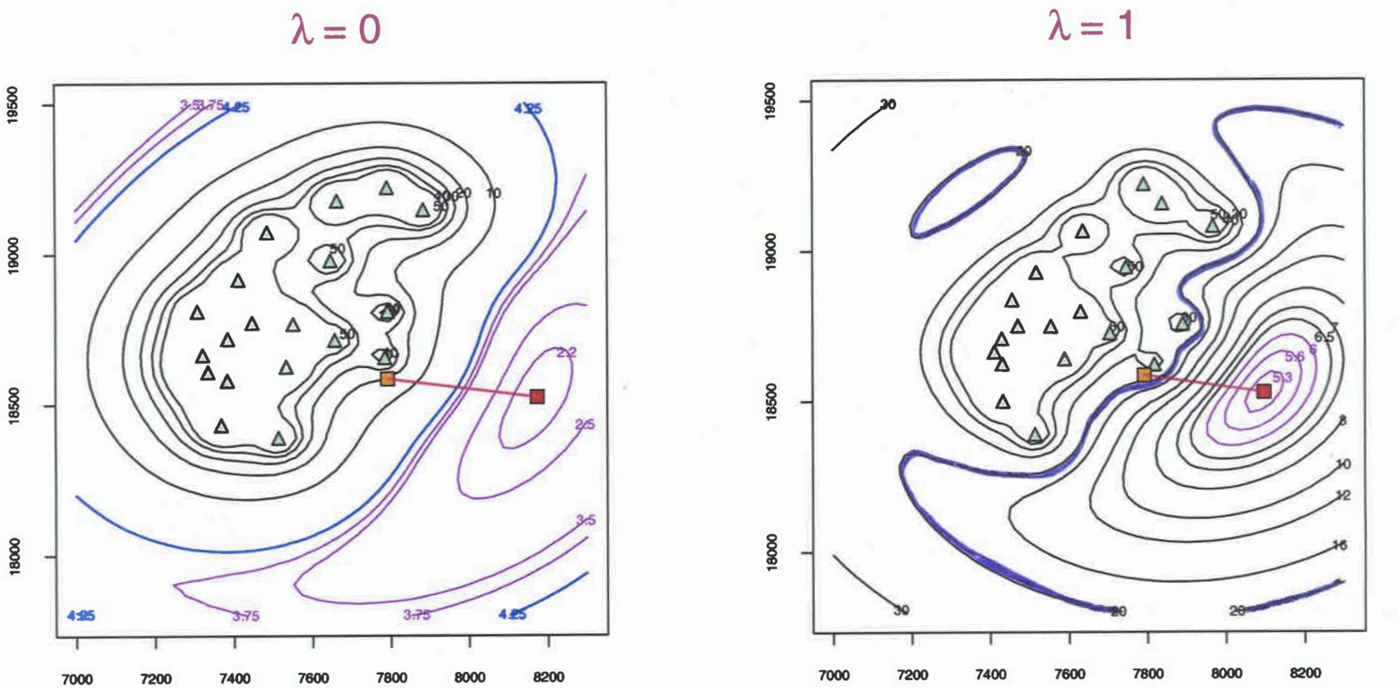
- **Alternating algorithm:**
  - Parameter estimation for D-space variogram
  - Estimation of D-space locations of monitoring sites

  N sites $\Longrightarrow$ **2N-4 dimensions**

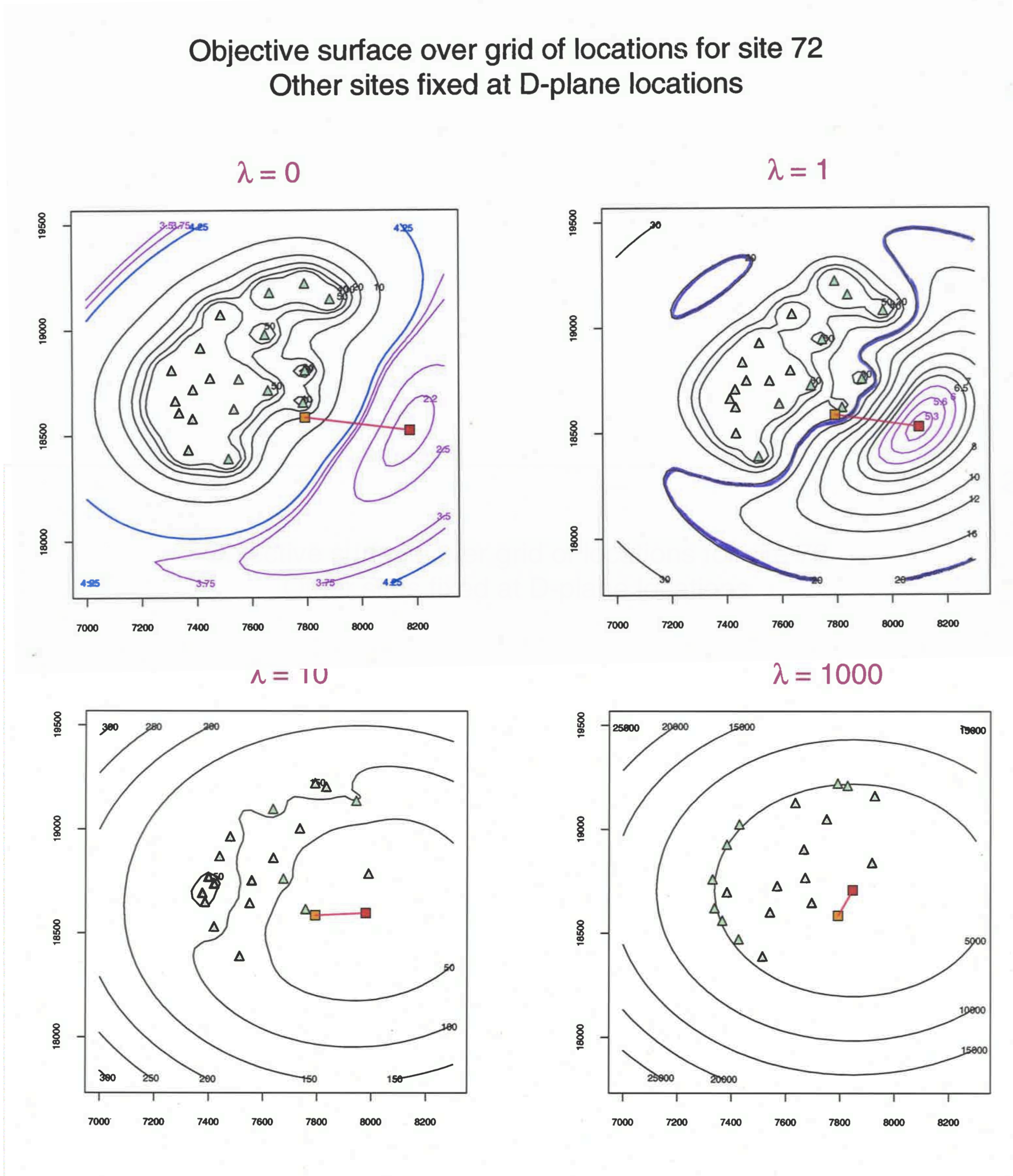
- **Scaling of coordinates**
  - Calculation of BEP
  - **Similar scales for optimization over variogram parameters**

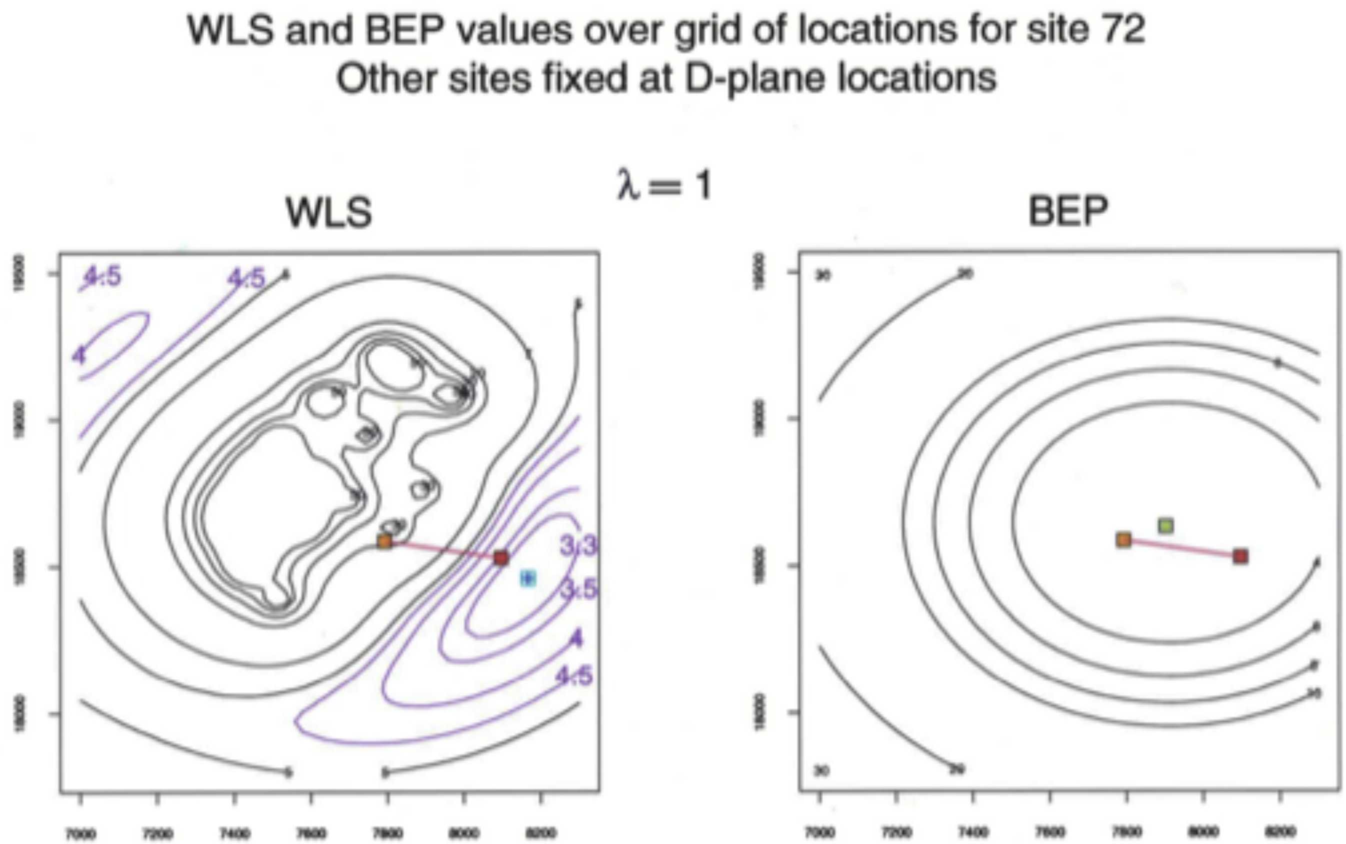
- **Starting values**
  - Locations (start at geographic locations)
  - Variogram parameters

Objective surface over grid of locations for site 72
Other sites fixed at D-plane locations



Complexity of the
Optimization
Surface decreases
As λ increases





Orange - G-plane location

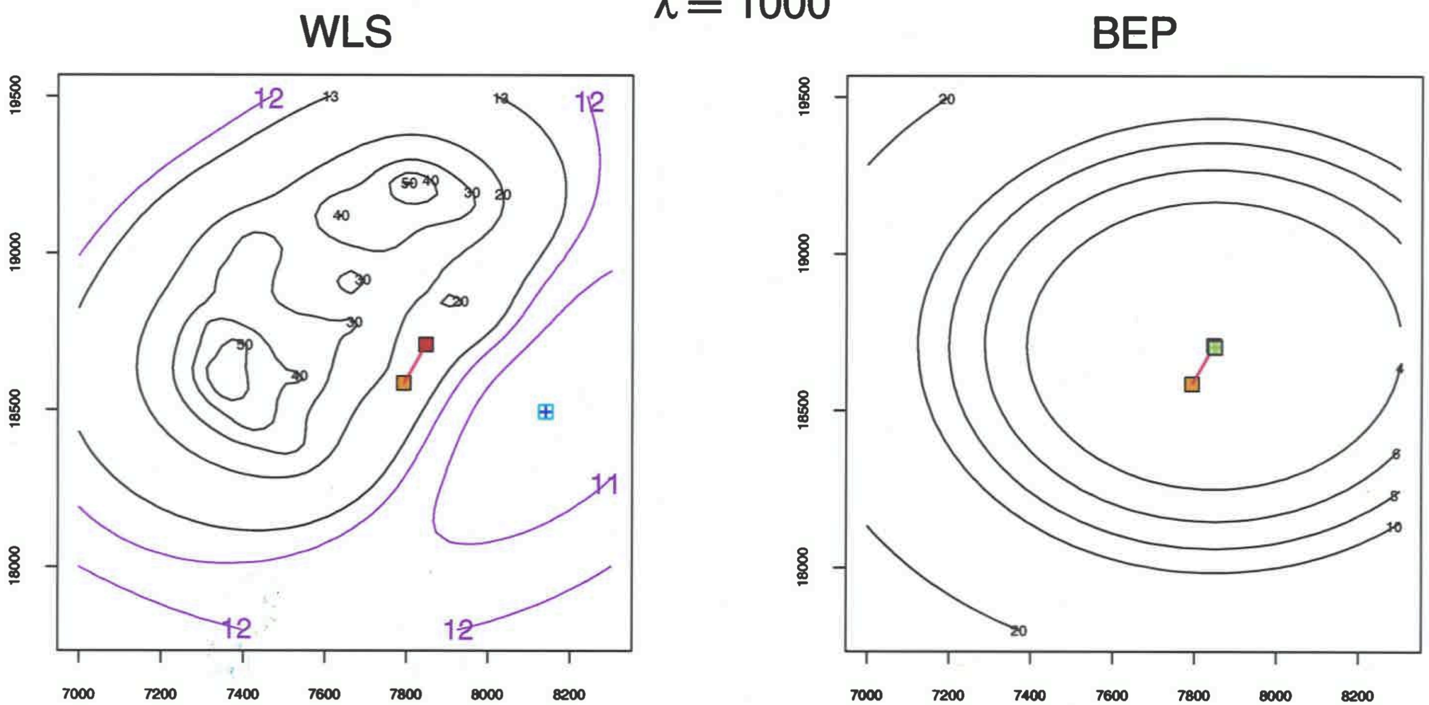
Red - D-plane location

Blue – minimizes WLS term (left)

Green – minimizes BEP term (right)

WLS and BEP values over grid of locations for site 72
Other sites fixed at D-plane locations

$\lambda = 1000$



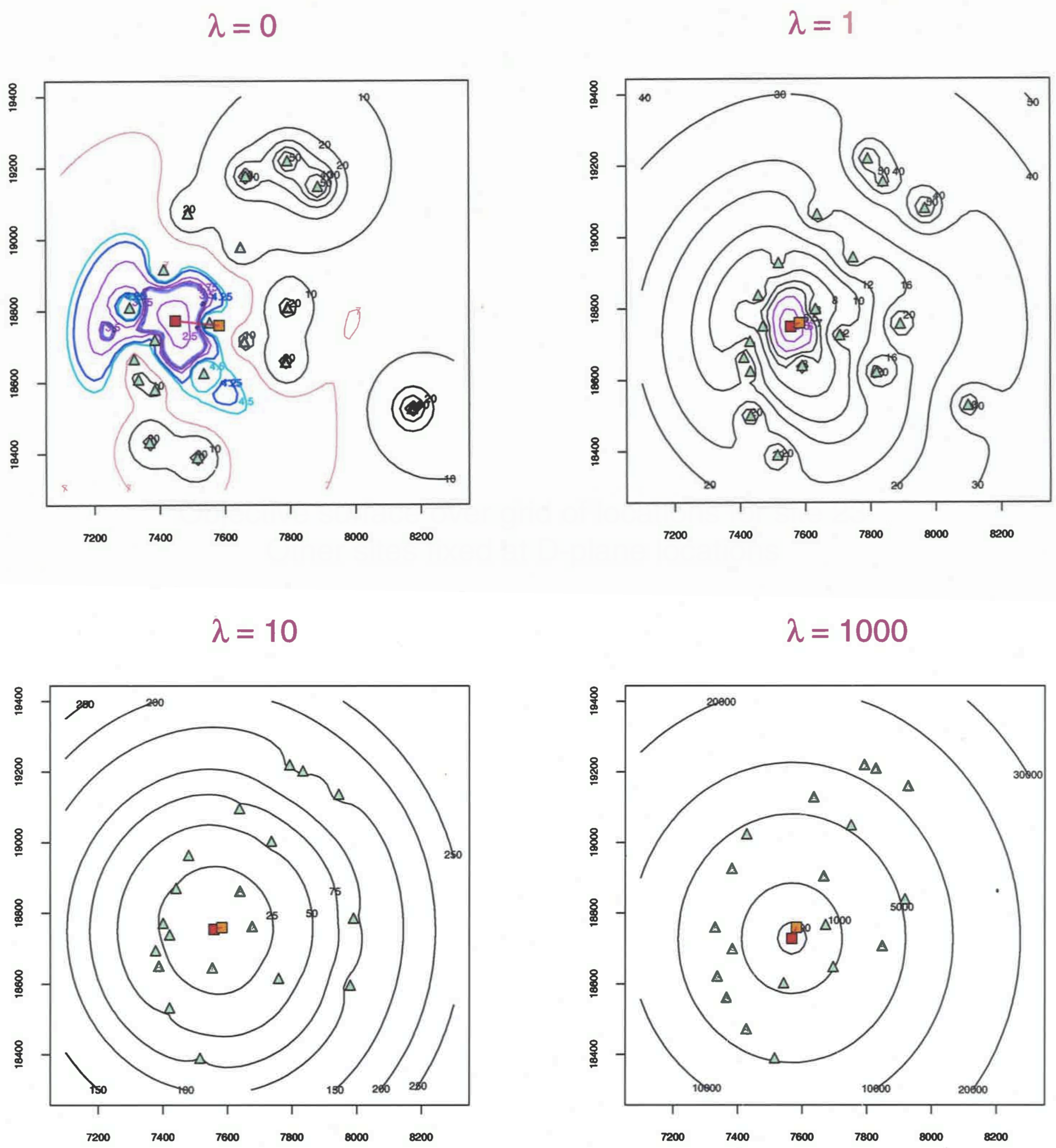
Orange - G-plane location

Red - D-plane location

Blue – minimizes WLS term (left)

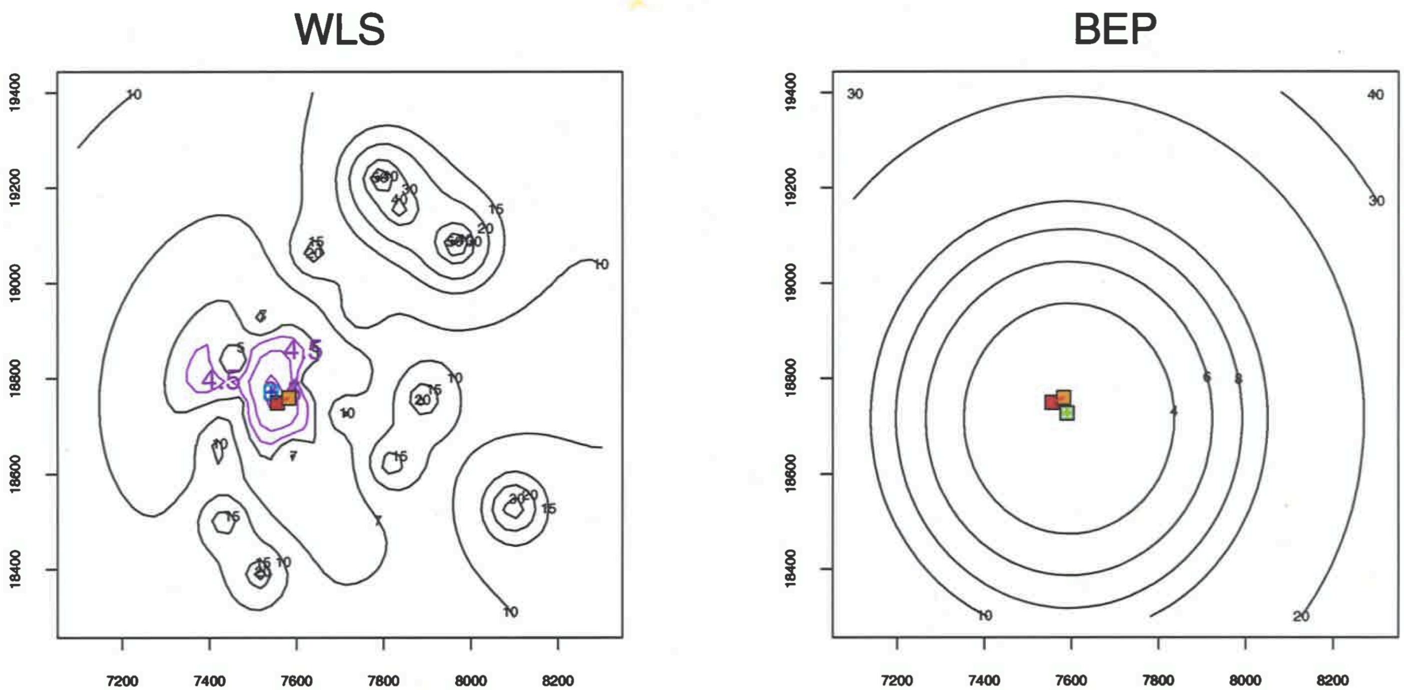
Green – minimizes BEP term (right)

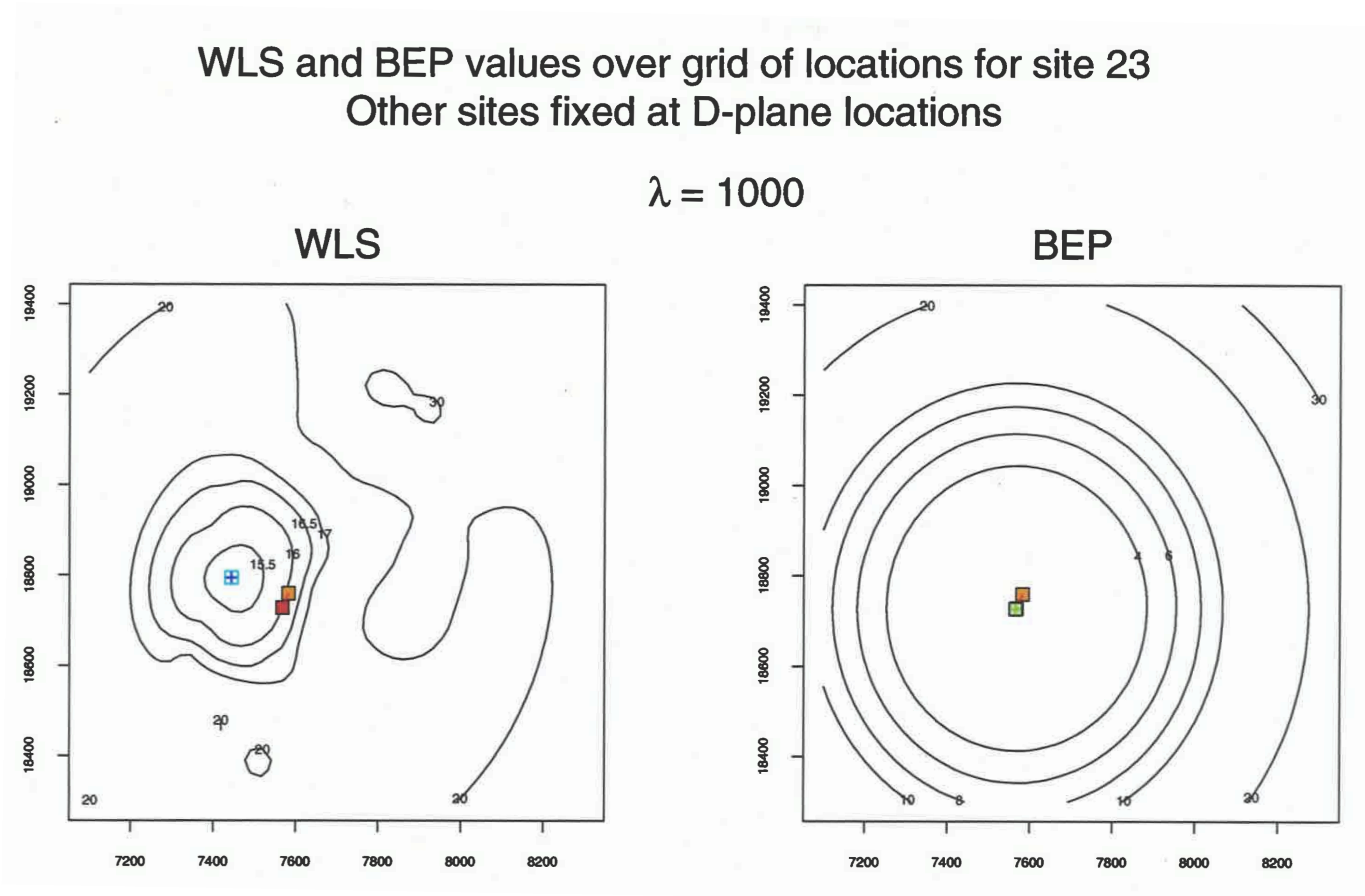
Objective surface over grid of locations for site 23
Other sites fixed at D-plane locations



WLS and BEP values over grid of locations for site 23
Other sites fixed at D-plane locations

$\lambda = 1$





Complexity of the optimization surface decreases as λ increases

Universal Kriging:
(here using s as spatial location instead of x)
Suppose

$$
\begin{aligned}
Z(\boldsymbol{s}) &= \sum_{j=1}^{p+1} f_{j-1}(\boldsymbol{s})\beta_{j-1} + \delta(\boldsymbol{s}), \qquad \boldsymbol{s} \in D. \\
\text{i.e.,} \quad \boldsymbol{Z} &= F\boldsymbol{\beta} + \boldsymbol{\delta}
\end{aligned}
$$

where

$$
\boldsymbol{Z} = \begin{bmatrix} \boldsymbol{Z}(\boldsymbol{s}_1) \\ \vdots \\ \boldsymbol{Z}(\boldsymbol{s}_n) \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \vdots \\ \beta_p \end{bmatrix}, \quad \text{and}
$$

$$
F = \begin{bmatrix} f_0(\boldsymbol{s}_1) & f_1(\boldsymbol{s}_1) & \dots & f_p(\boldsymbol{s}_1) \\ f_0(\boldsymbol{s}_2) & f_1(\boldsymbol{s}_2) & \dots & f_p(\boldsymbol{s}_2) \\ & & \vdots & \\ f_0(\boldsymbol{s}_n) & f_1(\boldsymbol{s}_n) & \dots & f_p(\boldsymbol{s}_n) \end{bmatrix}_{n\times(p+1)} .
$$

Known functions $\{f_0(\boldsymbol{s}), \dots, f_p(\boldsymbol{s})\}$.
Unknown parameters: $\boldsymbol{\beta} = (\beta_0, \dots, \beta_p)' \in \Re^{p+1}$.
$\delta(.)$ is a spatial residual process.

Aim: Predict $Z(\boldsymbol{s}_0) = \boldsymbol{f}'\boldsymbol{\beta} + \delta(\boldsymbol{s}_0)$ where
$\boldsymbol{f} = (f_0(\boldsymbol{s}_0), \dots, f_p(\boldsymbol{s}_0))'$.

Special case: Second order polynomial trend in $\Re^2$:

For $\boldsymbol{s} = (x, y)$,

$$\mu(\boldsymbol{s}) = a_{00} + a_{10}x + a_{01}y + a_{20}x^2 + a_{11}xy + a_{02}y^2$$

$$\begin{aligned} f_0(\boldsymbol{s}) &= 1 \\ f_1(\boldsymbol{s}) &= x \\ f_2(\boldsymbol{s}) &= y \\ f_3(\boldsymbol{s}) &= x^2 \\ f_4(\boldsymbol{s}) &= xy \\ f_5(\boldsymbol{s}) &= y^2 \end{aligned}$$

Minimize the mean square prediction error, subject to the uniform unbiasedness constraint.

mse

$$\begin{aligned}
&= E\left[\left(p\left(Z,\boldsymbol{s}_0\right)-Z\left(\boldsymbol{s}_0\right)\right)^2\right] \\
&= \mathrm{Var}\left(p\left(Z,\boldsymbol{s}_0\right)-Z\left(\boldsymbol{s}_0\right)\right)+\left[E\left(p\left(Z,\boldsymbol{s}_0\right)-Z\left(\boldsymbol{s}_0\right)\right)\right]^2. \\
&= \mathrm{Var}\left[\sum_{i=1}^{n}\lambda_i Z\left(\boldsymbol{s}_i\right)-Z\left(\boldsymbol{s}_0\right)\right] \\
&\quad +\left[E\left(\sum_{i=1}^{n}\lambda_i Z\left(\boldsymbol{s}_i\right)-Z\left(\boldsymbol{s}_0\right)\right)\right]^2
\end{aligned}$$

Minimizing the mse subject to the unbiasedness constraint is equivalent to minimizing

$$\begin{aligned}
Q &= E\left[\left(p\left(Z,\boldsymbol{s}_0\right)-Z\left(\boldsymbol{s}_0\right)\right)^2\right] \\
&\quad -2\sum_{j=1}^{p+1} m_{j-1}\left\{\sum_{i=1}^{n}\lambda_i f_{j-1}\left(\boldsymbol{s}_i\right)-f_{j-1}\left(\boldsymbol{s}_0\right)\right\}
\end{aligned}$$

with respect to $\lambda_1,\ldots,\lambda_n$, and $m_0,\ldots,m_p$

$$\begin{aligned}
\boldsymbol{\lambda}' &= \left\{\boldsymbol{c}+F(F'\Sigma^{-1}F)^{-1}\left(\boldsymbol{f}-F'\Sigma^{-1}\boldsymbol{c}\right)\right\}'\Sigma^{-1} \\
\boldsymbol{m}' &= \left(\boldsymbol{f}-F'\Sigma^{-1}\boldsymbol{c}\right)'\left(F'\Sigma^{-1}F\right)^{-1}
\end{aligned}$$

Universal kriging

Suppose $$Z(x) = \sum_{j=1}^{p+1} f_{j-1}(x)\beta_{j-1} + \delta(x),$$

for x in the region of interest D.

Assume $\{f_0(x), f_1(x), \ldots, f_p(x)\}$ are known functions of x, or of a related quantity at site x.

Suppose $\{\beta_0, \ldots, \beta_p\}$ are unknown,

$E[\delta(x)] = 0$ and $\delta(.)$ has known variogram $2\gamma(.)$.

Then there is a unique estimator of the form

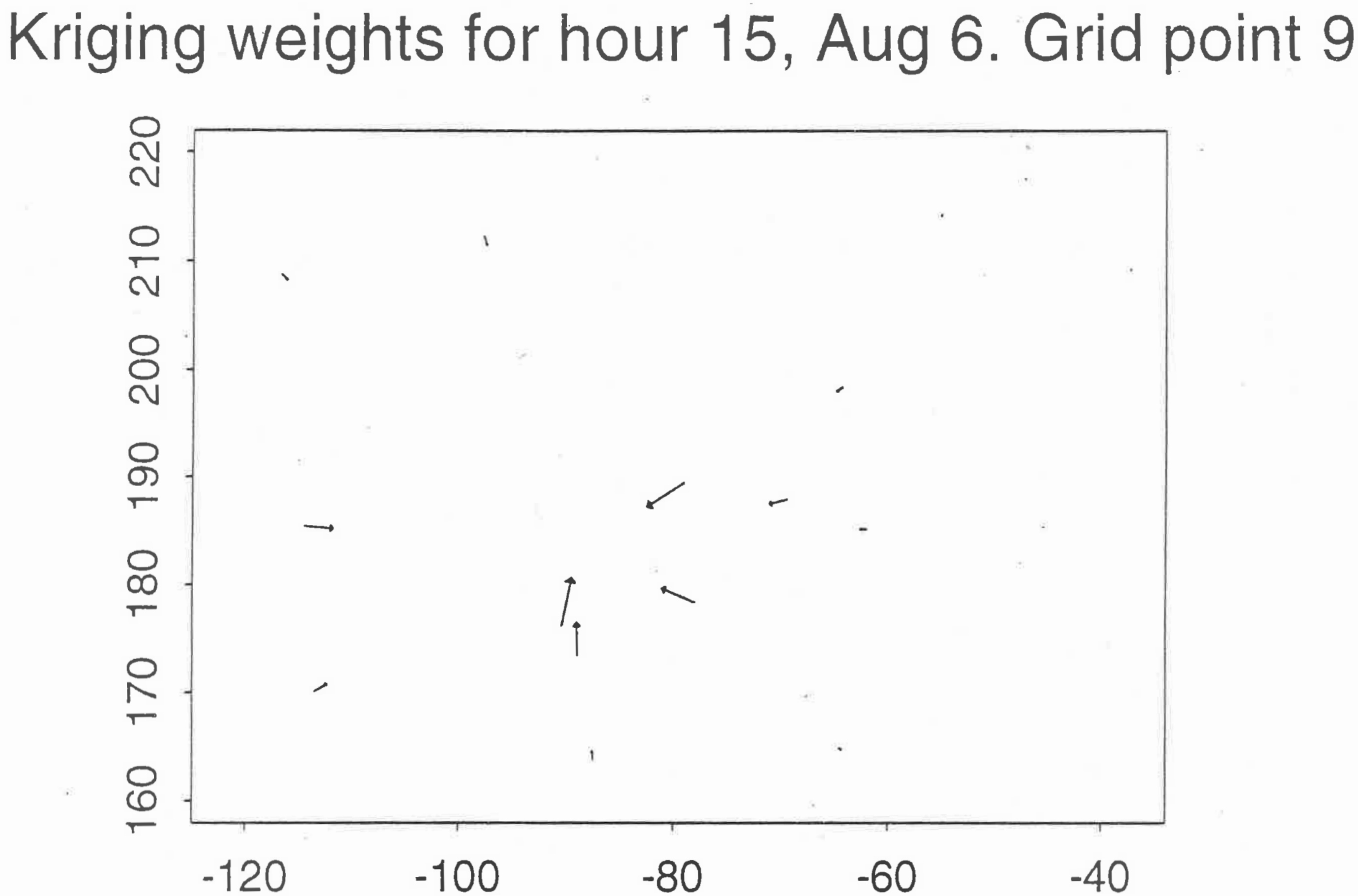
$$\hat{Z}(x_0) = \sum_{i=1}^{n} \lambda_i Z(x_i)$$

that minimizes the mean-square prediction error subject to an unbiasedness constraint on $\{\lambda_1, \ldots, \lambda_n\}$.

Last minute addition given other talks

Special case: $p = 0$ and $f_0(s) = 1$.

Ordinary Kriging Weights Illustration – although for different data



Spatial prediction via universal kriging

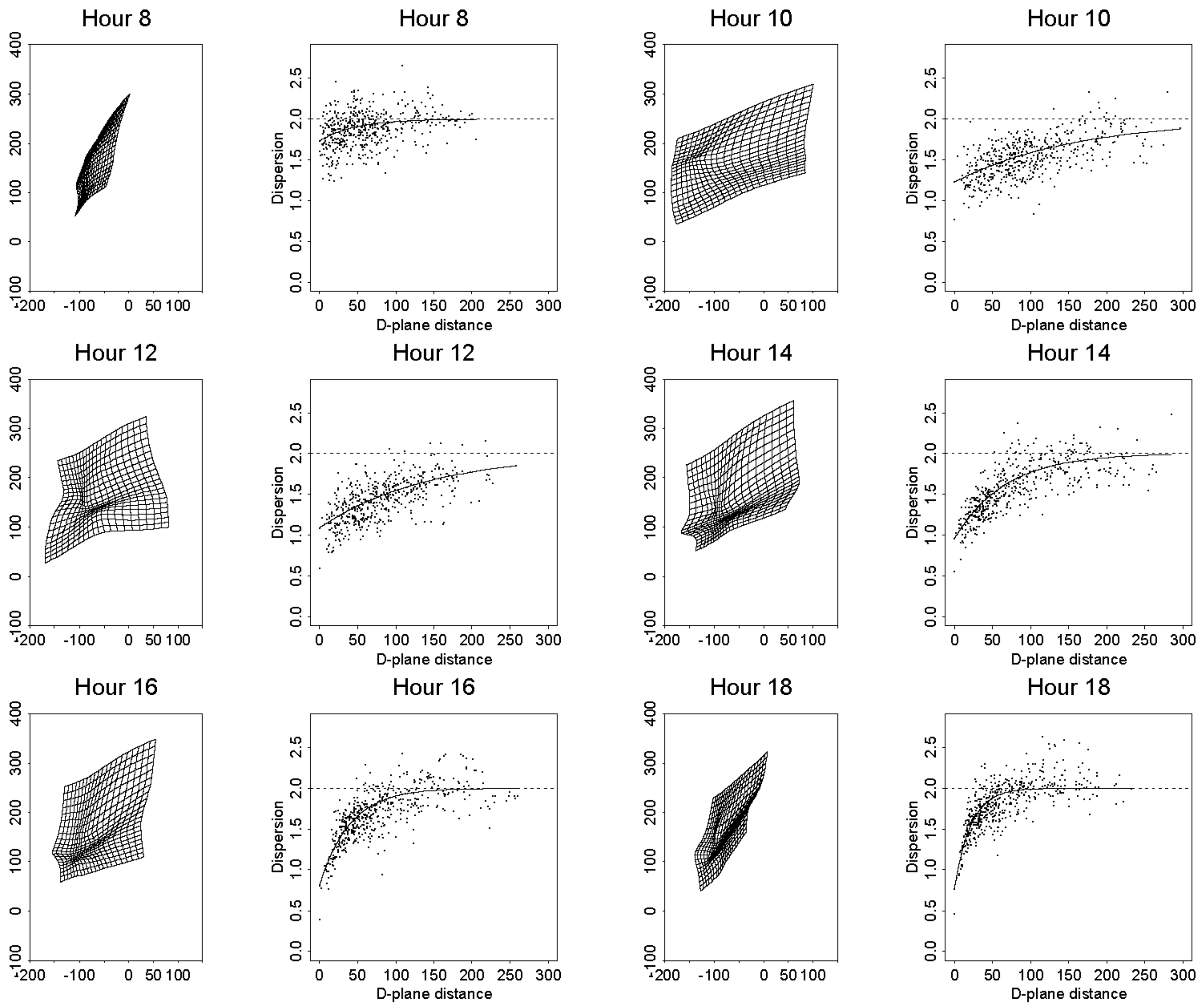
- Optimality results assume that the form and parameters of the spatial correlation function are known.

- **In practice, both the form and parameters are unknown.**

  - use Bayesian Kriging;

    or a bootstrap approach.

Space and Time Often Are Non-Separable. Ozone Example
Spatial Structure in Pre-whitened Residuals – varies by hour of day



Points for discussion/brain-storming

Extensions to space-time correlation.

Diagnostics for data that are different in their space-time second order structure from their neighbors – quality control (eg. Ozone eg. Guttorp et al., 1994)

Step 1 - Heterogeneous estimation approach can help identify and understand nature of anisotropy in spatial (or space-time) correlation, including changes in time such as seasonal.

Always motivates further study:
Is structure real?
Are there scientific explanations for these anisotropies?
Alexandra – including covariates in covariances.