Parameter Estimation

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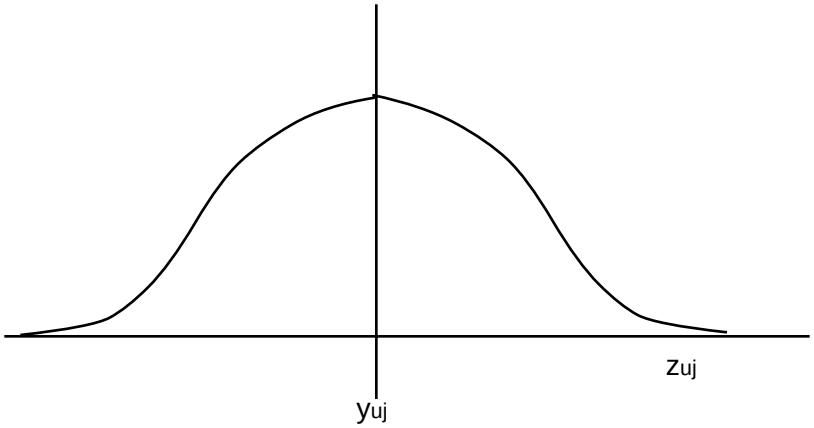
I. Motivation and Formulation

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^{th} component of data for u^{th} experiment

y_{uj} - corresponding (correct) model value

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

θ - adjustable parameters in model

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

Assume the following moment information:

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

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.

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

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

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 η_u, covariance V_u and experimental error distribution, ε_u

Then the joint probability distribution is given by:

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

and $p(\varepsilon_u)$ is:

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

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, ε_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, $V_u = E(\varepsilon_u \varepsilon_u^T)$
- 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:

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

and

$$\log L(\theta) = -nm/2 \log(2\pi) - n/2 \log(\det V)$$

$$- 1/2 \, Tr(V^{-1}M(\theta))$$

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

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., $V = v\, I$

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

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

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

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

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

What if V is not known?

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

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

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:

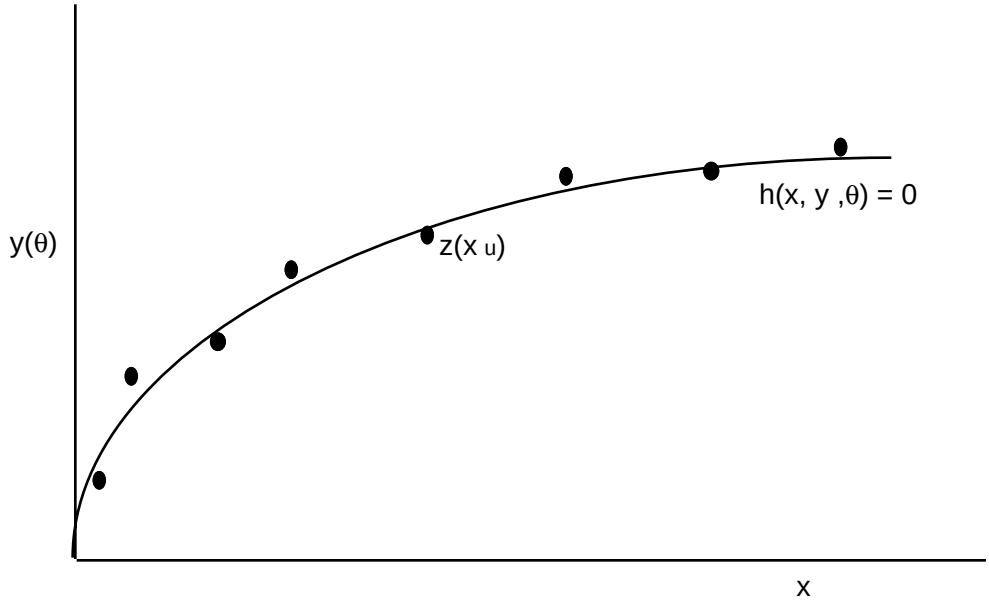
$$\log L(\theta) = -nm/2 \log(2\pi) + n/2 \log n - 1/2 \, m \, n$$
$$-n/2 \log(\det M(\theta))$$

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
$$V'' = n/(n-m \, n_\theta) \, V^*$$

II. Unconstrained Least Squares



Basic Problem:

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

$$\text{s.t. } h_u(x_u, y_u, \theta) = 0$$

$$a \le \theta \le b$$

- 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 θ,

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

and

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

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:

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

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

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

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 λ 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 λ be adjusted?

Trust region approach in MINPACK (More', 1980)

Choose $\Delta\theta$ and λ so that

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

is chosen by comparing τ = ared/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 λ.
- Evaluate actual reduction (ared) and predicted reduction (pred).
- Define τ = ared/pred

  a) If $\tau > \rho_1$, $\Delta = m_1\Delta$

  b) If $\tau < \rho_2$, $\Delta = \Delta / m_2$

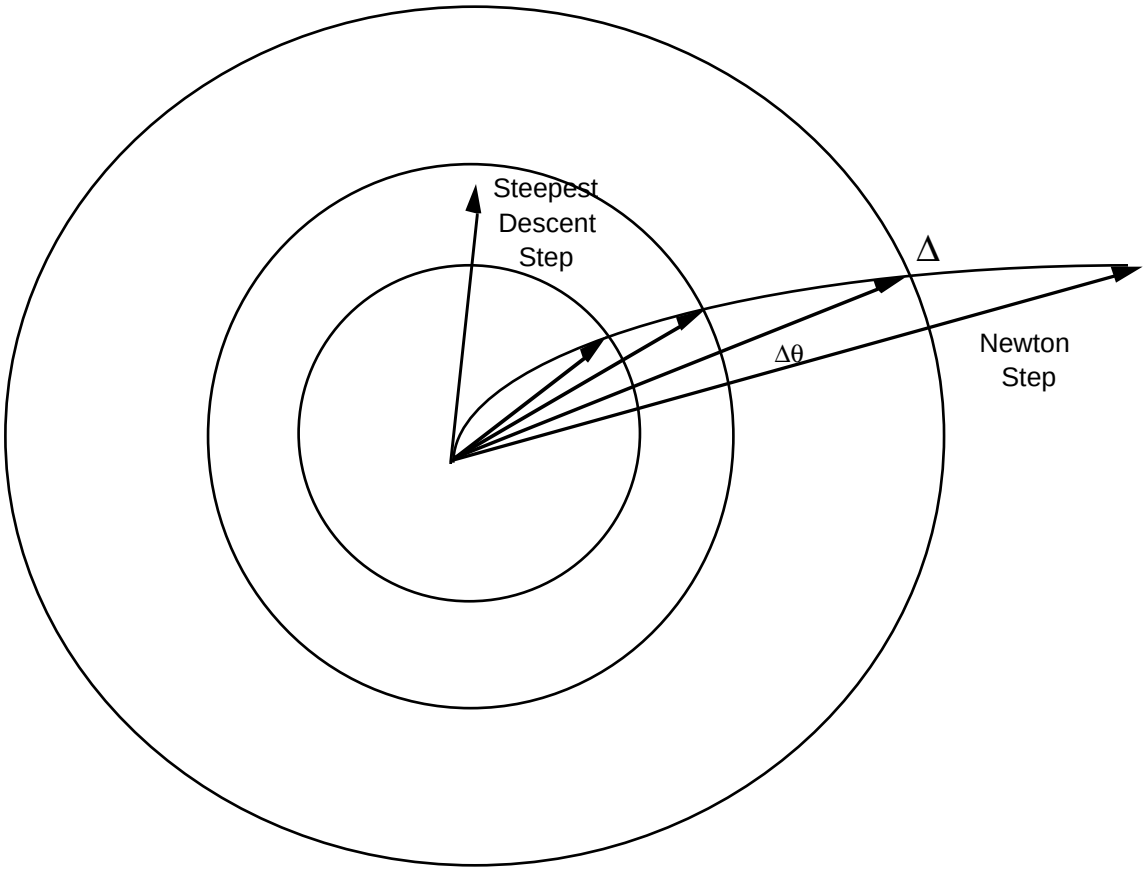
  c) If $\tau < \rho_3$ reset $\theta^{k+1} = \theta^k$

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

Typical values for the parameters:

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

Extremes of Trust Region Method:



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

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

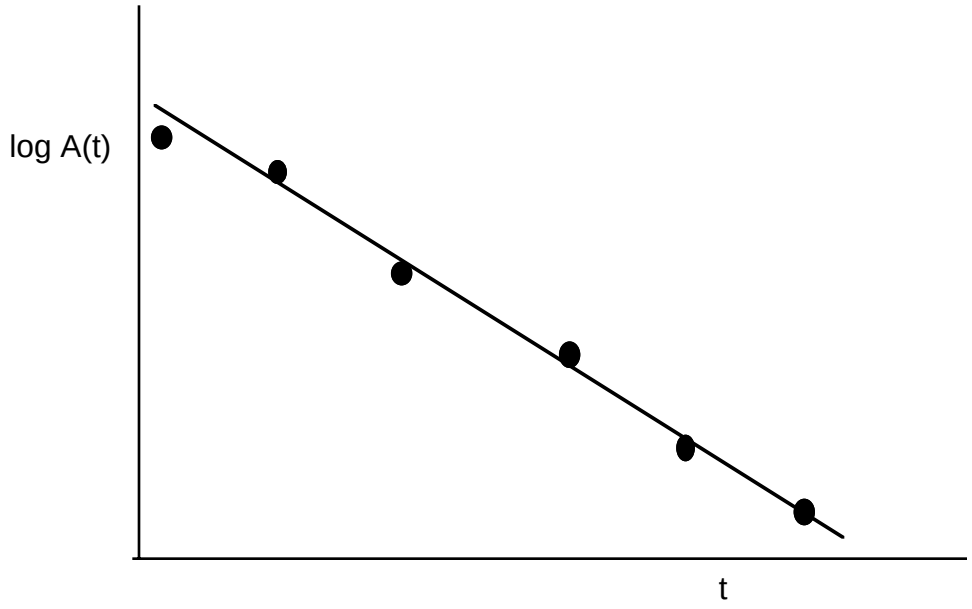
$\lambda \longrightarrow \infty$, $\Delta = 0$: $\Delta\theta$ is a small step in the steepest descent direction

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 --> 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)

$$A \xrightarrow{k_1} Q \qquad Q \xrightarrow{k_2} S \qquad A \xrightarrow{k_3} S$$

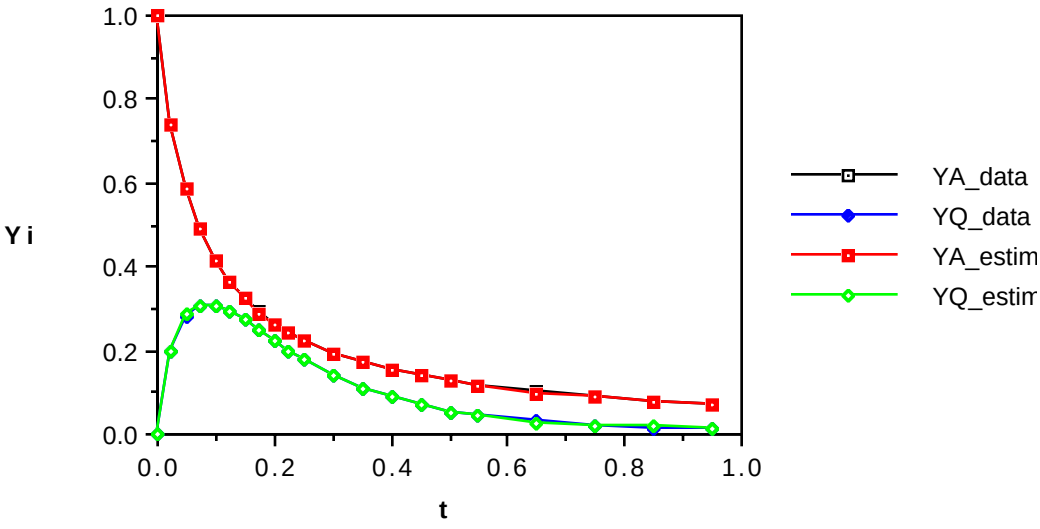
$$y_A' = -(k_1+k_3)\, y_A^2$$
$$y_Q' = -k_1 y_A^2 - k_2\, y_Q$$
$$y_A(0) = 1,\ y_Q(0) = 0$$

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

Apply Trust Region method (GREG):

$$(k_1, k_2, k_3)^0 = (6, 4, 1)$$
$$(k_1, k_2, k_3)^* = (11.95, 7.99, 2.02)$$
$$(k_1, k_2, k_3)^{true} = (12, 8, 2)$$

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 θ^*.

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 θ^*.

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 $\nabla_{\theta\theta}\Phi^* = \sum_{u=1}^{n} J_u^T W_u J_u + R_u$ 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: $\lim_{k\to\infty} \tau^k = 0$,

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

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

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:

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

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

Optimization Strategy: SQP method

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

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

The first order necessary conditions

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

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:

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

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

and select an n x n nonsingular matrix:

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

- 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: $d = Y p_Y + Z p_Z$.

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

Now defining X = diag [[Y | 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

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

where $L(\theta, y, v) = \Phi(y) + v^T h(\theta, y)$

$$\nabla_{\theta\theta} L = \sum_{j=1}^{m} v_j \nabla_{\theta\theta} h_j \qquad \nabla_{\theta y} L = \sum_{j=1}^{m} v_j \nabla_{\theta y} h_j$$

$$\nabla_{y\theta} L = \sum_{j=1}^{m} v_j \nabla_{y\theta} h_j \qquad \nabla_{yy} L = \nabla_{yy} \Phi + \sum_{j=1}^{m} v_j \nabla_{yy} h_j$$

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

$$v = - C^{-T} Y^T \nabla\Phi = - C^{-T} Y^T [\, 0 \mid \sum_{u=1}^{n} W_u e_u^T \,]^T$$

Assumption

If the residuals are *small*, then at convergence

$$e_u \approx 0 \quad \Rightarrow \quad v \approx 0$$

The Hessian becomes

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

$\Rightarrow$ *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: $\lim_{k\to\infty} \tau^k = 0$,

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

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

Use $Z^T B^{GN} Z$, $Z^T B^{GN} Y\ p_Y$ formula if $\tau^k > \varepsilon$

Choose $\varepsilon \sim 0.2$

'Zero' Residual Example

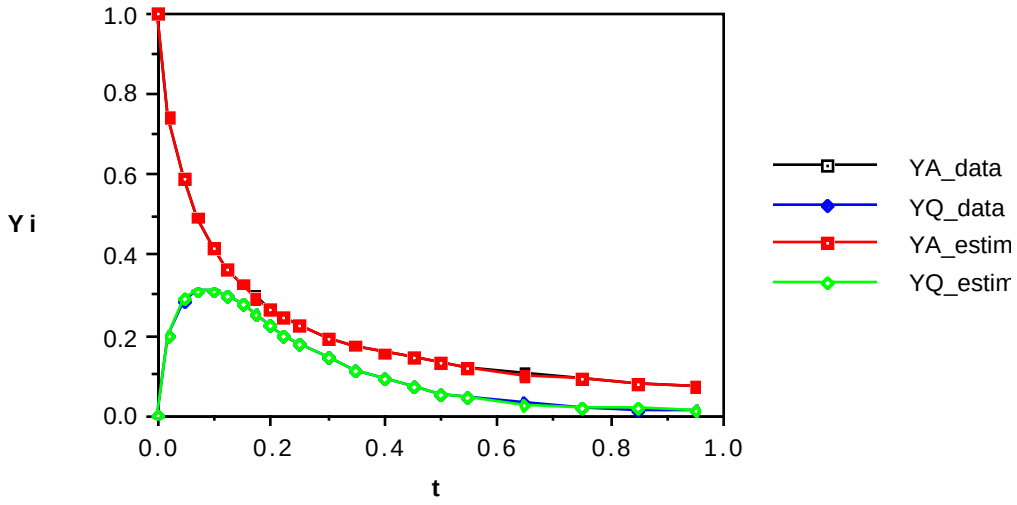
Catalytic Cracking of Gasoil (Tjoa, 1991)

$$A \xrightarrow{k_1} Q \qquad Q \xrightarrow{k_2} S \qquad A \xrightarrow{k_3} S$$

$$y_A' = -(k_1+k_3)\, y_A^2$$
$$y_Q' = -k_1 y_A^2 - k_2\, y_Q$$
$$y_A(0) = 1,\ y_Q(0) = 0$$

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

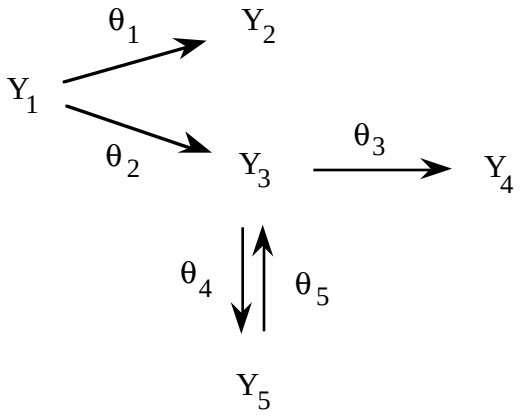
$$(k_1, k_2, k_3)^0 = (6, 4, 1)$$
$$(k_1, k_2, k_3)^* = (11.95, 7.99, 2.02)$$
$$(k_1, k_2, k_3)^{true} = (12, 8, 2)$$



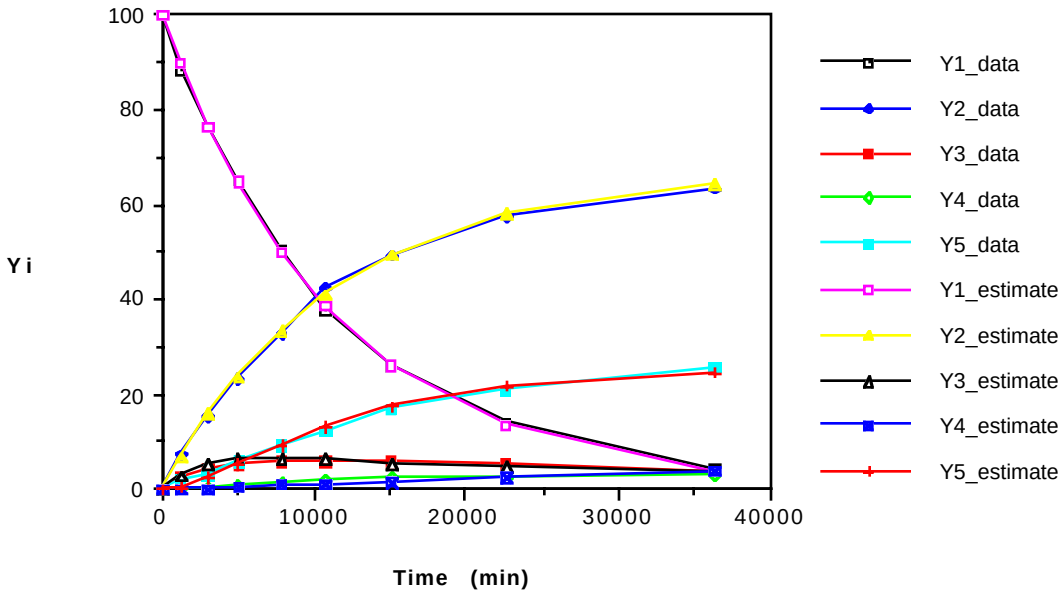
Method	Obj.	Iters.	CPU (s, Vax3200)
BFGS SQP	8.23e-5	10	4.31
Gauss-Newton	8.23e-5	4	2.25
Hybrid SQP	8.23e-5	4	2.31

Small Residual Example

α-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)

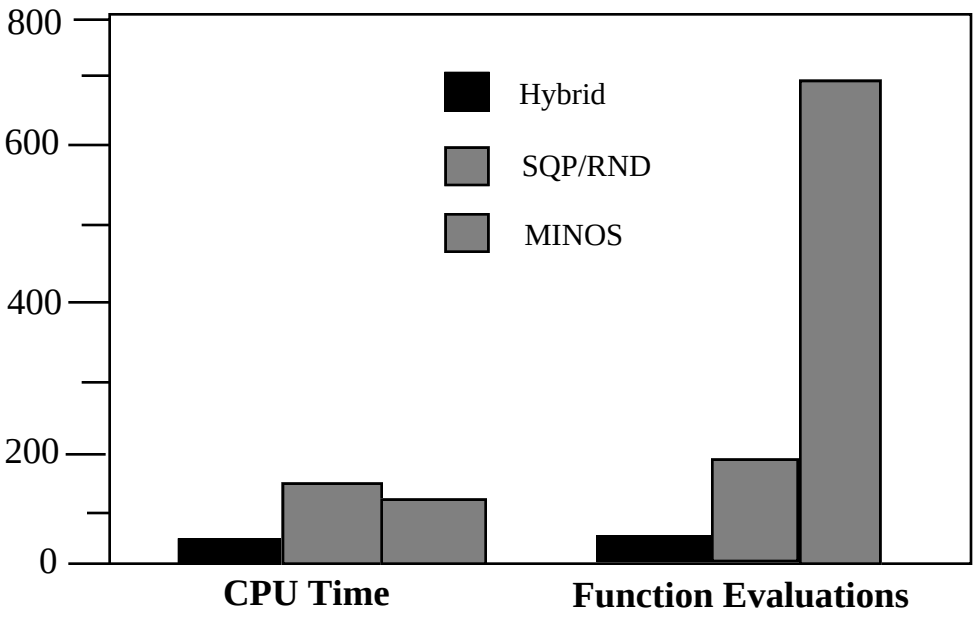
*: using least squares objective function

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

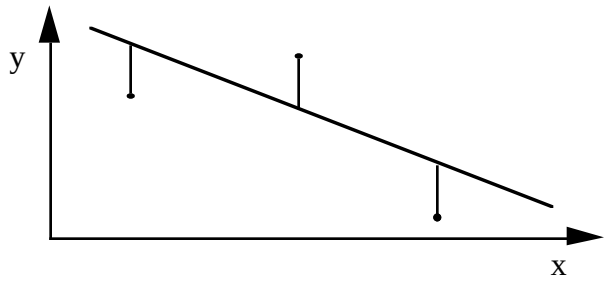
Comparison of Hybrid vs. General Purpose NLP Codes (Tjoa)



- 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 (θ) = 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

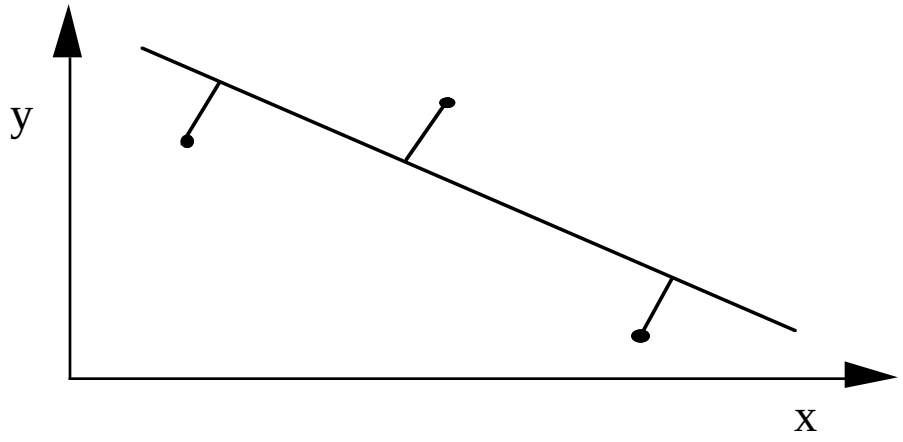
Minimize vertical distance, e.g. $(y_u - z_u)^2$

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

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

s.t. $f_u(w_u, \theta) = 0 \qquad u = 1,2, \ldots r$

$\theta^L \le \theta \le \theta^U$

where $w_u \equiv \begin{bmatrix} x_\mu \\ y_\mu \end{bmatrix}$

$e_{\mu k} \equiv w_{\mu k} - z_{\mu k}$

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: ζ_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.

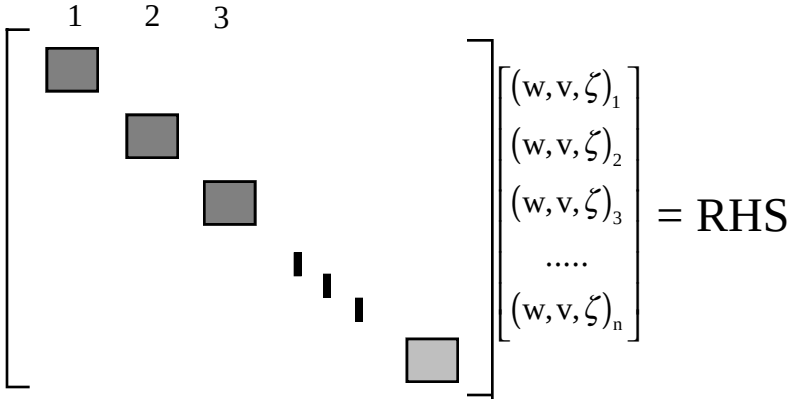
$$h_u(w_u, \zeta_u, \theta) = 0 \quad u = 1,2, \ldots r$$

$$\theta^L \le \theta \le \theta^U$$

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

KKT Conditions

Structure of the KKT matrix after decoupling:



The KKT conditions for each data set become:

$$\begin{bmatrix} B_u & \nabla h_u \\ \nabla h_u^T & 0 \end{bmatrix} \begin{bmatrix} \Delta d_u \\ v_u \end{bmatrix} = - \begin{bmatrix} \nabla \phi_u \\ h_u \end{bmatrix}$$

where

$$\nabla h_u = \begin{bmatrix} \nabla_w f_u & 0 \\ \nabla_\zeta f_u & I \end{bmatrix}, \Delta d_\mu = \begin{bmatrix} \Delta w_u \\ \Delta \zeta_u \end{bmatrix}, \; v_u = \begin{bmatrix} \lambda_u \\ \gamma_u \end{bmatrix}, \; h_u = \begin{bmatrix} f_\mu \\ -\Delta\theta \end{bmatrix}$$

- Can be solved independently for each data set, once θ is fixed.

Further decompositions

For each data set

- For ordinary least squares and small residuals

$$B_u = \begin{bmatrix} W_u & 0 \\ 0 & 0 \end{bmatrix}$$

  (Gauss-Newton Hessian approximation)

- Apply Range and Null space Decomposition
  - Define:

$$Z_u^T \nabla h_u = 0 \quad \text{and} \quad Y_u^T Z_u = 0$$

$$\Delta d_u = Z p_{y,u} + Y p_{y,u}$$

  - Subspace search directions:

Range space: $p_{y,u} = \cdot \left(\nabla h_u^T Y \right)^{-1} \begin{bmatrix} f_\mu \\ \cdot \Delta\theta \end{bmatrix}$

Null space: $p_{Z,u} = \cdot \left(Z_\mu^T B_\mu^{G \cdot N} Z_\mu \right)^{\cdot 1} Z_\mu^T \nabla \phi_\mu$

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

Reconstructed QP Subproblem

$\Rightarrow$ Sum up the contribution from all of the data sets

At each iteration:

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

$$\Delta\theta$$

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

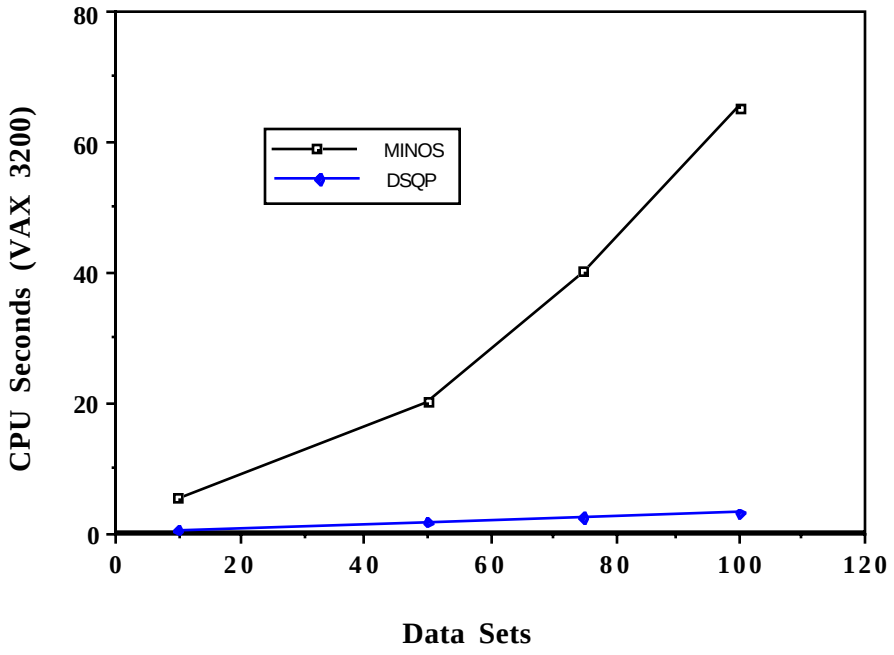
where

α_u and β_u --> only function of ∇h_u

$\Rightarrow$ Only in the space of actual parameters (θ).

EVM Examples

Example	Model	Number of Data sets	d.o.f
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:

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

How does θ change with data z?

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

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

2) If z_u is a scalar, then V_z is σ^2 and V_θ is given by:

$$V_\theta = \sigma^2 \sum_{u=1}^{n} \left(\frac{\partial f_u}{\partial \theta} \frac{\partial f_u^T}{\partial \theta}\right)^{-1}$$

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

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

4) For general likelihood functions:

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

is asymptotically correct for n --> ∞.

Elliptical Confidence Regions

For a given interval let

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

and for a single parameter this becomes:

$$|\theta_{true} - \theta^*| \le \zeta\, \sigma_\theta$$

where ζ is the confidence level for γ with σ_θ calculated with n --> ∞ and $\sigma_\theta^2 = \sigma_z^2 \sum_{u=1}^{n} \left(\frac{\partial f_u}{\partial \theta} \frac{\partial f_u^T}{\partial \theta} \right)^{-1}$

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

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

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

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

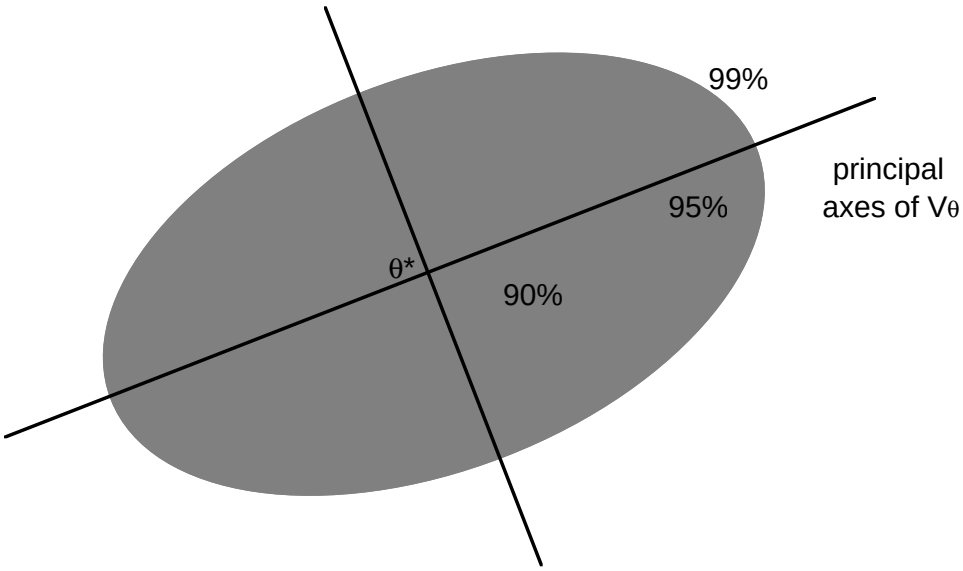
and this can be done using the principal directions of V_θ which leads to:

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

For normal, unbiased distributions, linear models and a known V_θ, this probability follows a χ^2 distribution so that the region can be defined by:

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

$c(\gamma)$ is χ^2 value for γ level of confidence with n_θ degrees of freedom.



Notes:

- For a scalar z, the χ^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, γ. 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 Hillstrom

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
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NAG Fortran Foundation Library

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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

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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