Early Fault-Tolerant Quantum Algorithms for Matrix Functions via Trotter Extrapolation

Arul Rhik Mazumder
Co-mentor: Samson Wang

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Motivation & Context

For a quantum system with Hamiltonian H, the time evolution of a state $|\psi(t)\rangle$ is governed by:

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- **Goal:** Improve precision scaling via classical extrapolation, without increasing quantum circuit depth.

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$2k$**-th-order (Recursive Suzuki Form):**

$$S_{2k}(t) = S_{2k-2}(p_k t)^2 \, S_{2k-2}((1-4p_k)t) \, S_{2k-2}(p_k t)^2$$

where $p_k = 1/(4 - 4^{1/(2k-1)})$

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- Higher-order Trotter reduces error:

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Basic Idea:

- Encode Hamiltonian $H = \sum_{j=1}^{m} a_j H_j$ using a block encoding.

$$U = \begin{bmatrix} H/\alpha & \cdot \\ \cdot & \cdot \end{bmatrix} \quad \text{where } \alpha = \sum_j |a_j|$$

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Challenges:

- Requires ancillary qubits.
- Needs oracles for state preparation and more complex to compile and implement on near-term devices.

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- **Theoretically intriguing:** Observed error often far below worst-case bounds, suggesting gaps in our theoretical understanding.

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- Choose α_i to cancel terms $\delta^p, \delta^{p+1}, \ldots$
- Only classical postprocessing — no circuit depth increase!

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$$F^{(1)}(\delta) = \frac{f(\delta/2) - \frac{1}{2}f(\delta)}{1 - \frac{1}{2}} = 2f(\delta/2) - f(\delta)$$

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This cancels the $\mathcal{O}(\delta)$ term, improving error to:

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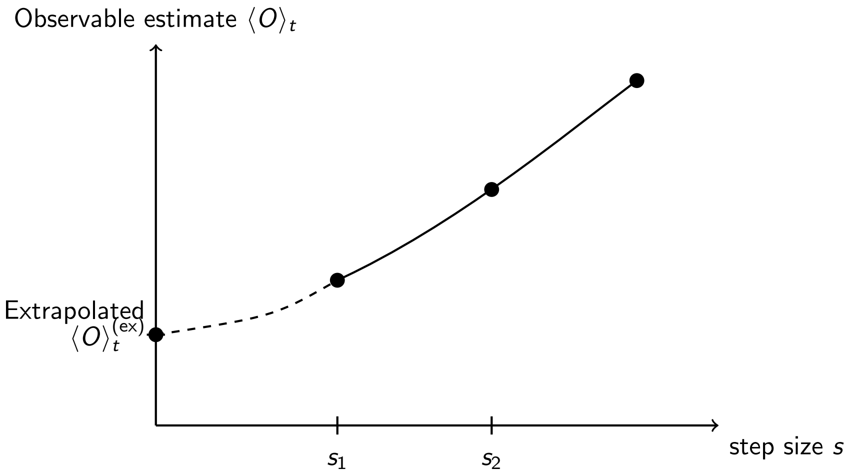
Trade-off:

- Requires multiple simulations at different δ_i.
- Sensitive to sampling noise — averaging must be precise.

Richardson Extrapolation of Observable Estimates



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We have it when $Z = \rho$, and extend to when $\|Z\|_1$ is bounded.

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Lemma (Observable Error Expansion)

For a staged p-th order product formula $\mathcal{P}$ of symmetry class σ, the observable satisfies:

$$\mathrm{Tr}\left[Z\,\mathcal{P}^{1/s}(sT)\right] = \mathrm{Tr}\left[Z\,e^{iAT}\right] + \sum_{j\in\sigma\mathbb{Z}_+\geq p} s^j\,\mathrm{Tr}[Z\,\tilde{E}_{j+1,K}(T)] + \mathrm{Tr}[Z\,\tilde{F}_K(T,s)]$$

- *s is the step size, so $r := 1/s$ is the number of steps*
- *$\tilde{E}, \tilde{F}$: operator-valued error terms*
- *Enables structured Richardson extrapolation of expectation values*

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Algorithm:

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Sample complexity $\mathcal{O}\left(\frac{\|\vec{c}\|_2^2 \|\vec{b}\|_2^2 \|Z\|_1^2 K^2 m^2}{\varepsilon^2} \cdot \log\left(\frac{1}{\delta}\right)\right)$

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Why is Randomized Better

Goal: Estimate weighted sum of traces:

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Why Faster? By Cauchy-Schwarz:

$$c^2 \leq Km \cdot \|c\|_2^2 \|b\|_2^2 \Rightarrow \text{Speedup up to factor of } Km$$

Richardson Extrapolation works for $\mathrm{Tr}[e^{iAt}\rho e^{-iAt'}O]$

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$$\left|\mathrm{Tr}\left[e^{iHt_1}\rho e^{-iHt_2}O\right] - \sum_{j=1}^{m}\sum_{r=1}^{m} b_j b_r \mathrm{Tr}\left[\mathcal{P}^{1/s_j}(s_j t_k)\rho\left(\mathcal{P}^{1/s_r}(s_r t_l)\right)^{\dagger} O\right]\right| =$$

$$\left|\mathrm{Tr}\left[Z_1\left(e^{-iHt_2} - \sum_{r=1}^{m}\mathcal{P}^{1/s_r}(s_r t_l)^{\dagger}\right)\right]\right| + \left|\mathrm{Tr}\left[\left(\sum_{j=1}^{m}\mathcal{P}^{1/s_j}(s_j t_k) - e^{iHt_1}\right) Z_2\right]\right.$$

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Lemma (Gate Complexity to estimate $\mathrm{Tr}(e^{iAt_k}\rho e^{-iAt_l}O)$)

We can estimate $\mathrm{Tr}(e^{iAt_k}\rho e^{-iAt_l}O)$ with Richardson error $\varepsilon_R \leq \varepsilon$ with gate complexity

$$C_{gate} = \mathcal{O}(\Gamma \cdot (\log(1/\varepsilon))(\log(c/\varepsilon)) \cdot (a_{\max}\Upsilon\lambda_{\mathrm{comm}} t_{max})^{1+\frac{1}{p}})$$

Estimating $\mathrm{Tr}(e^{iAt_k}\rho e^{-iAt_l}O)$

Use the same techniques as before (Hoeffding + Importance Sampling)

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Lemma (Sample Complexity to estimate $\mathrm{Tr}(f(A)\rho f(A)^\dagger O)$)

Suppose $\|O\| \leq 1$. Then, to estimate

$$\mathsf{Tr}[f(A)\rho f(A)^\dagger O]$$

to additive error ε with failure probability at most δ, the number of samples required satisfies

$$C_{\mathrm{sample}} = \mathcal{O}\left(\frac{c^4 \cdot (\log\log(1/\varepsilon))^4}{\varepsilon^2}\log\left(\frac{1}{\delta}\right)\right),$$

Putting it all together

Theorem (Estimating $\mathrm{Tr}(f(A)\rho(f(A))^\dagger O)$ with Richardson)

To estimate $\mathrm{Tr}[f(A)\rho(f(A))^\dagger O]$ *with error* $\leq \varepsilon$ *and success probability at least* $1-\delta$ *using the randomized Richardson-extrapolated method, the resource costs are:*

- **Gate complexity (per sample):**

$$C_{gate} = \mathcal{O}\left(\Gamma \cdot (\log(1/\varepsilon))^2 (\log(c(\varepsilon/3)/\varepsilon)) \cdot (a_{\max} \Upsilon \lambda_{\mathrm{comm}} t_{max}(\varepsilon/3))^{1+\frac{1}{p}}\right)$$

- **Sample complexity:**

$$C_{\mathrm{sample}} = \mathcal{O}\left(\frac{c(\varepsilon/3)^4 (\log\log(1/\varepsilon))^4}{\varepsilon^2} \log\left(\frac{1}{\delta}\right)\right)$$