Nonlinear Regression Programs

Interpretation of Program Output

Objectives

- To understand the output received from Nonlinear Regression Programs
  - Final Parameter Values
  - Data Values
  - Statistical Results
  - Plot Output

Final Parameter Values

- Final Values
- Standard Deviation / Coefficient of Variation
- Limits
- Correlation Matrix

Final Parameter Values

- Parameter Values
  - Value at each Iteration (Boomer/Damping Gauss-Newton)

```
Loop =     1
Damp =     1
P ( 1) =       .1130
P ( 2) =       22.80
WSS =       0.353223E-03

Loop =     2
Damp =     1
P ( 1) =       .1130
P ( 2) =       22.85
WSS =       0.333127E-03
```

Final Parameter Values

- Parameter Values
  Values (WSS) at each Iteration (Boomer/Simplex)

```
Loop   1 -
1>  0.4683E-02  2>  0.4503E-01  3>   .1010
Loop   2 -
1>  0.4683E-02  2>  0.4503E-01  3>  0.4543E-01
Loop   3 -
1>  0.4683E-02  2>  0.4503E-01  3>  0.3073E-01
Loop   4 -
1>  0.4683E-02  2>  0.1641E-01  3>  0.3073E-01
```

Final Parameter Values

- Final Values

```
# Name  Value       S.D.       C.V. %

1) kel  .11298      0.141E-02   1.2
2) V    22.854       .228       1.0
```

Final Parameter Values

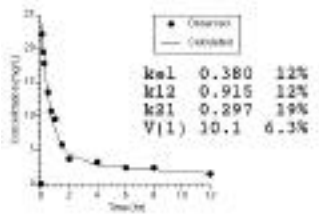
- Standard Deviation / Coefficient of Variation

#	Name	Value	S.D.	C.V. %
1)	kel	.11298	0.141E-02	1.2
2)	V	22.854	.228	1.0

- Used for Goodness of Fit and Model Identification
- Confidence Interval

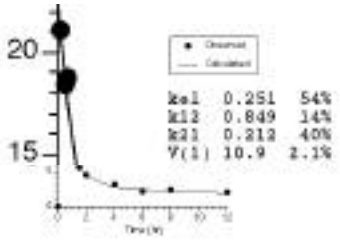
Final Parameter Values

- Coefficient of Variation



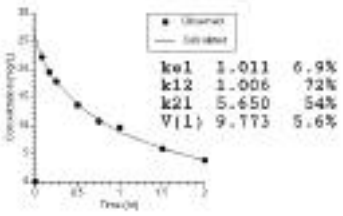
Final Parameter Values

- Coefficient of Variation



Final Parameter Values

- Coefficient of Variation



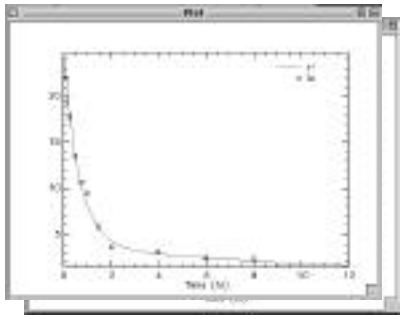
Final Parameter Values

- Limits to Parameter Values
  - Hit Limits - Distort Analysis
  - Refit with Wider Limits
  - Re-evaluate Fit

Final Parameter Values

- Limits to Parameter Values
  - SAAM II example

Final Parameter Values



Final Parameter Values

- Correlation Matrix
  - example from SAAM II

	V1	k(0,2)	k(1,2)	k(2,1)
V1	1.00000	-0.21503	-0.28737	-0.77344
k(0,2)	-0.21503	1.00000	0.85238	0.47760
k(1,2)	-0.28737	0.85238	1.00000	0.71964
k(2,1)	-0.77344	0.47760	0.71964	1.00000

  - High Correlation between Parameters
  - Too many Parameters?

Data Output

- Observed versus Calculated
- Residual
- Weight
- Weighted Residual

Data Output

- Observed versus Calculated

Time	Calculated	Observed
.0000	24.7939	.000000
.8300E-01	22.2898	22.0200
.1670	20.0542	19.4100
.2500	16.1854	17.7300
.5000	13.5866	13.5200
.7500	10.3380	10.6900
1.000	8.15879	9.52000
1.500	5.57542	5.79000
2.000	4.20505	3.64000
4.000	2.88426	3.15000
6.000	2.45898	2.42000
8.000	2.11862	2.33000
12.00	1.56835	1.49000

Data Output

– Weight Values

Observed	(Weight)
.000000	.000000
22.0200	.454133E-01
19.4100	.515198E-01
17.7300	.564016E-01
13.5200	.739645E-01
10.6900	.935454E-01
9.52000	.105042
5.79000	.172712
3.64000	.274725
3.15000	.317460
2.42000	.413223
2.33000	.429185
1.49000	.671141

Very High Weights with Very Low Values

Data Output

- Weighted Residuals

Observed	(Weight)	Weighted residual
.000000	.000000	.000000
22.0200	.454133E-01	-.122504E-01
19.4100	.515198E-01	-.331695E-01
17.7300	.564016E-01	-.211779E-01
13.5200	.739645E-01	.976105E-03
10.6900	.935454E-01	.328271E-01
9.52000	.105042	.143829
5.79000	.172712	.370599E-01
3.64000	.274725	-.182707
3.15000	.317460	.827731E-01
2.42000	.413223	-.128018E-01
2.33000	.429185	.340643E-01
1.49000	.671141	-.525910E-01

Random + and - Values

Similar Numbers

Statistical Output

- WSS
- R^2
- Correlation Coefficient
- AIC

Statistical Output

- Weighted Sum of Squares (WSS)

$$\sum_{i=1}^{i=n} \left(Y_{observed,i} - Y_{calculated,i}\right)^2 \cdot W_i$$

- Minimum Value with Same Weight Scheme
- Compare Different Models
- Compare Different Data Sets

Statistical Output

- R^2
  - Coefficient of Determination
- Correlation Coefficient

- Best fit Approaches Value of 1.00
- Indicates Goodness of Fit

Statistical Output

- AIC
  - Akaike's Information Criterion

    AIC = N • ln (WSS) + 2 • M

    N = number of data points
    M = number of parameters (adjustable)
  - Initially Used for Unweighted Comparison between Models
  - Used to Help Select the 'Correct' Model

Plot Output

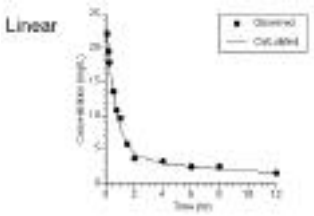
- Calculated and Observed versus Time
- Calculated versus Observed
- Weighted Residual versus Time
- Weighted Residual versus Calculated

Plot Output

- Calculated and Observed versus Time
  - Visual Inspection of Data
    (Maybe first time data is plotted)
  - Look for Systemic Deviations

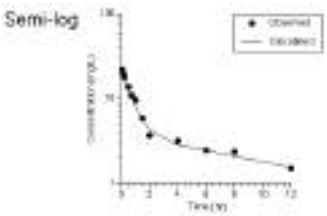
Plot Output

- Calculated and Observed versus Time
  - Two compartment Model - Wt(2)



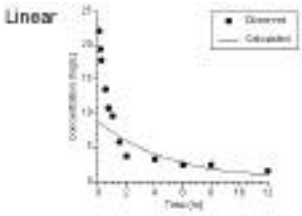
Plot Output

- Calculated and Observed versus Time
  - Two compartment Model - Wt(2)



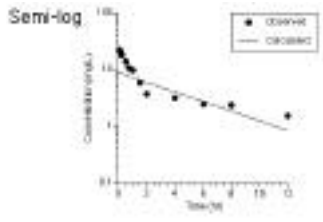
Plot Output

- Calculated and Observed versus Time
  - One compartment Model - Wt(2)



Plot Output

- Calculated and Observed versus Time
  - One compartment Model - Wt(2)

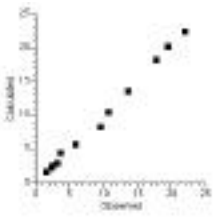


Plot Output

- Calculated versus Observed
  - Visual Inspection of Fit
  - Look for Systemic Deviations

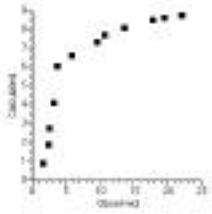
Plot Output

- Calculated versus Observed
  - Two Compartment Model - Wt(2)



Plot Output

- Calculated versus Observed
  - One Compartment Model - Wt(2)

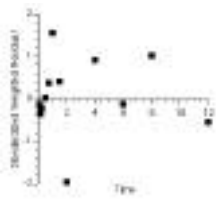


Plot Output

- Weighted Residual versus Time
  - Should Appear Random
  - Look for Patterns
  - Observe Outliers

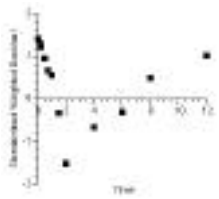
Plot Output

- Weighted Residual versus Time
  - Two compartment Model - Wt(2)



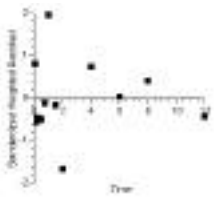
Plot Output

- Weighted Residual versus Time
  - One compartment Model - Wt(2)



Plot Output

- Weighted Residual versus Time
  - Two compartment Model - Wt(0)

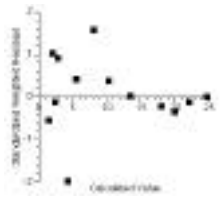


Plot Output

- Weighted Residual versus Calculated
  - Should Appear Random
  - Look for Patterns
  - Observe Outliers

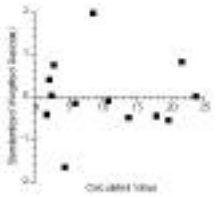
Plot Output

- Weighted Residual versus Calculated Value
  - Two compartment Model - Wt(2)



Plot Output

- Weighted Residual versus Calculated Value
  - Two compartment Model - Wt(0)



Plot Output

- Weighted Residual versus Calculated Value
  - One compartment Model - Wt(2)