Solving linear differential equations

Any linear diff. eq. can be reduced to first order system

$$x'(t) = A(t)x(t) + b(t) \in \mathbb{R}^{N_x}$$

$$x(0) = x_0$$

$A(t) \in \mathbb{R}^{N_x \times N_x}$ is s-sparse, $s \in \mathbb{N}$.

Idea 1: Lie-Trotter approach.

$\Rightarrow$ exponential cost in t

$\Rightarrow$ no inhomogeneous equations

Idea 2: Space-time approach

Feynman's clock: Encode time in basis states $|j\rangle$ and produce output state

$$|\psi\rangle := \sum_{j=0}^{N_t} |j\rangle |x_j\rangle$$

where $x_j \approx x(t_j)$

arXiv: 1010.2745
High-order q. alg. for solving ODEs

Here $N_t = T/\tau$ ... number of timesteps

T ... Final time

τ ... size of timestep.

Problem: Probability of measuring $x(T) \approx x_{N_t}$ is small. Idea: extend ODE beyond T with

$$A(t) := I \,, \quad b(t) = 0 \quad \forall\, t \in (T, 2T].$$

$\Rightarrow \quad x(t) = x(T) \quad \forall\, t \in [T, 2T]$

$\Rightarrow$ increased probability.

Example: Forward Euler

$$\frac{x_{j+1} - x_j}{\tau} = A(t_j)\, x_j + b(t_j) \qquad \forall\, t \in [0, 2T]$$

define
$$\vec{x} := \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{2N_t} \end{pmatrix}, \quad \vec{b} := \begin{pmatrix} x_0 \\ b_0 \tau \\ b_1 \tau \\ \vdots \\ b_{N_t} \tau \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\underline{A} = \begin{pmatrix} I & & & & & \\ -(I+A\tau) & I & & & O & \\ & \ddots & \ddots & & & \\ & & -(I+A\tau) & I & & \\ & O & & -I & I & \\ & & & & \ddots & \ddots \\ & & & & -I & I \end{pmatrix} \in \mathbb{R}^{2N_t N_x \times 2N_t N_x}$$

$$\sqrt{\sum_{i=1}^{n} i^2} \simeq \sqrt{n^3} = n^{\frac{3}{2}}$$

$\Rightarrow$ Euler $\Leftrightarrow$ $\underline{\underline{A}\vec{x} = \vec{b}}$

Informal Analysis: local Euler error $\simeq \tau^2$

$\Rightarrow$ Error at end-time $2N_t \tau^2 \simeq \frac{T^2}{N_t}$

to achieve error $\simeq \varepsilon$, we need $\underline{N_t \simeq \frac{T^2}{\varepsilon}}$

Use HHL Algorithm to solve linear system

$\Rightarrow$ require bounded cond. number

$$\|\underline{A}^{-1}\| \geq \frac{\|x\|}{\|b\|}$$

Consider $\begin{pmatrix} 1 & & 0 \\ -1 & \ddots & \\ 0 & \ddots & 1 \\ & -1 & 1 \end{pmatrix} \cdot \underbrace{\begin{pmatrix} 1 \\ 2 \\ 3 \\ \vdots \\ n \end{pmatrix}}_{x} = \underbrace{\begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}}_{b} \Rightarrow = \frac{\sqrt{\sum_{i=1}^{n} i^2}}{\sqrt{\sum_{i=1}^{n} 1}} \simeq \frac{n^{\frac{3}{2}}}{n^{\frac{1}{2}}} \simeq \underline{n}$

Hence $\kappa \simeq 2 M_t M_x \simeq T^2$

$\uparrow$ cond. number of $\underline{A}$

$\Rightarrow$ HHL Alg requires at least $\kappa^2 \simeq T^4$ operations

possible improvement:

<u>Multistep methods</u>

$$\sum_{e=0}^{k} \alpha_e x_{j+e} = \tau \sum_{e=0}^{k} \beta_e \left(A(t_{j+e}) x_{j+e} + b(t_{j+e}) \right)$$

Stability of method given by

$$\rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j \quad , \quad \sigma(\xi) = \sum_{j=0}^{k} \beta_j \xi^j$$

Let $R_j(\mu)$ denote the roots of

$$\rho(\xi) - \mu \sigma(\xi) = 0$$

and define

$$S := \left\{ \mu \in \mathbb{C} \;\middle|\; \begin{array}{l} \text{all roots } R_j(\mu) \text{ satisfy } |R_j(\mu)| \leq 1 \\ \text{multiple roots } R_j(\mu) \text{ satisfy } |R_j(\mu)| < 1 \end{array} \right\}$$

if all roots of σ satisfy $\Rightarrow$ method is stable at infinity.

In matrix form, the method reads

$$\underline{A}_{j,j} = I \qquad 0 \le j < k, \quad N_t < j \le 2N_t$$

$$\underline{A}_{j,j-1} = -(I + A\tau) \qquad 1 \le j < k$$

$$\underline{A}_{j,j-k+l} = \alpha_l I - \beta_l A\tau \qquad k \le j \le N_t, \quad 0 \le l \le k$$

$$\underline{A}_{j,j-1} = -I \qquad N_t < j \le 2N_t$$

$$b_0 = x_0$$

$$b_j = bh \qquad 1 \le j < k$$

$$b_j = \sum_{l=0}^{k} \beta_l bh \qquad k \le j \le N_t$$

$$b_j = 0 \qquad N_t < j \le N_t$$

Assume Oracles: $O_A |j,l\rangle |z\rangle = |j,l\rangle\, z \oplus A_{jl}$

binary rep.

$O_F |j,l\rangle = |j, f(j,l)\rangle$

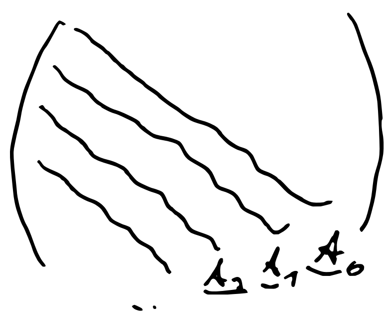
$\hookrightarrow$ lth nonzero in column j

Similar Oracle for ℓth nonzero in row j needed.

Lemma There holds $\|\underline{A}\| \lesssim 1$ if $\tau \lesssim \frac{1}{\|A\|}$.

Proof We write $\underline{\cancel{A}}$ as sum of block-diags

$$\underline{A} = \sum_{k=0}^{\ell} \underline{A}_k$$



$$\Rightarrow \quad \|\underline{A}_0\| \le \max\{1, |\alpha_k| + |\beta_k| h \|A\|\}$$

$$\|\underline{A}_1\| \le \max\{1 + h\|A\|, |\alpha_{k-1}| + |\beta_{k-1}| h \|A\|\}$$

$$\|\underline{A}_\ell\| \le |\alpha_\ell| + |\beta_\ell| h \|A\| \quad \forall\, 2 \le \ell \le k$$

$$\Rightarrow \|\underline{A}\| \le \sum_{\ell=0}^{k} \|\underline{A}_k\| \lesssim k \lesssim 1. \qquad \square$$

Lemma Assume that $A = VDV^{-1}$ with eigenvalues λ_i s.t. $|\arg(-\lambda_i)| \le \alpha$. Assume the multistep method is $A(\alpha)$-stable ($S \supseteq \{\lambda \in \mathbb{C} \,|\, |\arg(-\lambda)| < \alpha, \lambda \neq 0\}$).
Then, $\|\underline{A}^{-1}\| \lesssim N_t \kappa_V$, where $\kappa_V := \|V\| \|V^{-1}\|$

Proof Let $\underline{V}$ denote the block-diag matrix $\underline{V} = \begin{pmatrix} V & & & \\ & V & & \\ & & V & \\ & & & \ddots \\ & & & & V \end{pmatrix}$ and $\underline{D}$ the matrix $\underline{A}$ where we replace A with D. Then

$$\underline{A} = \underline{V}\,\underline{D}\,\underline{V}^{-1} \quad \text{and} \quad \|\underline{A}^{-1}\| \le \kappa_V \|\underline{D}^{-1}\|.$$

It remains to estimate $\|\underline{D}^{-1}\|$.

$$\underline{D} = \sum_{\ell=0}^{k} \underline{D}_\ell$$ with (off-diagonal) block-matrices $\underline{D}_\ell$

Case $\ell = 1$:

$$\underline{D}^{-1} = (\underline{D}_0 + \underline{D}_1)^{-1} = \underline{D}_0^{-1} (I + \underline{D}_1 \underline{D}_0^{-1})^{-1}$$

$$= \underline{D}_0^{-1} \sum_{k=0}^{\infty} (-\underline{D}_1 \underline{D}_0^{-1})^k$$

$\underline{D}_1 \underline{D}_0^{-1}$ is of form $\begin{pmatrix} 0 & & & 0 \\ * & \ddots & & \\ & \ddots & \ddots & \\ 0 & & * & 0 \end{pmatrix}$

$$\Rightarrow (\underline{D}_1 \underline{D}_0^{-1})^k = 0 \quad \forall k \geq 2N_t$$

The off-diagonal entries have the form

$$(1 + C\tau)^k \lesssim 1 \quad \forall k \leq \frac{1}{\tau} = N_t$$

$$\Rightarrow \underline{\| \underline{D}^{-1} \| \lesssim N_t}$$

<u>Case $\ell > 1$: (sketch)</u> $\underline{D}\, y = r$ corresponds to the discretization of the system

$$y^{(j)\prime}(t) = \lambda_j y^{(j)}(t) + r^{(j)}(t)$$

Since the method is α-stable, the numerical approximations $y_i^{(j)}$ can not grow unless forced by $r^{(j)}$

Let $\left(y_i^{(j,k)}\right)_{i=1}^{N_t}$ denote the solution with rhs $\left(r_i^{(j)} \delta_{ik}\right)_{i=1}^{N_t}$ and initial cond. $x_0 \delta_{k0}$

$$\Rightarrow \quad y_i^{(j)} = \sum_{k=0}^{N_t} y_i^{(j,k)}$$

stability shows $|y_i^{(j,k)}| \lesssim |r_k^{(j)}| \quad \forall i \geq k$

$$\Rightarrow \quad \|y^{(j)}\| \lesssim \sum_{k=0}^{N_t} \sqrt{(N_t - k)}\, |r_k^{(j)}|$$

$$\lesssim N_t \underbrace{\sqrt{\sum_{k=0}^{N_t} |r_k^{(j)}|^2}}_{\|r^{(j)}\|}$$

$$\Rightarrow \quad \|y\| \lesssim N_t \|r\| \qquad \square$$

Theorem Under the above assumptions the HHL Alg produces a state proportional to

$$|\psi\rangle = \sum_{j=0}^{N_t} |j\rangle|x_j\rangle$$

with error ε in

$$O\left(\log N_x \; s^{9/2} \left(\|A\| T\right)^{2+\frac{2}{p}} \kappa_V^5 \left(\|x_0\| + \frac{\|b\|}{\|A\|}\right) \varepsilon^{-2} \right)$$

calls to the oracles for A, b, and x_0

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arXiv:1701.03684 (Berry, Childs, Ostrander, Wang)

Theorem Suppose $A = VDV^{-1}$ with $\mathrm{Re}\, D \leq 0$. Assume $A(t) = A$ and $b(t) = b$.

There exists q-Alg which produces

$\frac{x(T)}{\|x(T)\|}$ up to error ε with

$$O\left(\kappa_V \, s \, g \, T \, \|A\| \operatorname{poly}\left(\log\left(\kappa_V \, s \, g \, \beta \, T \, \frac{\|A\|}{\varepsilon}\right)\right)\right)$$

$g = \max_{t \in [0,T]} \frac{\|x(t)\|}{\|x(T)\|}$ $\qquad\qquad$ $\beta = \frac{\|x_0\| + T\|b\|}{\|x(T)\|}$

Query calls.