Improved complexity estimation for Hamiltonian simulation with Trotter formula

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Overview

Hamiltonian simulation and Trotterization

Vector norm scaling

Adiabatic quantum computing

Hamiltonian simulation and Trotterization

Hamiltonian simulation

- Time-dependent Hamiltonian simulation:

$$i\frac{\partial}{\partial t}\psi(t) = H(t)\psi(t), \quad \psi(0) = \psi_{\text{in}} \tag{1}$$

  with control Hamiltonian

$$H(t) = f_1(t)H_1 + f_2(t)H_2 \tag{2}$$

  - $f_j(t)$: (scalar) control functions
  - H_j: time-independent Hamiltonians, $e^{-iH_j t}$ can be efficiently computed
- Applications:
  - Harmonic oscillator with time-dependent mass and frequency [Dantas-Pedrosa-Basei 1992]

$$H(t) = -\frac{1}{2M(t)}\Delta + \frac{1}{2}M(t)\omega^2(t)x^2 \tag{3}$$

  - Adiabatic quantum computing
  - Quantum (optimal) control
- Method: Trotter formula

Trotter formula

- Exact solution (involving time-ordering operator):

$$\psi(t) = \mathcal{T} e^{-i\int_0^t (f_1(s)H_1 + f_2(s)H_2)ds} \psi_{\text{in}} \tag{4}$$

- Standard Trotter [Lloyd 1996]:

$$\begin{aligned}\mathcal{T} e^{-i\int_0^h (f_1(s)H_1 + f_2(s)H_2)ds} &\approx e^{-i\int_0^h (f_1(s)H_1 + f_2(s)H_2)ds} \\ &\approx e^{-i(f_1(h)H_1 + f_2(h)H_2)h} \text{ (Quadrature step)} \\ &\approx e^{-if_1(h)H_2 h} e^{-if_1(h)H_1 h} \text{ (Splitting step)}\end{aligned}$$

- Assume that integrals can be accurately computed with negligible cost
- Generalized Trotter [Huyghebaert–De Raedt 1990]:

$$\begin{aligned}\mathcal{T} e^{-i\int_0^h (f_1(s)H_1 + f_2(s)H_2)ds} &\approx e^{-i\int_0^h (f_1(s)H_1 + f_2(s)H_2)ds} \\ &\approx e^{-i\int_0^h f_2(s)ds H_2} e^{-i\int_0^h f_1(s)ds H_1}\end{aligned}$$

Trotter formula

- Second order standard and generalized Trotter:

$$U_{s,2}(h,0) = e^{-if_1(h/2)H_1 h/2} e^{-if_1(h/2)H_2 h} e^{-if_1(h/2)H_1 h/2}$$

$$U_{g,2}(h,0) = e^{-i\int_{h/2}^{h} f_1(s)dsH_1} e^{-i\int_0^h f_2(s)dsH_2} e^{-i\int_0^{h/2} f_1(s)dsH_1}$$

- Higher order methods are also possible via Suzuki recursion [Suzuki 1993]: $U_{2k}(h) = U_{2k-2}(p_k h)^2 U_{2k-2}((1-4p_k)h) U_{2k-2}(p_k h)^2$
- Extremely high order methods are not preferable in practice: $O(5^k)$ terms
- Good approximations if h is small, long time simulation: $[0, T] \to [0, h], [h, 2h], \cdots, [(N-1)h, Nh]$

Trotter formula - Existing error bounds

- Most existing works measure the error using operator 2 norm, *i.e.*, $\|U_{\text{Trotter}} - U_{\text{exact}}\|$, and establish the error bound for generic Hamiltonian
- First order standard Trotter [Wecker-et Al. 2015]:

$$\|U_{s,1}(h,0) - U(h,0)\| \lesssim h^2 \left(\|f_1'\|_\infty \|H_1\| + \|f_2'\|_\infty \|H_2\| + \|f_1\|_\infty \|f_2\|_\infty \|[H_1, H_2]\|\right) \tag{5}$$

- High order standard Trotter [Wiebe-et Al. 2010]:

$$\|U_{s,2k}(h,0) - U(h,0)\| \lesssim (\Lambda_{2k} h)^{2k+1} \tag{6}$$

where $\Lambda_{2k} = \max_{p=0,1,\cdots,2k} \max_{s\in[0,T]} \left(\|f_1^{(p)}(s)H_1\| + \|f_2^{(p)}(s)H_2\|\right)^{1/(p+1)}$

- First order generalized Trotter [Huyghebaert–De Raedt 1990]:

$$\|U_{g,1}(h,0) - U(h,0)\| \lesssim h^2 \|f_1\|_\infty \|f_2\|_\infty \|[H_1, H_2]\| \tag{7}$$

- Lower bound in the time-independent case [Berry-et Al. 2007, Berry-Childs-Kothari 2015]: $\Omega(T\|H\|)$

Trotter formula - Existing error bounds

- Recent works focus more on deriving error estimates for simulating specific examples of practical interest, including
  - Time-dependent Schrödinger equation with constant Hamiltonian [Jahnke-Lubich 2000]
  - Low energy evolution [Şahinoğlu-Somma 2020]
  - System with interacting electrons [Su-Huang-Campbell 2020]
  - Quantum phase estimate [Yi-Crosson 2021]
  - Adiabatic evolution [Yi 2021]

Vector norm scaling

Motivation

- Assume that $\|H_1\| \gg \|H_2\|$
  - Example we have in mind: Hamiltonian with time-dependent mass and potential

$$H(t) = -\frac{1}{2M(t)}\Delta + \frac{1}{2}M(t)V(x) \tag{8}$$

- In practice, we may care more about the error within the obtained quantum state $|\psi(T)\rangle$, or the corresponding observable $\langle\psi(T)|O|\psi(T)\rangle$
- Bounds in terms of operator norms may overestimate the errors in the quantum state:

$$\|A\|_2 = \sup_{\||x\rangle\|_2=1} \|A\,|x\rangle\,\|_2 \tag{9}$$

Error bounds

$$\begin{aligned} U_{s,1}(h,0) &= e^{-if_2(h)H_2h}e^{-if_1(h)H_1h} \\ U_{g,1}(h,0) &= e^{-i\int_0^h f_2(s)dsH_2}e^{-i\int_0^h f_1(s)dsH_1} \end{aligned} \tag{10}$$

Theorem (Vector norm scaling [1])

Assume that for any vector $\vec{v}$, $\|[H_1,H_2]\vec{v}\| \lesssim \|H_1\vec{v}\| + \|\vec{v}\|$, then

1. *for any state $|v\rangle$, the local error can be bounded by*

$$\|U_1(h,0)|v\rangle - U_{exact}(h,0)|v\rangle\| \lesssim (\|H_1|v\rangle\| + 1)\, h^2 \tag{11}$$

2. *the global Trotter evolution operator, defines as $U_1 = \prod_{j=1}^N U_1(jh,(j-1)h)$, satisfies*

$$\|U_1 - U_{exact}\| \lesssim \frac{T^2}{N}\left(\sup_{t\in[0,T]} \|H_1|\psi(t)\rangle\| + 1\right) \tag{12}$$

[1] [An-Fang-Lin 2021] (arXiv:2012.13105)

Application

- The vector norm error bound can be much better than the operator norm error bound if
  - $\|[H_1, H_2]\vec{v}\| \lesssim \|H_1\vec{v}\| + \|\vec{v}\|$
  - $\sup_{t\in[0,T]} \|H_1 |\psi(t)\rangle \|$ is small
- For the example of Hamiltonian with time-dependent mass and smooth potential, $H_1 = \Delta$, $H_2 = V$
  - After spatial discretization with n basis functions, $\|H_1\| = \mathcal{O}(n^2)$, $\|H_2\| = \mathcal{O}(1)$
  - $\|H_1\|$ is large, but $\|H_1 |\psi(t)\rangle \|$ is $\mathcal{O}(1)$ if $|\psi(t)\rangle$ is sufficiently smooth

Application

	Work/Method	Scaling w. spatial discretization	Overall query complexity
Second order Trotter	[Huyghebaert-De Raedt 1990]	$\mathcal{O}(n)$	$\mathcal{O}(\epsilon^{-1})$
	[Wiebe-et al. 2010]	$\mathcal{O}(n^3)$	$\mathcal{O}(\epsilon^{-2})$
	[Wecker-et al. 2015]	$\mathcal{O}(n)$	$\mathcal{O}(\epsilon^{-1})$
	Our work [An-Fang-Lin 2021]	$\mathcal{O}(1)$	$\mathcal{O}(\epsilon^{-0.5})$
Higher order methods	p-th order Trotter [Wiebe-et al. 2010]	$\mathcal{O}(n^{2+2/p})$	$\mathcal{O}(\epsilon^{-1-2/p})$
	Truncated Dyson series [Berry-et al. 2015, Low-Wiebe 2019]	$\widetilde{\mathcal{O}}(n^2)$	$\widetilde{\mathcal{O}}(\epsilon^{-1})$
	Rescaled Dyson series [Berry-et al. 2020]	$\widetilde{\mathcal{O}}(n^2)$	$\widetilde{\mathcal{O}}(\epsilon^{-1})$

Numerical tests

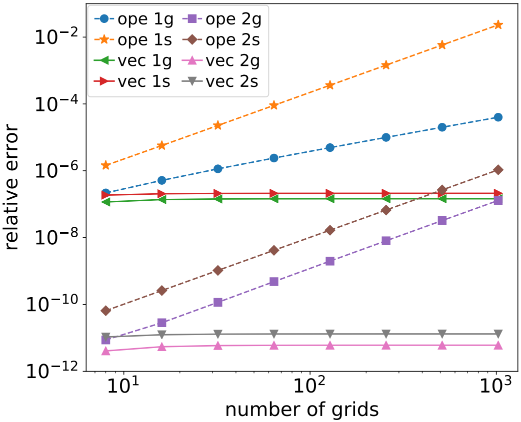


Figure: Relative Errors in the operator and vector norms. In the legend, “g” stands for the generalized Trotter formula and “s” for the standard Trotter formula. The error in operator norm is labeled as “ope” while the one in vector norm as “vec”.

Proof sketch

- Derive an exact representation of $(U_{\text{Trotter}}(h,0) - U_{\text{exact}})(h,0)$ by variation of parameters formula
  - linear combinations of integrals with integrand of the form

$$\left(\prod_{j=1}^{J} g_j\right) \left[\prod_{k=1}^{K} \exp\left(ih\xi_k H_{l_k}\right)\right] A \left[\prod_{k'=1}^{K'} \exp\left(ih\xi'_{k'} H_{l'_{k'}}\right)\right] \tag{13}$$

    where A can be H_1,H_2, $[H_1, H_2]$, and higher order commutators
- Multiplying the vector from the right gives the exact error representation with vector norm scaling
- Under certain assumptions, we can exchange the order of operators without much overhead, *e.g.*,

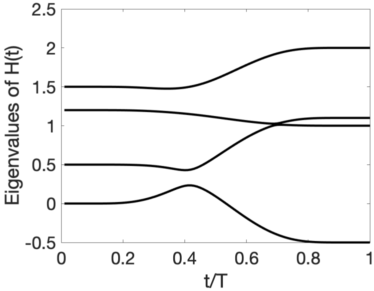
$$\left\| H_1 \left[\prod_{k=1}^{K} \exp\left(ih\xi_k H_{l_k}\right)\right] \vec{v} \right\| \leq \widetilde{C}(\|H_1 \vec{v}\| + \|\vec{v}\|) \tag{14}$$

Adiabatic quantum computing

Adiabatic Quantum Computing (AQC)

$$\imath \partial_t |\psi(t)\rangle = ((1 - t/T)H_0 + (t/T)H_1) |\psi(t)\rangle, \quad t \in [0, T] \tag{15}$$

- Goal: Solve eigenvalue problems
- Starting from the (easily prepared) eigenvector of H_0, the wavefunction at the final time will approximate the corresponding eigenvector of H_1 if
  - the Hamiltonian is slow enough (equivalently T is large enough)
  - gap condition is satisfied



Quantum Adiabatic Theorem

Theorem (Continuous Adiabatic theorem[2])

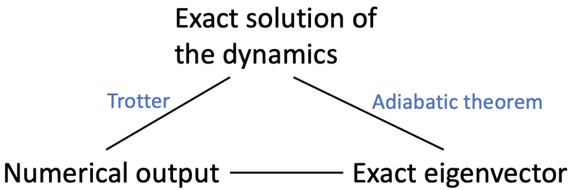
Assume an eigenpath $\lambda(s)$ of the Hamiltonian $H(s) = (1-s)H_0 + sH_1$ is separated from the rest by a gap $\Delta(s)$, then the distance between the dynamics and the eigenvector can be bounded by

$$\eta(1) = C\Big\{\frac{\|H'(0)\|_2}{T\Delta^2(0)} + \frac{\|H'(1)\|_2}{T\Delta^2(1)} + \frac{1}{T}\int_0^1 \left(\frac{\|H''(\tau)\|_2}{\Delta^2(\tau)} + \frac{\|H'(\tau)\|_2^2}{\Delta^3(\tau)}\right) d\tau\Big\}. \tag{16}$$

- To bound the error by ϵ: $T = \mathcal{O}(\Delta_*^{-3}\epsilon^{-1})$
- Cubic dependence on the gap

[2][Jansen-Ruskai-Seiler 2007]

Trotterization for adiabatic dynamics



- First order Trotter with $h = T/N$: $U(t+h,t) = e^{-i(t/T)H_1 h} e^{-i(1-t/T)H_0 h}$
- Trotter error $\sim Th \Longrightarrow h \sim \epsilon/T, \quad N \sim T^2/\epsilon$
- To bound the error between numerical solution and the exact eigenvector, combining with the estimate from adiabatic theorem than $T \sim 1/\epsilon$,
  - Time step: $h \sim \epsilon/T \sim \epsilon^2$
  - Total number of steps: $N \sim 1/\epsilon^3$
- However, numerical tests suggest a relatively large time step size

Discrete quantum adiabatic theorem

Theorem (Discrete adiabatic theorem[3])

Suppose that we are given a sequence of unitary operators $\{W_T(n/T) : n \in \mathbb{N}, 0 \leq n \leq T\}$ *such that*

1. *the difference between* $W_T(n/T)$ *and* $W_T((n+1)/T)$ *is bounded by* $\mathcal{O}(1/T)$*,*
2. *there is an eigenpath* $\lambda(s)$ *of* $W_T(s)$ *which is separated from the rest of the spectrum by a gap* $\Delta(s)$*.*

Then, starting from the eigenvector of $W_T(0)$ *corresponding to* $\lambda(0)$*, the final state* $W_T(1) \cdots W_T(1/T) W_T(0) |\psi(0)\rangle$ *is close to the eigenvector of* $W_T(1)$ *corresponding to* $\lambda(1)$ *with error bounded by*

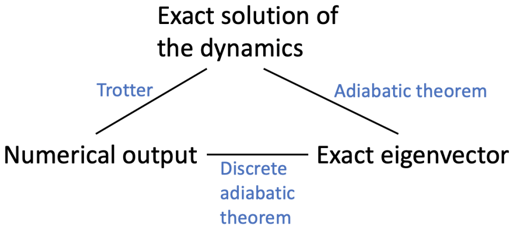
$$C \left(\frac{1}{T\Delta(0)^2} + \frac{1}{T\Delta(1)^2} + \sum_{n=1}^{T-1} \frac{1}{T^2 \Delta(n/T)^3} \right) \tag{17}$$

[3] [Dranov-Kellendonk-Seiler 1998, Costa-et al. 2021]

Continuous v.s. Discrete

	Continuous	Discrete
Evolution	$i\partial_t \|\psi(t)\rangle = H(t/T) \|\psi(t)\rangle$	$W_T(1)\cdots W_T(1/T)W_T(0) \|\psi_0\rangle$
Slow condition	$H(s+\Delta s)$ and $H(s)$ are close	Adjacent W_T's are close
Gap condition	Gap for $H(s)$	Gap for $W_T(s)$
Conclusion	From eigenvector of $H(0)$ to $H(1)$	From eigenvector of $W_T(0)$ to $W_T(1)$
Error bound	$\frac{1}{T\Delta(0)^2} + \frac{1}{T\Delta(1)^2} + \frac{1}{T}\int_0^1 \frac{d\tau}{\Delta(\tau)^3}$	$\frac{1}{T\Delta(0)^2} + \frac{1}{T\Delta(1)^2} + \frac{1}{T}\sum_{n=1}^{T-1} \frac{1}{T\Delta(n/T)^3}$

Trotterization for adiabatic dynamics



- Idea: View Trotter evolution operator $e^{-i(t/T)H_1 h}e^{-i(1-t/T)H_0 h}$ as discrete adiabatic walk operator
- Operator with $h=1$, *i.e.*, $W_T(t/T) = e^{-i(t/T)H_1}e^{-i(1-t/T)H_0}$ is slow enough
- Discrete adiabatic theorem directly tells us that the error is bounded by $\mathcal{O}(1/T)$,
  - Time step: $h = 1$
  - Total number of steps: $N = T \sim 1/\epsilon$
- Byproduct: Trotter error is negligible/not dominant
  - First order Trotter can even achieve exponential convergence
  - Adiabatic v.s. QAOA

Remarks

	Standard	Our work
Time step size	$\mathcal{O}(\epsilon/T)$	$\mathcal{O}(1)$
Trotter steps	$\mathcal{O}(1/\epsilon^3)$	$\mathcal{O}(1/\epsilon)$

- The discrete adiabatic perspective can also be applied to understand other time discretization approaches via deterministic short time evolution operators
- Compared to generic Trotter error bounds,
  - we require the gap condition
  - the gap condition is required for the unitary walk operator instead of the original Hamiltonian, *e.g.*,

$$\begin{aligned} H(s) &= (1-s)H_0 + sH_1 \\ W_T(s) &= e^{-i((1-s)H_0+sH_1)} = e^{-iH(s)} \\ W_T(s) &= e^{-isH_1}e^{-i(1-s)H_0} \end{aligned} \tag{18}$$

Thank you for your attention!