PEST - Beyond Basic Model Calibration

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science for a changing world

Purpose of Presentation

* Present advance techniques available in PEST for model calibration
* High level overview
* Inspire more people to use PEST!

*Any use of product names is for descriptive purposes only and does not imply endorsement by the U.S. Government.

PEST Overview

* PEST is a model-independent suite of software tools used throughout the environmental, hydraulic, and hydrologic modeling fields for parameter estimation in complex numerical models
* Adjusts model parameter in order to minimize an “objective function”
* Uses the Gauss-Marquardt-Levenberg optimization method

Objective Function

$$\Phi = \sum_{m} \left((h_m^{sim} - h_m^{obs}) \cdot w_m \right)^2$$

* Sum of the squared residuals
* Φ = The objective function to be minimized
* h_m^{sim} = Measured value of observation *m*
* h_m^{obs}= Simulated value corresponding to observation *m*
* w_m = Weight of the m’th observation
* *m* = Total number of observations

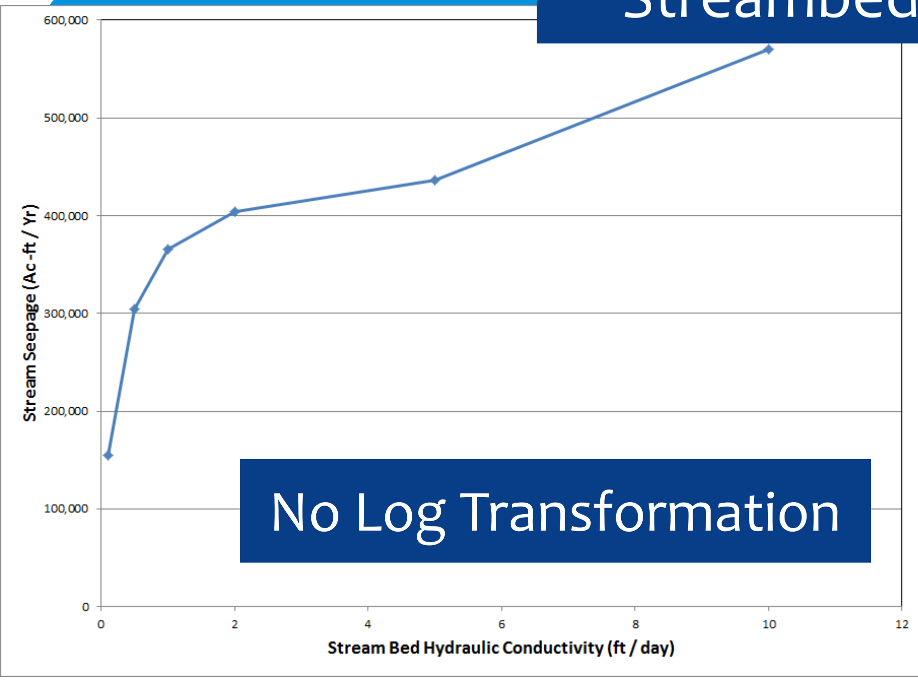
Overview of PEST Techniques

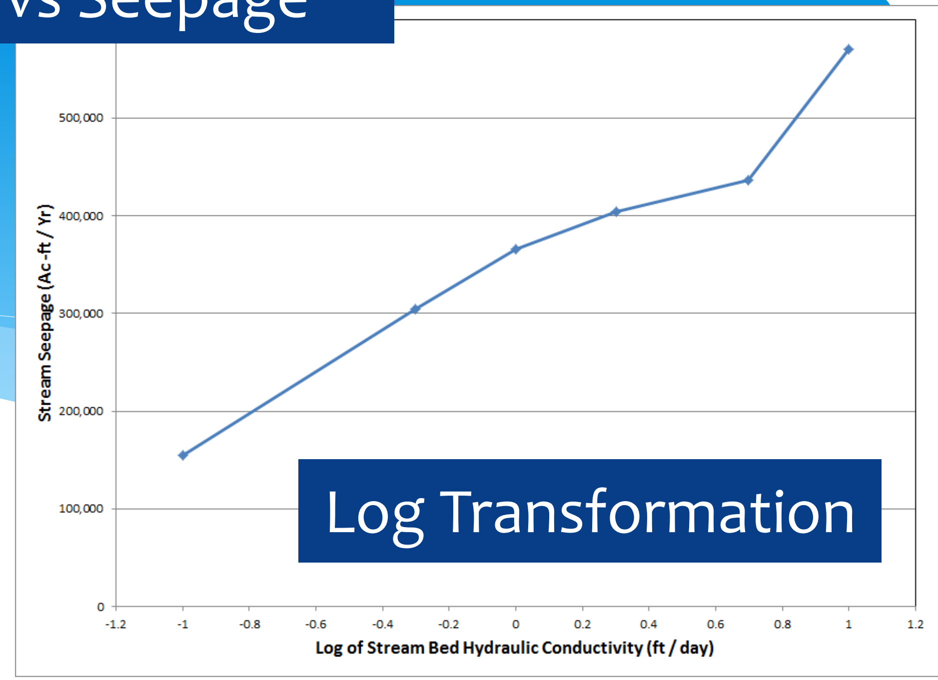
* PEST Control Variables
* BeoPEST
* Regularization though Prior Information
* Singular Value Decomposition
* Pilot Points
* Global Optimization Methods
* Sensitivity Analysis
* Predictive Uncertainty Analysis
* Pareto Mode
* Decision Analysis

Control Variables

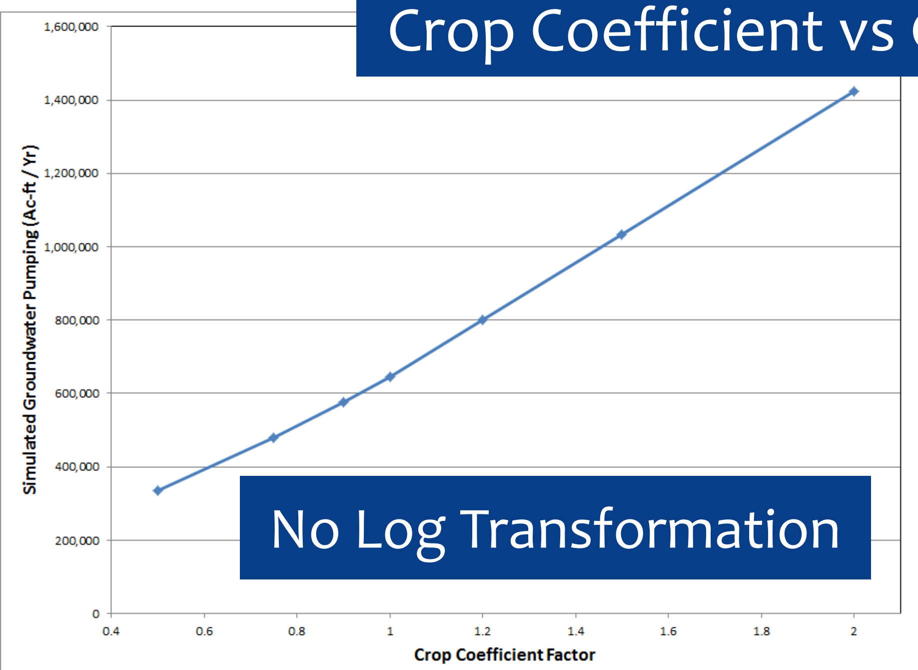
* Model solver variables
  * Precisions vs speed
* Log transformation of parameters
  * Linearize the relationship between parameter values and simulated values
* Observation weights
  * Weight your "best" data the highest
  * Remove spatial or temporal bias
* Many other control variables
* "Best PEST settings" document on PEST webpage
* Test if PEST can return to initial parameters

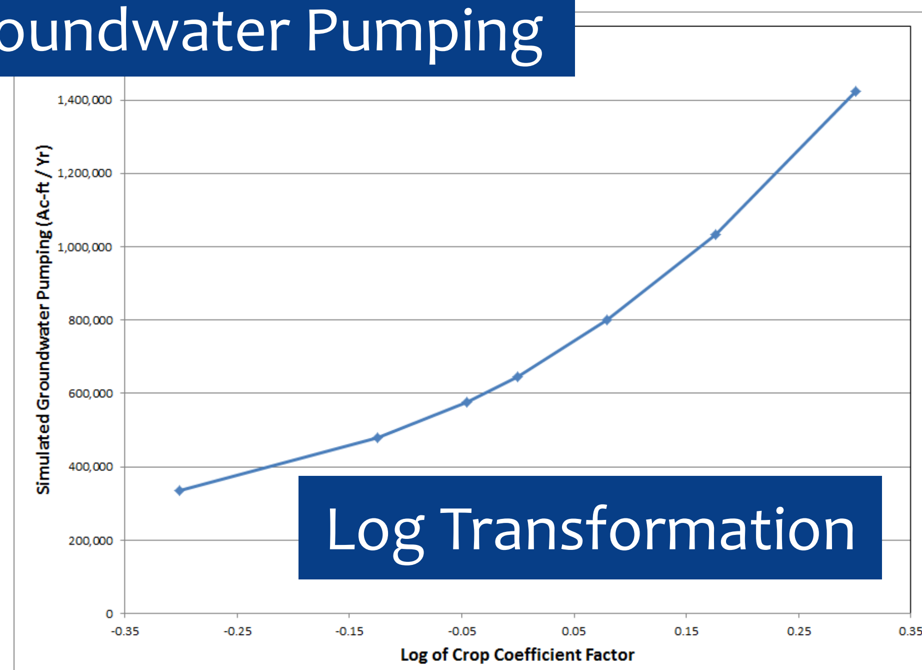
Streambed K vs Seepage





Crop Coefficient vs Groundwater Pumping





BeoPEST

* Allows execution of parallel model runs on one or more computers connected via TCP/IP
* Uses same PEST input files as a serial PEST run
* Fairly robust
* Extra computers can be added and removed mid PEST run
* Parameter values of every model run can be recorded
* Can use a “shotgun” approach to finding the optimal parameter upgrade vector

BeoPEST Examples

```
RUNNING MODEL WITH INITIAL PARAMETER VALUES AND FOR FIRST JACOBIAN.....

   Running model 99 times....

   Waiting for at least one slave to appear....

   New slave has appeared:-
   Slave host: "130.118.108.131"
   Slave working directory: "E:\PEST7b"
   Node number assigned to slave: 1
   Slave speed index:   35.612


   New slave has appeared:-
   Slave host: "130.118.108.131"
   Slave working directory: "E:\PEST7b\Slave3"
   Node number assigned to slave: 1
   Slave speed index:   40.064


   New slave has appeared:-
   Slave host: "130.118.108.131"
   Slave working directory: "E:\PEST7b\Slave2"
   Node number assigned to slave: 2
   Slave speed index:   40.064
```

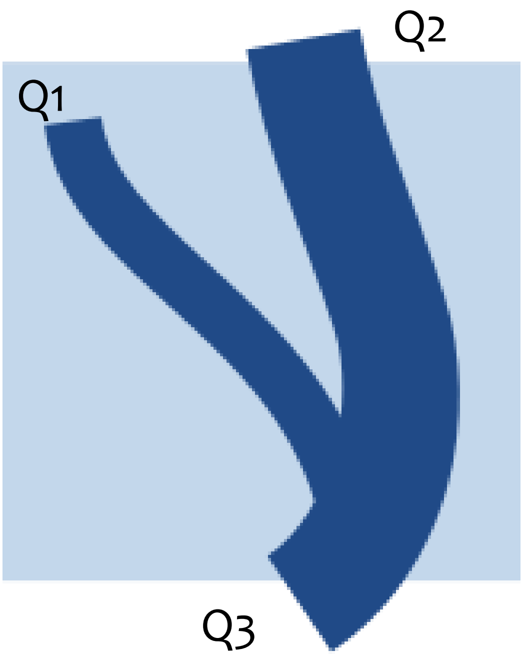
```
BEOSTATS:-
  Node   1  5169.860   61 130.118.108.131\
  Node   2  5325.113   60 130.118.108.131\
  Node   3  5122.886   60 130.118.108.131\
  Node   4  5134.213   60 130.118.108.131\
  Node   5  4392.372   61 130.118.108.131\
  Node   6  5078.254   61 130.118.108.131\
  Node   7  5200.139   60 130.118.108.131\
  Node   8  5230.872   60 130.118.108.131\
  Node   9  5365.565   60 130.118.108.131\
  Node  10  5112.216   60 130.118.108.131\
  Node  11  5237.939   61 130.118.108.131\
  Node  12  4307.615   77 130.118.109.133\
  Node  13  4285.462   79 130.118.109.133\
  Node  14  4151.190   74 130.118.109.133\
  Node  15  4373.090   74 130.118.109.133\
  Node  16  4152.283   76 130.118.109.133\
  Node  17  4283.903   77 130.118.109.133\
  Node  18  4215.667   78 130.118.109.133\
  Node  19  4240.284   79 130.118.109.133\
  Node  20  4213.545   76 130.118.109.133\
  Node  21  4253.435   75 130.118.109.133\
  Node  22  4133.734   76 130.118.109.133\
  Node  23  4129.086   76 130.118.109.133\
  Node  24  4250.034   60 130.118.108.178\
  Node  25  4254.761   60 130.118.108.178\
  Node  26  4169.552   60 130.118.108.178\
  Node  27  4260.424   60 130.118.108.178\
  Node  28  4278.473   60 130.118.108.178\
  Node  29  4189.754   60 130.118.108.178\
  Node  30  4214.466   60 130.118.108.178\
  Node  31  4242.312   60 130.118.108.178\
  Node  32  4171.970   60 130.118.108.178\
  Node  33  4248.272   60 130.118.108.178\
  Node  34  4168.382   60 130.118.108.178\
  Node  35  4169.396   60 130.118.108.178\
  Total CPU time           9795623.5
  Total elapsed time        333065.8
  Speedup                     29.410
```

Prior Information

* Set a “preferred value” for the parameters
* A “penalty” to the objective function is included if parameter values deviate from the prior information value
* Broadly defined as Tikhonov regularization
* Objective function with prior Information:
  * α can be estimated using PEST’s regularization mode

$$\Phi = \underbrace{\sum_{m} (h_m^{sim} - h_m^{obs}) \cdot w_m)^2}_{\text{Observation Component}} + \underbrace{\alpha * \sum_{k} (h_k^{sim} - h_k^{obs}) \cdot w_k)^2}_{\text{Prior Information Component}}$$

Simplest Model Ever
Example of Prior Information



* Two parameters: Q1 and Q2
* One output Q3
* If Q3 = 10, ware the optimized parameter values for Q1 and Q2?
* No unique solution

* Add a prior information equation
  * Q2 = 7
* Now a unique solution of
  * Q1 = 3 & Q2 = 7

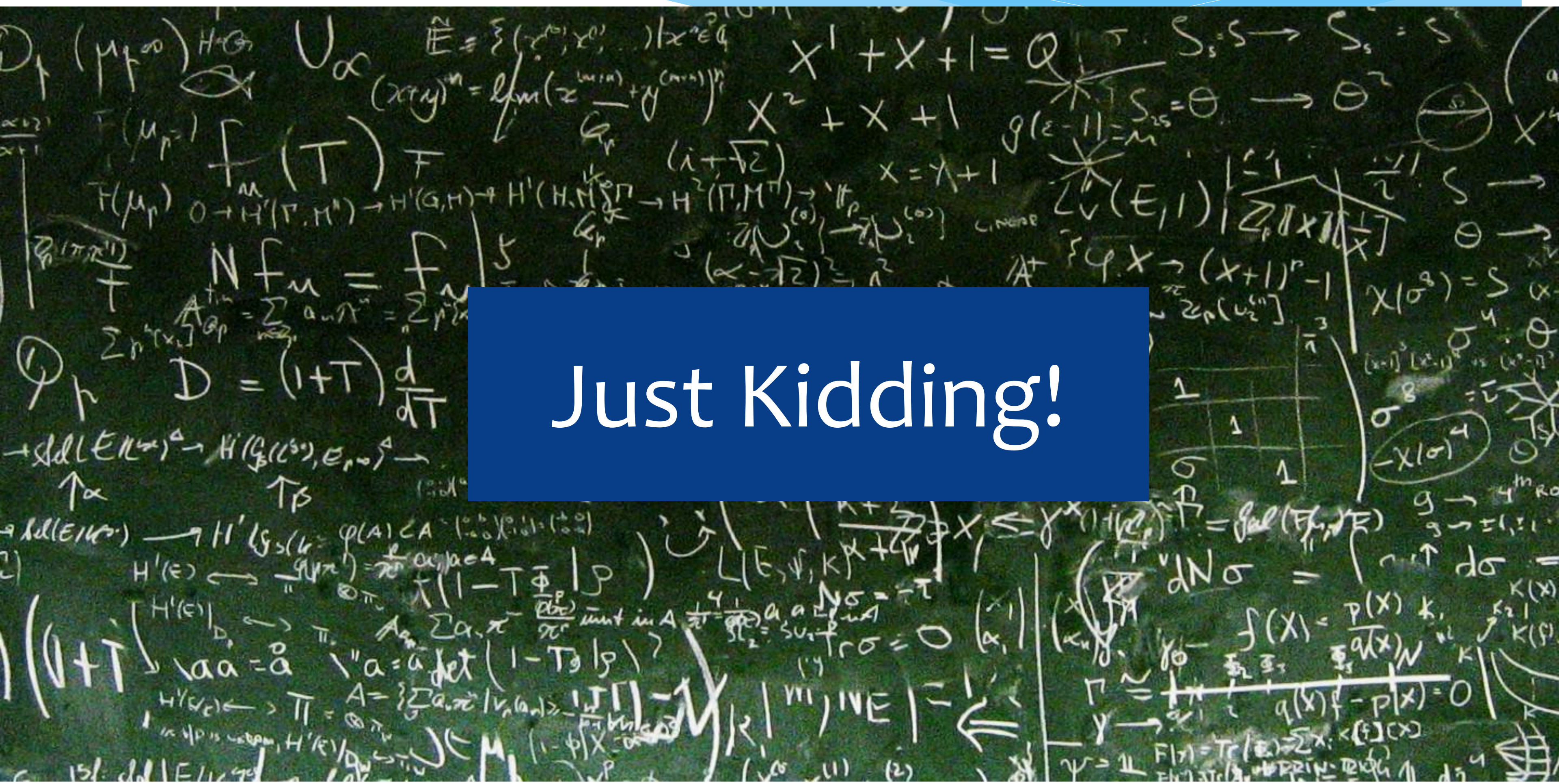
OR

* Add a prior information equation
  * Q2 / Q1 = 2
* Now a unique solution of
  * Q1 = 3.3 & Q2 = 6.7

Singular Value Decomposition

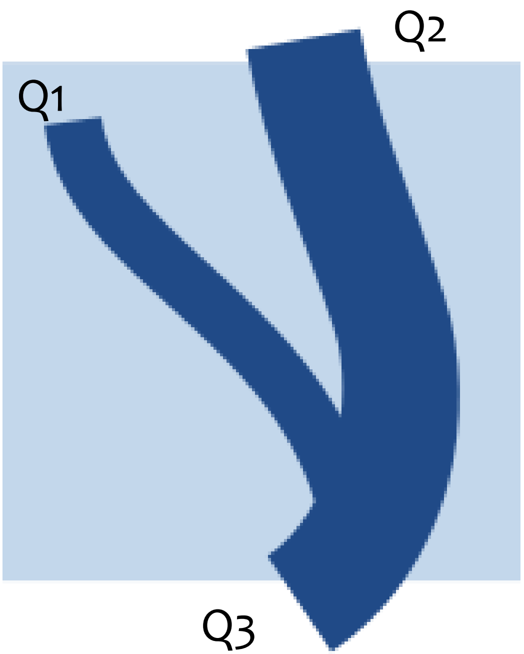
- Automates the removal of insensitive "super parameters" from the calibration problem
- "Super parameters" are orthogonal combinations of individual parameters
- Calculation done "behind the scenes" by PEST

Calculation of SVD and Null Space!



Just Kidding!

Simplest Model Ever Example of SVD

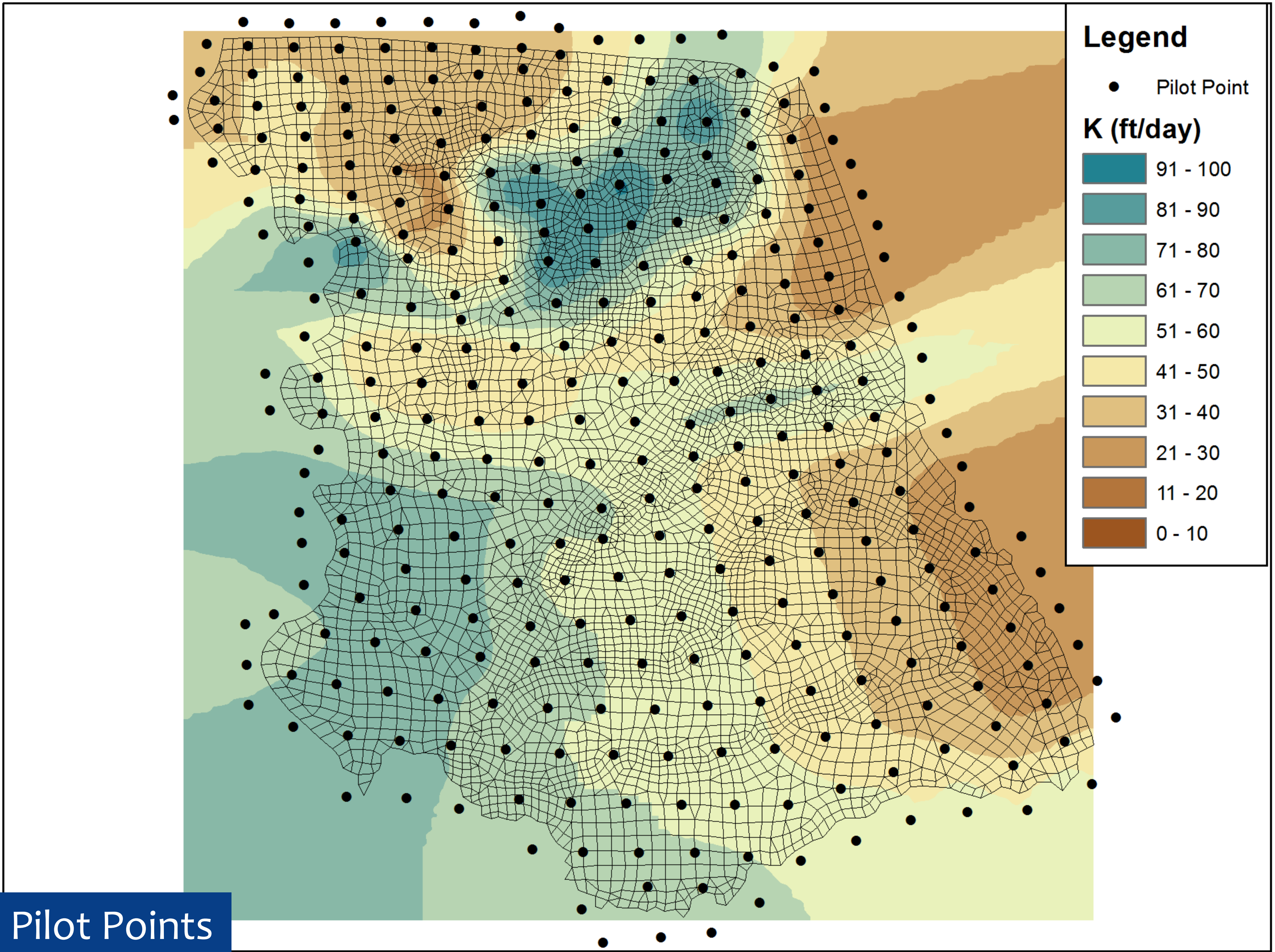


* Two parameters: Q1 and Q2
* One output Q3
* If Q3 = 10, what are the optimized parameter values for Q1 and Q2?
* No unique solution

* Using SVD, parameters are redefined as:
  * P1 = Q1 + Q2
  * P2 = Q1 – Q2
* P2 is insensitive and not solved
  * Null space!
* PEST only solves for P1
* If initially Q1 = 1 and Q2 = 3
* P2 = 2 (not estimated)
* P1 estimated as 10
* Resolve for Q1 and Q2 (Q1 = 4, Q2 = 6)
* Reminder: all done "behind the scenes"

Pilot Points

* Define model parameters using an independent grid of pilot points
* PEST estimates the value of the pilot points
* Value of pilot points are transferred to the model grid using kriging via using PEST tools
* PEST tools available for developing prior information for pilot point values
  * PPCOV utility "penalizes“ differences between nearby pilot points (tending towards a homogeneous parameter field)

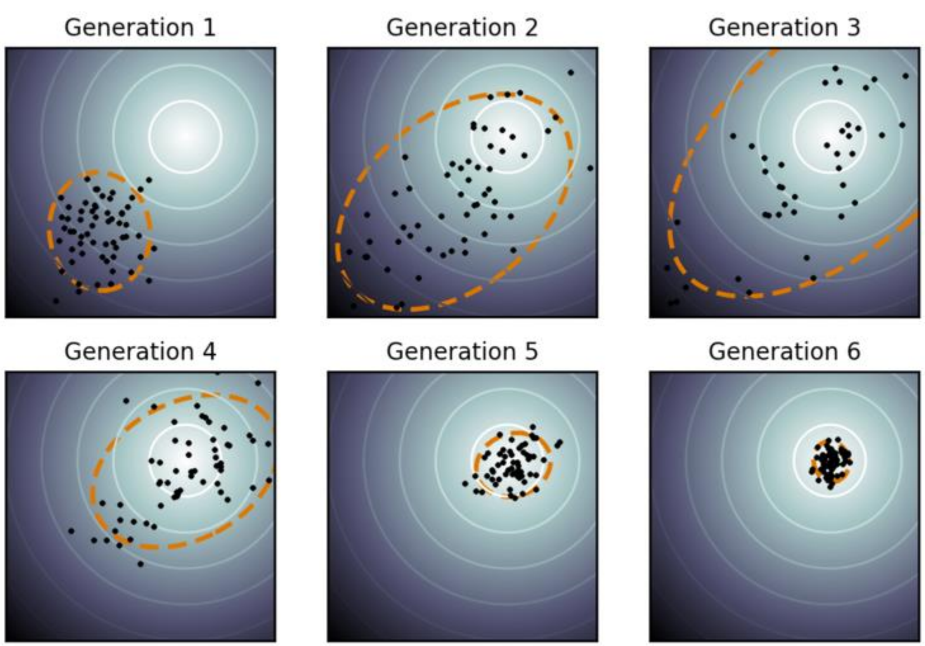


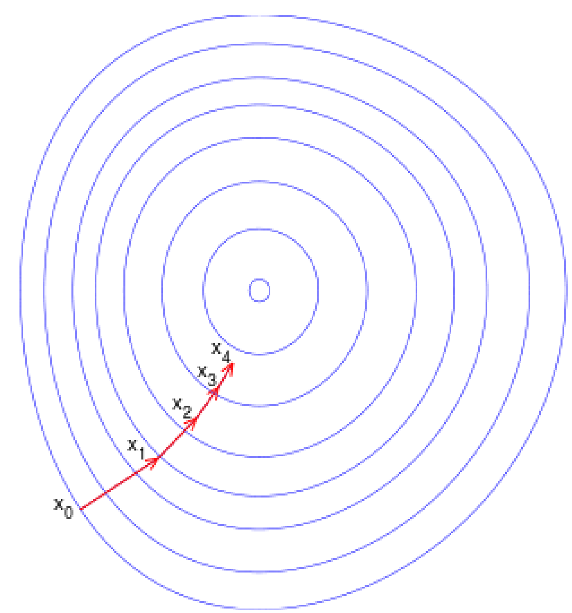
Pilot Points

Global Optimization Methods

Covariance Matrix Adaptation Evolution Strategy (global method)

Gauss-Marquardt-Levenberg (normal method)





Parameter Sensitivity Analysis

* Automatic calculation of parameter sensitivity statistics
* A number of other PEST utilities can be run for additional parameter statistics
  * GENLINPRED utility runs all of them
* Traditional Sensitivity Analysis using SENSAN utility

Examples of Files

SENSAN Input File

KGravel	KSand	KSilt	KClay	
500	100	20	4	copy Resust.txt Base.txt
2500	100	20	4	copy Resust.txt KGravelUp.txt
100	100	20	4	copy Resust.txt KGravelDown.txt
500	500	20	4	copy Resust.txt KSandUp.txt
500	20	20	4	copy Resust.txt KSandDown.txt
500	100	100	4	copy Resust.txt KSiltUp.txt
500	100	4	4	copy Resust.txt KSiltDown.txt
500	100	20	0.8	copy Resust.txt KClayUp.txt
500	100	20	20	copy Resust.txt KClayDown.txt

Composite Sensitivity Output File

Number of observations with non-zero weight = 24900

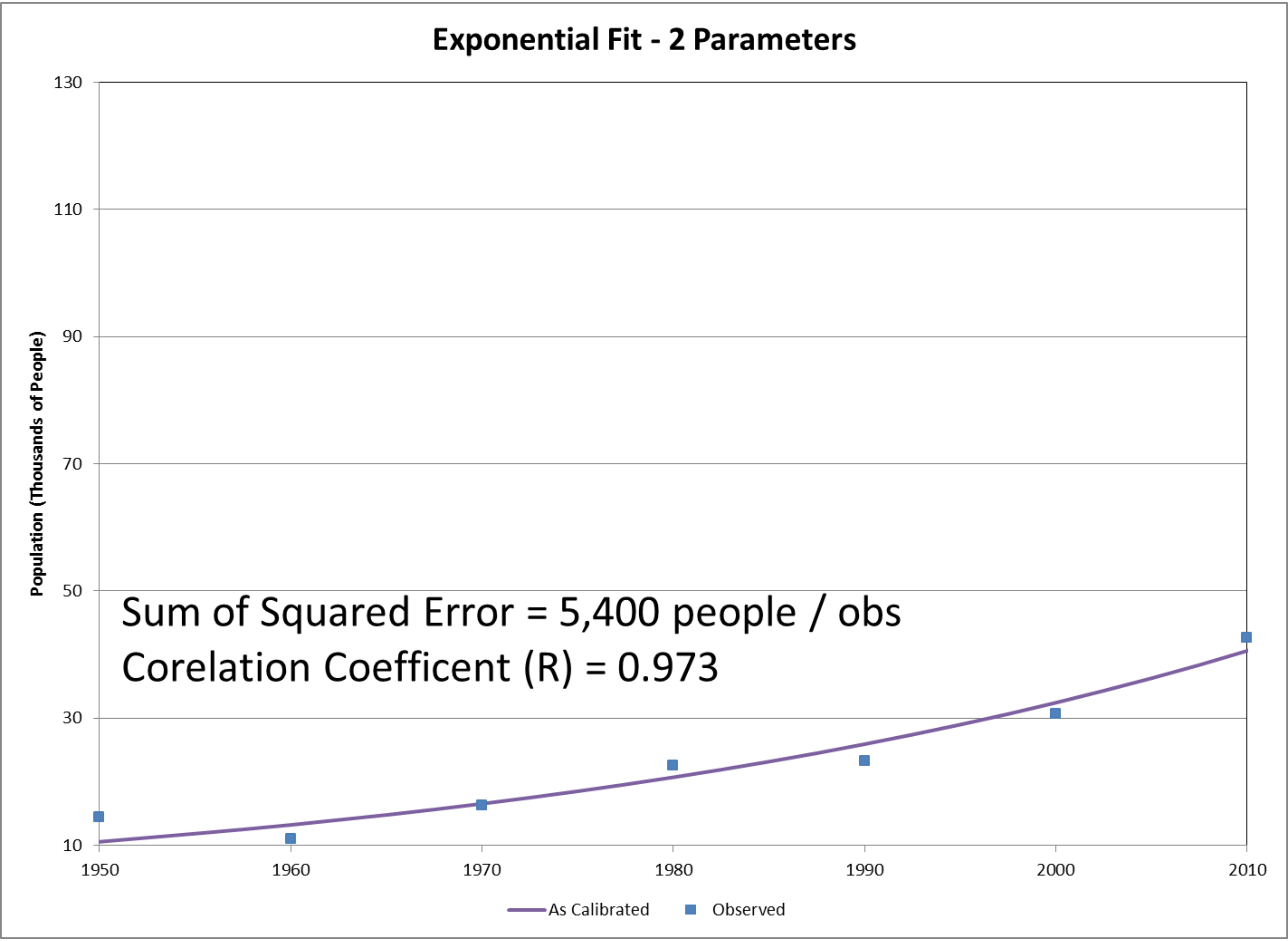
Parameter name	Group	Current value	Sensitivity
kgravel	hk	846.272	3.115821E-03
ksand	hk	248.330	6.729693E-03
ksilt	hk	20.0014	3.040856E-03
kclay	hk	2.822665	1.114168E-03

Parameter Confidence Intervals Output File

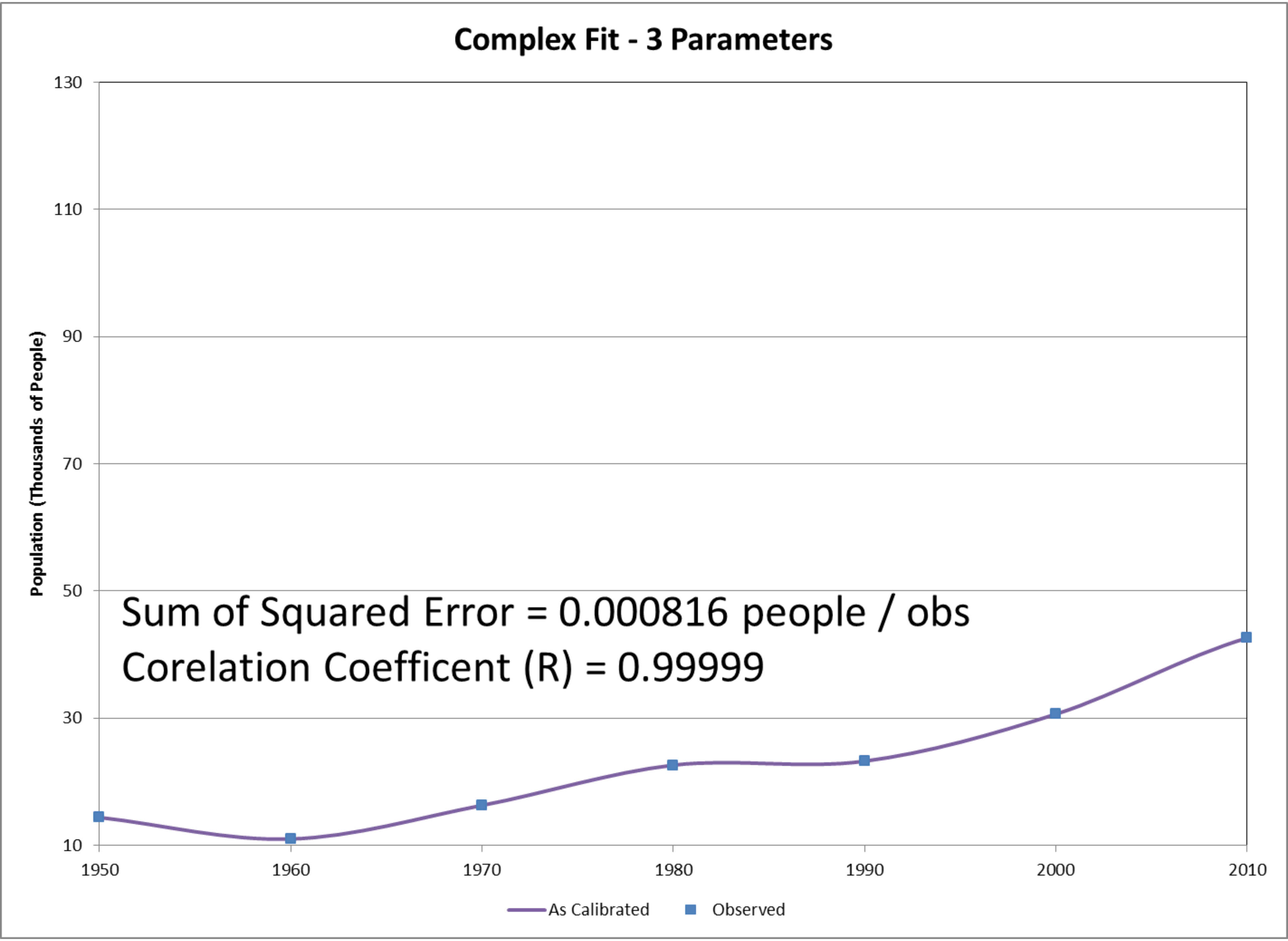
Parameter	Estimated value	95% percent confidence limits lower limit	upper limit
kc_01_01	1.32411	1.26474	1.38349
kc_01_02	0.872049	0.834381	0.909716
kc_01_03	1.13031	1.08010	1.18051
kc_01_04	0.210293	0.200577	0.220008
kc_01_05	1.15991	1.11782	1.20200
kc_01_06	0.208158	0.201743	0.214573
kc_01_07	0.207909	0.198025	0.217793

Predictive Uncertainty Analysis

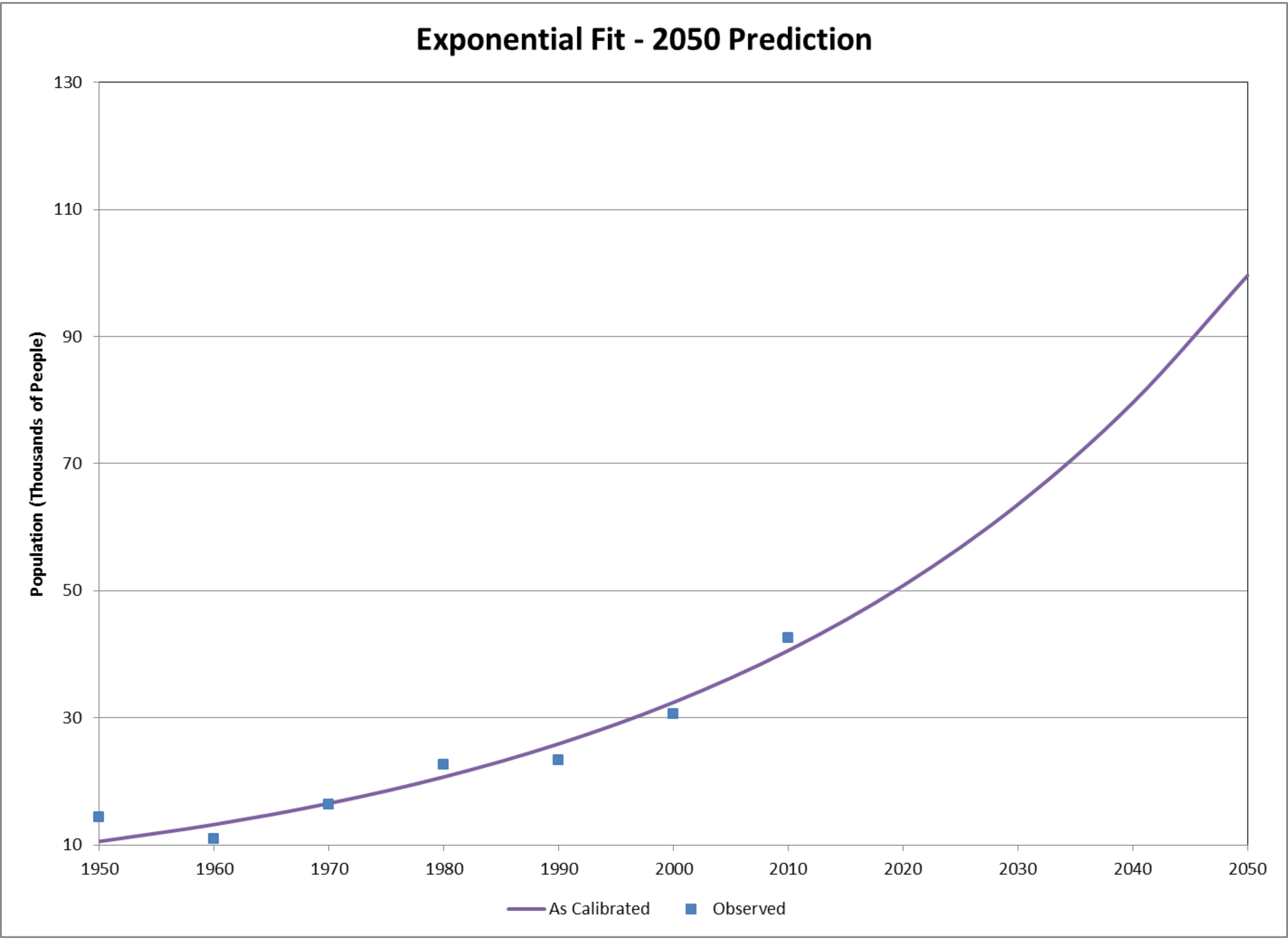
- Used to estimate the uncertainty in model predictions
- User defines a model output as observation to predict
- PEST maximizes (or minimizes) the prediction while keeping the model "almost calibrated"

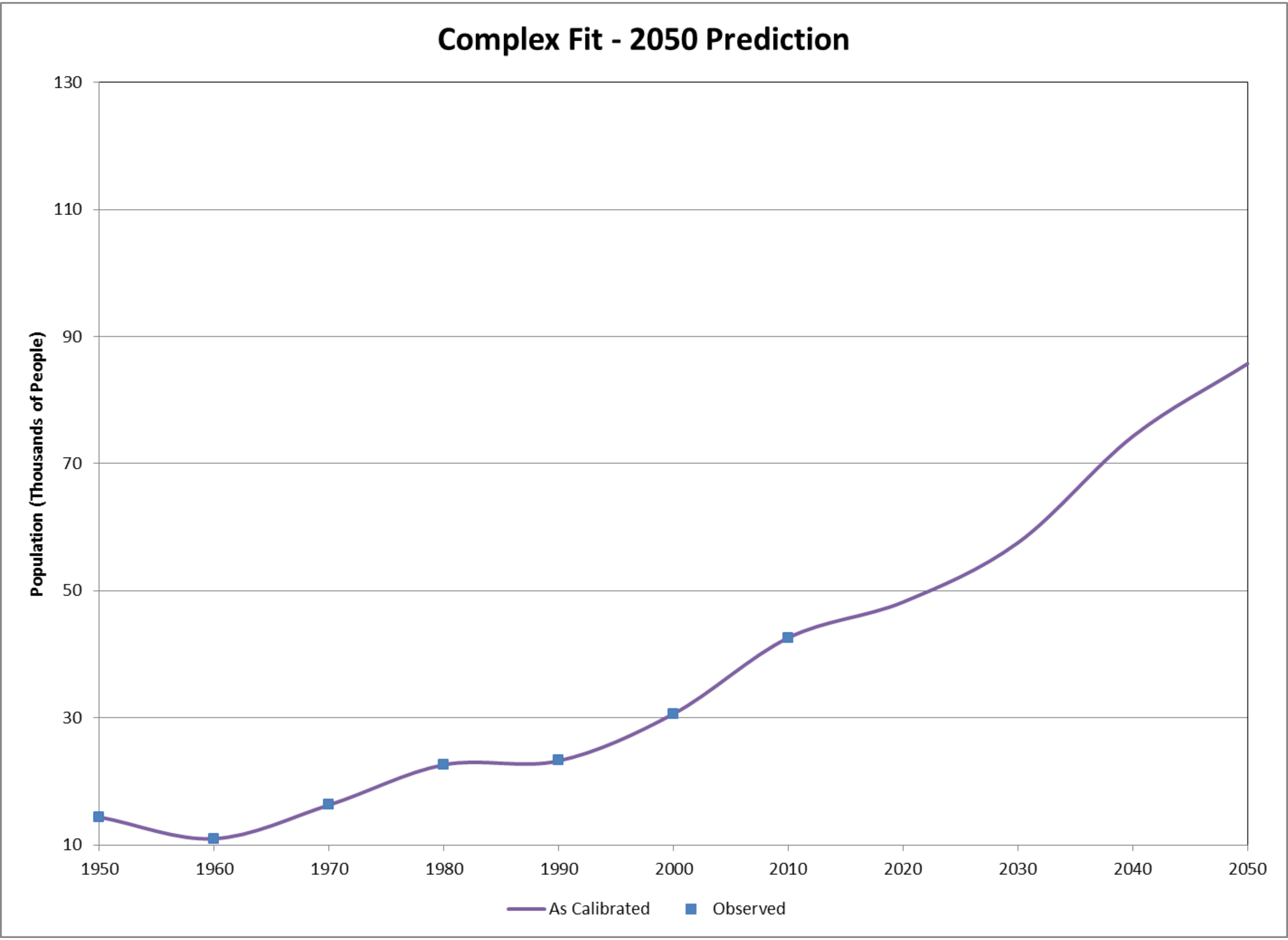


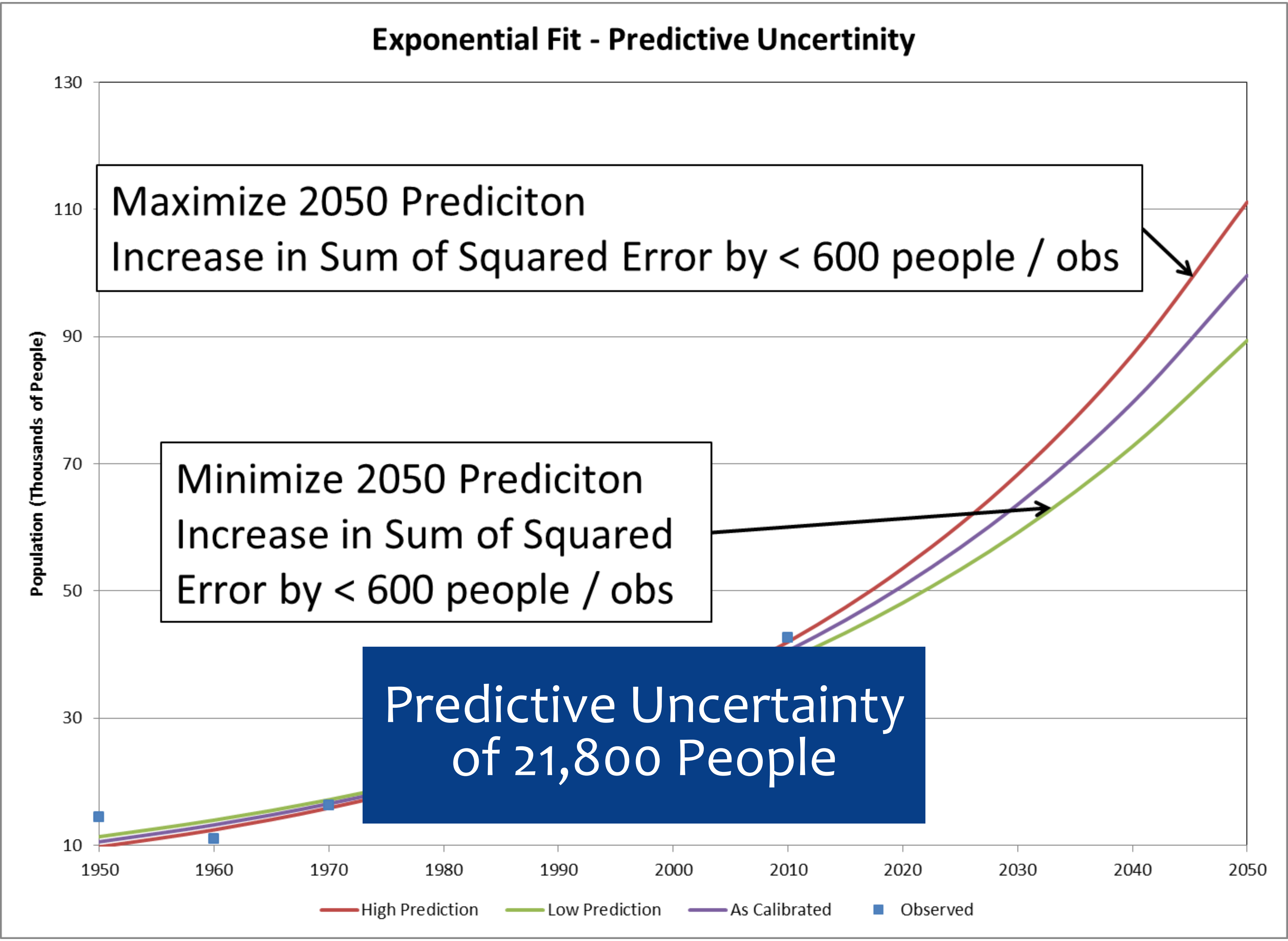
Exponential Fit - 2 Parameters
130
110
90
70
50
30
10
Population (Thousands of People)
Sum of Squared Error = 5,400 people / obs
Corelation Coefficent (R) = 0.973
1950
1960
1970
1980
1990
2000
2010
As Calibrated
Observed

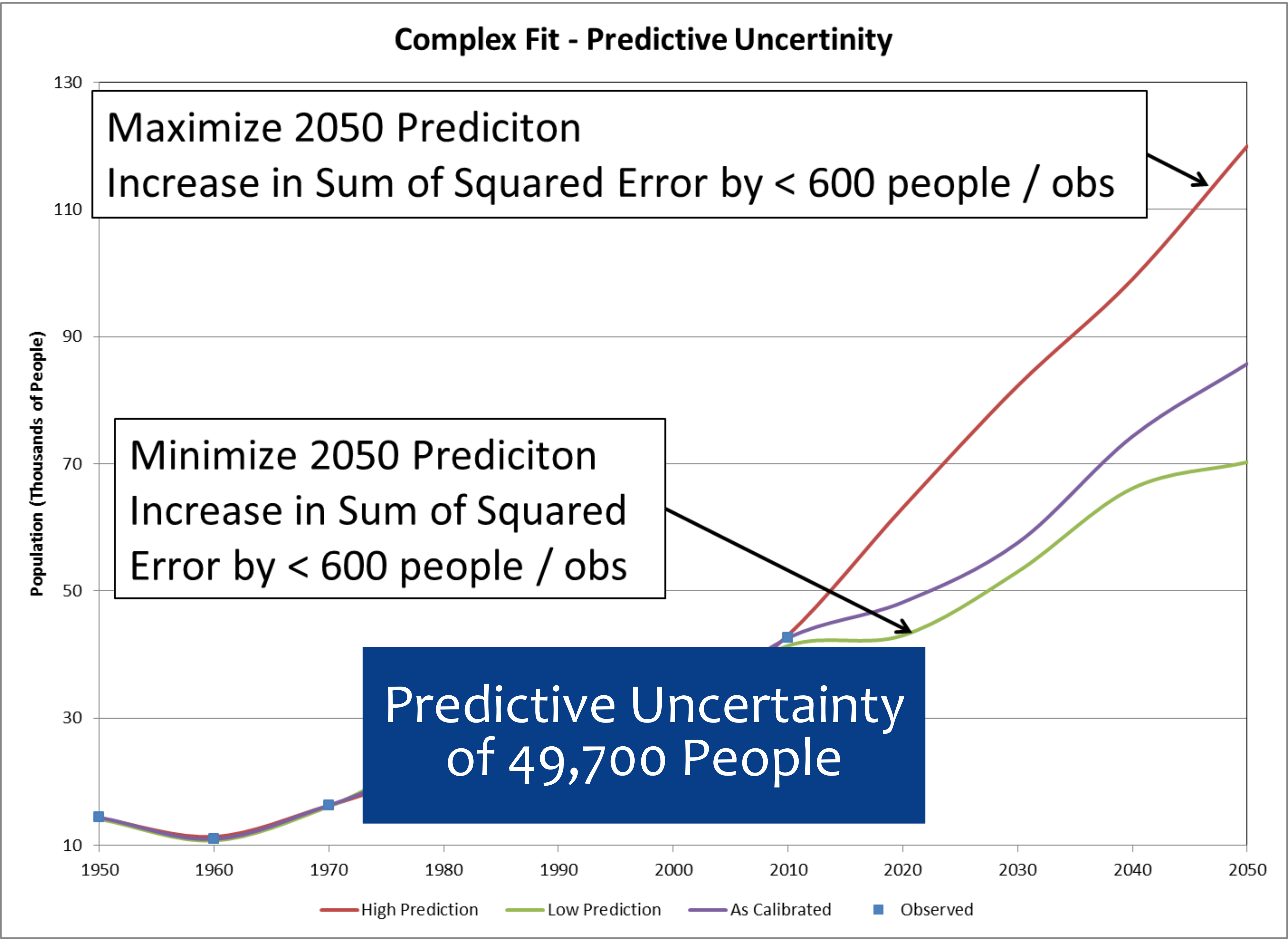


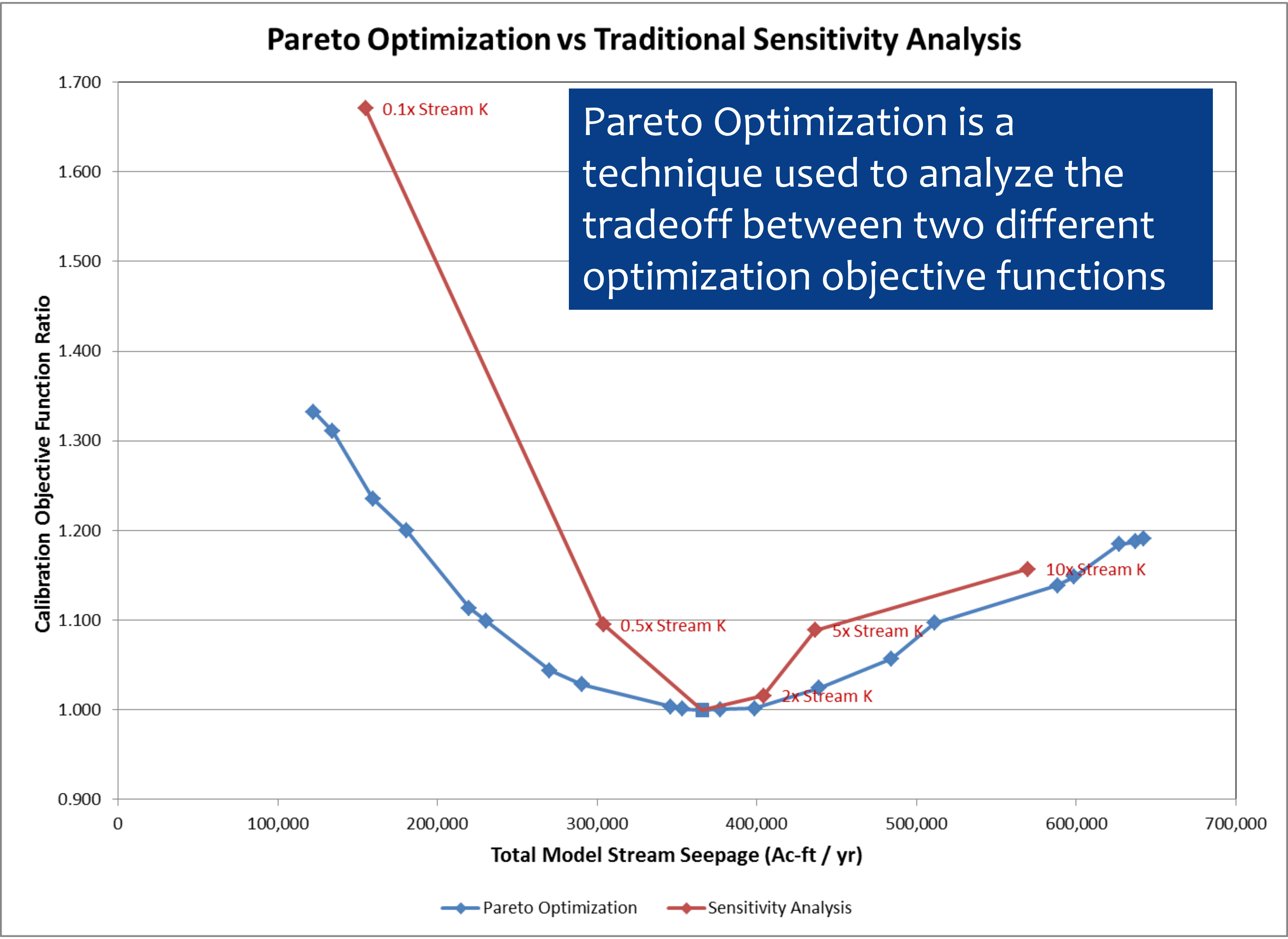
Complex Fit - 3 Parameters
Population (Thousands of People)
130
110
90
70
50
30
10
1950
1960
1970
1980
1990
2000
2010
Sum of Squared Error = 0.000816 people / obs
Corelation Coefficent (R) = 0.99999
As Calibrated
Observed


Exponential Fit - 2050 Prediction
Population (Thousands of People)
130
110
90
70
50
30
10
1950
1960
1970
1980
1990
2000
2010
2020
2030
2040
2050
As Calibrated
Observed


Complex Fit - 2050 Prediction
Population (Thousands of People)
130
110
90
70
50
30
10
1950
1960
1970
1980
1990
2000
2010
2020
2030
2040
2050
As Calibrated
Observed


Exponential Fit - Predictive Uncertinity
Maximize 2050 Prediciton
Increase in Sum of Squared Error by < 600 people / obs
Minimize 2050 Prediciton
Increase in Sum of Squared Error by < 600 people / obs
Predictive Uncertainty of 21,800 People
Population (Thousands of People)
130
110
90
70
50
30
10
1950
1960
1970
1980
1990
2000
2010
2020
2030
2040
2050
High Prediction
Low Prediction
As Calibrated
Observed


Complex Fit - Predictive Uncertinity
Maximize 2050 Prediciton
Increase in Sum of Squared Error by < 600 people / obs
Minimize 2050 Prediciton
Increase in Sum of Squared Error by < 600 people / obs
Predictive Uncertainty of 49,700 People
Population (Thousands of People)
130
110
90
70
50
30
10
1950
1960
1970
1980
1990
2000
2010
2020
2030
2040
2050
High Prediction
Low Prediction
As Calibrated
Observed


Pareto Optimization vs Traditional Sensitivity Analysis
Pareto Optimization is a technique used to analyze the tradeoff between two different optimization objective functions
Calibration Objective Function Ratio
1.700
1.600
1.500
1.400
1.300
1.200
1.100
1.000
0.900
0
100,000
200,000
300,000
400,000
500,000
600,000
700,000
Total Model Stream Seepage (Ac-ft / yr)
0.1x Stream K
0.5x Stream K
2x Stream K
5x Stream K
10x Stream K
Pareto Optimization
Sensitivity Analysis

Decision Analysis

* Start with a calibrated model
* Formulate an objective function to minimize negative effects and/or maximize benefits
  * Example: minimize groundwater drawdown
* Include constraints as observations
  * Example: total pumping must be greater than demand
* Replace model parameters with decision variables
  * Example: pumping rates from wells
* Obs2obs and Par2par utilities can be very helpful
* Resulting problem is often very non-linear (good use for global optimization methods)

Conclusions

* PEST has many capabilities, beyond those used for basic parameter estimation, for finding optimal parameter values and for performing additional analysis
* Read the documentation for details to prevent the misuse of these capabilities!
* Calibrated parameter values should make physical sense