NFSEG Version 1.1
Uncertainty Analysis

April 18, 2018
Outline

• Why do uncertainty analyses?
• How do we go about estimating uncertainty with the NFSEG model?
  • Theoretical basis
  • Methods of analysis
• What were our results?
Background and Motivation
The fundamental question that underpins all decision-making

What can go wrong?
**Model parameterization**

the two pillars on which it rests

**Expert knowledge**

Neither of these is very solid

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**Expert knowledge is a stochastic quantity**

The greater the detail that we express the less we know the exact value

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**History-matching**

There are infinite ways to fit a calibration dataset

Each can lead to different predictions
Bayes Equation

\[ P(k|h) \propto P(h|k) P(k) \]

History-matching

The possibilities that remain

Which of these possibilities fits the data

What is possible based on expert knowledge

What is possible based on expert knowledge
Before
History-Matching
After History-Matching
So what does the “calibrated model” give us?
History-Matching

A prediction of minimized error variance

After
What can go wrong?
After History-Matching

A prediction of minimized error variance
After History-Matching

A prediction of minimized error variance

stuff going wrong
After History-Matching

A prediction of minimized error variance

stuff going wrong

After
After History-Matching

A prediction of minimized error variance

stuff going wrong
Prior Probability Distribution
Geostatistics: generating realisations of prior probability distributions

Big problem: how do you get these parameter fields to fit a calibration dataset?
Parameterization device for NFSEG Model

Pilot points and model domain in layer 1
Pilot points and model domain in layer 2
Pilot points and model domain in layer 3
Pilot points and model domain in layer 4
Pilot points and model domain in layer 5
Pilot points and model domain in layer 6
Pilot points and model domain in layer 7
We require two things:–
• the uncertainty of each parameter
• the degree of spatial correlation between parameters

Hydraulic property value

not this high

In here somewhere

not this low
Select this. Why?

- No software/experience exists for building complex geostatistical models on a regional scale.
- Constraining random parameter fields to fit a calibration dataset is numerically difficult. Simplifying assumptions are needed.
Spatial Correlation

A variogram

\[ \gamma(h) = E \{(k(x) - k(x + h))^2\} \]
Pilot points are not statistically independent.

Spatial correlation depends on local pilot point spatial density.

Local pilot point density depends on local information content.
What is possible based on expert knowledge

Prior parameter covariance matrix

\[ P(k|h) \propto P(h|k) \ P(k) \]
Enforcing Calibration Constraints on Random Parameter Fields
**Step 1**

Calibrate model using PEST

- Fit the calibration dataset as well as possible
- Calculate a Jacobian matrix based on best-fit parameters...

\[
\begin{align*}
\frac{\partial o_1}{\partial p_1} & \quad \frac{\partial o_1}{\partial p_2} & \quad \frac{\partial o_1}{\partial p_3} & \quad \frac{\partial o_1}{\partial p_4} & \quad \text{etc} \\
\frac{\partial o_2}{\partial p_1} & \quad \frac{\partial o_2}{\partial p_2} & \quad \frac{\partial o_2}{\partial p_3} & \quad \frac{\partial o_2}{\partial p_4} \\
\frac{\partial o_3}{\partial p_1} & \quad \frac{\partial o_3}{\partial p_2} & \quad \frac{\partial o_3}{\partial p_3} & \quad \frac{\partial o_3}{\partial p_4} \\
\frac{\partial o_4}{\partial p_1} & \quad \frac{\partial o_4}{\partial p_2} & \quad \frac{\partial o_4}{\partial p_3} & \quad \frac{\partial o_4}{\partial p_4} \\
\frac{\partial o_5}{\partial p_1} & \quad \frac{\partial o_5}{\partial p_2} & \quad \frac{\partial o_5}{\partial p_3} & \quad \frac{\partial o_5}{\partial p_4} \\
\frac{\partial o_6}{\partial p_1} & \quad \frac{\partial o_6}{\partial p_2} & \quad \frac{\partial o_6}{\partial p_3} & \quad \frac{\partial o_6}{\partial p_4} \\
\frac{\partial o_7}{\partial p_1} & \quad \frac{\partial o_7}{\partial p_2} & \quad \frac{\partial o_7}{\partial p_3} & \quad \frac{\partial o_7}{\partial p_4} \\
\frac{\partial o_8}{\partial p_1} & \quad \frac{\partial o_8}{\partial p_2} & \quad \frac{\partial o_8}{\partial p_3} & \quad \frac{\partial o_8}{\partial p_4} \\
\end{align*}
\]

\[J_{i,j} = \frac{\partial o_i}{\partial p_j}\]
Use linearized form of Bayes equation to calculate a posterior (i.e. post-calibration) parameter covariance matrix from the prior parameter covariance matrix.

\[ C'(k) = C(k) - C(k)J^t[JC(k)J^t + C(\varepsilon)]^{-1}JC(k) \]

Prior covariance matrix

Reduced through history matching

Posterior covariance matrix
Step 3

Sample the linear approximation to the posterior parameter distribution:-
• Samples are centred on the calibrated parameter field
• Post-calibration standard deviations and spatial correlations expressed by $C'(k)$
• Run the model to obtain objective functions (quantify model-to-measurement misfit)

*Use RANDPAR1 utility from the PEST suite.*
Step 4

- undertaking singular value decomposition of the Jacobian matrix
- refine random parameter fields by extracting solution space components and replacing them with those of calibrated model.

*Use PNULPAR utility from the PEST suite.*

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![Graph showing realisation numbers and calibration points](image)

- **Acceptable φ**
- **Calibration φ**
Step 5

- adjust parameter fields using a single PEST iteration
- adjustment is numerically cheap; use same Jacobian matrix

*Run PEST with the “/i” switch*
Outcomes
Examples of Randomly Generated Parameters

Layer 3 Horizontal Hydraulic Conductivity
*Sim: kx3_001*

Layer 3 Horizontal Hydraulic Conductivity
*Sim: kx3_002*
Parameter Uncertainty: Estimated Probability Distributions

Estimated value for parameter, k3x496, in feet per day

Explanation
- Calibrated
- Mean
- Mean - 1 sd
- Mean + 1 sd
## Predictive Uncertainty

<table>
<thead>
<tr>
<th>Prediction Location and Type</th>
<th>Prediction Units</th>
<th>Mean of 2035 Predicted Value</th>
<th>Standard Deviation of 2035 Predicted Value</th>
<th>Mean of Predicted Change from 2009 to 2035</th>
<th>Standard Deviation of Predicted Change from 2009 to 2035</th>
</tr>
</thead>
<tbody>
<tr>
<td>UFA observation well near Lake Brooklyn</td>
<td>Feet</td>
<td>77.9</td>
<td>0.3</td>
<td>-1.8</td>
<td>0.1</td>
</tr>
<tr>
<td>UFA observation well near Lake Geneva</td>
<td>Feet</td>
<td>77.7</td>
<td>0.3</td>
<td>-1.9</td>
<td>0.1</td>
</tr>
<tr>
<td>Ichetucknee River at US HWY27 near Hildreth</td>
<td>Flow</td>
<td>-269.</td>
<td>4.8</td>
<td>7.5</td>
<td>0.3</td>
</tr>
<tr>
<td>Santa Fe River near Fort White</td>
<td>Flow</td>
<td>-707.</td>
<td>6.6</td>
<td>15.4</td>
<td>0.8</td>
</tr>
</tbody>
</table>
Predictive Uncertainty: Estimated Probability Distributions

Predicted 2035 head
w00202 UFA observation well near Lake Broklyn.
Predictive Uncertainty: Estimated Probability Distributions
Predictive Uncertainty: Estimated Probability Distributions
Predictive Uncertainty:
Estimated Probability Distributions

Predicted change in flow from 2009 to 2035
qd_2322700 Baseflow to the Ichetucknee River at US Highway 27 near Hildreth.
Predictive Uncertainty: Estimated Probability Distributions

Predicted change in flow from 2009 to 2035
q_{2322500} Baseflow to the Santa Fe River near Fort White.

Change in flow, in cubic feet per second