Mesh selection and conditioning for Boundary Value Problems

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outline

- Introduction
- Conditioning of Boundary Value Problems;
- Estimating the conditioning;
- Mesh selection based on conditioning;
- How to handle inhomogeneous problems;
- Examples;
- How to solve a problem using TOM;
- Conclusions

Introduction

- $\dfrac{dy}{dx} = f(x,y), \;\; a \leq x \leq b, y \in R^m, \quad g(y(a), y(b)) = 0.$
- Typically numerical methods attempt to control the error in the solution:
  - by estimating the pointwise local error at the mesh points;
  - by controlling the residual;
- In order to study the conditioning the standard approach is to examine the behaviour of the solutions in the neighborhood of an isolated solution;
- This leads us to consider linear equations.

Linear problems

- $\frac{dy}{dx} = A(x)y + q(x), \;\; a \leq x \leq b, \quad B_a y(a) + B_b y(b) = \beta.$
- the solution is given by

$$y(x) = Y(x)Q^{-1}\beta + \int_a^b G(x,t)q(t)dt.$$

$Q = B_a Y(a) + B_b Y(b)$

$G(x,t)$ is the Green's function

Conditioning parameters ∞-norm

- $$\frac{du}{dx} = A(x)u + q(x) + \delta(x), \ \ a \le x \le b,$$
  $$B_a u(a) + B_b u(b) = \beta + \epsilon.$$
- $u(x) - y(x) = Y(x)Q^{-1}\epsilon + \int_a^b G(x,t)\delta(t)dt.$
- $||u(x) - y(x)|| \le ||Y(x)Q^{-1}\epsilon|| + ||\int_a^b G(x,t)\delta(t)dt||$
- $\max_{a\le x\le b} ||u(x) - y(x)|| \le \kappa_1 ||\epsilon|| + \kappa_2 \max_{a\le x\le b} ||\delta(x)||$
- $\max_{a\le x\le b} ||u(x) - y(x)|| \le \kappa \max(||\epsilon||, \max_{a\le x\le b} ||\delta(x)||)$
- $\kappa_1 = \max_{a\le x\le b} ||Y(x)Q^{-1}||, \ \ \kappa_2 = sup_x \int_a^b ||G(x,t)||dt,$
- $\kappa = max_{a\le x\le b}(||Y(x)Q^{-1}|| + \int_a^b ||G(x,t)||dt).$

Conditioning parameters 1-norm

- $u(x) - y(x) = Y(x)Q^{-1}\epsilon + \int_a^b G(x,t)\delta(t)dt.$
- $||u(x) - y(x)|| \leq ||Y(x)Q^{-1}\epsilon|| + ||\int_a^b G(x,t)\delta(t)dt||$
- $\int_a^b ||u(x) - y(x)||dx \leq \gamma_1 ||\epsilon|| + \gamma_2 \max_{a \leq x \leq b} ||\delta(x)||$
- $\int_a^b ||u(x) - y(x)||dx \leq \gamma \max(||\epsilon||, \max_{a \leq x \leq b} ||\delta(x)||)$
- $\gamma_1 = \int_a^b ||Y(x)Q^{-1}||dx,$
- $\gamma_2 = \int_a^b \int_a^b ||G(x,t)||dtdx,$
- $\gamma = \int_a^b((||Y(x)Q^{-1}|| + \int_a^b ||G(x,t)||dt))dx.$

Classification of the problems

- If κ and γ are both of moderate size we are dealing with a well conditioned problem.
- Conversely if both are large we have an ill conditioned problem.
- A rather different case is when only κ is large and γ is small.
- This means that the problem is ill conditioned using the maximum norm and well conditioned using the 1 norm.
- The problems that fall into this class are typically those possessing different time scales.
- Brugnano and Trigiante, using κ_1 and γ_1, classified this class of problems as "stiff".

A stiff problem

$$\epsilon y'' + xy' = -\epsilon\pi^2 cos(\pi x) - \pi x sin(\pi x),$$
$$y(-1) = -2, y(1) = 0,$$
$$\epsilon = 10^{-10}.$$

This is a "stiff" problem: $\kappa_1 \approx 7.98e+4$ $\gamma_1 \approx 2.0$

Stiffness ratio: $\kappa_1/\gamma_1 \approx 3.95e+4$

$\kappa \approx 1.65e+5$

Estimating the conditioning

- Using a numerical method and the Newton scheme to solve the nonlinear algebraic equations arising at each step we obtain a linear system of algebraic equations of the form $Ax = b$;
- We set up the block matrix A so that the boundary conditions appear only in the first row block of b;
- Ascher, Mattheij and Russell proved that for one-step schemes $\|A^{-1}\| \approx \kappa$;
- The computation of the first m columns of A^{-1} allows us to have an estimating of κ_1 and γ_1;
- Note that numerical methods not only form A but also solve a linear system of algebraic equations. This means that we have the LU factorization of A at hand.

How to use the conditioning parameters

- Shampine and Muir use an estimate of the conditioning parameter κ in the solvers MIRKDC and BVP4c;
- If an appropriately scaled estimate of κ is larger than the inverse of the tolerance then this generates a warning that the solution may not be particularly accurate.
- In particular the global error in the solution may not be of the same order of magnitude as the local solution.
- An obvious drawback with the above approach is that the numerical algorithm may be badly conditioned even though the original continuous problem may be perfectly well conditioned.

How to use the conditioning parameters

- An alternative way of using the condition numbers was proposed by Brugnano and Trigiante and inserted in the MATLAB solver TOM.
- The conditioning parameters are also used in the mesh selection algorithm.

Mesh selection based on the conditioning

- We define the following matrices: $G = A^{-1}$, Ω having elements $\Omega_{ij} = ||G_{ij}||$.
- The discrete conditioning parameters are defined on the grid π in the following way:

$$\kappa_1(\pi) = \max_i \Omega_{i0}, \quad \gamma_1(\pi) = (\sum_{i=1}^{N} h_i \max(\Omega_{i-1,0}, \Omega_{i0}))/(b-a).$$

- Our aim is to choose the mesh so that: $\kappa_1(\pi) \approx \kappa_1$ and $\gamma_1(\pi) \approx \gamma_1$
- We define a monitor function based on both the local accuracy and on the conditioning estimate and then use equidistribution based on this monitor function.
- An estimating of κ is also computed.

Mesh selection based on conditioning

- The conditioning parameters κ_1 and γ_1 take into account only perturbations with respect to the boundary conditions ϵ;
- What happens to the perturbation $\delta(x)$?
- Suppose we are solving a boundary value problem where the boundary conditions are appropriate for handling the decreasing and the increasing modes, using a numerical method that properly handles the exponential growth and decay of the solution.
- In this case the information provided by κ_1 is sufficient to handle the perturbation $\delta(x)$ as well.
- A complete information about the conditioning is given by: κ_1, γ_1 and κ.

How to handle inhomogeneous problems

- An alternative mesh selection strategy, that takes into account also the inhomogeneous term, has been defined in term of the solution of the discrete problem, instead of the variational operator.
- Of course the information is less complete but in many cases the two approaches give similar results and the cheapest one should be preferable.

How to handle inhomogeneous problems

- Two parameters are defined on the grid π in the following way ($y_i \approx y(x_i)$):

$$\kappa_s(\pi) = \max_i \|y_i\|, \quad \gamma_s(\pi) = (\sum_{i=1}^{N} h_i \max(\|y_{i-1}\|, \|y_i\|))/(b-a).$$

- Our aim is to choose the mesh so that: $\kappa_s(\pi) \approx \max_{a \le x \le b} \|y(x)\|$ and $\gamma_s(\pi) \approx \int_a^b \|y(x)\| dx$
- We to define a monitor function based on both the local accuracy and on $\gamma_s(\pi)$ and then use equidistribution based on this monitor function.

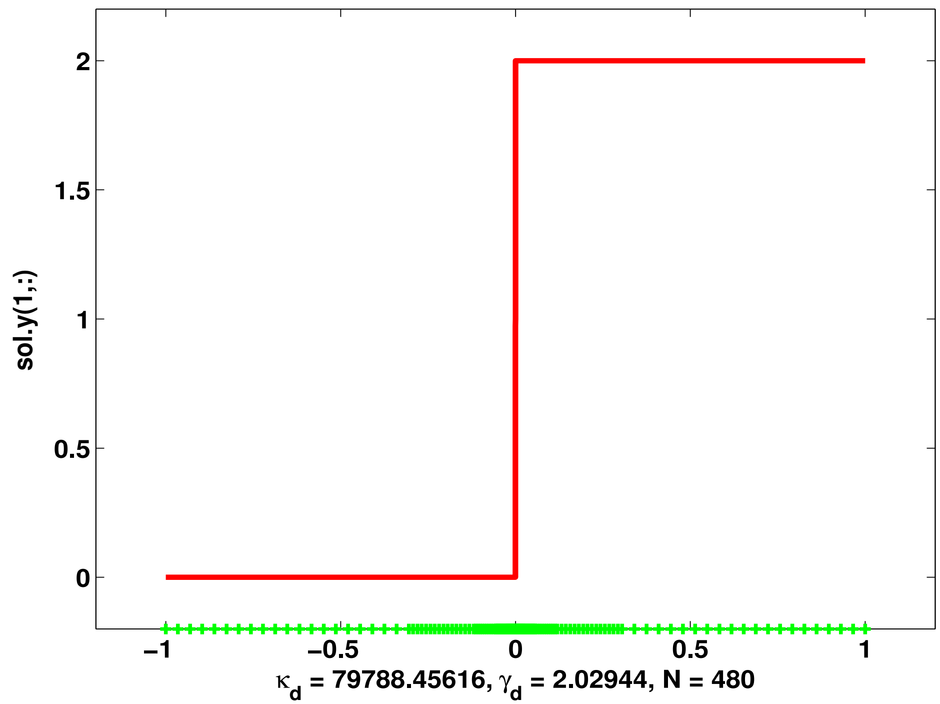
Mesh selections in the solver TOM

- It is possible to choose the mesh selection strategy:
  - WRCE (optimal with respect to the conditioning and the approximation of the error):
    we use information given by $\gamma_1(\pi)$, $\gamma_s(\pi)$ and the approximation of the error;
  - WRSE (optimal with respect to the solution and the approximation of the error):
    we use information given by $\gamma_s(\pi)$ and the approximation of the error;
  - WRE (optimal with respect to the approximation of the error):
    we use information given by the approximation of the error;

Mesh selections in the solver TWPBVP

- Strategy inserted in the known version of the solver:
  - WRE (optimal with respect to the approximation of the error): we use information given by the approximation of the error;
- Strategy inserted in the updated version of the solver (in preparation):
  - WRCE (optimal with respect to the conditioning and the approximation of the error):
    we use information given by $\gamma_1(\pi)$ and the approximation of the error;

A stiff problem



- $\epsilon y'' + xy' = 0, y(-1) = 0, y(1) = 2, \qquad \epsilon = 10^{-10}.$
- This is a "stiff" problem: $\kappa_1 \approx 7.98e + 4, \qquad \gamma_1 \approx 2.0$
- Stiffness ratio: $\kappa_1/\gamma_1 \approx 3.97e + 4$
- $\kappa \approx 1.65e + 5$

Numerical Solution using TOM (WRCE)

$\epsilon = 10^{-10}$, $Reltol = 10^{-3}$, $Abstol = 10^{-3}$.

$\kappa(\pi)$	$\kappa_1(\pi)$	$\gamma_1(\pi)$	N	$Error$	$order$
$2.09d+1$	$8.73d+0$	3.80	15	$2.40d+0$	6
$1.33d+2$	$6.33d+1$	2.97	60	$8.66d-2$	6
$1.53d+3$	$5.54d+2$	2.99	100	$3.84d-1$	6
$1.33d+4$	$6.63d+3$	3.00	130	$4.94d-1$	2
$1.23d+5$	$6.14d+4$	3.05	210	$8.79d-1$	2
$1.59d+5$	$7.95d+4$	2.10	230	$4.40d-1$	2
$1.59d+5$	$7.98d+4$	2.03	300	$7.63d-1$	2
$2.91d+5$	$7.98d+4$	2.03	430	$7.14d-6$	6

Numerical Solution using TOM (WRSE)

$\epsilon = 10^{-10}$, $Reltol = 10^{-3}$, $Abstol = 10^{-3}$.

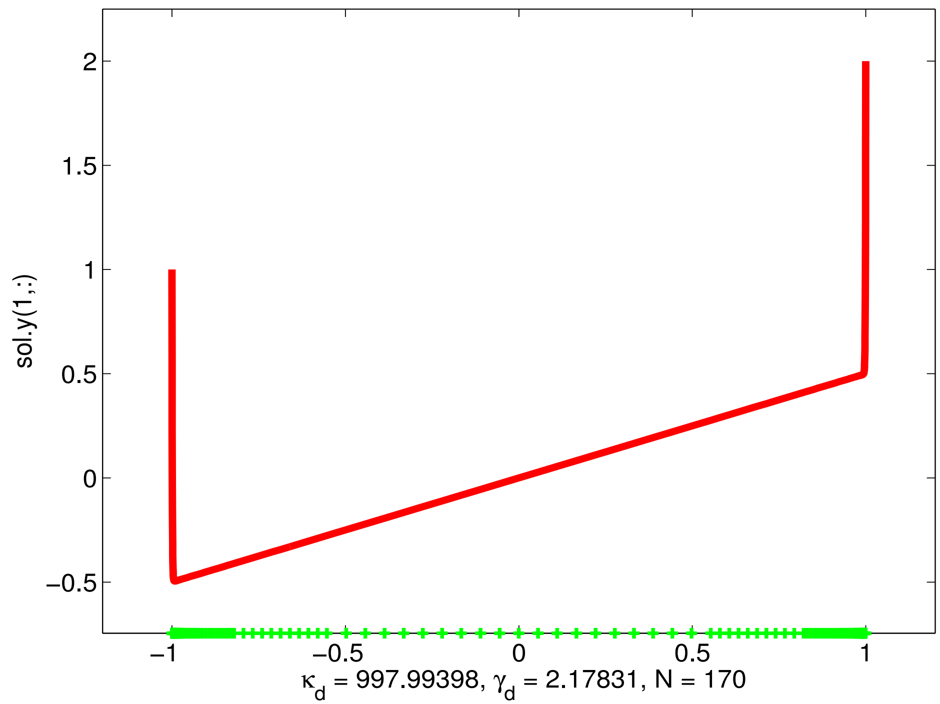
$\kappa(\pi)$	$\kappa_s(\pi)$	$\gamma_s(\pi)$	N	$Error$	$order$
$2.09d+1$	$8.73d+0$	3.94	15	$2.40d+0$	6
$1.34d+2$	$6.40d+1$	2.97	60	$8.66d-2$	6
$5.73d+2$	$2.12d+2$	32.05	105	$8.37d-1$	6
$4.88d+2$	$2.44d+2$	4.63	115	$6.81d-1$	2
$4.36d+2$	$2.18d+3$	6.84	140	$8.06d-1$	2
$7.03d+4$	$3.52d+4$	4.78	160	$8.95d-1$	2
$1.58d+5$	$7.92d+4$	2.13	210	$5.84d-1$	2
$1.59d+5$	$7.97d+4$	2.03	265	$9.08d-1$	2
$2.14d+5$	$7.98d+4$	2.03	325	$2.99d-1$	6
$2.09d+5$	$7.98d+4$	2.03	345	$3.56d-2$	6
$1.80d+5$	$7.97d+4$	2.03	430	$7.22d-3$	6

Numerical Solution using TWPBVP (WRC

$\epsilon = 10^{-6}, Reltol = 10^{-6}.$

κ_1	γ_1	Error in Order 4	Error in order 6
$0.18d+2$	$0.39d+1$	$0.32d-4$	$0.37d+0$
$0.36d+2$	$0.39d+1$	$0.22d-3$	$0.15d+1$
$0.71d+2$	$0.40d+1$	$0.12d-2$	$0.62d+1$
$0.14d+3$	$0.40d+1$	$0.27d-2$	$0.58d+1$
$0.25d+3$	$0.41d+1$	$0.14d-2$	$0.18d+2$
$0.38d+3$	$0.38d+1$	$0.38d-1$	$0.27d+2$
$0.40d+3$	$0.21d+1$	$0.17d-1$	$0.74d-1$
$0.40d+3$	$0.17d+1$	$0.57d-3$	$0.19d-1$
$0.40d+3$	$0.161d+1$	$0.14d-3$	$0.67d-2$
$0.40d+3$	$0.161d+1$	$0.80d-5$	$0.30d-5$

An ill conditioned linear problem



- $\epsilon y'' - xy' + y = 0, y(-1) = 1, y(1) = 2, \qquad \epsilon = 10^{-3}.$
- $\kappa_1 \approx 9.98d+2, \qquad \gamma_1 \approx 2.18$
- Stiffness ratio: $\kappa_1/\gamma_1 \approx 4.58d2$
- $\kappa \approx 8.53d+13$

Numerical Solution using TOM (WRCE)

$\epsilon = 10^{-3}, Reltol = 10^{-3}, Abstol = 10^{-3}.$

$\kappa(\pi)$	$\kappa_1(\pi)$	$\gamma_1(\pi)$	N	$Error$	$order$
$3.22d+00$	$1.02d+00$	1.01	15	$1.09d-1$	6
$1.33d+03$	$1.88d+02$	17.18	60	$8.87d-1$	6
$2.24d+04$	$6.08d+02$	4.43	100	$1.09d+0$	6
$8.53d+13$	$9.98d+02$	2.18	170	$5.70d-3$	6

Numerical Solution using TOM (WRSE)

$\epsilon = 10^{-3}, Reltol = 10^{-3}, Abstol = 10^{-3}.$

$\kappa(\pi)$	$\kappa_s(\pi)$	$\gamma_s(\pi)$	N	$Error$	$order$
$4.90d + 00$	$1.53d0$	1.51	15	$1.09d - 1$	6
$4.932d + 03$	$1.31d3$	114.91	60	$9.23d - 1$	6
$2.59d + 03$	$1.06d3$	7.33	100	$1.08d + 0$	6
$4.82d + 13$	$1.50d3$	2.27	170	$1.59d - 2$	6
$3.84d + 11$	$1.50d3$	2.05	230	$1.06d - 4$	6

Bratu problem

A problem with no solution

- $y'' = \lambda e^y, \quad y(0) = y(1) = 0, \lambda = 3.55$
- Numerical Solution using TOM (WRCE/WRSE)
- $Reltol = 10^{-3}, Abstol = 10^{-6}.$
  The solver is unable to give a solution.
- $Reltol = 10^{-2}, Abstol = 10^{-2}.$
  - the solver finds a pseudo solution on the given mesh with the warning that the conditioning parameters are not stabilized.
  - If we force the solver to find also the conditioning parameters, it fails to give any solution.

Troesh equation

- $y'' = \mu \sinh(\mu y) \;\; y(0) = 0, y(1) = 1.$
- Numerical Solution using TOM (WRCE),
  $Reltol = 1d-3, \;\; Abstol = 1d-3$
  Initial guess: $y = 0.5; y' = 0;$

μ	$\kappa(\pi)$	$\kappa_1(\pi)$	$\gamma_1(\pi)$	N	$itnl$
10	$7.66d+02$	$7.61d+02$	2.55	70	6
20	$2.20d+05$	$2.20d+05$	2.17	215	11
30	$4.91d+07$	$4.91d+07$	2.11	291	17
40	$9.72d+09$	$9.72d+09$	2.22	460	21
50	$1.80d+12$	$1.80d+12$	2.18	605	26

- Similar results are obtained with TOM (WRSE).

How to solve a problem using TOM

- The solver TOM is available on the web site:
  `http://www.dm.uniba.it/~mazzia/bvp/index.html`
- It is written in MATLAB, for uniformity the calling sequence is similar to the one of BVP4c:
  » sol = tom(odefun,bcfun,solinit)
- auxiliary function
  - tomget Get TOM OPTIONS parameters.
  - tomset Create/alter TOM OPTIONS structure.
  - tominit Form the initial guess for TOM.

Conclusions

- The purpose of this talk was to give an overview of the role of conditioning in the solution of two-point boundary value problems.
- We have shown how to estimate the condition number of a problem and how to incorporate this estimate into a mesh selection algorithm.
- We have show that the parameters κ_1, γ_1 and κ give all the information about the conditioning and the stiffness of the problem.
- We have also established the important concept that we need to wait until the condition constants have settled down before testing for accuracy and that this applies both to TOM and TWPBVP.

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