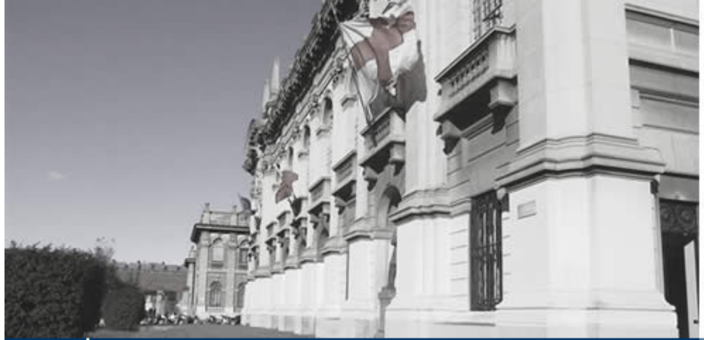

POLITECNICO DI MILANO

Analysis of Inverse Stochastic Moment Equations of Groundwater Flow in Heterogeneous Porous Media

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Objectives

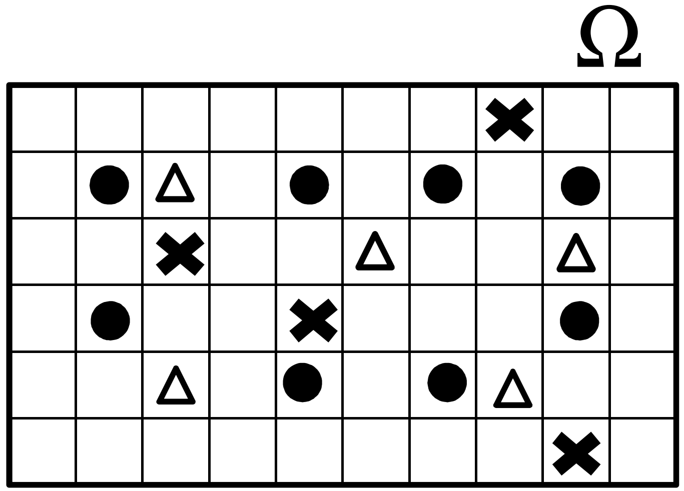
Available data:

- Log-conductivity ($Y=\ln(K)$) measurements
- Hydraulic head (h) measurements

Pilot points approach:

De Marsily, 1974

Log-conductivity measurements △
Pilot points ●
Hydraulic head measurements ✖



Estimation of:

- Spatial distribution of the parameters governing the groundwater flow equation $\ln(K)$
- Underlying variogram key parameters (I_Y, σ_Y^2)
- Statistical parameters (σ_{hE}^2, σ_{yE}^2)

Moment Equations of Groundwater Flow

Neuman and Orr, 1993
Tartakovsky and Neuman, 1998
Guadagnini and Neuman, 1999
Ye et al., 2004

Zero-order mean flow equation:

$$\left\langle \overline{\mathbf{q}}^{(0)}(\mathbf{x},\lambda) \right\rangle = -K_G(\mathbf{x}) \nabla \left\langle \overline{h}^{(0)}(\mathbf{x},\lambda) \right\rangle \qquad \mathbf{x} \in \Omega$$

$$\nabla \cdot \left\langle \overline{\mathbf{q}}^{(0)}(\mathbf{x},\lambda) \right\rangle + S(\mathbf{x})\lambda \left\langle \overline{h}^{(0)}(\mathbf{x},\lambda) \right\rangle = \left\langle \overline{f}(\mathbf{x},\lambda) \right\rangle + S(\mathbf{x}) \left\langle H_0(\mathbf{x}) \right\rangle \qquad \mathbf{x} \in \Omega$$

Second-order mean flow equation:

$$\left\langle \overline{\mathbf{q}}^{(2)}(\mathbf{x},\lambda) \right\rangle = -K_G(\mathbf{x}) \left[\nabla \left\langle \overline{h}^{(2)}(\mathbf{x},\lambda) \right\rangle + \frac{\sigma_Y^2(\mathbf{x})}{2} \nabla \left\langle \overline{h}^{(2)}(\mathbf{x},\lambda) \right\rangle \right] + \overline{\mathbf{r}}_c^{(2)}(\mathbf{x},\lambda) \qquad \mathbf{x} \in \Omega$$

$$\nabla \cdot \left\langle \overline{\mathbf{q}}^{(2)}(\mathbf{x},\lambda) \right\rangle + S(\mathbf{x})\lambda \left\langle \overline{h}^{(2)}(\mathbf{x},\lambda) \right\rangle = 0 \qquad \mathbf{x} \in \Omega$$

Maximum likelihood approach

Parameters:

$$\boldsymbol{\beta} = \left[\mathbf{Y}, \boldsymbol{\theta}\right]^T$$

Observations:

$$\mathbf{z}^* = \left[\mathbf{Y}^*, \mathbf{h}^*\right]^T$$

Maximum Likelihood Calibration (*Carrera and Neuman, 1986a*)
(*Hernandez et al., 2003, 2006*)

$$NLL = -2\ln\left[p\left(z^* \mid \hat{\beta}\right)\right] = \frac{J}{\sigma_{hE}^2} + \ln\left|\mathbf{V}_y\right| + \ln\left|\mathbf{V}_h\right| + N_h \ln\sigma_{hE}^2 + N_y \ln\sigma_{yE}^2 + N\ln 2\pi$$

For fixed value of $\boldsymbol{\theta} = \left[I_Y, \sigma_Y^2, \sigma_{hE}^2, \sigma_{yE}^2\right]^T$ (to avoid instability)

Objective function:

$$J = \left(\mathbf{h}^* - \hat{\mathbf{h}}\right)^T \mathbf{V}_h^{-1}\left(\mathbf{h}^* - \hat{\mathbf{h}}\right) + \mu\left(\mathbf{Y}^* - \hat{\mathbf{Y}}\right)^T \mathbf{V}_y^{-1}\left(\mathbf{Y}^* - \hat{\mathbf{Y}}\right)$$

($\mu = \sigma_{hE}^2 / \sigma_{yE}^2$: plausibility weight)

How to estimate $\boldsymbol{\theta} = \left[I_Y, \sigma_Y^2, \sigma_{hE}^2, \sigma_{yE}^2 \right]^T$?

NLL: no discriminatory power to select the optimum θ_k
(*Riva et al. 2010*)

Find the optimum θ_k minimizing:

$$AIC_k = -2\ln\left[L\left(\hat{\boldsymbol{\beta}}_k \middle| \mathbf{z}^* \right) \right] + 2N_k \qquad \textit{Akaike}, 1974$$

$$AICc_k = -2\ln\left[L\left(\hat{\boldsymbol{\beta}}_k \middle| \mathbf{z}^* \right) \right] + 2N_k + \frac{2N_k\left(N_k+1\right)}{N_z - N_k - 1} \qquad \textit{Hurvich and Tsai}, 1989$$

$$BIC_k = -2\ln\left[L\left(\hat{\boldsymbol{\beta}}_k \middle| \mathbf{z}^* \right) \right] + N_k \ln N_z \qquad \textit{Schwarz}, 1978$$

$$KIC_k = -2\ln\left[L\left(\hat{\boldsymbol{\beta}}_k \middle| \mathbf{z}^* \right) \right] - 2\ln\left[p\left(\hat{\boldsymbol{\beta}}_k \right) \right] + N_k \ln\left(N_z / 2\pi \right) + \ln\left| \overline{\mathbf{F}}_k \right| \qquad \textit{Kashyap}, 1982$$

Estimation of σ_Y^2

Minimization of NLL with respect to model parameters:

$$\nabla_{\mathbf{Y}_H} NLL \Big|_{\mathbf{Y}_H = \hat{\mathbf{Y}}_H} = \frac{2}{\sigma_{hE}^2} \mathfrak{J}^{\mathrm{T}} \mathbf{V}_h^{-1} \left(\hat{\mathbf{h}} - \mathbf{h}^* \right) + \frac{2}{\sigma_{YE}^2} \mathbf{V}_Y^{-1} \left(\hat{\mathbf{Y}}_H - \mathbf{Y}_H^* \right) = 0$$

$$\begin{cases} \hat{\mathbf{Y}}_M = \mathbf{Y}_M^* - \dfrac{\sigma_{YE}^2}{\sigma_{hE}^2} \mathbf{V}_{YM} \mathfrak{J}_{N_M}^{\mathrm{T}} \mathbf{V}_h^{-1} \left(\hat{\mathbf{h}} \left(\hat{\mathbf{Y}}_M , \hat{\mathbf{Y}}_P \right) - \mathbf{h}^* \right) \\ \hat{\mathbf{Y}}_P = \mathbf{Y}_P^* - \dfrac{\sigma_{YE}^2}{\sigma_{hE}^2} \mathbf{V}_{YP} \mathfrak{J}_{N_P}^{\mathrm{T}} \mathbf{V}_h^{-1} \left(\hat{\mathbf{h}} \left(\hat{\mathbf{Y}}_M , \hat{\mathbf{Y}}_P \right) - \mathbf{h}^* \right) \end{cases}$$

$$\lim_{\sigma_Y^2 \to 0} \left(\frac{J_h}{\sigma_{hE}^2} + \frac{J_{YM}}{\sigma_{yE}^2} + \frac{J_{YP}}{\sigma_{yE}^2} + N_t \ln \left| \mathbf{V}_x \right| + \ln \left| \mathbf{V}_Y \right| + N_h \ln \sigma_{hE}^2 + N_Y \ln \sigma_{YE}^2 + N \ln 2\pi \right)$$

Estimation of σ_Y^2

Minimization of NLL with respect to model parameters:

$$\nabla_{\mathbf{Y}_H} NLL\Big|_{\mathbf{Y}_H=\hat{\mathbf{Y}}_H} = \frac{2}{\sigma_{hE}^2}\mathfrak{I}^{\mathrm{T}}\mathbf{V}_h^{-1}\left(\hat{\mathbf{h}}-\mathbf{h}^*\right)+\frac{2}{\sigma_{YE}^2}\mathbf{V}_Y^{-1}\left(\hat{\mathbf{Y}}_H-\mathbf{Y}_H^*\right)=0$$

$$\begin{cases} \hat{\mathbf{Y}}_M = \mathbf{Y}_M^* - \dfrac{\sigma_{YE}^2}{\sigma_{hE}^2}\mathbf{V}_{YM}\mathfrak{I}_{N_M}^{\mathrm{T}}\mathbf{V}_h^{-1}\left(\hat{\mathbf{h}}\left(\hat{\mathbf{Y}}_M,\hat{\mathbf{Y}}_P\right)-\mathbf{h}^*\right) \\ \hat{\mathbf{Y}}_P = \mathbf{Y}_P^* - \dfrac{\sigma_{YE}^2}{\sigma_{hE}^2}\mathbf{V}_{YP}\mathfrak{I}_{N_P}^{\mathrm{T}}\mathbf{V}_h^{-1}\left(\hat{\mathbf{h}}\left(\hat{\mathbf{Y}}_M,\hat{\mathbf{Y}}_P\right)-\mathbf{h}^*\right) \end{cases}$$

$$\lim_{\sigma_Y^2\to 0}\left(\frac{J_h}{\sigma_{hE}^2}+\frac{J_{YM}}{\sigma_{yE}^2}+\frac{J_{YP}}{\sigma_{yE}^2}+N_t\ln\left|\mathbf{V}_x\right|+\ln\left|\mathbf{V}_Y\right|+N_h\ln\sigma_{hE}^2+N_Y\ln\sigma_{YE}^2+N\ln 2\pi\right)$$

Estimation of σ_Y^2

Kriging equations:

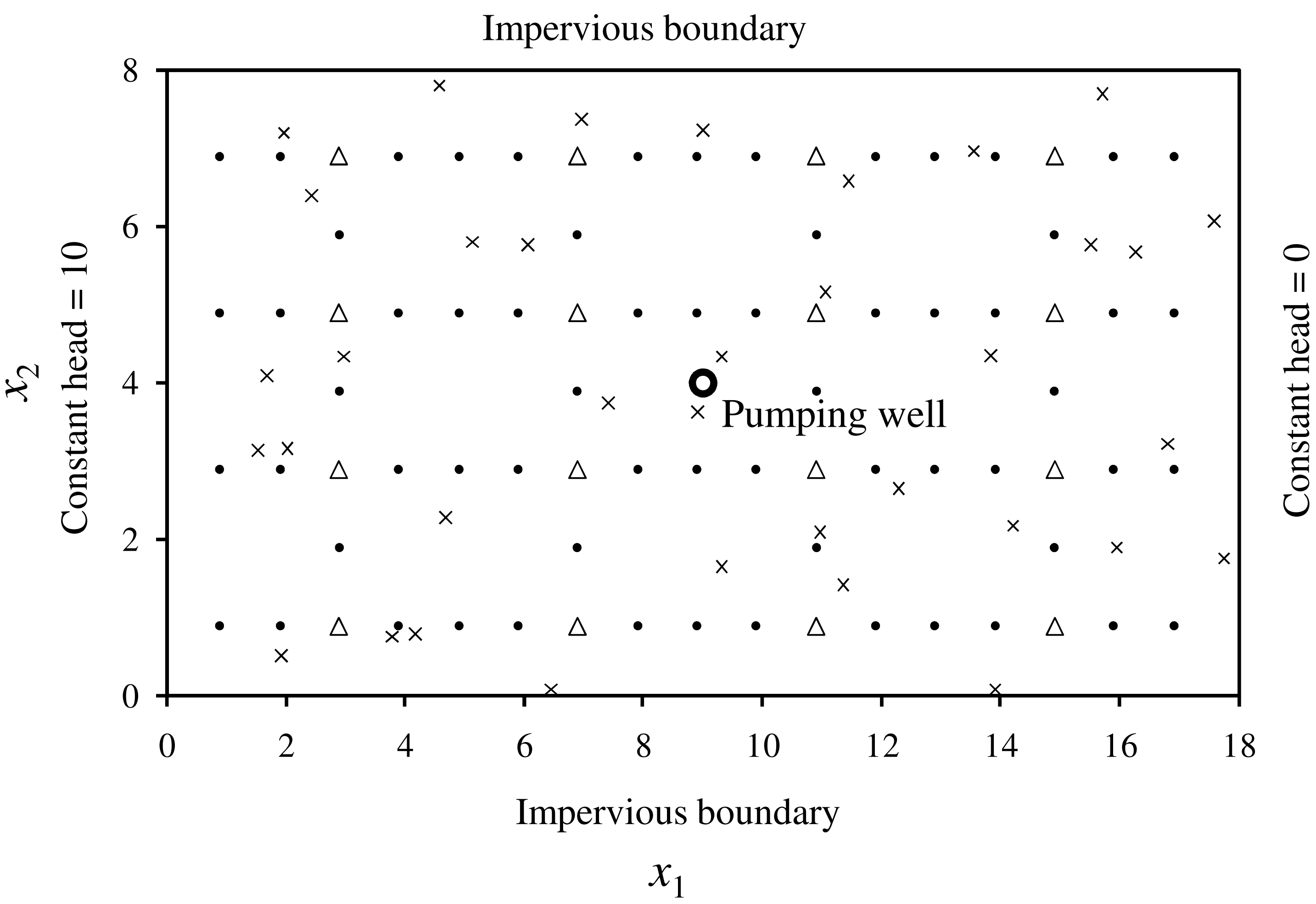
$$\begin{cases} \sum_{j=1}^{N_M} \varpi_j(\mathbf{x}_p) C_Y(\mathbf{x}_i - \mathbf{x}_j) + \varpi_i(\mathbf{x}_p)\sigma_{YE}^2 - \mu(\mathbf{x}_p) = C_Y(\mathbf{x}_i - \mathbf{x}_p) & i = 1,\ldots,N_M \\ \sum_{j=1}^{N_M} \varpi_j(\mathbf{x}_p) = 1 \end{cases}$$

$$\left\langle \varepsilon_{Yp}^* \varepsilon_{Yq}^* \right\rangle = C_Y(\mathbf{x}_p - \mathbf{x}_q) - \sum_{j=1}^{N_M} \varpi_j(\mathbf{x}_p) C_Y(\mathbf{x}_j - \mathbf{x}_q) + \mu(\mathbf{x}_p) \qquad p,\ q = 1,\ 2,\ldots,\ N_P$$

$$\begin{cases} \lim\limits_{\sigma_Y^2 \to 0} \varpi_j(\mathbf{x}_p) \to \dfrac{1}{N_M} \\ \lim\limits_{\sigma_Y^2 \to 0} \mu(\mathbf{x}_p) \to \dfrac{\sigma_{YE}^2}{N_M} \\ \lim\limits_{\sigma_Y^2 \to 0} \left\langle \varepsilon_{Yp}^* \varepsilon_{Yq}^* \right\rangle \to \dfrac{\sigma_{YE}^2}{N_M} \end{cases} \Rightarrow \begin{cases} \lim\limits_{\sigma_Y^2 \to 0} J = J\left(\sigma_Y^2 = 0\right) \\ \lim\limits_{\sigma_Y^2 \to 0} \left|\mathbf{V}_Y\right| = \lim\limits_{\sigma_Y^2 \to 0} \left|\mathbf{V}_{YM}\right| \left|\mathbf{V}_{YP}\right| = 0 \end{cases}$$

$$\lim_{\sigma_Y^2 \to 0} NLL = \lim_{\sigma_Y^2 \to 0} \frac{J}{\sigma_{hE}^2} + N_t \ln\left|\mathbf{V}_x\right| + \lim_{\sigma_Y^2 \to 0} \ln\left|\mathbf{V}_Y\right| + N_h \ln \sigma_{hE}^2 + N_Y \ln \sigma_{YE}^2 + N \ln 2\pi \to -\infty$$

Example: numerical model

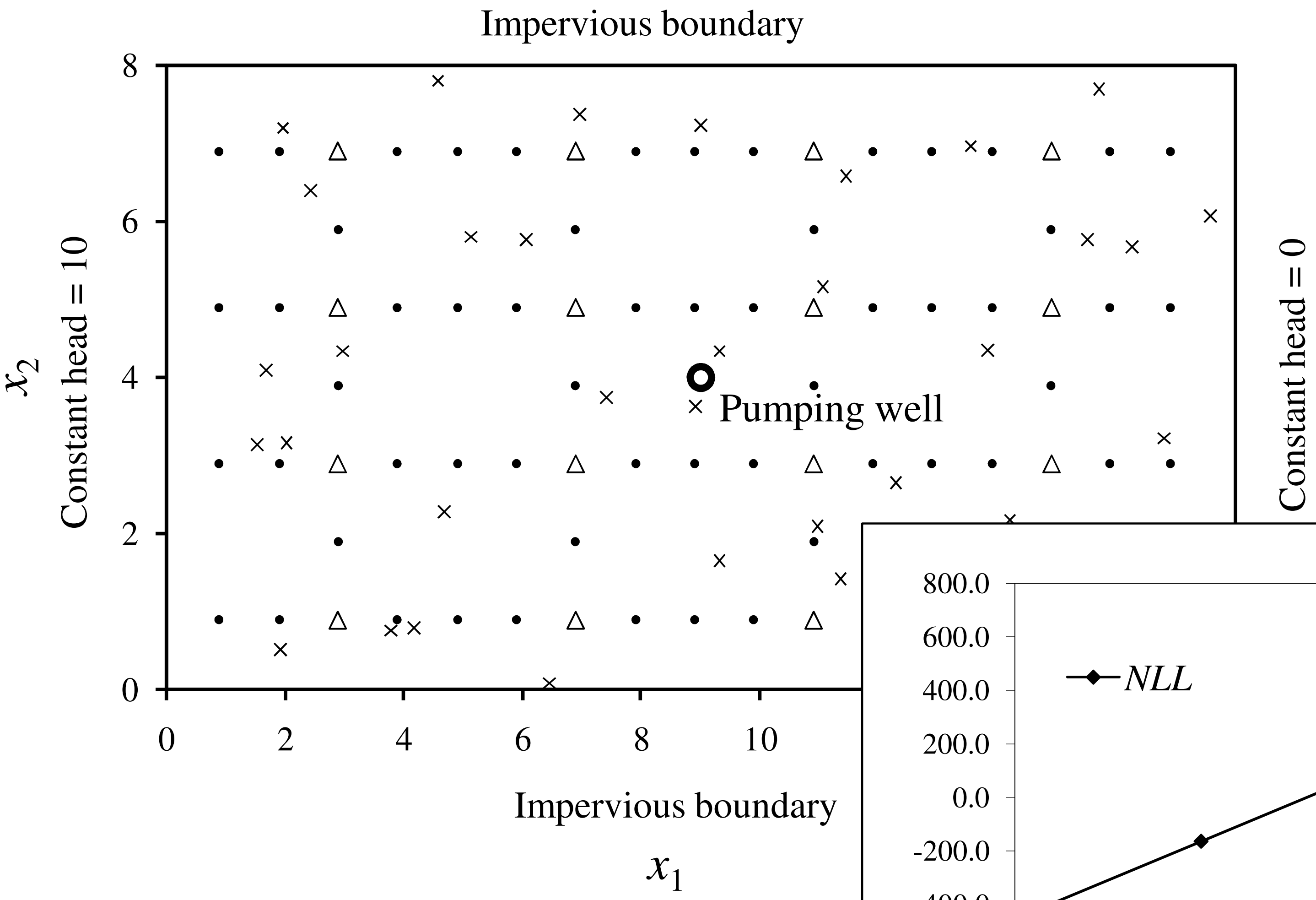


$\sigma^2_{hE} = 1.0$ m²
$\sigma^2_{yE} = 1.0$
$I_Y = 1.0$ m
$\sigma^2_Y = 4.0$

Reference properties

× 36 head measurements
Δ 16 log conductivity measurements
• 64 pilot points

Example: numerical model



σ^2_{hE} = 1.0 m²
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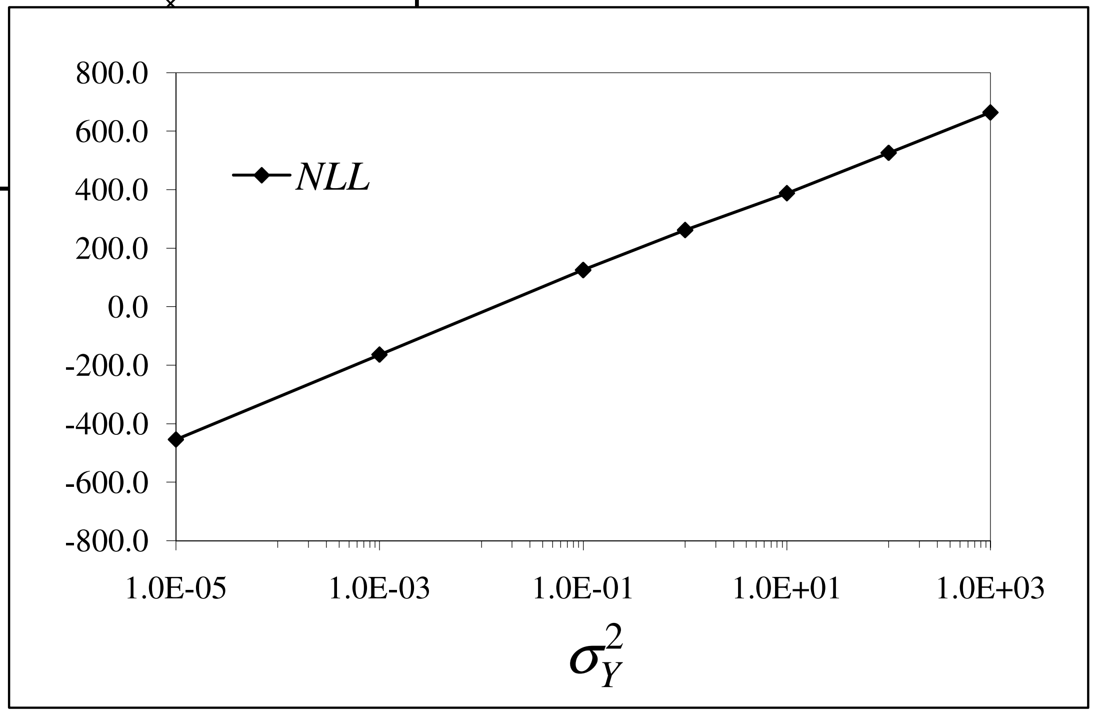
Reference properties



× 36 head measurements
Δ 16 log conductivity measurements
• 64 pilot points

Estimation of σ_Y^2

$$\ldots\ AIC,\ AICc \text{ and } BIC \text{ depends linearly on } NLL:$$

$$\lim_{\sigma_Y^2 \to 0} NLL = -\infty \Rightarrow \lim_{\sigma_Y^2 \to 0} AIC_k = \lim_{\sigma_Y^2 \to 0} AICc_k = \lim_{\sigma_Y^2 \to 0} BIC_k = -\infty$$

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

$$\begin{cases} \lim\limits_{\sigma_Y^2 \to 0} KIC = \lim\limits_{\sigma_Y^2 \to 0}\left(\dfrac{J}{\sigma_{hE}^2}\right) + N_t \ln\left|\mathbf{V}_x\right| + \lim\limits_{\sigma_Y^2 \to 0} \ln\left|\mathbf{V}_Y \mathbf{Q}^{-1}\right| + N_h \ln \sigma_{hE}^2 + N_Y \ln \sigma_{YE}^2 + N \ln 2\pi + N_Y \ln\left(N_z / 2\pi\right) \\ \lim\limits_{\sigma_Y^2 \to 0} \ln\left|\mathbf{V}_Y \mathbf{Q}^{-1}\right| = \lim\limits_{\sigma_Y^2 \to 0} \ln\left|\dfrac{1}{\sigma_{hE}^2} \mathbf{V}_Y \mathfrak{I}^{\mathbf{T}} \mathbf{V}_h^{-\mathbf{1}} \mathfrak{I} + \dfrac{1}{\sigma_{YE}^2} \mathbf{I}\right| \end{cases}$$

Positive definite matrix

Estimation of σ_Y^2

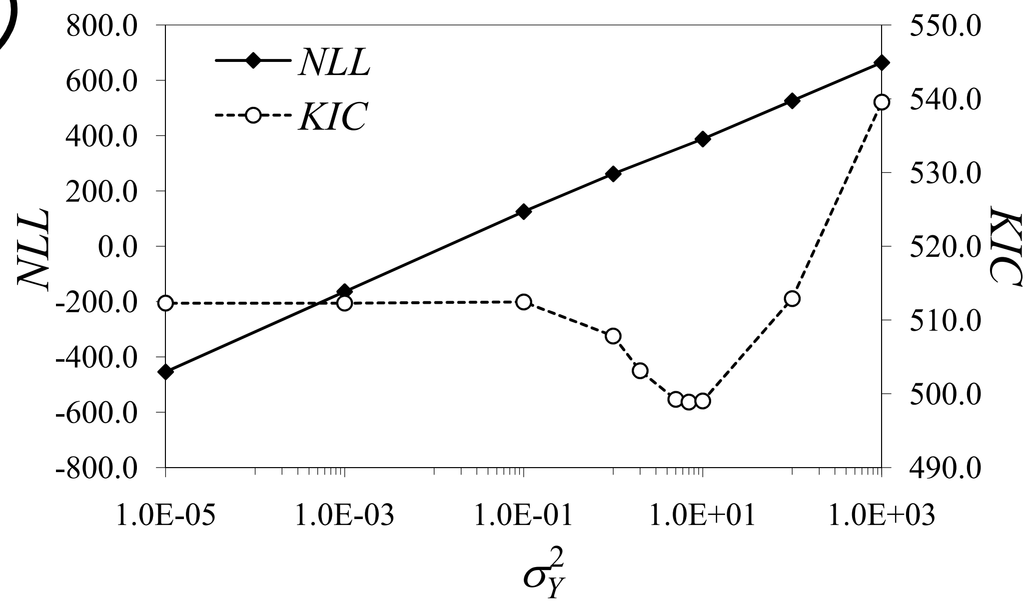
$$\ldots\ AIC\,,\ AICc\ \text{ and } BIC\ \text{depends linearly on } NLL:$$

$$\lim_{\sigma_Y^2 \to 0} NLL = -\infty \Rightarrow \lim_{\sigma_Y^2 \to 0} AIC_k = \lim_{\sigma_Y^2 \to 0} AICc_k = \lim_{\sigma_Y^2 \to 0} BIC_k = -\infty$$

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

$$\begin{cases} \lim\limits_{\sigma_Y^2 \to 0} KIC = \lim\limits_{\sigma_Y^2 \to 0}\left(\dfrac{J}{\sigma_{hE}^2}\right) + N_t \ln\left|\mathbf{V}_x\right| + \lim\limits_{\sigma_Y^2 \to 0} \ln\left|\mathbf{V}_Y\mathbf{Q}^{-1}\right| + N_h \ln\sigma_{hE}^2 + N_Y \ln\sigma_{YE}^2 + N \ln 2\pi + N_Y \ln\left(N_z/2\pi\right) \\ \lim\limits_{\sigma_Y^2 \to 0} \ln\left|\mathbf{V}_Y\mathbf{Q}^{-1}\right| = \lim\limits_{\sigma_Y^2 \to 0}\left(\ln\left|\dfrac{1}{\sigma_{hE}^2}\mathbf{V}_Y\mathfrak{J}^{\mathbf{T}}\mathbf{V}_h^{-1}\mathfrak{J} + \dfrac{1}{\sigma_{YE}^2}\mathbf{I}\right|\right) \end{cases}$$

Positive definite matrix



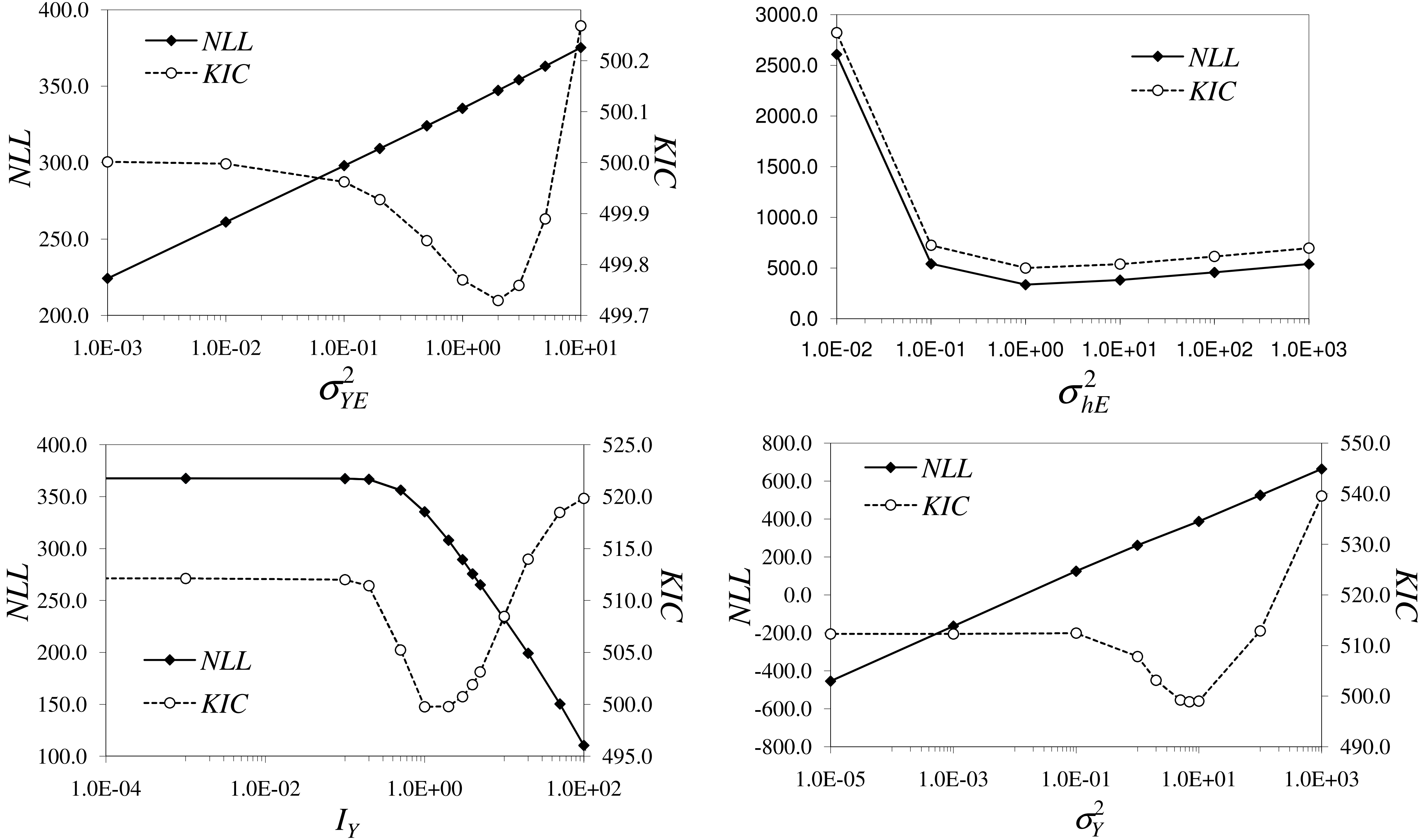
Estimation of θ

With an analogous procedure it is possible to obtain:

$$\lim_{I_Y \to \infty} NLL = \lim_{I_Y \to \infty} \frac{J}{\sigma_{hE}^2} + N_t \ln\left|\mathbf{V}_x\right| + \lim_{I_Y \to \infty} \ln\left|\mathbf{V}_Y\right| + \\ + N_h \ln \sigma_{hE}^2 + N_Y \ln \sigma_{YE}^2 + N \ln 2\pi \to -\infty$$

$$\lim_{\sigma_{YE}^2 \to 0} NLL = \lim_{\sigma_{YE}^2 \to 0} \frac{J}{\sigma_{hE}^2} + N_t \ln\left|\mathbf{V}_x\right| + \lim_{\sigma_{YE}^2 \to 0} \ln\left|\mathbf{V}_Y\right| + \\ + N_h \ln \sigma_{hE}^2 + N_Y \lim_{\sigma_{YE}^2 \to 0} \ln \sigma_{YE}^2 + N \ln 2\pi \to -\infty$$

Example: estimation of θ (zero-order)



Geostatistical Inverse algorithm (2)

Iterative inverse algorithm

$$\boldsymbol{\theta} = \left[I_Y, \sigma_Y^2, \sigma_{hE}^2, \sigma_{yE}^2 \right]^T$$

Initialization (G=1)**:**

- Set $\boldsymbol{\theta} = \boldsymbol{\theta}_{k,G}$ $\quad k=1, \dots Np$
- Find the optimum $\mathbf{Y}_k$ minimizing NLL_k (gradient-based algorithm)
- Compute $KIC_{k,G}$

Differentiation:

- Set $\boldsymbol{\chi}_k$ $\quad k=1, \dots Np$
- Compute $KIC_{k,G}$

Selection:

Select between $\boldsymbol{\chi}_k$ and $\boldsymbol{\theta}_{k,G}$ (parsimony principle)

$G = G + 1$

$\boldsymbol{\theta}_{k,G}$

Convergence?

Yes

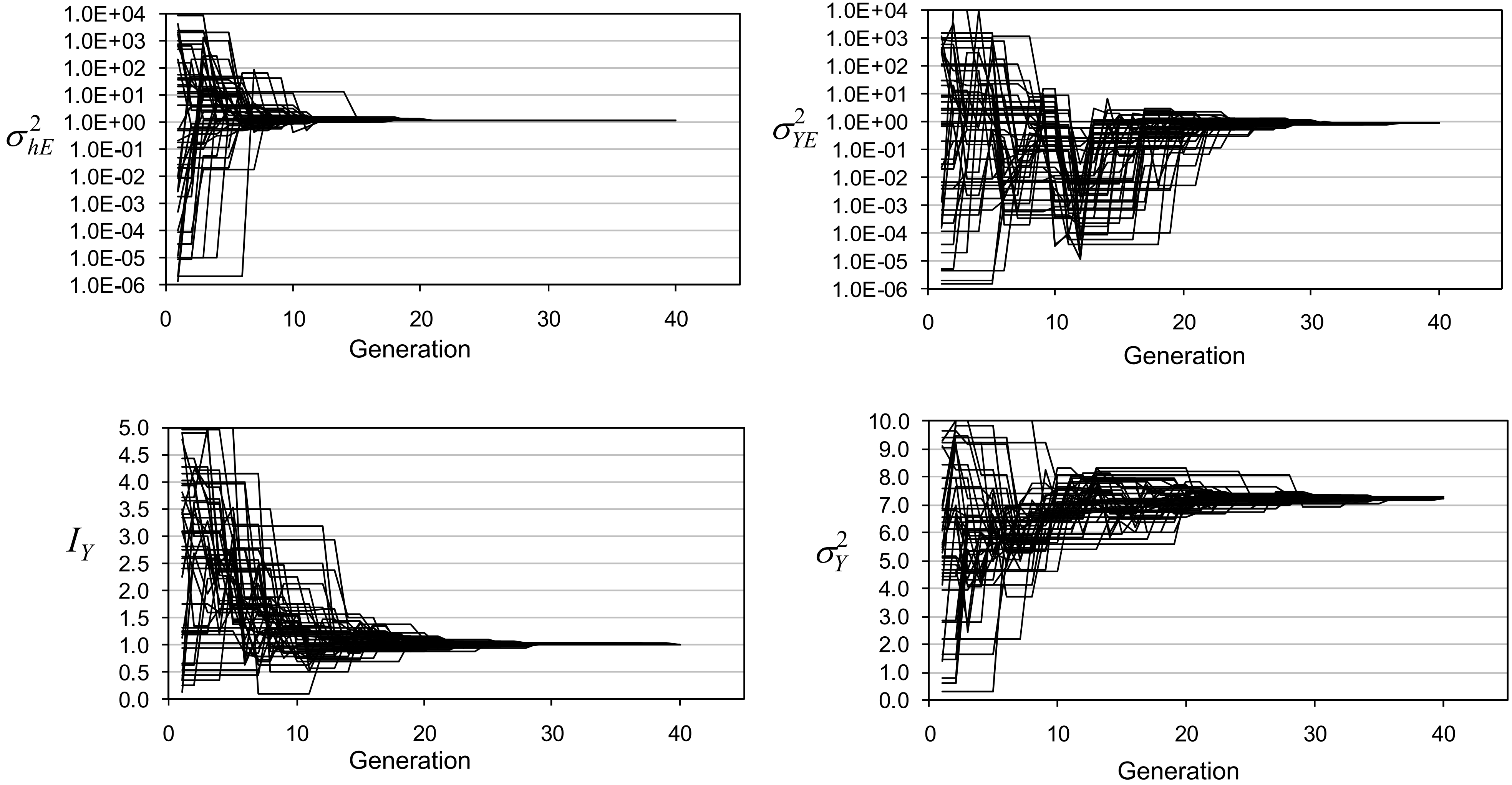
End

No

Example: estimation of θ (zero-order)

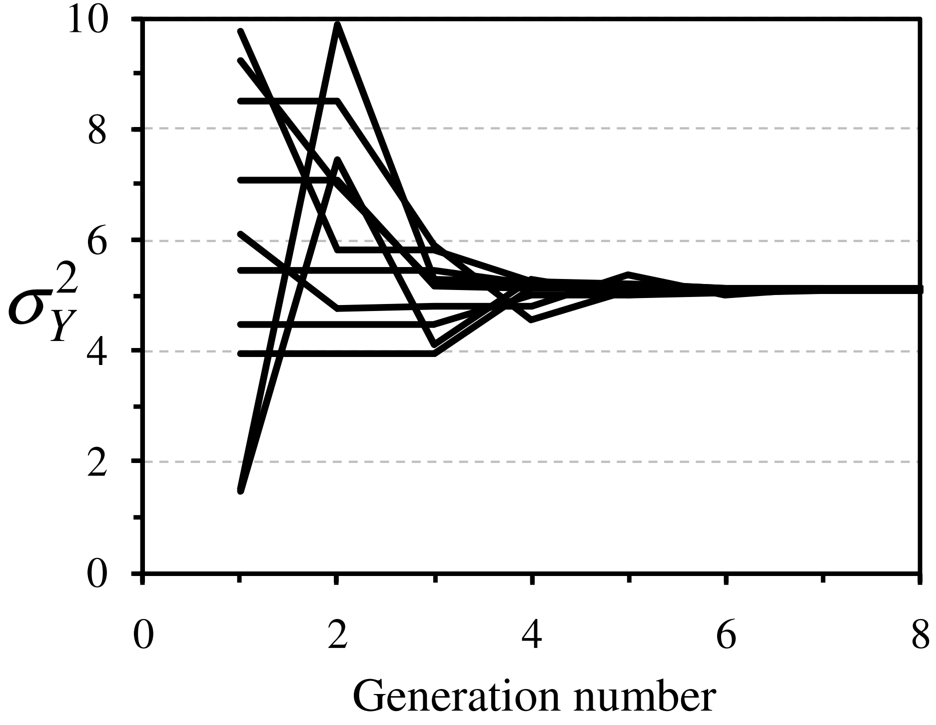
Joint estimation of $\boldsymbol{\theta} = \left[I_Y, \sigma_Y^2, \sigma_{hE}^2, \sigma_{yE}^2 \right]^T$

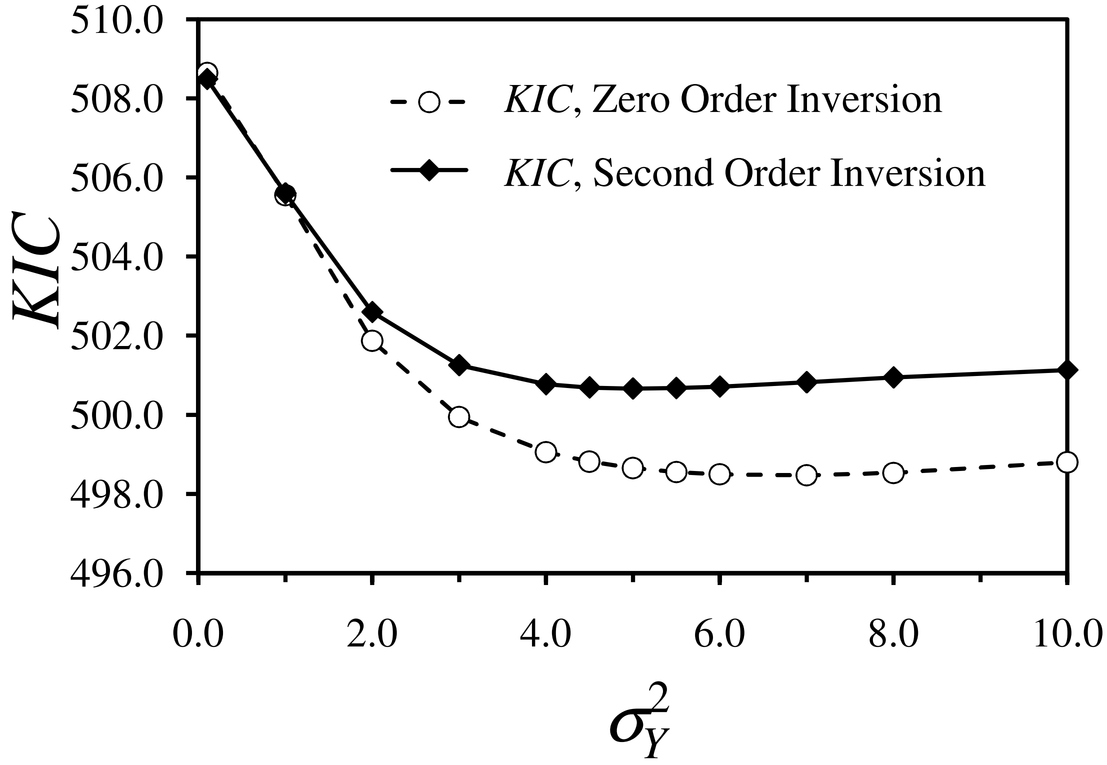
Reference properties
$$\begin{cases} \sigma_{hE}^2 = 1.0 \text{ m}^2 \\ \sigma_{yE}^2 = 1.0 \\ I_Y = 1.0 \text{ m} \\ \sigma_Y^2 = 4.0 \end{cases}$$



Example: estimation of σ_Y^2 (second-order)

$$I_Y = 1.02;\ \sigma_{hE}^2 = 1.17; \sigma_{YE}^2 = 0.89$$





Conclusions

- *KIC*: well suited for the estimation of statistical data- and model- parameters
- *NLL*, *BIC*, *AIC*, *AICc* and *HIC*: valid to estimate only one of the parameters we consider (variance of hydraulic head measurement errors)
- Minimization of KIC: accurately and efficiently performed by a genetic search algorithm based on DEM (Differential Evolution Algorithm)
- Statistical parameters and variogram integral scale: accurately estimated by means of zero-order approximations of conditional mean flow equation
- Variogram sill: requires second-order version of mean flow equation.