DUE TODAY COMPUTER FILES AND QUESTIONS for *Assgn#6*

Assignment # 6 Steady State Model Calibration: Calibrate your model. If you want to conduct a transient calibration, talk with me first. Perform **calibration using UCODE.** **Be sure your report addresses global, graphical, and spatial measures of error as well as common sense.** Consider more than one conceptual model and compare the results. **Remember to make a prediction with your calibrated models and evaluate confidence in your prediction.** Be sure to save your files because you will want to use them later in the semester.

Suggested Calibration Report Outline

- **Title**
- **Introduction**
  - **describe the system to be calibrated (use portions of your previous report as appropriate)**
- **Observations to be matched in calibration**
  - **type of observations**
  - **locations of observations**
  - **observed values**
  - **uncertainty associated with observations**
  - **explain specifically what the observation will be matched to in the model**
- **Calibration Procedure**
- **Evaluation of calibration**
  - **residuals**
  - **parameter values**
  - **quality of calibrated model**
- **Calibrated model results**
- **Predictions**
- **Uncertainty associated with predictions**
- **Problems encountered, if any**
- **Comparison with uncalibrated model results**
- **Assessment of future work needed, if appropriate**
- **Summary/Conclusions Summary/Conclusions**
- **References**

submit the paper as hard copy and include it in your zip file of model input and output
submit the model files (input and output for both simulations) in a zip file labeled:
ASSGN6_LASTNAME.ZIP

Calibration

(Parameter Estimation, Optimization, Inversion, Regression)

adjusting parameter values, boundary conditions, model conceptualization, and/or model construction until the model simulation matches field observations

We calibrate because

1. the field measurements are not accurate reflections of the model scale properties, and

2. calibration provides integrated interpretation of the available data

(e.g. the dependent observations tell us about the independent properties)

Calibrated model ~ provides minimized residuals (Observed – Simulated) without bias (N indicates the number of observations)

Global measures of error:

Mean Error: (Sum(Obs-Sim))/N

Mean Absolute Error: (Sum(ABS(Obs-Sim)))/N

Root Mean Squared Error: $((\text{Sum}((\text{Obs}-\text{Sim})^2))/N)^{0.5}$

Sum-of-Squared Weighted Residuals: $\text{Sum}(\text{weight}(\text{Obs}-\text{Sim})^2)$

Graphical measures of error

observed vs. simulated should form a 45° line passing through the origin

residual vs. simulated should form a uniform horizontal band around zero

ordered residuals on normal probability graph should form a straight line

Spatial and Temporal Distribution of Residuals

Map (obs-sim) in x, y, z space should exhibit a random pattern of positive and negative, as well as large and small, residuals

Graph of (obs-sim) vs. time OR vs. observation # should form a uniform horizontal band centered on zero

ALSO USE COMMON SENSE to spot errors

Optimal Parameter Values are the result of the calibration
They should correspond with field measured values

If they differ significantly carefully consider whether:

- such a difference is reasonable due to scale issues
- the conceptual model is in error, or
- there errors in the field data

Have expectations, question all aspects of the situation when calculations do not match expectations

We will use automated calibration (here nonlinear regression), it is a valuable tool for:

- finding the best fit to your field observations
- identifying the type and location of additional data that will be most helpful
- differentiating conceptual models
- identifying models that are most representative of the field

Unfortunately, many practicing ground-water professionals are still using trial-and-error but it is changing rapidly

Our objective is to minimize the sum of squared weighted residuals:

$$S(\underline{b}) = \sum_{i=1}^{ND} \omega_i \left[y_i - y_i'(\underline{b}) \right]^2$$

Objective Function

$\underline{b}$	**vector of estimated parameter values 1xNP**
ND	**number of observations**
NP	**number of parameters being estimated**
y_i	**i^{th} observation (head, flux, concentration)**
$y_i'(\underline{b})$	**modeled equivalent of the i^{th} observation**
ω_i	**weight of the i^{th} observation**

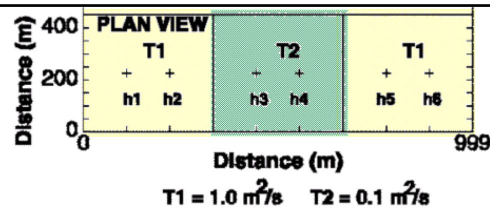
Weighting Squared Residuals because Observations are:

1. **not equally reliable** (some heads may have been determined from survey TOC (top of casing) while other TOCs were estimated from a topographic map)
2. **have different units** (a difference of 1 foot in head may not have the same importance as a difference of 1cfs flow rate)
3. **have true errors that are correlated** (e.g. many h obs @ one well but elevation of well or position of well is in error)

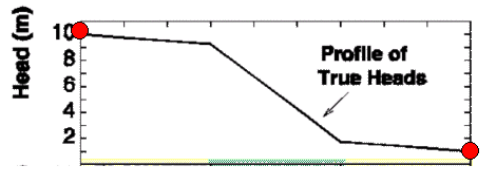
We deal with these issues through weighting observations. Research has indicated that ignoring the correlation of error between observations does not significantly influence the regression, but we can include them if we wish.

Using 1/variance of the measurement as the weight renders the weighted squared residuals unitless and assigns high weights to more accurate observations. THEREFORE we can sum weighted squared residuals and regardless of the units or magnitudes, they are of equal importance, except for their measurement certainty.

Let's look at some simple examples of the sum of squared weighted residuals



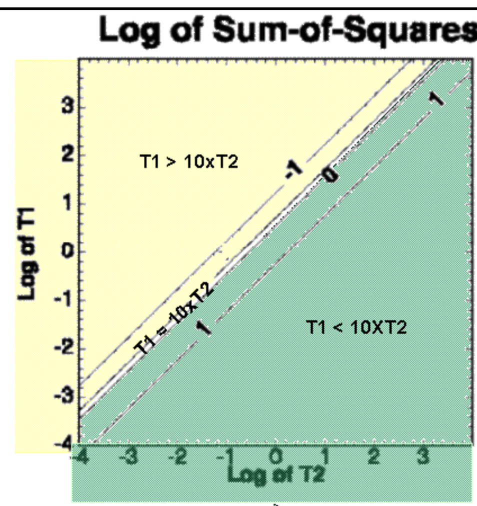
The heads are fixed at each end, on the left at 10m and on the right at 1m, for a gradient of 0.009.

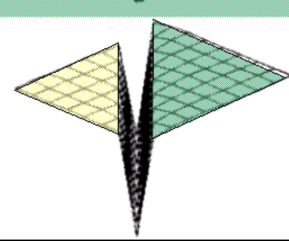


This results in the following accurate head observations from the system:

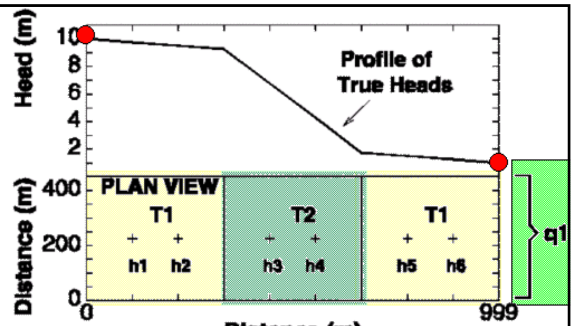
Observation Type and #	Value (m)
h1	9.75
h2	9.50
h3	6.75
h4	4.25
h5	1.50
h6	1.25

With the sum of squared weighted residuals being one value, for a simple 2 parameter estimation problem we can plot it on a graph and look at the surface





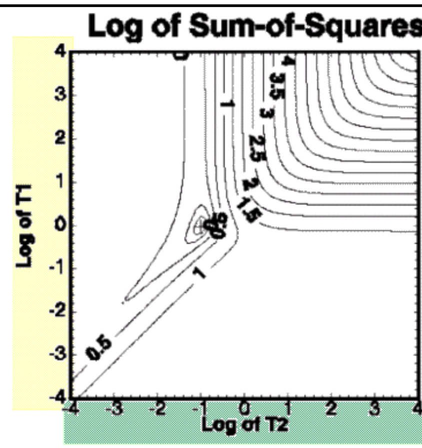
Here is the same example but now we add a flow observation and note the affect on the sum of squared weighted residuals

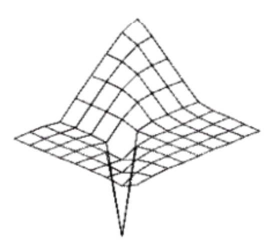


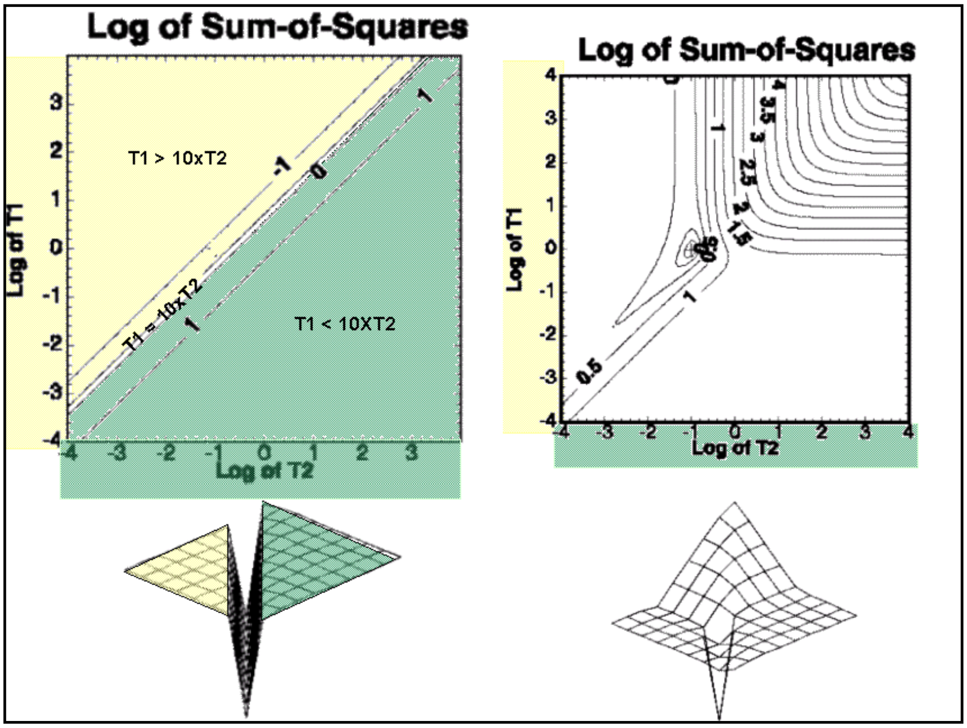
$T1 = 1.0\ m^2/s \quad T2 = 0.1\ m^2/s$

Observation Type and #	Value (m)
h1	9.75
h2	9.50
h3	5.75
h4	4.25
h5	1.50
h6	1.25
q1	-1.0135

Here is the sum of squared weighted residuals surface with the flow observation included. Note that now it is possible to find a unique solution







Sometimes we include prior knowledge of the parameter values from independent tests as observations (for diagonal weights):

$$S(b) = \sum_{i=1}^{ND} \omega_i \left[y_i - y_i^{'}(\underline{b}) \right]^2 + \sum_{p=1}^{NPR} \omega_p \left[P_p - P_p^{'}(\underline{b}) \right]^2$$

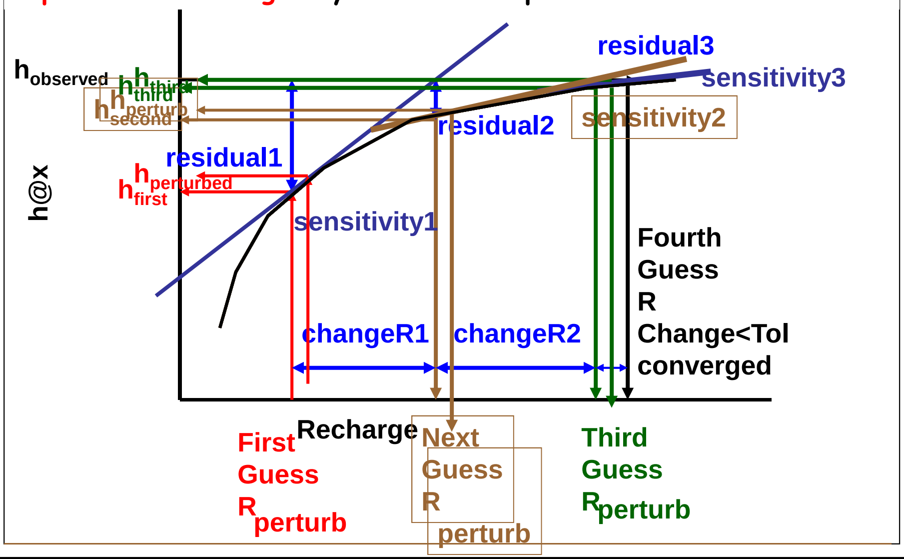
NPR number *of prior* information values

P_p pth prior estimate

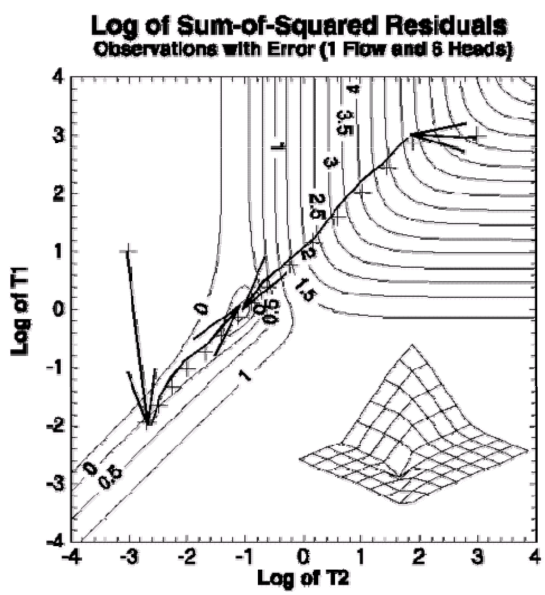
$P_p^{'}(\underline{b})$ pth modeled equivalent of prior estimate

ω_p weight on pth modeled equivalent of prior estimate

Consider how we could go about estimating parameter values for the following nonlinear model. We guess a recharge R, calculate h, determine residual, use that and the slope (sensitivity) to make a linear estimate of the best R, and because it is nonlinear, we repeat until R changes by less than a specified tolerance



An image of "the route" to the minimum:



CONSIDER the SENSITIVITY MATRIX

$y'(b)$ has ND + NPR elements

ND = # observations

NPR = # prior observations of parameters

b has NP elements

NP = # parameters

So the sensitivity matrix X has ND+NPR rows & NP columns

Each sensitivity is determined as:
[simulated(current b values)- simulated(perturbed b values)] / [(current b)-(perturbed b)]

i.e.

$$\frac{simulated(b_o) - simulated(b')}{b_o - b'}$$

NP →

ND + NPR ↓

$$\underline{\underline{X}} = \begin{bmatrix} \frac{\partial y'_1}{\partial b_1} & \frac{\partial y'_1}{\partial b_2} & \cdots & \frac{\partial y'_1}{\partial b_{NP}} \\ \frac{\partial y'_2}{\partial b_1} & \frac{\partial y'_2}{\partial b_2} & \cdots & \frac{\partial y'_2}{\partial b_{NP}} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \frac{\partial y'_{ND}}{\partial b_1} & \frac{\partial y'_{ND}}{\partial b_2} & \cdots & \frac{\partial y'_{ND}}{\partial b_{NP}} \end{bmatrix}$$

Estimating Parameter Values that Minimize the Sum of Weighted Squared Residuals via Nonlinear Regression using the Modified Gauss-Newton Gradient Method (also called Marquardt-Levenberg)

An iterative form of linear regression (i.e. solves normal equations like you do to fit a straight line to data, but repeatedly with updated parameter values)

To do this we minimize the objective function (i.e. we obtain the normal equations by assuming linearity and taking the derivative with respect to the parameters, then set the derivative equal to zero to find the parameter values that would minimize the function)

The ground water flow equations are not linear with respect to the parameters, so we repeat the process using the new parameter values and continue until there is little change in the parameter values

This only works well for non-linear problems IF MODIFIED to include:

* scaling
* adjusting to gradient correction
* damping

Gauss-Newton approach:

We solve iteratively for d:

$$\underline{d}_r = \left(\underline{\underline{X}}_r^T \underline{\underline{\omega}}\,\underline{\underline{X}}_r\right)^{-1} \underline{\underline{X}}_r^T \underline{\underline{\omega}}\left(\underline{y} - \underline{y}'(\underline{b}_r)\right)$$

Modified Gauss-Newton approach

scale(C) adjust direction(m) damp(ρ)

$$\underline{d}_r = \left(\underline{\underline{C}}^T \underline{\underline{X}}_r^T \underline{\underline{\omega}}\,\underline{\underline{X}}_r \underline{\underline{C}} + \underline{\underline{I}} m_r\right)^{-1} \underline{\underline{C}}\,\underline{\underline{C}}^T \underline{\underline{X}}_r^T \underline{\underline{\omega}}\left(\underline{y} - \underline{y}'(\underline{b}_r)\right)$$

And update b:

$$\underline{b}_{r+1} = \underline{b}_r + \rho_r \underline{d}_r$$

REPEAT UNTIL THE DISPLACEMENT VECTOR d
is LESS THAN TOLERANCE
Typically 1% change in parameters

Once optimal parameters are found, evaluate:
PARAMETER STATISTICS
RESIDUAL STATISTICS
To assess quality of the model

Table 1: Guidelines for effective model calibration (from Hill and Tiedeman, 2007 ; modified from Hill, 1998).

Model Development
1. Apply the principle of parsimony (start simple; build complexity slowly)
2. Use a broad range of information to constrain the problem
3. Maintain a well-posed, comprehensive regression problem
4. Include many types of observations in the regression
5. Use prior information carefully
6. Assign weights that reflect errors
7. Encourage convergence by improving the model and evaluating the observations
8. Consider alternative models
Test the Model
9. Evaluate model fit
10. Evaluate optimized parameters
Potential New Data
11. Identify new data to improve model parameter estimates and distribution
12. Identify new data to improve predictions
Prediction Accuracy and Uncertainty
13. Evaluate prediction uncertainty and accuracy using deterministic methods
14. Quantify prediction uncertainty using statistical methods

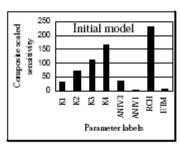
NOTE LINK TO THIS USGS REPORT ON CLASS WEB PAGE

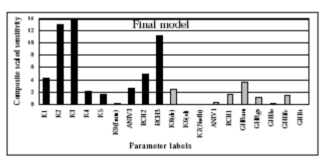
METHODS AND GUIDELINES FOR
EFFECTIVE MODEL CALIBRATION

by Mary C. Hill

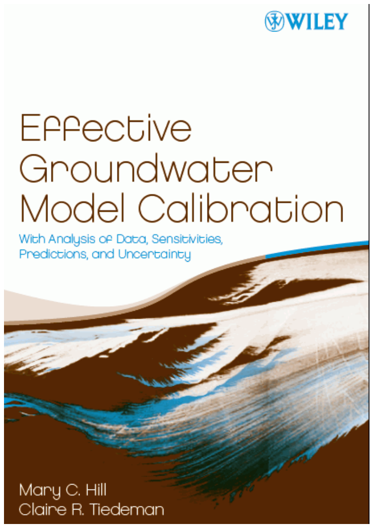
U.S. GEOLOGICAL SURVEY
WATER-RESOURCES INVESTIGATIONS REPORT 98-4005

With application to:
UCODE, a computer code for universal inverse modeling, and
MODFLOWP, a computer code for inverse modeling with MODFLOW





Learn much more about calibrating models via Hill and Tiedeman



REMEMBER

When you run a code, you should expect that there will be errors and be pleasantly surprised if there are not. When you see an error:

1) look closely at the error message, try to understand it, use any clue that may be provided (paths, directories, file names, numbers) to explore it
2) check the directory to see what files were created and view their contents, look at the dates and times on files to determine what was created recently
3) delete outputs and try it again and look at the new outputs
4) as Winston Churchill once said, "never, never, give up". If you do not find the error, keep thinking and experimenting to decipher the situation. Utilize "show me" skills.

Follow tutorial/see Ucode_main_out.#uout and _files

EVALUATING OUTPUT

Notice any errors in the command window and read the file to confirm everything is what you expected

The most common error is related to paths and file names
Next common error is improper substitution or extraction

Check that the UCODE input items are echoed correctly.
View the output (see Chapters 14 and 16)
fn.#uout & DataExchange files: fn._*

Note GWChart works for ucode _ files

Follow tutorial and use GWChart

Follow tutorial and use GWChart

EVALUATING OUTPUT

fn.#uout includes statistics, top portion of Fit Statistics Table 28

These reflect model fit
given the initial model configuration and starting values
<u>USE GWChart for convenient viewing of files</u>

Exceptionally large discrepancies between simulated and observed values may indicate that there is a conceptual error either in the model configuration or in the calculation of the simulated values

Fixing these now can eliminate many hours of frustration.

Data exchange files include residual informations at starting values Table 31

It is essential for UCODE to perform correctly in the forward mode.
Proceeding with errors will result in an invalid regression and wasted time.

Resolve any problems and continue

Follow tutorial for sensitivity run / see Ucode_main.in & Ucode_main_out.#uout

EXECUTE UCODE in the SENSITIVITY MODE

Look for the differences in the #uout file
What are the sensitivities?

Are there some parameters that will be difficult to estimate?
Dimensionless scaled sensitivity – 1 for each obs and parameter
dss = unscaledsens * (PARAMETER_VALUE * (wt**.5))
Composite Scaled Sensitivities – 1 for each parameter
css = ((SUM OF THE SQUARED DSS) / ND)**.5
Generally should be >1 AND
within ~ 2 orders of magnitude of the most sensitive parameter

Notice statistics are calculated for the starting parameter values as if they were optimal
This can be useful if you want to regenerate the statistics for an optimal parameter set

Follow tutorial for sensitivity run / see Ucode_main.in & Ucode_main_out.#uout

See "Perturbation Sensitivities" starting on p15

Accuracy of Sensitivities Depends on:

number of accurate significant figures in extracted simulated values
(print many significant figures and extract them all)

magnitude of the simulated values

magnitude of the substituted parameter values

size of the parameter perturbations, for nonlinear parameters

What if Sensitivities are zero?

If more than a few sensitivities equal zero, it may indicate extracted perturbed & unperturbed values are identical (given the significant figures) or perhaps the model did not execute

See "What to Do When Sensitivities Equal Zero" (p37) of the UCODE manual.

If sensitivities are zero for a Parameter:

If many other sensitivities are nonzero, observation is not very important, NO corrective action needed

If all sensitivities are zero, corrective action is needed (if there is a hydraulic reason for lack of sensitivity, do not estimate the parameter)

If many sensitivities are zero, corrective action MAY OR MAY NOT be needed

What if Sensitivities are zero?

Five possible corrective actions:
1) smaller solver convergence criteria can be specified in the application codes;
2) the extracted values can be printed with more significant figures in the application model output file if the values are calculated with sufficient accuracy;
3) the datum of the problem can be changed or a normalization can be applied;
4) the perturbation for the parameter can be changed; too small perturbations may result in negligible differences in extracted values, or differences that are obscured by round-off error; too large may yield inaccurate sensitivities for nonlinear parameters
5) the methods for coping with insensitive parameters discussed later can be employed.
- Reconsider the model construction
- Modify the defined parameters
- Eliminate observations or prior information, if biased
- Adjust weights either for groups of, or individual, observations

Sensitivities calculated for the values of the parameters just prior to failure can be investigated by substituting these parameter values as starting values in the prepare file and executing UCODE with sensitivities=yes, optimize=no. (add SenMethod=2 to also evaluate correlation)

Sensitivities for all intermediate sets of parameter values can be investigated by setting IntermedPrint=sensitivities in the input file and executing UCODE again with optimize=yes.

Follow tutorial for parameter estimation run/see Ucode_main.in & Ucode_main_out.#uout

Read through the resulting files

VERY IMPORTANT: USE YOUR COMMON SENSE

Most common trouble is lack of convergence, or progress toward it. Consider how to tackle that.

Have expectations for the results, question all aspects of the situation when calculations do not match expectations

Fix Problems

Evaluate Results

What do you make of the estimated parameter values? What of the confidence intervals?

EVALUATING PARAMETER ESTIMATION OUTPUT

OVERALL FIT, SUM OF SQUARED ERRORS

$$S(\underline{b}) = \sum_{i=1}^{ND} \omega_i \left[y_i - y_i^{'}(\underline{b}) \right]^2$$

CALCULATED ERROR VARIANCE (cev)

$$\mathbf{cev} \quad = \mathbf{s}^2 = \frac{\mathbf{S(b)}}{\mathrm{ND} - \mathrm{NP}}$$

STANDARD ERROR sqrt(cev)

$$\mathbf{s} = \sqrt{\mathbf{s}^2}$$

Model Selection Criteria

MLOF / AIC / AICc / BIC / KIC

SUM OF WEIGHTED SQUARED RESIDUALS

$$S(b) = \sum \omega \left(s_{RESIDUAL} \right)^2$$

CALCULATED ERROR VARIANCE

$$cev = s^2 = \frac{S(b)}{ND - NP}$$

STANDARD ERROR

$$\mathbf{s} = \sqrt{\mathbf{s}^2}$$

VARIANCE/COVARIANCE MATRIX

$$COV = cev \left(\underline{\underline{X}}^T \underline{\underline{\omega X}} \right)^{-1}$$

$$\begin{array}{c} \\ i=1 \\ \bullet \\ \bullet \\ i=NP \end{array} \begin{array}{c} \begin{array}{cccc} j=1 & \bullet & \bullet & j=NP \end{array} \\ \begin{bmatrix} 1,1 & 1,2 & \bullet & 1,NP \\ 2,1 & 2,2 & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ NP,1 & NP,2 & NP,3 & NP,NP \end{bmatrix} \end{array}$$

If 2 parameters were estimated:

$$\begin{array}{c} \\ b1 \\ b2 \end{array} \begin{array}{c} \begin{array}{cc} b1 & b2 \end{array} \\ \begin{bmatrix} Var_1 & Cov_{1,2} \\ Cov_{2,1} & Var_2 \end{bmatrix} \end{array}$$

VARIANCE (b1)

$$VAR(b1) = \left(\underline{\underline{X}}^T \underline{\underline{\omega}}\, \underline{\underline{X}}\right)^{-1}_{1,1} (EVAR)$$

$$Std\ Dev = \sqrt{VAR\ (b1)} \qquad 95\%\ Confid = b1 +/- 2 * StdDev$$

VARIANCE (b2)

$$VAR(b2) = \left(\underline{\underline{X}}^T \underline{\underline{\omega}}\, \underline{\underline{X}}\right)^{-1}_{2,2} (EVAR)$$

$$Std\ Dev = \sqrt{VAR\ (b2)} \qquad 95\%\ Confid = b2 +/- 2 * StdDev$$

Confidence interval on parameters

Later we use this for confidence interval on predictions

The regression is not extremely sensitive to the weights, thus the casual approach to their definition is not a problem

The weighting can be evaluated at the end of the regression by considering the cev (calculated error variance)

smaller values of s ^{2} and s indicate a better fit

values close to 1.0 indicate the fit is consistent with the data accuracy as described by the weighting

cev > 1 (eg 95% confidence intervals on cev completely above 1) indicates the modeler globally underestimated the variances (i.e. the model does not fit the observations as well as the variances assigned by the modeler would reflect)

cev < 1 (eg 95% confidence intervals on cev completely below 1) indicates the modeler globally overestimated the variances (i.e. the model fits better than expected)

The 95% confidence intervals on cev are calculated using the ChiSq distribution. Deviations from 1.0 are significant if 1.0 falls outside of the confidence limits.

The modeler could adjust weights to obtain 1, but it is not necessary as long as the cev is discussed along with the input variances

CONSIDER HOW THE PARAMETER UNCERTAINTY IS CALCULATED

Variance Optimal Parameters:

$$V(\underline{b}) = \frac{\text{Sum of Squared Weighted Residuals}}{\text{\#Observations - \#Parameters}} \left[\underline{X}^T \underline{w} \underline{X}\right]^{-1}$$

$$V(\underline{b}) = cev \left[\underline{X}^T \underline{w} \underline{X}\right]^{-1}$$

$\underline{b}$ vector of optimal parameters (e.g. K,S,R,H,Q)
$\underline{X}$ sensitivity matrix
$\underline{w}$ weight matrix for observations

Results in NPxNP matrix, with variances on the diagonal

$$V(\underline{b}) = \begin{pmatrix} K & KS & KR & KH & KQ \\ SK & S & SR & SH & SQ \\ RK & RS & R & RH & RQ \\ HK & HS & HR & H & HQ \\ QK & QS & QR & QH & Q \end{pmatrix}$$

VARIANCE (K)

$$VAR(K) = \left(\underline{\underline{X}}^T \underline{\underline{\omega}}\, \underline{\underline{X}}\right)^{-1}_{1,1} (EVAR)$$

$$Std\ Dev = \sqrt{VAR\ (K)} \qquad 95\ \%\ Confid = K +/- 2 * StdDev$$

VARIANCE (H)

$$VAR(H) = \left(\underline{\underline{X}}^T \underline{\underline{\omega}}\, \underline{\underline{X}}\right)^{-1}_{4,4} (EVAR)$$

$$Std\ Dev = \sqrt{VAR\ (H)} \qquad 95\ \%\ Confid = H +/- 2 * StdDev$$

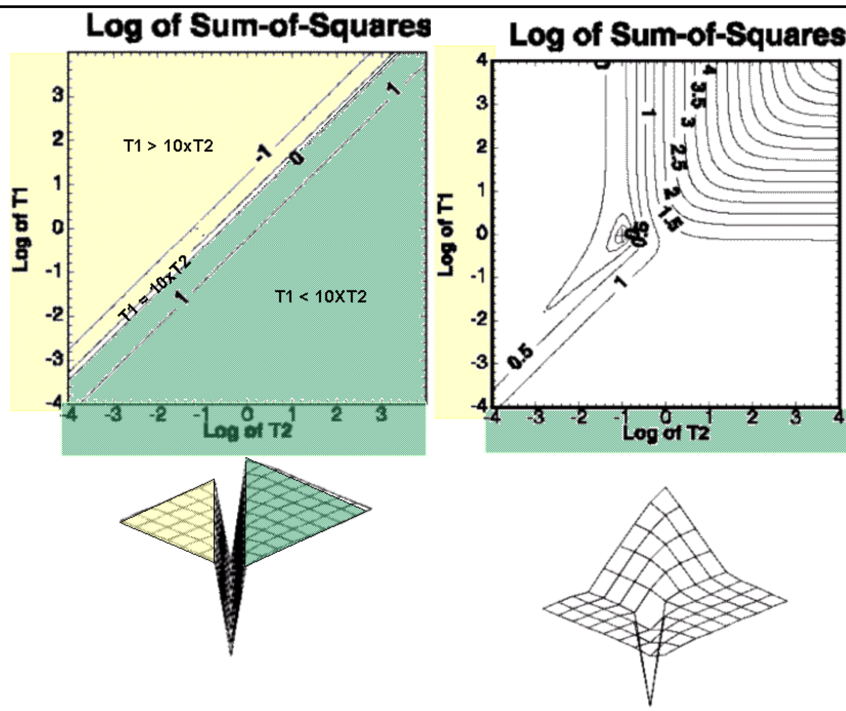
CORRELATION (normalized variance)

$$CORR(i,j) = \frac{COV(i,j)}{\sqrt{VAR(i)} * \sqrt{VAR(j)}}$$

$$\begin{array}{c} \\ i=1 \\ \bullet \\ \bullet \\ i=NP \end{array} \begin{array}{c} \begin{array}{cccc} j=1 & \bullet & \bullet & j=NP \end{array} \\ \begin{bmatrix} 1,1 & 1,2 & \bullet & 1,NP \\ 2,1 & 2,2 & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ NP,1 & NP,2 & NP,3 & NP,NP \end{bmatrix} \end{array}$$

If 2 parameters were estimated:

$$\begin{array}{c} \\ b1 \\ b2 \end{array} \begin{array}{c} \begin{array}{cc} b1 & b2 \end{array} \\ \begin{bmatrix} 1 & Cor_{b1,b2} \\ Cor_{b2,b1} & 1 \end{bmatrix} \end{array}$$



Follow tutorial for parameter estimation run/see Ucode_main.in Ucode_main_out.#uout and _files

As before parameter estimation view residual statistics / sensitivities

Using GWChart also

See previous items and more from

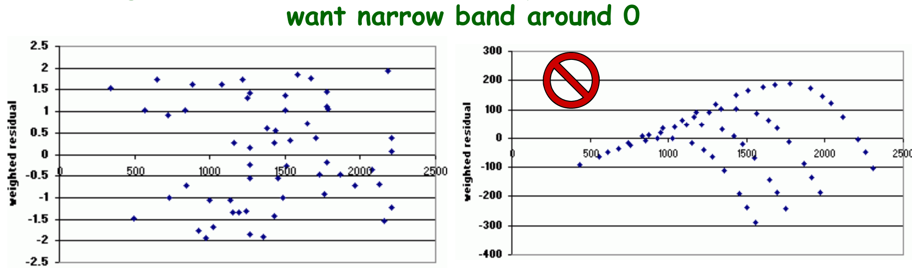
Tables 28 (p 176) and 31 (p 180)

EVALUATING PARAMETER ESTIMATION OUTPUT

RESIDUALS

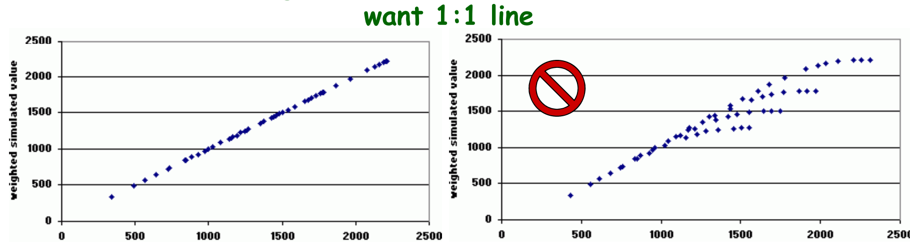
ws (weighted residuals vs simulated equivalents)

want narrow band around 0



ww (weighted observed versus simulated)

want 1:1 line

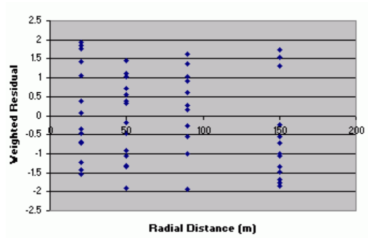


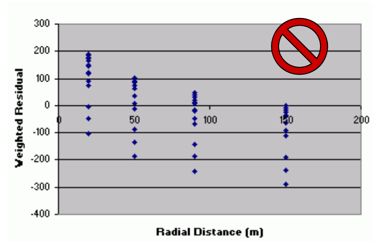
EVALUATING PARAMETER ESTIMATION OUTPUT

RESIDUALS (if you include a root.xyzt file)

wxyzt (weighted residuals vs space [1D distance in this illustration])

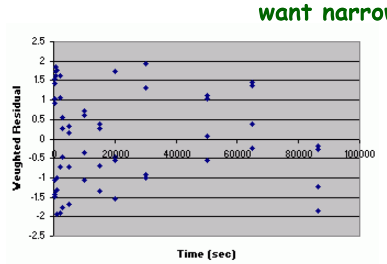
want narrow band around 0

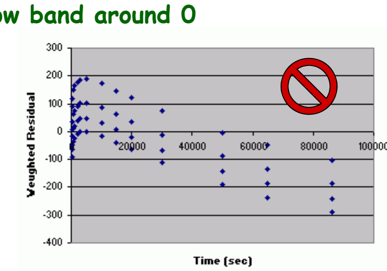




wxyzt (weighted observed versus time)

want narrow band around 0



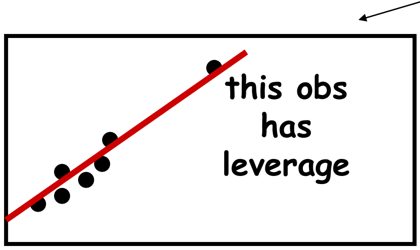


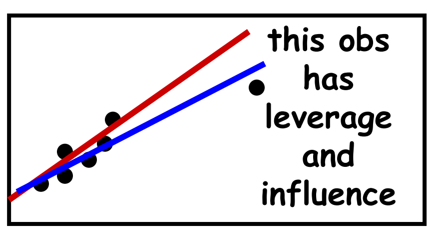
Extensive model analysis and development work can be accomplished by analyzing residuals

Explore the rest of the data exchange files

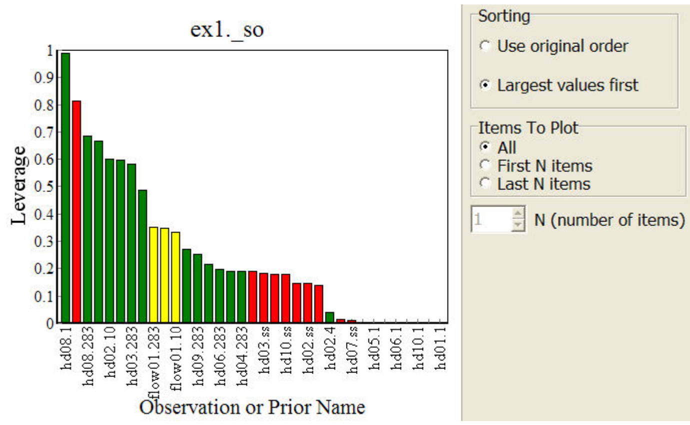
Various sensitivity representations (sc sd s1 so su)

Parameter Information (paopt pc pasub)





A typical _so



If the PARAMETER ESTIMATION is successful:
Further EVALUATE RESULTS
with UCODE's Residual_Analysis (p159 and on)
It only needs the data exchange files, but there is optional input described in the ucode manual

Create batch file for residual_analysis OR run in ModelMate

Additional Residual Analyses can be obtained running

residual_analysis.exe >>> fn.#resan

VIEW RESULTS WITH GW_CHART
_nm - want normally distributed residuals
If not a straight line compare to realizations of residuals:
Uncorrelated _rd – if these look like your nonlinear nm plot the cause is too few residuals
Correlated _rg – if these look like your nonlinear nm plot it is OK, due to correlation in the regression

ALSO see rdadv of residual_analysis_adv.exe on next slide

Create a batch file to run residual_analysis_adv or run in ModelMate

View _rdadv in GW_Chart

to see the theoretical confidence limits on the weighted residuals

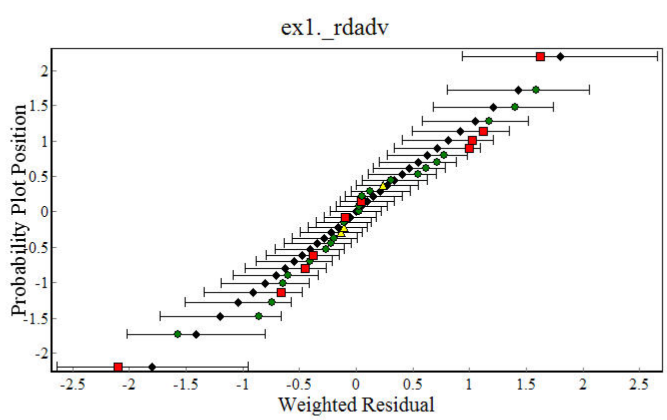
#resanadv

Mean Weighted Residual should be ~ 0
Slope should be ~ 0

INTRINSIC NONLINEARITY << Sum of Squared Residuals
If large Corfac_plus correction factors may not be accurate

CED correlation of weighted residuals and means of synthetic residuals
PROB – probability that a correlation would be <= CED if the residuals were normally distributed

A typical _rdadv



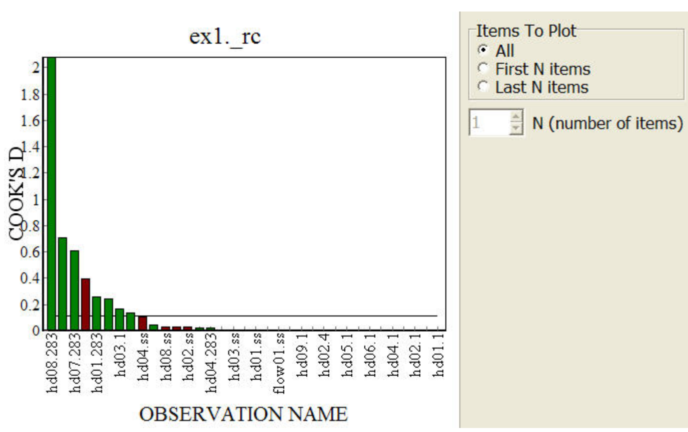
Back to:
EVALUATING PARAMETER ESTIMATION OUTPUT from
Residual_analysis fn.#resan _rc _rb

Cook'sD large values indicate observations that most influence all estimated parameter values

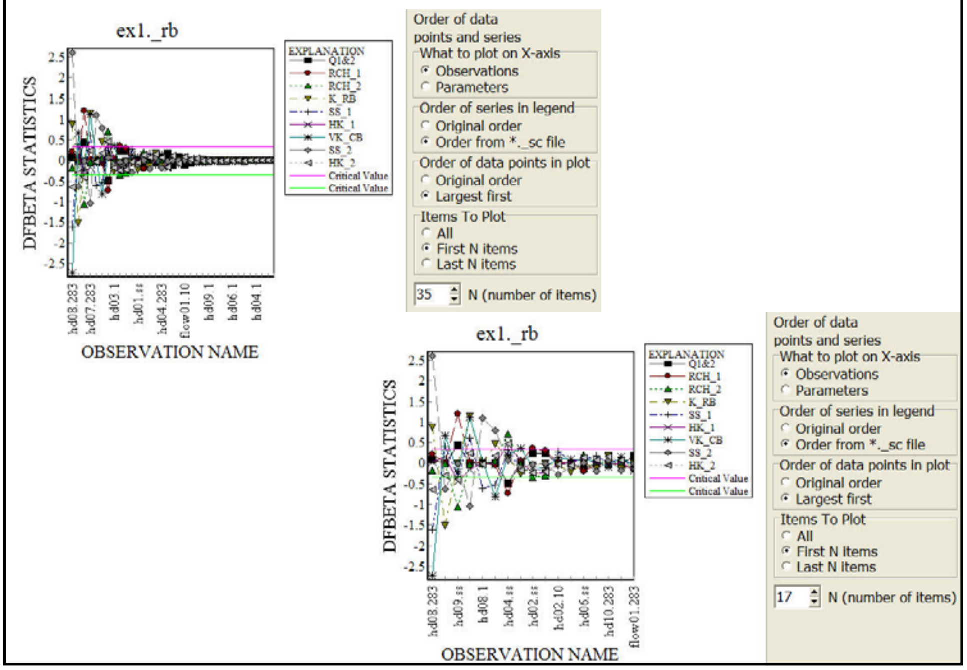
DFBetaS large values indicate observations important to individual parameters

Do you understand why the flow observation is so important? What would you be able to say about the parameter values without that observation?

A typical _rc



A typical _rb



Typical #resan results

```
*******************************************************************************
ANALYSIS OF COOKS D
FOR PLOTTING, COOKS D STATISTICS ARE LISTED IN THE _RC OUTPUT FILE

INFLUENTIAL OBSERVATIONS WITH COOKS D > CRITICAL VALUE (4/(NOBS+MPR)) = 0.114

OBS# OBSERVATION      PLOT-SYMBOL      COOK'S D
   3 hd01.283                   2       0.19920774E+00
  10 hd03.1                     2       0.16229212E+00
  11 hd03.283                   2       0.28741326E+00
  23 hd07.283                   2       0.69218923E+00
  25 hd08.1                     2       0.77273656E+00
  26 hd08.283                   2       0.19342235E+01
  27 hd09.ss                    1       0.41209141E+00
  29 hd09.283                   2       0.15028790E+00

NUMBER OF INFLUENTIAL OBSERVATIONS IDENTIFIED:    8
```

```
*******************************************************************************
ANALYSIS USING DFBETAS
FOR PLOTTING, DFBETA STATISTICS ARE LISTED IN THE _RB OUTPUT FILE

PARAMETER NUMBERS AND NAMES:

            1            2            3            4            5
            Q1&2         RCH_1        RCH_2        K_RB         SS_1
            6            7            8            9
            HK_1         VK_CB        SS_2         HK_2

INFLUENTIAL OBSERVATIONS WITH DFBETA >
                                     CRITICAL VALUE (2/(NOBS+MPR)**0.5) = 0.338

PARAMETERS INFLUENCED IDENTIFIED BY #

                                     PARAMETER NUMBER

OBS# ID                  PLOT-SYMBOL    1  2  3  4  5  6  7  8  9
   3 hd01.283                      2    -  -  -  #  #  -  #  #  -
   4 hd02.ss                       1    -  #  #  -  -  -  -  -  -
  10 hd03.1                        2    -  -  -  -  -  -  #  -  -
  11 hd03.283                      2    -  -  -  #  #  -  #  #  -
  12 hd04.ss                       1    #  #  #  -  -  #  -  -  #
  23 hd07.283                      2    -  -  -  #  #  -  #  #  -
  25 hd08.1                        2    -  -  -  -  #  -  -  #  -
  26 hd08.283                      2    -  -  -  #  #  -  #  #  #
  27 hd09.ss                       1    #  #  #  -  -  #  -  -  #

NUMBER OF INFLUENTIAL OBSERVATIONS IDENTIFIED:    9
```

EVALUATING PARAMETERIZATION

High parameter correlations calls for either
Additional data that will break the correlations
Or
Reparameterization

Barring the availability of additional data, consider reparameterization e.g. USING DERIVED_PARAMETERS Block
As an example you could define
rch2=0.5*rch1 and rch3=0.1*rch1
However, notice that the true values do not have those ratios

To evaluate if correlations are too high
try starting from different values
USE PARAMETER_VALUES Block
If results are the same (parameter values fall within one standard deviation of those determined with different starting values) **correlation is not an issue**
Thus parameters are being independently estimated

Overview of UCODE & Associated Codes

Modes that can be accomplished:

Forward Process Model run with Residuals

Conduct Sensitivity Analysis

Estimate Optimal Parameter values and associated linear uncertainty

Evaluate quality of the model

Estimate values of Predictions and associated linear uncertainty

Evaluate model linearity

Evaluate NonLinear uncertainty associated with
estimates of parameter values and predicted values

Auxiliary: Investigate Objective Function

See UCODE Manual Chapter 1 for overview and description of manual contents

When prediction=yes, UCODE calculates predictions and sensitivities (if sensitivities=yes) of the model parameters to those predicted values for the purpose of calculating 95-percent linear confidence and prediction intervals on the predictions. IN PREDICTION MODE WE CHANGE THE PROCESS MODEL TO THE PREDICTIVE CONDITIONS

We will get both
CONFIDENCE INTERVALS and PREDICTION INTERVALS
ON PREDICTED VALUES

CONFIDENCE INTERVALS are based on var-cov of parameters, reflecting certainty associated with the parameters

PREDICTION INTERVALS are based on var-cov of parameters AND the measurement error reflecting our ability to measure the predicted value

3 ALTERNATIVE METHODS OF CALCULATION OF INTERVALS for both CONFIDENCE INTERVALS AND PREDICTION INTERVALS on PREDICTIONS

Appropriate method depends on # of predictions jointly considered

1) INDIVIDUAL INTERVALS
2) SIMULTANEOUS INTERVALS - more than one interval
3) SIMULTANEOUS INTERVALS - undefined number of intervals (e.g. drawdown over an area must be limited to a given magnitude, but the location of the maximum drawdown cannot be determined a priori).

Only the critical values differ and are obtained from one of:

- Student-t Distribution
- Bonferroni-t Distribution
- Scheffe (based on the F-distribution)

UCODE tests for the appropriate method, then prints intervals for Individual and Both Simultaneous Intervals. Of these 3, the user selects the interval appropriate for their question.

INDIVIDUAL CONFIDENCE INTERVALS

$$z'_\ell \pm t_s\left(n, 1.0 - \frac{\alpha}{2}\right) s_{z'_\ell}$$

$z'_\ell = \ell^{th}$ simulated value

$t_s\left(n, 1.0 - \frac{\alpha}{2}\right)$ = critical value, value with $\frac{\alpha}{2}$ probability that a student-t distributed random value would be larger

n = degrees of freedom (ND + NPR - NP)

α = significance level, commonly 0.05 or 0.10 (5 or 10%)

$s_{z'_\ell}$ = standard deviation of the prediction

$$s_{z'} = \left[\sum_{i=1}^{NP}\sum_{j=1}^{NP} \frac{\partial z'}{\partial b_j} V(b_{ij}) \frac{\partial z'}{\partial b_i}\right]^{\frac{1}{2}}$$

Sensitivity of the simulated equivalent of the prediction to the parameters

Element ij of the variance/covariance matrix

SIMULTANEOUS CONFIDENCE INTERVALS

Two Methods: Bonferroni & Scheffe

- Both conservative with respect to significance level
- Both are calculated by UCODE and the smaller is used

Bonferroni: $z'_\ell \pm t_B\left(n, 1.0 - \frac{\alpha}{2k}\right) s_{z'_\ell}$

where k is the number of simultaneous intervals and t_B is the Bonferroni-t probability distribution for a given number of degrees of freedom and simultaneous intervals at the selected significance level

Scheffe: $z'_\ell \pm t_s(d, F_\alpha(d, n)) s_{z'_\ell}$

where d = k (# simultaneous intervals) OR the # of parameters (whichever is less) and F_α is the critical value from the F probability distribution for a given number of degrees of freedom at the selected significance level

PREDICTION INTERVALS are broader than confidence intervals because they include the probability that the MEASURED value will fall into the interval. Calculations are the same as for confidence intervals, however the standard deviation is increased to reflect the measurement error as follows:

$$z'_\ell \pm t_s\left(n\,,1.0-\frac{\alpha}{2}\right)\left(s_{z'_\ell}+s_a\right)$$

where s_a is the product of the

standard error of the regression

and the

expected measurement error of the prediction

EVALUATE PREDICTIVE UNCERTAINTY
using OPTIMAL PARAMETER VALUES with UCODE
Develop a predictive MODLFOW Model
Import to ModelMate as per instructions in PDF file
Run UCODE with prediction=yes, first to be sure all is functioning correctly
Then with sensitivity=yes
UCODE calculates the sensitivity of the predictions to the parameters at the optimal values
linear_uncertainty is executed in that folder with the ucode root file name as input, e.g.
C:\WRDAPP\UCODE_2005\bin\linear_uncertainty.exe ep_Ucode

NOTE IF you use different root names for calibration and prediction ucode runs you must use ucode 1.020 or later for the linear uncertainty run. ALWAYS USE THE LATEST VERSION OF ALL MODELING CODES

This ucode prediction execution does not overwrite previously created UCODE output files

It produces additional files

#upred
_p _pv _dmp _spu _sppp _sppr _spsp _spsr

The linear_uncertainty execution produces

#linunc and ._linp

You can view the results in GW_Chart

DUE TODAYCOMPUTER FILES AND QUESTIONS for Assgn#6

Assignment # 6 Steady State Model Calibration: Calibrate your model. If you want to conduct a transient calibration, talk with me first. Perform **calibration using UCODE.** **Be sure your report addresses global, graphical, and spatial measures of error as well as common sense.** Consider more than one conceptual model and compare the results. **Remember to make a prediction with your calibrated models and evaluate confidence in your prediction.** Be sure to save your files because you will want to use them later in the semester.

Suggested Calibration Report Outline

- **Title**
- **Introduction**
  - **describe the system to be calibrated (use portions of your previous report as appropriate)**
- **Observations to be matched in calibration**
  - **type of observations**
  - **locations of observations**
  - **observed values**
  - **uncertainty associated with observations**
  - **explain specifically what the observation will be matched to in the model**
- **Calibration Procedure**
- **Evaluation of calibration**
  - **residuals**
  - **parameter values**
  - **quality of calibrated model**
- **Calibrated model results**
- **Predictions**
- **Uncertainty associated with predictions**
- **Problems encountered, if any**
- **Comparison with uncalibrated model results**
- **Assessment of future work needed, if appropriate**
- **Summary/Conclusions**
- **References**

submit the paper as hard copy and include it in your zip file of model input and output
submit the model files (input and output for both simulations) in a zip file labeled:
ASSGN6_LASTNAME.ZIP