Convergence of Linear Multistep Methods on Smooth Nonuniform Grids

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- Statement of the problem
- Smooth nonuniform grids on compact intervals
- Zero stability on nonuniform grids
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Integrate $\dot{u} = f(u)$ on $[0, 1]$ using constant step size $h = 1/N$

$$\frac{1}{h}(\rho u)_n = \frac{1}{h}\sum_{j=0}^{k} \alpha_{k-j} u_{n-j} = \sum_{j=0}^{k} \beta_{k-j} f(u_{n-j}) = (\sigma f(u))_n$$

Linear difference equation can be interpreted as a *Toeplitz system*

$$N \cdot A_N U = B_N F(U)$$

with solution $U = \{u_j\}_{j=0}^{N}$ and $F_j(U) = f(U_j)$

0-stability *Are homogeneous solutions* $(N \cdot A_N)^{-1} U_0$ *bounded?*

Variable step size multistep methods

- Adaptive methods needed, especially for stiff problems
- Need *zero stability theory* on smooth nonuniform grids
- *Prove tolerance convergence of adaptive methods*

The extraneous operator

Constant step size

$$\frac{1}{h}(\rho y)_n = \frac{1}{h}\sum_{j=0}^{k} \alpha_{k-j} y_{n-j} = 0$$

- Characteristic polynomial $\rho(\zeta) = (\zeta - 1) \cdot \rho_{\mathcal{R}}(\zeta)$
- The *integrator* $\zeta - 1$ is present in all LMMs ("principal root")
- The *extraneous operator* $\rho_{\mathcal{R}}(\zeta)$ determines zero stability
- Adams methods, one-step methods have no extraneous operator but zero stability of interest in *BDF methods*

Uniform grids and operator factorization

Let $\nabla U = \{u_j - u_{j-1}\}_{j=1}^{N}$. Backward difference factorization

$$\rho = \mathcal{R}(\nabla) \cdot \nabla$$

where $\mathcal{R}(\nabla)$ is the *extraneous operator*

Example BDF2

$$\frac{1}{h}\left(\frac{3}{2}u_n - 2u_{n-1} + \frac{1}{2}u_{n-2}\right) = \frac{1}{h}\left(\nabla + \frac{\nabla^2}{2}\right)u_n = \left(1 + \frac{\nabla}{2}\right) \cdot \frac{\nabla}{h}\, u_n$$

Toeplitz operator factorization *BDF2*

$\rho u_n = 0$ in matrix–vector form, on uniform grid with $h = 1/N$

$$\frac{N}{2}\begin{pmatrix} 3 & 0 & 0 & 0 & 0 \\ -4 & 3 & \cdots & 0 & 0 \\ 1 & -4 & 3 & \cdots & 0 \\ & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1 & -4 & 3 \end{pmatrix} \begin{pmatrix} u_2 \\ u_3 \\ \vdots \\ \\ u_N \end{pmatrix} = \begin{pmatrix} 2Nu_1 - Nu_0/2 \\ -Nu_1/2 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Lower triangular Toeplitz operator $(NA_0)U = U_0$

Stability $\Leftrightarrow$ boundedness of inverse operator

Deflation and matrix factorization

BDF2 $\frac{1}{h}\left(\nabla + \frac{\nabla^2}{2}\right) u_n = \left(1 + \frac{\nabla}{2}\right) \cdot \frac{\nabla}{h}\, u_n$ is equivalent to

$$\frac{N}{2}\begin{pmatrix} 3 & 0 & 0 \\ -4 & 3 & \cdots \\ 1 & -4 & 3 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 3 & 0 & 0 \\ -1 & 3 & \cdots \\ 0 & -1 & 3 \end{pmatrix} \cdot N \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & \cdots \\ 0 & -1 & 1 \end{pmatrix}$$

Factorization into

- *Extraneous operator* $R_N(\mathbf{1})$
- *Backward difference operator* $\mathbf{D}_N$

Bounds on inverse lower triangular Toeplitz matrices

Lower triangular Toeplitz $\Rightarrow$ lower triangular *Toeplitz inverse*

$$\mathbf{D}_N^{-1} = \frac{1}{N}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & \cdots & 0 & 0 \\ 1 & 1 & 1 & \cdots & 0 \\ & \ddots & \ddots & \ddots & \vdots \\ 1 & \cdots & 1 & 1 & 1 \end{pmatrix} \quad \Rightarrow \quad \|\mathbf{D}_N^{-1}\|_\infty = 1$$

Strongly stable method $\rho_{\mathcal{R}}(\zeta) = 0 \Rightarrow |\zeta_j| < q < 1$ with bound

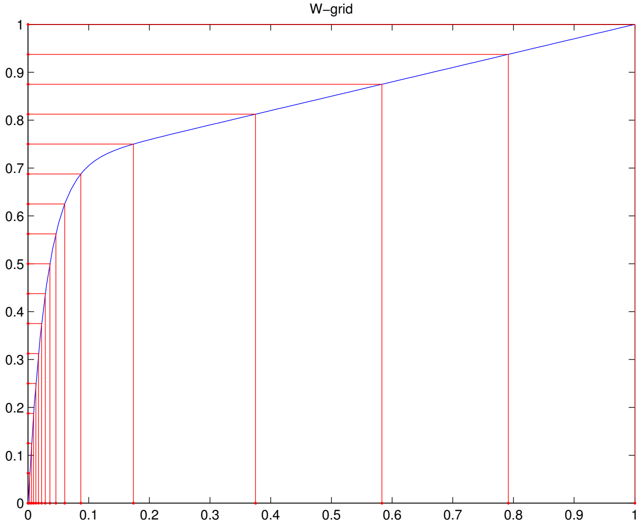
$$\|R_N^{-1}(\mathbf{1})\|_\infty \leq K_\infty \cdot \frac{q}{1-q}$$

1. Smooth nonuniform grids on compact intervals

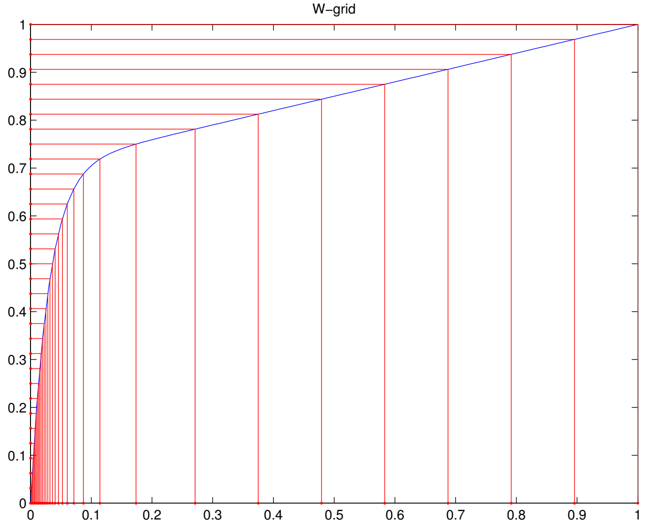
- Grid deformation map ('cdf') $\Phi : [0,1] \to [0,1]$
- $\Phi \in C^2[0,1]$, with 'pdf' $\Phi' = \varphi > 0$, and $\Phi(0) = 0$, $\Phi(1) = 1$
- Uniform grid $\tau_k = k/N$ maps to nonuniform grid $t_k = \Phi(\tau_k)$

$$h_k \;=\; t_{k+1} - t_k = \Phi(\tau_{k+1}) - \Phi(\tau_k) \;\approx\; \frac{\varphi(\tau_{k+1/2})}{N}$$

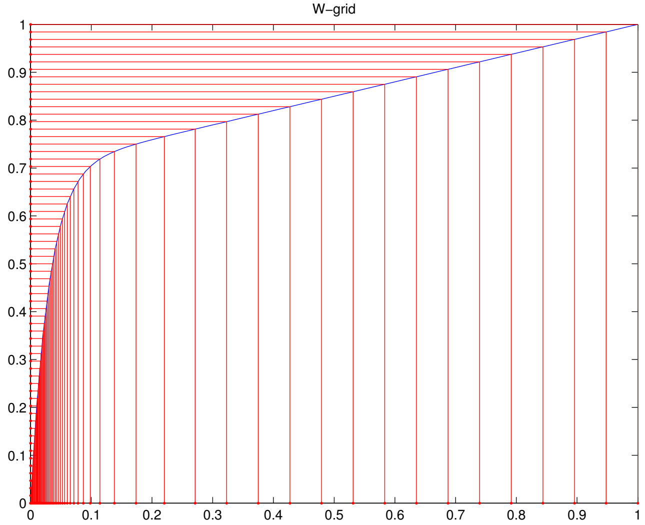
Grid deformation map $\Phi^{-1} : t \mapsto \tau$ $N = 15$



Grid deformation map $\Phi^{-1} : t \mapsto \tau$ $\quad N = 31$



Grid deformation map $\Phi^{-1} : t \mapsto \tau$ $\quad N = 63$



Grid smoothness as $N \to \infty$

Let $\Phi \in C^3[0,1]$ with derivative $\varphi = \Phi' > 0$, then

- Step sizes

$$h_k \approx \frac{\varphi}{N} \to 0$$

- Step ratios (cp. Gear & Tu, 1974)

$$r_{k-1} = \frac{h_k}{h_{k-1}} \approx 1 + \frac{1}{N} \cdot \frac{\varphi'}{\varphi} \to 1$$

- Consecutive ratios

$$\frac{r_k}{r_{k-1}} = \frac{h_{k+1} h_{k-1}}{h_k^2} \approx 1 + \frac{1}{N^2} \cdot \frac{\mathrm{d}^2 \log \varphi}{\mathrm{d}\tau^2} \to 1$$

Adaptive generation of smooth step sizes $\mu(t) = \varphi(\tau)$

Keeping $\|ch_n^p u^{(p+1)}\| = \mathrm{TOL}$, the ideal step size sequence has

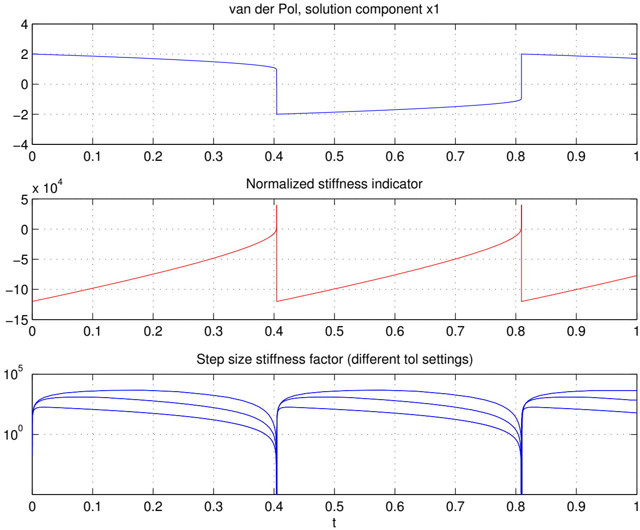
$$c \left(\frac{\mu(t_n)}{N} \right)^p \|u^{(p+1)}(t_n)\| = \mathrm{TOL}$$

Then

- $N \sim \mathrm{TOL}^{-1/p}$ implies $\mathrm{TOL} \to 0 \Rightarrow N \to \infty$
- $\mu(t) \sim \|u^{(p+1)}(t)\|^{-1/p}$ determines $\dot{\mu} = \varphi'/\varphi$

A well designed controller achieves high regularity if $u \in C^{p+2}[0, 1]$

Adaptively generated step sizes in van der Pol problem $\kappa = 200$



Variable step size method

$$\frac{1}{h_{n-1}} \sum_{j=0}^{k} \alpha_{n,k-j} u_{n-j} = \sum_{j=0}^{k} \beta_{n,k-j} f(u_{n-j})$$

Near-Toeplitz matrix-vector system $H_N^{-1} A_N(\bar{r}) U = B_N(\bar{r}) F(U)$

For $k = 2$, the system is a lower tridiagonal system

$$\begin{pmatrix} \frac{\alpha_{1,2}}{h_0} & 0 & 0 & 0 & 0 \\ \frac{\alpha_{2,1}}{h_1} & \frac{\alpha_{2,2}}{h_1} & \dots & 0 & 0 \\ \frac{\alpha_{3,0}}{h_2} & \frac{\alpha_{3,1}}{h_2} & \frac{\alpha_{3,2}}{h_2} & \dots & 0 \\ & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \frac{\alpha_{N,0}}{h_{N-1}} & \frac{\alpha_{N,1}}{h_{N-1}} & \frac{\alpha_{N,2}}{h_{N-1}} \end{pmatrix} \begin{pmatrix} u_2 \\ u_3 \\ \vdots \\ \vdots \\ u_N \end{pmatrix} = \dots$$

Example BDF2

$$\frac{1}{2h_{n-1}}\left(r_{n-2}^2 u_{n-2} - (1+r_{n-2})^2 u_{n-1} + (1+2r_{n-2})u_n\right) = f(u_n)$$

Factor out the integrator

$$\frac{-[-r_{n-2}^2 u_{n-2} + (1+2r_{n-2})u_{n-1}] + [-r_{n-2}^2 u_{n-1} + (1+2r_{n-2})u_n]}{2\varphi_{n-1/2}/N}$$

This is equivalent to

$$-\frac{r_{n-2}^2}{2\varphi_{n-1/2}}\frac{u_{n-1}-u_{n-2}}{1/N} + \frac{1+2r_{n-2}}{2\varphi_{n-1/2}}\frac{u_n-u_{n-1}}{1/N} = f(u_n)$$

This separates the *stable integrator* and the *extraneous operator*

Variable step size matrix factorization (deflation)

Theorem *Every strongly stable multistep method with step sizes* $h_n = \tilde{\varphi}_N / N$ *and* $H_N = \mathrm{diag}(h_{n-1})$*, has a factorization*

$$H_N^{-1} A_N(\varphi) = \tilde{\varphi}_N^{-1} R_N(\varphi) \cdot \mathbf{D}_N$$

with simple integrator $\mathbf{D}_N^{-1}$ *and extraneous operator* $\tilde{\varphi}_N^{-1} R_N(\varphi)$

Because $0 < \tilde{\varphi}_n < \infty$, zero stability is only a matter of having

$$\|R_N^{-1}(\varphi)\|_\infty \leq C_\varphi < \infty$$

as $N \to \infty$

It's complicated! BDF3 example

Difference equation (factorized operator) corresponding to $R_N(\varphi)$

$$\gamma_0(r_{n-2}, r_{n-3})z_{n-2} + \gamma_1(r_{n-2}, r_{n-3})z_{n-1} + \gamma_2(r_{n-2}, r_{n-3})z_n = 0$$

with coefficients

$$\gamma_2(r_2, r_1) = \frac{4r_1r_2 + r_2 + 3r_1^2r_2 + 2r_1 + 1}{r_2 + r_1^2r_2 + 2r_1r_2 + r_1 + 1}$$

$$\gamma_1(r_2, r_1) = -\frac{r_1^2(4r_1r_2^2 + r_1^2r_2^2 + 1 + 2r_1r_2 + 3r_2 + 3r_2^2)}{(r_2 + r_1^2r_2 + 2r_1r_2 + r_1 + 1)(r_2 + 1)}$$

$$\gamma_0(r_2, r_1) = \frac{(r_1 + 1)r_1^2r_2^3}{(r_2 + 1)(r_1r_2 + r_1 + 1)}$$

Write $r_n = 1 + s_n$ with $s_n = \mathrm{O}(N^{-1})$ and $s_n - s_{n-1} = \mathrm{O}(N^{-2})$

Step ratios $r_n = 1 + s_n$ with $S = \mathrm{diag}(s_n)$

$$s_n \approx \frac{\varphi_n'}{\varphi_n} \cdot \frac{1}{N} \quad \Rightarrow \quad \|S\|_\infty = \frac{1}{N} \left\| \frac{\varphi'}{\varphi} \right\|_\infty$$

Let $T_0 = R_N(\mathbf{1})$ and write *variable step size* extraneous operator

$$R_N(\varphi) = T_0 + S_1 T_1 + S_2 T_2 + \dots S_{k-1} T_{k-1} + \mathrm{O}(N^{-2})$$

Stability on smooth grid $S_j = S + \mathrm{O}(N^{-2})$

$$R_N^{-1}(\varphi) = R_N^{-1}(\mathbf{1}) \cdot (I + S \sum_{j=1}^{k-1} T_j T_0^{-1})^{-1} + \mathrm{O}(N^{-2})$$

All T_j are bounded Toeplitz operators and $\| T_j T_0^{-1} \|_\infty \le C_j < \infty$

3. Convergence analysis

Compare numerical and exact solutions

$$H_N^{-1} A_N(\bar{r}) U_N = B_N(\bar{r}) F(U_N)$$
$$H_N^{-1} A_N(\bar{r}) V_N = B_N(\bar{r}) F(V_N) - d_N$$

Global error $e_N = U_N - V_N$ satisfies

$$H_N^{-1} A_N(\bar{r}) e_N = B_N(\bar{r}) \cdot (F(V_N + e_N) - F(V_N)) + d_N$$

Error equation

All matrices involved,

$$
\begin{aligned}
H_N &= \tilde{\varphi}/N \\
A_N(\bar{r}) &= R_N(\bar{r}) \cdot \nabla \\
\mathbf{D}_N &= N \cdot \nabla
\end{aligned}
$$

are *lower triangular* and imply *componentwise inequality*

$$\nabla |e_N| \leq |R_N^{-1}(\bar{r})| \cdot \tilde{\varphi} \cdot |B_N(\bar{r})| \cdot L[f/N] \cdot |e_N| + |R_N^{-1}(\bar{r})| \cdot \tilde{\varphi} \cdot |d_N|$$

Note If $|R_N^{-1}(\bar{r})|$ is bounded and $L[f] < \infty$ then one can chose a large enough $N > N^*$ such that *there is a unique solution* $|e_N| > 0$

Preliminary error bound

Assume the uniform spectral radius bound

$$\frac{L[f]}{N} \cdot \rho[\,|R_N^{-1}(\bar{r})| \cdot \tilde{\varphi} \cdot |B_N(\bar{r})|\,] \leq \Theta < 1$$

The global error is majorized by $|e_N| \leq E_N$, where

$$\nabla E_N = |R_N^{-1}(\bar{r})| \cdot \tilde{\varphi} \cdot |B_N(\bar{r})| \cdot L[f/N] \cdot E_N + |R_N^{-1}(\bar{r})| \cdot \tilde{\varphi} \cdot |d_N|$$

with solution

$$E_N = \left(\nabla - |R_N^{-1}(\bar{r})| \cdot \tilde{\varphi} \cdot |B_N(\bar{r})| \cdot L[f/N]\right)^{-1} |R_N^{-1}(\bar{r})| \cdot \tilde{\varphi} \cdot |d_N|$$

Final result

$$\|e_N\|_\infty \leq C_\infty \cdot \|\tilde{\varphi} \cdot d_N\|_\infty \to 0$$

with

$$C_\infty = \|(\nabla - |R_N^{-1}(\bar{r})| \cdot \tilde{\varphi} \cdot |B_N(\bar{r})| \cdot L[f/N])^{-1}\|_\infty \cdot \|R_N^{-1}(\bar{r})\|_\infty$$

The result is far from the desired structure

Thank you!