

# Implementation of a Python-R interface for the assessment of simulation models

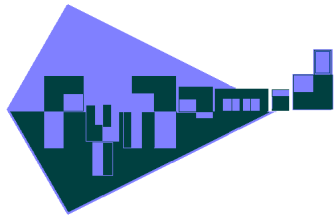
By Alisha Rossi

Internship Advisor: Dr. Jeffrey White



US Arid Land Agricultural Research Center (ALARC)  
of the United States department of agriculture  
(USDA)

Agricultural Research Service  
(ARS)



# Overview

## Section 1: Introduction

Simulation

Validation

Project Tasks

## Section 2: Literature Review

Validation

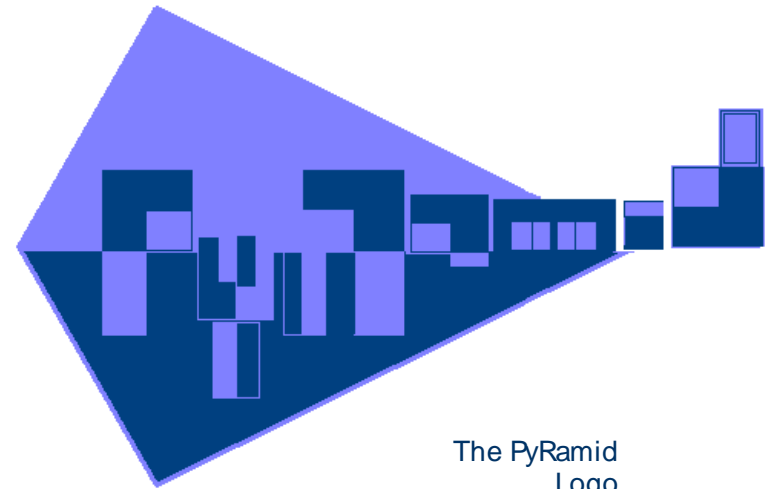
Programmed Model Validation

Statistical Validation

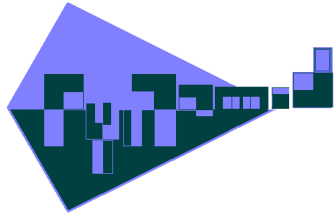
## Section 3: Project Implementation

Phase I: Learning Phase

Phase II: Tool Development



The PyRamid  
Logo



# Introduction

## Simulation

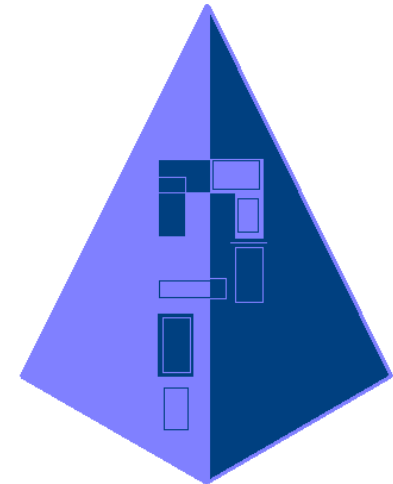
- What is a simulation?

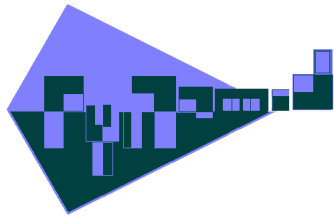
## Validation

- What is validation?
- What is statistical validation?

## Project Tasks

- Which statistical methods of validation are the most promising?
- Can we develop a tool that implements these procedures?





# Simulation

## A Simulation

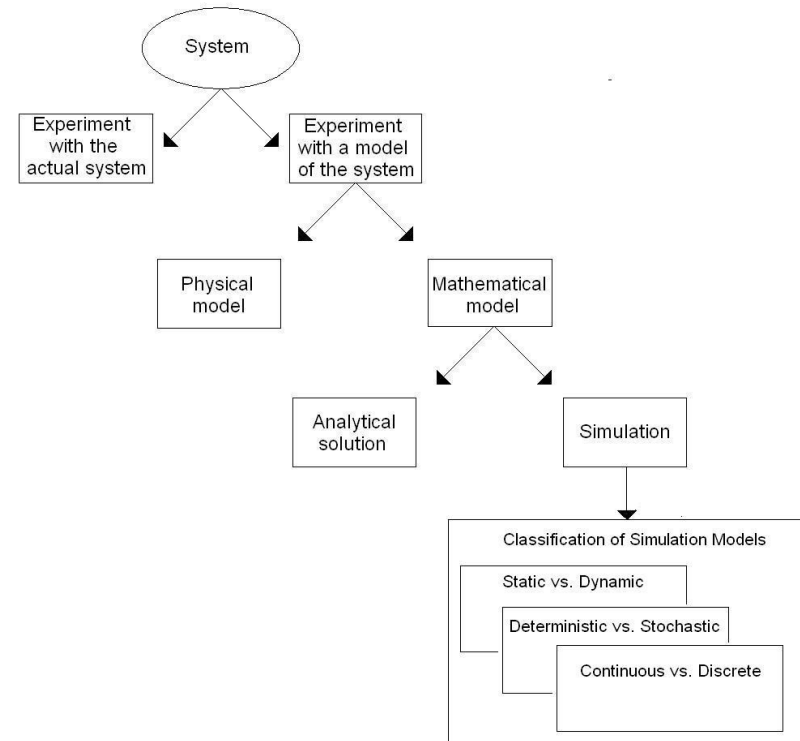
- the development of a computerized mathematical model of a system

## A Mathematical Model

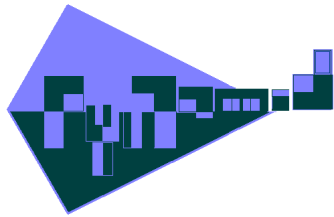
- a set of equations that collectively describe the dynamics of the system

## A System

- a collection of entities that interact to perform a particular task



Ways to study a system  
(modified from Law and Kelton, 2000)



# Classification of a Simulation

## Dynamic

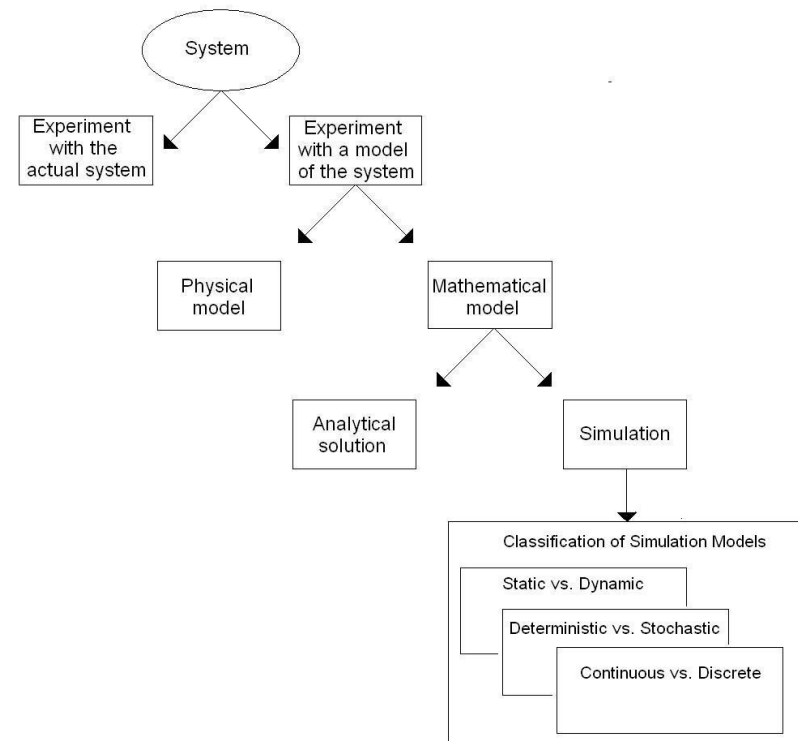
- represents the system as the system evolves

## Deterministic

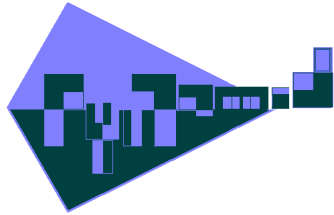
- does not contain probabilistic components

## Continuous

- state variables change continuously with respect to time



**Ways to study a system**  
(modified from Law and Kelton, 2000)



# The Simulation Life cycle

## Conceptual Model

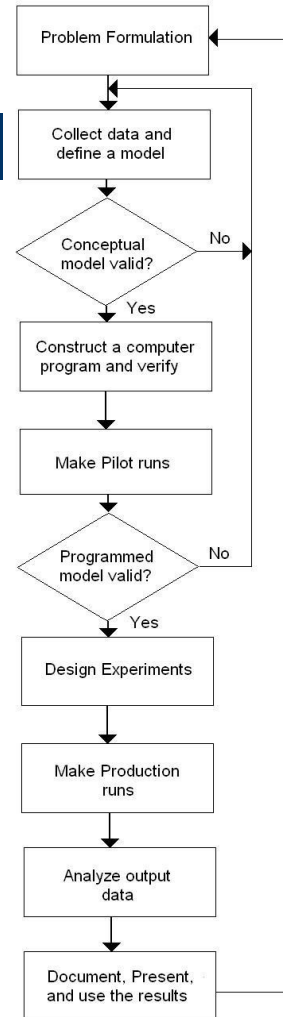
- the mathematical, logical, or verbal representation of the problem
- mimics reality within a limited set of assumptions

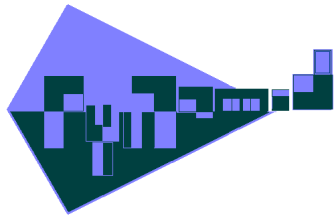
## Verification

- determine whether the model assumptions and mathematical formalisms are correctly translated into the computer program (i.e., debugging)

## Programmed Model

- the conceptual model translated onto a computer





# Validation

## Definition

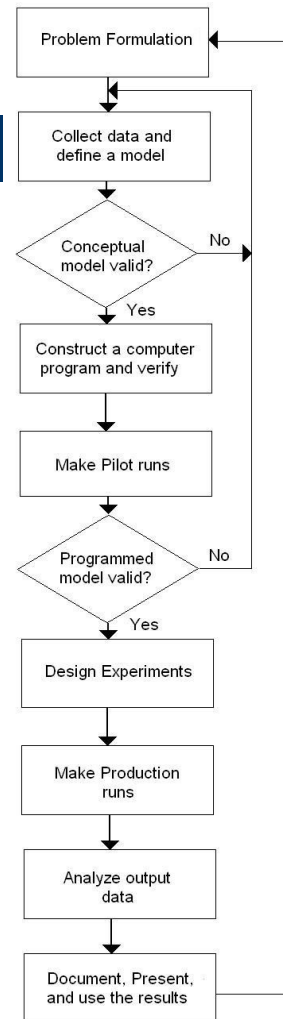
- Determining whether a simulation model is acceptable for its intended use given the specified performance requirements

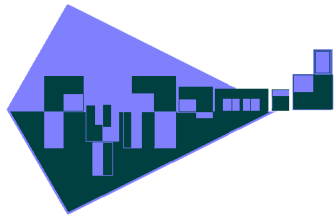
## Without validation

- the utility of any results produced by a simulation model can not be judged

## Validate the conceptual and programmed models

- Not required for development or exploration of the model





# Project Tasks

## Project Tasks

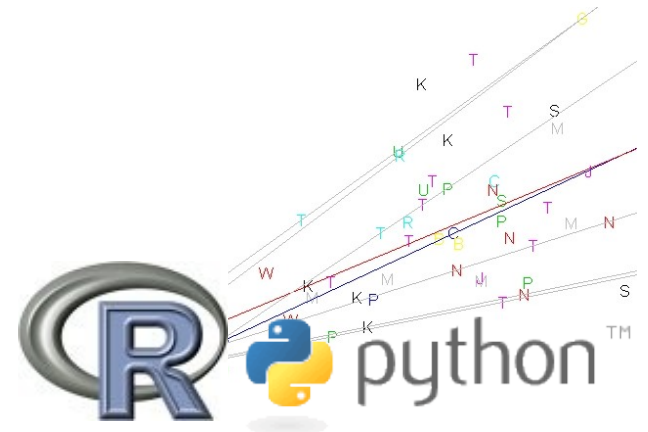
- Review literature on statistical validation
- Develop a tool

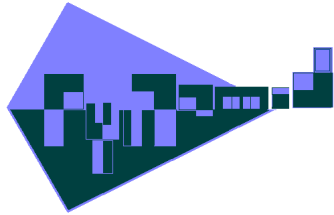
## Skills Acquired

- Programming in Python and R
- Regression Techniques
- Visual and Deviance measure techniques

## Project Deliverables

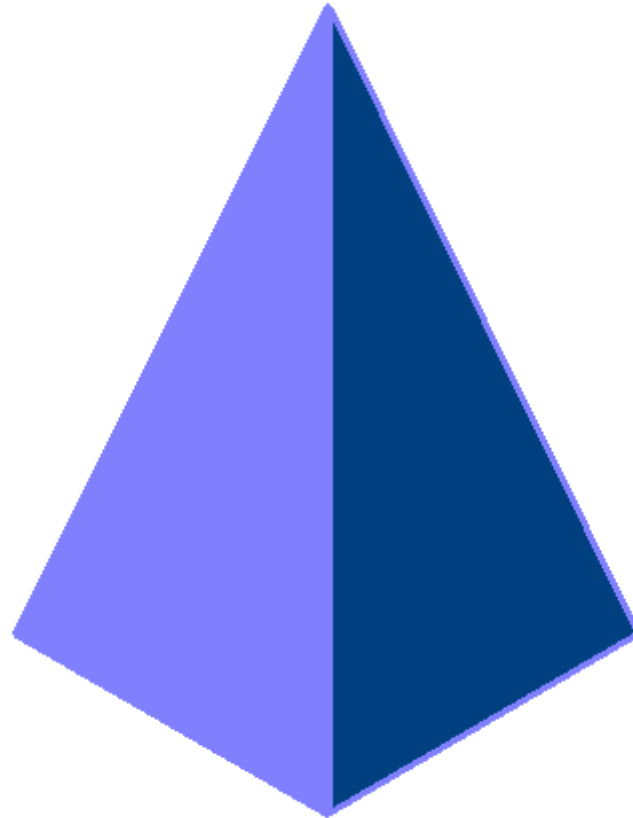
- Written report
- Prototype software

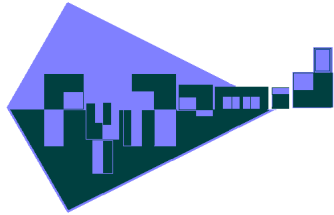




# Literature Review

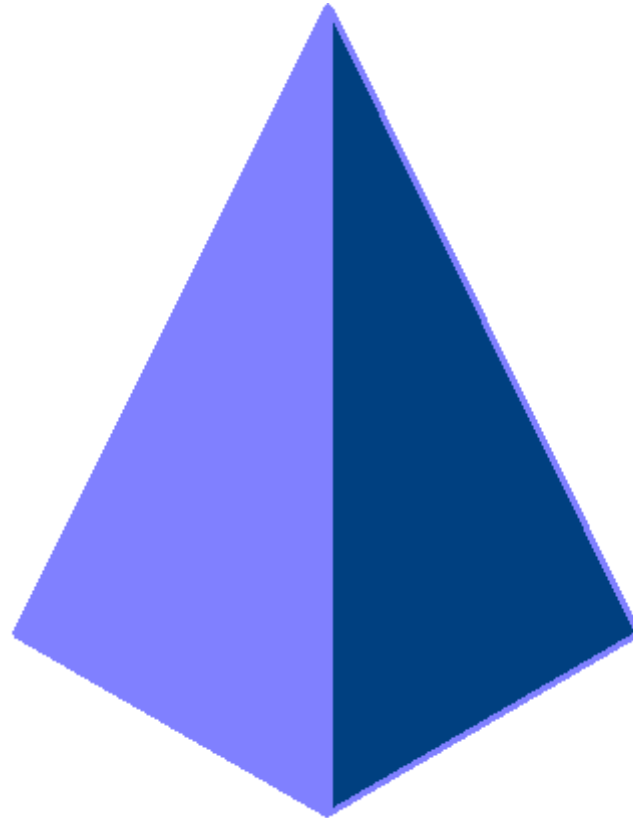
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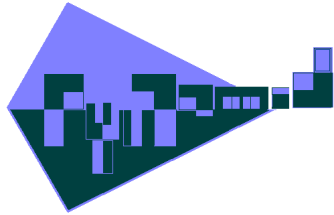




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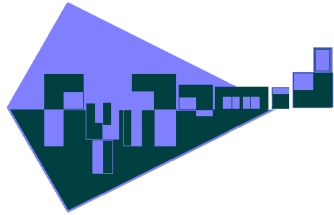
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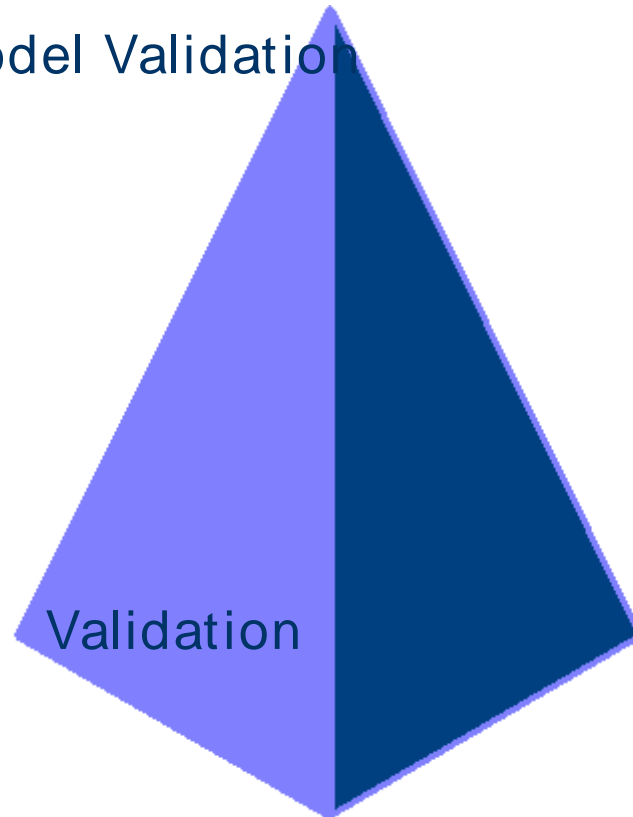
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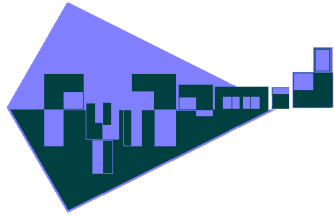
Validation



# Literature Review

Programmed Model Validation

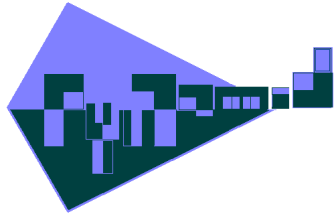




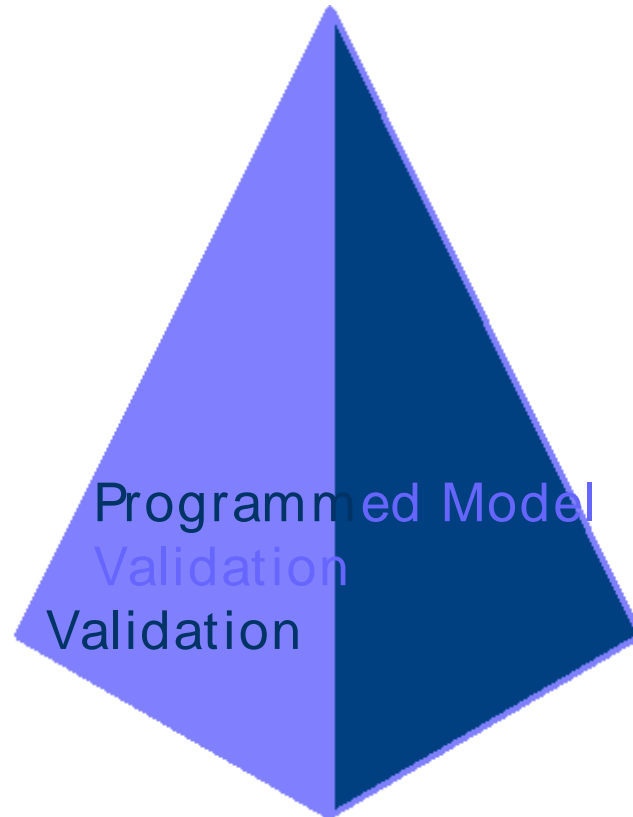
# Literature Review

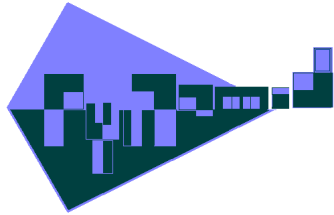
Programmed Model Validation

Validation



# Literature Review

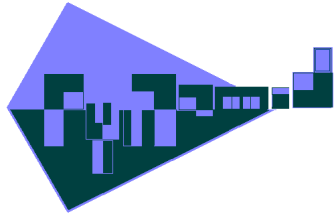




# Literature Review

Statistical Validation

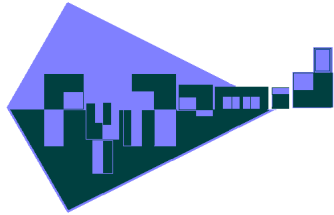
Programmed Model  
Validation  
Validation



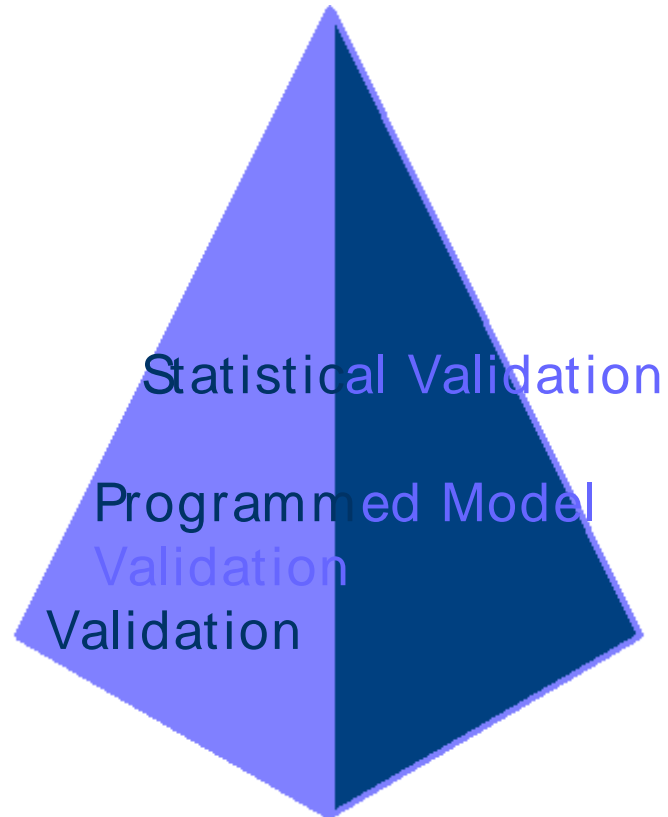
# Literature Review

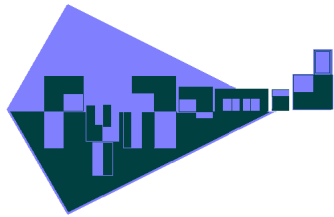
Statistical Validation

Programmed Model  
Validation  
Validation



# Literature Review





# Validation

## Credibility

- degree of belief in the validity of a model

## Calibration

- estimation and adjustment of model parameters

## Qualification

- domain of which the model has been validated

## Accreditation

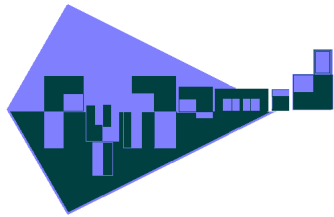
- Department of Defense (DOD) determines that a simulation model is valid

## Output Analysis

- estimate a model's true measures of performance (i.e., simulation run length and warm up time)

$$\begin{aligned} \mu_M &= |\mu_M - \mu_S| \\ \text{Error in } \mu_M &= |\mu_M - \mu_M + \mu_M - \mu_S| \\ &= |\mu_M - \mu_M| + |\mu_M - \mu_S| \end{aligned}$$

(Law and Kelton, 2000)



# Programmed Model Validation

## Statistical Validation

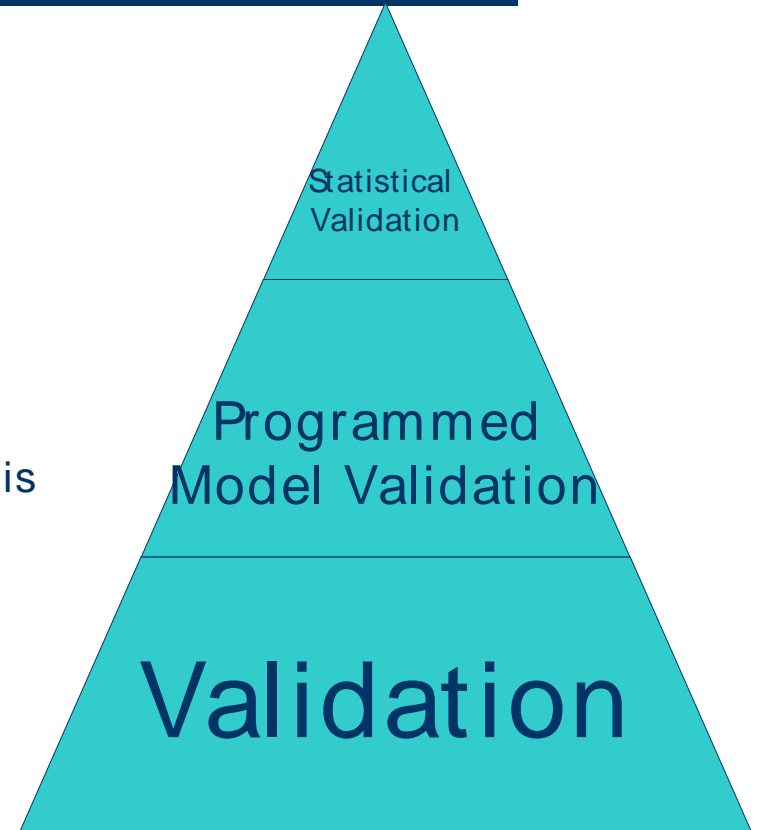
- Validation of a conceptual or programmed model using statistical tests

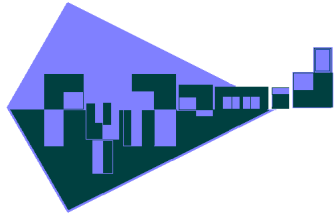
## Conceptual Model Validation

- determining the mathematical logic is reasonable for model assumptions (i.e., independence, normality)

## Programmed Model Validation

- comparing observations and simulated output (i.e., using visual techniques, regression techniques, and deviance measures )





# Statistical Validation

## Visualization Techniques

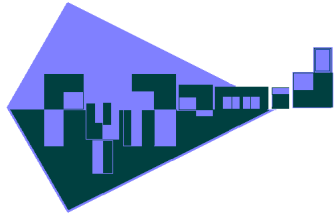
- Plot of observed vs. simulated values

## Regression Techniques

- Linear
- Quadratic
- F- Test

## Deviance Measures

- Modeling Efficiency
- Root Mean Squared Deviation
- Mean Absolute Error



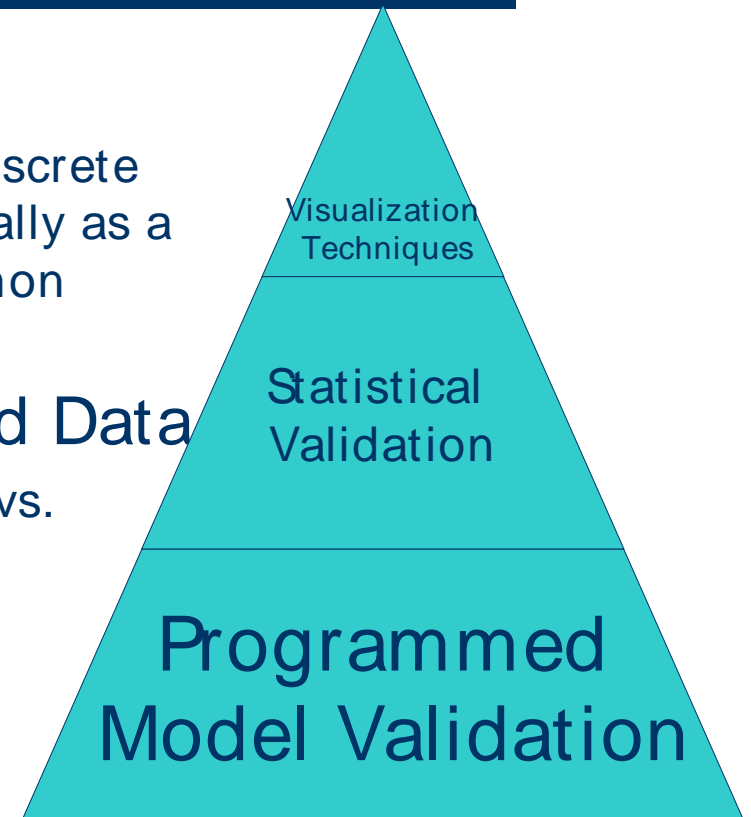
# Visualization Techniques

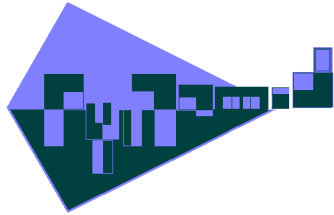
## Time Series Plots:

- Plot observed data (usually as discrete points) and simulated data (usually as a continuous line) against a common independent variable (time)

## Plot Observed vs. Simulated Data

- Plot  $y=x$  (1:1) line for observed vs. simulated data





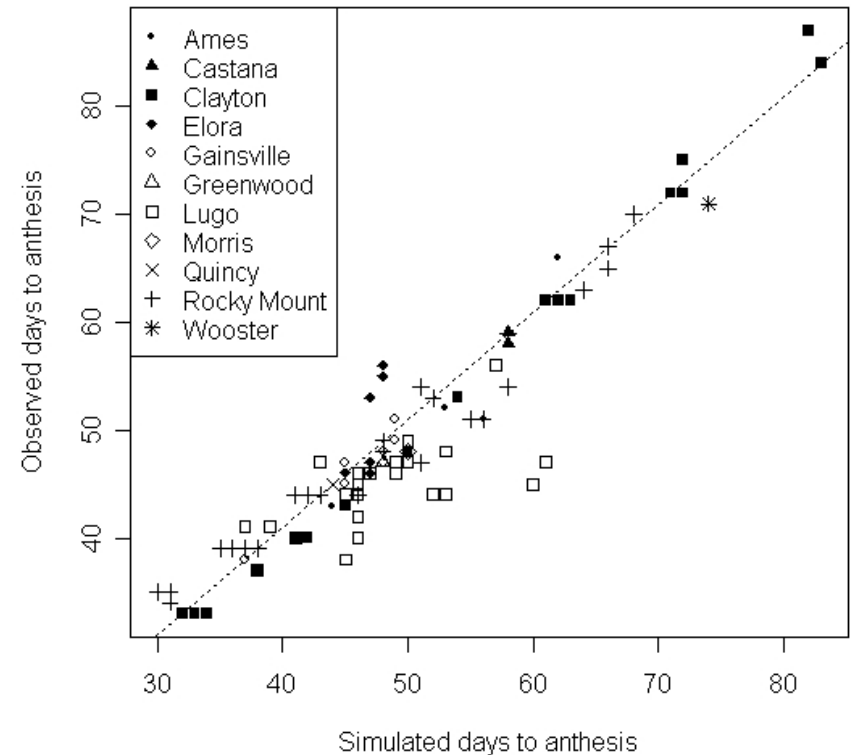
# Visualization Techniques

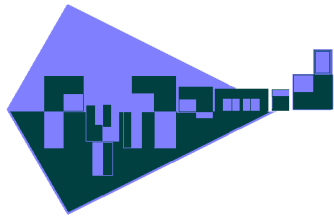
## Observed Vs. Simulated Plot with 1:1 line

- indicate any possible clustering of the data

## Use different characters to symbolize different stratum

- indicate lack of independence





# Regression Techniques

## Linear (Least Squares) Regression

- Plot equation:  $Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$

## Quantile Regression

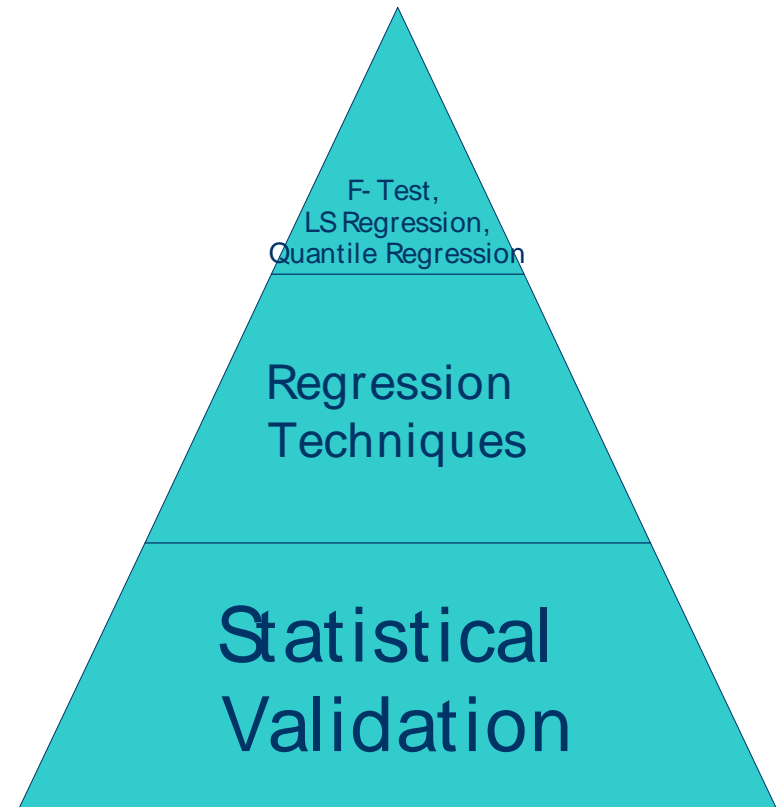
- Plot of  $X_i$  vs.  $F_i$ :  $F_i = i / (n + 1)$

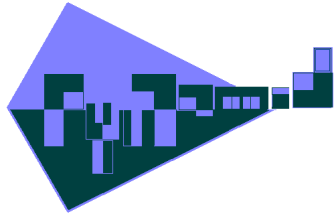
## F- test

- For observed vs. predicted values
- $$F^* = \frac{nb_1^2 + 2 \sum x_i b_1 (b_2 - 1) + \sum x_i^2 (b_2 - 1)^2}{2s^2}$$

$$F^* = \frac{\frac{SSR}{p-1}}{\frac{SSE}{n-p}} = \frac{MSR}{MSE}$$

- For LS regression





# Regression Techniques

F- test for fitted equation of  
observed vs. simulated values

- testing whether observed vs.  
predicted values vary constantly  
over 1:1 line

$$H_0: \beta_1 = 1, H_a: \beta_1 \neq 1$$

- test of zero intercept

$$H_0: \beta_0 = 0, H_a: \beta_0 \neq 0$$

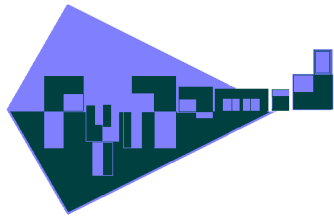
- Low values of  $F^*$  report  $H_0$
- Large Values of  $F^*$  (near 1) report  $H_a$

## Null and Alternative Hypotheses

$$H_0: \beta_1 = 1 \text{ and } \beta_0 = 0$$

$$H_a: \beta_1 \neq 1, \text{ or } \beta_0 \neq 0, \text{ or both}$$

$$F^* = \frac{\text{Test Statistic}}{2s^2} = \frac{nb_1^2 + 2 \sum x_i b_1 (b_2 - 1) + \sum x_i^2 (b_2 - 1)^2}{2s^2}$$



# Regression Techniques

## Least Squares Regression

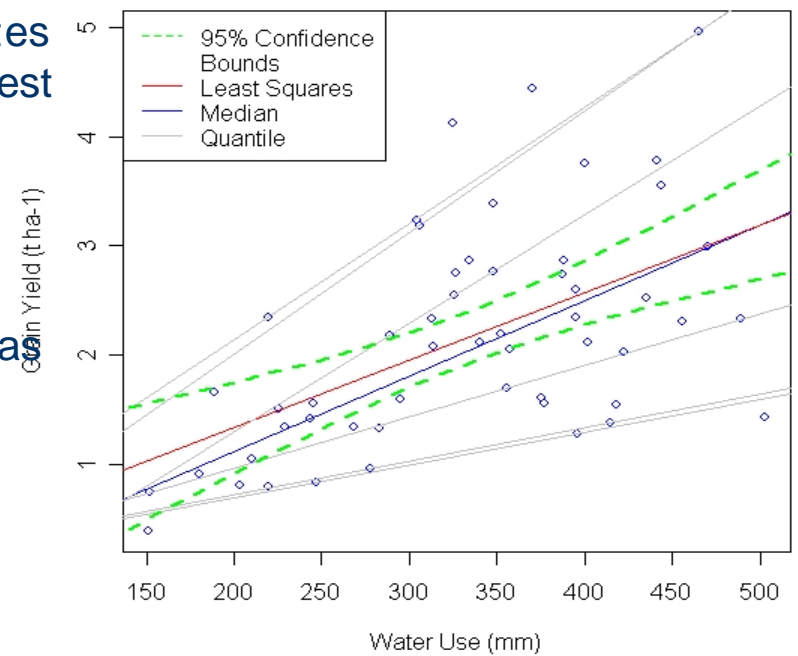
- Plot  $Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$
- F- Test:  $H_0: \beta_1 = 0$  and  $H_a: \beta_1 \neq 0$
- Too critical:

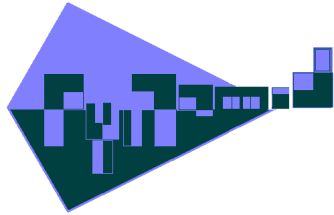
Case close to linear which deviates from the regression line - fails test  
Use confidence intervals  
Use quantile estimates

## Quantile Regression

- Explains variation in a model with bias
- More descriptive than inferential
- combine with other methods for validation

$$F^* = \frac{\frac{\sum (y_i - \hat{y}_i)^2}{p-1}}{\frac{\sum (y_i - \hat{y}_i)^2}{n-p}} = \frac{SSR}{SSE} = \frac{MSR}{MSE}$$





# Deviance Measures

## Modeling Efficiency

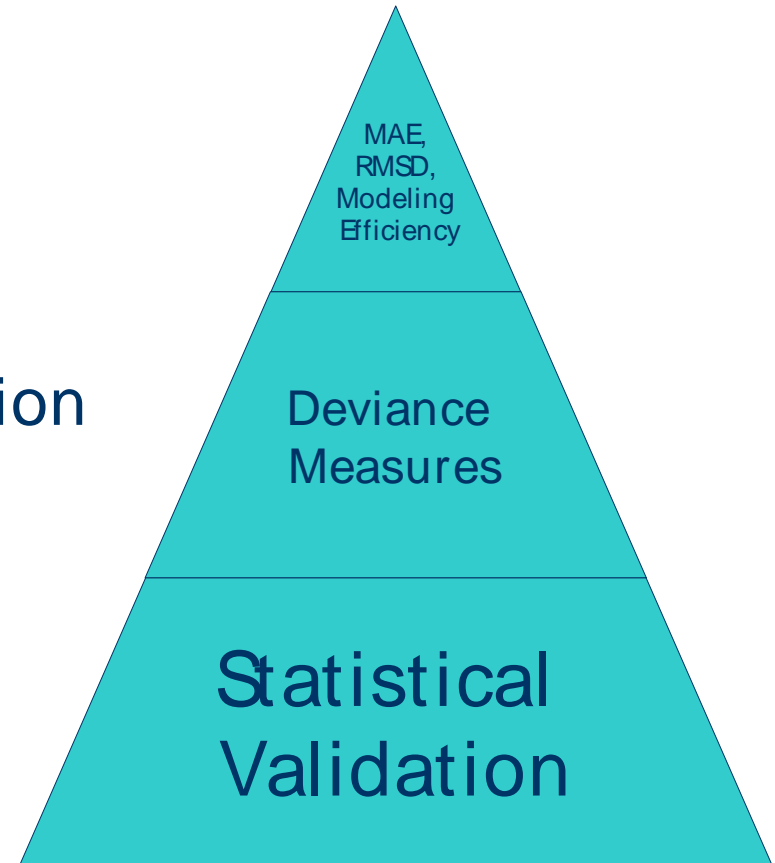
- Equation: 
$$EF = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}$$

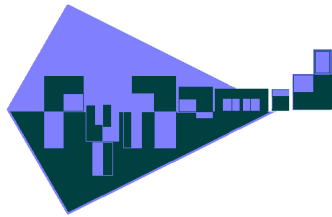
## Root Mean Squared Deviation

- Equation: 
$$RMSD = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_i - y_i)^2}$$

## Mean Absolute Error

- Equation: 
$$MAE = \frac{1}{n} \sum_{i=1}^n |x_i - y_i|$$





# Deviance Measures

## Coefficient of Determination

- the proportion of variation explained by the fitted line
- linear relationship between simulated and mean of observed value assumed

$$r^2 = \frac{SSR}{SSTO} = 1 - \frac{SSE}{SSTO} = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}$$

$$0 \leq r^2 \leq 1$$

$$EF = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}$$

## Modeling Efficiency

- 1 perfect fit
- EF= 0 simple average
- EF< 0 poor model
- $-1 \leq EF \leq 1$

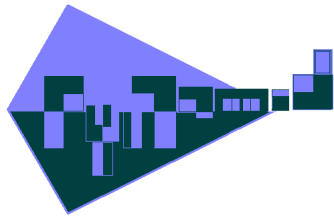
$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_i - y_i)^2}$$

## Root Mean Squared Deviation & Mean Absolute Error

$$MAE = \frac{1}{n} \sum_{i=1}^n |x_i - y_i|$$

- lower the value, closer the simulation is to it's measurement

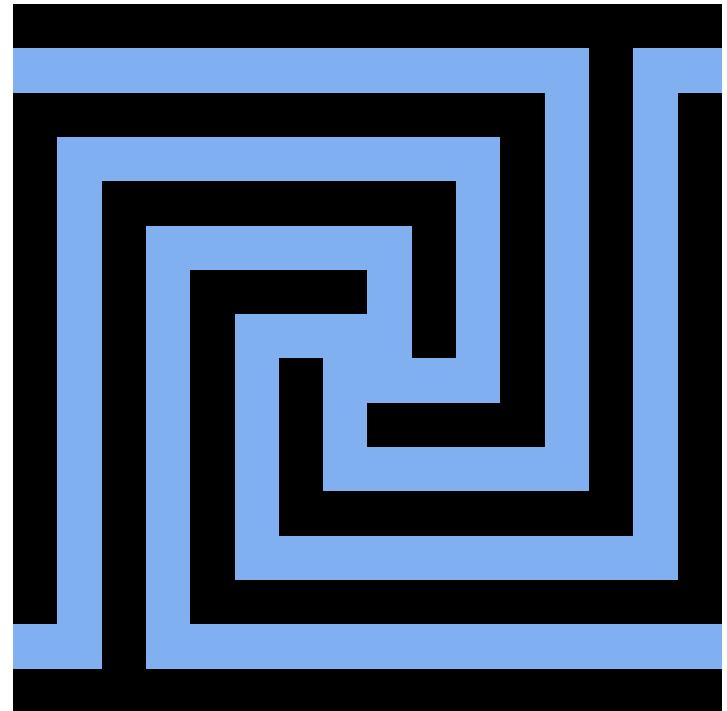
- Similar to RMSE. less sensitive to extreme values

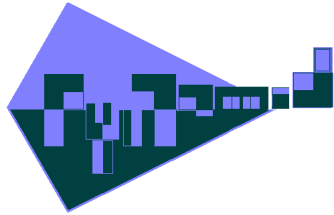


# Project Implementation

What exactly did I do?

- Phase I: The learning Phase
  - Review of the literature
  - Learning the R and Python Programming Languages
- Phase II: Tool Development
  - Creation of scripts
  - Combining scripts together
  - PyRamid Demo





## Phase I: The Learning Phase

### Review of the literature

- Validation

  - What validation is

  - What a simulation is

  - How to validate a simulation

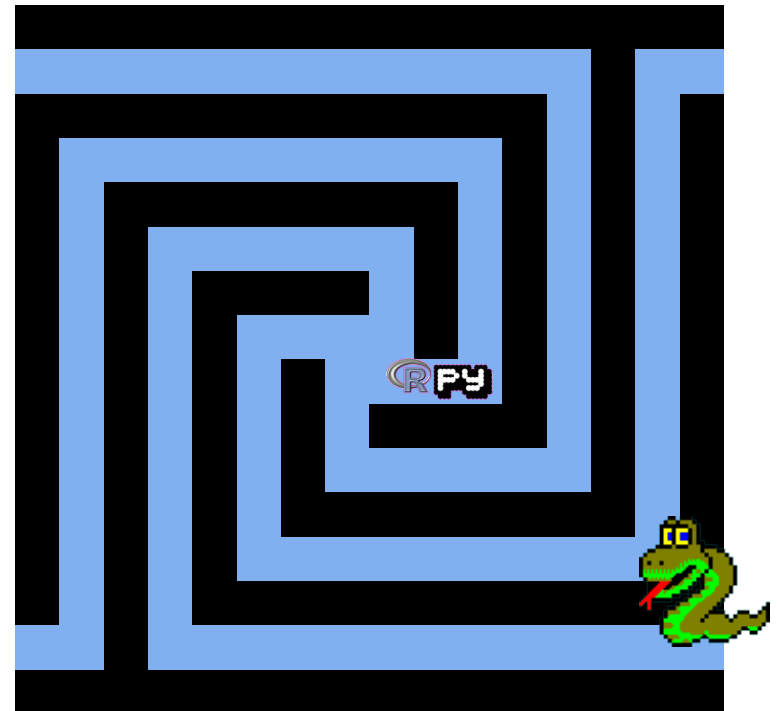
- Statistical Validation

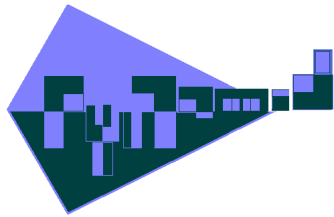
  - Visual Techniques

  - Regression Techniques  
(i.e., F-test)

  - Deviance Measures

Learning the R and Python  
Programming Languages





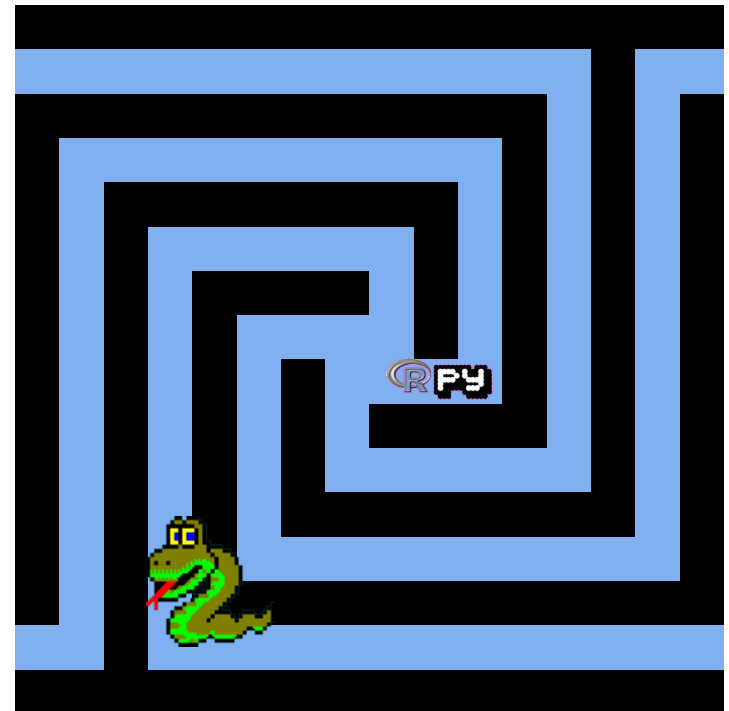
# Learning R and Python

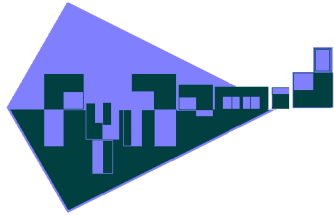
## Learning R Programming Language

- How to perform Visualization Techniques, Regression Techniques, and deviance measures in R

## Learning Python Programming Language

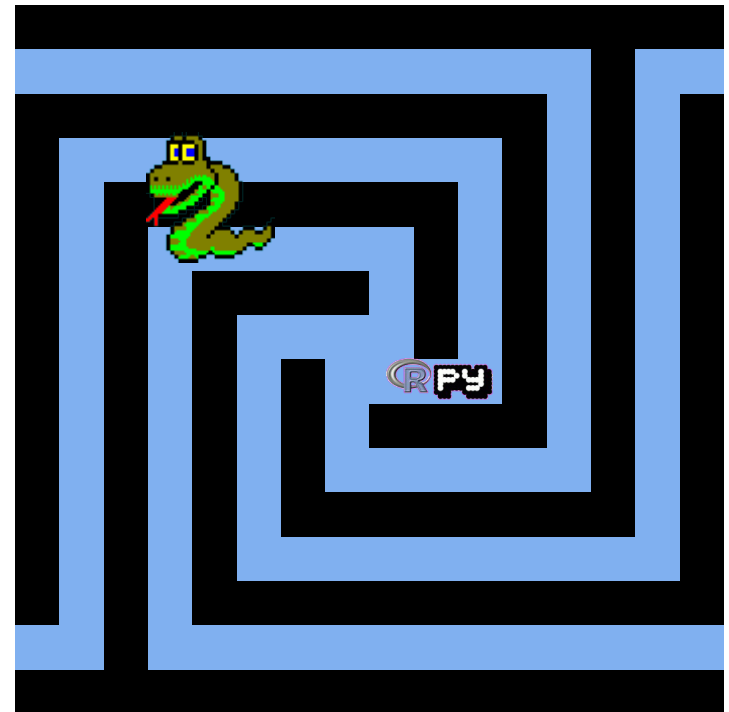
- How to create a GUI Interface
  - Tkinter, PMW extension toolkit
- How to use RPy to retrieve R objects and execute R commands

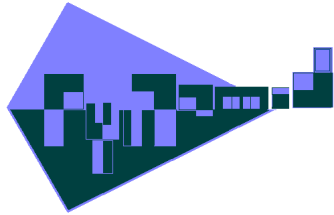




## Phase II: Tool Development

Creation of scripts  
Combining scripts  
together into one  
program  
PyRamid Demo



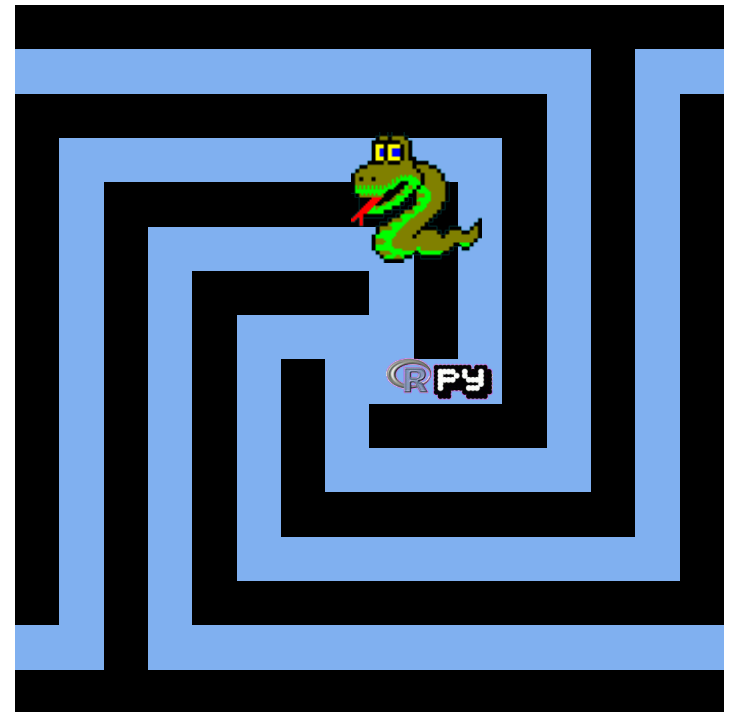


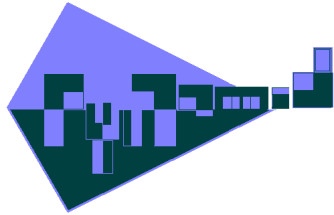
# The Creation of Scripts

## Creation window gadgets

- Message and entry
- Checkbuttons and Radiobuttons
- Building Frames and Popup Windows
- Menu options
- Dialogs
- Grids and packing

Creation of modified R scripts that use RPy to perform statistical techniques

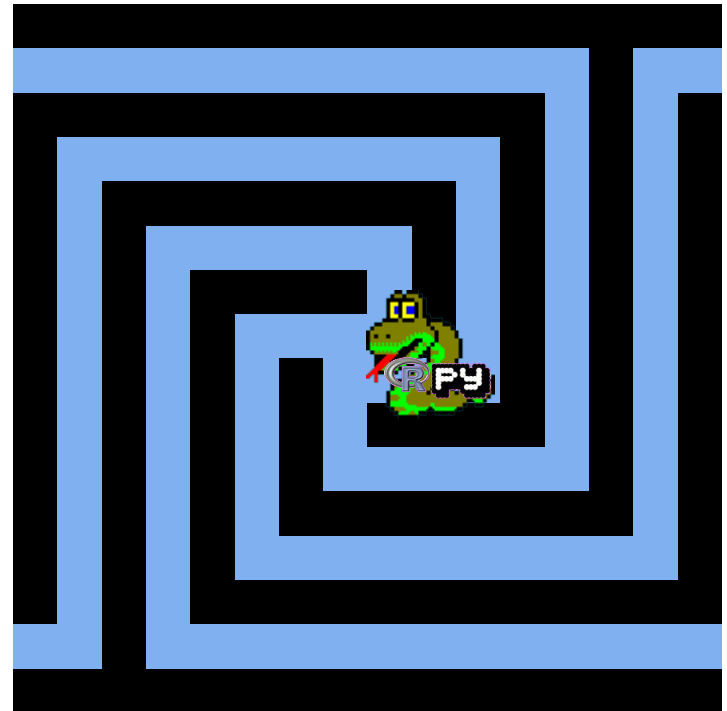


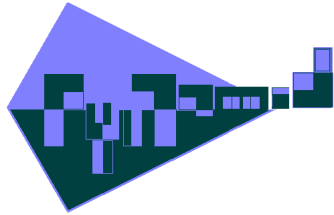


# Combining Scripts

Combine scripts into one program that can:

- Create data plots and diagnostic Plots
- Create ANOVA Tables and Statistics Tables
- Perform Least Squares, Quantile, and Multiple Regressions





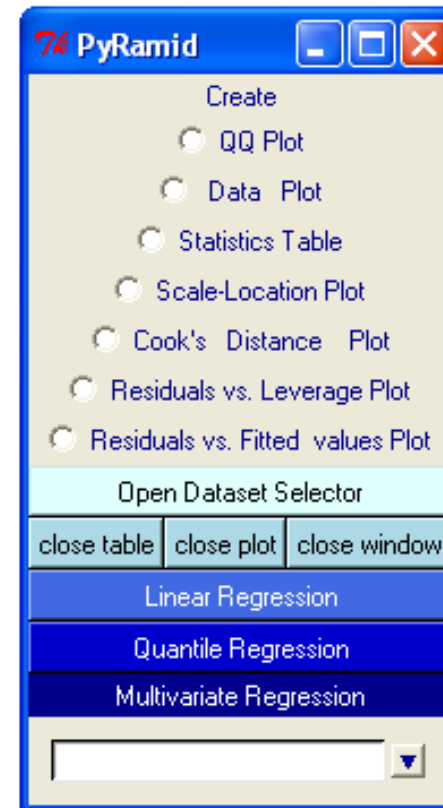
# The PyRamid Demo

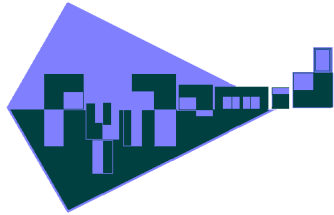
Main Window

Dataset Selector

Creating Data  
Plots

Creating  
Diagnostic Plots  
Statistics Tables





# The PyRamid Demo

Main Window

**Dataset  
Selector**

Creating Data  
Plots

Creating  
Diagnostic  
Plots

Statistics  
Tables

run	x2	y	x1	x3
94	NCRM8701	35	30	RANSOM
86	NCRM8701	35	31	CENTENN
102	NCRM8701	34	31	FORREST
78	NCCL8801	33	32	FORREST
72	NCCL8801	33	33	RANSOM
66	NCCL8801	33	34	CENTENN
101	NCRM8701	39	35	FORREST
93	NCRM8701	39	36	RANSOM
42	LUGD9501	41	37	LABR.
46	LUGD9501	41	37	MAJ.
85	NCRM8701	39	37	CENTENN
130	UFGA7902	38	37	WILLIAM
131	UFGA7902	38	37	WILLIAM
132	UFGA7902	38	37	WILLIAM
133	UFGA7902	38	37	WILLIAM

PyRamid software interface showing regression options and equations.

Create

- QQ Plot
- Data Plot
- Statistics Table
- Scale-Location Plot
- Cook's Distance Plot
- Residuals vs. Leverage Plot
- Residuals vs. Fitted values Plot

Open Dataset Selector

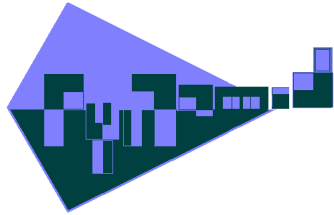
close table | close plot | close window

Linear Regression

Quantile Regression

Multivariate Regression

$y = b_0 + b_1x_1 + b_2x_2$   
 $y = b_0 + b_1x_1 + b_2x_2 + b_3x_1x_2$   
 $y = b_0 + b_1x_1 + b_2x_2 + b_3x_3$   
 $y = b_0 + b_1x_1 + b_2x_2 + b_3x_3/x_2$



# The PyRamid Demo

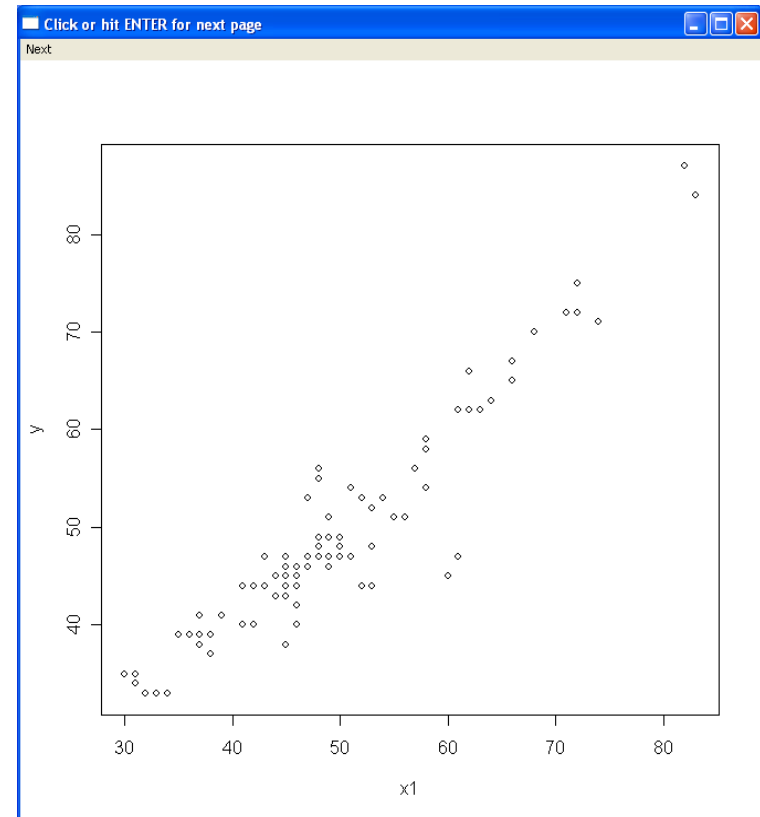
Main Window

Dataset Selector

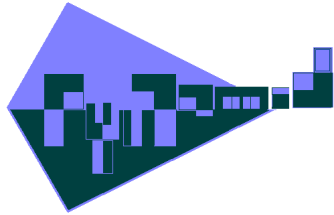
**Creating Data  
Plots**

Creating  
Diagnostic Plots

Statistics Tables



Plot appears in an R Graphics Window



# The PyRamid Demo

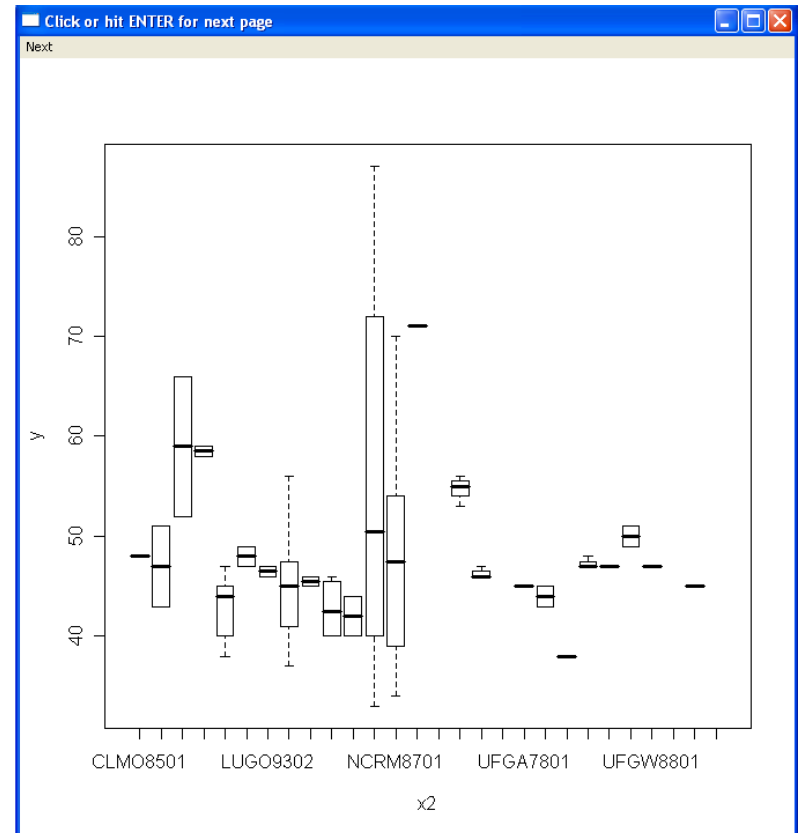
Main Window

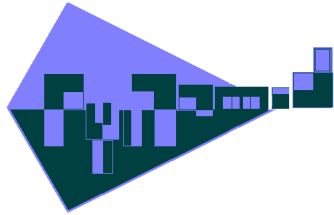
Dataset  
Selector

**Creating Data  
Plots**

Creating  
Diagnostic  
Plots

Statistics  
Tables





# The PyRamid Demo

Main Window

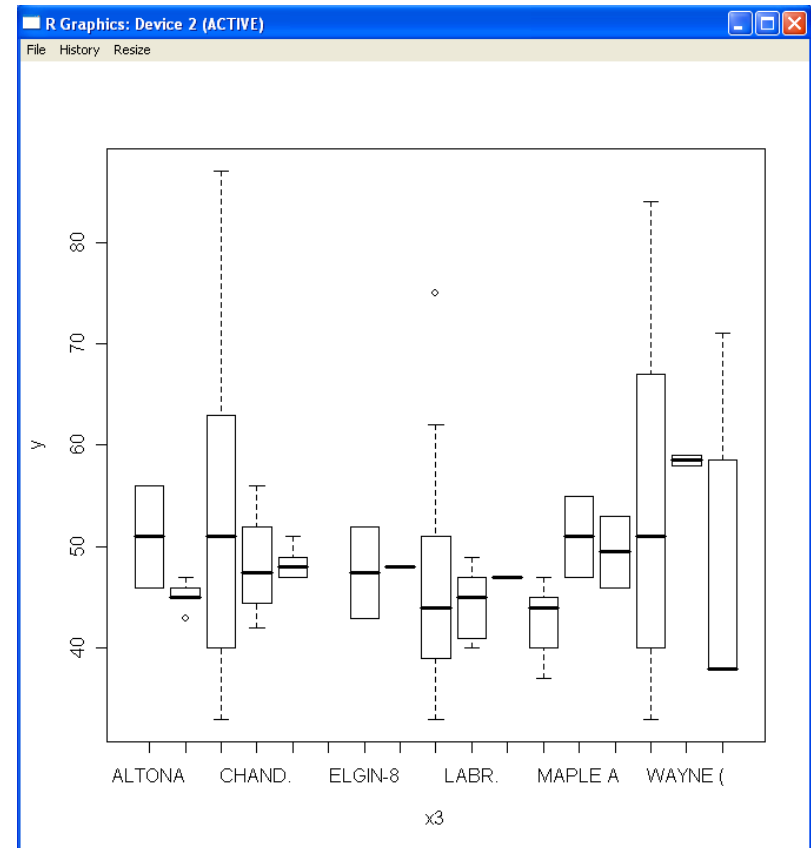
Dataset

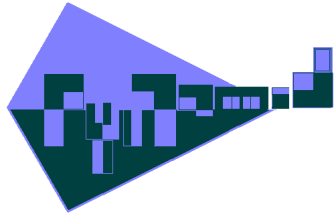
Selector

**Creating Data  
Plots**

Creating  
Diagnostic  
Plots

Statistics  
Tables

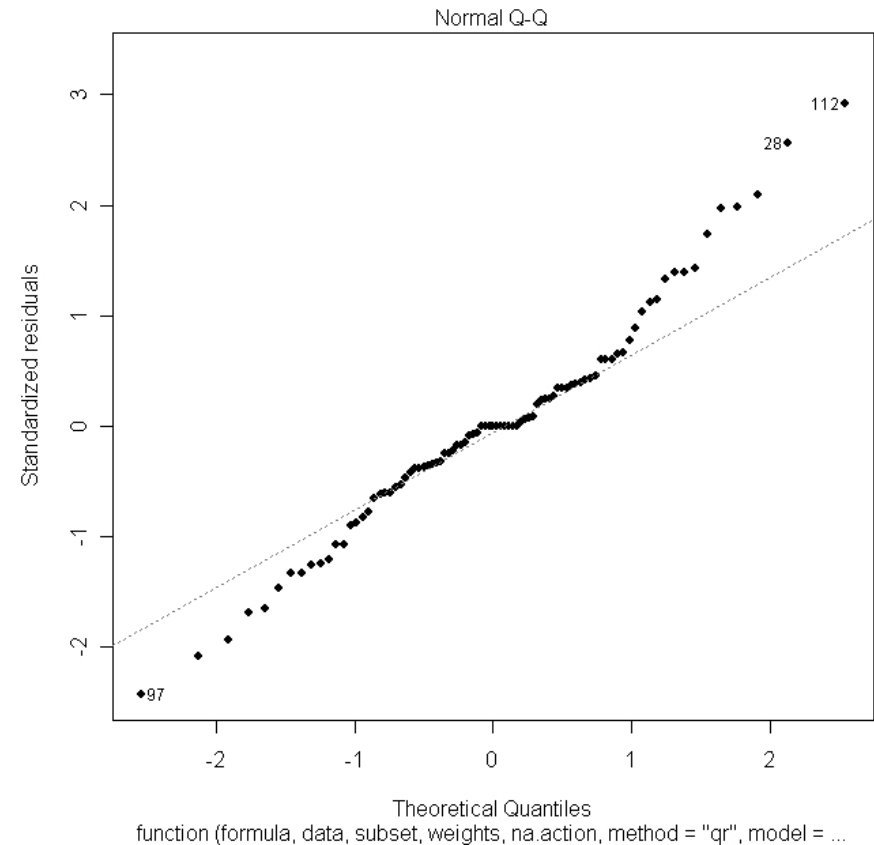


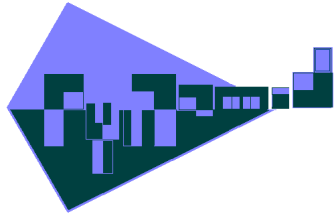


# The PyRamid Demo

Main Window  
Dataset Selector  
Creating Data Plots  
**Creating Diagnostic Plots**  
Statistics Tables

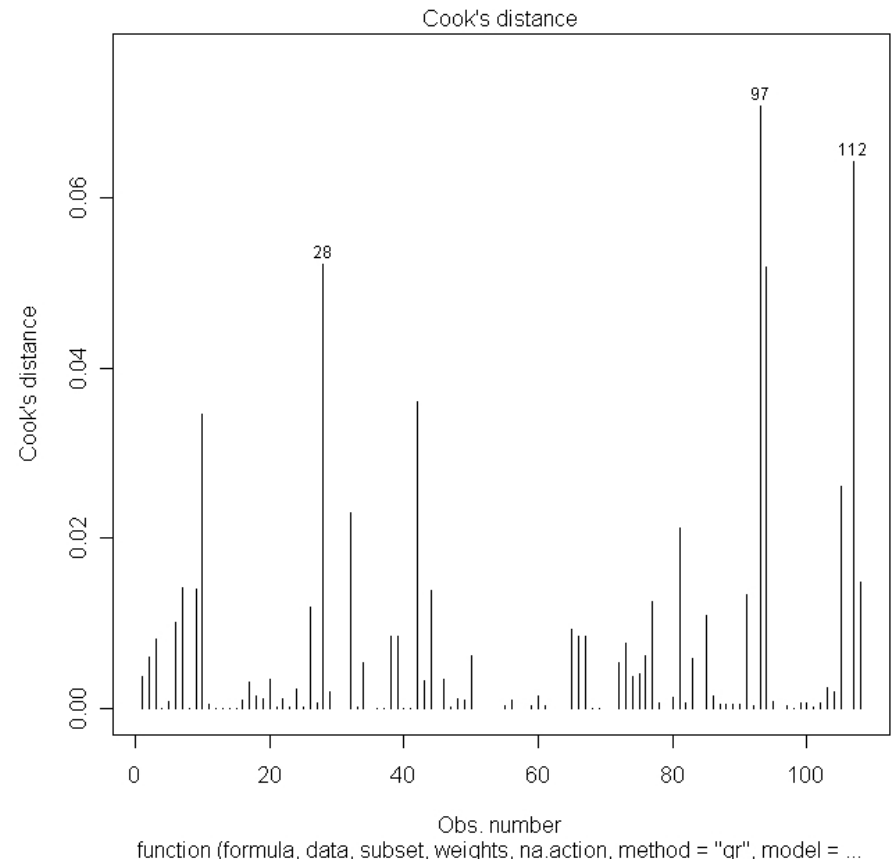
Plots can be saved in a variety of formats including metafile, postscript, PDF, PMG, BMP, and JPG

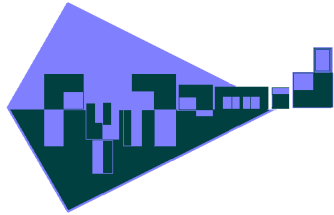




# The PyRamid Demo

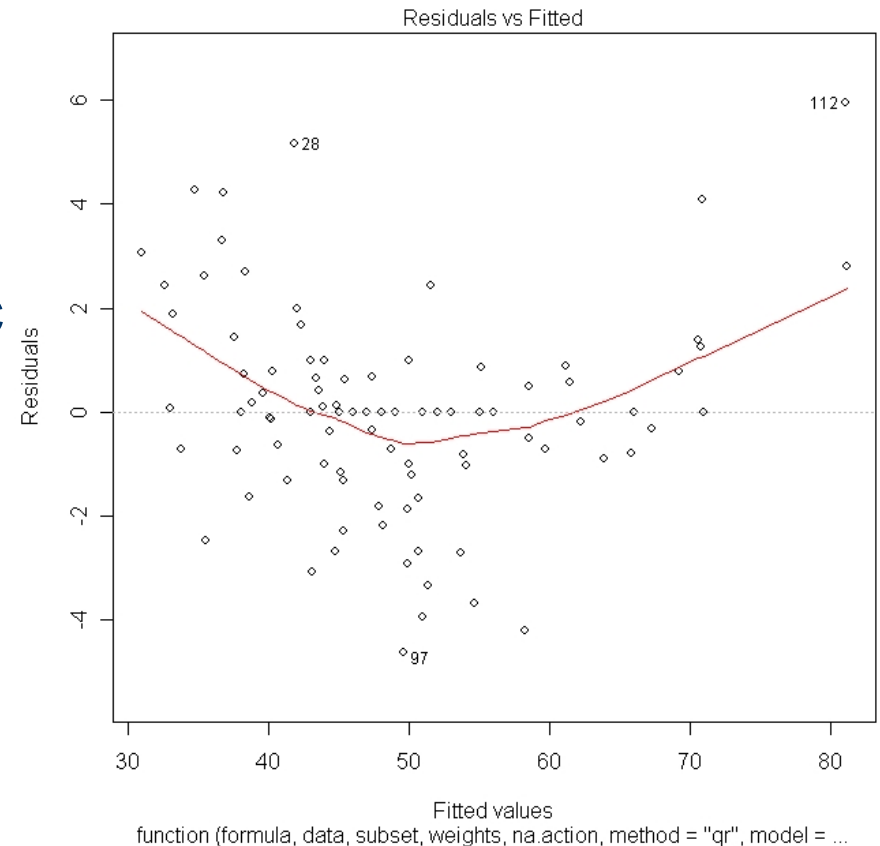
- Main Window
- Dataset Selector
- Creating Data Plots
- Creating Diagnostic Plots**
- Statistics Tables

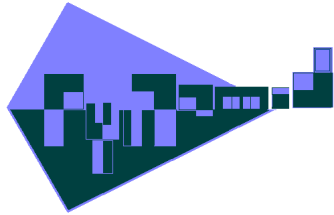




# The PyRamid Demo

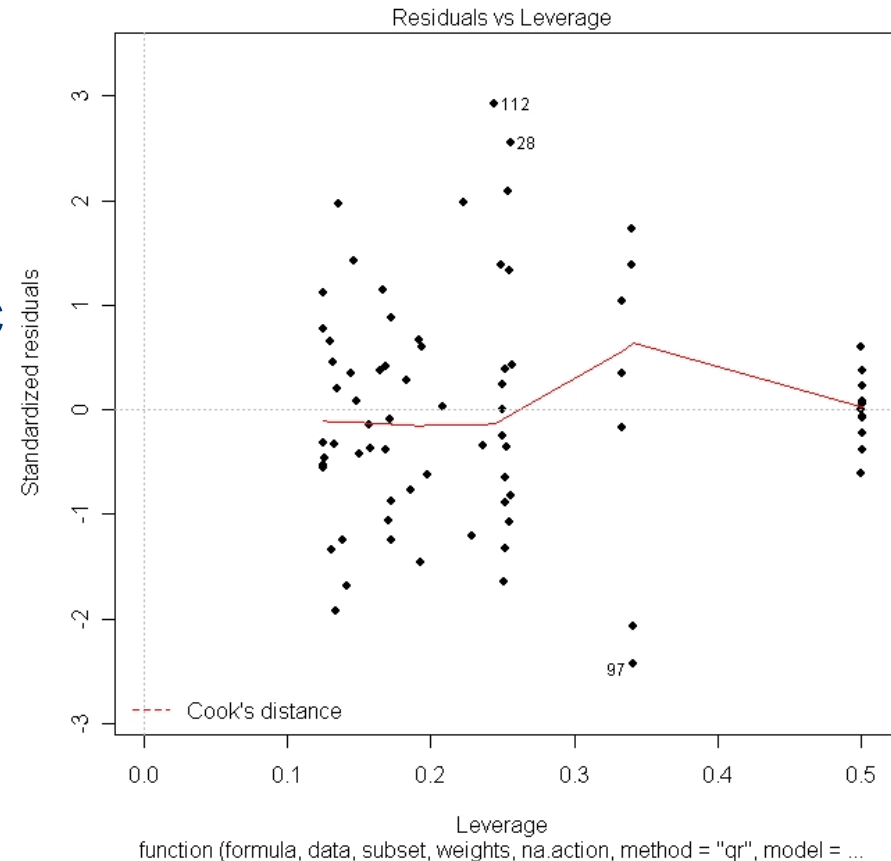
Main Window  
Dataset Selector  
Creating Data Plots  
**Creating Diagnostic  
Plots**  
Statistics Tables

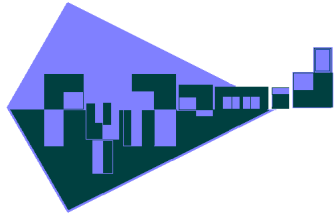




# The PyRamid Demo

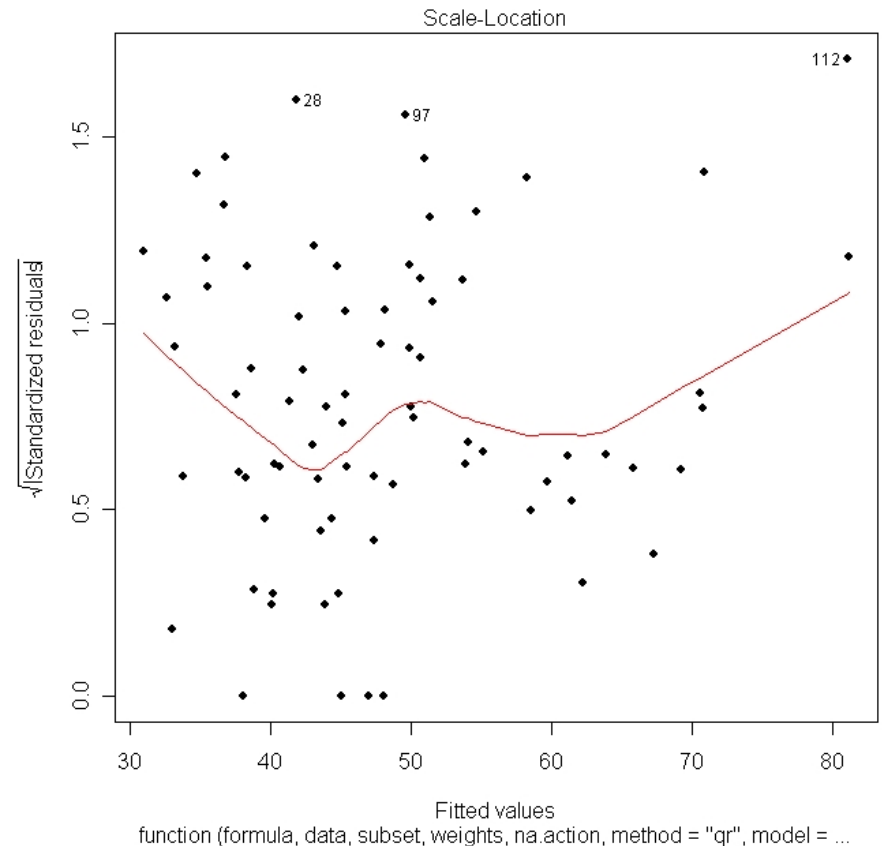
Main Window  
Dataset Selector  
Creating Data Plots  
**Creating Diagnostic  
Plots**  
Statistics Tables

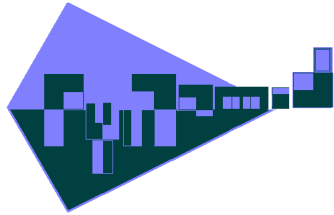




# The PyRamid Demo

Main Window  
Dataset Selector  
Creating Data Plots  
**Creating Diagnostic Plots**  
Statistics Tables



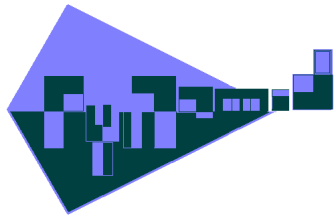


# The PyRamid Demo

Main Window Dataset  
Selector  
Creating Data Plots  
Creating Diagnostic Plots  
**Statistics Tables**

The screenshot shows a window titled "PyRamid Statistics Table" with a menu bar containing "File" and "Edit". The window displays an ANOVA table with the following data:

Anova.Table	Df	Sum.Sq	Mean.Sq	F.Value	Pr(>F)
-	1	10420	10420.433890	1905.493618	0.000000
X1	23	785.663002	34.159261	6.246405	0.000000
X2	18	77.405314	4.300295	0.786357	0.708004
X3\X2	65	355.460756	5.468627	-	-
Residuals					



# Summary

Determined the most appropriate statistical techniques to use for validating continuous, dynamic, and deterministic simulations

visual techniques

- Plot observed vs. simulated data

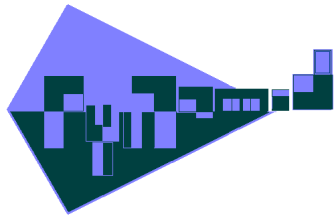
Regression techniques

- LS regression, quantile regression, and F-test

deviance measures

- EF, RMSD, MAE

Developed a tool that can be used to perform these techniques



# Acknowledgments

Thank you

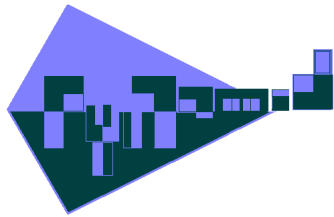
Dr. Gerrit Hoogenboom

Dr. Jeffery White

Dr. Rosemary Renaut

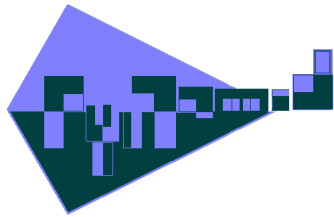
Dr. Zoé Lacroix

US Arid Land Agricultural Research Service



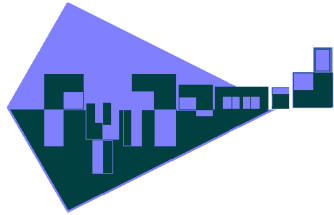
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# Questions?

