CS 59300 – Algorithms for Data Science

Classical and Quantum approaches

Lecture 20 (11/18)

Quantum linear algebra toolkits (IV)

https://ruizhezhang.com/course_fall_2025.html

The slides are partly based on Dong An and Lin Lin's talk

Quantum linear algebra toolbox

- Basic linear algebra operations
- Linear systems of equations
- Matrix functions
  - Functions of Hermitian matrices: quantum signal processing (QSP), qubitization
  - Functions of general matrices: quantum singular value transformation (QSVT), ~~linear combinations of Hamiltonian simulations (LCHS)~~
- Applications
  - Quantum walk
  - Hamiltonian simulation
  - Quantum ordinary differential equation (ODE) solvers

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Quantum walk

Classical random walk

- Let P be transition matrix of a Markov chain on a graph $G(V, E)$:

$$P_{ij} \geq 0, \qquad \sum_j P_{ij} = 1 \;\; \forall i \in V$$

- Let π be the stationary distribution, i.e., $\pi P = \pi$ (π is unique and positive if P is ergodic)
- P is reversible if

$$\pi_i P_{ij} = \pi_j P_{ji} \quad \forall i, j \in V$$

- The discriminant matrix D is a real symmetric matrix defined as:

$$D_{ij} := \sqrt{P_{ij} P_{ji}}$$

Quantum walk

Classical random walk

- The discriminant matrix D is a real symmetric matrix defined as:

$$D_{ij} \coloneqq \sqrt{P_{ij}P_{ji}}$$

Fact. Define the coherent version of the stationary state (i.e. qsample):

$$|\pi\rangle = \sum_i \sqrt{\pi_i}|i\rangle$$

Then, it holds that

- $D\sqrt{\pi} = \sqrt{\pi}$
- $D = \mathrm{diag}(\sqrt{\pi}) \cdot P \cdot \mathrm{diag}(\sqrt{\pi})^{-1}$, i.e. D and P have the same eigenvalues

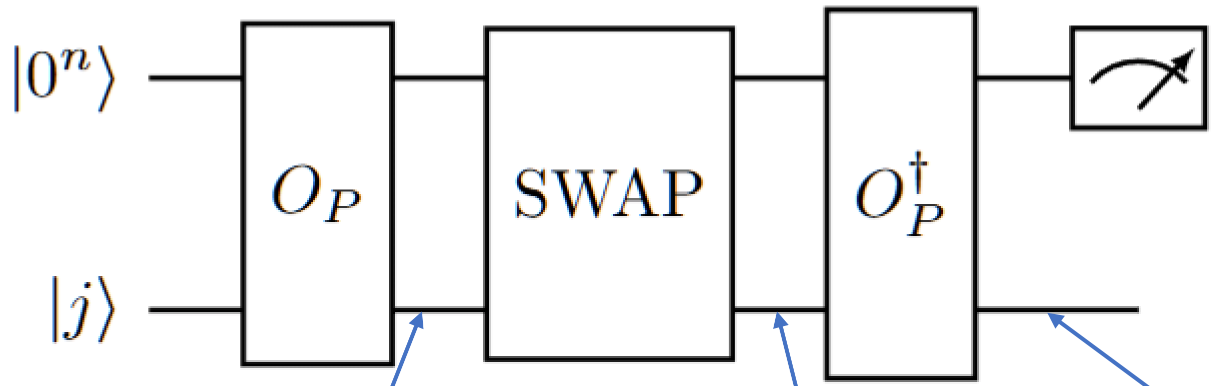
Block-encoding for the discriminant matrix

Assume that we have access to the transition matrix P via an oracle gate O_P:

$$O_P|0\rangle|j\rangle = \sum_k \sqrt{P_{jk}}|k\rangle|j\rangle$$

"coherent one-step walk from j"

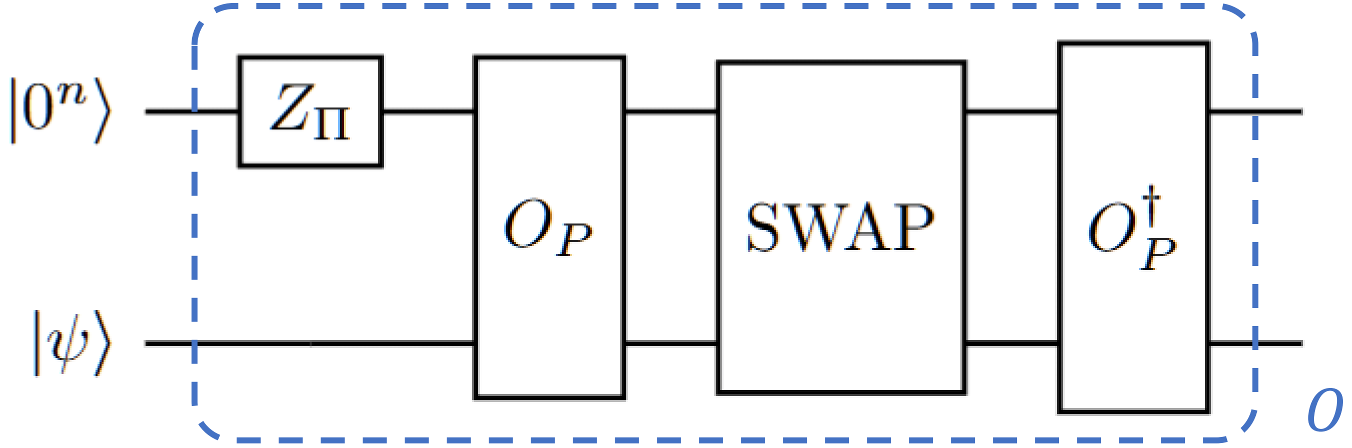
Then, the following quantum circuit is a Hermitian block-encoding for D:



$$\sum_k \sqrt{P_{jk}}|k\rangle|j\rangle \qquad \sum_k \sqrt{P_{jk}}|j\rangle|k\rangle \qquad \sum_k \sqrt{P_{jk}P_{kj}}|0\rangle|k\rangle + |\perp\rangle$$

Szegedy's quantum walk

Consider the qubitization for Hermitian block-encoding:



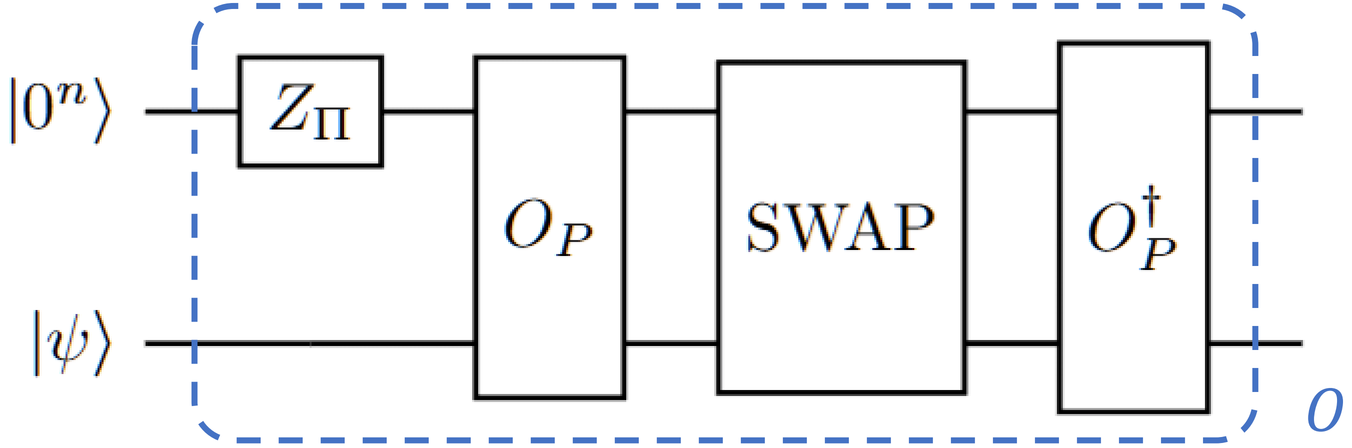
- O^k is a block-encoding for $T_k(D)$
- O has invariant subspaces $\{\mathcal{H}_i\}$ such that

$$[O]_{\mathcal{H}_i} = \begin{bmatrix} \lambda_i & -\sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & \lambda_i \end{bmatrix}$$

Eigenvalues: $e^{\pm \mathbf{i} \arccos(\lambda_i)}$

Szegedy's quantum walk

Consider the qubitization for Hermitian block-encoding:



- O^k is a block-encoding for $T_k(D)$ $\implies$ $\mathcal{O}\left(\sqrt{t}\right)$ cost to implement $D^t|v\rangle$ (fast-forwarding)
- The eigenvalues of O are $\left\{e^{\pm \mathbf{i} \arccos(\lambda_i)}\right\}$, where $\{\lambda_i\}$ are the eigenvalues of D
  - ➢ The largest eigenvalue of D is 1 (corresponding to $\sqrt{\pi}$), and $\arccos(1) = 0$
  - ➢ The other eigenvalues of $D \leq 1 - \delta$ (the spectral gap), and $\arccos(1-\delta) \approx \sqrt{2\delta}$

(spectral gap amplification)

Quadratically faster hitting

- Find a marked vertex in a graph (Szegedy '04; Magniez et al. '06; Belovs'13; Ambainis et al. '19; Piddock et al. '19): $\mathcal{O}(\text{hitting time}) \longrightarrow \mathcal{O}\left(\sqrt{\text{hitting time}}\right)$
- Element distinctness (Ambainis '03): $\mathcal{O}(n \log n) \longrightarrow \mathcal{O}\left(n^{2/3}\right)$
- Triangle finding (Magniez et al. '03): $\mathcal{O}(n^{\omega}) \longrightarrow \mathcal{O}(n^{1.3})$
- Matrix-product verification (Buhrman-Špalek '04): $\mathcal{O}(n^2) \longrightarrow \mathcal{O}\left(n^{5/3}\right)$
- Closest-pair problem (Aaronson et al. '20): $\mathcal{O}(n \log n) \longrightarrow \mathcal{O}\left(n^{2/3}\right)$

Quadratically faster "mixing" (qsample preparation)

- Partition function estimation (Harrow-Wei '20; Chakrabarti et al. '23), Logconcave sampling (Childs et al. '22), Approximate convex optimization (Li-**Z** '22), non-logconcave sampling (Ozgul et al. '23)

Fast-forwarding classical Markov chain

- Graph property testing (Apers-Sarlette '19; Apers '20)

MNRS framework for quantum walk search

Let P be a Markov chain on a graph V such that the vertices in $M \subset V$ are "marked". The goal is to decide whether M is empty or find a vertex $x \in M$

Consider three operations:

- Setup: preparing the initial state $|\pi\rangle = \frac{1}{\sqrt{|V|}} \sum_{x \in V} \sqrt{\pi_x} |x\rangle$ Cost: S
- Update: applying the transformation $|x\rangle|0\rangle \mapsto |x\rangle \sum_{y \in V} \sqrt{p_{xy}} |y\rangle$ Cost: U
- Checking: applying the transformation $|x\rangle \mapsto \begin{cases} -|x\rangle & \text{if } x \in M \\ |x\rangle & \text{otherewise} \end{cases}$ Cost: C

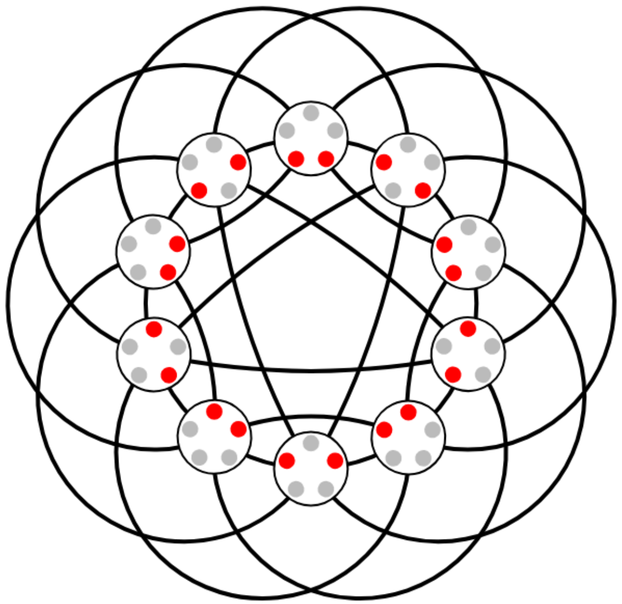
Let $\lambda \coloneqq \frac{\max\{|M|,1\}}{|V|}$ and δ be the spectral gap of P

Then, the quantum walk complexity is $\mathcal{O}\left(S + \frac{1}{\sqrt{\lambda}}\left(\frac{1}{\sqrt{\delta}} U + C\right)\right)$

Quantum walk for Element Distinctness

Problem: Given n numbers $(a_1, a_2, \dots, a_n)$, decide whether there exist $i \neq j$ such that $a_i = a_j$

- Johnson graph $\mathcal{J}(n, r)$
  - Vertices: r-subsets of $[n]$
  - Edges: $S \sim S'$ if and only if $|S \cap S'| = r - 1$
- S is marked if there are $i \neq j \in S$ such that $a_i = a_j$
- Let P be the "natural" random walk on $\mathcal{J}(n, r)$
- $\lambda \geq \binom{n-2}{r-2} / \binom{n}{r} = \mathcal{O}(r^2/n^2)$ and $\delta \geq 1/r$
- Apply the MNRS quantum walk on $|\pi\rangle \propto \sum_S |a_{i_1}, a_{i_2}, \cdots, a_{i_r}\rangle$
- Consider the query complexity: $S = r$, $U = 1$, and $C = 0$
- $\mathcal{O}\left(S + \frac{1}{\sqrt{\lambda}}\left(\frac{1}{\sqrt{\delta}} U + C\right)\right) = \mathcal{O}\left(r + \frac{n}{\sqrt{r}}\right) = \mathcal{O}(n^{2/3})$ if we choose $r = n^{2/3}$



Quantum linear algebra toolbox

- Basic linear algebra operations
- Linear systems of equations
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Hamiltonian simulation

Hamiltonian Simulation Problem: Given a description of the Hamiltonian $H(t)$, an evolution time t and an initial state $|\psi(0)\rangle$, to produce the final state $|\psi(t)\rangle$ within in some error tolerance ϵ

Time independent:

- $H(t) \equiv H$, a 2^n-by-2^n matrix
- Schrödinger equation: $\mathbf{i}\partial_t|\psi(t)\rangle = H|\psi(t)\rangle,\ |\psi(0)\rangle = |\psi\rangle$
- Equivalently, $|\psi(t)\rangle = e^{-\mathbf{i}Ht}|\psi\rangle$

Complexity:

- **BQP**-complete
- No fast-forwarding theorem: simulating the dynamics for time t requires $\Omega(t)$ cost

Quantum algorithms for Hamiltonian simulation

“Old” approach: Trotterization (= Product Formulae = Time/Operator Splitting)

- First-order Trotter formula for $H = H_1 + H_2$:

$$e^{-\mathbf{i}Ht} = \left(e^{-\mathbf{i}H_2 t/L} e^{-\mathbf{i}H_1 t/L}\right)^L + \mathcal{O}(\|[H_1, H_2]\| t^2/L)$$

$\mathcal{O}(\|[H_1, H_2]\| t^2 \epsilon^{-1})$ queries to $e^{-\mathbf{i}H_1 \Delta t}$ and $e^{-\mathbf{i}H_2 \Delta t}$

- High order (p-th): query complexity $\mathcal{O}\left(\alpha_H t^{1+1/p} \epsilon^{-1/p}\right)$

Proof of the (first-order) Trotter error bound

- $\widetilde{U}(t) \coloneqq e^{-\mathbf{i}tH_2} e^{-\mathbf{i}tH_1}$ satisfies the ODE:

$$
\begin{aligned}
\mathbf{i}\partial_t \widetilde{U}(t) &= H_2 e^{-\mathbf{i}tH_2} e^{-\mathbf{i}tH_1} + e^{-\mathbf{i}tH_2} H_1 e^{-\mathbf{i}tH_1} \\
&= (H_1 + H_2) e^{-\mathbf{i}tH_2} e^{-\mathbf{i}tH_1} - H_1 e^{-\mathbf{i}tH_2} e^{-\mathbf{i}tH_1} + e^{-\mathbf{i}tH_2} H_1 e^{-\mathbf{i}tH_1} \\
&= H\widetilde{U}(t) + \underbrace{\left[e^{-\mathbf{i}tH_2}, H_1\right] e^{-\mathbf{i}tH_1}}_{B(t)}
\end{aligned}
$$

  - Initial condition: $\widetilde{U}(0) = I$

- Duhamel's principle:

$$
\begin{aligned}
\widetilde{U}(t) &= e^{-\mathbf{i}tH} - \mathbf{i} \int_0^t e^{-\mathbf{i}(t-s)H} B(s) \mathrm{d}s \\
&= e^{-\mathbf{i}tH} - \mathbf{i} \int_0^t e^{-\mathbf{i}(t-s)H} \left[e^{-\mathbf{i}sH_2}, H_1\right] e^{-\mathbf{i}sH_1} \mathrm{d}s
\end{aligned}
$$

- $\left\| \widetilde{U}(t) - e^{-\mathbf{i}tH} \right\| \leq \int_0^t \left\| \left[e^{-\mathbf{i}sH_2}, H_1\right] \right\| \mathrm{d}s$

Proof of the (first-order) Trotter error bound

- $\left\|\widetilde{U}(t) - e^{-\mathbf{i}tH}\right\| \leq \int_0^t \left\|\left[e^{-\mathbf{i}sH_2}, H_1\right]\right\| \mathrm{d}s$
- Consider $G(t) \coloneqq \left[e^{-\mathbf{i}tH_2}, H_1\right] e^{\mathbf{i}tH_2} = e^{-\mathbf{i}tH_2} H_1 e^{\mathbf{i}tH_2} - H_1$, which satisfies the ODE:

$$\mathbf{i}\partial_t G(t) = e^{-\mathbf{i}tH_2}[H_2, H_1] e^{\mathbf{i}tH_2}$$

  - Initial condition: $G(0) = 0$
- We can directly bound the norm:

$$\left\|\left[e^{-\mathbf{i}tH_2}, H_1\right]\right\| = \|G(t)\| \leq \int_0^t \left\|e^{-\mathbf{i}sH_2}[H_2, H_1] e^{\mathbf{i}sH_2}\right\| \mathrm{d}s = t\|[H_1, H_2]\|$$

- Thus,

$$\left\|\widetilde{U}(t) - e^{-\mathbf{i}tH}\right\| \leq \int_0^t \left\|\left[e^{-\mathbf{i}sH_2}, H_1\right]\right\| \mathrm{d}s \leq t^2 \|[H_1, H_2]\|$$

■

Quantum algorithms for Hamiltonian simulation

Modern approach: QSVT

- Assume that we have access to U_H, the block-encoding for H
- $e^{\mathbf{i}tx} = \cos(tx) + \mathbf{i}\sin(tx)$
- Chebyshev expansion on $[-1,1]$:

$$\cos(tx) = J_0(t) + 2\sum_{k=1}^{\infty}(-1)^k J_{2k}(t) T_{2k}(x)$$

$$\sin(tx) = 2\sum_{k=1}^{\infty}(-1)^k J_{2k+1}(t) T_{2k+1}(x)$$

- The series converges rapidly so that we can truncate it after $\Theta\left(t + \frac{\log(1/\epsilon)}{\log(e+\log(1/\epsilon)/t)}\right)$ terms

Quantum algorithms for Hamiltonian simulation

Modern approach: QSVT

- Assume that we have access to U_H, the block-encoding for H
- $e^{\mathbf{i}tx} = \cos(tx) + \mathbf{i}\sin(tx)$
- By QSVT, we can implement $\cos(tH)$ and $\sin(tH)$ with complexity $\mathcal{O}(t + \log(1/\epsilon))$
- By LCU, we get a block-encoding for $\frac{1}{2}e^{\mathbf{i}tH}$, i.e. a $(2, a+2, \epsilon)$-block-encoding for $e^{\mathbf{i}tH}$
- How to convert $\frac{1}{2}e^{\mathbf{i}tH}$ to $e^{\mathbf{i}tH}$?
- Oblivious amplitude amplification (OAA)
  - $P(x) = 3x - 4x^3$, which maps $1/2$ to 1 and is bounded by 1 in $[-1,1]$
  - $P^{\mathrm{SV}}\left(\frac{1}{2}e^{\mathbf{i}Ht}\right) = e^{\mathbf{i}Ht}$

Quantum algorithms for Hamiltonian simulation

Modern approach: QSVT

- Assume that we have access to U_H, an $(\alpha, m, 0)$-block-encoding for H
- We can implement a $(1, m+2, \epsilon)$-block-encoding for $e^{-\mathbf{i}Ht}$ using $\mathcal{O}(\alpha t + \log(1/\epsilon))$ queries to U_H

Time-dependent Hamiltonian simulation

The goal is to implement

$$\mathcal{T}e^{-\mathbf{i}\int_0^t H(s)\mathrm{d}s}$$

- Trotterization (Wiebe et al. ’10):

  High order (p-th order) generalization: $\mathcal{O}\left(\sum_{j=1}^{m}\left\|\partial_t^p H_j\right\|\right)^{\frac{1}{p+1}}$

- Series truncation (Berry et al. ’15; Low-Wiebe ’18; Kieferova et al. ’18; An et al. ’22):

  Dyson series

$$\mathcal{T}e^{-\mathbf{i}\int_0^t H(s)\mathrm{d}s} = I - i\int_0^t \mathrm{d}t_1 H(t_1) - \int_0^t \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_1 H(t_2)H(t_1) + \cdots$$

  LCU cost: $\mathcal{O}\left(\frac{\alpha^2 t^2}{\epsilon}\right)$ where $\alpha = \max_{s\in[0,t]} \|H(s)\|$

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Quantum ODE solver

Quantum ODE Problem:

$$\frac{\mathrm{d}u(t)}{\mathrm{d}t} = -A(t)u(t) + b(t), \qquad u(0) = u_0$$

The goal is to prepare a quantum state encoding the solution in its amplitude:

$$|u(T)\rangle = \frac{1}{\|u(T)\|} \sum_{j=0}^{N-1} u_j(T)|j\rangle$$

Quantum ODE solver: finite difference method

- Discretization:

$$\frac{u(t+h)-u(t)}{h} \approx -A(t)u(t)+b(t) \qquad A_k \coloneqq A(kh), \qquad b_k \coloneqq b(kh)$$

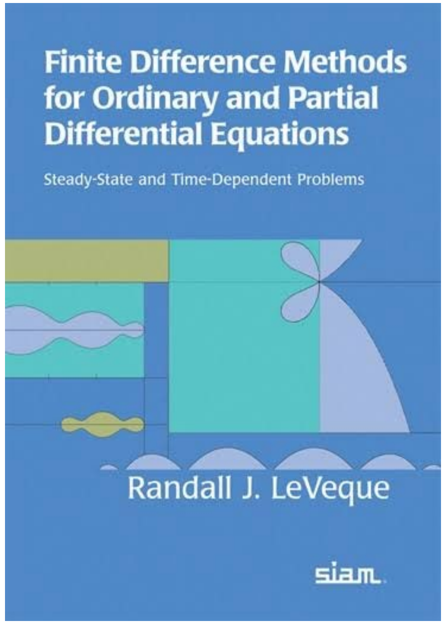
- Linear system:

$$\begin{bmatrix} I & & & & \\ -(I-hA_0) & I & & & \\ & -(I-hA_1) & I & & \\ & & \ddots & \ddots & \\ & & & -(I-hA_{n-1}) & I \end{bmatrix} \begin{bmatrix} u(0) \\ u(h) \\ u(2h) \\ \vdots \\ u(T) \end{bmatrix} = \begin{bmatrix} u_0 \\ b_0 h \\ b_1 h \\ \vdots \\ b_{n-1} h \end{bmatrix}$$

- QLSP + Dyson (Berry-Costa ’22):

$\tilde{O}\left(\tilde{q}\alpha T \log^2\left(\frac{1}{\epsilon}\right)\right)$ queries of A and $\tilde{O}\left(\tilde{q}\alpha T \log\left(\frac{1}{\epsilon}\right)\right)$ queries of u_0

$\tilde{q} \coloneqq \max_t \|u(t)\|/\|u(T)\|$ and $\alpha \coloneqq \max_t \|A(t)\|$



Linear combination of Hamiltonian simulation (LCHS)

This method is designed to map any non-unitary dynamics to Hamiltonian simulation problems

$$\frac{\mathrm{d}u(t)}{\mathrm{d}t} = -A(t)u(t), \qquad u(0) = u_0$$

- Suppose $A(t)$ is non-Hermitian, and can be decomposed into Hermitian and anti-Hermitian parts:

$$A(t) = L(t) + \mathbf{i}H(t), \qquad L(t) = \frac{A(t) + A^\dagger(t)}{2}, \qquad H(t) = \frac{A(t) - A^\dagger(t)}{2\mathbf{i}}$$

- We assume that $L(t) \succcurlyeq 0$ for stability

Linear combination of Hamiltonian simulation (LCHS)

Theorem (An-Liu-Lin '23; An-Childs-Lin '23).

Suppose $A(t) = L(t) + \mathbf{i}H(t)$ and $L(t) \succcurlyeq 0$, then

ODE solution: $$\mathcal{T}e^{-\int_0^t A(s)\mathrm{d}s} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} U_k(t)\mathrm{d}k$$

Here $U_k(t)$ are unitaries that solve the Schrödinger equation:

$$\frac{\mathrm{d}U_k(t)}{\mathrm{d}t} = -\mathbf{i}\big(kL(t) + H(t)\big)U_k(t), \qquad U(0) = I$$

Time-dependent Hamiltonian simulation: $$U_k(t) = \mathcal{T}e^{-\mathbf{i}\int_0^t \left(kL(s)+H(s)\right)\mathrm{d}s}$$

Special cases

$$\mathcal{T}e^{-\int_0^t (L(s)+\mathbf{i}H(s))\mathrm{d}s} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} \mathcal{T}e^{-\mathbf{i}\int_0^t (kL(s)+H(s))\mathrm{d}s}\mathrm{d}k$$

- $A(t) \equiv \mathbf{i}H$ (only the anti-Hermitian part):

$$e^{-\mathbf{i}Ht} = e^{-\mathbf{i}Ht}\int_{\mathbb{R}} \frac{1}{\pi(1+k^2)}\mathrm{d}k$$

  - ➢ $\frac{1}{\pi(1+k^2)}$ is the pdf of the Cauchy distribution

- $A(t) \equiv L$ (only the Hermitian part):

$$e^{-Lt} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} e^{-\mathbf{i}ktL}\mathrm{d}k$$

  - ➢ $\frac{1}{\pi(1+k^2)}$ is the Fourier transform of $e^{-|x|}$ and $L \succcurlyeq 0$

LCHS algorithm

LCHS identity + integral truncation ($K = \mathcal{O}(1/\epsilon)$) + quadrature

$$\mathcal{T}e^{-\int_0^t A(s)\mathrm{d}s} \approx \int_{-K}^{K} \frac{1}{\pi(1+k^2)} U_k(t)\mathrm{d}k \approx \sum_j c_j U_j$$

Plug-in any time-dependent Hamiltonian simulation algorithms and LCU

Method	Query complexity	
	A	u_0
Dyson [8]	$\widetilde{\mathcal{O}}\left(\widetilde{q}\alpha T \log^2\left(\frac{1}{\epsilon}\right)\right)$	$\mathcal{O}\left(\widetilde{q}\alpha T \log\left(\frac{1}{\epsilon}\right)\right)$
LCHS	$\widetilde{\mathcal{O}}\left(q^2\alpha T/\epsilon\right)$	$\mathcal{O}(q)$

Table: Comparison between LCHS and the state-of-the-art truncated Dyson series method. Here $\alpha = \max_t \|A(t)\|$, $q = \|u_0\|/\|u(T)\|$ and $\widetilde{q} = \max_t \|u(t)\|/\|u(T)\|$ (we have $q \leq \widetilde{q}$)

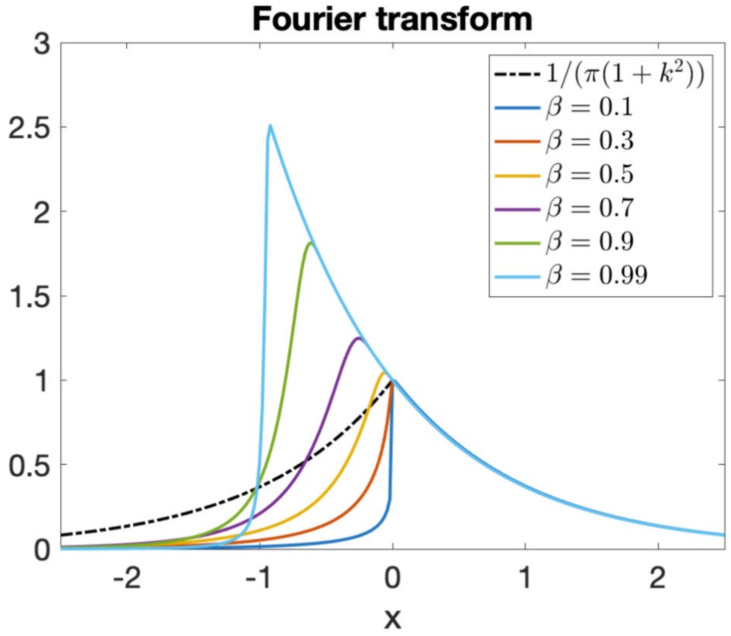
Change kernel function

$$e^{-(L+\mathbf{i}H)t} = \int_{\mathbb{R}} \frac{f(k)}{1-\mathbf{i}k} e^{-\mathbf{i}(kL+H)t} \mathrm{d}k$$

- $L \geqslant 0$, and when $H = 0$, we need:

$$e^{-x} = \int_{\mathbb{R}} \frac{f(k)}{1-\mathbf{i}k} e^{-\mathbf{i}kt} \mathrm{d}k\,, \qquad x \geq 0$$

- The same Fourier transform on the positive real axis
- Design freedom on the negative real axis



Improved LCHS

Theorem (An-Childs-Lin ’23).

Suppose $f(z)$ is a function of $z \in \mathbb{C}$ satisfying the following conditions:

- Analyticity: $f(z)$ is analytic on the lower half plane $\{z : \mathrm{Im}(z) < 0\}$ and continuous on $\{z : \mathrm{Im}(z) \leq 0\}$
- Decay: $|f(z)| = \mathcal{O}(|z|^{-\alpha})$ for $\mathrm{Im}(z) \leq 0$
- Normalization: $\int_{\mathbb{R}} \frac{f(k)}{1-\mathbf{i}k} \mathrm{d}k = 1$

Then, for $L(t) \succcurlyeq 0$, the LCHS identity holds:

$$\mathcal{T} e^{-\int_0^t A(s)\mathrm{d}s} = \int_{\mathbb{R}} \frac{f(k)}{1-\mathbf{i}k} \mathcal{T} e^{-\mathbf{i}\int_0^t (kL(s)+H(s))\mathrm{d}s} \mathrm{d}k$$

Nearly-optimal quantum ODE solver

- Nearly exponential decay kernel function:

$$f(z) \propto e^{-(1+\mathbf{i}z)^{\beta}}, \qquad \beta \in (0,1)$$

  (the sub-exp decay rate $e^{-c|z|^{\beta}}$ is near optimal within the LCHS framework)

- The integral can be truncated with $K \sim \log^{1+1/\beta}(1/\epsilon)$

- By using a non-uniform quadrature (the composite Gaussian quadrature), the number of queries to A can be improved to

$$\tilde{O}\left(q\alpha T \log^{1+1/\beta}(1/\epsilon)\right)$$

- **Low-Somma '25:** $\log^{1+1/\beta}(1/\epsilon) \longrightarrow \log(1/\epsilon)$ by extending the LCHS framework to an approximate version, which allows them to use an exp decay kernel

Proof of the LCHS identity

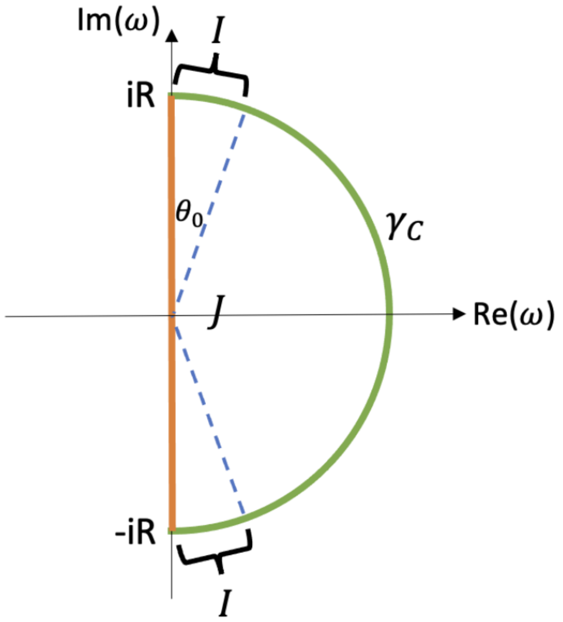
Time-independent case:

$$O_L(t) \coloneqq e^{-(L+\mathbf{i}H)t} = \int_{\mathbb{R}} \frac{f(k)}{1-\mathbf{i}k} e^{-\mathbf{i}(kL+H)t} \mathrm{d}k \eqqcolon O_R(t)$$

We'll show that $O_L(t)$ and $O_R(t)$ follow the same ODE

- $\frac{\mathrm{d}}{\mathrm{d}t} O_L(t) = -(L+\mathbf{i}H) O_L(t)$
- $$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} O_R(t) &= \mathrm{p.v.} \int_{\mathbb{R}} \frac{f(k)}{1-\mathbf{i}k} (-\mathbf{i}kL - \mathbf{i}H) e^{-\mathbf{i}(kL+H)t} \mathrm{d}k \\ &= \mathrm{p.v.} \int_{\mathbb{R}} \frac{f(k)}{1-\mathbf{i}k} (-L - \mathbf{i}H + (1-\mathbf{i}k)L) e^{-\mathbf{i}(kL+H)t} \mathrm{d}k \\ &= -(L+\mathbf{i}H) O_R(t) + L \underbrace{\left(\mathrm{p.v.} \int_{\mathbb{R}} f(k) e^{-\mathbf{i}(kL+H)t} \mathrm{d}k \right)}_{\equiv 0} \end{aligned}$$

Proof of the LCHS identity



- Change of variable $\omega = \mathbf{i}k$:

$$\mathrm{p.v.}\int_{\mathbb{R}} f(k)e^{-\mathbf{i}(kL+H)t}\mathrm{d}k = -\mathbf{i}\lim_{R\to\infty}\int_{-\mathbf{i}R}^{\mathbf{i}R} f(-\mathbf{i}\omega)e^{-\omega Lt-\mathbf{i}Ht}\mathrm{d}\omega$$

- Consider the curve $\gamma_C \coloneqq \{\omega = Re^{\mathbf{i}\theta} : \theta \in [-\pi/2, \pi/2]\}$

- f is analytic on $\{z : \mathrm{Im}(z) < 0\}$ implies that:

$$\int_{\gamma_C \cup [-\mathbf{i}R,\mathbf{i}R]} f(-\mathbf{i}\omega)e^{-\omega Lt-\mathbf{i}Ht}\mathrm{d}\omega = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathbf{i}Re^{\mathbf{i}\theta} f\left(-\mathbf{i}Re^{\mathbf{i}\theta}\right)e^{-Re^{\mathbf{i}\theta}Lt-\mathbf{i}Ht}\mathrm{d}\theta + \int_{\mathbf{i}R}^{-\mathbf{i}R} f(-\mathbf{i}\omega)e^{-\omega Lt-\mathbf{i}Ht}\mathrm{d}\omega = 0$$

$$\mathrm{p.v.}\int_{\mathbb{R}} f(k)e^{-\mathbf{i}(kL+H)t}\mathrm{d}k = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} Re^{\mathbf{i}\theta} f\left(-\mathbf{i}Re^{\mathbf{i}\theta}\right)e^{-Re^{\mathbf{i}\theta}Lt-\mathbf{i}Ht}\mathrm{d}\theta$$

- Divide $[-\pi/2, \pi/2]$ into $I \cup J$ where $I = [-\pi/2, -\theta_0] \cup [\theta_0, \pi/2]$

Proof of the LCHS identity

- Integral over J:

$$\left\|\int_J Re^{\mathbf{i}\theta} f\left(-\mathbf{i}Re^{\mathbf{i}\theta}\right) e^{-Re^{\mathbf{i}\theta}Lt-\mathbf{i}Ht}\mathrm{d}\theta\right\| \le \int_J R\left|f\left(-\mathbf{i}Re^{\mathbf{i}\theta}\right)\right| \left\|e^{-Re^{\mathbf{i}\theta}Lt}\right\| \mathrm{d}\theta$$

$(L \succcurlyeq \lambda_0)$
$$\le \int_J R\left|f\left(-\mathbf{i}Re^{\mathbf{i}\theta}\right)\right| e^{-R\lambda_0 t\cos\theta}\mathrm{d}\theta \le \int_J R\left|f\left(-\mathbf{i}Re^{\mathbf{i}\theta}\right)\right| e^{-R\lambda_0 t\frac{2}{\pi}\theta_0}\mathrm{d}\theta$$
($\cos\theta \ge \frac{2}{\pi}\theta_0$ for $\theta \in J$)

(decay of f)
$$\le \int_J R\mathcal{O}(R^{-\alpha})e^{-R\lambda_0 t\frac{2}{\pi}\theta_0}\mathrm{d}\theta = R^{1-\alpha}e^{-\Omega(\theta_0 R)} \to 0 \text{ as } R\to\infty$$

- Integral over I:

$$\left\|\int_I Re^{\mathbf{i}\theta} f\left(-\mathbf{i}Re^{\mathbf{i}\theta}\right) e^{-Re^{\mathbf{i}\theta}Lt-\mathbf{i}Ht}\mathrm{d}\theta\right\| \le \int_I R\left|f\left(-\mathbf{i}Re^{\mathbf{i}\theta}\right)\right|\mathrm{d}\theta = \mathcal{O}(R^{1-\alpha}\theta_0) \to 0 \text{ as } R\to\infty$$

- We can take $\theta_0 = R^{-1+\alpha/2}$

Proof of the LCHS identity

Time-independent case:

$$O_L(t) := e^{-(L+\mathbf{i}H)t} = \int_{\mathbb{R}} \frac{f(k)}{1-\mathbf{i}k} e^{-\mathbf{i}(kL+H)t} \mathrm{d}k =: O_R(t)$$

We'll show that $O_L(t)$ and $O_R(t)$ follow the same ODE

- $\frac{\mathrm{d}}{\mathrm{d}t} O_L(t) = -(L + \mathbf{i}H) O_L(t)$
- $\frac{\mathrm{d}}{\mathrm{d}t} O_R(t) = -(L + \mathbf{i}H) O_R(t) + L\left(\text{p.v.} \int_{\mathbb{R}} f(k) e^{-\mathbf{i}(kL+H)t} \mathrm{d}k\right) = -(L + \mathbf{i}H) O_R(t)$

$\blacksquare$

Improved LCHS with user-friendly conditions

Theorem (Huang-An ’25).

Suppose $f(k)$ is a function of $k \in \mathbb{R}$, and $F(x)$ is the Fourier transform of $\frac{f(k)}{1-\mathbf{i}k}$

- $F(x) = e^{-x}$ when $x \geq 0$
- Smoothness and integrability: $F(x) \in C^2(\mathbb{R}) \cap W^{2,1}(\mathbb{R})$

Then, for $L(t) \succcurlyeq 0$, the LCHS identity holds:

$$\mathcal{T}e^{-\int_0^t A(s)\mathrm{d}s} = \int_{\mathbb{R}} \frac{f(k)}{1-\mathbf{i}k} \mathcal{T}e^{-\mathbf{i}\int_0^t (kL(s)+H(s))\mathrm{d}s} \mathrm{d}k$$

To design a good kernel, we want to minimize:

- Truncation parameter K
- Overall complexity $K \int_{-K}^{K} \left| \frac{f(k)}{1-\mathbf{i}k} \right| \mathrm{d}k$