Non-linear Regression Analysis with Fitter Software Application

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Agenda

- 1. Introduction
- 2. TGA Example
- 3. NLR Basics
- 4. Multicollinearity
- 5. Prediction
- 6. Testing
- 7. Bayesian Estimation
- 8. Conclusions



1. Introduction



Linear and Non-linear Regressions



2. Thermo Gravimetric Analysis Example



TGA Experiment and Data



TGA Example Variables



Plasticizer Evaporation Model

Evaporation Law

$$\frac{dy}{dt} = -kC, \ y(0) = y_0$$



$$T=T_0+vt$$

Temperature growth



Fitter Worksheet for TGA Example

	А	В	С	D	E	F	G	Н	1	J	К	L	М	N	0	
1																
2	Data															
3		V	TO	С	F	t	y	f	Left		Fitt	er	×			
4		3	373	0.3	2.4	0.00	1.000	1.001	1.001		ත්					
5		3	373	0.3	2.4	1.	1 000		1 01							
6		3	373	0.3	2.4	$\frac{ay}{1}$ =	=-kC,	$y(\theta) =$	yo 200			TGA T	btion M			
7		3	373	0.3	2.4	dt			[*] 00		lvl/	$D[t] = k^*[$		$v_{\rm v} = v_{\rm v}$		
8		3	373	0.3	2.4		. 1-0	2	200			*ext k0	- J],](),]		
9		3	373	0.3	2.4	C =	$C = l - \underline{0}$					T=T0+v	t i i i			
10		3	373	0.3	2.4		y					P.987	17			
11		3	373	0.3	2.4	4	-	. E		1		у0=?				
12		3	373	0.3	2.4	k=1	$k = F \exp\left[k_0 - \frac{1}{RT}\right] \frac{1}{100}$					k0=?				
13		3	373	0.3	2.4							E=?				
14					-:	T=7	r + vt									
15		0	293	0.4	2	1 1	1 10 ⁺ ¹					Parameters estimation				
16		0	293	0.4	2	JE 100		0.011	0.844		Name	Initial	Final	Deviation		
17		0	293	0.4	2	8E+06		0.821	0.788		у0	1	1.00088	0.0002		
18		0	293	0.4	2	1E+07		0.781	0.746		k0	10	13.9964	0.24016		
19		0	293	0.4	2	1E+07		0.748	0.714		E	10000	18052.3	225.424		
20																

Service Life Prediction by TGA Data



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3. NLR Basics



Data and Errors





Data & Model Prepared for Fitter





Objective Function Q(a)

Sum of squares

$$S(a) = \sum_{i=1}^{N} w_i^2 (y_i - f_i)^2 g_i^2$$

Bayesian terms
$$s_0^2$$
 Function Q
Is a sum = $Q_a f_+ B$ squares
Objection for the bayes of the bayes
Weighted variance estimate

$$\hat{a} = \arg\min Q(a)$$
 $s^2 = \frac{S(\hat{a})}{N_f}$ $N_f = N - p$

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Very Important Matrix *A*



$$A_{\alpha\beta} = \frac{1}{2} \frac{\partial^2 Q(\boldsymbol{a})}{\partial a_{\alpha} \partial a_{\beta}}, \quad \alpha, \beta = 1, \mathbb{X} \quad , p$$



Quality of Estimation



Final Objective Value

$$s^2 = \frac{S(\hat{a})}{N_f}$$
 $N_f = N - p$

08. Error Variance and Number Degrees of Freedom

Search by Gradient Method



Local minima

4. Multicollinearity





Multicollinearity: View

Multicollinearity is degradation of matrix AObjective function Q(a)Spread of eigenvalues $N(A) = \log_{10} \left(\frac{\lambda_{\max}}{\lambda_{\max}} \right)$ enei is a measure of degradation a_2 a_1 N(A) = 708/12/2023 20

Multicollinearity: Source

"Hard" multicollinearity

"Soft" multicollinearity

$$y = a_1 a_2 x$$
 $y = a_1 (1 - e^{-a_2 x}) \approx a_1 a_2 x$ at $a_2 x << 1$



Data & Model Preprocessing



Example: The Arrhenius Law



Derivative Calculation and Precision



2) Auto calculation of analytical derivatives

$$f=exp(-a*t)$$

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5. Prediction



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Reliable Prediction



Nonlinearity and Simulation

$$\boldsymbol{a}^* \sim N(\hat{\boldsymbol{a}}, \boldsymbol{C}) \rightarrow \boldsymbol{a}_1^*, \mathbb{R}, \boldsymbol{a}_M^* \rightarrow f_1^*, \mathbb{R}, f_M^* \rightarrow r(\boldsymbol{P}, \boldsymbol{x})$$



Prediction: Example



6. Testing





Hypotheses Testing



Lack-of-Fit and Variances Tests

These hypotheses are based on variances and they <u>can't be</u> tested without **replicas**!



Outlier and Series Tests



7. Bayesian Estimation



Bayesian Estimation





Posterior and Prior Information. Type I



Posterior and Prior Information. Type II







8. Conclusions

Mysterious Nature





NLR Model



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