Boundary value problems with very sharp structures: numerical challenges



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Introduction

- Singular perturbation problems depend on a small parameter ε which typically premultiplies the highest derivative.
- As $\varepsilon \to 0$, the problems exhibit localized structures such as boundary layers, corner layers, spikes, interfaces.
- Typically, the localized structure has the size O(ε); the solution is relatively smooth outside the localized region.
- Standard codes to solve BVP may have difficulty resolving localized structures: typically, meshsize scales with $1/\varepsilon$.
- Example: a standard code requires 10,000 meshpoints when $\varepsilon = 10^{-5}$?

Problem 1

Solve the problem

$$\varepsilon^2 u'' - u + (1 + x^2) u^2 = 0; \quad u'(0) = 0; \quad \varepsilon u'(1) = -u(1).$$



• Note that

$$w \sim O(1) \quad \text{for} \quad y = O(1)$$

but it decays,

$$w \sim 6e^{-y}$$
 for large y .

- This exponential decay can cause trouble for BVP solvers.
- The solution exhibits two different spatial scales.
- Maple BVP solver: meshsize scales like $1/\varepsilon$.
- Matlab does much better [see below]

Split-range method

Split-range method

• Choose $l \in [0, 1]$,

$$\varepsilon \ll l \ll 1$$

• On [0, l], (inner problem) transform:

$$x = ly, \ u(t) = \hat{u}(y)$$

• On [l, 1], (outer problem) transform:

$$x = l + (1 - l)y, \ u(t) = \exp\left(\frac{\tilde{u}(y)}{\varepsilon}\right)$$

• We get a 4-dimensional BVP for \hat{u}, \tilde{u} on $y \in [0, 1]$. The boundary conditions become:

$$\begin{split} \hat{u}'(0) &= 0, \quad \tilde{u}'(1) = -1 \\ \hat{u}(1) &= \exp\left(\frac{\tilde{u}(0)}{\varepsilon}\right) \text{ (continuity of } u) \\ \frac{\hat{u}'(1)}{l} &= \frac{1}{\varepsilon(1-l)} \exp\left(\frac{\tilde{u}(0)}{\varepsilon}\right) \tilde{u}'(0) \text{ (continuity of } u') \end{split}$$

• The parameter l is chosen by trial and error. Global tolerance is set to 10^{-6} ; Maple's dsolve/bvp is used with adaptive gridding.

Meshsize scaling laws

	split range	split range	Standard Maple	Standard Matlab
2	$(l = 9\varepsilon)$	$(l = 4\varepsilon \ln \frac{1}{\varepsilon})$	(adaptive mesh)	(adaptive mesh)
0.1	21	21	51	50
0.05	21	24	87	37
0.025	21	21	106	41
$2^{-3} \times 0.1$	21	26	178	38
$2^{-4} \times 0.1$	21	29	376	41
$2^{-5} \times 0.1$	30	30	792	42
$2^{-6} \times 0.1$	58	32	error	50
$2^{-7} \times 0.1$	119	31		39
$2^{-8} \times 0.1$	226	32		35
$2^{-9} \times 0.1$	472	33		35
$2^{-10} \times 0.1$	946	34		93
$2^{-11} \times 0.1$	error	35		61
$2^{-16} \times 0.1$		41		36
$2^{-17} \times 0.1$		42		38

• The "good" l scales like $l = O(\varepsilon \ln \varepsilon)!$

Understanding $l = O(\varepsilon \ln \varepsilon)$

• Consider a simple problem

$$\varepsilon u_{xx} + u_x = 1, \quad u(0) = 0 = u(1).$$
 (1)

• Asymptotic composite solution is:

$$u \sim \exp\left(-x/\varepsilon\right) + x - 1$$
 (2)

• There is a boundary layer at 0 as $\varepsilon \to 0$:



Error analysis, uniform mesh

• Discretize: let
$$h = 1/N$$
 and approximate $\varepsilon u_{xx} + u_x = 1$ by
 $\varepsilon \frac{\hat{u}_{i-1} + \hat{u}_{i+1} - 2u_i}{h^2} + \frac{\hat{u}_{i+1} - \hat{u}_{i-1}}{2h} = 1; \quad \hat{u}_0 = 0 = \hat{u}_N.$

• Interpolate \hat{u} so it is defined on the whole interval [0,1] with $\hat{u}(ih) = \hat{u}_i$.

• Next, note that

$$\frac{\hat{u}_{i+1} + \hat{u}_{i-1} - 2\hat{u}_i}{h^2} = \hat{u}'' + h^2 \frac{\hat{u}''''}{12} + O(h^4);$$
$$\frac{\hat{u}_{i+1} - \hat{u}_{i-1}}{2h} = \hat{u}' + h^2 \frac{\hat{u}'''}{6} + O(h^4);$$

• So consider the error

$$w = u - \hat{u};$$

Then

$$\varepsilon w_{xx} + w_x \sim h^2 \left(\varepsilon \frac{\hat{u}''''}{12} + \frac{\hat{u}'''}{6} \right)$$
$$\sim h^2 \left(\varepsilon \frac{u''''}{12} + \frac{u'''}{6} \right)$$
$$\sim -\frac{1}{12} \frac{h^2}{\varepsilon^3} \exp\left(-x/\varepsilon\right)$$

• The error $w = u - \hat{u}$ satisfies

$$\varepsilon w_{xx} + w_x \sim -\frac{1}{12} \frac{h^2}{\varepsilon^3} \exp\left(-x/\varepsilon\right); \quad w(0) = 0 = w(1)$$

Note the resonance! The solution is

$$w \sim \frac{1}{12} \frac{h^2}{\varepsilon^3} x \exp\left(-x/\varepsilon\right);$$

Maximum occurs at $x = \varepsilon$; max error is

$$\max w = \left(\frac{h}{\varepsilon}\right)^2 \frac{e^{-1}}{12}$$

Conclusion: $N=O(1/\varepsilon)$ for uniform mesh!!!

A two-sized mesh:

Take $l \in (0, 1)$ and discretize using uniform mesh of N_1 points inside [0, l] and another uniform mesh of $N_2 = N - N_1$ points inside [l, 1].

The error function $w = u - \hat{u}$ then satisfies:

$$\varepsilon w'' + w' \sim -\frac{1}{12} \begin{cases} \frac{l^2}{N_1^2 \varepsilon^3} e^{-x/\varepsilon}, & x \in (0, l) \\ \frac{(1-l)^2}{N_2^2 \varepsilon^3} e^{-x/\varepsilon}, & x \in (l, 1) \end{cases}$$

Define

$$r := N_2/N_1;$$

and write

$$N_1 = N \frac{1}{1+r}; \quad N_2 = N \frac{r}{1+r}$$

Assuming $l, \varepsilon \ll 1$, solving for w we obtain:

$$\begin{split} w &\sim \frac{1}{12} \frac{(1+r)^2}{N^2} \left\{ e^{-x/\varepsilon} \frac{xl^2}{\varepsilon^3} + e^{-l/\varepsilon} \frac{l^2}{\varepsilon^2} \left(\frac{1}{r^2} \frac{1}{l^2} - 1 \right) \left(1 - e^{-x/\varepsilon} \right) \right\}, x \in [0, l] \\ &\sim \frac{1}{12} \frac{(1+r)^2}{N^2} \left\{ \frac{e^{-x/\varepsilon}}{r^2} \frac{x}{\varepsilon^3} + (1 - \frac{1}{r^2 l^2}) \frac{l^2 e^{-x/\varepsilon}}{\varepsilon^2} \left(e^{-l/\varepsilon} - 1 + \frac{l}{\varepsilon} \right) \right\}, x \in [l, 1] \end{split}$$

Given ε , N, we want to determine l, r which minimizes the maximum of w.

The proper scaling is

$$l = \varepsilon \ln \frac{1}{\varepsilon} p;$$

The maximum of w is attained at $x^{\star} \sim \varepsilon \ll l;$ given by

$$w(x^{\star}) \sim \frac{1}{12} \frac{(1+r)^2}{N^2} \left\{ \exp\left(-1\right) \left(\ln\frac{1}{\varepsilon}\right)^2 p^2 + \varepsilon^{p-2} \frac{1}{r^2} \left(1 - \exp(-1)\right) \right\}$$

Minimizing with respect to p and r, we get:

$$p = 2; \ r = \left(\frac{e-1}{4}\right)^{1/3} \left(\frac{1}{\ln(1/\varepsilon)}\right)^{2/3};$$
$$\min_{l,r} \max_{x} w \sim \frac{1}{3e} \left(\frac{\ln\frac{1}{\varepsilon}}{N}\right)^{2}$$

Conclusion: $N=O(\ln(1/\varepsilon))$ for two-sized mesh!!! [this is exponentially better than $N=O(1/\varepsilon)$ scaling of the uniform mesh!!ç

Example 1: $\varepsilon := 10^{-8}$; N = 200.

• The optimal two-sized mesh is:

$$l = 3.6 \times 10^{-6}$$

 $r = 0.108 \implies N_1 = 180, N_2 = 20$

• Numerical error = 0.0013. Predicted error = 0.0014. Uniform mesh: Would need $N = 10^9$ meshpoints to get same accuracy!

Example 2: Direct comparison of uniform vs. split-range:

	N	error	error	
ε		(unif. mesh)	(optimal two-sided mesh)	
0.02	100	0.0080	0.00053	
0.01	100	0.035	0.00072	
0.005	100	0.14	0.00092	
0.0025	100	FAIL	0.0011	
10^{-3}	100		0.0012	
10 ⁻⁴	100		0.0028	
10^{-6}	100		0.0031	
10 ⁻⁶	200		0.00082	

Problem 2

Same ODE as problem 1:

$$\varepsilon^2 u'' - u + (1 + x^2) u^2 = 0; \quad u'(0) = 0; \quad \varepsilon u'(1) = -u(1).$$

but it has another solution of the form $u = w(\frac{x-x_0}{\varepsilon})$ where x_0 is approximately scales like

$$x_0 \sim \varepsilon \frac{1}{2} \ln \left(\frac{30}{\varepsilon x_0} \right) + O(1/\ln(\varepsilon))$$



Three different scales

- To leading order, $x_0 \sim \frac{1}{2} \varepsilon \ln(30/\varepsilon)$ has $O(\varepsilon \ln 1/\varepsilon)$
- The extent of the spike has $O(\varepsilon)$
- The outer problem has extend ${\cal O}(1)$
- The relative error in the asymptotics of x_0 is $O(1/\ln \varepsilon^{-1})$;
- This means that to asymptotics with numerics, we must take $1/\ln\varepsilon^{-1}\sim 0.1\implies\varepsilon\sim 10^{-5}!!!!$
- Challenge: can you compute with $\varepsilon \sim 10^{-4}$?
- Maple, matlab all fail for this problem when $\varepsilon \sim 10^{-3}$.

Problem 3

$$0 = u_{rr} + \frac{2}{r}u_r - u + u^2(\varepsilon + r), \quad u'(0) = 0, \, u'(\infty) = 0.$$
(3)

• **THEOREM:** In the limit $\varepsilon \ll 1$, Let $r_0 \gg 1$ be the large solution to the equation

$$\varepsilon \sim 30r_0^2 \exp\left(-2r_0\right).$$

Then there exists solutions of (3) of the form

$$u(r) \sim \frac{1}{r_0} w(r - r_0)$$

- Error is expected to be of $O(1/\ln(1/\varepsilon))$. To validate results, must take externely small ε ; for example if $\varepsilon = 10^{-3}$ then $r_0 \sim 5$, is not so small
- Standard codes [matlab, maple] all fail even for $\varepsilon = 10^{-2}$ [$r_0 \sim 5.5$].

Solve for ε instead

- Instead of fixing ε and solving for r_0 , fix r_0 then solve numerically the problem (3) first on $[0, r_0]$ with $u'(r_0^+) = 0$ and on $[r_0, \infty]$; with $u'(r_0^-) = 0$.
- Additional constraint $u\left(r_{0}^{-}\right) = u(r_{0}^{+})$ determines ε .
- Can get an accurate answer up to $r_0 \sim 9.5$. The method fails for bigger values of r_0 since the difference between $u(r_0^-) u(r_0^+)$ becomes smaller than the machine tolerance.

r_0	ε	Solution r_0 to $\varepsilon = 30r_0^2 e^{-2r_0}$	% err
4	0.05544	4.603	15.09%
4.5	0.02965	5.018	11.52%
5	0.015065	5.451	9.02%
5.5	0.007326	5.898	7.24%
6	0.003441	6.357	5.95%
6.5	0.001569	6.825	5.00%
7	0.0007028	7.297	4.25%
7.5	0.0003080	7.776	3.68%
8	0.0001336	8.256	3.20%
8.5	5.704e-5	8.74	2.83%
9	2.41e-5	9.227	2.52%

Discussion

- When splitting the integration range, take the splitting point to have order $l = O(\varepsilon \ln \varepsilon)$
- Problems with sharp interior boundary layers whose location depends on ε are difficult for standard solvers
- Matlab byp solver is currently better than maple's [as of Aug 2010]
- The asymptotics of the problem should be reflected in the numerics; the analytical insight is invaluable when looking for numerical solution, especially for nonlinear problems.