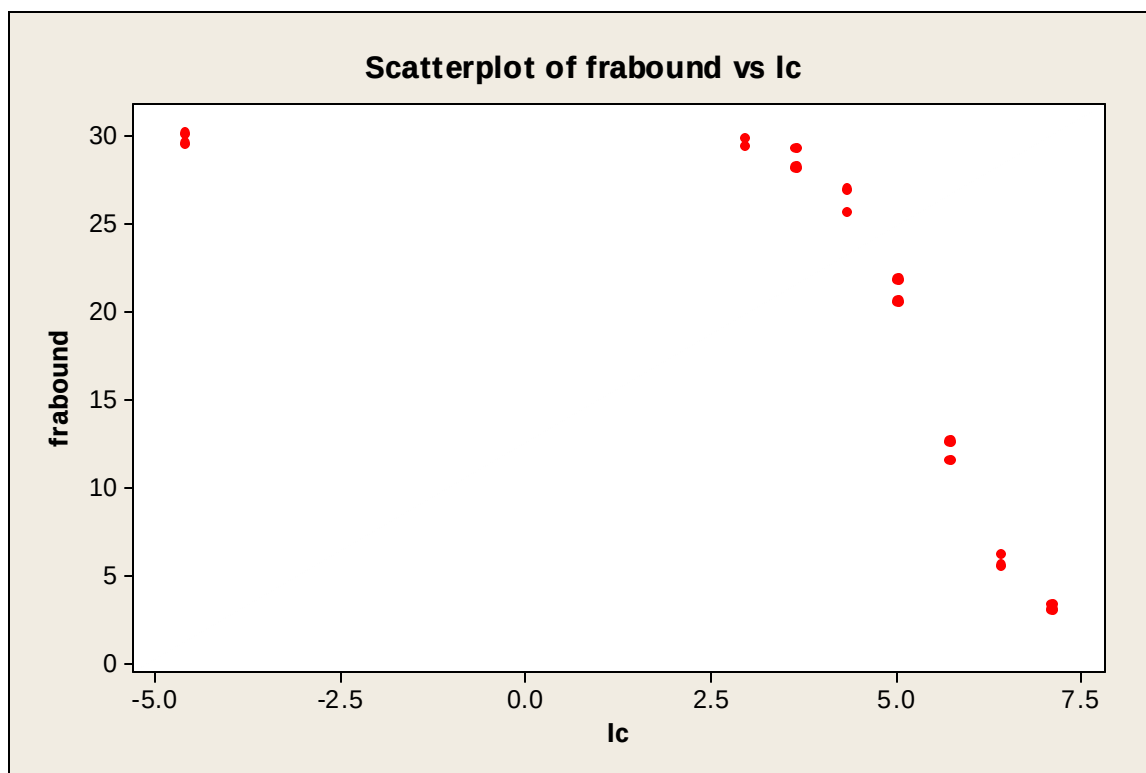




conc	frabound	lc
0.0	30.16	-4.60517
0.0	29.58	-4.60517
19.4	29.87	2.96579
19.4	29.43	2.96579
38.8	28.19	3.65868
38.8	29.33	3.65868
77.5	26.96	4.35041
77.5	25.72	4.35041
155.0	21.82	5.04349
155.0	20.59	5.04349
310.0	12.62	5.73660
310.0	11.57	5.73660
620.0	5.56	6.42974
620.0	6.17	6.42974
1240.0	3.33	7.12287
1240.0	3.07	7.12287

```

proc nlin data=one;
  parms th1=30 th2=0 th3=300 th4=2;
  if conc=0 then do;
    rhs=th1;
  end;
  else do;
    t=(conc/th3)**th4;
    rhs=th2+(th1-th2)/(1+t);
  end;
  model frabound=rhs;
  output out=two r=r p=p;
run;
proc print noobs; var r p; run;

```

Dependent Variable frabound

Method: Gauss-Newton

Iterative Phase

Iter	th1	th2	th3	th4	Sum of Squares
0	30.0000	0	300.0	2.0000	39.5202
1	29.7547	1.7626	236.1	1.7641	4.1840
2	29.8066	2.0042	232.1	1.8567	3.6505
3	29.8038	1.9915	232.4	1.8615	3.6471
4	29.8033	1.9928	232.4	1.8619	3.6471
5	29.8033	1.9929	232.4	1.8619	3.6471

NOTE: Convergence criterion met.

Estimation Summary

Method	Gauss-Newton
Iterations	5
R	2.794E-6
PPC(th2)	1.471E-6
RPC(th2)	0.000025
Object	2.965E-9
Objective	3.647137
Observations Read	16
Observations Used	16
Observations Missing	0

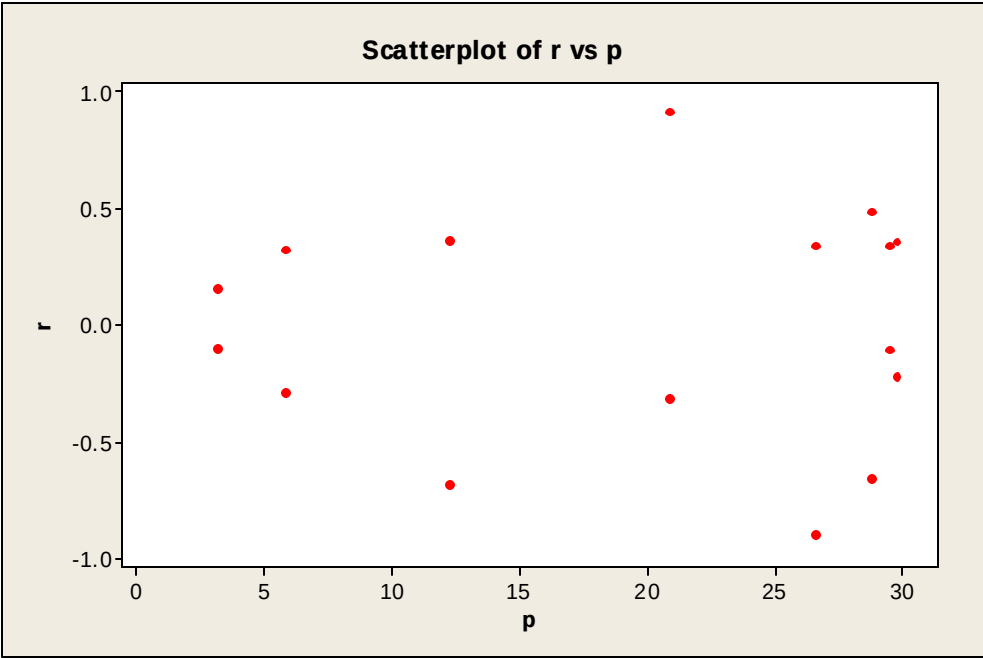
Source	DF	Sum of Squares	Mean Square	F Value	Approx Pr > F
Model	3	1704.2	568.1	1869.08	<.0001
Error	12	3.6471	0.3039		
Corrected Total	15	1707.8			

Parameter	Estimate	Std Error	Approximate	95% Confidence Limits
th1	29.8033	0.2658	29.2242	30.3823
th2	1.9929	0.5667	0.7582	3.2276
th3	232.4	8.6272	213.6	251.2
th4	1.8619	0.1122	1.6174	2.1065

Approximate Correlation Matrix

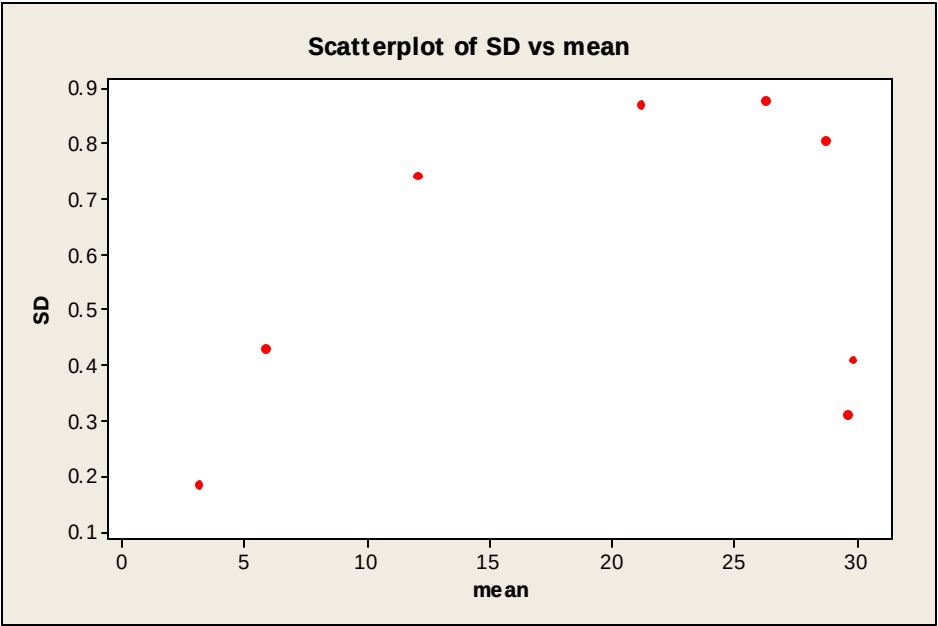
	th1	th2	th3	th4
th1	1.0000000	-0.3033530	-0.1517961	-0.5459955
th2	-0.3033530	1.0000000	-0.7268311	0.7460833
th3	-0.1517961	-0.7268311	1.0000000	-0.4125604
th4	-0.5459955	0.7460833	-0.4125604	1.0000000

r	p
0.35675	29.8033
-0.22325	29.8033
0.33705	29.5329
-0.10295	29.5329
-0.65525	28.8452
0.48475	28.8452
0.34247	26.6175
-0.89753	26.6175
0.91179	20.9082
-0.31821	20.9082
0.36251	12.2575
-0.68749	12.2575
-0.28828	5.8483
0.32172	5.8483
0.15796	3.1720
-0.10204	3.1720



```
proc sort data=one; by conc; run;  
proc means noprint; var frabound; by conc; output out=three mean=m stddev=s; run;  
data three; set three; drop _TYPE_ _FREQ_;  
proc print; run;
```

Obs	conc	m	s
1	0.0	29.870	0.41012
2	19.4	29.650	0.31113
3	38.8	28.760	0.80610
4	77.5	26.340	0.87681
5	155.0	21.205	0.86974
6	310.0	12.095	0.74246
7	620.0	5.865	0.43134
8	1240.0	3.200	0.18385



```

proc nlmixed data=one; *** NLMIXED # 1 ***;
parms th1=30 th2=0 th3=300 th4=2 se=1;
if conc=0 then do;
  rhs=th1;
end;
else do;
  t=(conc/th3)**th4; den=1+t;
  rhs=th2+(th1-th2)/den;
end;
var=se*se;
model frabound ~ normal(rhs,var);
run;

```

The NLMIXED Procedure

Iteration History

Iter	Calls	NegLogLike	Diff	MaxGrad	Slope
22	39	10.8738466	0.000103	0.004516	-0.00021
23	41	10.8738465	1.446E-7	0.000804	-3.4E-7
24	43	10.8738465	3.317E-9	7.301E-6	-6.64E-9

NOTE: GCONV convergence criterion satisfied.

Fit Statistics

-2 Log Likelihood	21.7
AIC (smaller is better)	31.7
AICC (smaller is better)	37.7
BIC (smaller is better)	35.6

Parameter Estimates

Parameter	Estimate	Standard Error	DF	t Value	Pr > t	Alpha	Lower	Upper	Gradient
th1	29.8033	0.2329	16	127.97	<.0001	0.05	29.3095	30.2970	1.531E-7
th2	1.9929	0.4927	16	4.04	0.0009	0.05	0.9484	3.0374	-1.97E-6
th3	232.44	7.4175	16	31.34	<.0001	0.05	216.72	248.17	-7.76E-8
th4	1.8619	0.09942	16	18.73	<.0001	0.05	1.6512	2.0727	7.301E-6
se	0.4774	0.08440	16	5.66	<.0001	0.05	0.2985	0.6564	2.854E-7

```

proc nlmixed data=one; *** NLMIXED # 2 ***;
parms th1=30 th2=0 th3=300 th4=2 se=.01 rho=0;
if conc=0 then do;
  rhs=th1;
end;
else do;
  t=(conc/th3)**th4; den=1+t;
  rhs=th2+(th1-th2)/den;
end;
var=se*se*(rhs)**rho;
model frabound ~ normal(rhs,var);
run;

```

The NLMIXED Procedure

Iteration History

Iter	Calls	NegLogLike	Diff	MaxGrad	Slope
84	198	9.68738811	1.119E-9	0.0002	-1.8E-6
85	201	9.68738811	1.36E-10	0.000189	-2.11E-7
86	202	9.68738811	1.79E-10	0.000129	-1.07E-9

NOTE: GCONV convergence criterion satisfied.

Fit Statistics

-2 Log Likelihood	19.4
AIC (smaller is better)	31.4
AICC (smaller is better)	40.7
BIC (smaller is better)	36.0

Parameter Estimates

Parameter	Estimate	Standard Error	DF	t Value	Pr > t	Alpha	Lower	Upper	Gradient
th1	29.7840	0.2777	16	107.24	<.0001	0.05	29.1952	30.3728	-2.57E-6
th2	2.0618	0.2811	16	7.33	<.0001	0.05	1.4659	2.6577	0.000037
th3	231.74	5.6829	16	40.78	<.0001	0.05	219.69	243.79	6.445E-7
th4	1.8784	0.08705	16	21.58	<.0001	0.05	1.6939	2.0629	-0.00013
se	0.1223	0.09460	16	1.29	0.2144	0.05	-0.07822	0.3229	0.000046
rho	0.9410	0.5501	16	1.71	0.1065	0.05	-0.2252	2.1071	7.497E-6

```
proc nlmixed data=one; *** NLMIXED # 3 ***;
  parms th1=30 th2=2 th3=250 th4=2 se=.01 rho1=5 rho2=4;
  if conc=0 then do;
    rhs=th1;
  end;
  else do;
    t=(conc/th3)**th4; den=1+t;
    rhs=th2+(th1-th2)/den;
  end;
  var=.00001*se*se*((rhs)**rho1)*((1.1*th1-rhs)**rho2);
  model frabound ~ normal(rhs,var);
run;
```

The NLMIXED Procedure

Iteration History

Iter	Calls	NegLogLike	Diff	MaxGrad	Slope
44	90	7.71820293	3.782E-8	0.027773	-6.64E-8

NOTE: GCONV convergence criterion satisfied.

Fit Statistics

-2 Log Likelihood	15.4
AIC (smaller is better)	29.4
AICC (smaller is better)	43.4
BIC (smaller is better)	34.8

Parameter Estimates

Parameter	Estimate	Standard Error	DF	t Value	Pr > t	Alpha	Lower	Upper	Gradient
th1	29.8710	0.1771	16	168.64	<.0001	0.05	29.4955	30.2464	-0.00012
th2	1.9814	0.2295	16	8.63	<.0001	0.05	1.4948	2.4680	0.00012
th3	230.04	6.7797	16	33.93	<.0001	0.05	215.67	244.42	-0.00032
th4	1.8332	0.08383	16	21.87	<.0001	0.05	1.6555	2.0109	-0.00032
se	0.2476	0.6171	16	0.40	0.6936	0.05	-1.0606	1.5557	-0.02777
rho1	2.9106	1.0545	16	2.76	0.0139	0.05	0.6751	5.1461	-0.00009
rho2	2.0161	0.9914	16	2.03	0.0589	0.05	-0.08554	4.1176	-0.00011