A fundamental inverse problem in geosciences

Predict the values of a spatial random field (SRF) using a set of observed values of the same and/or other SRFs.

$$y_i = L_i(u) + v_i \ , \quad i = 1,\ldots,n \quad \longrightarrow \quad u(P) = ?$$

$L_i(u)$: linear functionals $\qquad$ v_i : random noise

$E\{u(P)\} = m(P)$ trend of the unknown field

$E\{(u(P) - m(P))\,(u(Q) - m(Q))\} = C_u(P,Q)$ CV function

Setting the stage ...

$$y_i = \underbrace{L_i(u)}_{s(P_i)} + v_i = s_i + v_i \;, \quad i = 1,\ldots,n$$

$$\mathbf{y} = \mathbf{s} + \mathbf{v}$$

Auxiliary hypotheses:

1) $E\{u(P)\} = 0\,, \quad E\{s_i\} = 0\,, \quad E\{\mathbf{s}\} = \mathbf{0}$

2) $\mathbf{C_{sv}} = \mathbf{0} \longrightarrow \mathbf{C_y} = \mathbf{C_s} + \mathbf{C_v}$

3) $\mathbf{C_s}[i,j] = L_i L_j C_u(P_i, P_j)$

$\mathbf{c}^{T}_{u(P)\mathbf{s}}[i] = L_i C_u(P, P_i)$

} Signal CV model + CV propagation law

4) $\mathbf{C_v}[i,j] = E\{v_i v_j\} = \sigma_{v_i v_j}$ ⟶ Noise CV model

Optimal generalized interpolation

$$y_i = \underbrace{L_i(u)}_{s(P_i)} + v_i = s_i + v_i \;, \quad i = 1, \ldots, n$$

$$\mathbf{y} = \mathbf{s} + \mathbf{v}$$

Linear unbiased prediction of the unknown field with minimum mean squared error

$$\hat{u}(P) = \mathbf{c}^{\mathrm{T}}_{u(P)\mathbf{s}} \left(\mathbf{C_s} + \mathbf{C_v}\right)^{-1} \mathbf{y}$$

$$\hat{\mathbf{u}} = \mathbf{C_{us}} \left(\mathbf{C_s} + \mathbf{C_v}\right)^{-1} \mathbf{y}$$

– Least-squares collocation (LSC)

– Kriging

– Wiener-Kolmogorov (WK) theory

"Hidden" characteristics of the LSC solution

The signal prediction algorithm is not affected by the spatial distribution of the prediction points

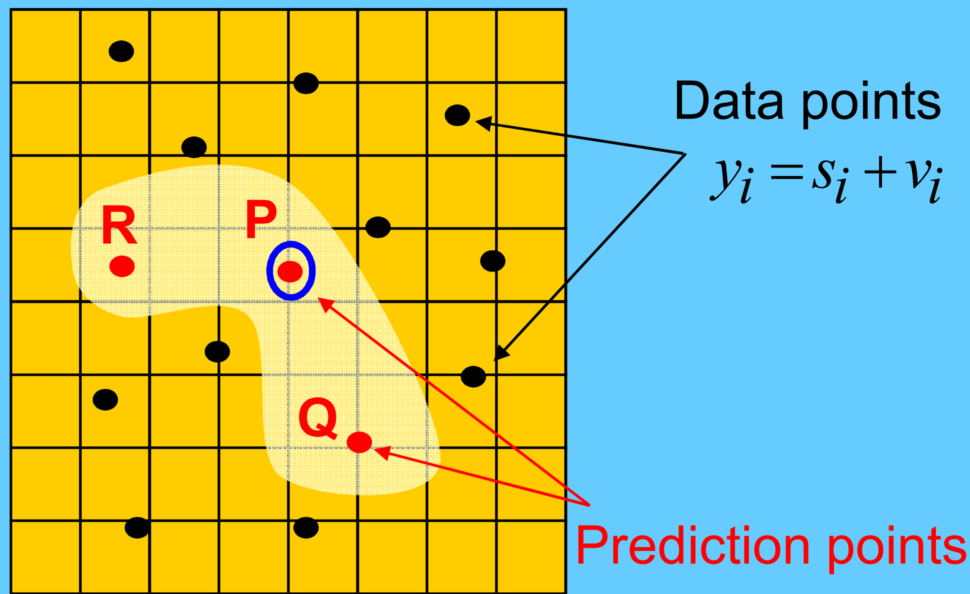
(the LSC estimate at P is the same, regardless of the number and/or the geometry of other prediction points).

$$\hat{u}(P) = \mathbf{c}^{T}_{u(P)\mathbf{s}} (\mathbf{C_s} + \mathbf{C_v})^{-1} \mathbf{y}$$

$$\hat{u}(Q) = \mathbf{c}^{T}_{u(Q)\mathbf{s}} (\mathbf{C_s} + \mathbf{C_v})^{-1} \mathbf{y}$$

$$\hat{u}(R) = \ldots$$

$$\hat{\mathbf{u}} = \mathbf{C_{us}} (\mathbf{C_s} + \mathbf{C_v})^{-1} \mathbf{y}$$



"Hidden" characteristics of the LSC solution

$$\hat{\mathbf{u}} = \mathbf{C}_{\mathbf{us}} (\mathbf{C}_{\mathbf{s}} + \mathbf{C}_{\mathbf{v}})^{-1} \mathbf{y}$$

Model-denial occurs through the LSC estimation procedure, in the sense that:

$$\mathbf{C}_{\mathbf{u}}[i,j] = C_u(P_i, P_j)$$

$$\mathbf{C}_{\hat{\mathbf{u}}} = \mathbf{C}_{\mathbf{us}} (\mathbf{C}_{\mathbf{s}} + \mathbf{C}_{\mathbf{v}})^{-1} \mathbf{C}_{\mathbf{us}}^{\mathrm{T}} \neq \mathbf{C}_{\mathbf{u}}$$

$$\mathbf{e} = \hat{\mathbf{u}} - \mathbf{u}$$

$$\mathbf{C}_{\hat{\mathbf{u}}} = \mathbf{C}_{\mathbf{u}} - \mathbf{C}_{\mathbf{e}}$$

The auto-covariance structure of the estimated SRF is different from the auto-covariance structure of the corresponding true SRF (field smoothing).

Due to the fact that:

$$\mathbf{C}_{\hat{\mathbf{u}}} = \mathbf{C}_{\mathbf{u}} - \mathbf{C}_{\mathbf{e}} \neq \mathbf{C}_{\mathbf{u}}$$

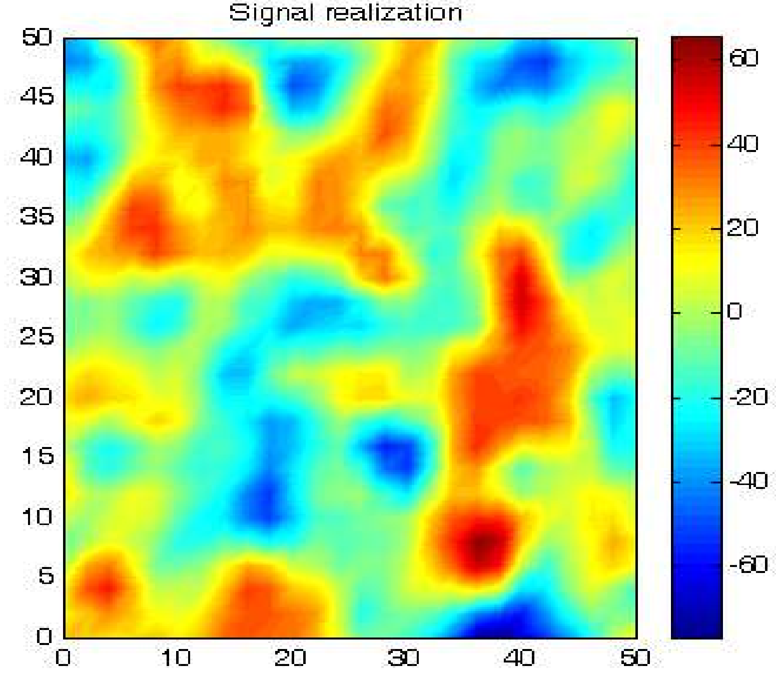
- Smoothing effect in the field estimate $\hat{u}(P)$.

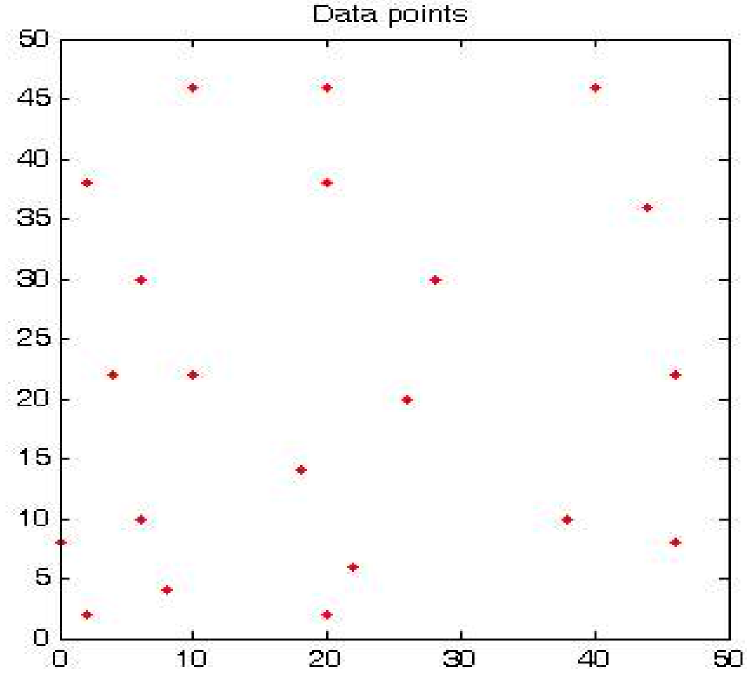
- Field "images" based on LSC are unsuitable for applications where the spatial signal variability is a key element for scientific inference.

- Signal details not inherent or proven by the actual data (i.e. artifacts) are not produced, but ..

- Inability to reproduce even the empirically determined CV function model $C_u(P,Q)$.

Example



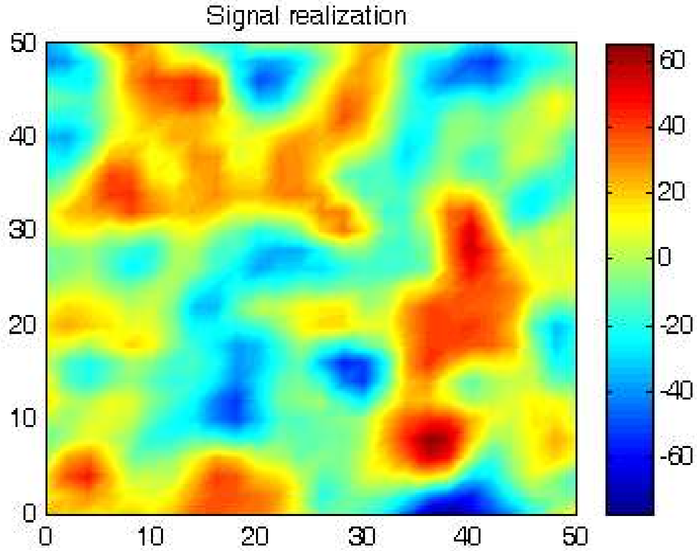


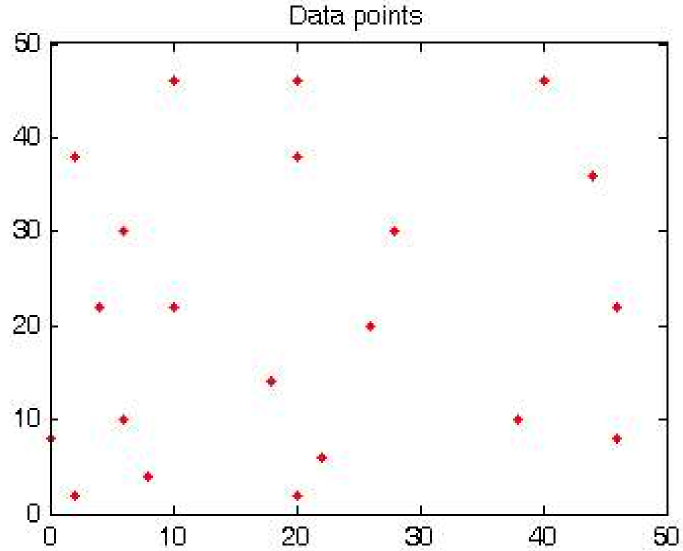
$$C_u(P,Q) = C_u(\tau = |P-Q|) = \frac{C_o}{1+(\frac{\tau}{a})^2}$$

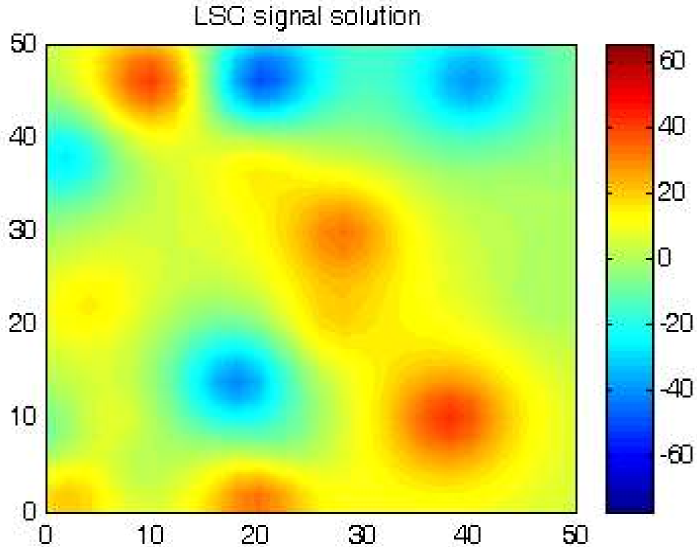
$$C_o = 750\ \text{mgal}^2$$

$$\xi = 9.5\ \text{km}$$

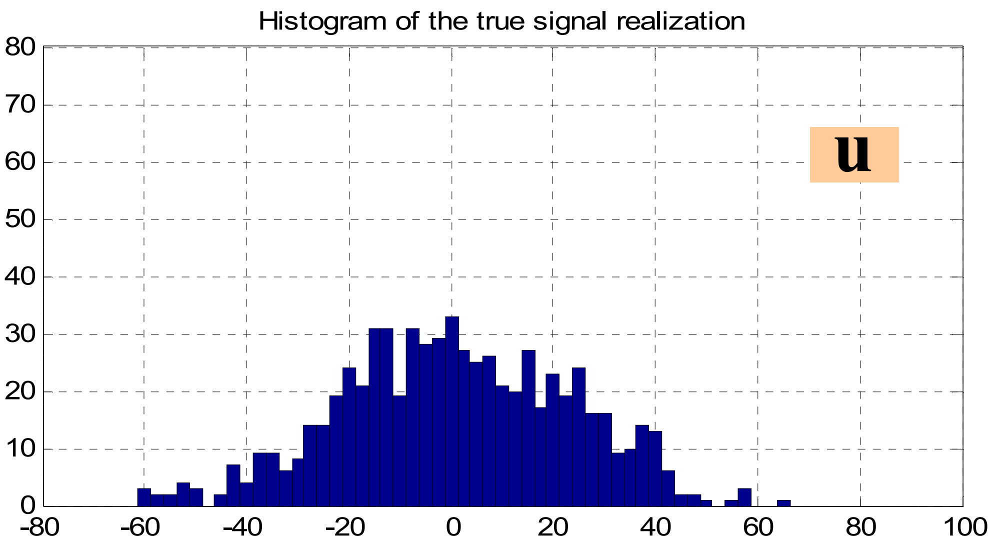
Spatial resolution: 2 km







Smoothed image that does represent realistically the spatial variability of the underlying field



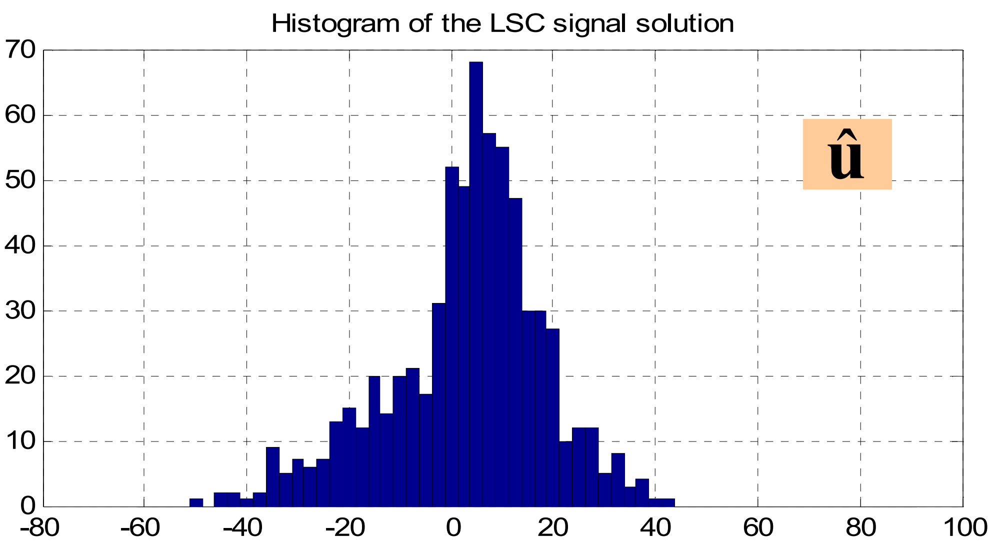
Signal realization

Max = 65.30

Min = -76.85

Mean = 0.70

σ = 22.71



LSC solution

Max = 42.62

Min = -49.86

Mean = 2.95

σ = 15.39

theoretical σ = 27.39 mgal

Preliminary conclusions

- Signal predictions from LSC should be listed, not mapped!
- LSC is the optimal prediction method for localized signal recovery (minimum pointwise MSE).
- LSC is unsuitable for spatial field mapping (fails to reproduce the model-based spatio-statistical variability of the unknown field).
- The final result of LSC denies its fundamental building component (i.e. the CV function of the underlying unknown signal)!

A revised formulation

Apply a post-processing "correction" algorithm (de-smoothing transformation) on the LSC solution

$$\hat{\mathbf{u}}' = \Re\{\hat{\mathbf{u}}\}$$

such that:

1) The CV structure of the SRF is preserved

$$\mathbf{C}_{\hat{\mathbf{u}}'} = \mathbf{C}_{\mathbf{u}}$$

2) The estimation error remains small in some sense

$$\mathbf{e}' = \hat{\mathbf{u}}' - \mathbf{u}$$

i.e. minimize some functional of $\mathbf{C}_{\mathbf{e}'}$

A linear revised formulation

Linear transformation of the LSC solution

$$\hat{\mathbf{u}}' = \mathbf{R} \cdot \hat{\mathbf{u}}$$

where $\mathbf{R}$ is a filtering matrix that needs to be determined according to some optimality criteria

Note that:

$\mathbf{e} = \hat{\mathbf{u}} - \mathbf{u}$ LSC estimation error

$\mathbf{e}' = \hat{\mathbf{u}}' - \mathbf{u}$ (LSC & $\mathbf{R}$-filtering) estimation error

$$\mathbf{C}_{\mathbf{e}'} = \mathbf{C}_{\mathbf{e}} + (\mathbf{I} - \mathbf{R})\mathbf{C}_{\hat{\mathbf{u}}}(\mathbf{I} - \mathbf{R})^{\mathrm{T}}$$

Filtering optimization

Determine the transformation matrix $\mathbf{R}$

$$\hat{\mathbf{u}}' = \mathbf{R}\,\hat{\mathbf{u}}$$

$$\mathbf{e}' = \hat{\mathbf{u}}' - \mathbf{u}$$

such that

$$\mathbf{C}_{\hat{\mathbf{u}}'} = \mathbf{R}\mathbf{C}_{\hat{\mathbf{u}}}\mathbf{R}^{\mathrm{T}} = \mathbf{C}_{\mathbf{u}}$$

CV-matching constraint

subject to the optimal prediction criterion

$$\mathbf{C}_{\mathbf{e}'} = \mathbf{C}_{\mathbf{e}} + \underbrace{(\mathbf{I}-\mathbf{R})\mathbf{C}_{\hat{\mathbf{u}}}(\mathbf{I}-\mathbf{R})^{\mathrm{T}}}_{\delta\mathbf{C}_{\mathbf{e}'}}$$

From LSC

$$\mathit{trace}\,\delta\mathbf{C}_{\mathbf{e}'} = \text{minimum}$$

The optimal matrix $\mathbf{R}$

Solving the previous optimization problem, we get the result:

$$\mathbf{R} = \mathbf{C}_{\mathbf{u}}^{1/2}(\mathbf{C}_{\mathbf{u}}^{1/2}\mathbf{C}_{\hat{\mathbf{u}}}\mathbf{C}_{\mathbf{u}}^{1/2})^{-1/2}\mathbf{C}_{\mathbf{u}}^{1/2}$$

or equivalently

$$\mathbf{R} = \mathbf{C}_{\hat{\mathbf{u}}}^{-1/2}(\mathbf{C}_{\hat{\mathbf{u}}}^{1/2}\mathbf{C}_{\mathbf{u}}\mathbf{C}_{\hat{\mathbf{u}}}^{1/2})^{1/2}\mathbf{C}_{\hat{\mathbf{u}}}^{-1/2}$$

- Symmetric

- Positive definite

Alternative forms for the optimal filtering matrix $\mathbf{R}$

Using the matrix identity: $\mathbf{S}\mathbf{T}^{1/2}\mathbf{S}^{-1} = (\mathbf{S}\mathbf{T}\mathbf{S}^{-1})^{1/2}$

we obtain the equivalent compact expressions for the matrix $\mathbf{R}$

$$\mathbf{R} = (\mathbf{C_u}\mathbf{C_{\hat{u}}})^{-1/2}\mathbf{C_u}$$

$$\mathbf{R} = \mathbf{C}_{\hat{\mathbf{u}}}^{-1}(\mathbf{C_{\hat{u}}}\mathbf{C_u})^{1/2}$$

$$\mathbf{R} = (\mathbf{C_u}\mathbf{C_{\hat{u}}})^{1/2}\mathbf{C}_{\hat{\mathbf{u}}}^{-1}$$

$$\mathbf{R} = \mathbf{C_u}(\mathbf{C_{\hat{u}}}\mathbf{C_u})^{-1/2}$$

Prediction error

Co-variance matrix of the prediction error

$$\mathbf{C}_{\mathbf{e}'} = \mathbf{C}_{\mathbf{e}} + (\mathbf{I}-\mathbf{R})\mathbf{C}_{\hat{\mathbf{u}}}(\mathbf{I}-\mathbf{R})^{\mathrm{T}}$$

If all eigenvalues of the filtering matrix $\mathbf{R}^*$ are larger than one, i.e.

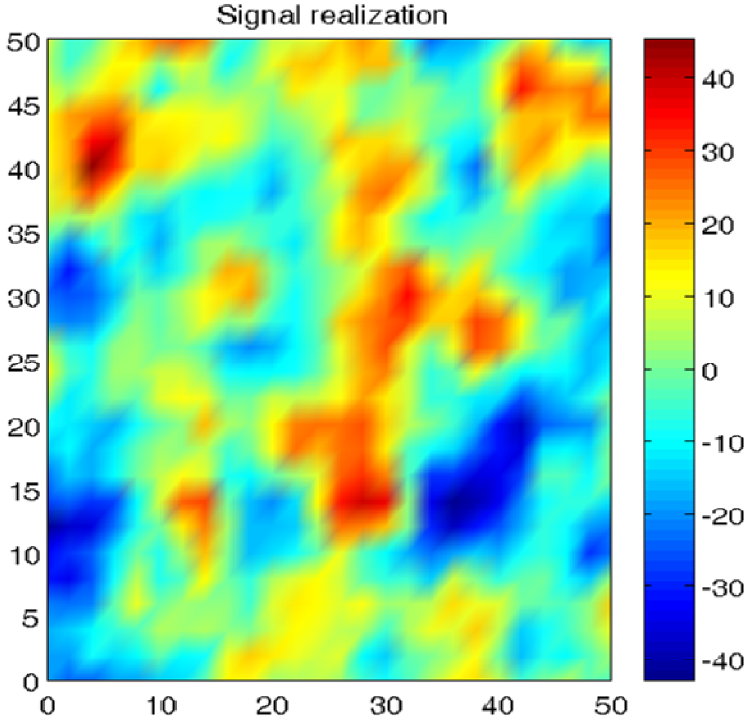
$$\mathbf{R} = \mathbf{I} + \delta\mathbf{R} \longrightarrow$$ positive definite matrix

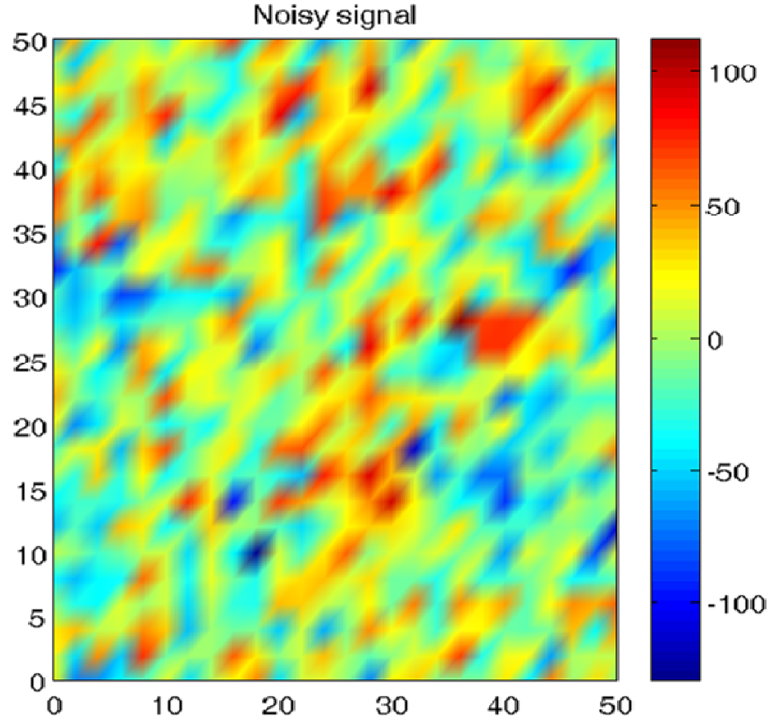
then it can be shown that

$$trace(\mathbf{C}_{\mathbf{e}'}) \leq 2 \times trace(\mathbf{C}_{\mathbf{e}})$$

* not necessarily optimal..

Test 1 (noise filtering)





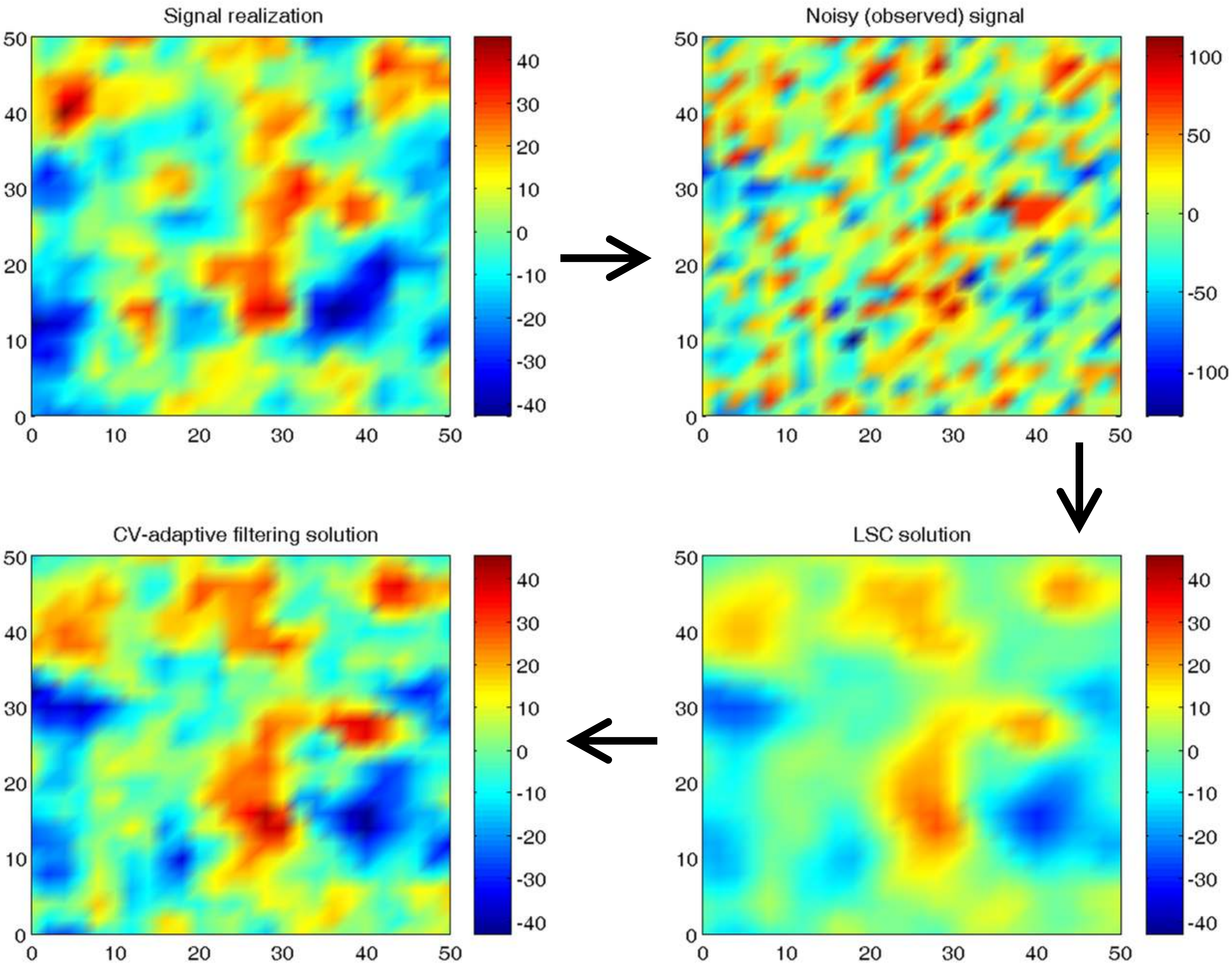
$$C_u(\tau) = \frac{C_o}{1+(\frac{\tau}{a})^2}$$

Spatial resolution: 2 km

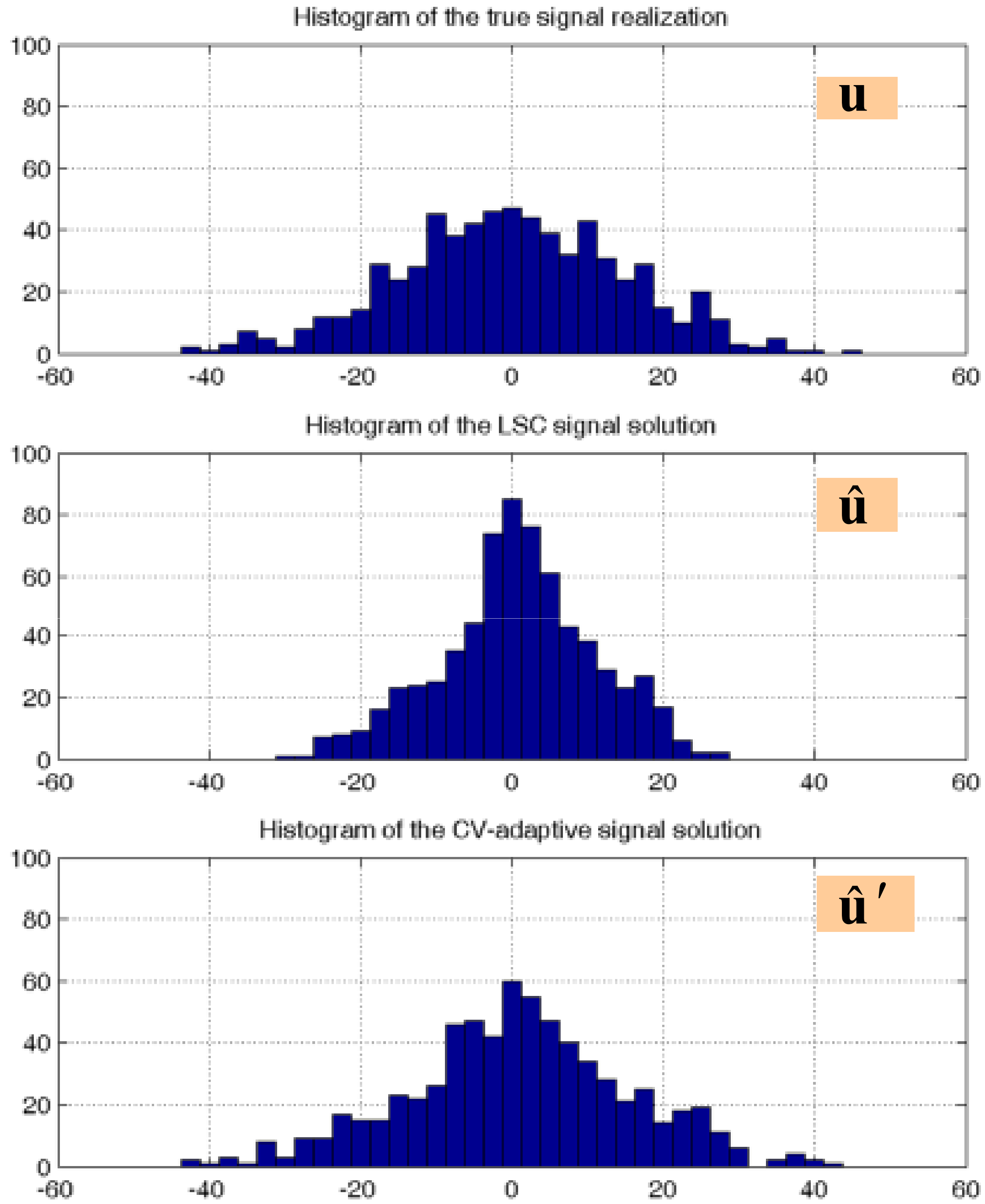
$$\sigma_v = 35 \text{ mgal} \quad \text{(white noise)}$$

$$C_o = 220 \text{ mgal}^2$$

$$\xi = 7 \text{ km}$$



Signal realization
Noisy (observed) signal
CV-adaptive filtering solution
LSC solution
0
10
20
30
40
50
-40
-30
-20
-10
0
10
20
30
40
-100
-50
0
50
100



theoretical σ = 14.83 mgal

Signal realization

Max = 45.33

Min = -42.88

Mean = -0.04

σ = 14.96

LSC solution

Max = 27.42

Min = -29.10

Mean = 0.74

σ = 10.29

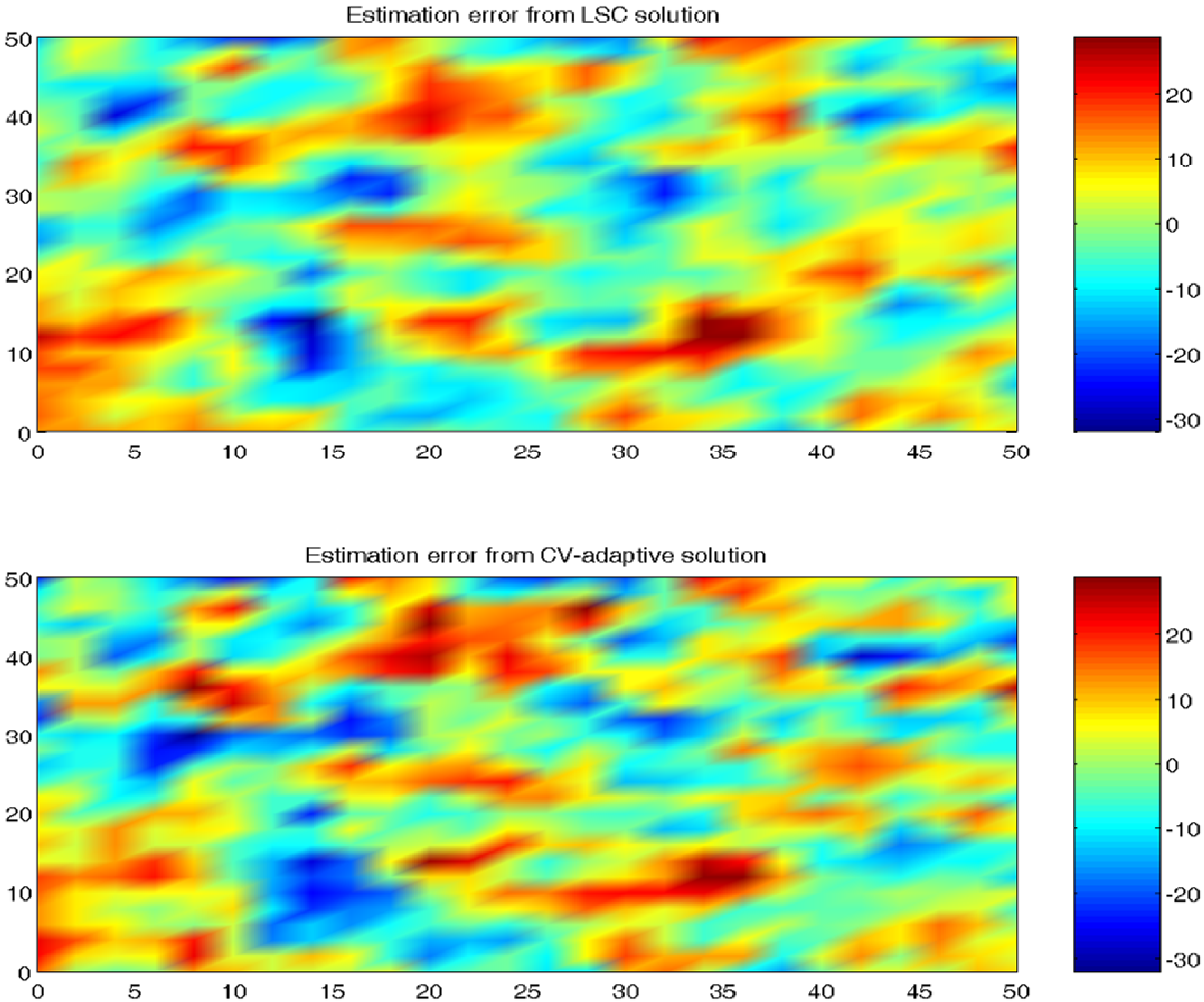
CV-adaptive solution

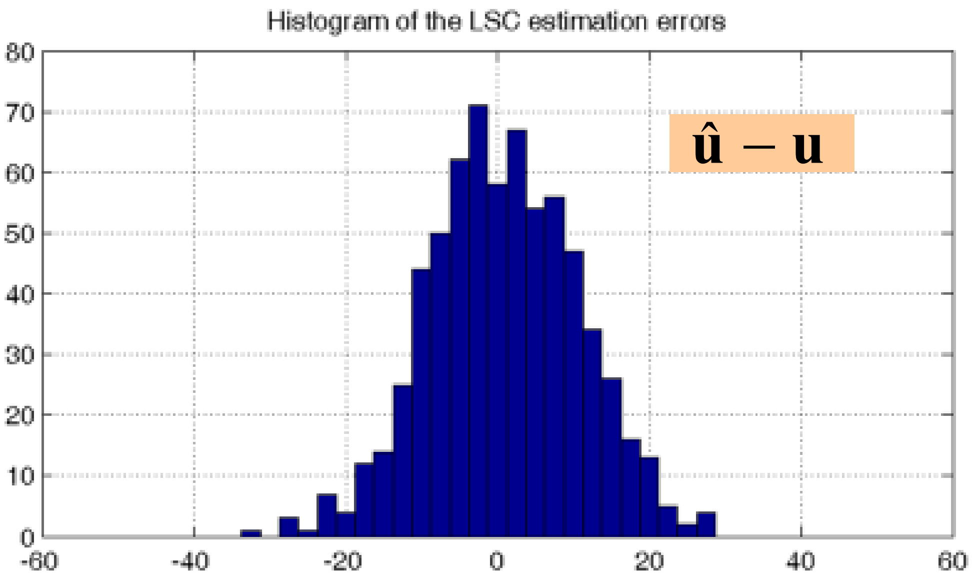
Max = 41.47

Min = -42.48

Mean = 0.73

σ = 14.64


Estimation error from LSC solution
50
40
30
20
10
0
0
5
10
15
20
25
30
35
40
45
50
20
10
0
-10
-20
-30
Estimation error from CV-adaptive solution
50
40
30
20
10
0
0
5
10
15
20
25
30
35
40
45
50
20
10
0
-10
-20
-30



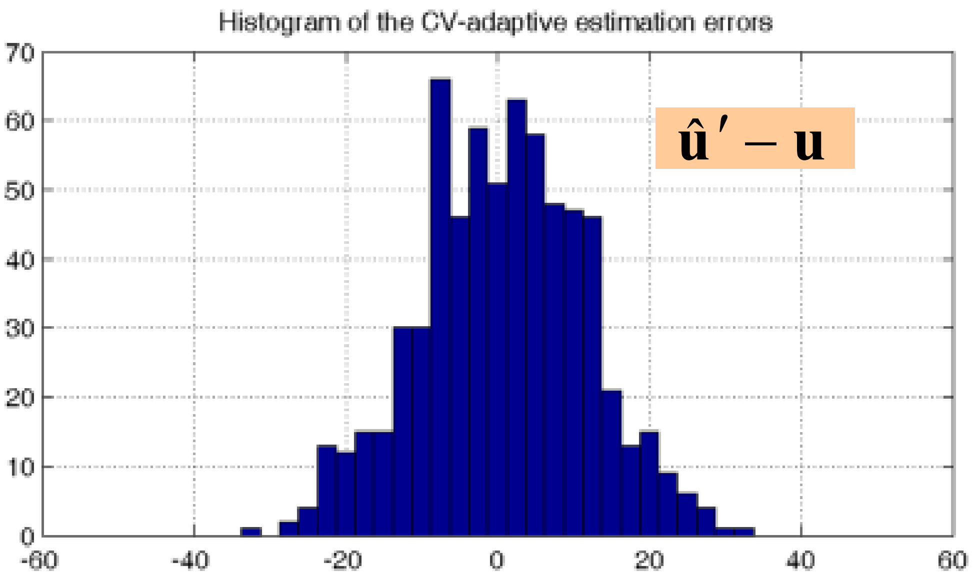
LSC estimation errors

Max = 28.70

Min = -31.94

Mean = 0.78

σ = 9.88



CV-adaptive estimation errors

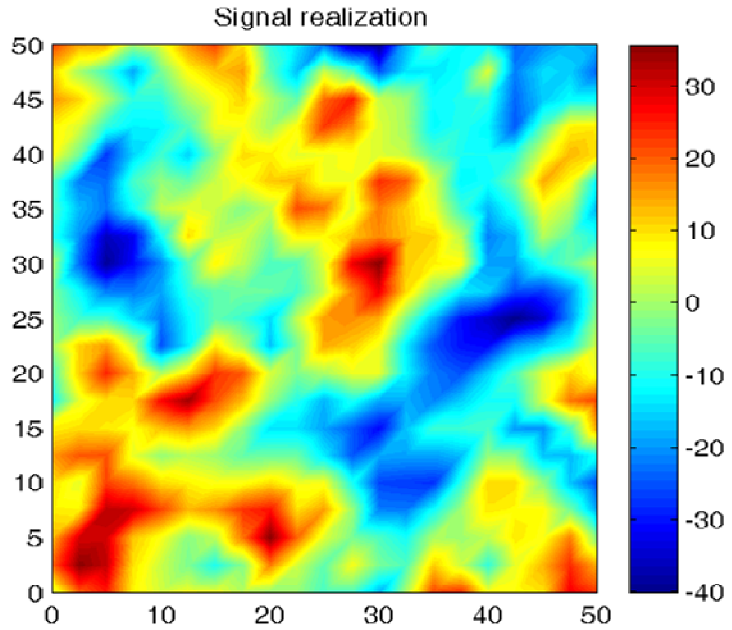
Max = 31.98

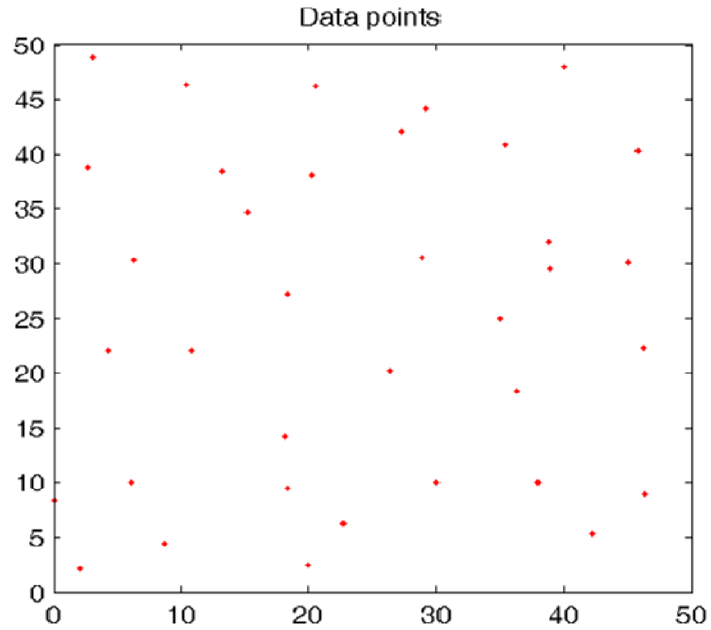
Min = -32.05

Mean = 0.77

σ = 11.01

Test 2
(noise filtering + spatial interpolation)





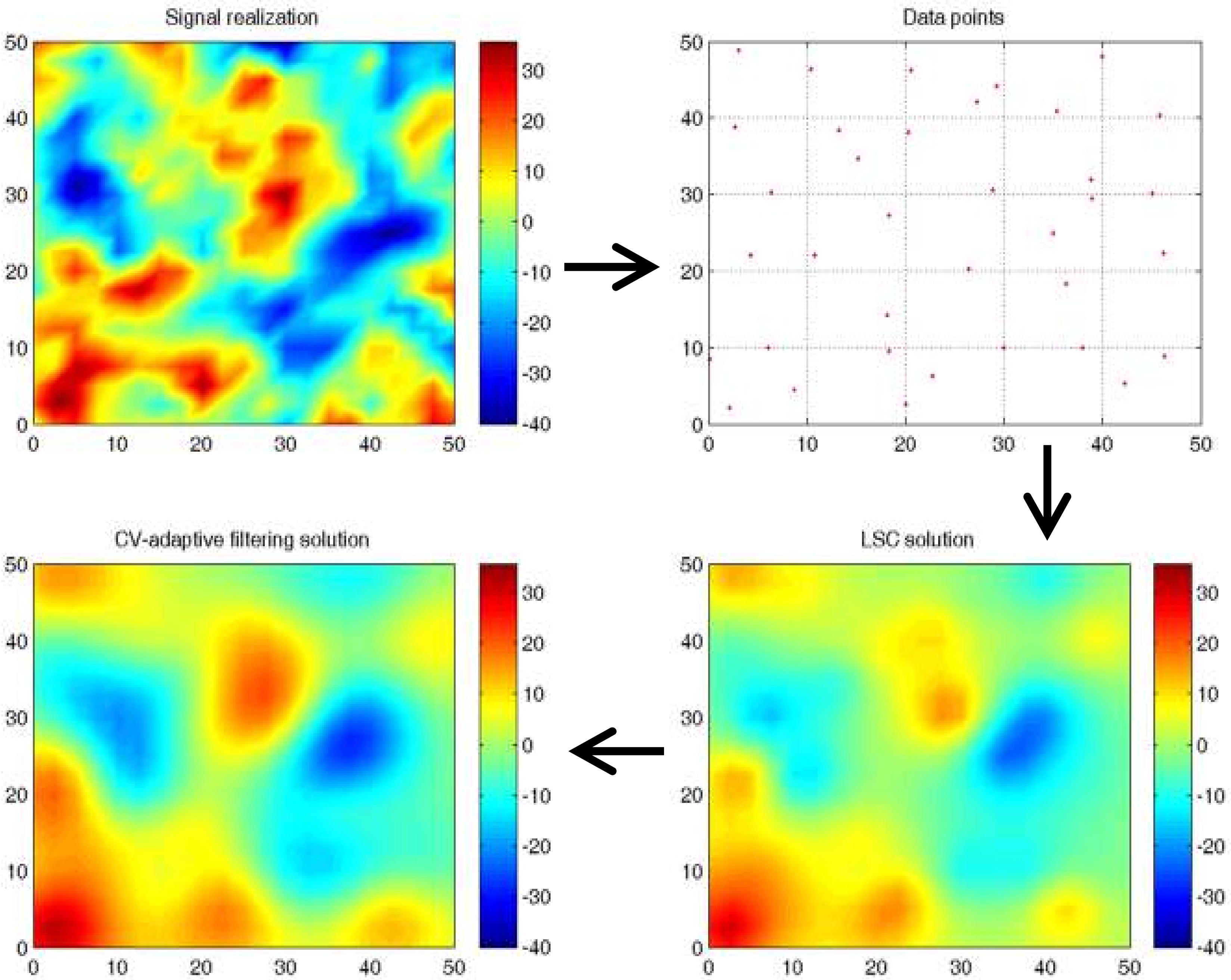
$$C_u(\tau) = \frac{C_o}{1+(\frac{\tau}{a})^2}$$

Spatial resolution: 2 km

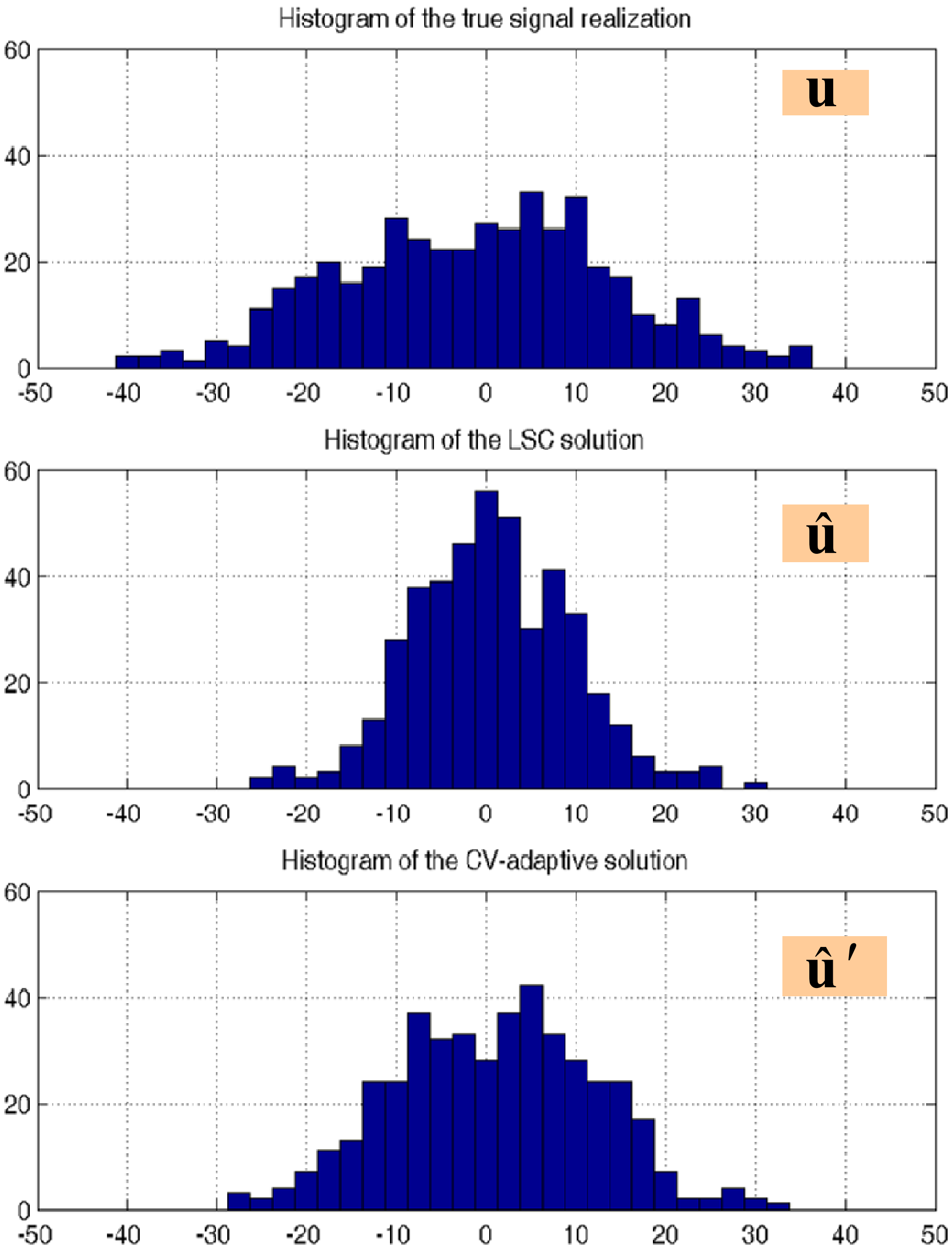
$$\sigma_v = 5 \text{ mgal} \quad \text{(white noise)}$$

$$C_o = 220 \text{ mgal}^2$$

$$\xi = 8 \text{ km}$$



Signal realization
Data points
CV-adaptive filtering solution
LSC solution



theoretical σ = 14.83 mgal

Signal realization

Max = 35.76

Min = -40.09

Mean = -1.19

σ = 14.94

LSC solution

Max = 31.04

Min = -24.38

Mean = 0.67

σ = 8.85

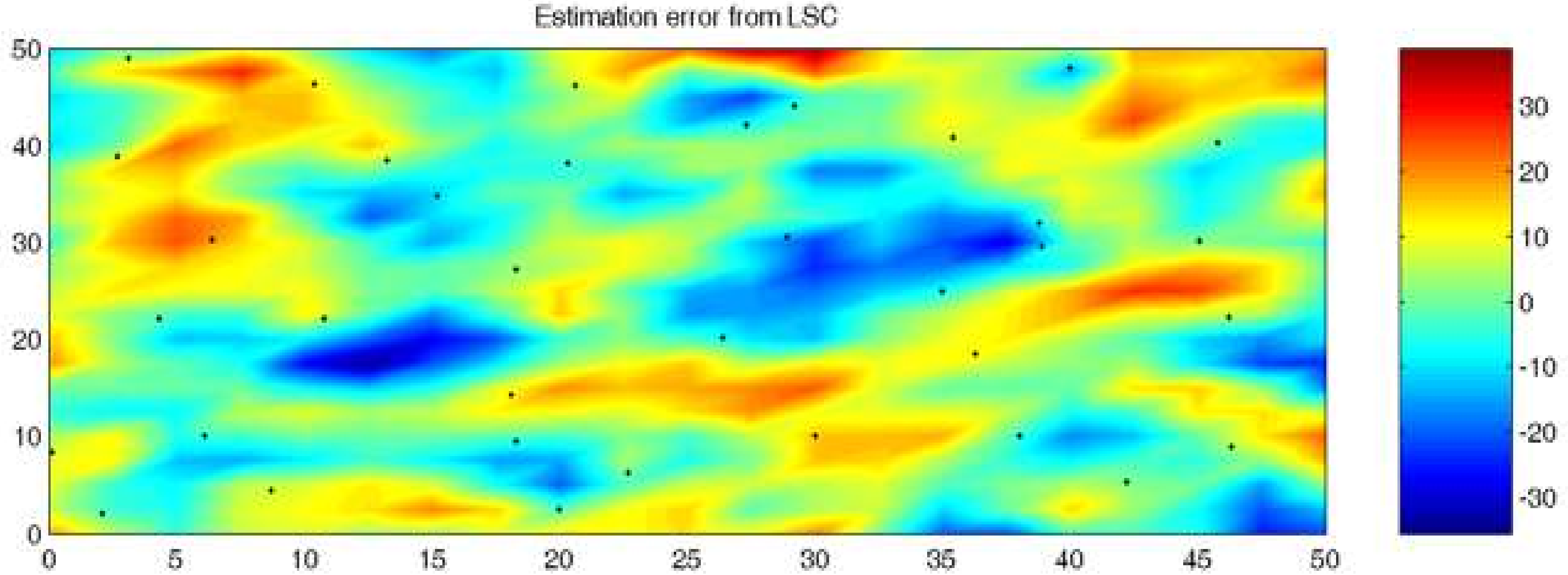
CV-adaptive solution

Max = 32.48

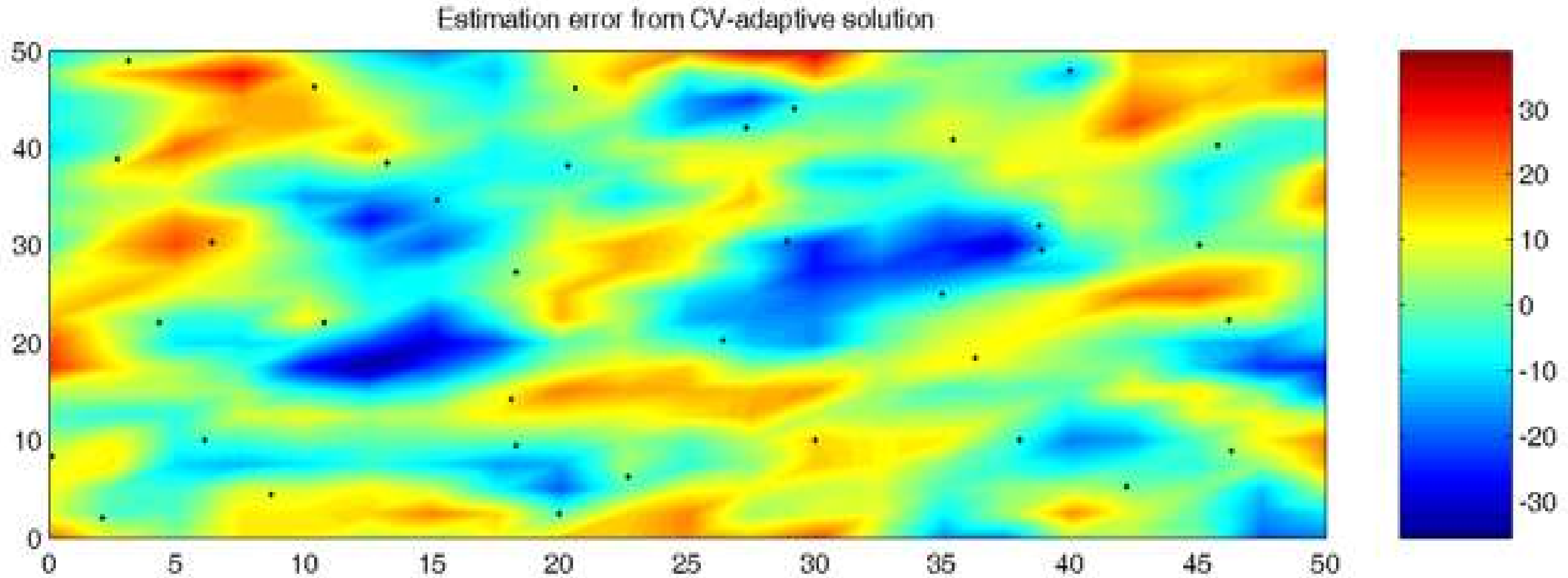
Min = -28.56

Mean = 0.94

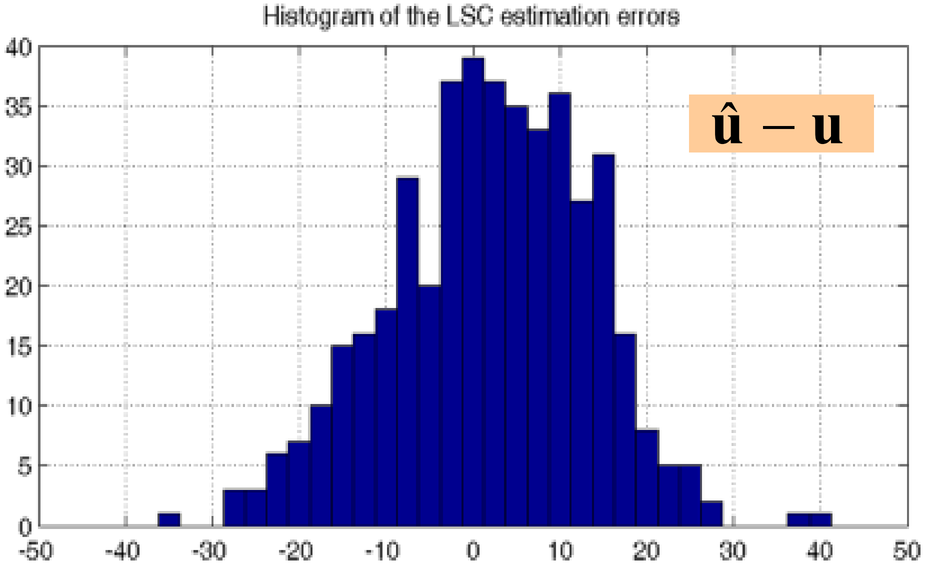
σ= 11.18



Estimation error from LSC
50
40
30
20
10
0
0
5
10
15
20
25
30
35
40
45
50
30
20
10
0
-10
-20
-30



Estimation error from CV-adaptive solution
50
40
30
20
10
0
0
5
10
15
20
25
30
35
40
45
50
30
20
10
0
-10
-20
-30



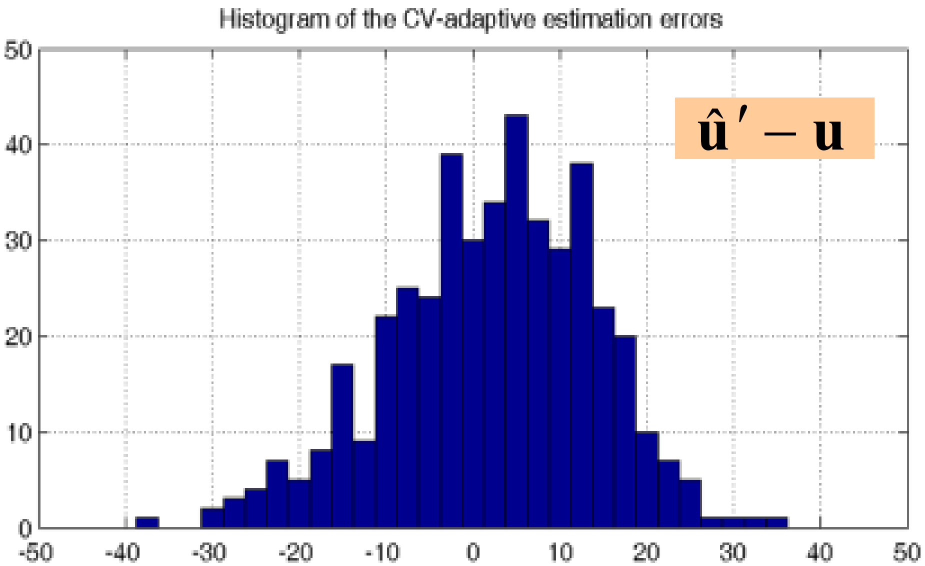
LSC estimation errors

Max = 39.01

Min = -35.59

Mean = 1.86

σ = 11.58



CV-adaptive estimation errors

Max = 34.25

Min = -36.92

Mean = 2.13

σ = 11.81

Conclusions

– LSC provides optimal **local** accuracy, yet poor **global** spatial rendering in SRF prediction problems.

– New prediction approach based on **optimal de-smoothing** through **CV-matching filtering**;

i.e. reproduce the signal CV function with minimum loss in the MSE accuracy

– Identify relevant application areas where **global spatial accuracy** is an important issue (preserving non-stationary patterns, spatial field mapping,…)

– Are there any “fundamental” issues hidden on the trade-off between local and global accuracy in SRF estimation from discrete data?

Thanks for your attention!