A Controlled Experiment for Investigating
*Prediction Accuracy* and
*Prediction Uncertainty*
in Groundwater Flow Modeling

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Problem Statement

- **Groundwater predictions** can be made by different model parameterization.

  - What parameterization and what level of parameterization would produce accurate predictions are not universally agreed on.

- **Predictions** are accompanied with uncertainty.

- Prediction uncertainty can be evaluated using *inferential statistics* and *sampling methods*.

- For both techniques, some **assumptions** are needed to exactly evaluate the prediction uncertainty.

  - Which assumption would cause more serious problem has not been demonstrated.
Methods Considered

- Parameterization
  - Homogeneous to highly parameterized: Zones, Interpolation, Kriging

- Uncertainty measures: individual confidence intervals on predictions
  (intervals with stated probability of including true value)
  - Linear
  - Nonlinear
  - Markov Chain Monte Carlo

Individual Linear Confidence Intervals

- Assumptions:
  - The model is correct;
  - The errors are normally distributed;
  - The model is linear and the prediction is linear.

- Calculation:

\[
\hat{z}_m \pm s_{\hat{z}_m} \times t_{s} \left( n + npr - p, 1.0 - \alpha / 2 \right)
\]

where

\[
s_{\hat{z}_m} = \left[ \sum_{i=1}^{p} \sum_{j=1}^{p} \frac{\partial}{\partial b_j} \frac{\partial}{\partial b_i} V(b) \frac{\partial}{\partial b_i} \hat{z}_m \right]^{1/2}
\]

\( V(b) \) is the parameter covariance matrix;
Individual Nonlinear Confidence Intervals

- **Assumptions:**
  - The model is correct;
  - The errors are normally distributed;
  - The model intrinsic nonlinearity is small.

- **Procedure:** The upper and lower limits of the confidence interval for a function $g(b)$ are calculated as the maximum and minimum value of $g(b)$ under the constraint:

$$S(b) \leq S(b^*) + d_{1-\alpha}^2 \frac{S(b^*)}{(n+npr-p)}$$

where

$$d_{1-\alpha} = t_{\alpha / 2}(n+npr-p, 1.0 - \alpha / 2)$$

Markov Chain Monte Carlo

- **Assumption:**
  - The model is correct;
  - Linearity not required;
  - Normality not required.

- **Procedure:**
  - The values drawn for each parameter start from its prior distribution and converge, as iterations progress, to a data-adjusted posterior distribution.

- **Key in Metropolis-Hastings algorithm:** acceptance rate (AR)
  - If AR is too large, low probability regions will be undersampled;
  - If AR is too small, MCMC will be quite inefficient.
True Groundwater Flow Model

- 3D (3810m x 6096m x 80m);
- Confining unit;
- Areal recharge;
- Groundwater interacts with lake and stream;
- Pumping well at P3;
- Top: free-surface;
- Four sides and bottom: no-flow;
- Heterogeneous K;

Same for all Models

- **Calibration data**
  - 54 heads (white noise with $\sigma=0.1$)
  - 1 elevation of lake stage (white noise with $\sigma=0.1$)
  - 2 measurements of stream flow (no noise added)
  - 1 prior information of net lake recharge (no noise added)

- **Calibrated parameters**
  - 5 parameters for recharge, KRB, confining unit KV, net lake recharge, and vertical anisotropy.

- **Prediction under pumping conditions**
  - Drawdown at pumping well P3.
Parameterization in K Field

- **HO**: Homogeneous; 1 K parameter
- **3Z**: 3 Zones; 3 K parameters
- **Int**: FE interpolation; 21 K parameters

**Krig**: Kriging with 229 pilot points

\[ S(b) = e^T \omega e + \mu \times e^T \omega R e \]

- **Krig-\( \mu \)=1**: Error-based weighting of observations and regularization;
- **Krig-mod**: \(e^T \omega e\)=#obs. Model fit consistent with obs weighting, \( \mu = 0.13 \);
- **Krig-close**: \(e^T \omega e\)=20. Close fit to observations, \( \mu = 0.0095 \).

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Hydraulic Conductivity Distributions

- **True**
- **3Z**
- **Int**

- **Krig-\( \mu \)=1**
- **Krig-mod**
- **Krig-close**
Hydraulic Conductivity Distributions

prediction error and parameterization

There is a trade-off between model fit and prediction accuracy with respect to the number of parameters.
A highly parameterized model that is tightly constrained by regularization performs like a simply parameterized model (Fienen et al., 2009).

Given a similar level of fit to observations, the simpler model gives better prediction.
Models with good prediction are constructed using many types of parameterization (zones, FE interpolation, kriging).

Biased confidence intervals occur for models with evident model error. Here, model error is suggested from the standard error of regression.

<table>
<thead>
<tr>
<th></th>
<th>HO</th>
<th>3Z</th>
<th>Int</th>
</tr>
</thead>
<tbody>
<tr>
<td>Error</td>
<td>1.49 (1.25-1.84)</td>
<td>1.27 (1.06-1.57)</td>
<td>1.00 (0.84-1.24)</td>
</tr>
<tr>
<td>Intrinsic nonlinearity</td>
<td>0.09</td>
<td>0.02</td>
<td>0.26</td>
</tr>
<tr>
<td>$R_N^2$</td>
<td>0.99</td>
<td>0.99</td>
<td>0.98</td>
</tr>
</tbody>
</table>
Conclusions

- Models with good prediction were constructed using many types of parameterization (zones, FE interpolation, kriging).
- Here, model error is the most serious problem in evaluation of prediction uncertainty. We expect this to be true for other systems, but more examples are needed.

Influence of Acceptance Rate on MCMC Results

Linear model:  \( y = ax + b + e \), where \( e \sim N(0,1) \), \( x=1,2,\ldots,20 \);
Linear prediction:  \( y = a \times 30 + b \);

<table>
<thead>
<tr>
<th></th>
<th>Prediction</th>
<th>LowerLimit</th>
<th>UpperLimit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analytical solution</td>
<td>63.765</td>
<td>62.265</td>
<td>65.265</td>
</tr>
<tr>
<td>Linear confidence interval</td>
<td>63.765</td>
<td>62.265</td>
<td>65.265</td>
</tr>
<tr>
<td>Nonlinear confidence interval</td>
<td>63.765</td>
<td>62.265</td>
<td>65.265</td>
</tr>
<tr>
<td>Simple MC (N=1000000)</td>
<td>63.765</td>
<td>62.265</td>
<td>65.265</td>
</tr>
<tr>
<td>MCMC (N=1000000) (acceptance rate: 20-30%)</td>
<td>63.764</td>
<td>62.223</td>
<td>65.306</td>
</tr>
<tr>
<td>MCMC (N=1000000) (acceptance rate: 20-50%)</td>
<td>63.766</td>
<td>62.301</td>
<td>65.232</td>
</tr>
</tbody>
</table>
Influence of Acceptance Rate on MCMC Results

AR: 20–30%

AR: 20–50%