Analysis of Experiments With Functional Responses

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- Joint work with Dr. Qing Shen (Edmunds.com Inc.)

Outline

- Introduction
- Linear models with functional responses
- Diagnostics
- An Example
- Summary

Introduction

- Many designed experiments have functional responses.
  - Robust parameter designs with a signal factor.
- Functional linear models are useful for such experiments
  - functional response, scalar predictors
- Ramsay and Silverman (1997, 2005):
  Introduction to Functional Data Analysis
- Ramsay and Silverman (2002):
  Applied Functional Data Analysis: Methods and Case Studies
- Nair, Taam and Ye (2002, JQT) analyzed three real robust design experiments with functional responses.

Example: Alternator Experiment

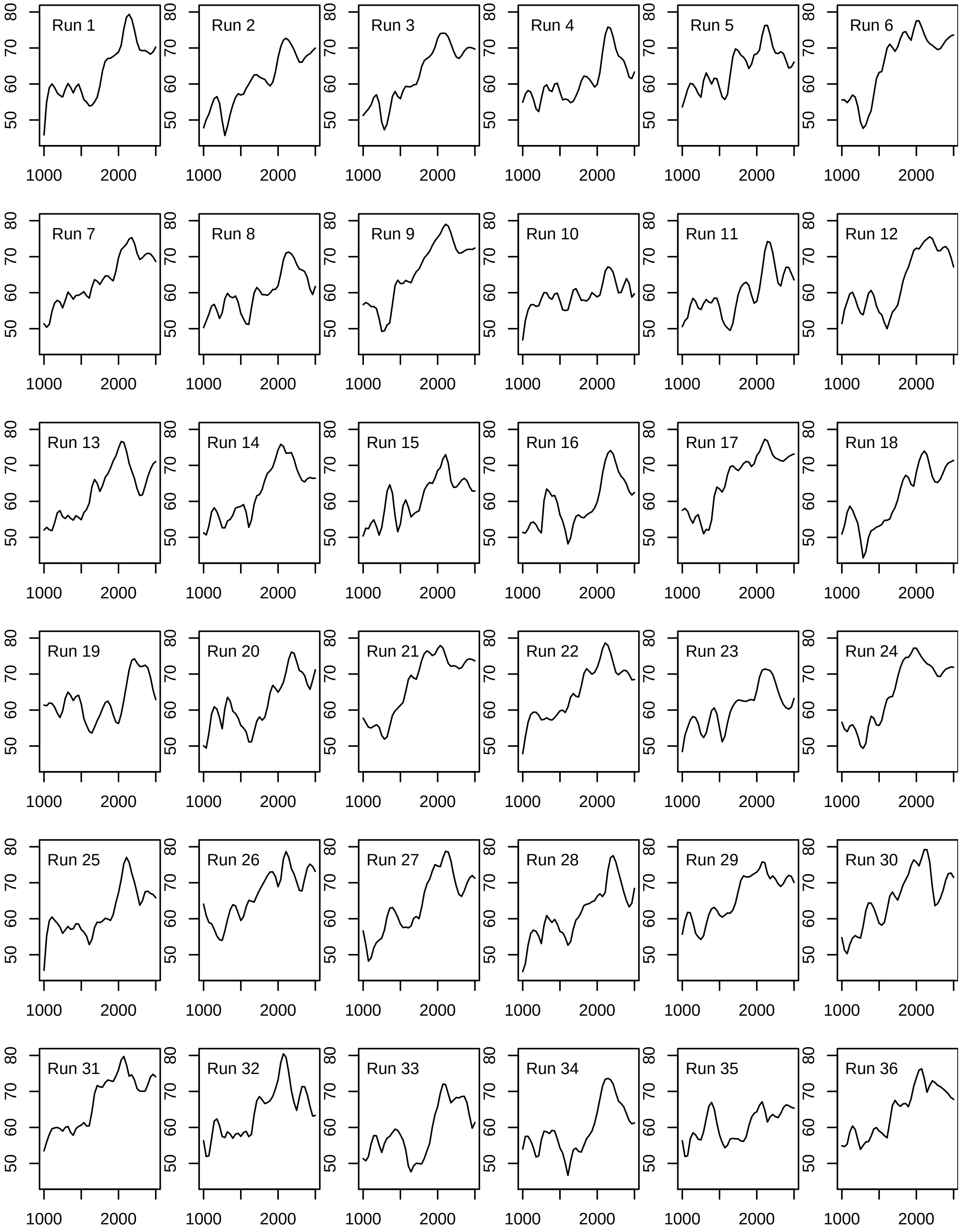
- A robust design experiment from Nair, Taam and Ye (2002)
- Study the effects of 7 process assembly parameters (factors A–G) on the audible noise levels of alternators.
- Noise factor: D.
- A 2_{IV}^{7-2} design plus 4 additional runs at the high levels
- signal factor: rotating speed
- recorded 43 measurements of sound pressure levels (responses) at rotating speeds ranging from 1000 to 2500 revolution per minute.

(Fig. Observed response curves)

Factor	Description
A	Through Bolt Torque
B	Rotor Balance
C	Stator Varnish
D	Air Gap Variation
E	Stator Orientation
F	Housing Stator Slip Fit
G	Shaft Radial Alignment

Run	A	B	C	D	E	F	G
1	-1	-1	-1	-1	-1	1	1
2	-1	-1	-1	-1	1	1	-1
3	-1	-1	-1	1	-1	-1	-1
4	-1	-1	-1	1	1	-1	1
5	-1	-1	1	-1	-1	-1	1
6	-1	-1	1	-1	1	-1	-1
7	-1	-1	1	1	-1	1	-1
8	-1	-1	1	1	1	1	1
9	-1	1	-1	-1	-1	-1	-1
10	-1	1	-1	-1	1	-1	1
11	-1	1	-1	1	-1	1	1
12	-1	1	-1	1	1	1	-1
13	-1	1	1	-1	-1	1	-1
14	-1	1	1	-1	1	1	1
15	-1	1	1	1	-1	-1	1
16	-1	1	1	1	1	-1	-1
17	1	-1	-1	-1	-1	-1	-1
18	1	-1	-1	-1	1	-1	1
19	1	-1	-1	1	-1	1	1
20	1	-1	-1	1	1	1	-1
21	1	-1	1	-1	-1	1	-1
22	1	-1	1	-1	1	1	1
23	1	-1	1	1	-1	-1	1
24	1	-1	1	1	1	-1	-1
25	1	1	-1	-1	-1	1	1
26	1	1	-1	-1	1	1	-1
27	1	1	-1	1	-1	-1	-1
28	1	1	-1	1	1	-1	1
29	1	1	1	-1	-1	-1	1
30	1	1	1	-1	1	-1	-1
31	1	1	1	1	-1	1	-1
32	1	1	1	1	1	1	1
33	1	1	1	1	1	1	1
34	1	1	1	1	1	1	1
35	1	1	1	1	1	1	1
36	1	1	1	1	1	1	1

Observed Response Curves



Linear Models With Functional Responses

Model:

$$\mathbf{Y}(t) = \mathbf{X}\boldsymbol{\beta}(t) + \boldsymbol{\epsilon}(t), \quad t \in [a, b]$$

- $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)^T$ is an $n \times p$ matrix
- $\boldsymbol{\beta}(t) = (\beta_1(t), \cdots, \beta_p(t))^T$
- $\boldsymbol{\epsilon}(t) = (\epsilon_1(t), \cdots, \epsilon_n(t))^T$
- each $\epsilon_i(t)$ is an independent realization of a Gaussian process with mean 0 and covariance function $\gamma(s, t)$.
- eigen-decomposition

$$\gamma(s, t) = \sum_{i=1}^{\infty} \lambda_i \phi_i(s) \phi_i(t),$$

where λ_i are eigenvalues and ϕ_i are orthonormal eigenfunctions.

Estimation

- Each curve is a point in a functional space.
- The least squares estimates minimize the residual SS in L_2.

$$\hat{\boldsymbol{\beta}}(t) = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}(t)$$

- This is point-wise l.s. estimation.
- Fitted responses: $\hat{y}_i(t) = \mathbf{x}_i^T\hat{\boldsymbol{\beta}}(t)$
- Residuals: $\hat{\epsilon}_i(t) = y_i(t) - \hat{y}_i(t)$.
- Residual SS: $rss = \sum_{i=1}^n \|\hat{\epsilon}_i\|^2 = \sum_{i=1}^n \int \hat{\epsilon}_i(t)^2 dt$.

Testing Nested Linear Hypothesis

$$H_0(\omega): \qquad \mathbf{Y}(t) = \mathbf{X}_1\boldsymbol{\beta}_1(t) + \boldsymbol{\epsilon}(t)$$

$$H_1(\Omega): \qquad \mathbf{Y}(t) = \mathbf{X}_1\boldsymbol{\beta}_1(t) + \mathbf{X}_2\boldsymbol{\beta}_2(t) + \boldsymbol{\epsilon}(t)$$

- Traditional multivariate tests are not appropriate.
- Ramsay and Silverman (1997) used pointwise t statistics
  - problem of multiple comparison and correlated responses
- Faraway (1997) proposed a bootstrap based test
  - heavy computation
- Fan and Lin (1998) proposed adaptive transform-based tests
- Shen and Faraway (2004) proposed a functional F test
  - similar to an ordinary F test
  - easy to use

Functional F Test

$$F = \frac{(rss_\omega - rss_\Omega)/(p-q)}{rss_\Omega/(n-p)}$$

- Under the null hypothesis,

$$F \sim \frac{\sum_{i=1}^{\infty} \lambda_i \chi^2_{p-q}/(p-q)}{\sum_{i=1}^{\infty} \lambda_i \chi^2_{n-p}/(n-p)},$$

  where λ_i are eigenvalues of $\gamma(s,t)$ and the χ^2 random variables are independent.

- approximate it by an ordinary F distribution,

$$F \approx F(\lambda(p-q), \lambda(n-p))$$

  where

$$\lambda = (\sum \lambda_i)^2 / \sum \lambda_i^2$$

  is the *degrees-of-freedom-adjustment-factor*.

Testing Individual Predictors

$$H_0 : \beta_j(t) = 0 \text{ vs. } H_1 : \beta_j(t) \neq 0$$

- Functional F test statistic

$$F_j = \frac{rss_j - rss}{rss/(n-p)}$$

where rss_j is the residual SS under H_0.

$$F_j = \frac{\|\hat{\beta}_j\|^2}{(rss/(n-p))(\mathbf{X}^T\mathbf{X})^{-1}_{jj}} = \frac{\|\hat{\beta}_j\|^2}{(se)^2}.$$

- approximated by an ordinary F distribution

$$F_j \approx F(\lambda, \lambda(n-p))$$

In Practice

- only observe $y_i(t)$ for $t_1, \ldots, t_m$,

$$y_i(t_j) = \mathbf{x}_i^T \boldsymbol{\beta}(t_j) + \epsilon(t_j), i = 1, \ldots, n, j = 1, \ldots, m,$$

- do point-wise estimation and regression.
- compute $\|\hat{\epsilon}_i\|^2 = \sum_{k=1}^m \hat{\epsilon}_i(t_k)^2/m$
- compute $\|\hat{\beta}_j\|^2 = \sum_{k=1}^m \hat{\beta}_j(t_k)^2/m.$
- estimate the covariance function $\gamma(s, t)$ by the empirical covariance matrix $\hat{\Sigma}$
- estimate the degrees-of-freedom-adjustment-factor by

$$\hat{\lambda} = \text{trace}\,(\hat{\Sigma})^2/\text{trace}\,(\hat{\Sigma}^2).$$

- A large sample size ($n \geq 30$) is desired.

Diagnostics

- Outliers exist not only in observational studies but also in designed experiments.
- Outliers and influential cases often lead to misleading conclusions.
- Point-wise diagnostics are useful, but
  - residuals are correlated over time.
  - inconsistence often emerges from different time points.
- Truly functional diagnostics is desired

Studentized Residuals

- Hat matrix: $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$
- Leverage h_{ii} is the ith diagonal element of $\mathbf{H}$.

Studentized residuals (for scalar regression):

$$s_i = \frac{\hat{\epsilon}_i}{\sqrt{1 - h_{ii}}\hat{\sigma}}$$

Studentized residuals (for functional regression):

$$S_i = \frac{\|\hat{\epsilon}_i\|}{\sqrt{1 - h_{ii}}\hat{\Delta}}$$

where $\hat{\Delta}^2 = rss/(n-p)$ is an unbiased estimate of total variance $\Delta^2 = \int \gamma(t,t)dt = \sum \lambda_k$.

- S_i and $\|\hat{y}_i\|$ are uncorrelated.

Studentized Residuals

- If the error process is Gaussian,

$$\frac{\|\hat{\epsilon}_i\|^2}{1-h_{ii}} \sim \sum_{k=1}^{\infty} \lambda_k \chi_1^2,$$

  where λ_k are eigenvalues of $\gamma(s,t)$ and the χ^2 random variables are independent.

$$\frac{\|\hat{\epsilon}_i\|^2}{1-h_{ii}} \approx c\chi_\lambda^2,$$

- $\lambda = (\sum \lambda_k)^2 / (\sum \lambda_k^2)$ is the adjustment factor.

Residual plots:

- Residual vs. Fitted Plot: S_i against $\|\hat{y}_i\|$.
- Chi-square Q-Q plot: S_i^2 against quantiles of a χ^2 distribution with df $=\hat{\lambda}$.

Outliers and Jackknife Residuals

Scalar:

$$j_i = \frac{y_i - \tilde{y}_i}{\hat{\sigma}_{(i)}\sqrt{1 + \mathbf{x}_i^T(\mathbf{X}_{(i)}^T\mathbf{X}_{(i)})^{-1}\mathbf{x}_i}}$$

Functional:

$$J_i = \frac{\|y_i - \tilde{y}_i\|}{\sqrt{1 + \mathbf{x}_i^T(\mathbf{X}_{(i)}^T\mathbf{X}_{(i)})^{-1}\mathbf{x}_i}\hat{\Delta}_{(i)}}$$

where $\hat{\Delta}_{(i)}^2$ is an unbiased estimate of total variance Δ^2 without the ith case.

Outliers and Jackknife Residuals

To test whether the ith case is an outlier, consider the *mean shift outlier model*:

$$y_j(t) = \mathbf{x}_j^T \boldsymbol{\beta}(t) + \epsilon_j(t), \qquad j \neq i,$$

$$y_i(t) = \mathbf{x}_i^T \boldsymbol{\beta}(t) + \delta(t) + \epsilon_i(t).$$

- The ith case is not an outlier is equivalent to $\delta(t) = 0$.
- A functional F test can be used for the latter.
- $F_i = J_i^2$.

Outliers and Jackknife Residuals

- If the ith case is not an outlier,

$$J_i^2 \sim \frac{\sum_{k=1}^{\infty} \lambda_k \chi_1^2}{\sum_{k=1}^{\infty} \lambda_k \chi_{n-p-1}^2/(n-p-1)},$$

  where λ_k are eigenvalues of $\gamma(s,t)$ and the χ^2 random variables are independent.

- Use functional F test to formally detect outliers.

$$J_i^2 \approx F(\lambda, \lambda(n-p-1))$$

- Formula for computation:

$$J_i = S_i \sqrt{\frac{n-p-1}{n-p-S_i^2}}$$

Influential Cases and Cook's Distance

Scalar:

$$d_i = \frac{(\hat{\boldsymbol{\beta}}_{(i)} - \hat{\boldsymbol{\beta}})^T (\mathbf{X}^T \mathbf{X}) (\hat{\boldsymbol{\beta}}_{(i)} - \hat{\boldsymbol{\beta}})}{p \hat{\sigma}^2}$$

Functional:

$$D_i = \frac{\int (\hat{\boldsymbol{\beta}}_{(i)}(t) - \hat{\boldsymbol{\beta}}(t))^T (\mathbf{X}^T \mathbf{X}) (\hat{\boldsymbol{\beta}}_{(i)}(t) - \hat{\boldsymbol{\beta}}(t)) dt}{p \hat{\Delta}^2}.$$

Formula for computation:

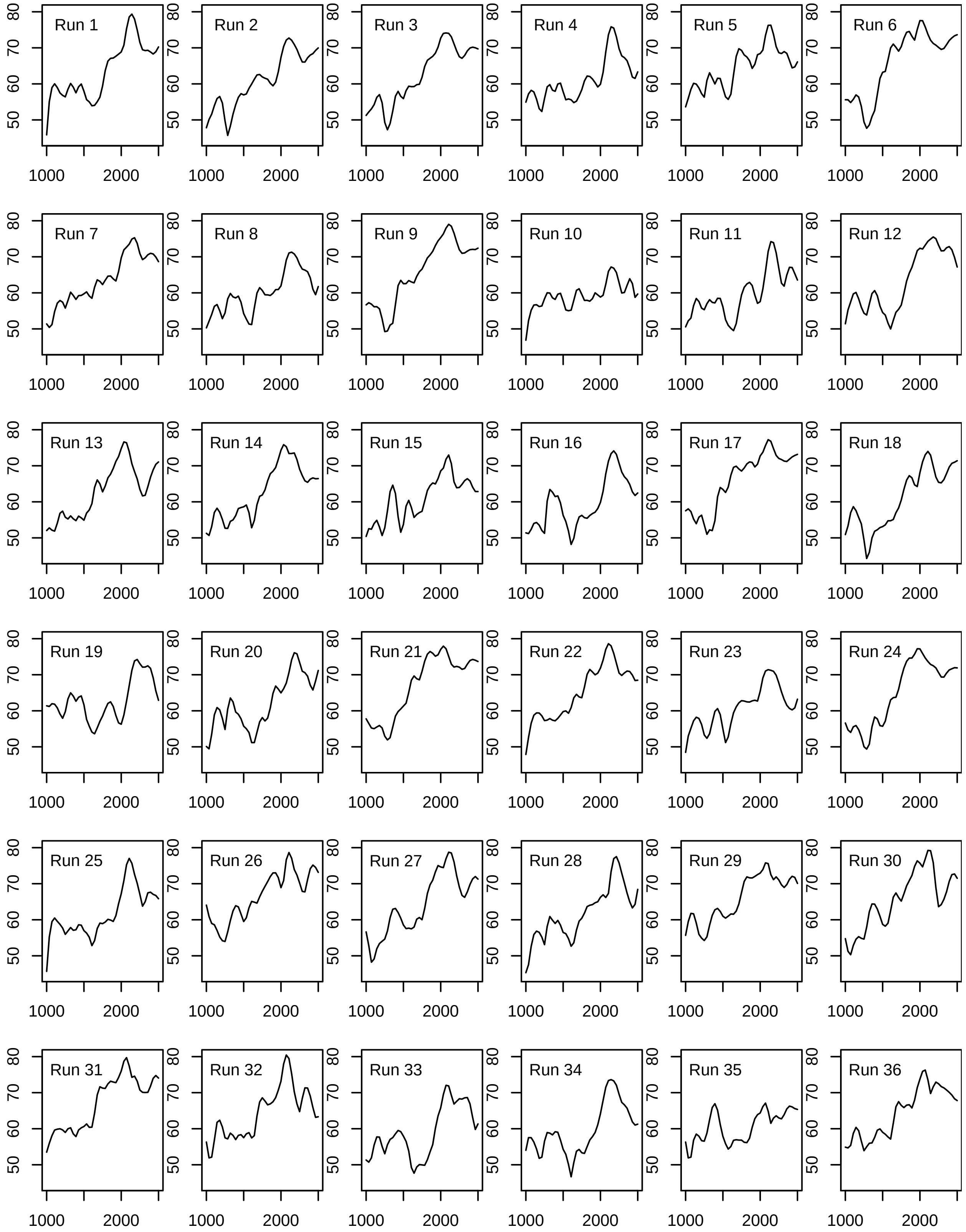
$$D_i = \frac{1}{p} \frac{h_{ii}}{1 - h_{ii}} S_i^2.$$

Example: Alternator Experiment

- A 2_{IV}^{7-2} design with defining relation
  $I = CEFG = ABCDF = ABDEG$.
- It allows the clear estimation of all 7 main effects and 15 two-factor interactions.
- The 6 remaining 2-factor interactions are aliased in three pairs (i.e., $CE = FG$, $CF = EG$, $CG = EF$).
- For simplicity, ignore the last four runs in the analysis.
- Start with a main effects model.
- Indeed, none of the 2-factor interactions is significant.

(Fig. Observed response curves)

Observed Response Curves



Main Effects Model

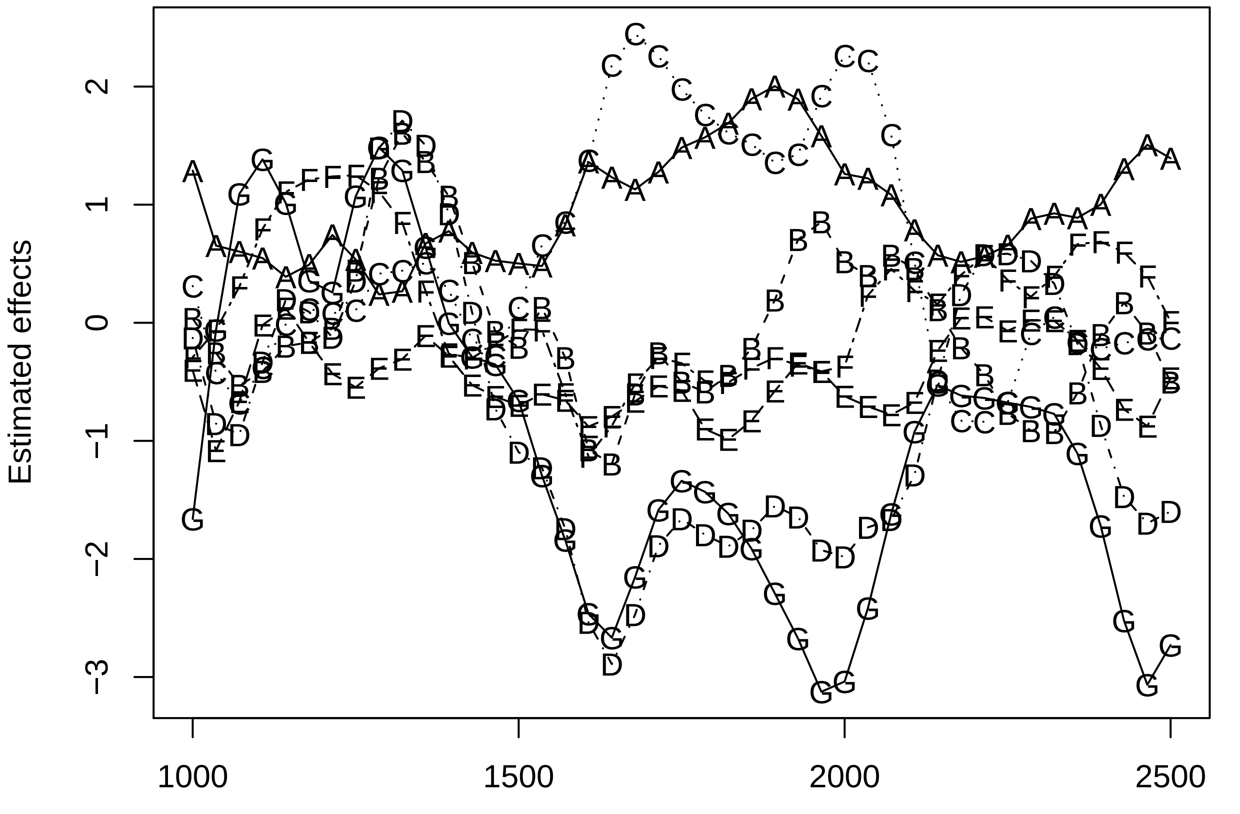
	Numerator	Denominator	F Value	P-Value
Intercept	4035.1	0.3556	11348	0.0000
A	1.1633	0.3556	3.2716	0.0093
B	0.4084	0.3556	1.1485	0.3388
C	1.2838	0.3556	3.6103	0.0051
D	1.9419	0.3556	5.4611	0.0002
E	0.3225	0.3556	0.9071	0.4762
F	0.3602	0.3556	1.0130	0.4117
G	2.7768	0.3556	7.8091	0.0000

```
Average residual SS: 273.0895 on 24 degrees of freedom
Adjustment factor: 4.808803 (for 43 grids)
```

- D and G are very significant.
- A and C are significant at 1% margin.

(Fig. Estimated effect curves from the main effects model)

Estimated Effect Curves (Main Effects Model)



Reduced Model

	Numerator	Denominator	F Value	P-Value
Intercept	4035.1	0.3565	11319	0.0000
A	1.1633	0.3565	3.2633	0.0076
C	1.2838	0.3565	3.6012	0.0040
D	1.9419	0.3565	5.4473	0.0001
G	2.7768	0.3565	7.7893	0.0000

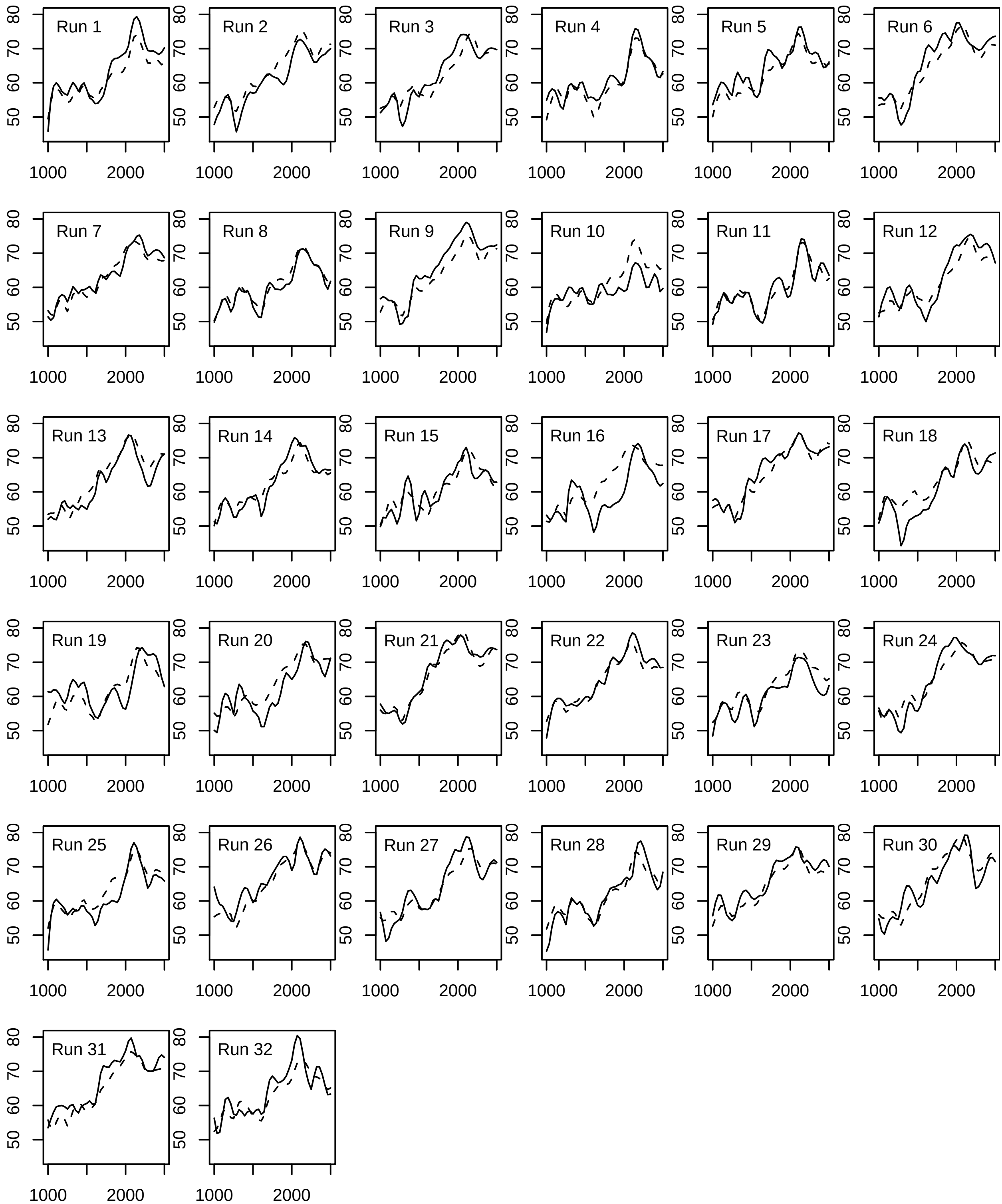
```
Average residual SS: 308.0066 on 27 degrees of freedom
Adjustment factor: 5.135548 (for 43 grids)
```

ANOVA Table

```
              DF Resid SS Mean SS   F
Reduced       27 308.0066 11.4077  1.02
Main-Effects  24 273.0895 11.3787
Adjusted DF:  14.4 and 115.4,  p-value: 0.4365
Adjustment factor: 4.808803 (for 43 grids)
```

(Fig. Observed and fitted curves for the reduced model)

Observed and Fitted Curves (Reduced Model)



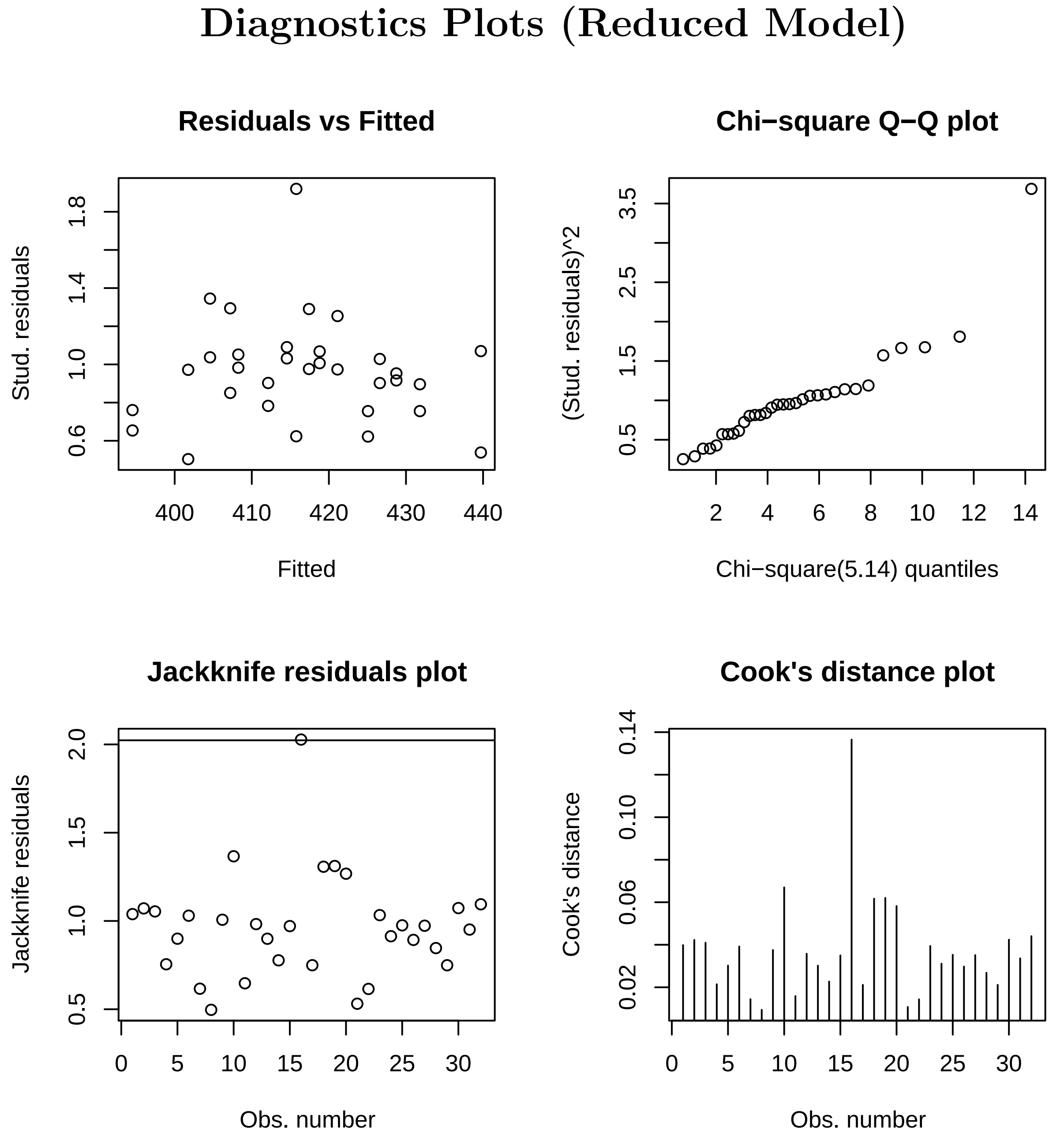
Observed (solid), fitted (dashed)

Diagnosics

(Fig. Diagnostics plots for the reduced model)

- The formal outlier test declares that case 16 is an outlier.
- The horizontal line on the jackknife plot shows the (Bonferoni adjusted) critical value at the 5% level.

(Fig. Observed and fitted curves for the reduced model)


Diagnostics Plots (Reduced Model)
Residuals vs Fitted
Stud. residuals
Fitted
Chi−square Q−Q plot
(Stud. residuals)^2
Chi−square(5.14) quantiles
Jackknife residuals plot
Jackknife residuals
Obs. number
Cook's distance plot
Cook's distance
Obs. number

Reduced Model Without Case 16

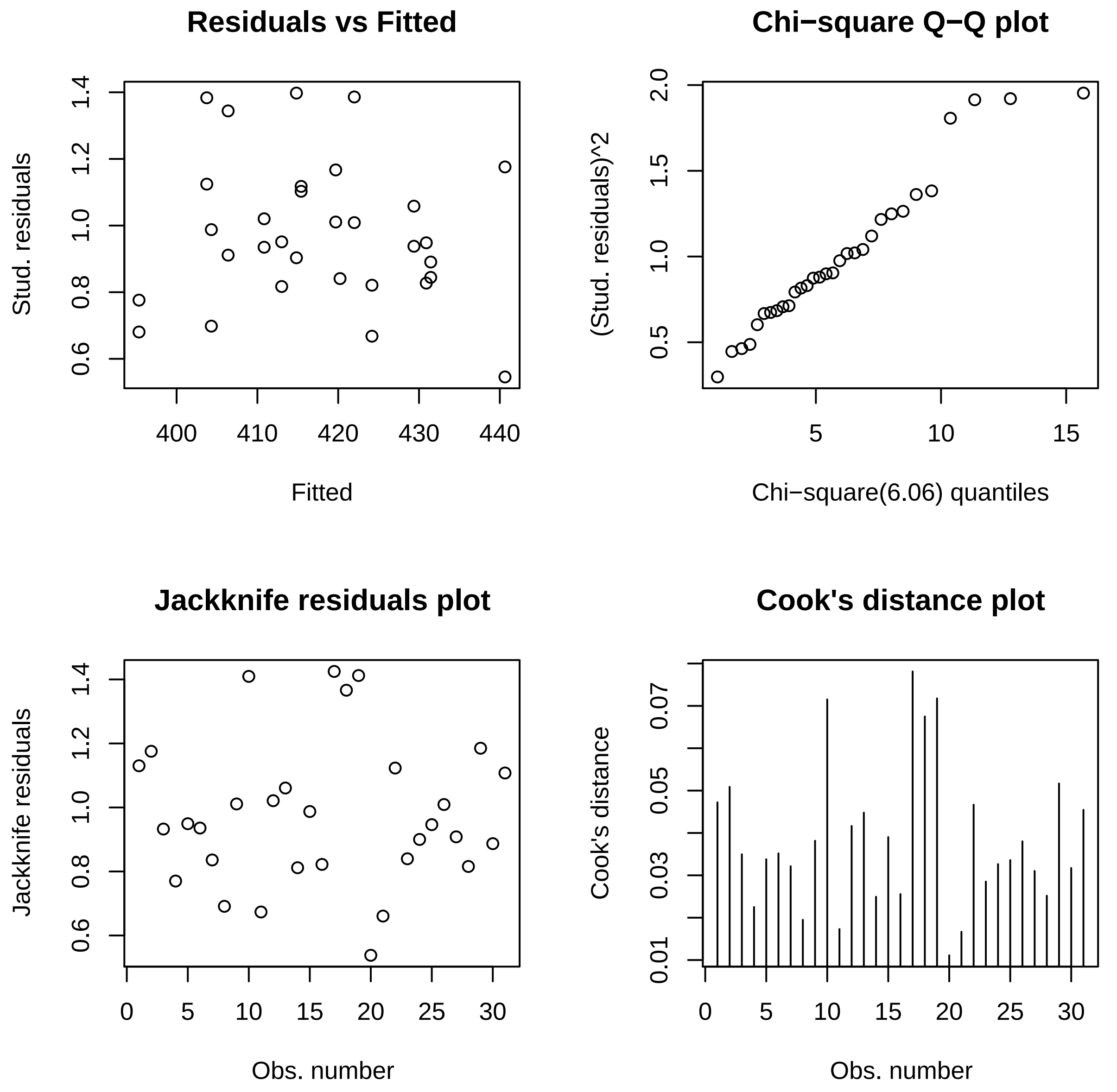
	Numerator	Denominator	F Value	P-Value
Intercept	4052.1	0.3315	12224	0.0000
A	0.8192	0.3315	2.4712	0.0256
C	1.7529	0.3315	5.2879	0.0001
D	1.4225	0.3315	4.2911	0.0005
G	3.4725	0.3315	10.4753	0.0000

```
Average residual SS: 265.9543 on 26 degrees of freedom
Adjustment factor: 6.055215 (for 43 grids)
```

- G is still most significant,
- but C is more significant than D,
- A becomes less significant (p-value increases from .0076 to .0256).

(Fig. Diagnostics plots for the reduced model w/o case 16)

Diagnostics Plots (reduced model w/o case 16)



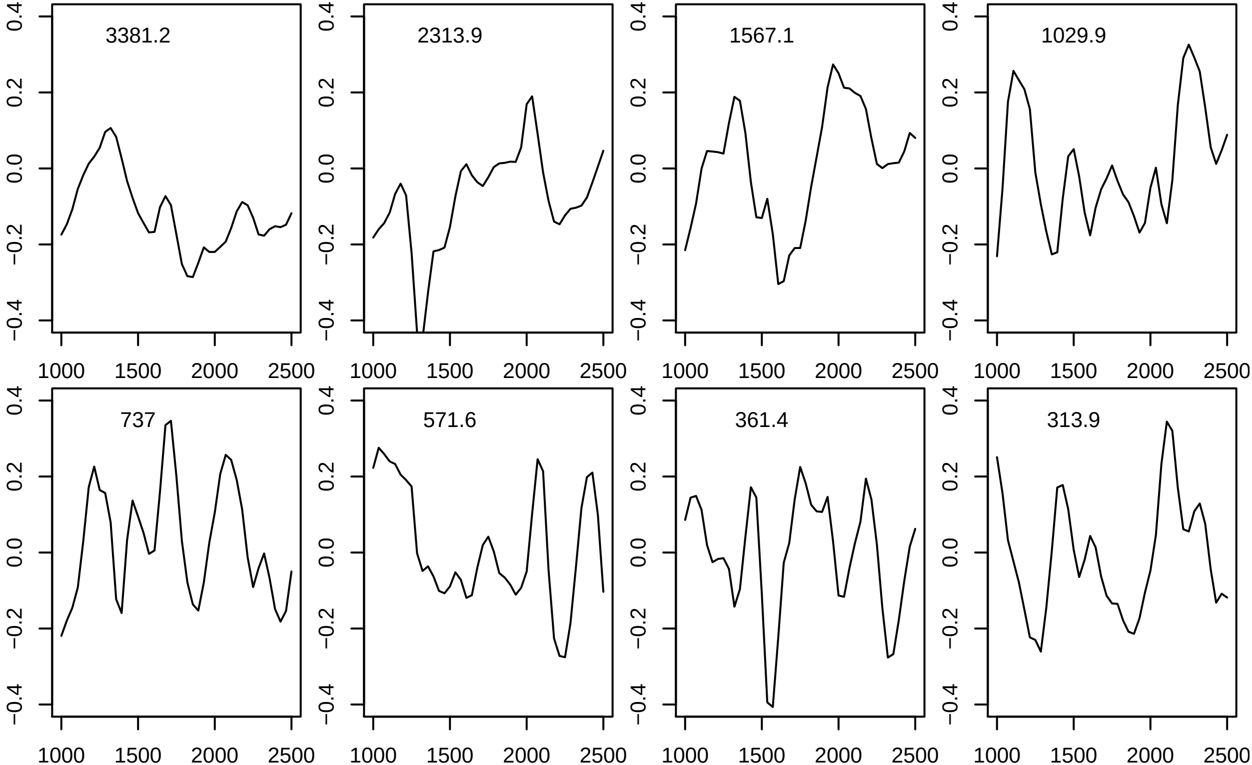
Discussion

- Nair, Taam and Ye (2002)
  - used point-wise CI to declare significant effects.
  - did not perform diagnostics.

(Fig. Estimated eigenfunctions and their associated eigenvalues)

- The error process is rather complicated.
- The first 8 eigenvalues explain 90% variation of the residual functions.
- Difficult to decide the dimension of the error process.
- The functional F test does not suffer from this difficulty.

Estimated Eigenfunctions and Associated Eigenvalues (reduced model w/o case 16)



Summary

Functional linear regression models

- functional responses and scale predictors
- functional F test
  - simple and flexible
  - results are not sensitive to small eigenvalues
- diagnostics
  - studentized residuals (chi-square Q-Q plot)
  - jackknife residuals (formal test for outliers)
  - Cook's distance
  - easy computation formulas

References

1. Nair, V. N., Taam, W., and Ye, K. Q. (2002), “Analysis of Functional Responses From Robust Design Studies,” *Journal of Quality Technology*, 34, 355–370.

2. Shen, Q. and Faraway, J. (2004). An F Test for Linear Models With Functional Responses. *Statistica Sinica* **14** 1239–1257.

3. Shen, Q. and Xu, H. (2005). Diagnostics for Linear Models With Functional Responses. UCLA Department of Statistics, preprint 439.