Solvers for Systems of Nonlinear Algebraic Equations; Where are we TODAY?

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Presentation Plan

- Introduction
- Problem description
- Search for the ultimate solver
    - algorithms and solvers
    - test problems
    - method
  - small problems
  - large problems
- Original problem revisited

Background (1)

- Work originated in early 1990’s
- Computer simulation of the behavior of airplanes under action of atmospheric gusts
- Two possible approaches
  - method of harmonic (S. O. Rice)
  - method of filtration (N. Wiener and independently Y. A. Kchinchin)
- Method of filtration used in original study

Background (2)

- Result $\rightarrow$ system of nonlinear algebraic equations
  - central/computational/difficult part of the problem
  - “independent” of other parts (well-defined and self-contained)
  - no preexisting knowledge about the solution
    - no simple way to suggest a starting vector
    - no simple way to reduce the “search area”

The Avionics Problem $\rightarrow$ Filter Equation

- Impulsive characteristics of a non-recursive filter h(t) as related to the correlation function $K(\tau)$ of the stochastic process {y(t)} obtained via filtering of the input white noise {x(t)}:

- $K(\tau) = E\left[\ \sum_{k=0}^{N} h(k)x(t-k) \sum_{k=0}^{N} h(n)x(t+\tau-n)\ \right]$

Filter Equation (2)

- Since input {x(t)} is a white noise we can rewrite the problem as:

- $K(\tau) = \sum_{n=0}^{N} h(n)h(n+\tau)$ for $\tau = 0, 1, \ldots, N$

- In its explicit form we have a system of nonlinear algebraic equations

Explicit Problem Formulation

$K(0) = h(0)h(0) + h(1)h(1) + h(2)h(2) + \ldots + h(N)h(N)$

$K(1) = h(0)h(1) + h(1)h(2) + h(2)h(3) + \ldots + h(N-1)h(N)$

$K(2) = h(0)h(2) + h(1)h(3) + h(2)h(4) + \ldots + h(N-2)h(N)$

…

$K(N-2) = h(0)(N-2) + h(1)h(N-1)+h(2)h(N)$

$K(N-1) = h(0)h(N-1) + h(1)h(N)$

$K(N) = h(0)h(N)$

Initial Work (1)

- Requirements for success (engineering-estimate)
  - minimum N = 512
  - potentially N = 1024 (?)
  - reached N = 64 using modified Powell's Method (1994)
- Encountered problems
  - computer hardware
    - for N = 64 solution time 10 minutes on a PC-486
  - robustness of solution methods

Initial Work (2)

- Research re-started $\rightarrow$ questions:
  - how to solve the system for very (?) large N?
  - how to select the starting vector?
- Search directions
  - to find (an) ultimate solver(s)
  - use modern hardware

Back to the Basics

- System of N nonlinear algebraic equations
- Large number of algorithms and implemented solvers
  - iterative methods
- How to find the best?
  - use existing/agreed on test problems
  - compare performance

- **NAÏVE!**

“Available” Algorithms

- Newton’s method
- Powell’s algorithm
- Brown’s method
- Secant method
- Bisection
- Steepest Descent
- Trust Region
- Line Search
- Continuation
- Homotopy
- Augmented Lagrangian
- Reduced-Gradient
- Tensor

“Available” Solvers (1)

Solver	**Algorithm**	**Source**
Brown	Brown’s method	In-house implementation
QuasiA	Hybrid Powell (Newton/Trust Region)	In-house implementation
CHABIS	Characteristic Bisection	ACM TOMS
SOS	Brown’s method	NETLIB
HOMPACK	Homotopy	ACM TOMS/NETLIB

“Available” Solvers (2)

Solver	**Algorithm**	**Source**
CONTIN	Continuation	ACM TOMS/NETLIB
HYBRD	Hybrid Powell (Newton/Trust Region)	NETLIB
TENSOLVE	Tensor/Line Search	NETLIB
LANCELOT	Projected Gradient	NEOS
MINOS	Reduced Gradient	NEOS

Test Problems

- **LACK of an "all-agreed" test library !**

- Test set → 22 frequently used problems
  - some artificially generated (with properties not typical for real-life applications)
  - most popular → More Test Set
  - typically small systems → $N \leq 10$
    - only few can be extended to larger N
    - no problems with absolute value

22 Test Problems

- Rosenbrock's
- Powell singular
- Powell badly scaled
- Wood
- Helical Valley
- Watson*
- Chebyquad*
- Brown Almost-linear*
- Discrete Boundary Value*
- Discrete integral equation*
- Trigonometric*
- Variably dimensioned*
- Broyden tri-diagonal*
- Broyden banded*
- Exponential/Sine Function
- The Freudenstein-Roth Function
- Semiconductor Boundary Condition
- Brown Badly Scaled
- Powell singular Extended
- Rosenbrock Extended
- Matrix Square Root Problem
- Dennis, Gay, Vu Problem

Methodological Considerations (1)

- Default settings for all solvers used
  - “engineering” approach
    - solver as black-box software
  - controversial choice

- Test problems contain default starting vectors
  - additional starting vectors used
    - zero
    - one
    - random [0,1]

Methodological Considerations (2)

- Computational cost
  - number of iterations
  - number of function evaluations
  - time

- Two steps
  - problems in their default formulation
  - increasing the size of amenable problems

Results (1)

- Easy test problems (solved easily by all solvers)
  - Rosenbrock's
  - Helical valley
  - The Freudenstein-Roth Function
  - Powell badly scaled
  - Broyden banded function
- USELESS(?!) as test problems
- Time so short that practically immeasurable
- In house codes only slightly less efficient than library solvers
  - implementation is not the "important" issue

Results (2)

- Weakest solvers (solve only few problems outside of the easy five):
  - bisection
  - variations of Newton’s method
- TENSOLVE results are slightly less accurate
- Homotopy should not be used as a black-box solver
  - requires proper problem mapping
  - makes it less of a “general-purpose” solver than others

Solution of Large Problems

- Test problems that can have the default number of equations increased
  - Watson
  - Brown Almost-linear
  - Discrete integral equation
  - Variably dimensioned
  - Broyden banded
  - Chebyquad
  - Discrete Boundary Value
  - Trigonometric
  - Broyden tri-diagonal
- Five solvers left after initial selection
  - CONTIN
  - HYBRD
  - MINOS
  - LANCELOT
  - TENSOLVE

Results

- Test problems can be divided into three groups (results for any tried starting vector):
  - Difficult Problems - solution only for small N (≤ 31)
  - Medium Difficult Problems - some solvers fail to reach N=1000
  - Easy Problems - all solvers reach N=1000

Difficult Problems

Solver	Watson Max N	Chebyquad Max N
CONTIN	6	2
HYBRD	14	9
TENSOLVE	23	18
LANCELOT	31	18
MINOS	31	20

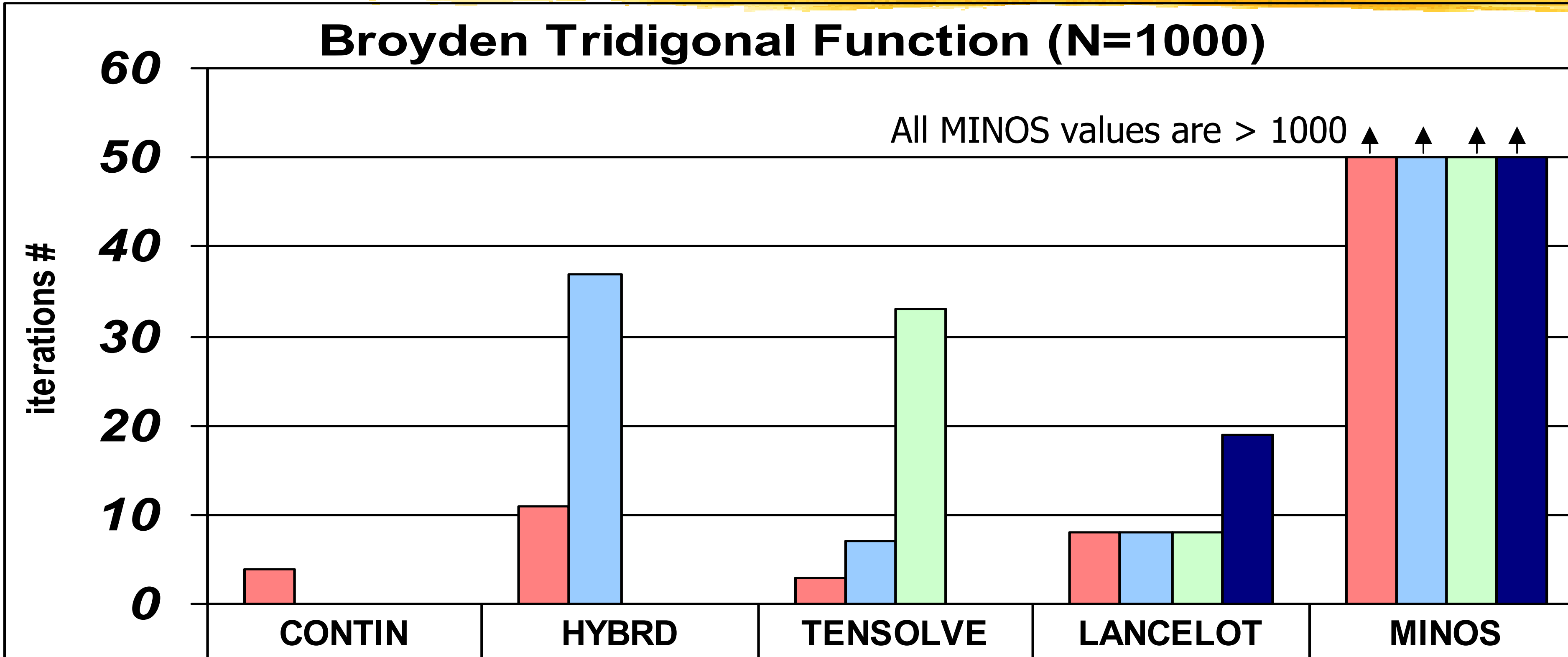
Difficult Problem Example
Watson Function

Solver	**Max N**	**IT**	**FC**	**Time/ Sec**
CONTIN	6	6	256	0
HYBRD	14	54	120	0
TENSOLVE	23	180	5351	2.00
LANCELOT	31	44	44	1.03
MINOS	31	49	115	0.16

Medium Difficult

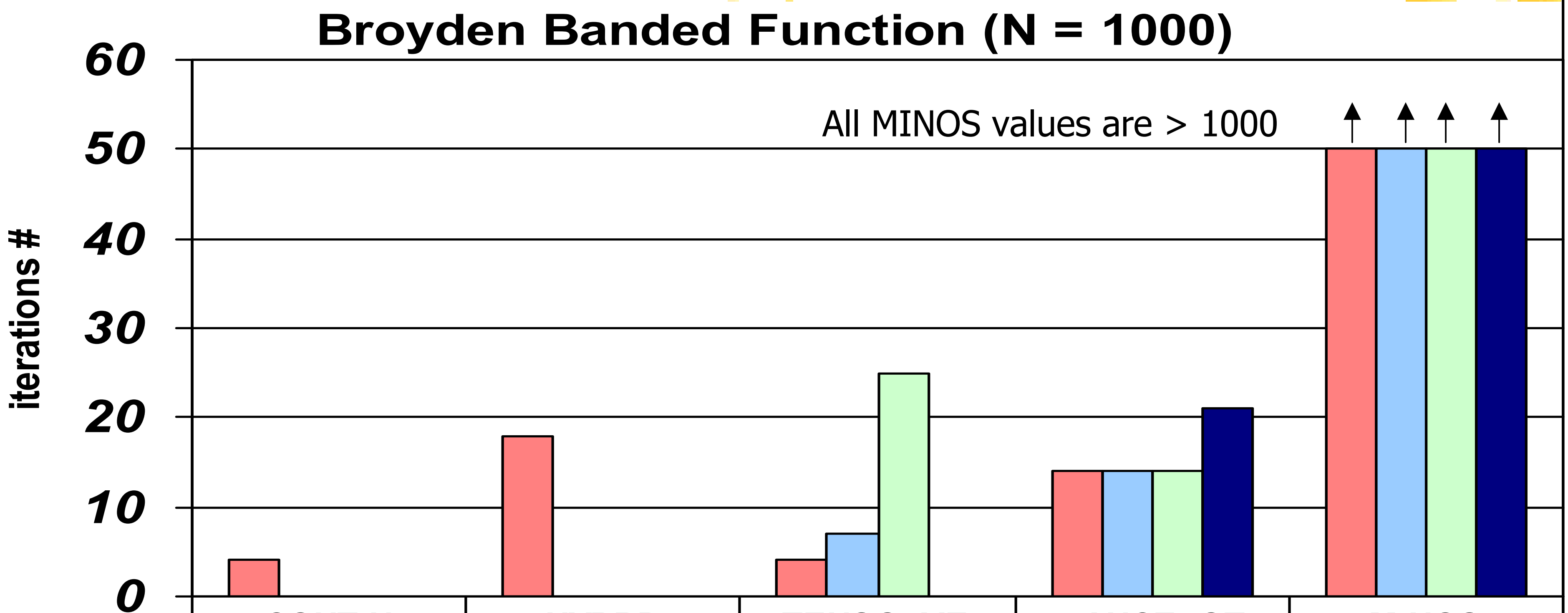
Solver	Brown Almost Linear Max N/ Time/Sec	Discrete Boundary Value Max N/ Time/Sec	Discrete Integral Equation Max N/ Time/Sec	Trigono-metric Max N/ Time/Sec	Variably Dimen-sioned Max N Time/Sec
CONTIN	1000/ 300	11/ 0	4/ 0	23/ 0	4/ 0
HYBRD	22/ 0	1000/ 350	1000/ 497	40/ 0	42/ 0
TENSOLVE	1000/ 228	1000/ 1	1000/ 547	1000/ 2	200/ 31
LANCELOT	1000/ 220	1000/ 61	600/ 2826	1000/ 10506	1000/ 15
MINOS	1000/ 1094	1000/ 4	600/ 1804	1000/ 3737	1000/ 234

Sensitivity to starting vector (1)



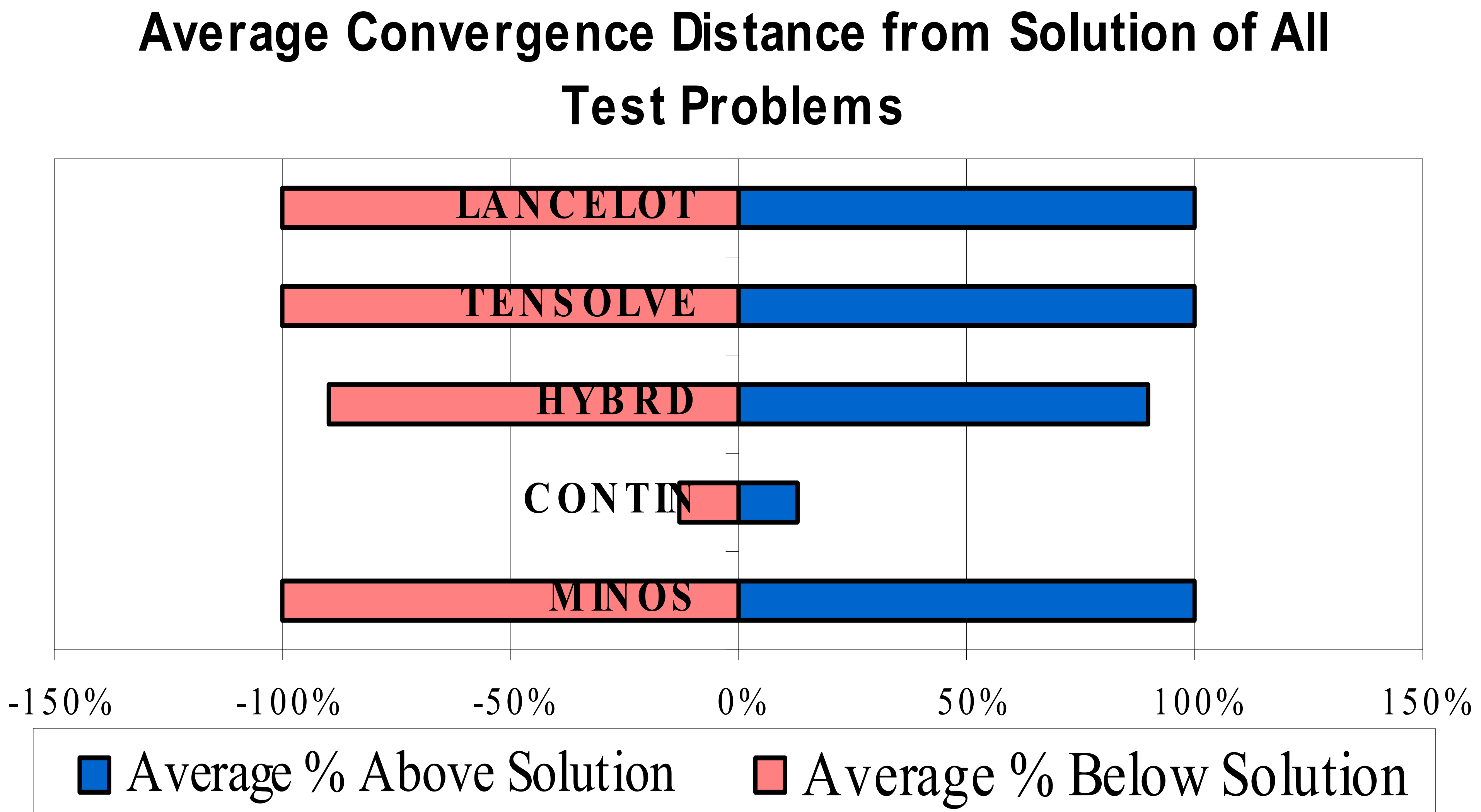
	CONTIN	HYBRD	TENSOLVE	LANCELOT	MINOS
Default	4	11	3	8	50
Zeros	0	37	7	8	50
Ones	0	0	33	8	50
Random	0	0	0	19	50

Sensitivity to starting vector (2)



	CONTIN	HYBRD	TENSOLVE	LANCELOT	MINOS
Default	4	18	4	14	50
Zeros	0	0	7	14	50
Ones	0	0	25	14	50
Random	0	0	0	21	50

Summary


Average Convergence Distance from Solution of All Test Problems
LANCELOT
TENSOLVE
HYBRD
CONTIN
MINOS
-150%
-100%
-50%
0%
50%
100%
150%
Average % Above Solution
Average % Below Solution

Observations (1)

- Solvability of the problem depends on interaction between
  - problem
  - solver
  - starting vector

- Problems not solvable using one solver with one starting vector may be solvable by another solver, or when a different starting vector is used

Observations (2)

- How to detect **true lack of solution** to the problem? (A. Grievank, Rousse 2000)
- Of the solvers tested, TENSOLVE, LANCELOT, and MINOS are most robust followed by HYBRD
  - CONTIN and HYBRD converge best with “default”
  - TENSOLVE converges best with “one”
  - LANCELOT and MINOS converges best with “zero”

Observations (3)

- Six popular test problems:
  - Rosenbrock's
  - Helical valley
  - The Freudenstein-Roth function
  - Powell badly scaled
  - Broyden banded function
  - Broyden tridiagonal

  are "easily solvable" by more robust solvers → provide no useful information for performance measuring
- Watson and Chebyquad seem to be very hard to solve → can be recommended as real benchmarks for the robustness of new solvers
- New test problems needed(?)

Original Problem Revisited

- Four most robust solvers found earlier to be used:
  - HYBRD
  - TENSOLVE
  - LANCELOT
  - MINOS
- Other solvers tried and similar behavior/weakness as for the test problems observed

Initial Numerical Test

- Example used in original papers has solutions expressed by integers; for example
- For N=2:
  - K(1) = 34 and K(2) = 5
  - Basic solution: h(1) = 5 and h(2) = 3
- For N=4:
  - K(1)=30, K(2) = 20, K(3) = 11, and K(4)=4
  - Basic solution: h(1)=1, h(2)=2, h(3)=3, h(4)=4
    - alternate solution(!)
    - h(1)≈1.65, h(3≈1.58, h(3) ≈4.35, h(4) ≈2.24

Test Cases

- System of equations:
  - $K(\tau) = \sum_{i=0}^{N} h(i)h(j)$ for j=0,1,…,N
- Problem 1 $\rightarrow$ Integer Data
  - coefficient vector created so that:
  - exact solution: $h_f(i) = i$
  - starting vector: $h_0(i) = 1$
- Problem 2 $\rightarrow$ Floating Point Data
  - coefficient vector: real world data
  - starting vector: $h_0(i) = 1$
- Other starting vectors used; “one” seems best-overall

Results for Problem 1 (1)

	HYBRD			LANCELOT		
N	**IC**	**FC**	**Time/ sec**	**IC**	**FC**	**Time/ sec**
2	8	10	0	10	11	.01
4	19	27	0	8	9	.02
8	8	16	0	11	12	.04
32	10	42	0	14	15	.40
64	10	74	0	23	24	2.89
128	10	110	1	49	50	34.68
256	10	160	2	161	162	905.4
512	10	210	3	nc		
1024	10	310	12	nc		

Results for Problem 1 (2)

	MINOS			TENSOLVE		
N	**IC**	**FC**	**Time/ sec**	**IC**	**FC**	**Time/ sec**
2	11	27	.01	9	23	.01
4	18	42	.01	18	42	.01
8	40	97	.01	40	94	.01
32	274	624	.32	88	201	.04
64	602	1357	2.47	274	624	2.97
128	1977	4182	19.2	602	1367	2.44
256	7340	14771	564.07	1216	2646	11.75
512	24205	47580	8346.04	4591	9422	171.02
1024	nc			nc		

Comments

- **HYBRD**
  - Converges for the largest number of equations (N = 1024)
  - Extremely fast
  - Best accuracy
- **LANCELOT**
  - Converges only for up to N = 256
  - Slowest
  - Different solution(!)
- **MINOS**
  - Converges for up to N = 512
  - Different solution(!)
- **TENSOLVE**
  - Converges for up to N = 512
  - Second fastest
  - Solution less accurate than HYBRD

Results for Problem 2 (1)

	HYBRD			LANCELOT		
N	IC	FC	Time/ sec	IC	FC	Time/ sec
128	10	110	1	161	162	111.5
256	10	160	2	164	165	633.09
512	21	2095	90	201	206	5140.05

Results for Problem 2 (2)

	MINOS			TENSOLVE		
N	**IC**	**FC**	**Time/ sec**	**IC**	**FC**	**Time/ sec**
128	**1068**	**2737**	**19.22**	**28**	**3818**	**4**
256	**1383**	**3881**	**131.52**	**16**	**4381**	**20**
512	**2310**	**6508**	**1068.88**	**12**	**6692**	**117**

Error Estimate

- Error estimate $\rightarrow$ comparison between the actual coefficient vector K(i) and the computed $\underline{K}$(i) obtained by substituting computed $\underline{h}$(i) to the problem

Solver	Minimum Error	Maximum Error	Average Error
HYBRD	4.40E-07	7.15E-05	1.87E-05
LANCELOT	1.25E-07	5.42E-05	1.83E-05
MINOS	4.16E-07	4.45E-05	1.80E-05
TENSOLVE	4.51E-07	2.83E-03	2.86E-04

Partial View of Solution Vectors (N = 512)

	LANCELOT	MINOS	TENSOLVE	HYBRD
i	**x(i)**	**x(i)**	**x(i)**	**x(i)**
1	-0.0596631	0.141907	-0.135745775	-0.137628574
2	-0.0336641	0.072495	-0.080370211	-0.079030645
3	-0.0176408	0.077313	-0.074520022	-0.075754926
4	0.0450654	0.054729	-0.044292743	-0.041200875
⋮				
509	0.289799	-0.02806	0.044774790	0.042478349
510	0.417939	-0.03148	0.043859563	0.046436000
511	0.139752	-0.02624	0.027990174	0.027022607
512	0.133402	-0.06305	0.054905619	0.056642195

Observations

- HYBRD
  - Convergence only if TENSOLVE results used as starting vector
    - very fast then
- LANCELOT
  - Converges to a different solution
- MINOS
  - Converges to yet another different solution
  - Slowest of the three globally converging solvers
- TENSOLVE
  - Converges fast
  - Least accurate solution
  - Accuracy improved by HYBRD as post-processor

Future Work

- Analysis of the three results (engineering aspects)
  - which/any/all solutions are “correct"?
  - is N = 512 enough?
  - what do these results mean?
- Interval solver (INTLIB) for verification
- Commercial solvers $\rightarrow$ will they introduce anything new?

Big Picture

- PROBLEM vs. SOLVER vs. STARTING VECTOR
- EXISTENCE vs. NON-EXISTENCE vs. SOLUTION #
- UNCONSTRAINED vs. CONSTRAINED PROBLEMS

THANK YOU!

QUESTIONS?