Reducing Uncertainty when Approximating Solutions of ODEs [a]

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The Focus of this Talk

Tools for Reducing Uncertainty when Investigating Mathematical Models described by Systems of ODEs

- “Investigating” – not only “Approximating the Solution”.
  1. Sensitivity Analysis - (of solution wrt parameters defining the problem)
  2. Global Error Estimation
  3. Estimating the "Conditioning" of a problem
- “ODEs” includes IVPs, BVPs, DDEs, DAEs and VIDEs.

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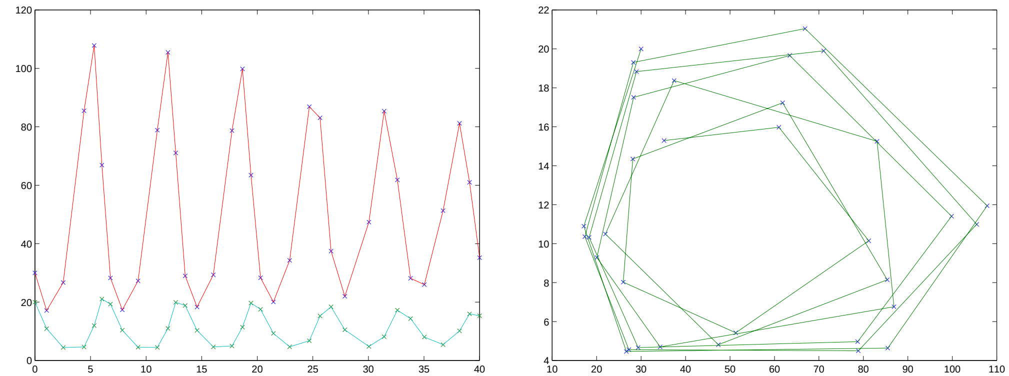
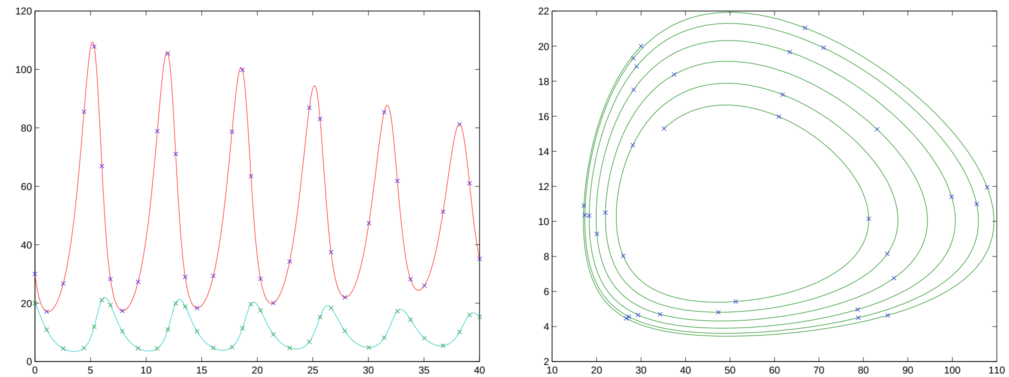
An Effective ODE Solver

Minimum Requirements:

- An Accurate Discrete Approximation is not Enough



- An Accurate Continuous Extension is Necessary (aka Dense Output)



Outline of Talk

- Current Scientific Computing Paradigm and its implications:
  - Acceptability of an approximate solution
- Continuous RK Methods provide dense output for ODEs
- Defect Error Control for CRK Methods
- Measuring or quantifying the Reliability of a CRK Method
- Classes of ODE problems that can be Investigated by CRK-based Methods (IVPs, BVPs, DDEs, DAEs, and VIDEs)
- Useful Software Tools for Investigating and quantifying Important Properties of the Mathematical Model and its Approximate Solution. (sensitivity analysis, global error estimation, parameter fitting and condition number estimation.)
- Some Numerical Examples
- What is Next?

Scientific Computing Paradigm

Mathematical Modelling in a Problem Solving Environment:

- Formulate the mathematical model of the system being investigated. (The model may involve parameters.)
- Approximate the exact solution of this model relative to a specified accuracy parameter, TOL.
- Visualize the <u>approximate</u> solution.
- Is the mathematical model well-posed and is the approximate solution stable? (may involve sensitivity analysis).

Implications for ODE Methods

What is an acceptable approximate solution?

- An approximate solution must be easy to represent, display and manipulate.
- The accuracy (or *quality*) of an approximate solution must be easy to measure and interpret.

What are the implications for an ODE method?

- Solver must be easy to invoke –(only need specify those parameters necessary to define the problem).
- A discrete solution is not sufficient (as it is difficult to visualize and its accuracy is difficult to interpret).
- It should have a generic calling sequence so it is easy to adopt in a PSE.

Continuous Runge-Kutta Methods

- Consider an IVP defined by the system

$$y' = f(x, y), \;\; y(a) = y_0, \;\; \text{on} \;\; [a, b].$$

- A numerical method will introduce a partitioning $a = x_0 < x_1 < \cdots < x_N = b$ and corresponding discrete approximations $y_0, y_1 \cdots y_N$. The y_i's are usually determined sequentially.

- On step i let $z_i(x)$ be the solution of the local IVP:

$$z_i' = f(x, z_i(x)), \;\; z_i(x_{i-1}) = y_{i-1}, \;\; \text{on} \;\; [x_{i-1}, x_i].$$

CRK methods (cont)

A classical p^{th}-order, s-stage, discrete RK formula determines

$$y_i = y_{i-1} + h_i \sum_{j=1}^{s} \omega_j k_j,$$

where $h_i = x_i - x_{i-1}$ and the j^{th} stage is defined by,

$$k_j = f(x_{i-1} + h_i c_j,\ y_{i-1} + h_i \sum_{r=1}^{s} a_{jr} k_r).$$

A Continuous extension (CRK) is determined by introducing $(\tilde{s} - s)$ additional stages to obtain an order p approximation for any $x \in (x_{i-1}, x_i)$

$$u_i(x) = y_{i-1} + h_i \sum_{j=1}^{\tilde{s}} b_j(\frac{x - x_{i-1}}{h_i}) k_j,$$

where $b_j(\tau)$ is a polynomial of degree at least p and $\tau = \frac{x - x_{i-1}}{h_i}$.

CRK methods (cont)

- We consider $O(h^p)$ extensions, satisfying:

$$u_i(x) = y_{i-1} + h_i \sum_{j=1}^{\tilde{s}} b_j(\tau) k_j = z_i(x) + O(h_i^{p+1}).$$

- The $[u_i(x)]_{i=1}^{N}$ define a piecewise polynomial $U(x)$ for $x \in [x_0, x_F]$. This is the approximate solution generated by the CRK method.
- $U(x) \in C^0[x_0, x_F]$ and will interpolate the underlying discrete RK values, y_i, if $b_j(1) = \omega_j$ for $j = 1, 2 \cdots s$ and $b_{s+1}(1) = b_{s+2}(1) = \cdots b_{\tilde{s}}(1) = 0$.
- Similarly a simple set of constraints on the $\frac{d}{d\,\tau}(b_j(\tau))$, and requiring that $k_{s+1} = f(x_i, y_i), k_1 = f(x_{i-1}, y_{i-1})$, will ensure $U'(x)$ interpolates $f(x_i, y_i), f(x_{i-1}, y_{i-1})$ and therefore $U(x) \in C^1[x_0, x_F]$.

Defect Error Control for CRKs

$U(x)$, the approximate solution, has an associated defect or residual,

$$\delta(x) \equiv f(x, U(x)) - U'(x) \equiv f(x, u_i(x)) - u_i'(x), \quad \text{for} \quad x \in [x_{i-1}, x_i].$$

It can be shown that, for sufficiently differentiable f,

$$\delta(x) = G(\tau) h_i^p + O(h_i^{p+1}),$$

$$G(\tau) = \tilde{q}_1(\tau) F_1 + \tilde{q}_2(\tau) F_2 + \cdots + \tilde{q}_k(\tau) F_k,$$

where the $\tilde{q}_j$ are polynomials in τ that depend only on the CRK formula while the F_j are constants (elementary differentials) that depend only on the problem.

Methods can be implemented to adjust h_i in an attempt to ensure that the maximum magnitude of $\delta(x)$ is bounded by TOL. The quality of an approximate solution can then be described in terms of the max of $||\delta(x)||/TOL$.

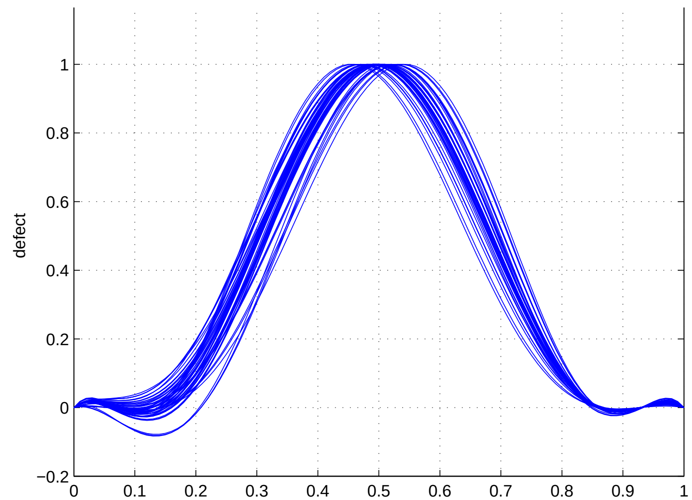
Defect Error Control (cont)

$$\delta(x) = G(\tau)h_i^p + O(h_i^{p+1}),$$

$$G(\tau) = \tilde{q}_1(\tau)F_1 + \tilde{q}_2(\tau)F_2 + \cdots + \tilde{q}_k(\tau)F_k.$$

- As $h_i \to 0$ the defect will then look like a linear combination of the known polynomials $\tilde{q}_j(\tau)$ over $[x_{i-1}, x_i]$.
- In the special case where $k = 1$ the shape of the defect will be the same (as $h_i \to 0$) for all problems and all steps. That is, the defect will almost always 'converge' to a multiple of $\tilde{q}_1(\tau)$, in which case the maximum should occur (as $h_i \to 0$) at $\tau = \tau^*$ where τ^* is the location of the local extremum of $\tilde{q}_1(\tau)$. In this case we will refer to the defect control strategy as **Strict Defect Control (SDC)**.

Typical Shape of SDC Defects



Plot of scaled defect vs τ (ie. $\delta(\tau)/\delta(\tau^*)$ vs τ) for each step required to solve a typical problem with SDC CRK6 and $TOL = 10^{-6}$.

Cost of Strict Defect Control

$$p^{th} - \text{order, explicit, discrete RK} : y_i = y_{i-1} + h_i \sum_{j=1}^{s} \omega_j k_j,$$

$$SDC: \quad \tilde{u}_i(x) = y_{i-1} + h_i \sum_{j=1}^{\tilde{s}} \tilde{b}_j(\tau) k_j = z_i(x) + O(h_i^{p+1}).$$

Formula	p	s	$\tilde{s}$
CRK4	4	4	8
CRK5	5	6	12
CRK6	6	7	15
CRK7	7	9	20
CRK8	8	13	27

Table 1: Cost per step of some SDC-CRK formulas
(Note that $\tilde{s} \approx 2\ s$.)

Strict Defect Control

SDC CRKs are not unique (for a given discrete RK formula).
Each SDC-CRK satisfies,

$$\delta(x) = \tilde{q}_1(\tau) F_1 h_i^p \; + \; (\hat{q}_1(\tau)\hat{F}_1 + \hat{q}_2(\tau)\hat{F}_2 + \cdots\cdots \hat{q}_{\hat{k}}(\tau)\hat{F}_{\hat{k}}) h_i^{p+1} + O(h_i^{p+2})$$

Potential Difficulties:

- $\tilde{q}_1(\tau)$ may have a large maximum ($\tilde{q}_1(0) = \tilde{q}_1(1) = 0$ and its 'average' value must be one).
- The $\hat{q}_j(\tau)$ may be large in magnitude relative to $\tilde{q}_1(\tau)$ (and therefore h_i would have to be small before the estimate is justified). (That is, before $|h_i \hat{q}_j(\tau)| << |\tilde{q}_1(\tau)|$.)
- $|F_1|$ may be zero (or very small) on isolated steps.

For each p we have identified a particular SDC-CRK that minimizes these difficulties.

Optimal SDC CRK6

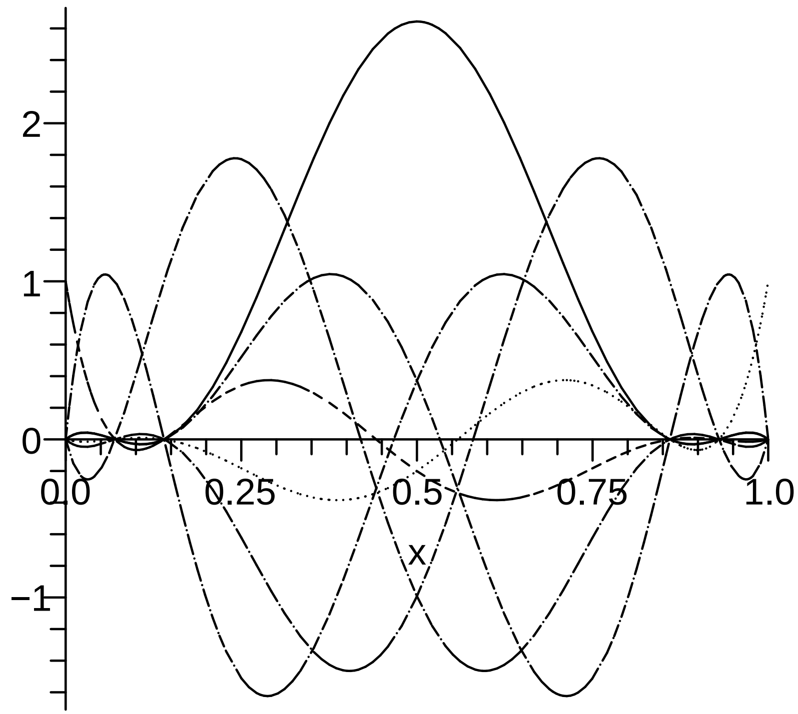


Figure 1: Plots of $\tilde{q}_1$ and $\hat{q}_2 \cdots \hat{q}_7$ for SDC CRK6. $\tilde{q}_1$ is represented by the solid line and has the highest magnitude.

Optimal SDC CRK8

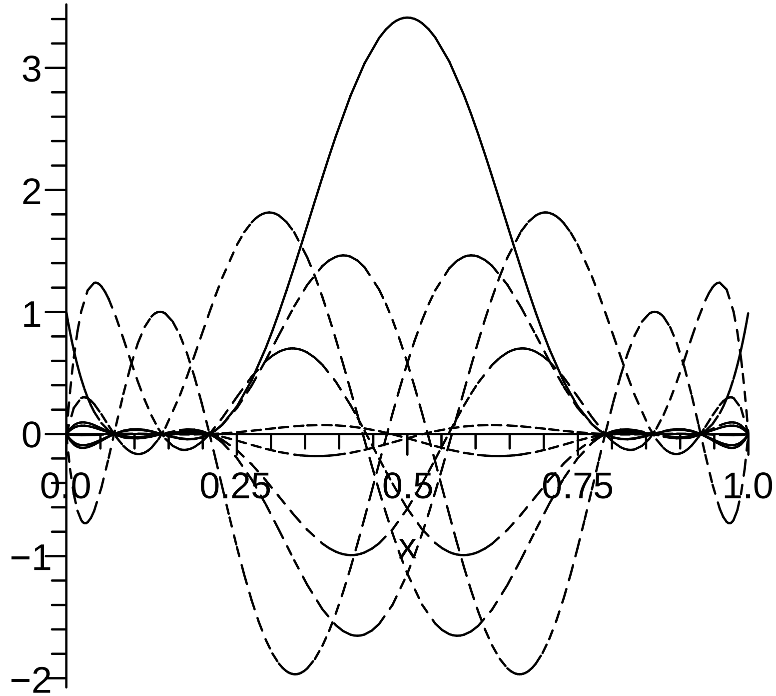


Figure 2: Plots of $\tilde{q}_1$ and $\hat{q}_2 \cdots \hat{q}_9$ for SDC CRK8. $\tilde{q}_1$ is represented by the solid line and has the highest magnitude.

Quantifying Reliability

Consider two measures of reliability of a CRK method:

- How well does the **Method** control the maximum magnitude of the defect? We can measure the ratio of the max defect to TOL on each step and the fraction of steps where this ratio is greater than 1 ?
- How well does the **Estimate** of the max defect reflect its true value? We can measure both the ratio of the true maximum defect (on a successful step) to its estimated value and the fraction of attempted steps where the estimated maximum is within <u>one percent</u> of the true maximum.

We will use these measures of reliability to demonstrate that SDC error control can significantly reduce the uncertainty of approximate solutions to ODE problems.

Reliability of SDC Methods

- We have implemented SDC versions of CRK5, CRK6 and CRK8.
- We have run these three methods on the 25 IVP test problems of DETEST (all non-stiff), at 9 tolerances from 10^{-1} to 10^{-9}.
- We report summaries only. We report two measures of cost: NSTP and NFCN, two measures of the reliability of the method : DMAX and Frac-D (max defect and fraction of steps where this exceeded TOL), and two measures of the reliability of the estimate: R-Max and Frac-G (maximum ratio of the true maximum defect to the estimate and the fraction of steps where this was bounded by 1.01).

Numerical Results for SDC CRKs

Results on the 25 DETEST Problems for SDC5, SDC6 and SDC8

TOL	CRK	NSTP	NFCN	DMAX	Frac-D	R-Max	Frac-G
10^{-2}	SDC5	625	11709	0.97	.000	1.05	.67
	SDC6	549	12300	1.00	.000	1.43	.71
	SDC8	333	12793	1.01	.003	1.65	.35
10^{-4}	SDC5	1065	19033	1.01	.001	1.12	.78
	SDC6	931	19819	1.00	.001	1.08	.87
	SDC8	465	17319	1.05	.004	1.47	.45
10^{-6}	SDC5	2099	35703	1.01	.002	1.08	.86
	SDC6	1748	35073	1.01	.001	1.08	.96
	SDC8	712	26253	1.02	.001	1.34	.59
10^{-8}	SDC5	4566	66937	1.01	.001	1.07	.95
	SDC6	3547	65148	1.01	.001	1.07	.98
	SDC8	1081	38251	1.12	.007	2.60	.62

SDC-CRK based methods developed for

- IVPs:

$$y' = f(x, y), \;\; y(a) = y_0, \;\; x \in [a, b],$$

  where $y, y_0 \in \Re^n$ and $f : \Re \times \Re^n \rightarrow \Re^n$.

- BVPs:

$$y' = f(x, y), \;\; x \in [a, b],$$

  with

$$g(y(a), y(b)) = 0, \;\; g : \Re^n \times \Re^n \rightarrow \Re^n.$$

- DAEs (with low index):

$$F(x, y, y') = 0, \;\; y(x) \in \Re^n, \;\; y(a) = y_0,$$

  for $x \in [a,\ b]$. With $\frac{\partial F}{\partial y'}$ singular but of constant rank in some neighborhood of $y(x)$.

Classes of ODEs (cont)

- DDEs (both retarded and neutral problems):

$$\begin{aligned} y' &= f(x, y(x), y(x-\sigma_1) \cdots y(x-\sigma_k), y'(x-\sigma_{k+1}), \\ &\cdots y'(x-\sigma_{k+\ell})), \text{ for } x \in [a,b], \end{aligned}$$

  where $y(x) \in \Re^n$ and,

$$y(x) = \phi(x), \;\; y'(x) = \phi'(x), \;\; \text{for } \; x \le a,$$

$$\sigma_i \equiv \sigma_i(x, y(x)) \ge 0 \;\text{ for }\; i = 1, 2 \cdots k + \ell.$$

- VIDEs (with a time dependent delay):

(1) $$y'(x) = f(x, y(x)) + \int_{x-\sigma(x)}^{x} K(x, s, y(s), y'(s))ds,$$

  for $x \in [a,b]$, $f : \Re \times \Re^n \to \Re^n$ and $K : \Re \times \Re \times \Re^n \times \Re^n \to \Re^n$ and $y(x) = \phi(x)$ for $x \le a$.

Effective Tools for Investigating ODEs

For each Class of ODEs we can develop a CRK method and define an associated defect of the approximate solution. For these methods we are implementing effective tools for:

- Estimating the Global Error
- Detecting, Locating and Coping with Discontinuous Problems
- Estimating the Conditioning of the Problem
- Sensitivity analysis of the Problem (eg., $\frac{\partial y_i(x)}{\partial p_j}$)
- Solving Problems which depend on parameters (parameter continuation and/or parameter fitting – an inverse problem)

Global Error Estimates for IVPs

Cost is comparable to that of computing $U(x)$. We will consider a typical IVP test problem:
Predator – Prey Problem:

$$\begin{aligned} y_1' &= y_1 - 0.1 y_1 y_2 + 0.02x, \\ y_2' &= -y_2 + 0.02 y_1 y_2 + 0.008x, \end{aligned}$$

with $y_1(0) = 30$, $y_2(0) = 20$, and $x \in [0, 40]$.

Quality of the Global Error Estimate

For each SDC method we monitor performance of the GE estimate over a range of tolerances and report the following:

- NS – The number of steps to determine $U(x)$.
- DEFUM – The maximum magnitude of the defect $\delta(x)$, (associated with $U(x)$), in units of TOL.
- G-ESTM – The maximum value of the global error estimate associated with $U(x)$ in units of TOL.
- G-ERRM – The maximum global error associated with $U(x)$ in units of TOL.

SDC on pred-prey problem

Method	TOL :	10^{-2}	10^{-4}	10^{-6}	10^{-8}
SDC5:	NS	70	148	315	705
	DEFUM	1.8	1.1	1.2	1.2
	G-ESTM	3.7	7.3	11.4	14.6
	G-ERRM	3.7	7.3	11.4	14.4
SDC6:	NS	65	134	277	585
	DEFUM	1.3	1.0	1.0	1.2
	G-ESTM	2.2	4.6	2.5	3.6
	G-ERRM	2.2	4.6	2.5	3.5
SDC8:	NS	34	53	83	127
	DEFUM	1.3	1.1	0.9	2.1
	G-ESTM	9.5	6.1	6.1	13.9
	G-ERRM	9.5	6.1	6.1	14.4

Reliability of Error Control and Global Error Estimate

The Next Steps

1. Implement a CRK for an implicit Runge-Kutta method that is suitable for stiff equations.
   (a) The additional RK stages can be explicit and SDC methods can be developed.
   (b) Requiring
   $$\max_{x \in [x_{i-1}, x_i]} ||\delta(x)|| \leq TOL$$
   may be too strong.
2. Multiple Shooting for BVPs based on CRK IVP methods.
3. Parameter fitting and sensitivity analysis for IVPs and DDEs arising in Chemical Kinetics and Biochemical simulations.

Implementation for DDEs

In his PhD thesis, Hossein Zivaripiran [University of Toronto, 2009] began the implementation of a PSE (DDEM) for the investigation of DDEs. (see `http://www.cs.utoronto.ca/~hzp`).

DDEM includes modules for:

1. Accurate location of all significant discontinuities.
2. Reliable simulation and visualization of a problem.
3. Efficient solution of the discrete approximations when delay is small or the underlying discrete RK formula is implicit.
4. Reliable approximation of first order sensitivities. (No other method we know of can do this.)
5. Parameter fitting from noisy data (using a “nonsmooth Newton” approach to achieve superlinear convergence.

Example: Parameter Fitting for DDEs

Consider the Kermack-McKendrick model of an infectious disease with periodic outbreaks:

$$\begin{aligned} y_1' &= -y_1(x)y_2(x-\sigma) \; + \; y_2(x-\rho), \\ y_2' &= y_1(x)y_2(x-\sigma) \; - \; y_2(x), \\ y_3' &= y_2(x) \; - \; y_2(x-\rho), \end{aligned}$$

with $x \in [0, 55]$, and $y_1(x) = 5.0, y_2(x) = 0.1, y_3(x) = 1.0,$ for $x \leq 0$.

The exact solution to this problem is unknown. Each delay introduces a C^2 discontinuity in the objective function whenever it is evaluated at a multiple of σ or ρ. We generate the data to be "fit" by computing an accurate solution with parameter values, $\sigma^* = 1$ and $\rho^* = 10$. We perturb these values by up to a 10% random perturbation to determine our initial guess for each parameter and we use 10 equally spaced sample points to define the prescribed data to be fit.

Parameter Fitting Results

Newton Jac	FCN	ITER	TIME	OBJ
DivDiff	783092	393.2	54.9	$7.4 \cdot 10^{-13}$
SenJac	37344	13.8	2.3	$1.3 \cdot 10^{-9}$
ConSenJac	5293	2.1	0.31	$1.3 \cdot 10^{-9}$

We report the total number of derivative evaluations FCN, The number of Newton iterations ITER, and the CPU time TIME (each averaged over 10 runs) for solving this problem with standard divided differences used to approximate the Newton Jacobian (DivDiff); with the Newton Jacobian approximated using an accurate Sensitivity Analysis (SenJac); and with the Newton Jacobian approximated using a constrained Newton step (ConSenJac). We also report the value of the objective function OBJ at the computed optimum point.