

# Parameter Estimation

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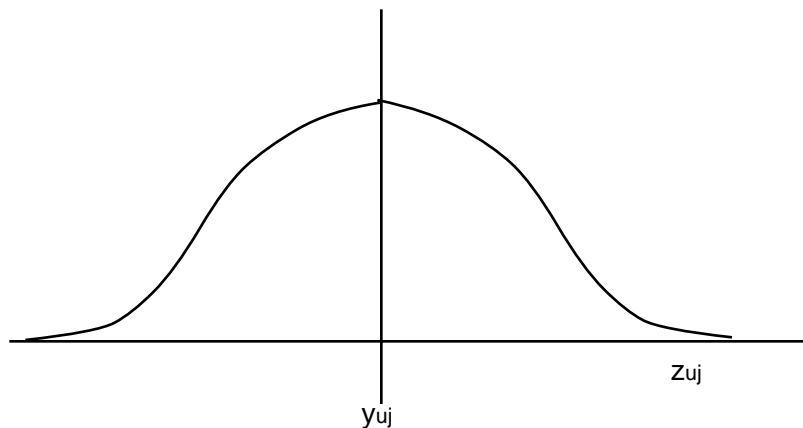
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# I. Motivation and Formulation

## Motivation:

- fit models to data to find 'optimal' parameters
- determine levels of confidence of fitted parameters
- evaluate suitability of models

## Derivation of Objective Function



Let

$$z_{uj} = y_{uj}(\theta) + \varepsilon_{uj}$$

$z_{uj}$  -  $j^{\text{th}}$  component of data for  $u^{\text{th}}$  experiment

$y_{uj}$  - corresponding (correct) model value

$\varepsilon_{uj}$  - observation error following probability distribution function (pdf),  $p(z)$

$\theta$  - adjustable parameters in model

What is  $p(z)$ ? For a scalar  $z$ , how is it derived?

Assume the following moment information:

$$p(z) \geq 0 \quad \int_{-\infty}^{\infty} p(z) dz = 1 \quad \int_{-\infty}^{\infty} z p(z) dz = \eta \quad \int_{-\infty}^{\infty} (z - \eta)^2 p(z) dz = \sigma^2$$

Define measure of information (Shannon, 1948) and find the distribution function that maximizes the information assuming only the moment information:

$$\text{Max } (I(p) = E(\log p) = \int_{-\infty}^{\infty} p(z) \log p(z) dz$$

s.t.

$$p(z) \geq 0 \quad \int_{-\infty}^{\infty} p(z) dz = 1$$

$$\int_{-\infty}^{\infty} z p(z) dz = \eta \quad \int_{-\infty}^{\infty} (z - \eta)^2 p(z) dz = \sigma^2$$

Problem can be solved analytically to yield:

$$p(z) = \frac{1}{(2\pi)^{1/2}\sigma} \exp(-1/2(z-\eta)^2/2\sigma^2)$$

If  $z$  is an  $m$ -vector for a single experiment, this can be extended to a joint multivariable distribution to give:

$$p(z) = (2\pi)^{-m/2} \det(V)^{-1/2} \exp(-1/2(z-\eta)^T(V)^{-1}(z-\eta))$$

where  $V$  is a covariance matrix defined by:

$$V = \int_{-\infty}^{\infty} (z-\eta)(z-\eta)^T p(z) dz$$

Now let's consider n multiple experiments (with index u). Each experiment has a mean  $\eta_u$ , covariance  $V_u$  and experimental error distribution,  $\epsilon_u$

Then the joint probability distribution is given by:

$$p(\epsilon_u) = (2\pi)^{-m/2} \det(V_u)^{-1/2} \exp(-1/2(\epsilon_u)^T(V_u)^{-1}(\epsilon_u))$$

and  $p(\epsilon_u)$  is:

$$\prod_{u=1}^n p(\epsilon_u) = (2\pi)^{-mn/2} \left[ \prod_{u=1}^n \det(V_u)^{-1/2} \right] \exp(-1/2 \sum_{u=1}^n (\epsilon_u)^T(V_u)^{-1}(\epsilon_u))$$

This distribution now needs to be converted into an objective function that 'maximizes information' about our data.

Let's make the following assumptions:

- Replace distributional errors,  $\epsilon_u$  by the actual residuals,  $e_u = (z_u - y_u(\theta))$
- Experiments u are independent and  $V_u$  is the same for all experiments,  $V_u = E(\epsilon_u \epsilon_u^T)$
- Define likelihood function  $L(\theta) = p(e)$  and we maximizes this function (or its log).

This leads to the general form:

$$\log L(\theta) = -nm/2 \log(2\pi) - n/2 \log(\det V) - 1/2 \sum_{u=1}^n e_u^T V^{-1} e_u$$

# Choice of Objective Function

Let's specialize these objectives based on what we know about the error distributions. Define moment matrix:

$$M(\theta) = \sum_{u=1}^n e_u e_u^T, \text{Tr}(V^{-1}M(\theta)) = \sum_{u=1}^n e_u^T V^{-1} e_u$$

and

$$\log L(\theta) = -nm/2 \log(2\pi) - n/2 \log(\det V) \\ - 1/2 \text{Tr}(V^{-1}M(\theta))$$

Since first two terms do not contain  $\theta$ , we simply minimize  $\text{Tr}(V^{-1}M(\theta))$

Some special cases:

- Ordinary Least Squares:  $V$  is known, all component errors  $e_{uj}$  are about the same and independent of each other, i.e.,  $V = v I$

$$\text{Min Tr}(M(\theta)) = \sum_u \sum_j e_{ju}^2$$

- Simple Weighted Least Squares:  $V$  is known and diagonal, all component errors  $e_{uj}$  are independent of each other, i.e.,  $V = \text{diag}\{\sigma_j^2\}$

$$\text{Min Tr}(V^{-1}M(\theta)) = \sum_u \sum_j e_{ju}^2 / \sigma_j^2$$

- Weighted Least Squares:  $V$  is known but general, all component errors  $e_{uj}$  depend on each other:

$$\text{Min Tr}(V^{-1}M(\theta)) = \sum_u \sum_j e_u^T V^{-1} e_u$$

## What if $V$ is not known?

Maximize  $L(\theta)$  wrt  $V$  as well as  $\theta$ .

$$\begin{aligned}\log L(\theta) = & -nm/2 \log(2\pi) - n/2 \log(\det V) \\ & - 1/2 \text{Tr}(V^{-1}M(\theta))\end{aligned}$$

Assuming  $V$  is symmetric and nonsingular, we can get:

$$\frac{\partial \log L(\theta)}{\partial V} = -n/2 (V^{-1}) + 1/2 (V^{-1}M(\theta)V^{-1}) = 0$$

which leads to:

$$V^* = 1/n M(\theta)$$

Substitution into  $L(\theta)$  leads to:

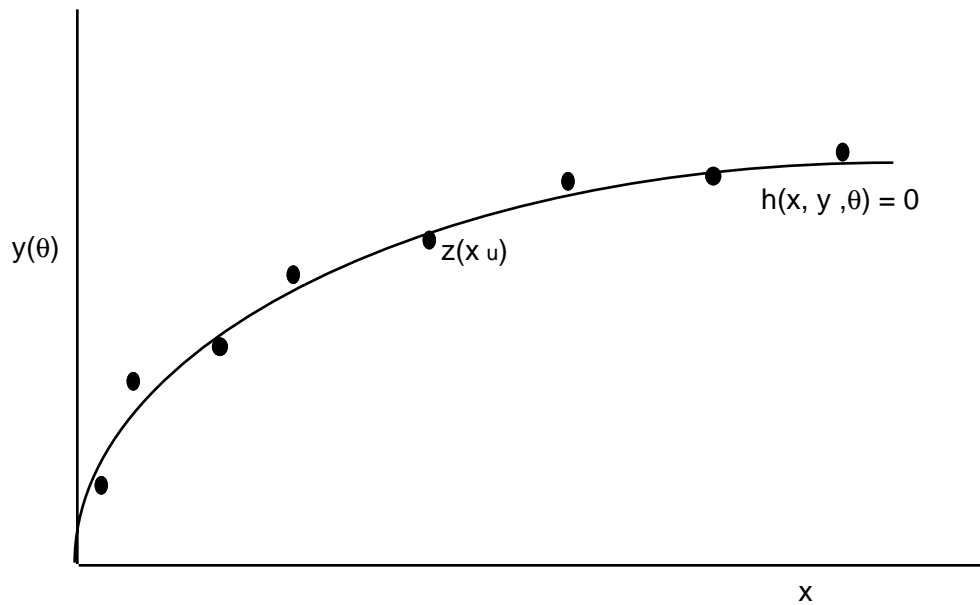
$$\begin{aligned}\log L(\theta) = & -nm/2 \log(2\pi) + n/2 \log n - 1/2 m n \\ & - n/2 \log(\det M(\theta))\end{aligned}$$

so we minimize:  $n/2 \log \det(M(\theta))$

Notes:

- If the form of  $V$  is known, we can further specialize the objective for unknown covariance (e.g., diagonal covariance, same covariance)
- $V^*$  is biased but can be corrected by using
$$V'' = n/(n-m) V^*$$

## II. Unconstrained Least Squares



Basic Problem:

$$\begin{aligned} \text{Min } \Phi(\theta, y, z) &= \frac{1}{2} \sum_{u=1}^n (z_u - y_u)^T W_u (z_u - y_u) \\ \text{s.t. } h_u(x_u, y_u, \theta) &= 0 \\ a &\leq \theta \leq b \end{aligned}$$

- $W_u$  can be chosen to be  $(V_u)^{-1}$
- $h_u(x_u, y_u, \theta) = 0$  is a model for the system
- $x_u$  are fixed independent variables
- Bounds are not expected to be active

Consider the case where  $y_u$  is an explicit function of  $\theta$ ,

$$h_u(x_u, y_u, \theta) = 0 \implies y_u = f_u(x_u, \theta)$$

and

$$\text{Min } \Phi(\theta, z) = \frac{1}{2} \sum_{u=1}^n (z_u - f_u(\theta))^T W_u (z_u - f_u(\theta))$$

# Methods of Solution

## 1. Linear Least Squares

Model is given by:  $y_u = A_u \theta + b_u$

$$\text{Min } \Phi(\theta, z) = 1/2 \sum_{u=1}^n (z_u - A_u \theta - b_u)^T W_u (z_u - A_u \theta - b_u)$$

From  $\nabla_{\theta} \Phi(\theta, z) = 0$ , we get the normal equation:

$$\sum_{u=1}^n (A_u^T W_u A_u) \theta = - \sum_{u=1}^n A_u^T W_u (z_u - b_u)$$

and this leads to:

$$\theta = - \left( \sum_{u=1}^n A_u^T W_u A_u \right)^{-1} \sum_{u=1}^n A_u^T W_u (z_u - b_u)$$

Note: A better way to solve this linear system is to do a QR factorization on  $(W_u)^{1/2} A_u$ .

## 2. Nonlinear Least Squares

Model is given by:  $y_u = f_u(x_u, \theta)$

$$\text{Min } \Phi(\theta, z) = 1/2 \sum_{u=1}^n (z_u - f_u(\theta))^T W_u (z_u - f_u(\theta))$$

and we solve this unconstrained problem with Newton's method.

Apply  $\nabla_{\theta}\Phi(\theta^k, z) + \nabla_{\theta\theta}\Phi(\theta^k, z)\Delta\theta = 0$ , where we have:

$$\nabla_{\theta}\Phi = \sum_{u=1}^n J_u^T W_u (z_u - f(x_u, \theta))$$

$$\nabla_{\theta\theta}\Phi = \sum_{u=1}^n J_u^T W_u J_u + R_u$$

with

$$\{R_u\}_{ij} = -(\nabla_{\theta_i}\theta_j f_u)^T W_u (z_u - f(x_u, \theta)), \quad J_u = \nabla_{\theta} f_u^T$$

Now assume that  $(z_u - f(x_u, \theta)) \sim 0$  and therefore  $R_u \sim 0$  at the solution  $\theta^*$ . Then the Hessian simplifies to:

$$\nabla_{\theta\theta}\Phi = \sum_{u=1}^n J_u^T W_u J_u$$

and we have the Gauss-Newton method

$$\Delta\theta = - \left( \sum_{u=1}^n J_u^T W_u J_u \right)^{-1} \left( \sum_{u=1}^n J_u^T W_u (z_u - f(x_u, \theta)) \right)$$

Note: A better way to solve this linear system is to do a QR factorization on  $(W_u)^{1/2} J_u$ .

# Globalization of Gauss-Newton Method

To ensure convergence from poor starting points:

## Line search method

Choose  $\alpha \in (0, 1]$  so that a sufficient decrease is found for  $\Phi(\theta)$  with:

$$\theta^{k+1} = \theta^k + \alpha \Delta\theta$$

This will converge to a stationary point ( $\nabla_{\theta}\Phi = 0$ ) as long as  $\left(\sum_{u=1}^n J_u^T W_u J_u\right)$  is sufficiently positive definite.

What if is  $\left(\sum_{u=1}^n J_u^T W_u J_u\right)$  singular?

Add  $\lambda I$  to Hessian to get the LevenbergMarquardt method.

$$\Delta\theta = -\left(\sum_{u=1}^n J_u^T W_u J_u + \lambda I\right)^{-1}\left(\sum_{u=1}^n J_u^T W_u (z_u - f(x_u, \theta))\right)$$

How should  $\lambda$  be adjusted?

## Trust region approach in MINPACK (More', 1980)

Choose  $\Delta\theta$  and  $\lambda$  so that

$$\left\| \Delta\theta = - \left( \sum_{u=1}^n J_u^T W_u J_u + \lambda I \right)^{-1} \left( \sum_{u=1}^n J_u^T W_u (z_u - f(x_u, \theta)) \right) \right\| \leq \Delta.$$

is chosen by comparing  $\tau = \text{ared}/\text{pred}$

actual reduction (ared):  $\Phi(\theta^k) - \Phi(\theta^{k+\Delta\theta})$

predicted reduction (pred):  $\nabla_{\theta\theta}\Phi^T \Delta\theta + 1/2 \Delta\theta^T \nabla_{\theta\theta}\Phi \Delta\theta$

At iteration k:

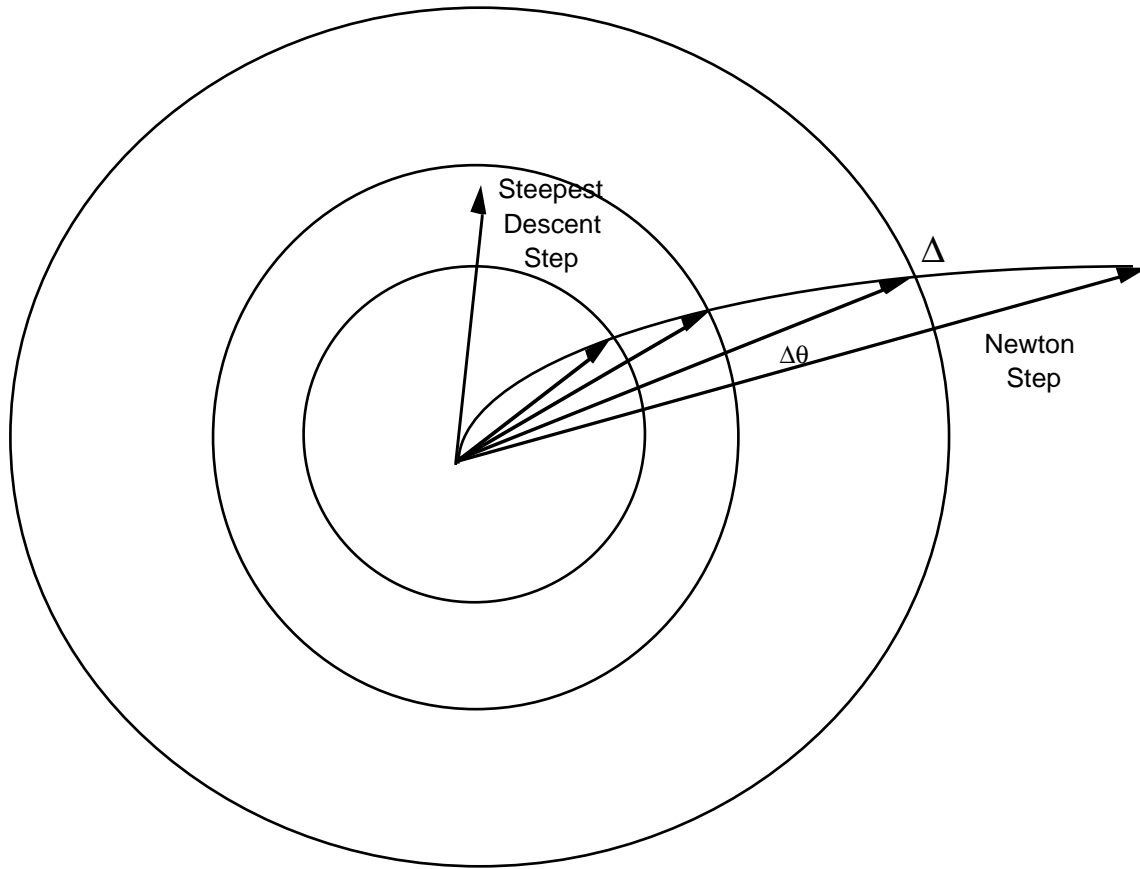
- Calculate  $\Delta\theta$  for given value of  $\lambda$ .
- Evaluate actual reduction (ared) and predicted reduction (pred).
- Define  $\tau = \text{ared}/\text{pred}$ 
  - a) If  $\tau > \rho_1$ ,  $\Delta = m_1 \Delta$
  - b) If  $\tau < \rho_2$ ,  $\Delta = \Delta / m_2$
  - c) If  $\tau < \rho_3$  reset  $\theta^{k+1} = \theta^k$

Else,  $\theta^{k+1} = \theta^k + \Delta\theta$

Typical values for the parameters:

$$m_1 = m_2 = 2 \text{ and } \rho_1 = 0.75, \rho_2 = 0.25, \rho_3 = 0.$$

## Extremes of Trust Region Method:



For given  $\Delta$ , solves for  $1/\|\Delta\theta(\lambda)\| - 1/\Delta = 0$  directly:

$\lambda = 0, \Delta$  large:  $\Delta\theta$  is the Gauss-Newton Step

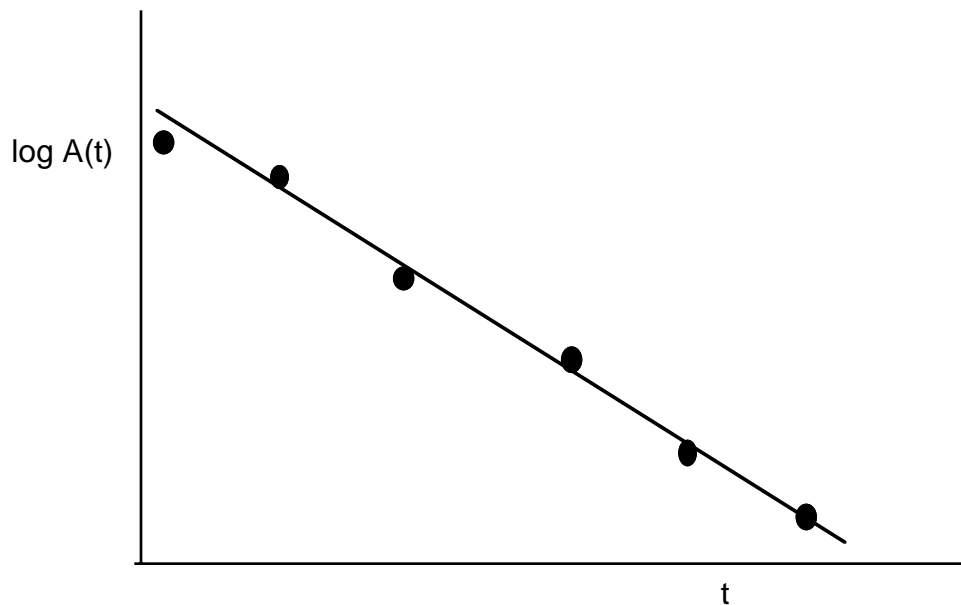
$\lambda \rightarrow \infty, \Delta = 0$ :  $\Delta\theta$  is a small step in the steepest descent direction

Trust Region Methods are guaranteed to converge to stationary points, under mild assumptions.

# Why is trust region required for parameter estimation?

Example:

Consider batch reaction system:  $A \rightarrow B$



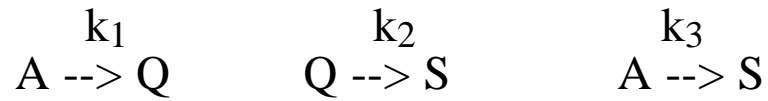
First order reaction:  $A(t) = A(0) \exp(-k t)$   
 $k = k_0 \exp(-E/RT)$

Data available only at one temperature.

Results:

- Nonunique parameter estimates,  $k_0$ ,  $E$
- Singular  $\left( \sum_{u=1}^n J_u^T W_u J_u \right)$
- Can be due to poor model and/or poor data
- Trust region methods will ensure convergence to some solution, other methods won't
- Postoptimality analysis will establish nonuniqueness, insensitivity

Example: Catalytic Cracking of Gasoil (Tjoa, 1991)



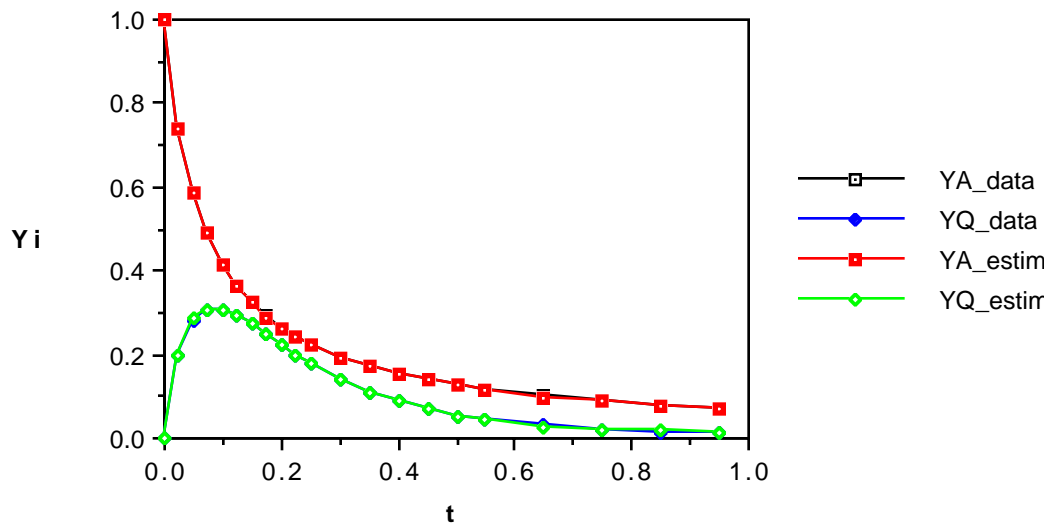
$$\begin{aligned} y_A' &= -(k_1+k_3) y_A^2 \\ y_Q' &= -k_1 y_A^2 - k_2 y_Q \\ y_A(0) &= 1, y_Q(0) = 0 \end{aligned}$$

ODEs can be solved to yield explicit form:  $y = f(\theta, t)$

Apply Trust Region method (GREG):

$$\begin{aligned} (k_1, k_2, k_3)^0 &= (6, 4, 1) \\ (k_1, k_2, k_3)^* &= (11.95, 7.99, 2.02) \\ (k_1, k_2, k_3)^{\text{true}} &= (12, 8, 2) \end{aligned}$$

Converges in 5 iterations (11 function calls)



# Rates of Convergence for Gauss-Newton Methods

Small Residuals at Solution (Good Model Fit):

$$e_u^* = 0, R_u^* = 0, \nabla_{\theta\theta}\Phi^* = \sum_{u=1}^n J_u^T W_u J_u$$

- Gauss-Newton method is quadratically convergent.
- Trust region will be inactive if Hessian is nonsingular
- L-M is also quadratically convergent for unique  $\theta^*$ .

Large Residuals at Solution (Poor Model Fit):

$$e_u^* \neq 0, R_u^* \neq 0, \nabla_{\theta\theta}\Phi^* = \sum_{u=1}^n J_u^T W_u J_u + R_u$$

- Gauss-Newton method is linearly convergent.
- Trust region may not be inactive if Hessian is nonsingular
- L-M is also linearly convergent for unique  $\theta^*$ .

# Hybrid Methods

## Quasi-Newton Methods

- DFP and BFGS Methods apply secant formula, symmetry and positive definiteness for Hessian
- Do not exploit structure of least squares problem

## Dennis, Gay and Welsh (1981) - NL2SOL

- Approximates  $\nabla_{\theta} \Phi^* = \sum_{u=1}^n J_u^T W_u J_u + R_u$  since  $\sum_{u=1}^n J_u^T W_u J_u$  is known
- Specialized, self-scaling Q-N method developed that approximates  $R_u$
- Incorporates Trust Region Approach of More'
- Leads to superlinear convergence

## Fletcher and Xu (1987)

- Applies specialized Q-N method to approximate  $R_u$
- Uses a switching rule to monitor if there are small or large residuals

$$\tau^k = (\Phi(\theta^k) - \Phi(\theta^{k+1})) / \Phi(\theta^k)$$

Large residuals:  $\lim_{k \rightarrow \infty} \tau^k = 0,$

Use specialized Q-N update if  $\tau^k \leq \varepsilon$

Small residuals:  $\lim_{k \rightarrow \infty} \tau^k = 1,$

Use specialized G-N formula if  $\tau^k > \varepsilon$

Choose  $\varepsilon \sim 0.1$

### III. Constrained Least Squares

#### Motivation:

- Model cannot be reformulated as  $y = f(\theta)$
- Too expensive to converge  $h_u(y_u, \theta) = 0$  for each parameter value

#### Basic Formulation:

$$\begin{aligned} \text{Min } \Phi(\theta, y, z) &= 1/2 \sum_{u=1}^n (z_u - y_u)^T W_u (z_u - y_u) \\ \text{s.t. } h_u(y_u, \theta) &= 0 \\ a &\leq \theta \leq b \end{aligned}$$

- Any NLP method can be used to solve this problem
- SQP can be tailored to take advantage of special form of  $\Phi$  allows for tailored algorithm.
- Leads to faster algorithm than standard SQP with BFGS updates

## Optimization Strategy: SQP method

Let  $\mathbf{x}^T = [\theta^T, \mathbf{y}^T]$  and consider QP subproblems for SQP:

$$\begin{aligned} \min_{\mathbf{d}} \quad & \nabla\Phi^T(\mathbf{x}^k)\mathbf{d} + 1/2 \mathbf{d}^T\mathbf{B} \mathbf{d} \\ \text{s.t.} \quad & \mathbf{h}(\mathbf{x}^k) + \nabla\mathbf{h}^T(\mathbf{x}^k)\mathbf{d} = 0 \\ & \mathbf{x}^L \leq \mathbf{x}^k + \mathbf{d} \leq \mathbf{x}^U \end{aligned}$$

The first order necessary conditions

$$\begin{bmatrix} \mathbf{B} & \nabla\mathbf{h} \\ \nabla\mathbf{h}^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{d} \\ \mathbf{v} \end{bmatrix} = - \begin{bmatrix} \nabla\Phi \\ \mathbf{h} \end{bmatrix}$$

### Problems:

- How to deal with a larger QP problems
- How to calculate the Hessian

### Strategies:

- Use Range and Null space Decomposition strategy to decompose the search direction into:
  - Null space movement
  - Range space movement
- Use a hybrid Gauss-Newton and BGFS update formula
- Analogy to unconstrained approaches

## Range and Null Space Decomposition

Define the linear system from the QP as  $M s = f$  to give:

$$\begin{bmatrix} B & \nabla h \\ \nabla h^T & 0 \end{bmatrix} \begin{bmatrix} d \\ v \end{bmatrix} = - \begin{bmatrix} \nabla \Phi \\ h \end{bmatrix}$$

$$x^T = [\theta^T, y^T], \quad \nabla h^T = [N \mid C]$$

and select an  $n \times n$  nonsingular matrix:

$$H = [Y \mid Z], \quad \text{where } \nabla h^T Z = 0.$$

- $Z$  and  $Y$  form null and range space bases for the linearized equality constraints.
- Search direction with range ( $p_Y$ ) and null space ( $p_Z$ ) components:  $d = Y p_Y + Z p_Z$ .

$$Y^T = [0 \mid I] \quad Z^T = [I \mid N^T C^{-T}]$$

Now defining  $X = \text{diag} [ [Y \mid Z], I ]$ , we can consider the equivalent system  $X^T M X z = X^T f$  (with  $X z = s$ ) as:

$$\begin{bmatrix} Y^T B Y & Y^T B Z & Y^T \nabla h \\ Z^T B Y & Z^T B Z & 0 \\ \nabla h^T Y & 0 & 0 \end{bmatrix} \begin{bmatrix} p_Y \\ p_Z \\ v \end{bmatrix} = - \begin{bmatrix} Y^T \nabla \Phi \\ Z^T \nabla \Phi \\ h \end{bmatrix}$$

Standard assumptions: set  $Y^T B Y = 0$  and  $Y^T B Z = 0$

## Structure of the Hessian

$$\mathbf{B}^k = \begin{bmatrix} \nabla_{\theta\theta}\mathbf{L} & \nabla_{\theta y}\mathbf{L} \\ \nabla_{y\theta}\mathbf{L} & \nabla_{yy}\mathbf{L} \end{bmatrix}$$

where

$$\mathbf{L}(\theta, y, \mathbf{v}) = \Phi(y) + \mathbf{v}^T \mathbf{h}(\theta, y)$$

$$\nabla_{\theta\theta}\mathbf{L} = \sum_{j=1}^m \mathbf{v}_j \nabla_{\theta\theta} \mathbf{h}_j \quad \nabla_{\theta y}\mathbf{L} = \sum_{j=1}^m \mathbf{v}_j \nabla_{\theta y} \mathbf{h}_j$$

$$\nabla_{y\theta}\mathbf{L} = \sum_{j=1}^m \mathbf{v}_j \nabla_{y\theta} \mathbf{h}_j \quad \nabla_{yy}\mathbf{L} = \nabla_{yy}\Phi + \sum_{j=1}^m \mathbf{v}_j \nabla_{yy} \mathbf{h}_j$$

The K-T multipliers (based on first order estimates) are given by:

$$\mathbf{v} = -\mathbf{C}^{-T}\mathbf{Y}^T\nabla\Phi = -\mathbf{C}^{-T}\mathbf{Y}^T\left[0 \mid \sum_{u=1}^n \mathbf{W}_u \mathbf{e}_u^T\right]^T$$

Assumption

If the residuals are *small*, then at convergence

$$\mathbf{e}_u \approx 0 \quad \Rightarrow \quad \mathbf{v} \approx 0$$

The Hessian becomes

$$\mathbf{B}^{\text{G-N}} = \begin{bmatrix} 0 & 0 \\ 0 & \text{diag}(\mathbf{W}_u) \end{bmatrix}$$

$\Rightarrow$  *Newton-like* rate of convergence

# Least Squares Hybrid SQP Method

Motivation: Combine best Hessian approximation for different types of problems

Strategies: Develop a switching rule to decide if Q-N or G-N approximation should be made for B. (Fletcher and Xu, 1987)

- Define merit function:

$$L^*(x^k) = \Phi(x^k) + v^T h(x^k) + 1/2 \gamma \|h(x^k)\|^2$$

- Uses a switching rule to monitor if there are small or large residuals

$$\tau^k = (L^*(x^k) - L^*(x^{k+1})) / L^*(x^k)$$

Large residuals:  $\lim_{k \rightarrow \infty} \tau^k = 0,$

Use specialized Q-N for  $Z^T B Z$  if  $\tau^k \leq \epsilon$

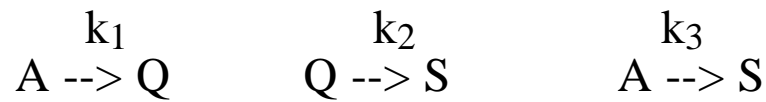
Small residuals:  $\lim_{k \rightarrow \infty} \tau^k = 1,$

Use  $Z^T B^{GN} Z, Z^T B^{GN} Y$  p<sub>Y</sub> formula if  $\tau^k > \epsilon$

Choose  $\epsilon \sim 0.2$

# 'Zero' Residual Example

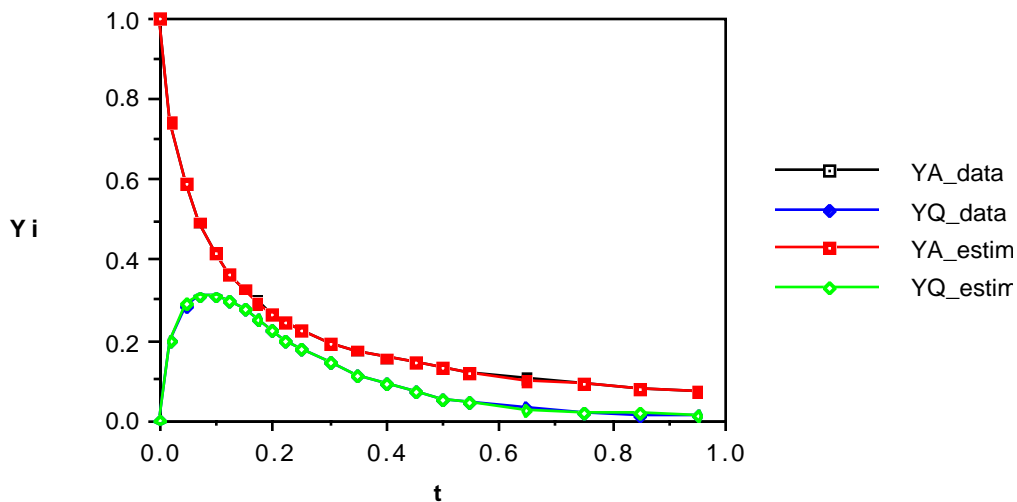
Catalytic Cracking of Gasoil (Tjoa, 1991)



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number of ODEs: 2  
 number of parameters: 3  
 discretized ODEs: 68 variables

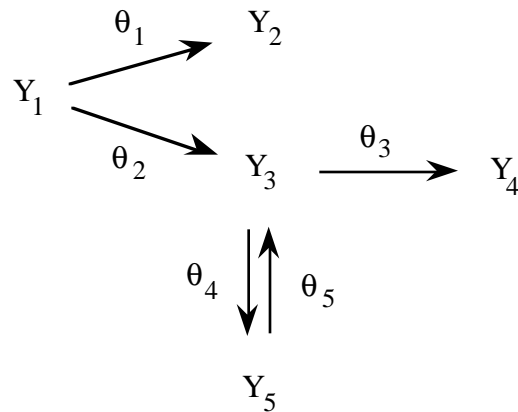
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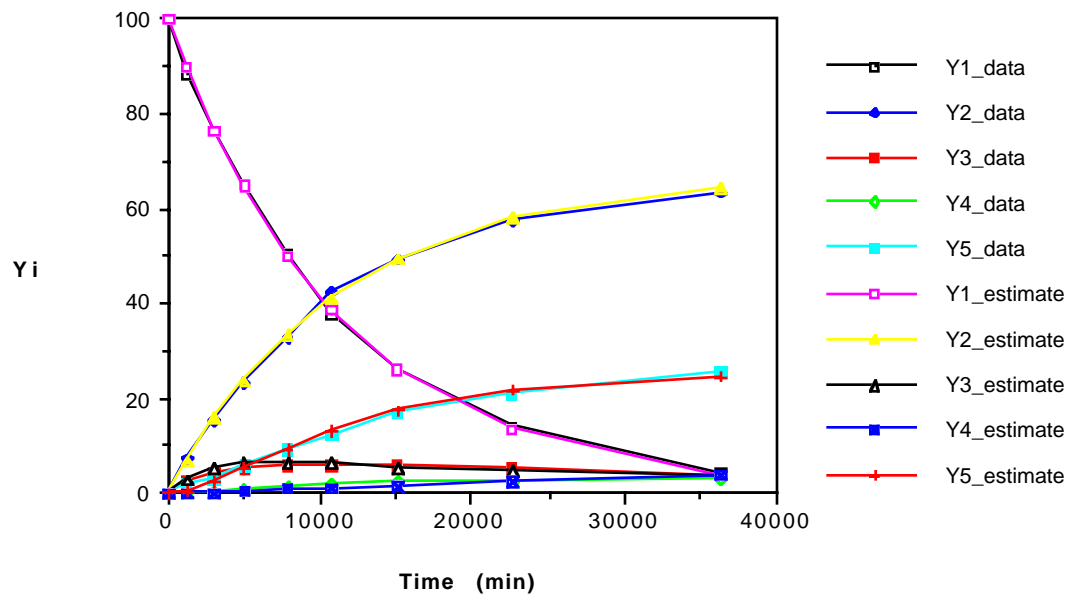
Method	Obj.	Iters.	CPU (s, Vax3200)
BFGS SQP	8.23e-5	10	4.31
Gauss-Newton	8.23e-5	4	2.25
Hybrid SQP	8.23e-5	4	2.31

# Small Residual Example

## $\alpha$ -Pinene Kinetics



number of ODEs: 5  
 number of parameters: 5  
 discretized ODEs: 245 variables



Method	Iterations.	CPU (s, Vax3200)
BFGS SQP	37	90.8
MINOS	21	64.8
Gauss-Newton	6	23.5
Hybrid SQP	6	23.6

# Further Results (Tjoa and Biegler,1990)

## Number of Iterations (Function Evaluations)

Problem	GREG	MINOS	SQP based methods		
			BFGS	GN	Hybrid
1	6 (12)	8 (41)	8 (10)	3 (3)	3 (3)
2	14 (34)	8 (72)	14 (17)	3 (3)	3 (3)
3	6 (12)	8 (55)	30 (31)	3 (3)	3 (3)
4	7 (20)	13 (95)	14 (15)	6 (6)	6 (6)
5	7 (19)	15 (236)	fail	13 (16)	13 (16)
6	5 (10)*	7 (72)	13 (21)	5 (5)	5 (5)
7	8 (16)	10 (150)	24 (30)	5 (5)	6 (6)
8	fail	21 (271)	37 (61)	6 (6)	6 (6)
9	26 (95)*	33 (320)	19 (24)	fail	18 (18)

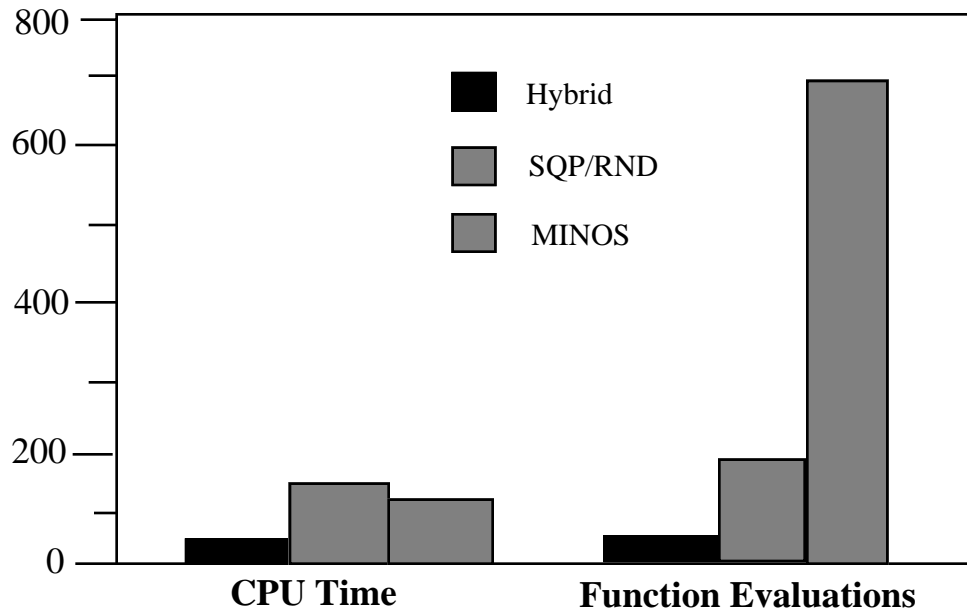
\*: using least squares objective function

## CPU Times (s, Vax 3200)

Problem	GREG	MINOS	SQP based methods		
			BFGS	GN	Hybrid
1	2.1	3.8	2.4	1.1	1.0
2	9.6	10.0	9.0	2.7	2.7
3	3.7	5.7	12.1	1.7	1.7
4	5.2	3.8	2.8	1.4	1.4
5	26.7	149.0	fail	50.8	51.1
6	3.5*	2.9	2.1	0.9	0.9
7	9.6	9.4	7.7	2.8	3.3
8	fail	64.8	90.8	23.5	23.6
9	0.9*	5.6	1.7	fail	1.6

\*: using least squares objective function

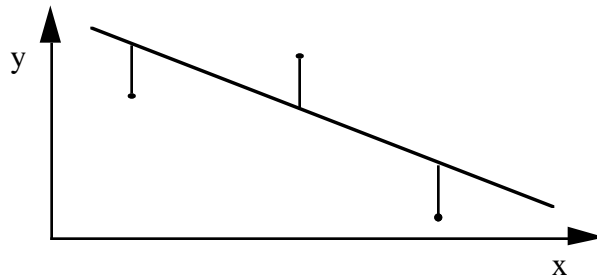
## Comparison of Hybrid vs. General Purpose NLP Codes (Tjoa)



- Summary on 10 parameter estimation (kinetics) problems
- Few parameters, degrees of freedom
- Hybrid method for Hessian structure: (Fletcher and Xu) quasi-Newton method.

## IV. Errors in Variables Models (EVM)

*Conventional model:*  $y = f(x, \theta)$  or  $h(x, y, \theta) = 0$



No. of independent variables ( $x$ ) =  $s_1$

No. of dependent variables ( $y$ ) =  $s_2$

No. of parameters ( $\theta$ ) =  $p$

No. of constraints =  $m$

No. of data sets =  $r$

$\Rightarrow$  *No error in the "independent" variables,  $x$*

Number of degrees of freedom for optimization =  $p$

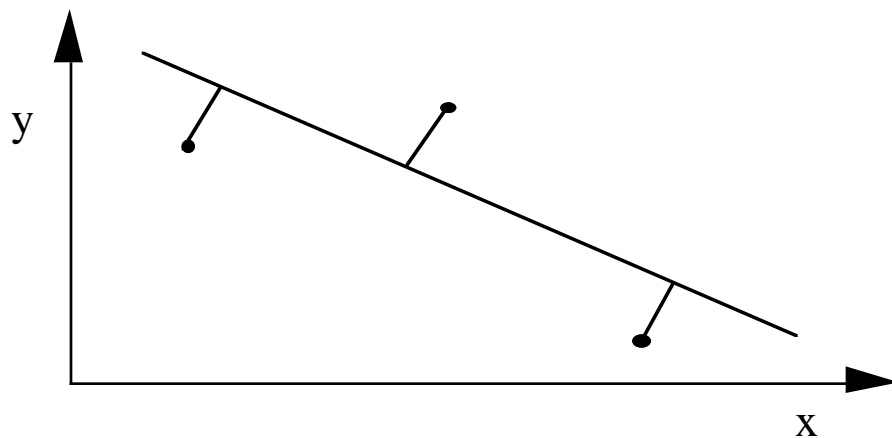
Minimize vertical distance, e.g.  $(y_u - z_u)^2$

*Implicit Model:*  $f(x,y,\theta) = 0$

Both  $x$  and  $y$  have inherent measurement errors

$\Rightarrow$  under-determined system

(e.g., pressure vs. temperature data)



Number of degrees of freedom for optimization

$$= p + (s-m)r$$

$\Rightarrow$  NLP size grows linearly with the number of data sets

Minimize a *nonvertical* distance

## Problem Statement

$$\min \Phi \equiv \sum_{u=1}^r \phi_u = \frac{1}{2} \sum_{u=1}^r \mathbf{e}_u^T \mathbf{W} \mathbf{e}_u$$

$$\text{s.t. } f_u(\mathbf{w}_u, \theta) = 0 \quad u = 1, 2, \dots, r$$
$$\theta^L \leq \theta \leq \theta^U$$

where  $\mathbf{w}_u \equiv \begin{bmatrix} x_\mu \\ y_\mu \end{bmatrix}$

$$\mathbf{e}_{\mu k} \equiv \mathbf{w}_{\mu k} - \mathbf{z}_{\mu k}$$

*Formulation:*

- Least squares nonlinear constraints with many degrees of freedom

*Current Approaches*

- Nonlinear Programming Strategies - Expensive
- Linearized Least Squares - Not robust

*Solution Strategy*

- Apply decoupling strategies to the optimality conditions of SQP method
- Overcomes disadvantages of current approaches

## Decoupling Strategies

*Introduce*

New variables:  $\zeta_u$

New constraints:  $g_u = \zeta_u - \theta = 0$ .

*Reformulated Problem:*

$$\min_w \Phi(w) \equiv \sum_{\mu=1}^r \phi_{\mu} = \frac{1}{2} \sum_{\mu=1}^r e_{\mu}^T W e_{\mu}$$

s.t.

$$\begin{aligned} h_u(w_u, \zeta_u, \theta) &= 0 \quad u = 1, 2, \dots, r \\ \theta^L &\leq \theta \leq \theta^U \end{aligned}$$

$$\text{where } h_{\mu} \equiv \begin{bmatrix} f_{\mu} \\ g_{\mu} \end{bmatrix}$$



## Further decompositions

For each data set

- For ordinary least squares and small residuals

$$\mathbf{B}_u = \begin{bmatrix} \mathbf{W}_u & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

(Gauss-Newton Hessian approximation)

- Apply Range and Null space Decomposition

- Define:

$$\mathbf{Z}_u^T \nabla \mathbf{h}_u = \mathbf{0} \quad \text{and} \quad \mathbf{Y}_u^T \mathbf{Z}_u = \mathbf{0}$$

$$\Delta \mathbf{d}_u = \mathbf{Z} \mathbf{p}_{y,u} + \mathbf{Y} \mathbf{p}_{y,u}$$

- Subspace search directions:

$$\text{Range space: } \mathbf{p}_{y,u} = \cdot \left( \nabla \mathbf{h}_u^T \mathbf{Y} \right)^{-1} \begin{bmatrix} \mathbf{f}_\mu \\ \cdot \Delta \theta \end{bmatrix}$$

$$\text{Null space: } \mathbf{p}_{z,u} = \cdot \left( \mathbf{Z}_\mu^T \mathbf{B}_\mu^{\text{G.N}} \mathbf{Z}_\mu \right)^{-1} \mathbf{Z}_\mu^T \nabla \phi_\mu$$

- $\mathbf{p}_{Y,u}$  is dependent on  $\Delta \theta$ ,  $\mathbf{p}_{Z,u}$  is not!

## Reconstructed QP Subproblem

⇒ Sum up the contribution from all of the data sets

At each iteration:

$$\min \left( \sum_{\mu=1}^r \alpha_{\mu} \right) \Delta\theta + \frac{1}{2} \Delta\theta^T \left( \sum_{\mu=1}^r \beta_{\mu} \right) \Delta\theta$$

$$\Delta\theta$$

$$\text{s.t.} \quad \Delta\theta L \leq \Delta\theta \leq \Delta\theta U$$

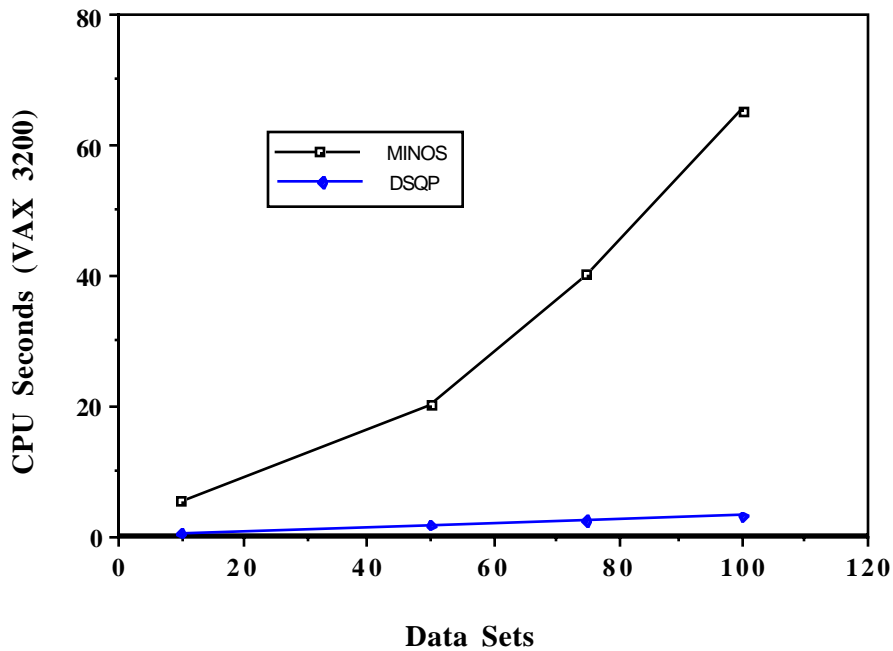
where

$\alpha_u$  and  $\beta_u$  --> only function of  $\nabla h_u$

⇒ Only in the space of actual parameters ( $\theta$ ).

# EVM Examples

<u>Example</u>	<u>Model</u>	<u>Data sets</u>	<u>Number of d.o.f</u>
1	$y = \theta_1 + \theta_2 x$	10	12
2	$y = \theta_1 + \theta_2 x + \theta_3 x^2 + \theta_4 x^3$	10	14
3	$\exp(-\theta_1 t \exp(-\theta_2/T)) - y = 0.$	15	32
4	$x_3 = \frac{\theta_1 \theta_2^2 \theta_3 x_1 x_2^2}{(1 + \theta_1 x_1 + \theta_2 x_2)^3}$	28	59
5, Case 1	$x_2 = \theta_1 + \frac{1}{x_1 - \theta_2}$	25	27
5, Case 2		50	52
5, Case 3		75	77
5, Case 4		100	102



## V. Statistical Inference of Estimated Parameters

### Covariance of Optimal Parameters

Given an error distribution for the data (assumed Gaussian with covariance,  $V_z$ ) how does this affect the accuracy of the estimated parameters?

Recall:

$$V_z = E(\delta z \delta z^T) \quad \text{and} \quad V_\theta = E(\delta \theta^* \delta \theta^{*T})$$

How does  $\theta$  change with data  $z$ ?

$$\frac{\partial \Phi(\theta^*, z)}{\partial \theta} = 0 \quad \frac{\partial \Phi(\theta^* + \delta \theta, z + \delta z)}{\partial \theta} = 0$$

Approximate by:

$$\frac{\partial^2 \Phi}{\partial \theta \partial z} \delta z + \frac{\partial^2 \Phi}{\partial \theta^2} \delta \theta^* = 0$$

and

$$\delta \theta^* = - \left( \frac{\partial^2 \Phi}{\partial \theta^2} \right)^{-1} \frac{\partial^2 \Phi}{\partial \theta \partial z} \delta z$$

$$V_\theta = E(\delta \theta^* \delta \theta^{*T}) = \left( \frac{\partial^2 \Phi}{\partial \theta^2} \right)^{-1} \left[ \frac{\partial^2 \Phi}{\partial \theta \partial z} \right] E(\delta z \delta z^T) \left[ \frac{\partial^2 \Phi}{\partial \theta \partial z} \right]^T \left( \frac{\partial^2 \Phi}{\partial \theta^2} \right)^{-T}$$

$$V_\theta = \left( \frac{\partial^2 \Phi}{\partial \theta^2} \right)^{-1} \left[ \frac{\partial^2 \Phi}{\partial \theta \partial z} \right] V_z \left[ \frac{\partial^2 \Phi}{\partial \theta \partial z} \right]^T \left( \frac{\partial^2 \Phi}{\partial \theta^2} \right)^{-T}$$

## Special Cases

1) If we use an objective where the measurements are independent in  $u$ :

$$\sum_{u=1}^n (z_u - f(x_u, \theta))^T V_z^{-1} (z_u - f(x_u, \theta))$$

Then we have: 
$$V_{\theta} = \sum_{u=1}^n (J_u^T V_z^{-1} J_u)^{-1}$$

2) If  $z_u$  is a scalar, then  $V_z$  is  $\sigma^2$  and  $V_{\theta}$  is given by:

$$V_{\theta} = \sigma^2 \sum_{u=1}^n \begin{pmatrix} \frac{\partial f_u}{\partial \theta} & \frac{\partial f_u^T}{\partial \theta} \end{pmatrix}^{-1}$$

3) If the covariance for  $z$  is unknown, it can be estimated from the moment matrix  $V_z = M(\theta)/n$  and then:

$$V_{\theta} = \sum_{u=1}^n (J_u^T V_z^{-1} J_u)^{-1}$$

4) For general likelihood functions:

$$V_{\theta} = -(\nabla_{\theta} \theta (\log L(\theta^*)))^{-1}$$

is asymptotically correct for  $n \rightarrow \infty$ .

# Elliptical Confidence Regions

For a given interval let

$$\gamma = \Pr( a \leq \theta^* \leq b ) = \int_a^b p(\theta^* | \theta_{\text{true}}) d\theta$$

and for a single parameter this becomes:

$$|\theta_{\text{true}} - \theta^*| \leq \zeta \sigma_{\theta}$$

where  $\zeta$  is the confidence level for  $\gamma$  with  $\sigma_{\theta}$  calculated

with  $n \rightarrow \infty$  and  $\sigma_{\theta}^2 = \sigma_z^2 \sum_{u=1}^n \left( \frac{\partial f_u}{\partial \theta} \quad \frac{\partial f_u^T}{\partial \theta} \right)^{-1}$

Otherwise, with a small sample size:  $|\theta_{\text{true}} - \theta^*| \leq t s_{\theta}$

$$s_z = \frac{\left[ \sum_{u=1}^n (z_u - f(x_u, \theta))^2 \right]^{1/2}}{n-1} \text{ and } s_{\theta}^2 = s_z^2 \sum_{u=1}^n \left( \frac{\partial f_u}{\partial \theta} \quad \frac{\partial f_u^T}{\partial \theta} \right)^{-1}$$

For multiple parameters, we map out a region  $S(\theta)$  so that

$$\gamma = \Pr(\theta_{\text{true}} \in S(\theta))$$

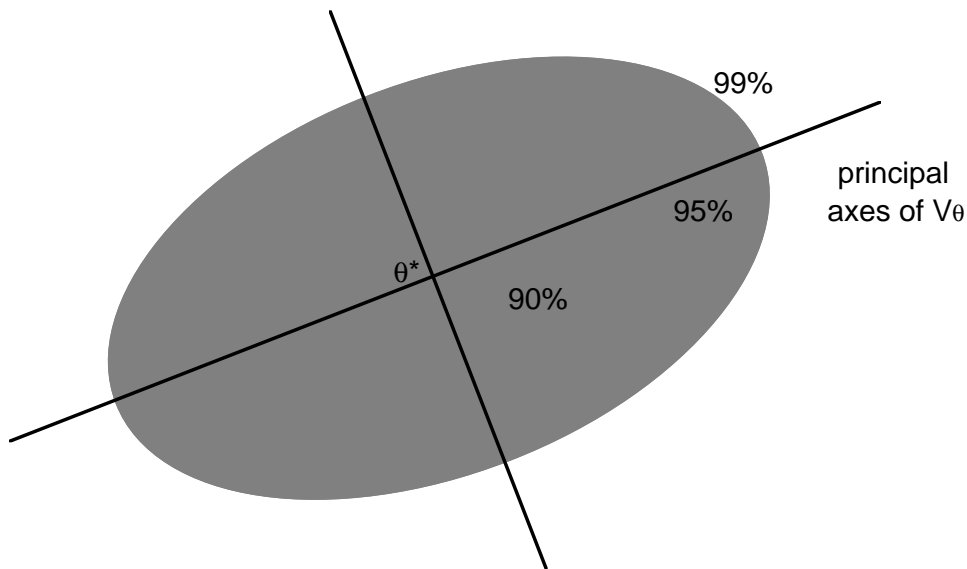
and this can be done using the principal directions of  $V_{\theta}$  which leads to:

$$\gamma = \Pr((\theta_{\text{true}} - \theta^*)^T V_{\theta}^{-1} (\theta_{\text{true}} - \theta^*))$$

For normal, unbiased distributions, linear models and a known  $V_{\theta}$ , this probability follows a  $\chi^2$  distribution so that the region can be defined by:

$$(\theta_{\text{true}} - \theta^*)^T V_{\theta}^{-1} (\theta_{\text{true}} - \theta^*) \leq c(\gamma)$$

$c(\gamma)$  is  $\chi^2$  value for  $\gamma$  level of confidence with  $n_{\theta}$  degrees of freedom.



Notes:

- For a scalar  $z$ , the  $\chi^2$  test simplifies to an F-test for determination of  $c(\gamma)$ .
- Elliptical confidence regions are correct if the model is linear or for small levels of confidence,  $\gamma$ . Otherwise, the confidence regions can deviate significantly from ellipses.
- Elliptical confidence regions are most commonly used. Other nonlinear confidence regions are rarely calculated.

## VI. References

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## Software

### Netlib

<http://www.netlib.org/toms/573>

NL2SOL by Dennis, Gay and Welsh

Given a p-vector  $x$  of parameters, `calcr` computes an n-vector  $r = r(x)$  of residuals corresponding to  $x$ . ( $r(x)$  probably arises from a nonlinear model involving  $p$  parameters and  $n$  observations.) this routine interacts with `nl2itr` to seek a parameter vector  $x$  that minimizes the sum of the squares of (the components of)  $r(x)$ , i.e., that minimizes the sum-of-squares function  $f(x) = (r(x)**t) * r(x) / 2$ .  $r(x)$  is assumed to be a twice continuously differentiable function of  $x$ .

<http://www.netlib.org/minpack/readme>

MINPACK by Jorge More', Burt Garbow, and Ken Hillstom

Minpack includes software for solving nonlinear equations and nonlinear least squares problems. Five algorithmic paths each include a core subroutine and an easy-to-use driver. The algorithms proceed either from an analytic specification of the Jacobian matrix or directly from the problem functions. The paths include facilities for systems of equations with a banded Jacobian matrix, for least squares problems with a large amount of data, and for checking the consistency of the Jacobian matrix with the functions.

<http://www.netlib.org/odrpack>

ODRPACK by Boggs et al. (1987)

Orthogonal distance regression for nonlinear least squares problems with many degrees of freedom due to errors in all variables.

*NAG Fortran Library*

E04YCF - Covariance matrix for nonlinear least-squares problem

G02GAF - Fits a generalized linear model with Normal errors

NAG FL90plus Library

E04YCF - Covariance matrix for nonlinear least-squares problem

G02GAF - Fits a generalized linear model with Normal errors

NAG Fortran Foundation Library

E04YCF - Covariance matrix for nonlinear least-squares problem

NAG Fortran Library, Mark 17

E04FCF - Unconstrained minimum of a sum of squares, combined Gauss-Newton and modified Newton algorithm using function values only (comprehensive)

E04FDF - Unconstrained minimum of a sum of squares, combined Gauss-Newton and modified Newton algorithm using function values only (easy-to-use)

E04UNF - Minimum of a sum of squares, nonlinear constraints, sequential QP method, using function values and optionally 1st derivatives

#### NAG FL90plus Library

E04FCF - Unconstrained minimum of a sum of squares, combined Gauss-Newton and modified Newton algorithm using function values only (comprehensive)

E04FDF - Unconstrained minimum of a sum of squares, combined Gauss-Newton and modified Newton algorithm using function values only (easy-to-use)

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#### NAG Fortran Foundation Library

E04FDF - Unconstrained minimum of a sum of squares, combined Gauss-Newton and modified Newton algorithm using function values only (easy-to-use)

## Summary

- Trust Region (Levenberg-Marquardt) methods are standard for unconstrained problem formulations - see MINPACK, NaG, NL2SOL, Harwell
- Constrained problem formulations allow for more flexibility with models.
- SQP codes can be adapted to exploit least squares structure, leads to faster methods
- EVM problems can be very expensive for convention parameter estimation codes
  - many degrees of freedom for optimization
  - decomposition of KKT conditions required
  - ODRPACK (netlib) developed for  $y = f(x, \theta)$
- Large-scale SQP methods developed for:
  - Parameter estimation
  - Data Reconciliation
  - EVM methods