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Lecture 5 ODE solvers, stiff ODE, stability.

Large linear system of ODE

$$\dot{u} = Au$$

eigenvalues of A:

Parabolic (heat eqn)

$$\lambda_1 = -1, \quad \lambda_2 = -4, \quad \ldots, \quad \lambda_n = -n^2, \quad \sim -\frac{1}{\Delta x^2}.$$

negative real axis

Hyperbolic (acoustics)

$$\lambda_1, \lambda_2 = \pm i$$

$$\lambda_3 \; \lambda_4 = \pm 2i$$

$$\vdots$$

$$\lambda_{n-1}, \lambda_n = \pm \frac{n}{2} i = \pm \frac{i}{\Delta x}$$

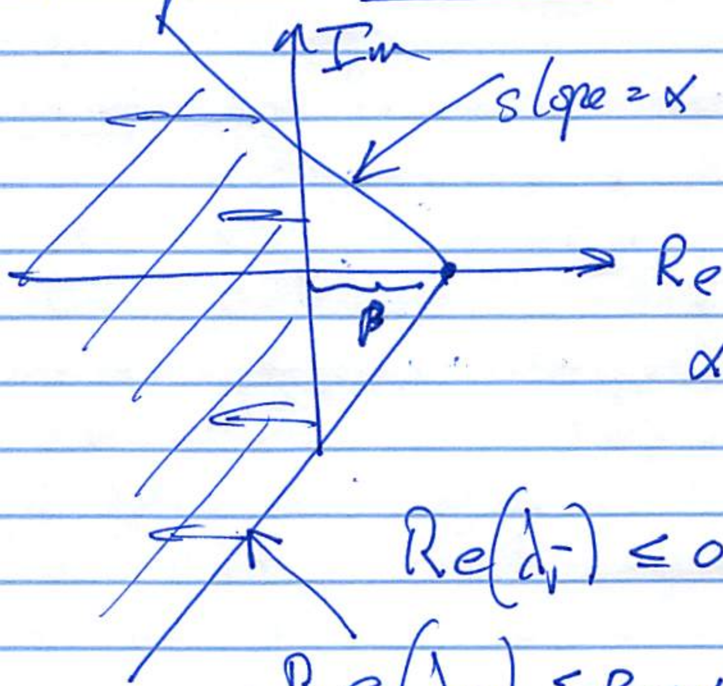
Imaginary axis

More general Stable: $Re(\lambda_j) \le 0$

(2)

stiff: some $|\lambda_j|$ much smaller than other $|\lambda_j|$

Parabolic PDE with advection & other things: <u>Sectorial</u>



$\alpha > 0$.

$\mathrm{Re}(\lambda_j) \le 0$

$\mathrm{Re}(\lambda_j) \le \beta - \alpha\,|\mathrm{Im}(\lambda_j)|$

<u>Hyperbolic</u> problems are not sectorial.

Assume (for now) A is diagonalizable

$$A = Q \Lambda Q^{-1}.$$

Runge Kutta method

$\xi_1 = \Delta t\, A u$

② ③

$$\xi_2 = \Delta t A(U + b_{11}\Delta t A U)$$
$$= \Delta t A U + b_{11}(\Delta t A)^2 U$$

$$\xi_3 = \Delta t A(U + b_{21}\Delta t A U + b_{22}\Delta t A U + b_{11}(\Delta t A)^2 U)$$
$$= \Delta t A U + c\,\Delta t^2 A^2 U + d\,\Delta t^3 A^3 U$$

etc.

r-stage explicit RK:

$$U_{k+1} = P_r(\Delta t A)\cdot U_k$$

polynomial degree r.

Diagonalize

$$Q^{-1}AQ = \Lambda$$

$$Q^{-1}P_r(\Delta t A)Q = P_r(\Delta t \Lambda)$$
$$= \mathrm{diag}(\Delta t \lambda_j).$$

$$W_{k+1} = P_r(\Delta t \Lambda)W_k$$

$W_k = Q^{-1}U_k =$ vector of eigenvector coefficients.

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$$W_{k+1,j} = P_r(\Delta t\,\lambda_j)\,W_{k,j}$$

k = time step

j = component

Consider the generic drop j.

$$w_{k+1} = P_r(\mu)\,w_k, \qquad \mu = \lambda\,\Delta t$$

<u>Stability region</u> $\Sigma \subseteq \mathbb{C}$

$$\mu \in \Sigma \text{ if } |P_r(\mu)| \leq 1.$$

- For stiff problems, we want Σ to be large
- For specific kinds of stiff problems we want Σ to be large in specific ways
- Mainly interested in whether μ with $Re(\mu) \leq 0$ is in Σ, do not

seek to stabilize unstable systems, though this does happen.

e.g. forward Euler

$$U_{k+1} = (I + \Delta t A) U_k$$

$$P(\mu) = 1 + \mu$$

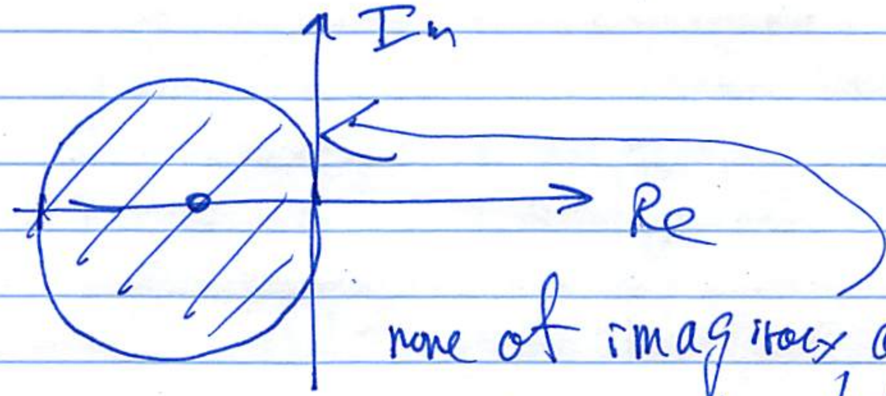
if $\mu = \tau + i\omega$, for what τ, ω

is $|1 + \tau + i\omega| \le 1$.

$$(1+\tau)^2 + \omega^2 \le 1$$

= ~~circle in co~~ disk in complex plane

center $= -1$, radius $= 1$



none of imaginary axis

$\Longrightarrow$ always unstable for hyperbolic problems.

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real axis stability to $\tau = -2$

$\Rightarrow$ CFL stability limit for forward Euler for heat eqn (more on that coming).

e.g. Predictor/corrector mid point rule

$$w_{k+\frac{1}{2}} = \left(1 + \tfrac{1}{2}\mu\right) w_k$$

$$\begin{aligned} w_{k+1} &= w_k + \mu\, w_{k+\frac{1}{2}} \\ &= w_k + \mu\left(1 + \tfrac{1}{2}\mu\right) w_k \\ &= \underbrace{\left(1 + \mu + \tfrac{1}{2}\mu^2\right)}_{\text{1st 3 terms of Taylor formula for } e^{\mu}} w_k \end{aligned}$$

Any 2-stage 2nd order method has the same:

$$u_{k+1} = \left(I + \Delta t A + \frac{\Delta t^2}{2} A^2\right) u_k$$

- It must be polynomial degree 2 (2 stages)
- It must agree with $e^{\Delta t A}$ up to 2^{nd} order terms $\Rightarrow$

must be terms up to 2^{nd} order.

Same reasoning for 3-stage 3^{rd} order and 4 stage 4^{th} order.

2^{nd} order stability diagram:

$$\left| 1 + \tau + i\omega + \tfrac{1}{2}(\tau + i\omega)^2 \right| \le 1$$

$$\left| 1 + \tau + i\omega + \tfrac{1}{2}\tau^2 + i\tau\omega - \tfrac{1}{2}\omega^2 \right| \le 1$$

$$\left(1 + \tau + \tfrac{1}{2}(\tau^2 - \omega^2)\right)^2 + \cancel{\omega \tfrac{1}{2}\omega}\,(\omega - \tau\omega)^2 \le 1$$

complicated - degree 4 in 2 variables

Make pictures numerically.

analytically, explore real + imaginary axes.

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Real: $\omega = 0$

$$|1 + \tau + \tfrac{1}{2}\tau^2| \le 1$$

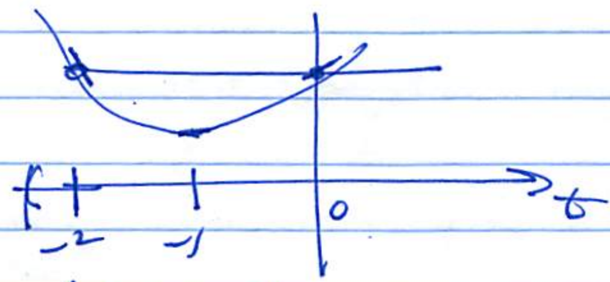
look at the fn $1 + \tau + \frac{1}{2}\tau^2$:

it's quadratic in τ, $= 1$ when $\tau = 0$

min at $1 + \tau = 0$, $\tau = -1$

Symmetric: $= 1$ when $\tau = -2$

min value: $\tau = -1 \Rightarrow 1 + \tau + \frac{1}{2}\tau^2 = \frac{1}{2}$



stable for $-2 \le \tau \le 0$

same stability region as forward Euler

Imag (hyperbolic problems) $\mu = i\omega$

$$\left| 1 + i\omega + \tfrac{1}{2}(i\omega)^2 \right| \le 1$$

$$\left| 1 + i\omega - \tfrac{1}{2}\omega^2 \right|^2 \le 1$$

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$$\left(1-\tfrac{1}{2}\omega^2\right)^2+\omega^2\le 1$$

$$1-\omega^2+\tfrac{1}{4}\omega^4+\omega^2\le 1$$

$1+\tfrac{1}{4}\omega^4\le 1$ never happens.

2^{nd} order 2-stage explicit RK

is <u>unstable for</u> hyperbolic problems.

3^{rd} order 3 stage, hyperbolic

$\mu=i\omega$ $\quad \left|1+\mu+\tfrac{1}{2}\mu^2+\tfrac{1}{6}\mu^3\right|\le 1.$

$$\left|1+i\omega-\tfrac{1}{2}\omega^2-\tfrac{1}{6}i\omega^3\right|\le 1$$

$$\left(1-\tfrac{1}{2}\omega^2\right)^2+\left(\omega-\tfrac{1}{6}\omega^3\right)^2\le 1$$

$$1-\cancel{\omega^2}+\tfrac{1}{4}\omega^4+\cancel{\omega^2}-\tfrac{1}{3}\omega^4+\tfrac{1}{36}\omega^6\le 1$$

$$\cancel{1}-\tfrac{1}{12}\omega^4+\tfrac{1}{36}\omega^6\le\cancel{1}$$

$$-\tfrac{1}{12}\omega^4+\tfrac{1}{36}\omega^6\le 0$$

find roots:

$$-\omega^4+\tfrac{1}{3}\omega^6=0$$

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$\omega = 0$ or $\omega^2 = 3$

$\omega = \sqrt{3}$ ~ 3 stages

Imaginary axis stability 1.7

stable for $\mu = i\omega$ with $|\omega| \le \sqrt{3}$.

Stable for hyperbolic problems.

~~advan~~ advance ~ $1.7/3 = .56$

per stage.

4th order 4 stage, $\mu = i\omega$

similar analysis, stability if $|\omega| \le 2\sqrt{2}$
$= 2.8$

$\approx .7$ per stage = slightly

better than 3-stage.

Linear multi-step methods:

$$u_{k+1} = a_0 u_k + \cdots + a_s u_{k-s}$$
$$+ \delta t \left(b_0 A u_k + \cdots + b_s A u_{k-s} \right)$$

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diagonalize as before

$$w_{k+1} = a_0 w_k + \cdots + a_s w_{k-s}$$
$$+ \mu (b_0 w_0 + \cdots + b_s w_{k-s})$$

(*) $$w_{k+1} = c_0 w_k + \cdots + c_s w_{k-s}$$

$$c_j = a_j + \mu b_j$$

stability $\rightarrow$ $\sup_k |w_k| \le C \left(|w_0| + \cdots + |w_s| \right)$

There is a C so that ← initial data

solution → $|w_k| \le C \left(|w_0| + \cdots + |w_s| \right)$

the solution is bounded by the initial data uniformly in k.

(Recall: we take $\Delta t \to 0$, $k \to \infty$ with t_k fixed)

Characteristic roots of (*) numbers z so that $w_k = z^k$ satisfy (*).

$$z^{k+1} = c_0 z^k + \cdots + c_s z^{k-s}$$

divide out z^{k-s}

$$z^{s+1} = c_0 z^s + \cdots + c_s$$

$$z^{s+1} - c_0 z^s - \cdots - c_s = 0$$

$p(z) = z^{s+1} - \cdots - c_s$ = characteristic polynomial

degree $s+1$

roots (with multiplicity) $z_0, \dots, z_s$

Thm The recurrence relation (*) is stable if & only if the roots are stable in the sense that

(i) $|z_j| \leq 1$ for all roots z_j

(ii) if $|z_j| = 1$ then z_j is a simple root: $p'(z_j) = (s+1)z^s - s c_0 z^{s-1} - \cdots - s_1 \neq 0$.

Proof: Only if: (i) or (ii) is violated

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it is not stable. Because...

if (i) is violated & there is a $|z|>1$ with $p(z)=0$, then ~~z^k grow~~ $|w_k| = |z^k| \to \infty$ as $k \to \infty$ (exponentially).

if (ii) is violated then

$$p(z)=0, \quad p'(z)=0, \quad |z|=1.$$

Then $w_k = k z^k$ satisfies ⊛

check:

$$(k+1) z^{k+1} \stackrel{?}{=} c_0 k z^k + \dots + c_s (k-s) z^{k-s}$$

check: $k+1 = k-s+s+1$
$k = k-s+s$

$$\underline{(k-s) z^{k+1}} + \underline{\underline{(s+1) z^{k+1}}} \stackrel{?}{=} c_0 \underline{(k-s) z^k} + \underline{\underline{c_0 s z^k}} + \dots + c_s \underline{(k-s) z^{k-s}}$$

← The single underline terms are

$$(k-s) z^{k+1} \stackrel{?}{=} c_0 (k-s) z^k + \dots + c_s (k-s) z^{k-s}$$

yes, because $p(z)=0$

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The double underline terms

$$(s+1)\,z^{k+1} \stackrel{?}{=} c_0\, s\, z^{k} + \cdots + c_{s-1}\, z^{k-s+1}$$

divide by z^{k-s+1} (not z^{k-s})

$\cancel{(s+1)\, z^{k} \stackrel{?}{=}}$

$$(s+1)\,z^{s} \stackrel{?}{=} c_0\, s\, z^{s-1} + \cdots + c_1$$

yes, because $p'(z_j)=0$.

This is the "only if" part

if there is a $|z_j|>1$ or a $|z_j|=1$ that is not simple the recurrence is unstable.

The "if" part: I do this more generally using matrices rather than in the special case of scalar recurrence relations.

Consider the vector $x_k \in \mathbb{C}^{s+1}$ given by

$$x_k = \begin{pmatrix} w_k \\ w_{k-1} \\ \vdots \\ \\ w_{k-s} \end{pmatrix}$$

Then $x_{k+1} = M x_k$, where the companion matrix is

$$M = \begin{pmatrix} c_0 & c_1 & \cdots & & c_s \\ 1 & 0 & & & \\ 0 & 1 & & 0 & \\ & & \ddots & & \\ & 0 & & & \\ 0 & & & 1 & 0 \end{pmatrix}$$

It is easy to see that an eigenvalue of M is a characteristic root of the recurrence relation. It is also easy (≤ 30 min) that ~~of M~~ any double or higher ~~order~~ multiplicity eigenvalue of M corresponds to a Jordan block of M.

<u>Review of the relevant algebra</u>

$$p(z) = z^{s+1} - c_0 z^s - \cdots - c_s$$

factors as a product of the roots

$$p(z) = \prod_{k=0}^{s} (z - z_k)$$

characteristic roots

If, say z_1 is a double root, then

$$p(z) = (z - z_1)^2 \, g(z)$$

product of the remaining $s-1$ factors

Therefore

$$\cancel{p(z_k)} \Rightarrow p(z_1) = 0$$

and $p'(z_1) = 2(z - z_1) g(z) + (z - z_1)^2 g'(z)$

$= 0.$

Thus $k z_1^k$ also satisfies the recurrence relation.

If $|z_1| = 1$ then $|k z_1^k| = k \to \infty$

as $k \to \infty \Longrightarrow$ unstable.

So suppose $|z_j| \le 1$ for all

z_j eigenvalue of M

$|z_j| = 1 \Longrightarrow z_j$ is a simple eigenvalue.

Then there is a C so that

$\|M^k\| \le C$ for all k.

bounded total growth, same C for all k.

<u>Proof</u>: Lemma: If z_1 is a simple eigenvalue of M then there is a basis of $\mathbb{C}^{s+1}$ so that in this basis M has elements $\tilde{M}_{ij}$

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$$\left(\begin{array}{c|ccc} z_1 & 0 & \text{—} & 0 \\ \hline 0 & & & \\ | & & \tilde{M}_{s\times s} & \\ 0 & & & \end{array}\right)$$

z_1 not an eigenvalue of $\tilde{M}$

<u>Proof of Lemma</u>: suppose first $z_1 = 0$

The hypothesis in this case is that M is singular (an eigenvalue equal to zero) but ① if $x \in \text{Range}(M) = R \subseteq \mathbb{C}^{s+1}$ then $Mx \neq 0$ ② $\dim(R) = s$

To see ②, if $\dim(R) < s$ then there are two linearly independent eigenvectors of M with eigenvalue zero.

To see ① if $x \in \text{Range}(M)$, then $x = My$ for some $y \in \mathbb{C}^{s+1}$.

if $Mx = 0$ then $x = c\,v$, where

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$Mv = 0$, $v \neq 0$ (v is "the" eigenvector with eigenvalue zero).

Thus, $My = c \cdot v$. This makes y part of the Jordan block of M for eigenvalue zero.

~~(Lemma, if zero is~~

Therefore M defines a linear map $R \to R$. Pick a basis for R and add the eigenvector v to get a basis of $\mathbb{C}^{s+1}$.

~~This proves~~ Done with $z_1 = 0$ case.

Now if $z_1 \neq 0$, apply to $M - z_1 I$.

Therefore, if $z_1, \ldots, z_k$ are the eigenvalues of M with $|z_j| = 1$ and

$|z_j| < 1$ for $j > k$ ~~so~~ there is a basis of ~~the with~~ when M takes the form

$$\left(\begin{array}{c|c} \begin{matrix} z_1 & & 0 \\ & \ddots & \\ 0 & & z_k \end{matrix} & 0 \\ \hline 0 & \tilde{M} \end{array}\right)$$

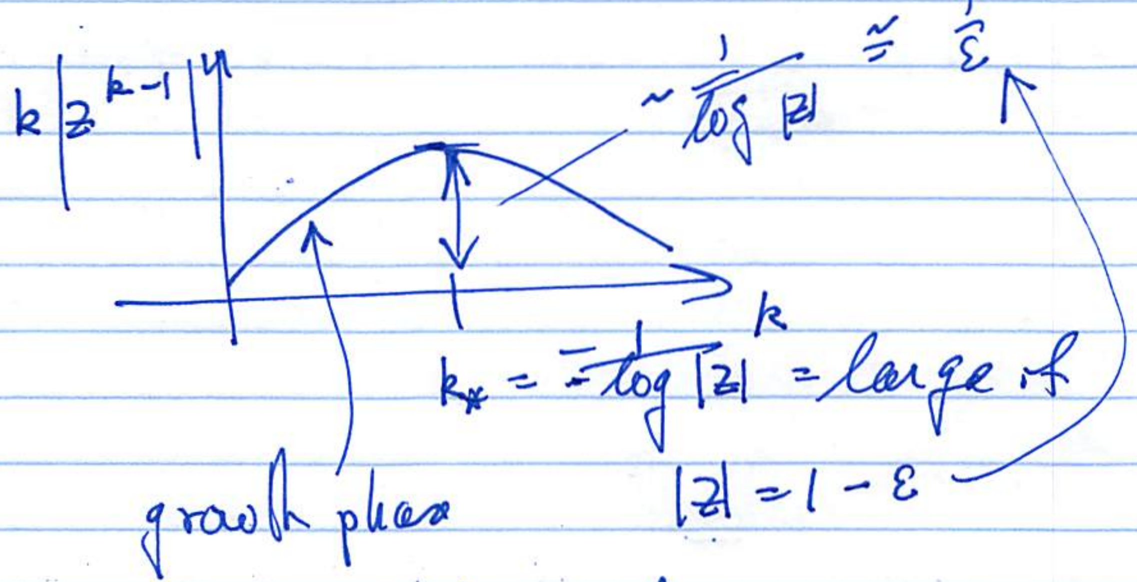
<u>Lemma</u> (the main point): If M is a matrix with $|z_j| < 1$ for all j, then there is a norm $\|\cdot\|$ in which M is a contraction:

$$\|M x\| < \|x\| \quad \text{if} \quad x \neq 0.$$

<u>Proof</u>: You can think of this as being related to Jordan blocks. Suppose

$$M = \begin{pmatrix} z & 1 \\ 0 & z \end{pmatrix}$$

Then $M^k = \begin{pmatrix} z^k & k z^{k-1} \\ 0 & z^k \end{pmatrix}$



transient growth

changing, doesn't last forever

Write the recurrence relation

$$\begin{pmatrix} x_{k+1} \\ y_{k+1} \end{pmatrix} = \begin{pmatrix} z & 1 \\ 0 & z \end{pmatrix} \begin{pmatrix} x_k \\ y_k \end{pmatrix}$$

$x_{k+1} = z x_k + y_k$

$y_{k+1} = z y_k$

(2D)

The x component can grow because it is "forced" by the y component. The y component doesn't grow. The growth of the x component depends on the size of the y component. Want a function $f(x,y)$ that measures progress toward zero. Give a lot of weight to y so that the benefit from y-progress outweighs the setback of x increasing

$$\|(x,y)\| = \cancel{x^2+w} \; |x| + r|y|$$

$$\|(x_{k+1}, y_{k+1})\| = |z x_k + y_k| + r|z||y_k|$$

$$\leq |x_k| + |y_k| + \cancel{2r(1-|z|)} \; r|z||y_k|$$

$$\leq |x_k| + r|y_k| \text{ if}$$

$$|y_k| + r|z||y_k| \le r|y_k|$$

$$\frac{1}{r} + |z| \le 1 \qquad \underline{r \ge \frac{1}{1-|z|}}.$$

(as the calculation suggested.

(Rest as exercise).

Convergence proofs for ~~Adams~~

<u>Linear multistep methods:</u>

$$U_{k+1} = a_0 U_k + \dots + a_s U_{k-s}$$
$$+ \Delta t\left(b_0 F(U_k) + \dots + b_s F(U_{k-s})\right)$$

The method is zero-stable if the a-recurrence relation is stable (simple roots with $|z|=1$, all roots $|z| \le 1$). This is the same as being "linearly" stable when applied

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to $\dot{w} = \lambda w$ with $\lambda = 0$.

Thm if the LMM is zero-stable and formally accurate of order p, and if $F(U)$ is globally Lipschitz, and if $U_j = U(t_j)$ for $0 \le j \le s$, then

$$|U_k - U(t_k)| \le C_T \Delta t^p \quad \text{for } t_k \le T$$

uniformly as $\Delta t \to 0$.

Proof: Define $X_k = (U_k, U_{k-1}, \dots, U_{k-s})$

$X_k \in \mathbb{R}^{s \cdot d}$ if $U_k \in \mathbb{R}^d$.

Let $\|X\|$ be the norm in which the a-recurrence relation is stable

~~if~~ $\cancel{X_{k+1} = a_0 X_k + \dots +}$

if $U_{k+1} = a_0 U_k + \dots + a_s U_{k-s}$

then $\|X_{k+1}\| \le \|X_k\|$.

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Let L_F be the Lipschitz constant for F in this norm (see below).

Then

$$X_{k+1} = \tilde{M} X_k + \Delta t \tilde{F}(X_k)$$

where

$$\tilde{F}(X_k) = b_0 F(U_k) + \cdots + b_s F(U_{k-s})$$

$$X(t_{k+1}) = \tilde{M} X(t_k) + \tilde{F}(X(t_k)) + \Delta t \tilde{R}_k$$

and the proof is as before.

A-stable methods:

Stable whenever applied to $\dot{w} = \lambda w$ for $\Delta t = 1$, $Re(\lambda) \le 0$.

<u>Must be implicit:</u>

e.g. Backward Euler

$$U_{k+1} = U_k + \Delta t\, F(U_{k+1})$$

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$$U_{k+1} = U_k + \mu U_{k+1} \quad \left(F(U) = \lambda U, \; \mu = \lambda \Delta t \right)$$

$$U_{k+1} = \frac{1}{1-\mu} U_k$$

$$\mu = \tau + i\omega$$

$$\left| \frac{1}{1-\mu} \right| = \frac{1}{(1-\tau)^2 + \omega^2} < 1$$

if $\tau \le 0$, any ω.

Trapezoid rule (2nd order)

$$U_{k+1} = U_k + \frac{\Delta t}{2}\left(F(U_k) + F(U_{k+1}) \right)$$

$$U_{k+1} = U_k + \frac{\mu}{2} U_k + \frac{\mu}{2} U_{k+1}$$

$$U_{k+1} = \frac{1+\frac{\mu}{2}}{1-\frac{\mu}{2}} U_k$$

$$= \frac{1 + \frac{\tau}{2} + \frac{i\omega}{2}}{1 - \frac{\tau}{2} - \frac{i\omega}{2}} U_k$$

(27)

Note: $M = \dfrac{1+\frac{\tau}{2}+\frac{i\omega}{2}}{1-\frac{\tau}{2}-\frac{i\omega}{2}} \to -1$

as $\tau \to -\infty$. This is "ringing".
The mode that is supposed to disappear very fast: $\dot{u} = -\lambda u$, λ large, is instead "rings" $u_{k+1} \approx -u_k$.

Calculation:

$$|M|^2 = \frac{\left(1+\frac{\tau}{2}\right)^2+\omega^2}{\left(1-\frac{\tau}{2}\right)^2+\omega^2}$$

$$= \frac{1+\frac{\tau^2}{4}+\omega^2+\tau}{1+\frac{\tau^2}{4}+\omega^2-\tau}$$

The bottom is larger than the top ($|M|<1$) if $\tau<0$.

Trap is stable for the heat equation with any CFL: make \$ on Wall Street with this.

BDF (Backward differentiation formula)

$$\dot{u}(t+\Delta t) = \frac{1}{\Delta t}\left(\frac{3}{2}u(t+\Delta t) - 2u(t) + \frac{1}{2}u(t-\Delta t)\right) + O(\Delta t^2)$$

(second order

$\cancel{u_{k+1} = \frac{1}{\Delta t}}$

$$\frac{1}{\Delta t}\left(\frac{3}{2}u_{k+1} - 2u_k + \frac{1}{2}u_{k-1}\right) = F(u_{k+1})$$

is second order.

also A-stable - complicated but not hard.

Dahlquist saturation theorem

A linear multistep method that is A-stable is at most second order accurate.