POLITECNICO DI MILANO

GEOSTATISTICAL INVERSION OF MOMENT EQUATIONS OF GROUNDWATER FLOW

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Flow in Heterogeneous Media

Governed by:

$$\mathbf{q}(\mathbf{x},t) = -K(\mathbf{x})\nabla h(\mathbf{x},t) \qquad \mathbf{x}\in\Omega$$

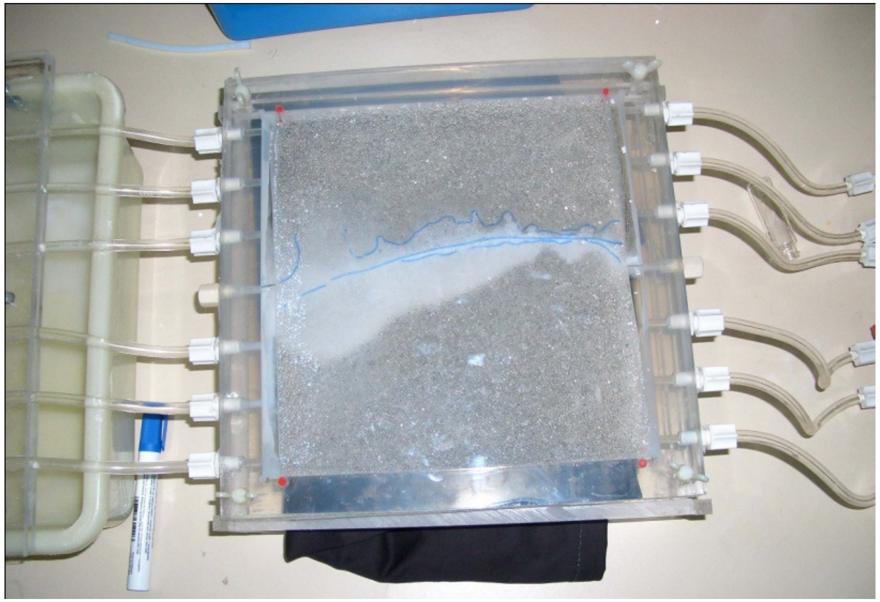
$$S_s(\mathbf{x})\frac{\partial h}{\partial t} = -\nabla\cdot\mathbf{q}(\mathbf{x},t) + f(\mathbf{x},t) \qquad \mathbf{x}\in\Omega$$

$$h(\mathbf{x},0) = H_0(\mathbf{x}) \qquad \mathbf{x}\in\Omega$$

$$h(\mathbf{x},t) = H(\mathbf{x},t) \qquad \mathbf{x}\in\Gamma_D$$

$$-\mathbf{q}(\mathbf{x},t)\cdot\mathbf{n}(\mathbf{x}) = Q(\mathbf{x},t) \qquad \mathbf{x}\in\Gamma_N$$

Problem of Aquifer Characterization

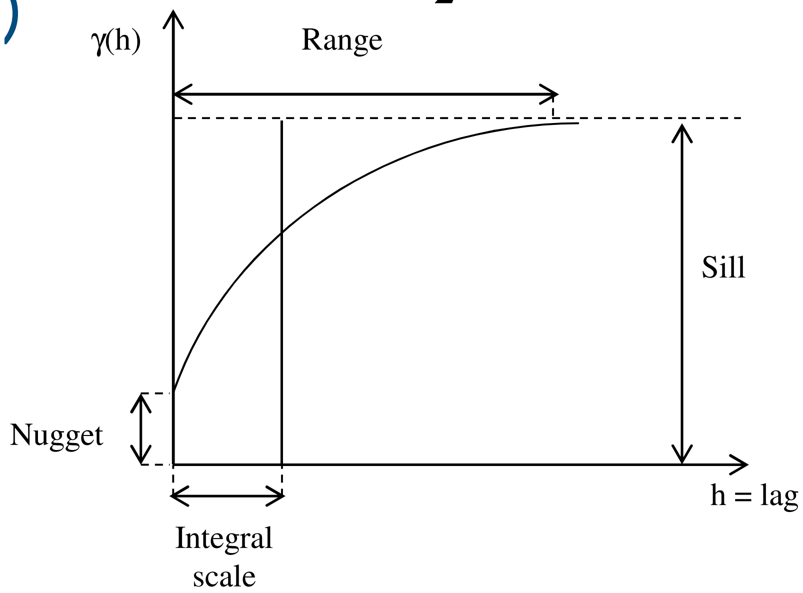


Achilles' heel in Hydro !

Random Heterogeneous Media

$$\gamma(\mathbf{h}) = \frac{1}{2} E\left[\left(z(\mathbf{h}) - z(x+\mathbf{h}) \right)^2 \right]$$

- Models:
  - Pure Nugget $\gamma(h) = C_0$
  - Spherical $\gamma(h) = \sigma^2((1.5h/a) - 0.5(h/a)^3)$
  - Exponential $\gamma(h) = \sigma^2(1 - \exp(-h/a))$
  - Gaussian $\gamma(h) = \sigma^2(1 - \exp(-h^2/a^2))$
  - Power $\gamma(h) = ah^b$



- **Moment Equation Solution consists of:**
  - **mean (optimum prediction) head/state variables**
  - **covariance (predictive uncertainty measure) of head/state variables**

conditioned on measured *K*, h/state variables:

Mean of flow equations

$$\nabla \cdot [< \mathrm{K}(\boldsymbol{x}) >_c \nabla < \mathrm{h}(\boldsymbol{x}) >_c - \boldsymbol{r_c}(\boldsymbol{x})] + < f(\boldsymbol{x}) > = 0 \qquad \text{on } \Omega$$

$$<\mathrm{h}(\boldsymbol{x}) >_c = <\mathrm{H}(\boldsymbol{x}) > \qquad \text{on } \Gamma_{\mathrm{D}}$$

$$[< \mathrm{K}(\boldsymbol{x}) >_c \nabla < \mathrm{h}(\boldsymbol{x}) >_c - \boldsymbol{r_c}(\boldsymbol{x})] \cdot \mathbf{n}(\boldsymbol{x}) = < \mathrm{Q}(\boldsymbol{x}) > \qquad \text{on } \Gamma_{\mathrm{N}}$$

<u>where</u>

$<\mathbf{q}(\boldsymbol{x})>_c$ = **conditional mean flux** = $- < \mathrm{K}(\boldsymbol{x}) >_c \nabla < \mathrm{h}(\boldsymbol{x}) >_c + \boldsymbol{r_c}(\boldsymbol{x})$

$$\boldsymbol{r_c}(\boldsymbol{x}) = \langle K'(\boldsymbol{x}) \nabla_x h'(\boldsymbol{x}) \rangle_c$$

$$\boldsymbol{r_c}(\boldsymbol{x}) = \int_\Omega \boldsymbol{a_c}(\boldsymbol{y}, \boldsymbol{x}) \nabla_y < \mathrm{h}(\boldsymbol{y}) >_c d\boldsymbol{y} + \int_\Omega \boldsymbol{d_c}(\boldsymbol{y}, \boldsymbol{x}) \boldsymbol{r_c}(\boldsymbol{y}) \, d\boldsymbol{y}$$

Covariance of head predictions

$$C_{hc}(\boldsymbol{x}, \boldsymbol{y}) = \langle h'(\boldsymbol{x})\, h'(\boldsymbol{y})\rangle_c$$

$$\nabla_x \cdot [< K(\boldsymbol{x}) >_c \nabla_x C_{hc}(\boldsymbol{x}, \boldsymbol{y}) + \boldsymbol{p_c}(\boldsymbol{x}, \boldsymbol{y}) + C_{hKc}(\boldsymbol{x}, \boldsymbol{y}) \nabla_x < h(\boldsymbol{x}) >_c] = - < f'(\boldsymbol{x})\, h'(\boldsymbol{y}) >_c \quad \text{on } \Omega$$

$$C_{hc}(\boldsymbol{x}, \boldsymbol{y}) = < H'(\boldsymbol{x})\, h'(\boldsymbol{y}) >_c \quad \text{on } \Gamma_D$$

$$[< K(\boldsymbol{x}) >_c \nabla_x C_{hc}(\boldsymbol{x}, \boldsymbol{y}) + \boldsymbol{p_c}(\boldsymbol{x}, \boldsymbol{y}) + C_{hKc}(\boldsymbol{x}, \boldsymbol{y}) \nabla_x < h(\boldsymbol{x}) >_c] \cdot \mathbf{n}(\boldsymbol{x}) = < Q'(\boldsymbol{x})\, h'(\boldsymbol{y}) >_c \quad \text{on } \Gamma_N$$

$\boldsymbol{p_c}(\boldsymbol{x}, \boldsymbol{y}) = \langle K'(\boldsymbol{x})\, \nabla_x h'(\boldsymbol{x})\, h'(\boldsymbol{y})\rangle_c$ = mixed third-order moment

$C_{hKc}(\boldsymbol{x}, \boldsymbol{y})$ = conditional cross-covariance between head and conductivity

Methodology

1. **Reynolds' decomposition**

$$A(\boldsymbol{x}) = \langle A(\boldsymbol{x})\rangle + A'(\boldsymbol{x}) \qquad\qquad \langle A'(\boldsymbol{x})\rangle = 0$$

2. **Exact ME for $\langle h\rangle$, $\langle q\rangle$, C_h, C_q, ……**

3. **Recursive approximations:**
   Expansions in power series of σ_Y (Y = ln (K))

$$\langle A(\boldsymbol{x})\rangle = \langle A(\boldsymbol{x})\rangle^{(0)} + \langle A(\boldsymbol{x})\rangle^{(2)} \ldots$$

$$\langle A(\boldsymbol{x})\rangle^{(i)} \propto (\sigma_Y)^{i}$$

Approximated equations need knowledge of $\langle Y(x)\rangle$, C_Y as input

Geostatistical Inversion

Conditions head/state variables on *measurements*

Entails:

- **(Pilot point) Parameterization of *Y***
- **Prior/posterior universal kriging of *Y***
- **Forward simulation of head/flux**
- **Nonlinear Maximum Likelihood estimation of**
  - ✓ ***Y* at pilot points**
  - ✓ **Statistical parameters of variogram of *Y***

Parameterization of *Y*

Parameterization via kriging:

$$\langle Y(\mathbf{x})\rangle = \sum_{i=1}^{N_Y} \lambda_i(\mathbf{x}) Y_{H_i} \qquad N_Y = N_M + N_P$$

N_M = **number of** Y **measurement points**

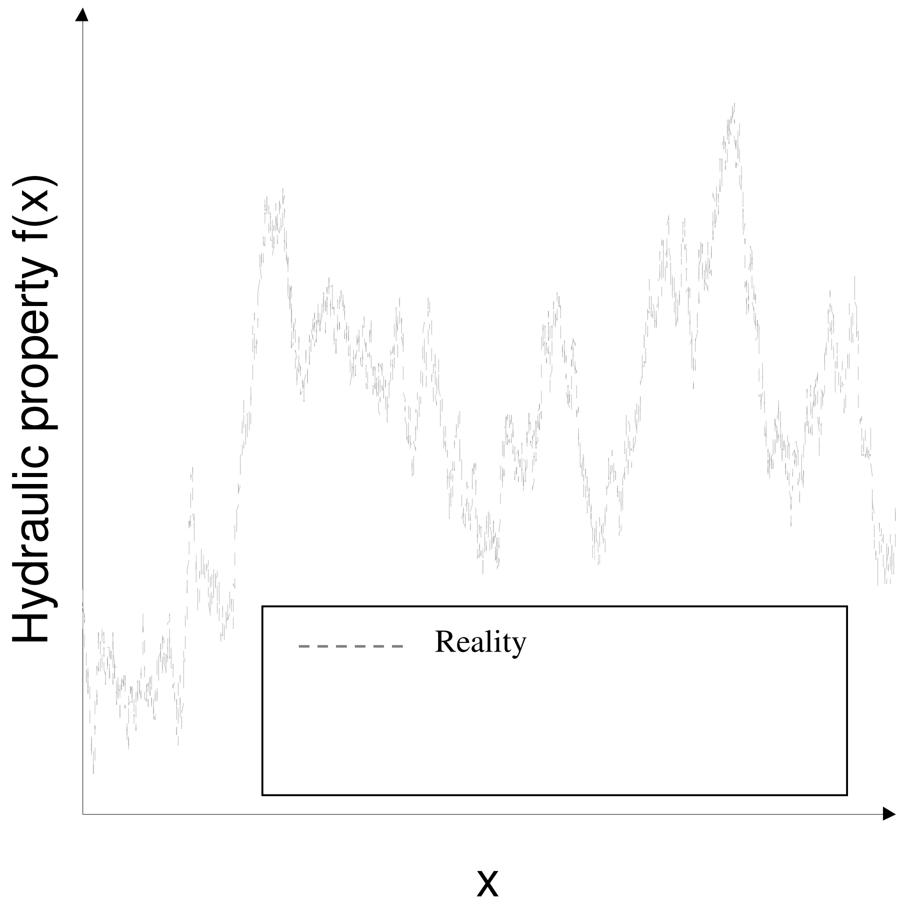
N_p = **number of pilot points**

$\mathbf{Y}_H = (\mathbf{Y}_M, \mathbf{Y}_P)^T =$ **"measured", pilot values**

λ_i = **kriging weights**

The pilot points are additional locations at which the parameter must be calibrated. The pilot point method consists of describing a conductivity field by kriging based on (1) the inferred variogram obtained from the data, (2) the measured values of conductivity and (3) a set of additional conductivity values at selected unmeasured locations in the aqwhich are unknown prior to calibration. uifer, called the "pilot points",

The Pilot Points Method



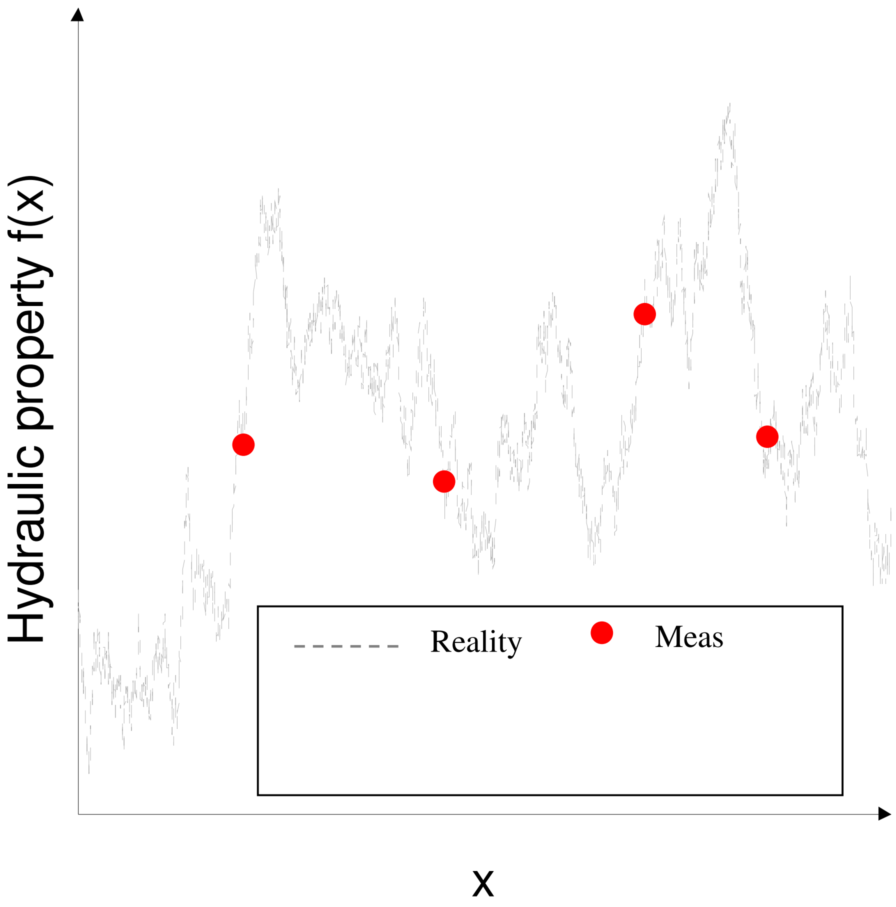
Parameterize hydraulic property

Residual

Parameterization of hydraulic property: $f(x,t) = \underbrace{f_D(x,t)}_{\text{Drift}} + \overbrace{f_p(x,t)}^{\text{Residual}}$

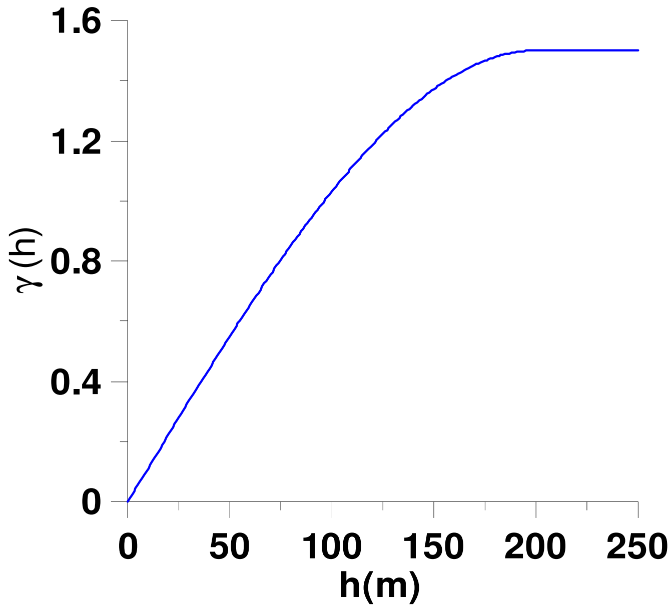
Drift

The Pilot Points Method



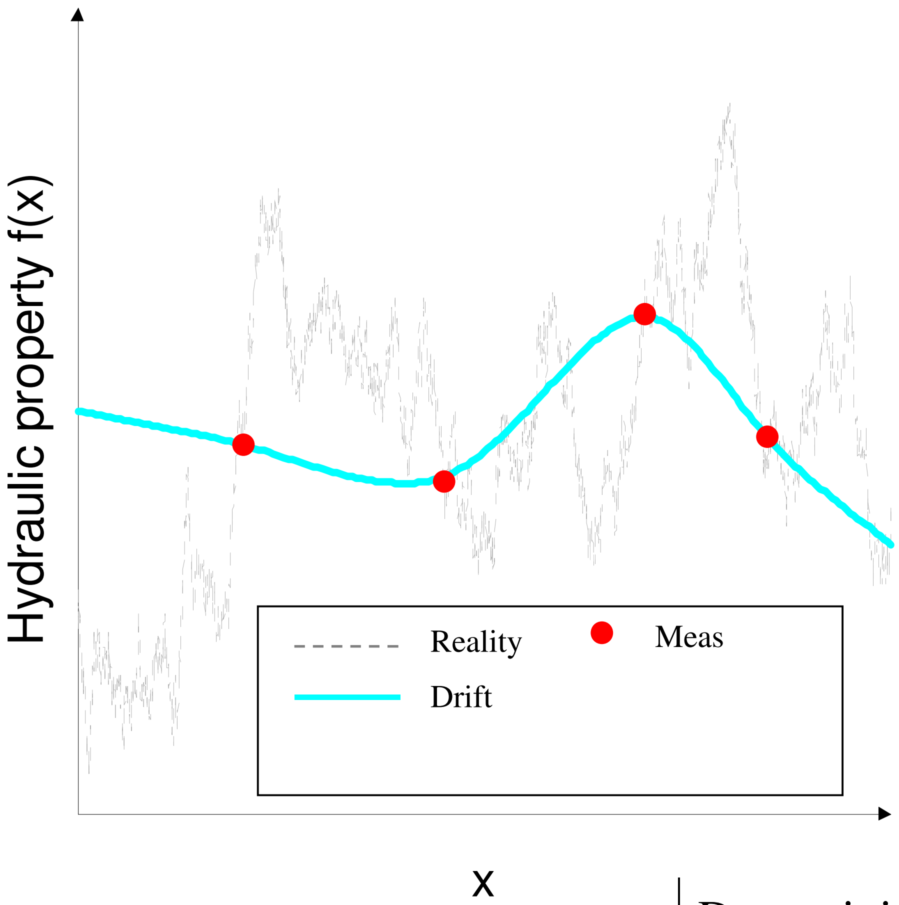
Parameterize hydraulic property

- **Definition of a geostatistical model**



Definition of a geostatistical model from available information

The Pilot Points Method



Parameterize hydraulic property

- Definition of a geostatistical model
- **Parameterize drift**

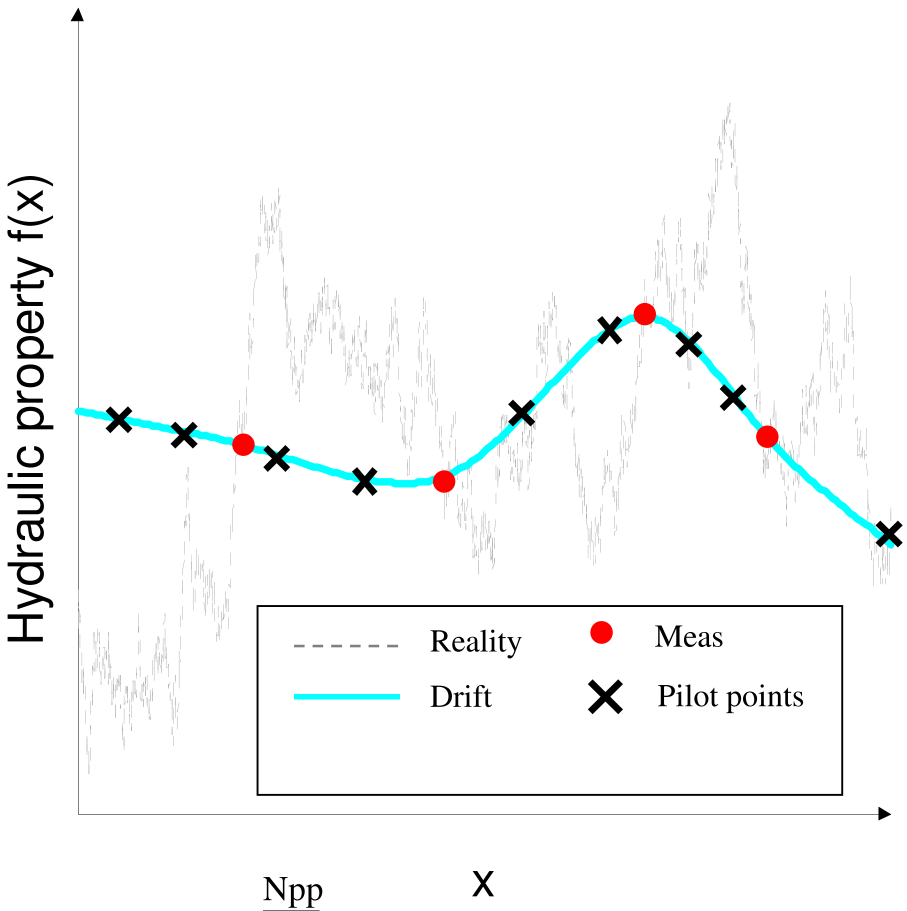
$$f_D(\mathbf{x}, t) = \sum_{i=1}^{\dim Z} \lambda_i^Z(\mathbf{x}) f^*(\mathbf{x_i}, t)$$

Deterministic (CE):

- Simple kriging
- Ordinary kriging
- Residual kriging
- Kriging locally varying mean
- Kriging external drift
- Simple cokriging
- Ordinary cokriging

Stochastic (CS) : sequential simulation

The Pilot Points Method



Parameterize hydraulic property

- Definition of a geostatistical model
- Parameterize drift
- **Parameterize residual**

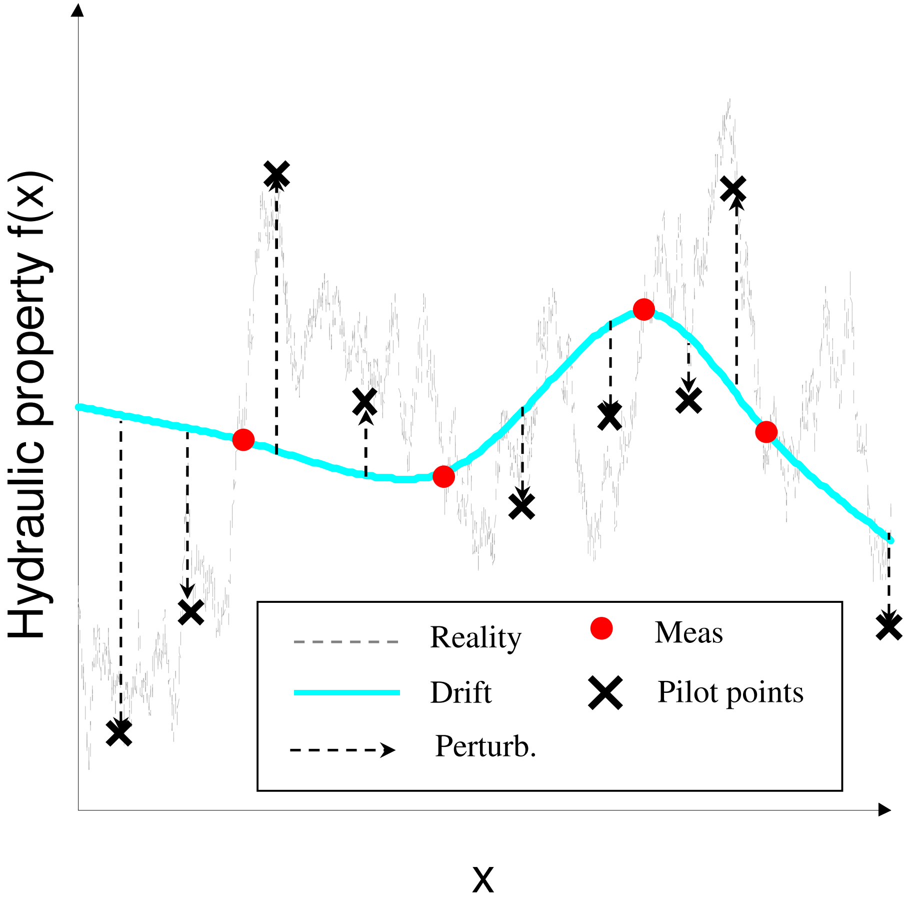
$$f_p(\mathbf{x}) = \sum_{j=1}^{Npp} \lambda_j^{pp}(\mathbf{x})\, p_j$$

Weights λ^{pp} and λ^{Z} calculated jointly

$$p_j^* = p^*(\mathbf{x}_j) = \sum_{k=1}^{\dim Z} \beta_k(\mathbf{x}_j)\, f_{k_*}$$

Prior information calculated from measurements

The Pilot Points Method

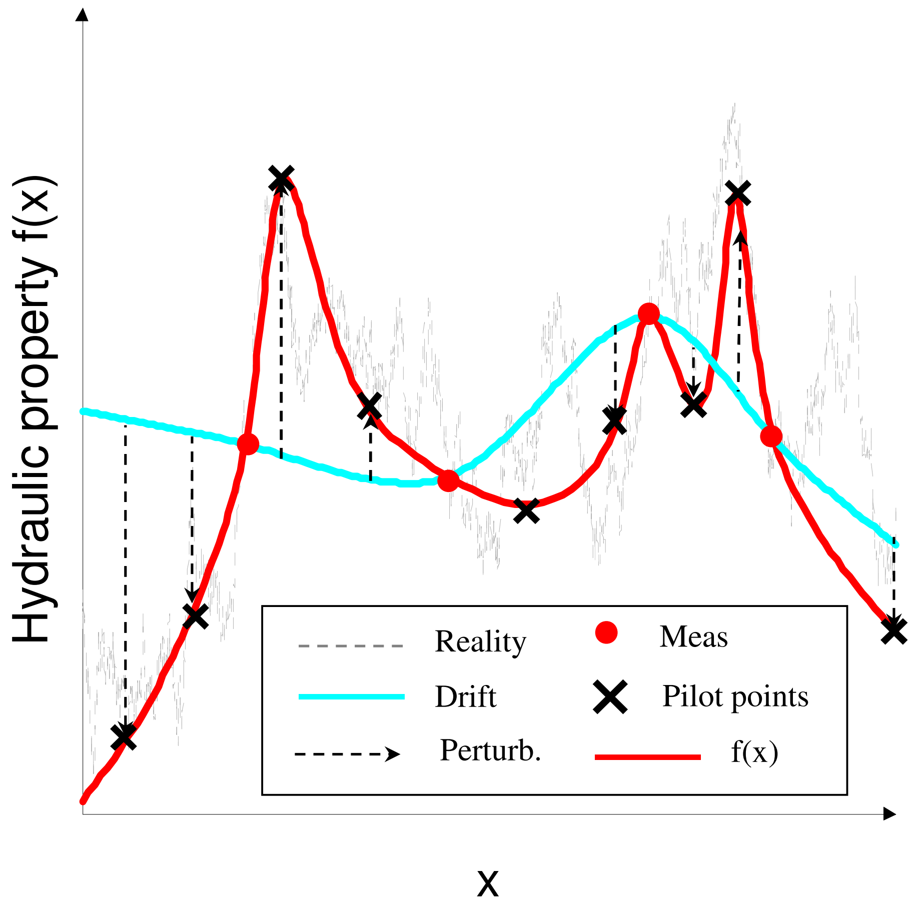


Parameterize hydraulic property

- Definition of a geostatistical model
- Parameterize drift
- Parameterize residual
- **Optimize model parameters**

Minimization of an objective function

The Pilot Points Method



Parameterize hydraulic property

- Definition of a geostatistical model
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Geostatistical Inversion

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Kriging estimation covariance

$$\left\langle Y'(\mathbf{x})Y'(\mathbf{y})\right\rangle = -\sum_{j=1}^{N_Y}\lambda_j(\mathbf{x})\sum_{i=1}^{N_Y}\lambda_i(\mathbf{y})\left[\gamma\left(\mathbf{x}_j-\mathbf{x}_i,\theta\right)-Q_{ji}\right]$$

$$-\gamma\left(\mathbf{x}-\mathbf{y},\theta\right)+\sum_{i=1}^{N_Y}\lambda_i(\mathbf{x})\gamma\left(\mathbf{y}-\mathbf{x}_i,\theta\right)+\sum_{i=1}^{N_Y}\lambda_i(\mathbf{y})\gamma\left(\mathbf{x}-\mathbf{x}_i,\theta\right)$$

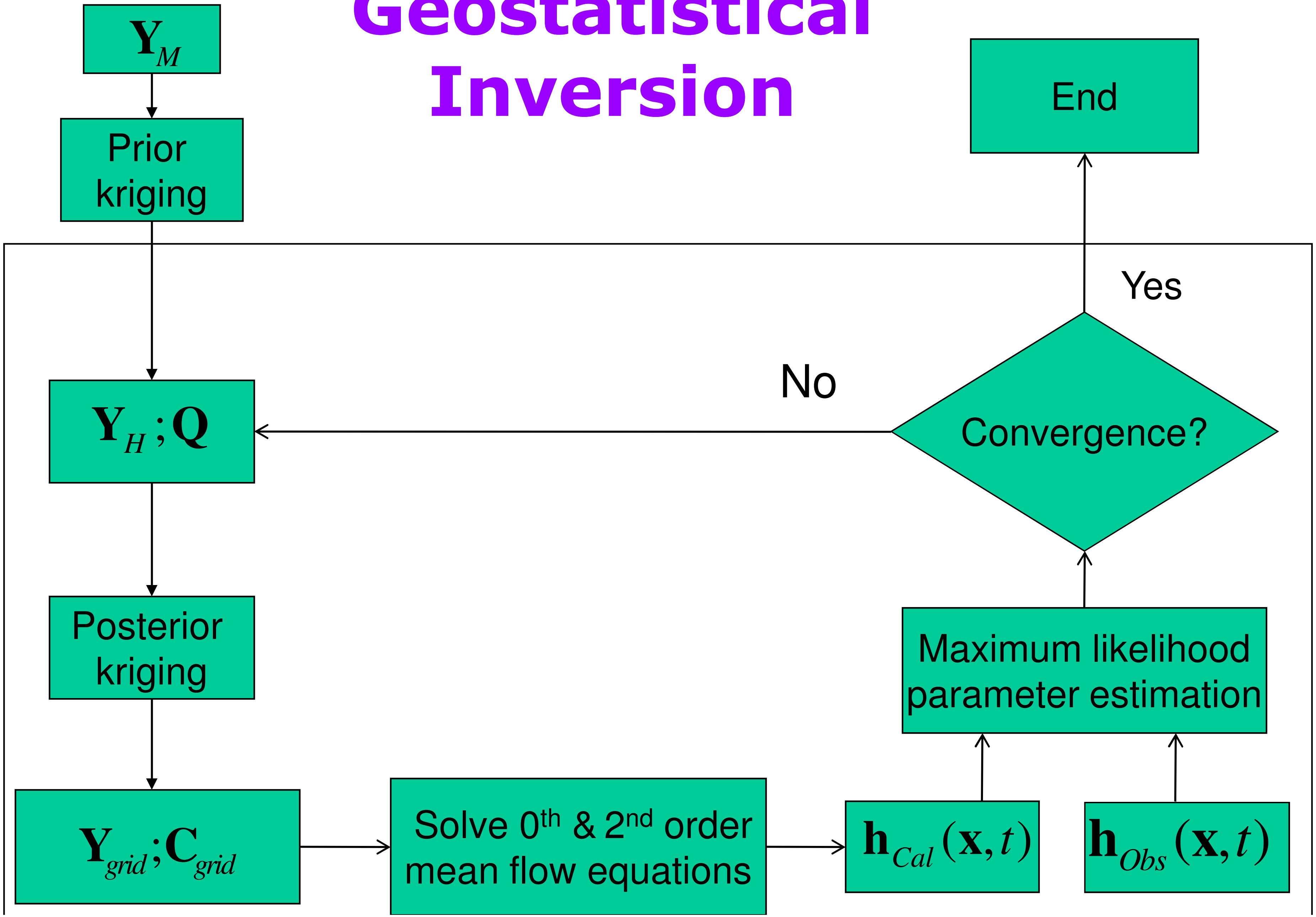
$\gamma(s,\theta) =$ **variogram of *Y***

$s =$ **separation distance (lag)**

$\theta =$ **variogram (statistical) parameters**

$\mathbf{Q} =$ **parameter estimation covariance**

Geostatistical Inversion



Maximum likelihood parameter estimation

Estimate $\beta = \left(\mathbf{Y}_H, \theta\right)^T$ **by minimizing**

$$NLL = \left(\boldsymbol{v}^* - \boldsymbol{v}\right)^T \boldsymbol{C}_v^{-1}\left(\boldsymbol{v}^* - \boldsymbol{v}\right) + \left(\mathbf{Y}^* - \mathbf{Y}\right)^T \boldsymbol{C}_Y^{-1}\left(\mathbf{Y}^* - \mathbf{Y}\right) + M \ln 2\pi$$

$\boldsymbol{M} = \boldsymbol{N_v} + \boldsymbol{N_Y}$

$\boldsymbol{v}^* =$ **measured state variable**

$\boldsymbol{Y}^* =$ **prior (measured + pilot)** ***Y*** **values**

$\mathbf{C}_v = \sigma_{vE}^2 \mathbf{V}_v =$ **Prior** $N_v \times N_v$ **covariance of** $\boldsymbol{v}$ **meas. errors**

$\sigma_{vE}^2 =$ **known or unknown variance of** $\boldsymbol{v}$ **meas. errors**

Maximum likelihood parameter estimation

Prior *Y* covariance:

$$\mathbf{C}_{\mathbf{Y}} = \begin{bmatrix} \mathbf{C}_{YM} & 0 \\ 0 & \mathbf{C}_{YP} \end{bmatrix} = \sigma_{YE}^2 \begin{bmatrix} \mathbf{V}_{YM} & 0 \\ 0 & \mathbf{V}_{YP} \end{bmatrix}$$

$\mathbf{V}_{YM}$ = **diagonal**

$\mathbf{V}_{YP}$ = **non-diagonal**

σ_{YE}^2 = **known or unknown variance of *Y* mesur. errors**

If $\theta, \sigma_{vE}^2, \sigma_{YE}^2$ **are known minimize**

$$F = \underbrace{\left(\boldsymbol{v}^* - \boldsymbol{v}\right)^{\mathrm{T}} \mathbf{V}_v^{-1} \left(\boldsymbol{v}^* - \boldsymbol{v}\right)}_{F_v} + \mu \underbrace{\left(\boldsymbol{Y}^* - \boldsymbol{Y}\right)^{\mathrm{T}} \mathbf{V}_Y^{-1} \left(\boldsymbol{Y}^* - \boldsymbol{Y}\right)}_{F_Y}$$

$\mu = \sigma_{vE}^2 / \sigma_{YE}^2 =$ **Plausibility weight**

Otherwise iterate to overcome instability:

- **For range of θ and μ values**
  - **Estimate Y_H by minimizing F**
  - **Estimate** $\sigma_{vE}^2 = F_{MIN} / M$
  - **Estimate** $\sigma_{YE}^2 = \sigma_{hE}^2 / \mu$

Find optimum θ, μ *a posteriori* based on following criteria:

1. NLL

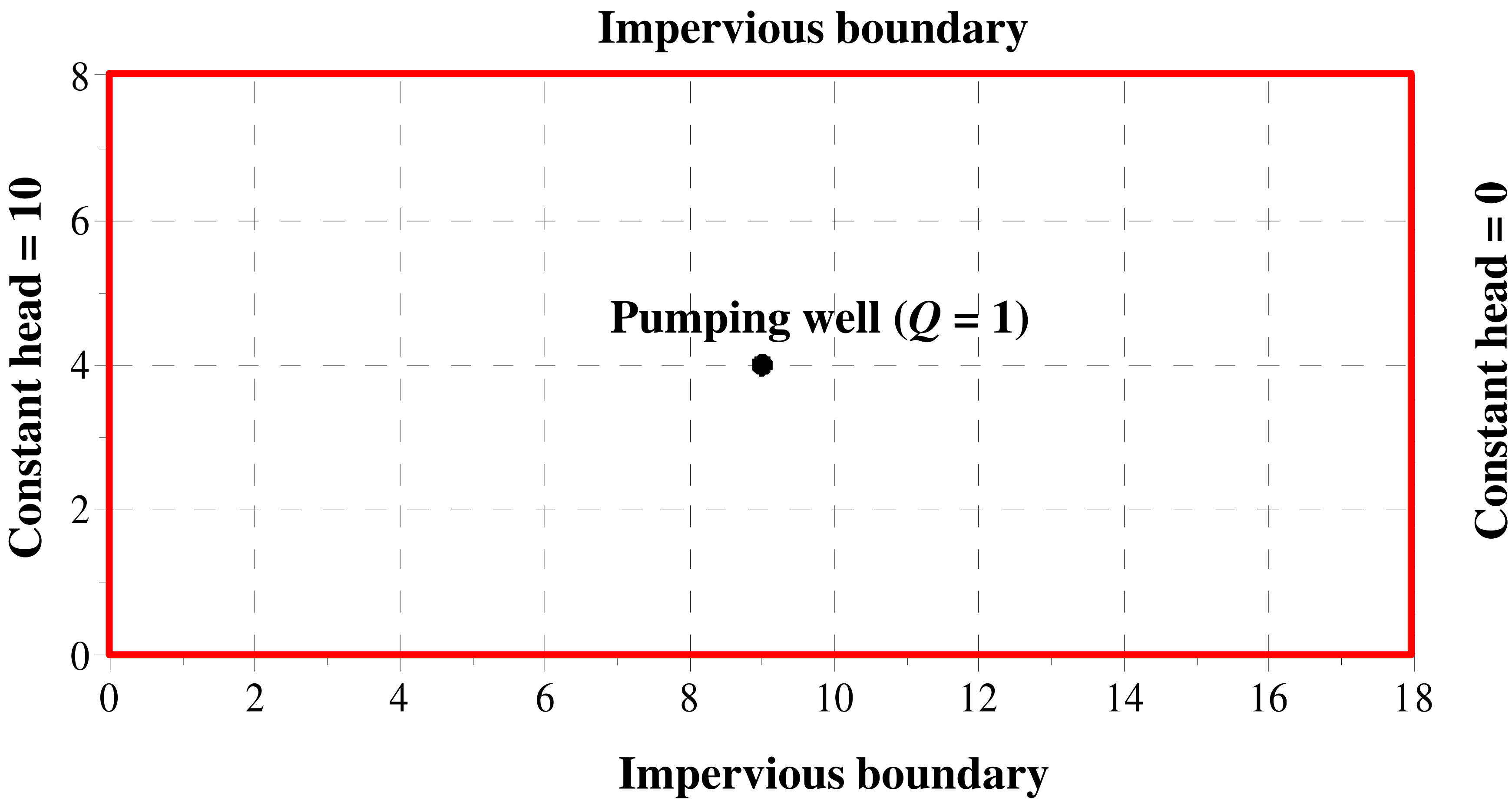
2. Model discrimination criteria

$$KIC = NLL + N_Y \ln\left(\frac{M}{2\pi}\right) - \ln|\mathbf{Q}|$$

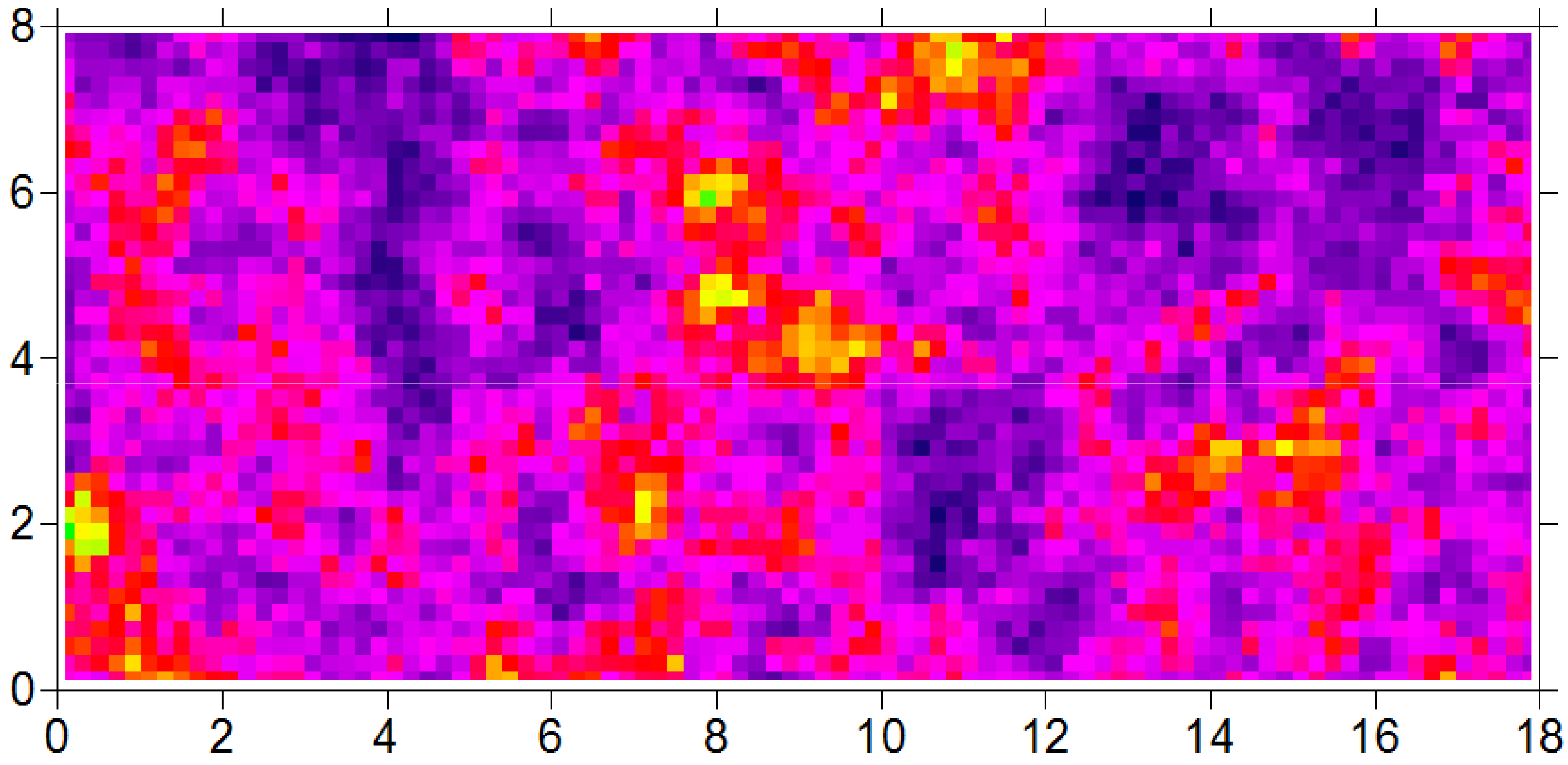
$$\mathbf{Q} = \sigma_{vE}^2 \left[\mathbf{J}^{\mathbf{T}} V_h^{-1} \mathbf{J} + \mu V_Y^{-1} \right]^{-1} \qquad J_{nm} = \partial v_n / \partial Y_m$$

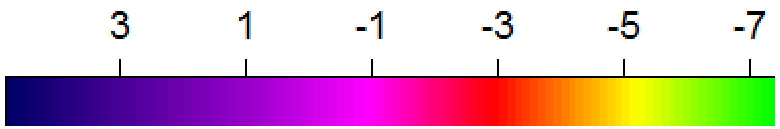
parameter estimation covariance

Synthetic Example



Synthetic Example

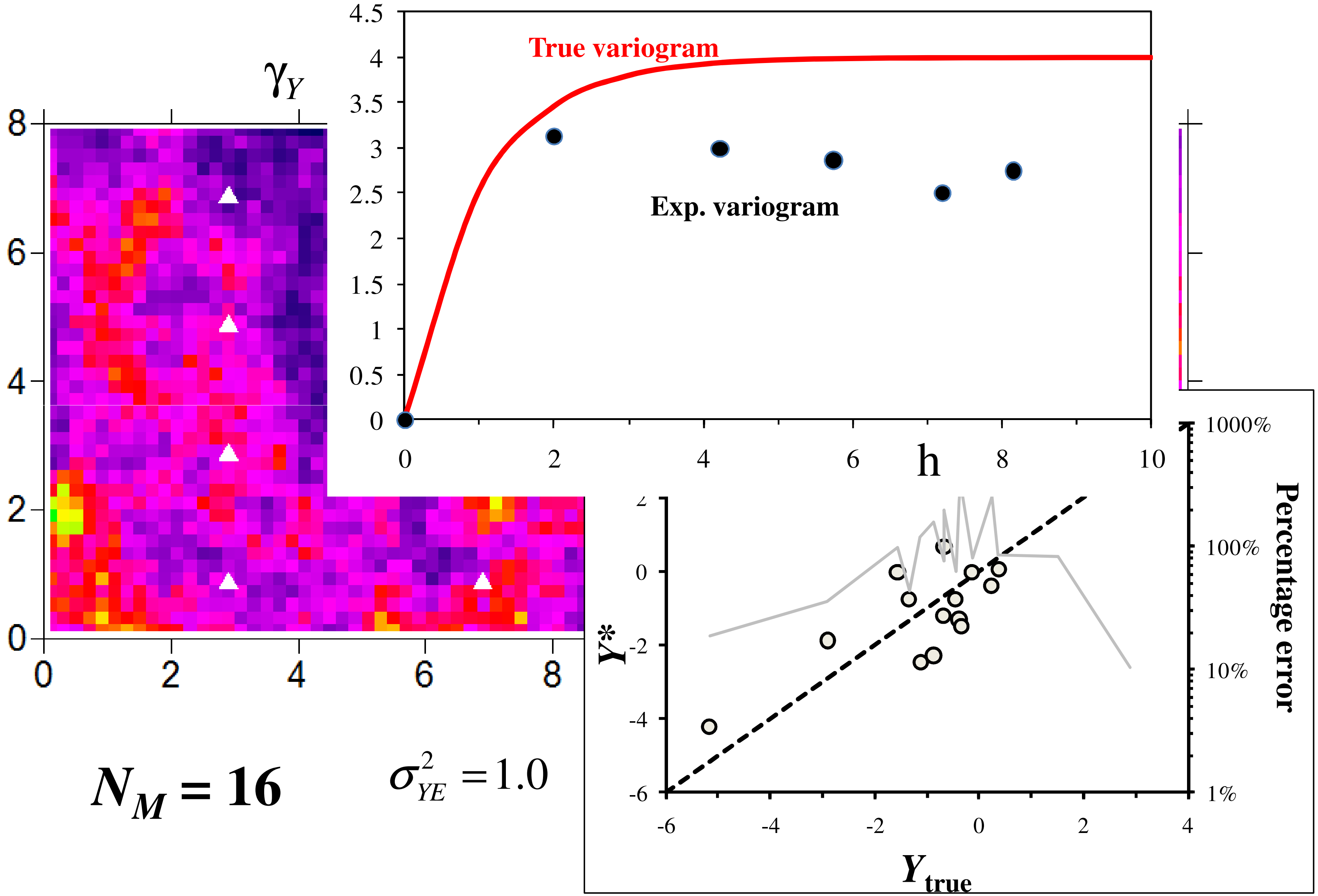




$$\gamma(s;\theta) = \sigma_Y^2 \left[1 - \exp\left(-\frac{s}{I_Y} \right) \right]$$

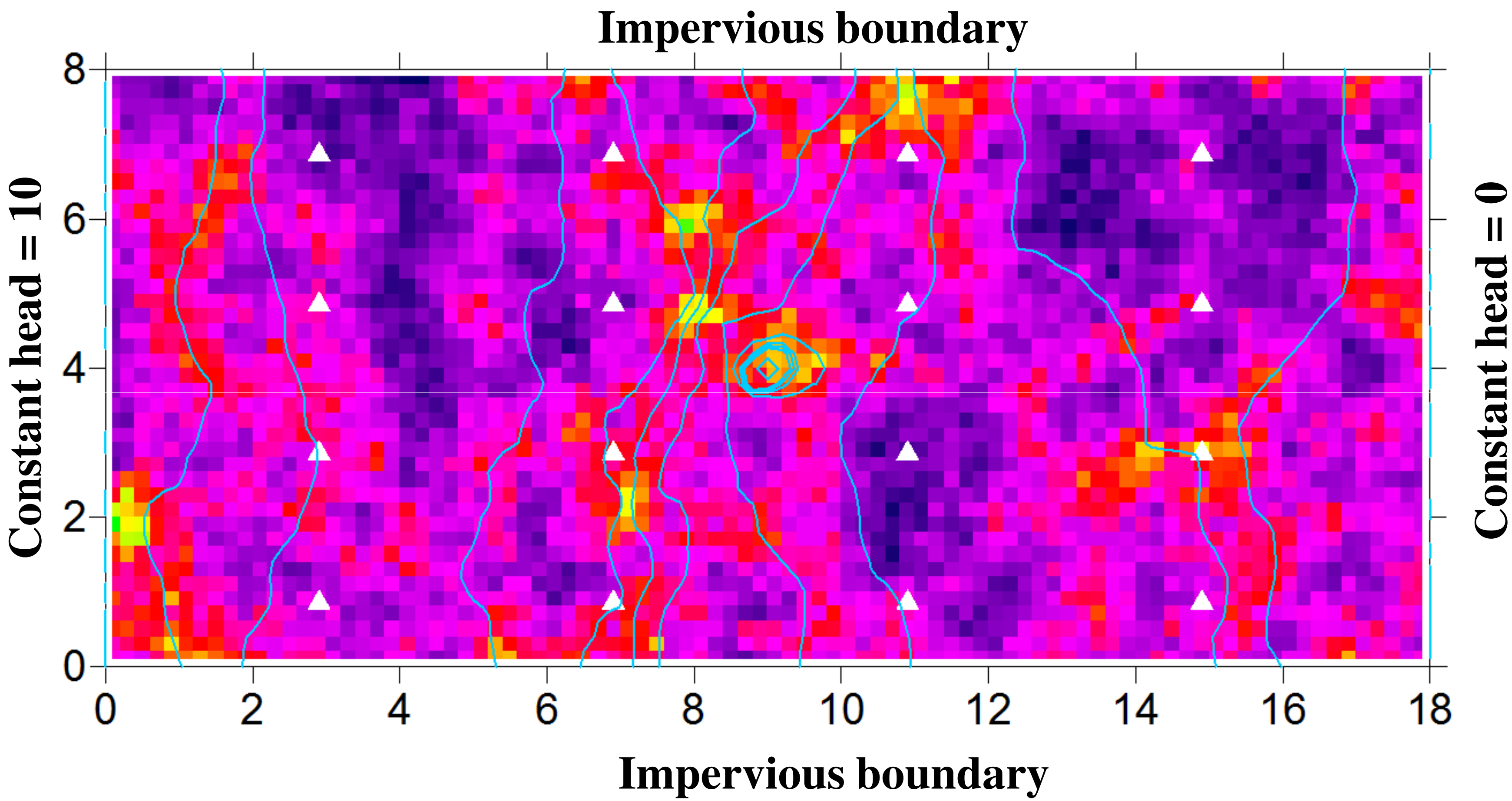
$I_Y = 1.0$ m; $\sigma_Y^2 = 4.0$

Synthetic Example

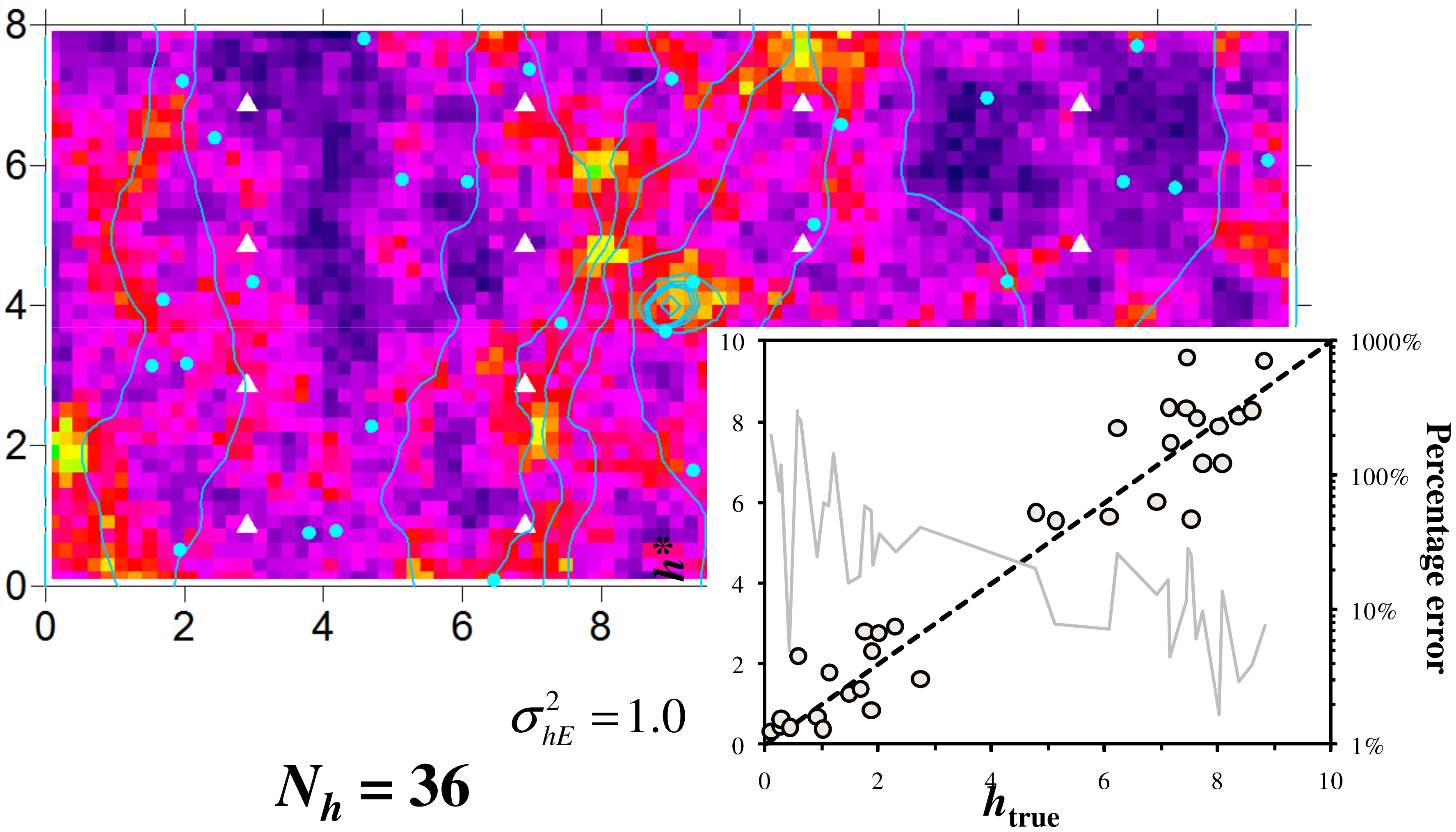


$N_M = 16$ $\sigma^2_{YE} = 1.0$

Synthetic Example



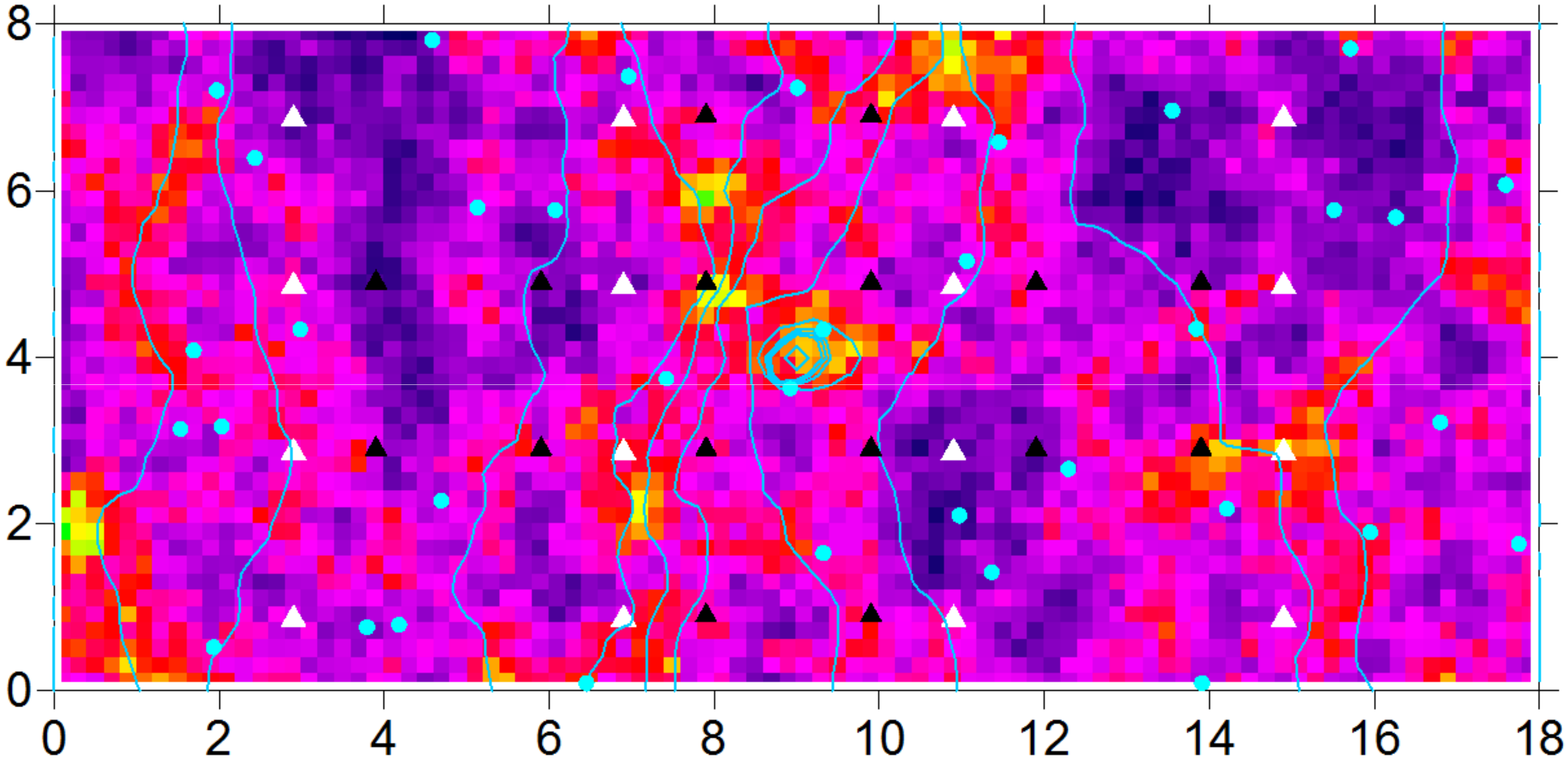
Synthetic Example



$\sigma^2_{hE} = 1.0$

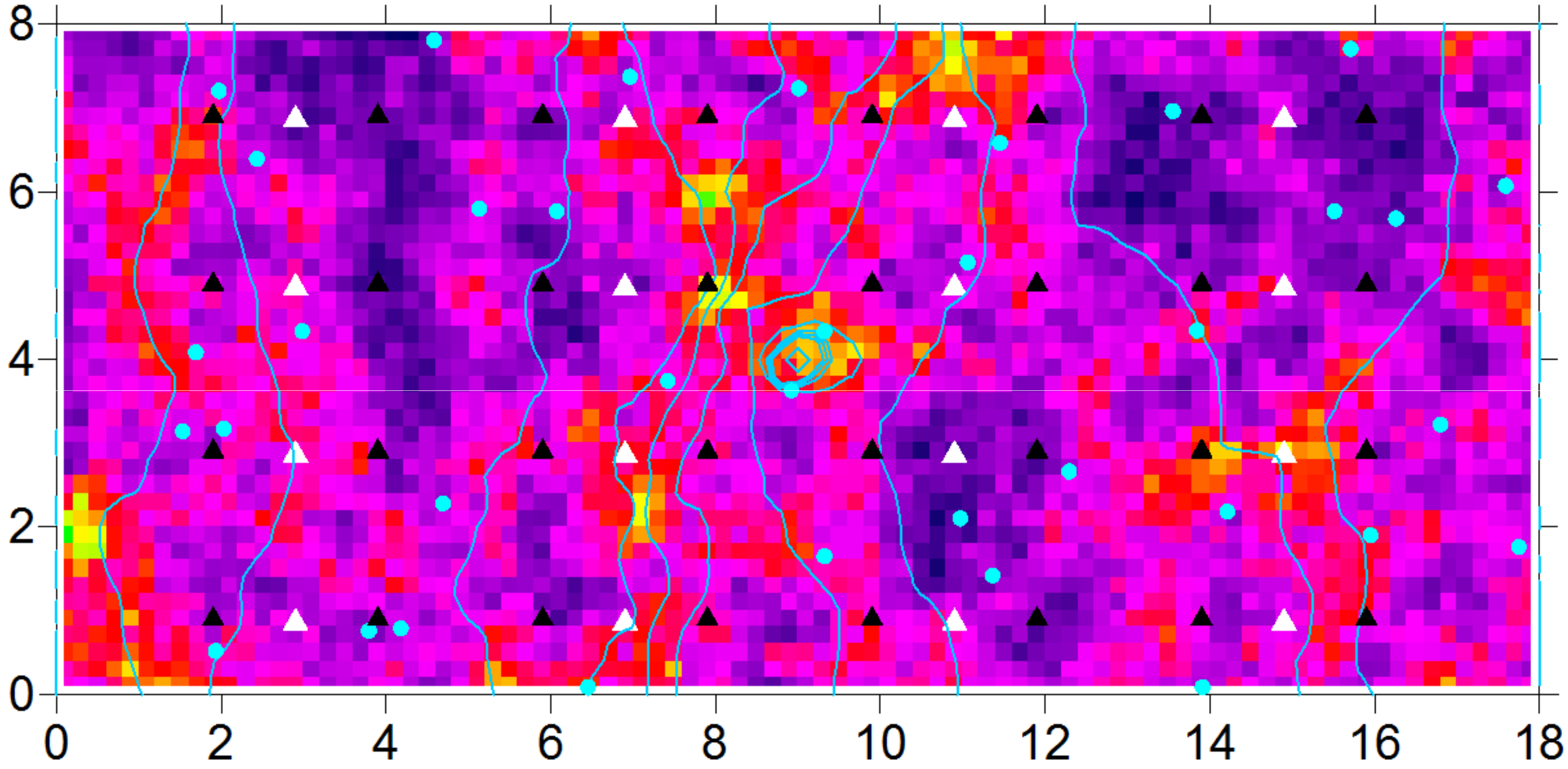
$N_h = 36$

Synthetic Example



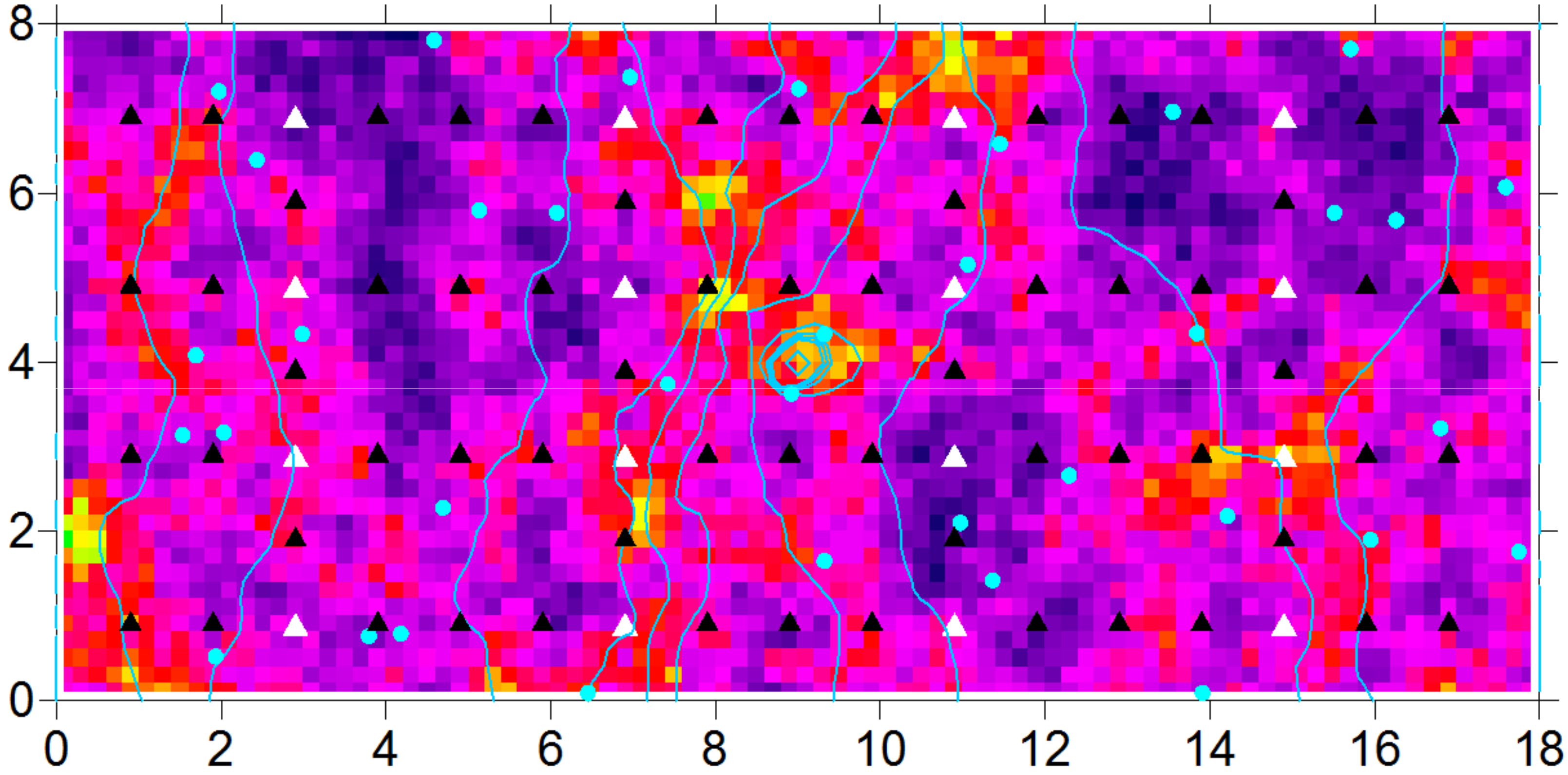
$N_p = 16$

Synthetic Example



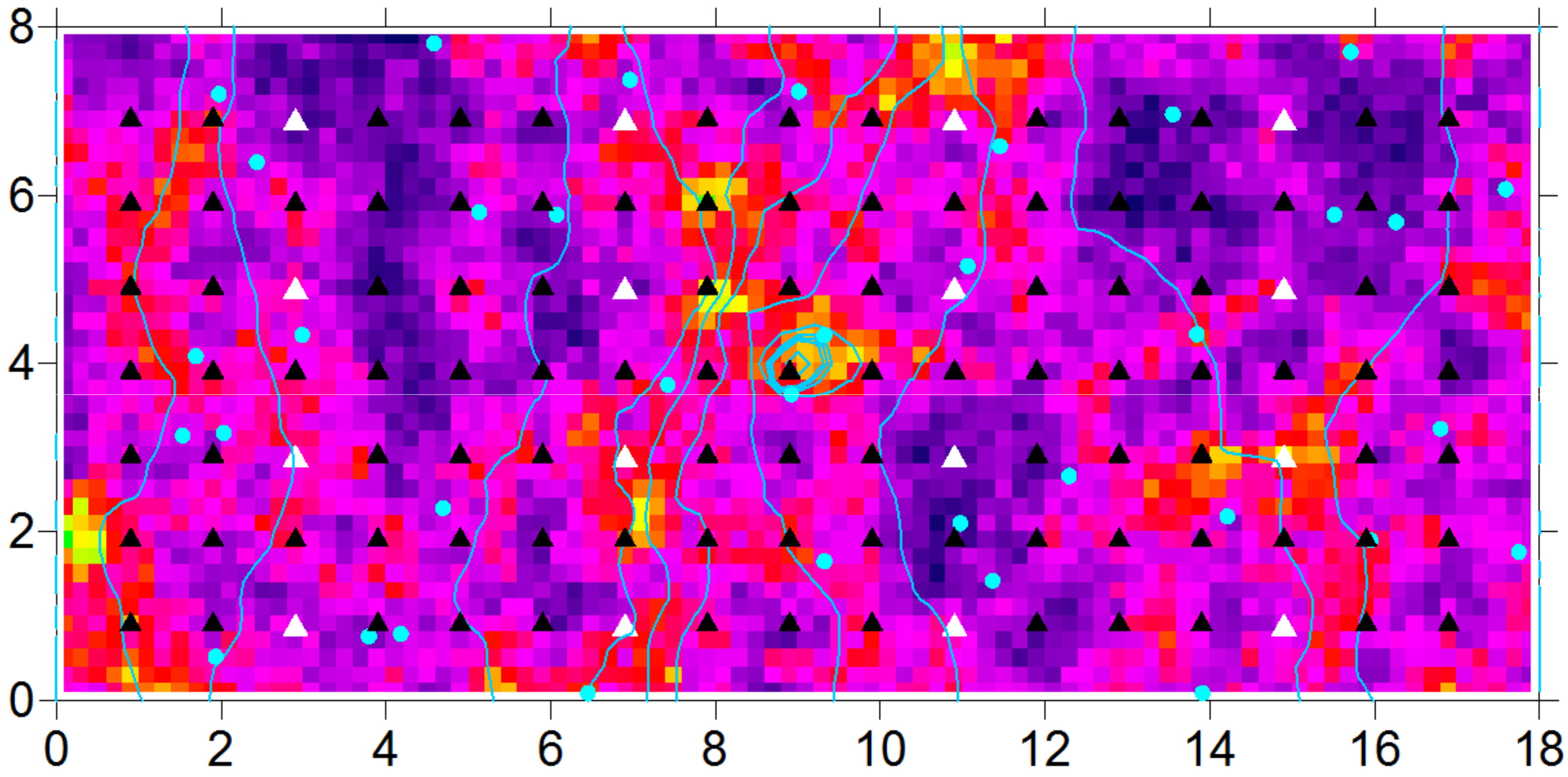
$N_p = 32$

Synthetic Example



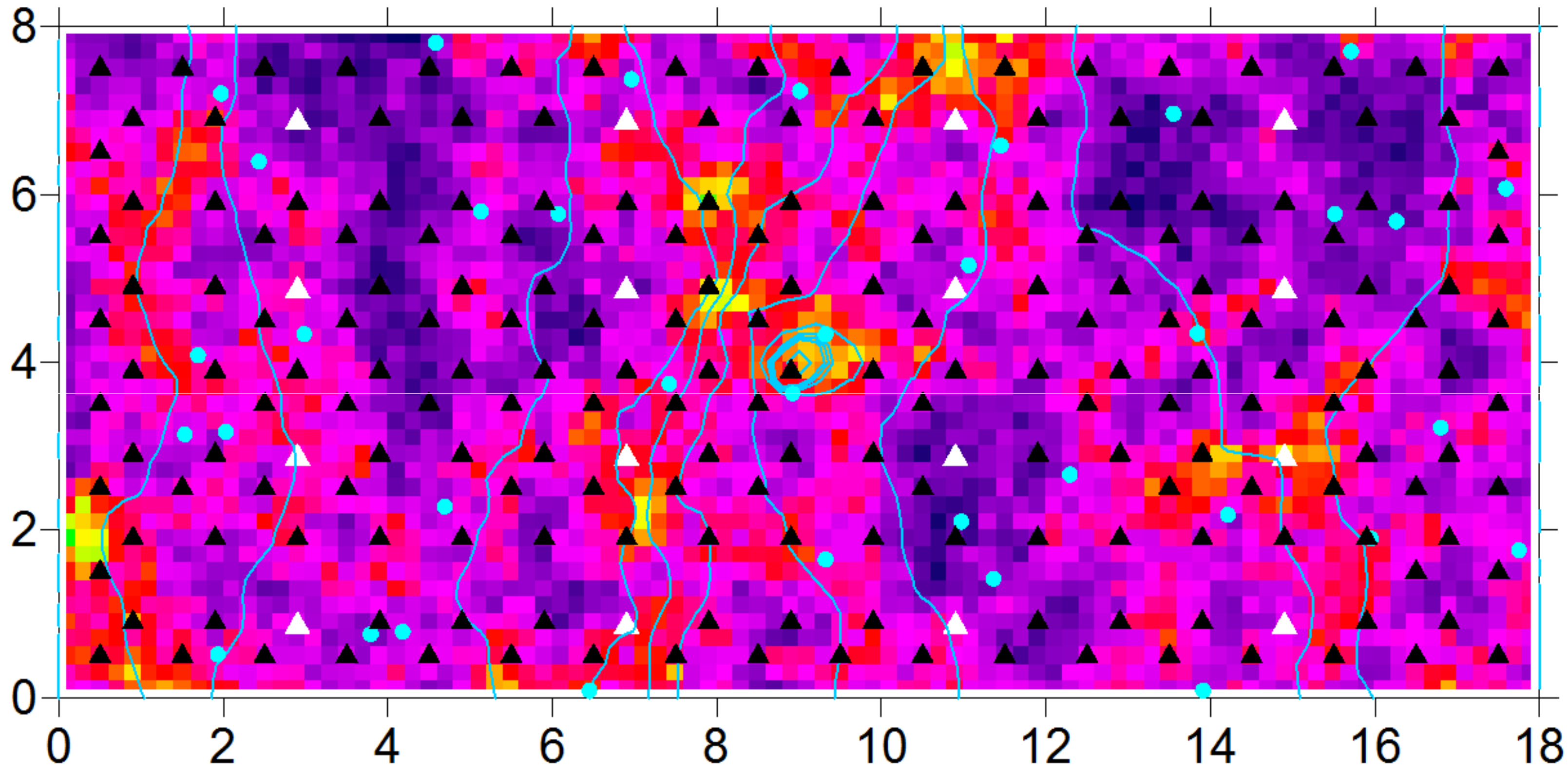
$$N_p = 64$$

Synthetic Example

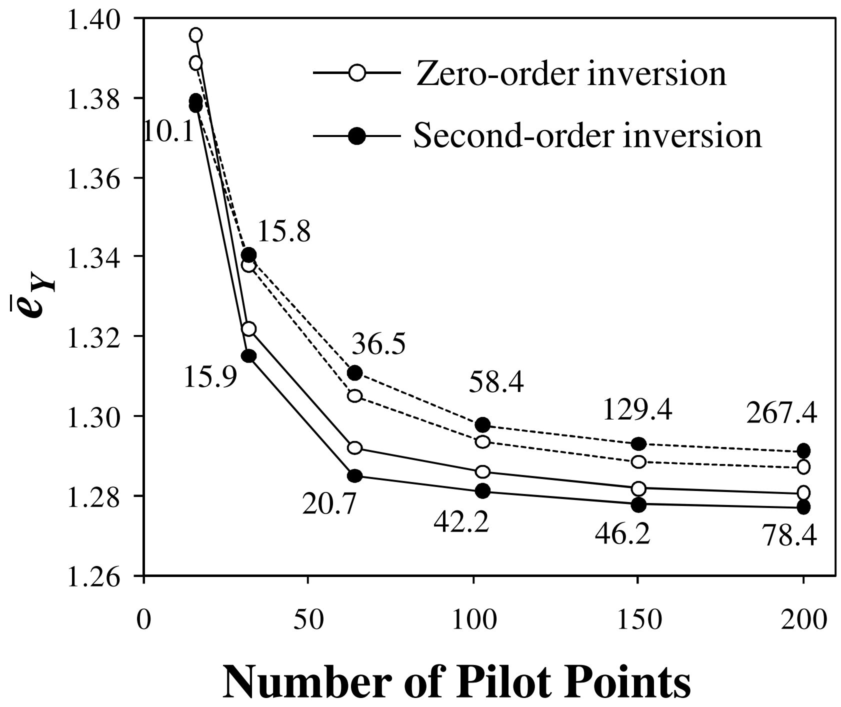


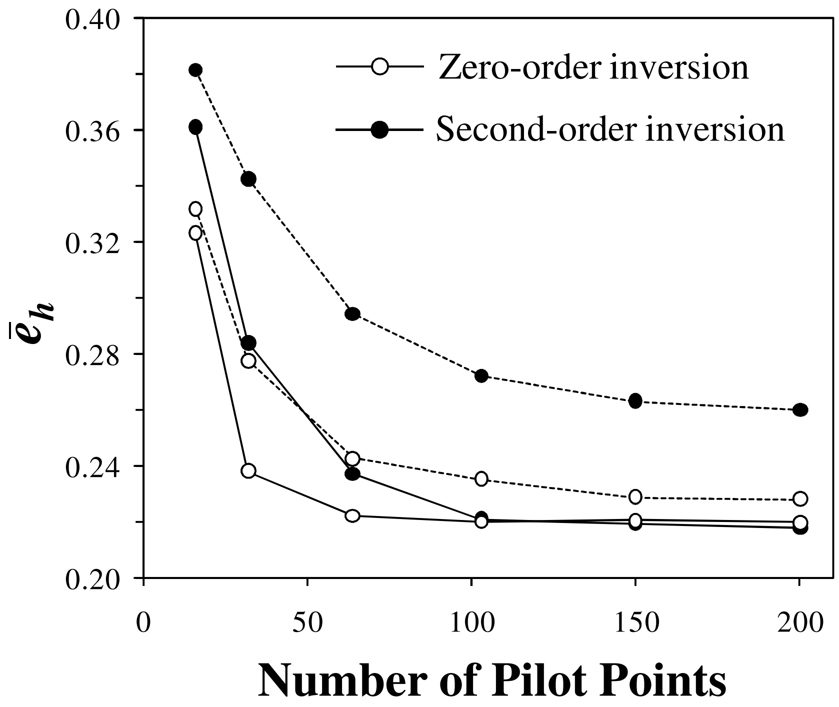
$$N_p = 100$$

Synthetic Example



$N_p = 200$





$$\overline{e}_Y = \frac{1}{N_e} \sum_{i=1}^{N_e} \left| \left\langle Y(\mathbf{x}_i^e) \right\rangle_c^{[a]} - Y_{ref}(\mathbf{x}_i^e) \right|$$

$$\overline{e}_h = \frac{1}{N_g} \sum_{j=1}^{N_g} \left| \left\langle h^{[a]}(\mathbf{x}_j) \right\rangle_c - h_{ref}(\mathbf{x}_j) \right|$$

Identification of μ

Various combinations of (*i*) values of the plausibility weight (0.01 ≤ μ ≤ 100), (*ii*) variogram sill (0.5 ≤ σ_Y^2 ≤ 6.0), (*iii*) integral scale (0.25 ≤ I_Y ≤ 4.0) for each network of pilot points selected.

	Zero-order inversion				Second-order inversion			
Best μ	$N_p = 16$	$N_p = 32$	$N_p = 64$	$N_p = 103$	$N_p = 16$	$N_p = 32$	$N_p = 64$	$N_p = 103$
0.01	2%	0%	0%	0%	0%	0%	0%	0%
0.1	13%	9%	9%	9%	22%	7%	7%	7%
0.5	60%	60%	42%	51%	56%	67%	53%	44%
0.75	4%	11%	13%	9%	2%	7%	16%	20%
1.0	18%	7%	22%	31%	20%	20%	24%	29%
5.0	2%	13%	13%	0%	0%	0%	0%	0%
10	0%	0%	0%	0%	0%	0%	0%	0%
	82%	**78%**	**78%**	**91%**	**78%**	**93%**	**93%**	**93%**

Identification of variogram parameters

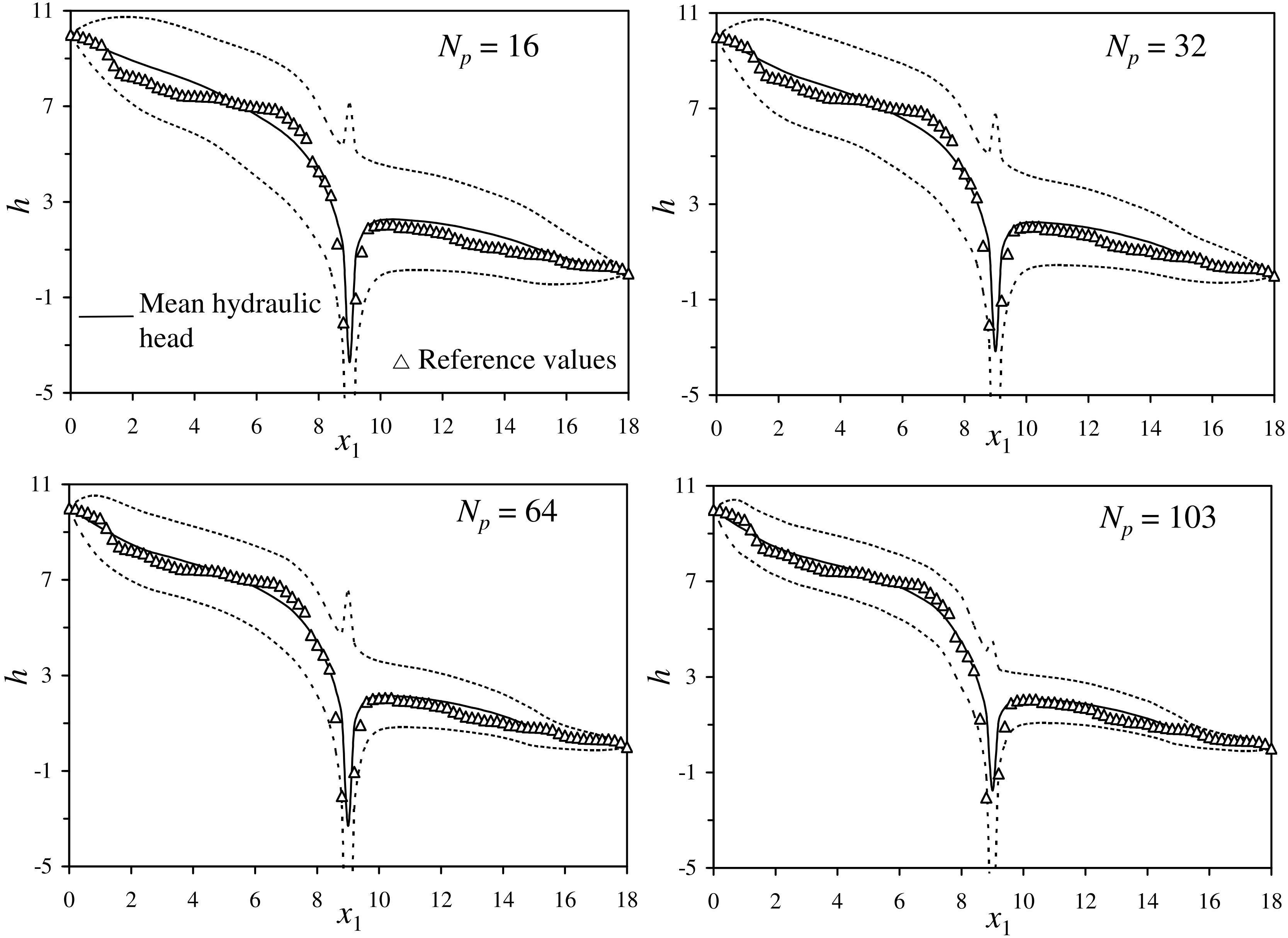
$0.5 \leq \mu \leq 1.0$

	Zero-order inversion			Second-order inversion		
Best I_Y	$N_p = 16$	$N_p = 32$	$N_p = 64$	$N_p = 16$	$N_p = 32$	$N_p = 64$
0.25	17%	6%	0%	6%	6%	0%
0.5	6%	0%	0%	22%	0%	0%
1.0	78%	89%	100%	72%	56%	100%
2.0	0%	6%	0%	0%	33%	0%
4.0	0%	0%	0%	0%	6%	0%

The use of a large number of pilot points does not necessarily renders a more accurate identification of all the parameters of interest. Fitting the model to noise!

Min KIC

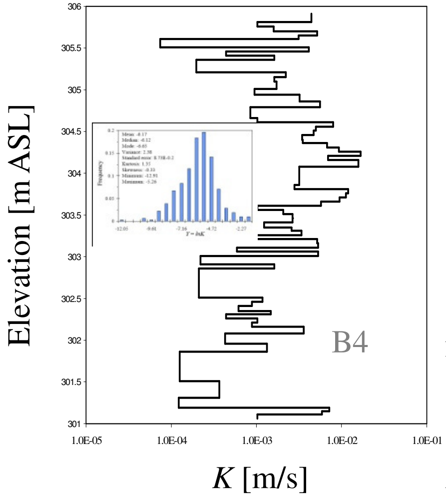
	Zero-order inversion					Second-order inversion				
N_p	μ	σ_Y^2	I_Y	σ_{hE}^2	σ_{YE}^2	μ	σ_Y^2	I_Y	σ_{hE}^2	σ_{YE}^2
16	0.5	4.0	1.0	0.7	1.4	0.5	3.0	1.0	0.7	1.5
32	0.5	4.5	1.0	0.5	1.0	0.5	4.0	1.0	0.5	1.1
64	0.5	3.0	1.0	0.4	0.7	0.5	3.0	1.0	0.4	0.7
103	0.5	2.0	1.0	0.3	0.5	0.5	2.0	1.0	0.3	0.6


$N_p = 16$
$N_p = 32$
$N_p = 64$
$N_p = 103$
Mean hydraulic head
△ Reference values
h
x_1
11
7
3
-1
-5
0
2
4
6
8
10
12
14
16
18

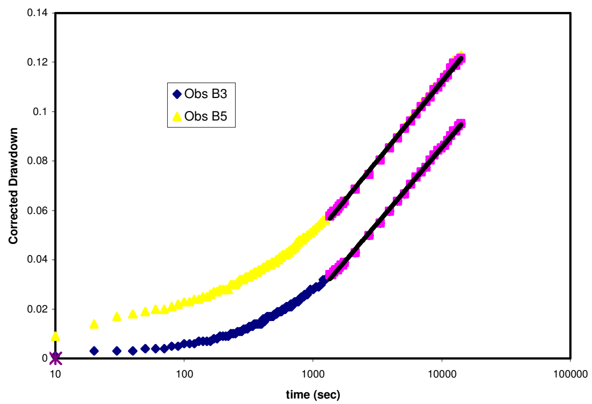
Field case application

Data available

K from flow-meters

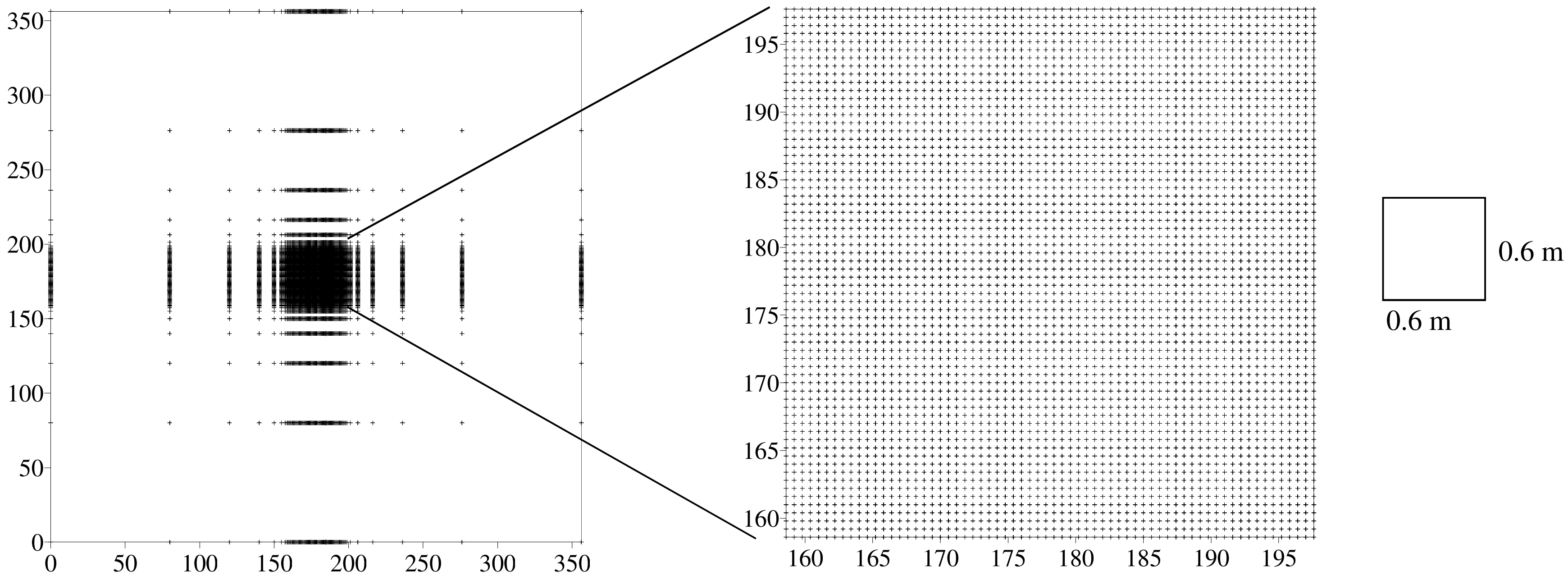


Drawdown data from 4 pumping tests in B2 – B5.



5 transmissivity measurments;
16 pseudo steady state drawdowns

Numerical grid



79 × 79 elements

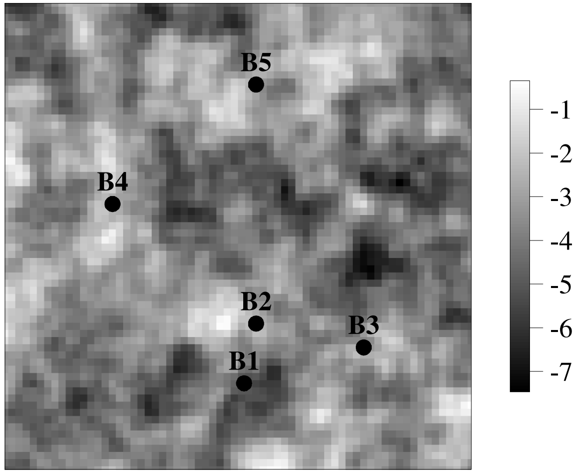
365.2 m × 365.2 m

65 × 65 elements

39 m × 39 m

Field case application

Synthetic case:



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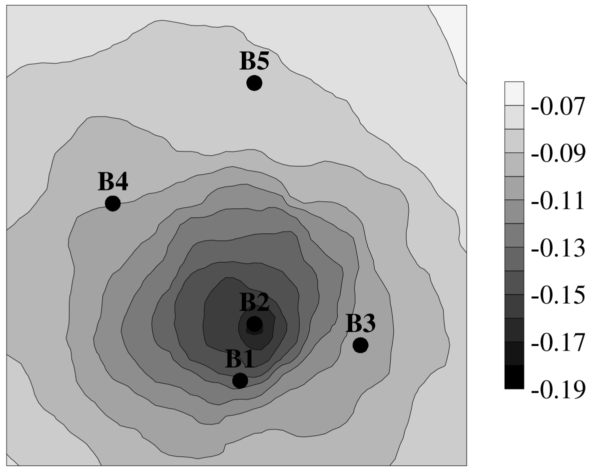
$I_Y = 2.5$ m; $\sigma_Y^2 = 1.5$

$Y^{TRUE} \Rightarrow h^{TRUE}$

$$\sigma_{YE} = \pm 1 \longrightarrow Y^*$$

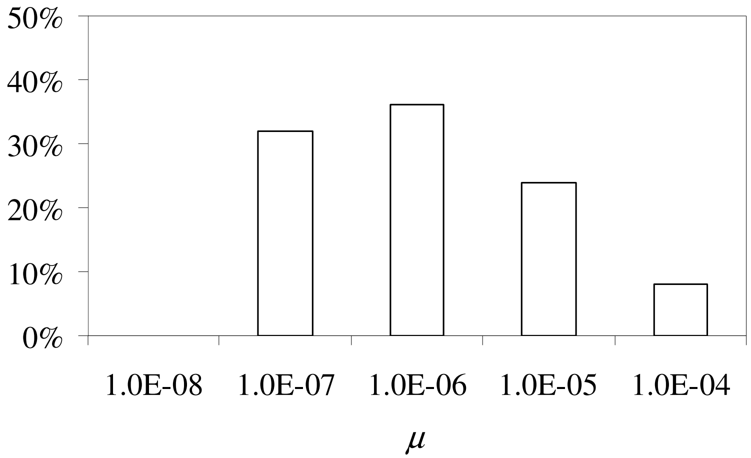
$$\sigma_{hE} = \pm 0.001\,\text{m} \longrightarrow h^*$$

$$\mu = \frac{\sigma_{hE}^2}{\sigma_{YE}^2} = 10^{-6}$$



Synthetic case

Zero Order Inversion

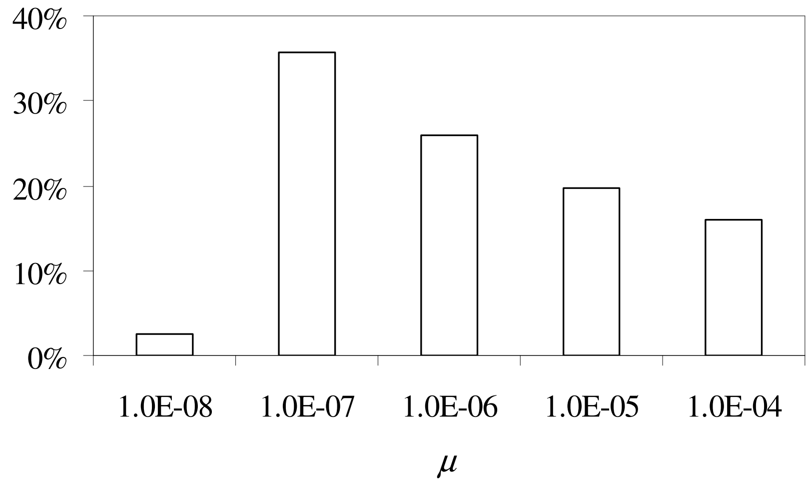


$\mu = 10^{-6}$

$\mu = 10^{-6}; I_Y = 2.5\text{ m}; \sigma_Y^2 = 5.0$

Field case application

Zero Order Inversion



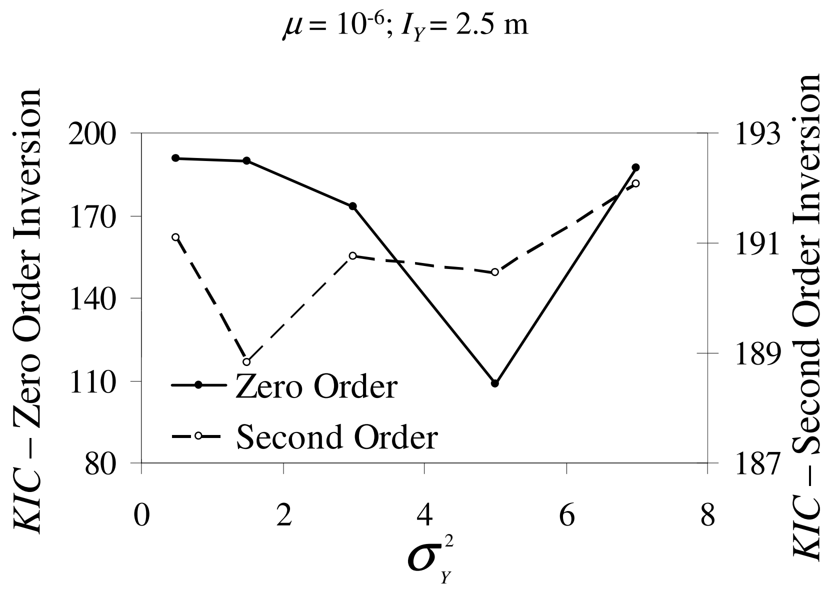
$\mu = 10^{-7}$

$\mu = 10^{-5}; I_Y = 3.0\text{ m}; \sigma_Y^2 = 1.0$

Synthetic case

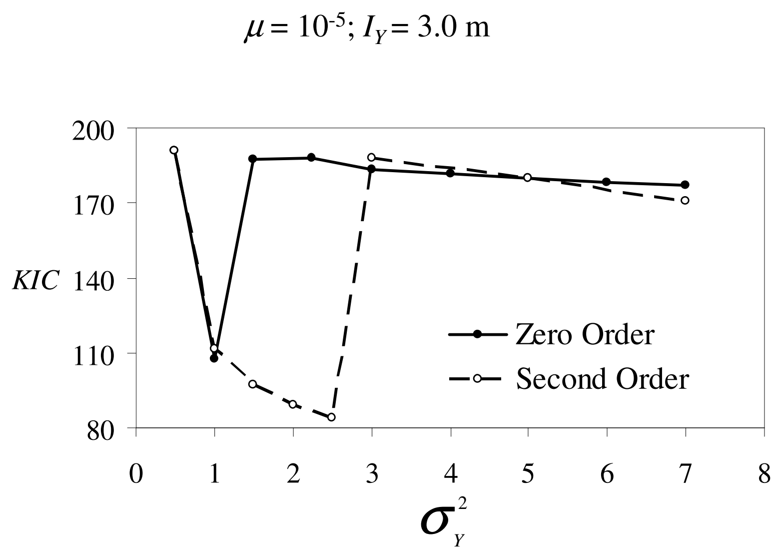
Field case application

Second Order Inversion



$\mu = 10^{-6}; I_Y = 2.5$ m; $\sigma_Y^2 = 1.5$

Second Order Inversion

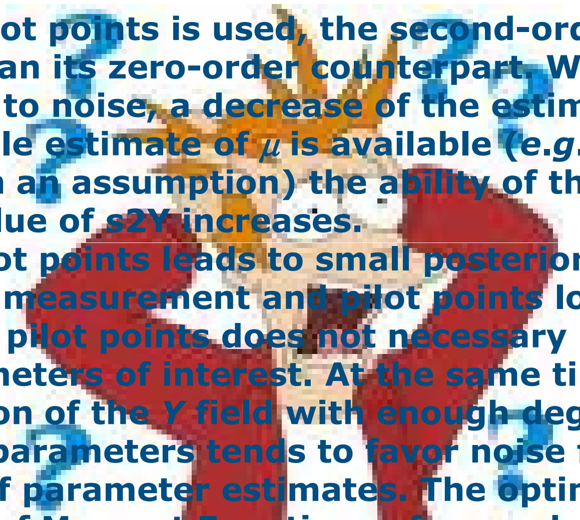


$\mu = 10^{-5}; I_Y = 3.0$ m; $\sigma_Y^2 = 2.5$

Conclusions

The mean absolute error between the reconstructed and true *Y* fields tends to be slightly smaller for a second- than for a zero-order inversion. Values of tend to decrease when the number of pilot points, N_p, increases, until they reach a plateau which is practically insensitive to N_p.

Estimation of the plausibility weight and integral scale of *Y* is quite robust and can be performed with a limited number of pilot points and with a low order approximation of the Moment Equations. The ability of *KIC* to identify *μ* tends to increase with N_p and (slightly) with the order of inversion, regardless of the assumed statistical parameters of the underlying *Y* field.



When a limited number of pilot points is used, the second-order solution can identify the optimum sill more sharply than its zero-order counterpart. When N_p becomes so large that the model starts being fitted to noise, a decrease of the estimated sill value is noted with N_p. When a sufficiently reliable estimate of μ is available (*e.g.*, when experimental information can support such an assumption) the ability of the second-order inversion to correctly identify the true value of s2Y increases.

Increasing the number of pilot points leads to small posterior variance of *Y* and *h*, especially in the vicinity of *Y* measurement and pilot points locations.

The use of a large number of pilot points does not necessary imply a more accurate identification of all the parameters of interest. At the same time, it must be large enough to provide the characterization of the *Y* field with enough degrees of freedom. However, a very large number of model parameters tends to favor noise fitting, thus causing a deterioration of the quality of parameter estimates. The optimum number of pilot points to be adopted during inversion of Moment Equations of groundwater flow depends on the quantity one desires to determine (*i.e.*, the spatial distribution of mean *Y*, the parameters of the *Y* variogram, the measurement error associated with the experimental data) and on the adopted flow model (zero- or second-order equations). Our example indicates that one should gradually increase N_p until the desired quantities become insensitive to it.

Our results suggest that the geostatistical inversion of groundwater flow Moment Equations can benefit from successive inversions of zero- and second-order equations to provide a robust and computationally affordable estimate of hydraulic and (geo-)statistical parameters (including the number of pilot points) of the problem.