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Organised by:

Computational Mathematics Group of the Australian Mathematics Society
School of Mathematical and Physical Sciences, James Cook University

A conference on aspects of computational mathematics; scientific, technical, and industrial applications; and high performance computing

About the CTAC Meetings:

CTAC is organised by the special interest group in computational techniques and applications of ANZIAM, the Australian and New Zealand Industrial & Applied Mathematics Division of the Australian Mathematical Society. The meeting will provide an interactive forum for researchers interested in the development and use of computational methods applied to engineering, scientific and other problems.

The CTAC meetings have been taking place biennially since 1981, the most recent being held in 2004. CTAC'06 is the 13th meeting in the series and is the first to be held in tropical North Queensland.
CTAC'06 is hosted by the School of Mathematical and Physical Sciences, James Cook University.

Stability problems in ODE estimation

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Outline

Estimation

Given the ODE:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}\left(t, \mathbf{x}, \boldsymbol{\beta}\right),$$

where $\mathbf{x} \in R^m$, $\boldsymbol{\beta} \in R^p$, $\mathbf{f} \in R \times R^m \times R^p \to R^m$ smooth enough, together with data

$$\mathbf{y}_i = H\mathbf{x}(t_i, \boldsymbol{\beta}^*) + \boldsymbol{\varepsilon}_i, \quad i = 1, 2, \cdots, n,$$

where $H : R^m \to R^k$, $\boldsymbol{\varepsilon}_i \sim N\left(0, \sigma^2 I\right)$, estimate $\boldsymbol{\beta}$.

Equivalent smoothing problem: $\mathbf{x} \leftarrow \begin{bmatrix} \mathbf{x}(t) \\ \boldsymbol{\beta} \end{bmatrix}$, $\mathbf{f} \leftarrow \begin{bmatrix} \mathbf{f}(t, \mathbf{x}) \\ 0 \end{bmatrix}$.

Assume problem has a well determined solution for n, the number of observations, large enough.

The problem setting

Mesh selection for integrating the ODE system is conditioned by two important considerations:

- The asymptotic analysis of the effects of noisy data on the parameter estimates shows that this gets small no faster than $O\left(n^{-1/2}\right)$.
- It is not difficult to obtain ODE discretizations that give errors at most $O\left(n^{-2}\right)$.

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This suggests:

- That the trapezoidal rule provides an adequate integration method.
- That it should be possible even to integrate the ODE on a mesh coarser than that provided by the observation points $\{t_i\}$ (here we wont!).

The objective

Estimation principles (least squares, maximum likelihood) consider the objective:

$$F\left(\mathbf{x}_c,\beta\right)=\sum_{i=1}^{n}\left\|\mathbf{y}_i-H\mathbf{x}\left(t_i,\beta\right)\right\|^2.$$

Methods differ in manner of generating comparison function values $\mathbf{x}(t_i,\beta),\ i=1,2,\cdots,n$.

Embedding: $\mathbf{x}(t_i,\beta,\mathbf{b})$ satisfies BVP

$$\frac{d\mathbf{x}}{dt}=\mathbf{f}(t,\mathbf{x},\beta),\quad B_0\mathbf{x}(0)+B_1\mathbf{x}(1)=\mathbf{b}.$$

Introduces extra parameters $\mathbf{b}$. Needs method for choosing $B_0,\ B_1$. Must solve boundary value problem at each step. go GNM

The objective

Estimation principles (least squares, maximum likelihood) consider the objective:

$$F\left(\mathbf{x}_c, \beta\right) = \sum_{i=1}^{n} \left\| \mathbf{y}_i - H\mathbf{x}\left(t_i, \beta\right) \right\|^2 .$$

Methods differ in manner of generating comparison function values $\mathbf{x}(t_i, \beta),\ i = 1, 2, \cdots, n$.

Simultaneous: ODE discretization information added as constraints

$$\mathbf{c}_i(\mathbf{x}_c) = \mathbf{x}_{i+1} - \mathbf{x}_i - \frac{h}{2}\left(\mathbf{f}_{i+1} + \mathbf{f}_i\right), \quad i = 1, 2, \cdots, n-1,$$

with $\mathbf{x}_i = \mathbf{x}(t_i, \beta)$. Methods typically correct solution and parameter estimates simultaneously. go SQP

Initial value stability (IVS)

Here the problem considered is:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(t, \mathbf{x}), \quad \mathbf{x}(0) = \mathbf{b}.$$

The stability requirement is that solutions with close initial conditions $\mathbf{x}_1(0)$, $\mathbf{x}_2(0)$ remain close in an appropriate sense.

- $\|\mathbf{x}_1(t) - \mathbf{x}_2(t)\| \to 0, \; t \to \infty$. strong IVS.

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- $\|\mathbf{x}_1(t) - \mathbf{x}_2(t)\| \to 0,\ t \to \infty$. strong IVS.
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- $\|\mathbf{x}_1(t) - \mathbf{x}_2(t)\| \to 0, \ t \to \infty$. strong IVS.
- $\|\mathbf{x}_1(t) - \mathbf{x}_2(t)\|$ remains bounded as $t \to \infty$. weak IVS.
- Computation introduces idea of stiff discretizations which preserve the stability characteristics of the original equation. Computations not limited by IVS. Important for multiple shooting - permits reasonably accurate fundamental matrices to be computed over short enough time intervals in relatively unstable problems by taking h small enough.

Constant coefficient case

Here

$$\mathbf{f}(t, \mathbf{x}) = A\mathbf{x} - \mathbf{q}$$

If A is non-defective then weak IVS requires the eigenvalues $\lambda_i(A)$ to satisfy $Re\lambda_i \leq 0$ while this inequality must be strict for strong IVS.
A one-step discretization of the ODE (ignoring q contribution) can be written

$$\mathbf{x}_{i+1} = T_h(A)\,\mathbf{x}_i.$$

where $T_h(A)$ is the amplification matrix. Here a stiff discretization requires the stability inequalities to map into the condition $|\lambda_i(T_h)| \leq 1$.
For the trapezoidal rule

$$|\lambda_i(T_h)| = \left|\frac{1 + h\lambda_i(A)/2}{1 - h\lambda_i(A)/2}\right|,$$
$$\leq 1 \text{ if } Re\{\lambda_i(A)\} \leq 0.$$

Boundary value stability (BVS)

Here the problem is

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(t, \mathbf{x}), \quad B(\mathbf{x}) = B_0\mathbf{x}(0) + B_1\mathbf{x}(1) = \mathbf{b}.$$

Behaviour of perturbations about a solution trajectory $\mathbf{x}^*(t)$ is governed to first order by the linearized equation

$$L(\mathbf{z}) = \frac{d\mathbf{z}}{dt} - \nabla_x \mathbf{f}(t, \mathbf{x}^*(t))\,\mathbf{z} = 0.$$

Here (computational) stability is closely related to existence of a modest bound for the Green's matrix:

$$\begin{aligned} G(t,s) &= Z(t)\left[B_0 Z(0) + B_1 Z(1)\right]^{-1} B_0 Z(0) Z^{-1}(s), \quad t > s, \\ &= -Z(t)\left[B_0 Z(0) + B_1 Z(1)\right]^{-1} B_1 Z(1) Z^{-1}(s), \quad t < s. \end{aligned}$$

Where $Z(t)$ is a fundamental matrix for the linearised equation. Let α be a bound for $|G(t,s)|$.

Dichotomy

Weak form: $\exists$ projection P depending on choice of Z such that, given

$$S_1 \leftarrow \{ZP\mathbf{w},\ \mathbf{w} \in R^m\}, \quad S_2 \leftarrow \{Z(I-P)\mathbf{w},\ \mathbf{w} \in R^m\},$$

$$\phi \in S_1 \Rightarrow \frac{|\phi(t)|}{|\phi(s)|} \le \kappa, \quad t \ge s,$$
$$\phi \in S_2 \Rightarrow \frac{|\phi(t)|}{|\phi(s)|} \le \kappa, \quad t \le s.$$

Computational context requires modest κ for $t, s \in [0, 1]$. If Z satisfies $B_0 Z(0) + B_1 Z(1) = I$ then $P = B_0 Z(0)$ is a suitable projection in sense that for separated boundary conditions can take $\kappa = \alpha$. There is a basic equivalence between stability and dichotomy. Key paper is de Hoog and Mattheij.

BVS restricts possible discretizations

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- This requires solutions of ODE which are increasing (decreasing) in magnitude to be mapped into solutions of discretization which are increasing (decreasing) in magnitude.

This property called di-stability by England and Mattheij who show the TR is di-stable in constant coefficient case.

$$\lambda(A) > 0 \Rightarrow \left| \frac{1 + h\lambda(A)/2}{1 - h\lambda(A)/2} \right| > 1.$$

Bob Mattheij's example

Consider the differential system defined by

$$A(t) = \begin{bmatrix} 1 - 19\cos 2t & 0 & 1 + 19\sin 2t \\ 0 & 19 & 0 \\ -1 + 19\sin 2t & 0 & 1 + 19\cos 2t \end{bmatrix},$$

$$\mathbf{q}(t) = \begin{bmatrix} e^t\left(-1 + 19\left(\cos 2t - \sin 2t\right)\right) \\ -18e^t \\ e^t\left(1 - 19\left(\cos 2t + \sin 2t\right)\right) \end{bmatrix}.$$

Here the right hand side is chosen so that $\mathbf{z}(t) = e^t\mathbf{e}$ satisfies the differential equation. The fundamental matrix displays the fast and slow solutions:

$$Z(t,0) = \begin{bmatrix} e^{-18t}\cos t & 0 & e^{20t}\sin t \\ 0 & e^{19t} & 0 \\ -e^{-18t}\sin t & 0 & e^{20t}\cos t \end{bmatrix}.$$

go OBC

Bob Mattheij's example

For boundary data with two terminal conditions and one initial condition :

$$B_0 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \; B_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \; \mathbf{b} = \begin{bmatrix} e \\ e \\ 1 \end{bmatrix},$$

the trapezoidal rule discretization scheme gives the following results.

	$\Delta t = .1$			$\Delta t = .01$		
$\mathbf{x}(0)$	1.0000	.9999	.9999	1.0000	1.0000	1.0000
$\mathbf{x}(1)$	2.7183	2.7183	2.7183	2.7183	2.7183	2.7183

Table: Boundary point values - stable computation

These computations are apparently satisfactory.

Bob Mattheij's example

For two initial and one terminal condition:

$$B_0 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \; B_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \; \mathbf{b} = \begin{bmatrix} 1 \\ e \\ 1 \end{bmatrix}.$$

The results are given in following Table.

	$\Delta t = .1$			$\Delta t = .01$		
$\mathbf{x}(0)$	1.0000	.9999	1.0000	1.0000	1.0000	1.0000
$\mathbf{x}(1)$	-7.9+11	2.7183	-4.7+11	2.03+2	2.7183	1.31+2

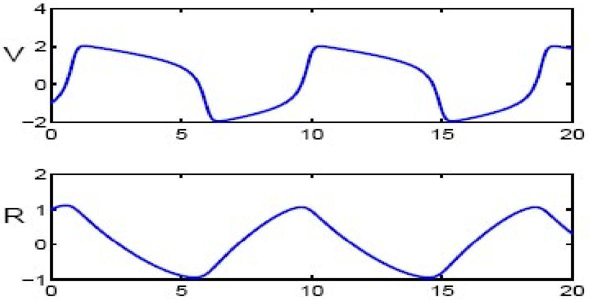
Table: Boundary point values - unstable computation

The effects of instability are seen clearly in the first and third solution components.

Nonlinear stability - preprint Hooker et al

FitzHugh-Nagumo equations $\alpha = .2$, $\beta = .2$.

$$\frac{dV}{dt} = \gamma\left(V - \frac{V^3}{3} + R\right),$$
$$\frac{dR}{dt} = -\frac{1}{\gamma}\left(V - \alpha - \beta R\right).$$



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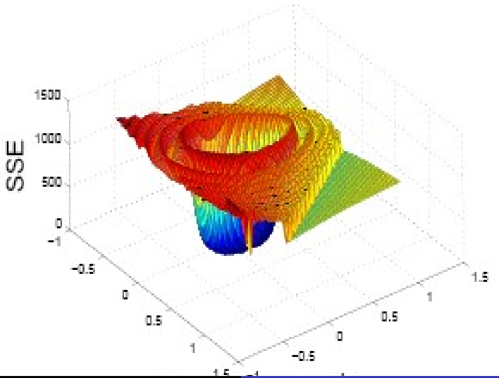

System factorization

go OPT1 First problem is to set suitable boundary conditions. Expect good boundary conditions should lead to a relatively well conditioned linear system. Assume the ODE discretization is

$$\mathbf{c}_i\left(\mathbf{x}_i, \mathbf{x}_{i+1}\right) = \mathbf{c}_{ii}(\mathbf{x}_i) + \mathbf{c}_{i(i+1)}(\mathbf{x}_{i+1}).$$

Consider the factorization of the difference equation (gradient) matrix with first column permuted to end:

$$\left[\begin{array}{cccc|c} C_{12} & & & & C_{11} \\ C_{21} & C_{22} & & & \\ & & & & \\ \hline & & C_{(n-1)(n-1)} & C_{(n-1)n} & 0 \end{array}\right] \rightarrow Q\left[\begin{array}{ccc|c} & U & & V \\ \hline 0 & \cdots & H & G \end{array}\right]$$

This step is independent of the boundary conditions. go SVE

Optimal boundary conditions

The boundary conditions can be inserted at this point. This gives the system with matrix $\begin{bmatrix} H & G \\ B_1 & B_0 \end{bmatrix}$ to solve for $\mathbf{x}_1$, $\mathbf{x}_n$. Orthogonal factorization again provides a useful strategy.

$$\begin{bmatrix} H & G \end{bmatrix} = \begin{bmatrix} L & 0 \end{bmatrix} \begin{bmatrix} S_1^T \\ S_2^T \end{bmatrix}$$

It follows that the system determining $\mathbf{x}_1$, $\mathbf{x}_n$ is best conditioned by choosing

$$\begin{bmatrix} B_1 & B_0 \end{bmatrix} = S_2^T.$$

The conditions depend only on the ODE.

BC's for Mattheij example

go MatEx The "optimal" boundary matrices corresponding to $h = .1$ are given in the Table. These confirm the importance of weighting the boundary data to reflect the stability requirements of a mix of fast and slow solutions. The solution does not differ from that obtained when the split into fast and slow was correctly anticipated.

B_1			B_2		
.99955	0.0000	.02126	-.01819	0.0000	-.01102
0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
.02126	0.0000	.00045	.85517	0.0000	.51791

Table: Optimal boundary matrices when $h = .1$

Gauss-Newton details

Let $\nabla_{(\beta,b)}\mathbf{x} = \left[\frac{\partial \mathbf{x}}{\partial \boldsymbol{\beta}}, \frac{\partial \mathbf{x}}{\partial \mathbf{b}}\right]$, $\mathbf{r}_i = \mathbf{y}_i - H\mathbf{x}(t_i, \boldsymbol{\beta}, \mathbf{b})$ then the gradient of F is

$$\nabla_{(\beta,b)}F = -2\sum_{i=1}^{n} \mathbf{r}_i^T H \nabla_{(\beta,b)}\mathbf{x}_i .$$

The gradient terms wrt $\boldsymbol{\beta}$ are found by solving the BVP's

$$B_0 \frac{\partial \mathbf{x}}{\partial \boldsymbol{\beta}}(0) + B_1 \frac{\partial \mathbf{x}}{\partial \boldsymbol{\beta}}(1) = 0,$$

$$\frac{d}{dt}\frac{\partial \mathbf{x}}{\partial \boldsymbol{\beta}} = \nabla_x \mathbf{f} \frac{\partial \mathbf{x}}{\partial \boldsymbol{\beta}} + \nabla_\beta \mathbf{f},$$

Gauss-Newton details

Let $\nabla_{(\beta,b)}\mathbf{x} = \left[\frac{\partial \mathbf{x}}{\partial \boldsymbol{\beta}}, \frac{\partial \mathbf{x}}{\partial \mathbf{b}}\right]$, $\mathbf{r}_i = \mathbf{y}_i - H\mathbf{x}(t_i, \boldsymbol{\beta}, \mathbf{b})$ then the gradient of F is

$$\nabla_{(\beta,b)}F = -2\sum_{i=1}^{n} \mathbf{r}_i^T H \nabla_{(\beta,b)}\mathbf{x}_i.$$

while the gradient terms wrt **b** satisfy the BVP's

$$B_0\frac{\partial \mathbf{x}}{\partial \mathbf{b}}(0) + B_1\frac{\partial \mathbf{x}}{\partial \mathbf{b}}(1) = I,$$

$$\frac{d}{dt}\frac{\partial \mathbf{x}}{\partial \mathbf{b}} = \nabla_x \mathbf{f}\frac{\partial \mathbf{x}}{\partial \mathbf{b}}.$$

Embedding: Again the Mattheij example

Consider the modification of the Mattheij problem with parameters $\beta_1^* = \gamma$, and $\beta_2^* = 2$ corresponding to the solution $\mathbf{x}(t, \boldsymbol{\beta}^*) = e^t \mathbf{e}$:

$$A(t) = \begin{bmatrix} 1 - \beta_1 \cos \beta_2 t & 0 & 1 + \beta_1 \sin \beta_2 t \\ 0 & \beta_1 & 0 \\ -1 + \beta_1 \sin \beta_2 t & 0 & 1 + \beta_1 \cos \beta_2 t \end{bmatrix},$$

$$\mathbf{q}(t) = \begin{bmatrix} e^t \left(-1 + \gamma \left(\cos 2t - \sin 2t\right)\right) \\ -(\gamma - 1)e^t \\ e^t \left(1 - \gamma \left(\cos 2t + \sin 2t\right)\right) \end{bmatrix}.$$

In the numerical experiments optimal boundary conditions are set at the first iteration. The aim is to recover estimates of $\boldsymbol{\beta}^*, \mathbf{b}^*$ from simulated data $e^{t_i} H\mathbf{e} + \varepsilon_i$, $\varepsilon_i \sim N(0, .01I)$ using Gauss-Newton, stopping when $\nabla F \mathbf{h} < 10^{-8}$.

Embedding: Again the Mattheij example

$$H = \begin{bmatrix} 1/3 & 1/3 & 1/3 \end{bmatrix} \qquad H = \begin{bmatrix} .5 & 0 & .5 \\ 0 & 1 & 0 \end{bmatrix}$$

$n = 51,\ \gamma = 10,\ \sigma = .1$
14 iterations
$n = 51,\ \gamma = 20,\ \sigma = .1$
11 iterations
$n = 251,\ \gamma = 10,\ \sigma = .1$
9 iterations
$n = 251,\ \gamma = 20,\ \sigma = .1$
8 iterations

$n = 51,\ \gamma = 10,\ \sigma = .1$
5 iterations
$n = 51,\ \gamma = 20,\ \sigma = .1$
9 iterations
$n = 251,\ \gamma = 10,\ \sigma = .1$
4 iterations
$n = 251,\ \gamma = 20,\ \sigma = .1$
5 iterations

Here $\| \begin{bmatrix} B_1 & B_2 \end{bmatrix}_1 \begin{bmatrix} B_1 & B_2 \end{bmatrix}_k^T - I \|_F < 10^{-3}$, $k > 1$.

Lagrangian

go OPT2 Associated with the equality constrained problem is the Lagrangian

$$\mathcal{L} = F(\mathbf{x}_c) + \sum_{i=1}^{n-1} \boldsymbol{\lambda}_i^T \mathbf{c}_i.$$

The necessary conditions give:

$$\nabla_{\mathbf{x}_i} \mathcal{L} = 0, \; i = 1, 2, \cdots, n, \quad \mathbf{c}(\mathbf{x}_c) = 0.$$

The Newton equations determining corrections $\mathbf{dx}_c, \mathbf{d}\boldsymbol{\lambda}_c$ are:

$$\begin{aligned} \nabla^2_{\mathbf{xx}} \mathcal{L} \mathbf{dx}_c + \nabla^2_{\mathbf{x}\boldsymbol{\lambda}} \mathcal{L} \mathbf{d}\boldsymbol{\lambda}_c &= -\nabla_{\mathbf{x}} \mathcal{L}^T, \\ \nabla_{\mathbf{x}} \mathbf{c}(\mathbf{x}_c) \mathbf{dx}_c = C \mathbf{dx}_c &= -\mathbf{c}(\mathbf{x}_c), \end{aligned}$$

Note sparsity! $\nabla^2_{\mathbf{xx}} \mathcal{L}$ is block diagonal, $\nabla^2_{\mathbf{x}\boldsymbol{\lambda}} \mathcal{L} = C^T$ is block bidiagonal.

SQP formulation

The Newton equations also correspond to necessary conditions for the QP:

$$\min_{\mathbf{dx}} \nabla_{\mathbf{x}} F \mathbf{dx}_c + \frac{1}{2}\mathbf{dx}_c^T M \mathbf{dx}_c; \quad \mathbf{c} + C\mathbf{dx}_c = 0,$$

in case $M = \nabla^2_{\mathbf{xx}}\mathcal{L}$, $\boldsymbol{\lambda}^u = \boldsymbol{\lambda}_c + \mathbf{d}\boldsymbol{\lambda}_c$. A standard approach is to use the constraint equations to eliminate variables. go GNM

$$\mathbf{dx}_i = \mathbf{v}_i + V_i \mathbf{dx}_1 + W_i \mathbf{dx}_n, \quad i = 2, 3, \cdots, n-1.$$

The reduced constraint equation is

$$G\mathbf{dx}_1 + H\mathbf{dx}_n = \mathbf{w}.$$

Is this variable elimination restricted by BVS considerations?

Null space method

Standard SQP approach. Let $C^T = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} U \\ 0 \end{bmatrix}$ then Newton equations can be written

$$\begin{bmatrix} Q^T \nabla^2_{\mathbf{xx}} \mathcal{L} Q & \begin{bmatrix} U \\ 0 \end{bmatrix} \\ \begin{bmatrix} U^T & 0 \end{bmatrix} & 0 \end{bmatrix} \begin{bmatrix} Q^T \mathbf{dx}_c \\ \lambda^u \end{bmatrix} = - \begin{bmatrix} Q^T \nabla_{\mathbf{x}} F^T \\ \mathbf{c} \end{bmatrix}.$$

These can be solved in sequence

$$\begin{aligned} U^T Q_1^T \mathbf{dx}_c &= -\mathbf{c}, \\ Q_2^T \nabla^2_{\mathbf{xx}} \mathcal{L} Q_2 Q_2^T \mathbf{dx}_c &= -Q_2^T \nabla^2_{\mathbf{xx}} \mathcal{L} Q_1 Q_1^T \mathbf{dx}_c - Q_2^T \nabla_{\mathbf{x}} F^T, \\ U \lambda^u &= -Q_1^T \nabla^2_{\mathbf{xx}} \mathcal{L} \mathbf{dx}_c - Q_1^T \nabla_{\mathbf{x}} F^T. \end{aligned}$$

Stability test using Mattheij problem

$Q_1^T \mathbf{dx}_c$ estimates $Q_1^T \text{vec}\left\{e^{t_i}\right\}$ when $\mathbf{x}_c = 0$.

test results $n = 11$

.87665	-.97130	-1.0001
.74089	-1.0987	-1.3432
.47327	-1.2149	-1.6230
.11498	-1.3427	-1.8611
-.32987	-1.4839	-2.0366
-.85368	-1.6400	-2.1250
-1.4428	-1.8125	-2.1018
-2.0773	-2.0031	-1.9444
-2.7309	-2.2137	-1.6330
-3.3719	-2.4466	-1.1526

particular integral $Q_1^T x$

.87660	-.97134	-1.0001
.74083	-1.0988	-1.3432
.47321	-1.2150	-1.6231
.11491	-1.3428	-1.8612
-.32994	-1.4840	-2.0367
-.85376	-1.6401	-2.1250
-1.4429	-1.8125	-2.1019
-2.0774	-2.0032	-1.9444
-2.7310	-2.2138	-1.6331
-3.3720	-2.4467	-1.1527

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- The variable eliminations form of the simultaneous method partitions variables into sets $\{\mathbf{x}_1, \ \mathbf{x}_n\}$, and $\{\mathbf{x}_2, \cdots, \mathbf{x}_{n-1}\}$ which are found sequentially. It relies implicitly on a form of BVS although the system is special.

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- The variable eliminations form of the simultaneous method partitions variables into sets $\{\mathbf{x}_1, \ \mathbf{x}_n\}$, and $\{\mathbf{x}_2, \cdots, \mathbf{x}_{n-1}\}$ which are found sequentially. It relies implicitly on a form of BVS although the system is special.
- The null space variant partitions the variables into the sets $\{Q_1^T \mathbf{x}_c\}$, $\{Q_2^T \mathbf{x}_c\}$. It appears at least as stable as the variable elimination procedure. Sparsity preserving implementation is straightforward.