

CS 59300 – Algorithms for Data Science

Classical and Quantum approaches

Lecture 17 (11/6)

Quantum linear algebra toolkits (II)

https://ruizhezhang.com/course_fall_2025.html

Quantum linear algebra toolbox

- Basic linear algebra operations
 - Input models for vectors and matrices
 - Matrix-vector multiplication
 - Matrix/vector addition: linear combination of unitaries (LCU)
 - Matrix multiplication
- Linear systems of equations

Quantum linear system problem (QLSP)

Classical version: given an N -by- N Hermitian matrix A , and a vector b , compute

$$x = A^{-1}b$$

- For non-Hermitian A , consider dilation: $\begin{bmatrix} 0 & A \\ A^\dagger & 0 \end{bmatrix} \begin{bmatrix} 0 \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$

Quantum version: given a block-encoding for A (assuming $\|A\| = 1$) and a state preparation oracle for $|b\rangle$, compute an ϵ -approximation of the **quantum state**:

$$\| |\tilde{x}\rangle - |x\rangle \| \leq \epsilon \quad |x\rangle = \frac{A^{-1}|b\rangle}{\|A^{-1}|b\rangle\|}$$

Parameters:

- Condition number: $\kappa := \|A\| \|A^{-1}\| = \|A^{-1}\|$
- Accuracy ϵ

Harrow-Hassidim-Lloyd (HHL)

QLSP as an **eigenvalue transformation problem**:

- Consider the eigen-decomposition: $A = \sum_j \lambda_j |v_j\rangle\langle v_j|$
- $|b\rangle = \sum_j \beta_j |v_j\rangle$

$$A^{-1}|b\rangle = \left(\sum_j \lambda_j^{-1} |v_j\rangle\langle v_j| \right) \left(\sum_j \beta_j |v_j\rangle \right) = \sum_j \frac{\beta_j}{\lambda_j} |v_j\rangle$$

Need to do:

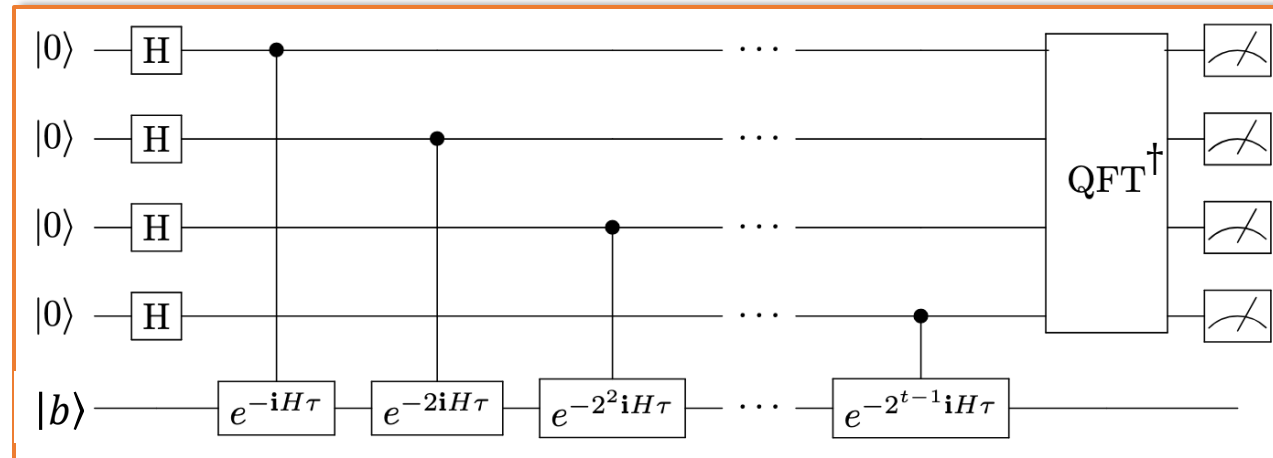
1. Store the information (binary encoding) of λ_j 's in an ancilla register coherently
2. Multiply the factor λ_j^{-1} to each eigenvector $|v_j\rangle$

← QPE

Harrow-Hassidim-Lloyd (HHL)

Need to do:

1. Store the information (binary encoding) of λ_j 's in an ancilla register coherently



$$U_{\text{QPE}}|0\rangle|b\rangle = \sum_j \beta_j |\tilde{\lambda}_j\rangle |v_j\rangle$$

Harrow-Hassidim-Lloyd (HHL)

Need to do:

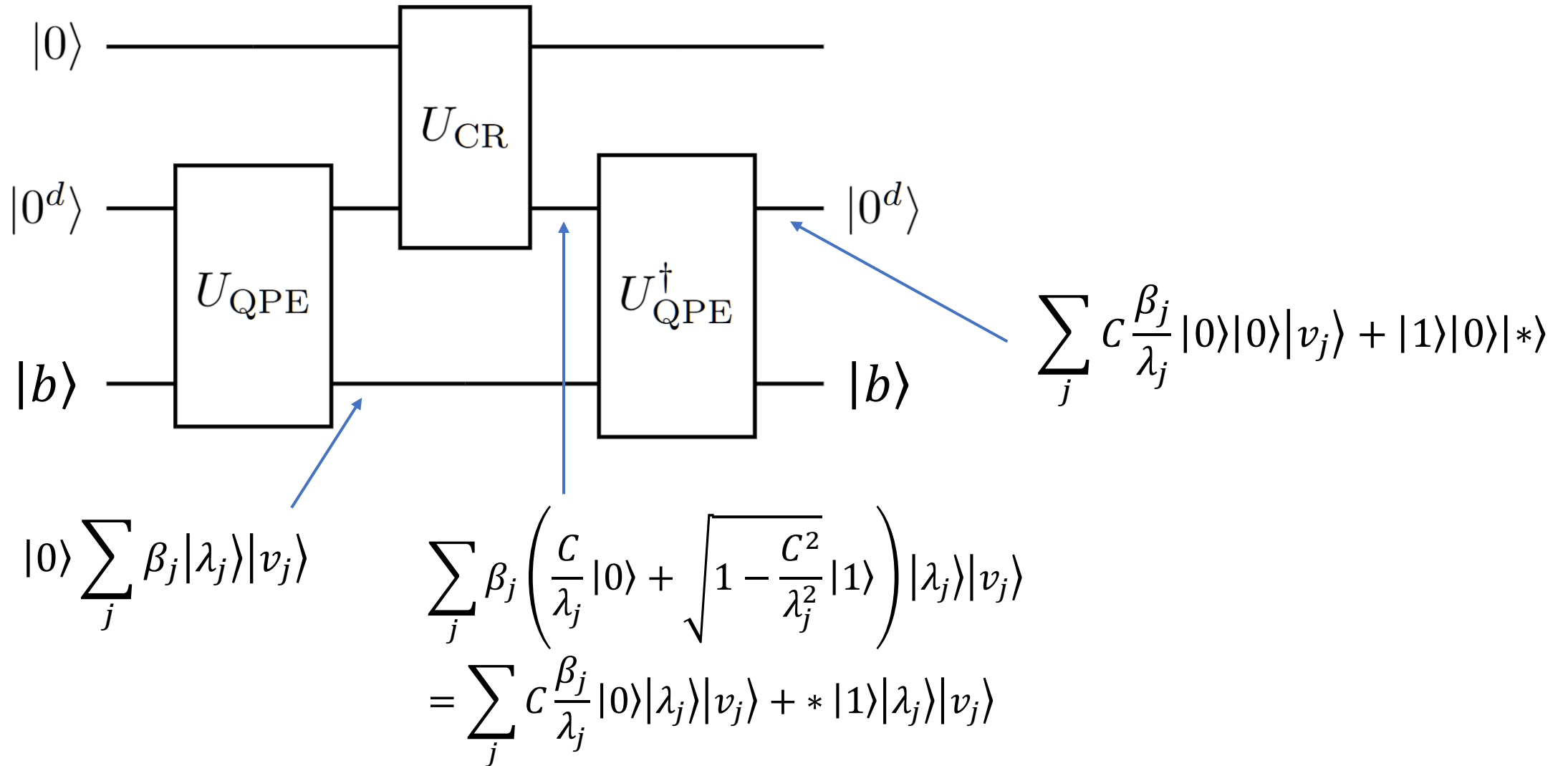
1. Store the information (binary encoding) of λ_j 's in an ancilla register coherently
2. Multiply the factor λ_j^{-1} to each eigenvector $|v_j\rangle$

Controlled rotation:

$$U_{\text{CR}}|0\rangle|\lambda_j\rangle = \left(\frac{C}{\lambda_j}|0\rangle + \sqrt{1 - \frac{C^2}{\lambda_j^2}}|1\rangle \right) |\lambda_j\rangle$$

- See Sec. 4.3.2 of *QASC* if you want to know how to implement U_{CR}

Harrow-Hassidim-Lloyd (HHL)



Harrow-Hassidim-Lloyd (HHL)

Final state of HHL:

$$|0\rangle \sum_j C \frac{\beta_j}{\lambda_j} |v_j\rangle + |\perp\rangle = |0\rangle C A^{-1} |b\rangle + |\perp\rangle$$

- We need to choose C so that $\left| \frac{C}{\lambda_j} \right| \leq 1$, i.e., $C \leq |\lambda_0|$
 - The success probability $= \|CA^{-1}|b\rangle\|^2 = C^2 \|x\|^2$, so we want C to be large
- } $C \sim 1/\kappa$

$$\text{Pr}[\text{succ}] = \|CA^{-1}|b\rangle\|^2 = \kappa^{-2} \cdot \|A^{-1}|b\rangle\|^2 \geq \kappa^{-2} \cdot \frac{\| |b\rangle \|^2}{\|A\|^2} = \kappa^{-2}$$

- Number of repeats: $\mathcal{O}(\kappa^{-1})$
- What is the cost of QPE?

Harrow-Hassidim-Lloyd (HHL)

Due to the approximation errors from QPE, the actual final state is

$$|0\rangle \sum_j c \frac{\beta_j}{\tilde{\lambda}_j} |v_j\rangle + |\perp\rangle \approx |0\rangle C A^{-1} |b\rangle + |\perp\rangle$$

where $\tilde{\lambda}_j = \lambda_j(1 + e_j)$ with $|e_j| \leq \epsilon/4$

- For the unnormalized solution,

$$\|\tilde{x} - x\| = \left\| \sum_j \beta_j \left(\frac{1}{\tilde{\lambda}_j} - \frac{1}{\lambda_j} \right) |v_j\rangle \right\| \leq \left\| \sum_j \frac{\beta_j}{\lambda_j} \left(\frac{-e_j}{1 + e_j} \right) |v_j\rangle \right\| = \mathcal{O}(\epsilon) \|x\|$$

- For the normalized solution state,

$$\| |\tilde{x}\rangle - |x\rangle \| = \left\| \frac{\tilde{x}}{\|\tilde{x}\|} - \frac{x}{\|x\|} \right\| \leq \left| 1 - \frac{\|\tilde{x}\|}{\|x\|} \right| + \frac{\|\tilde{x} - x\|}{\|x\|} \leq \epsilon$$

Harrow-Hassidim-Lloyd (HHL)

Due to the approximation errors from QPE, the actual final state is

$$|0\rangle \sum_j c \frac{\beta_j}{\tilde{\lambda}_j} |v_j\rangle + |\perp\rangle \approx |0\rangle C A^{-1} |b\rangle + |\perp\rangle$$

where $\tilde{\lambda}_j = \lambda_j(1 + e_j)$ with $|e_j| \leq \epsilon/4$

- Thus, QPE requires an addition error to within $\epsilon_{\text{QPE}} = \mathcal{O}(\lambda_0 \epsilon) \leq \epsilon/\kappa$
- The cost of U_{QPE} is $\mathcal{O}(\kappa/\epsilon)$
- Overall complexity of HHL: $\mathcal{O}(\kappa^2/\epsilon)$
- **Caveat:** QPE requires **Hamiltonian simulation** $e^{-i\tau A}$ and the $1/\epsilon$ in the complexity

QLSP via LCU (Fourier approach)

- Key identity:

$$\frac{1}{x} = \frac{\mathbf{i}}{\sqrt{2\pi}} \int_0^\infty dy \underbrace{\int_{-\infty}^\infty z e^{-z^2/2} e^{-ixyz} dz}_{-\sqrt{2\pi} \mathbf{i} t e^{-t^2/2} \Big|_{t=xy}}$$

$$\forall \text{ odd } f(y) \text{ s. t. } \int_0^\infty f(y) dy = 1, \quad \int_0^\infty f(xy) dy = \frac{1}{x}$$

QLSP via LCU (Fourier approach)

- Key identity:

$$\frac{1}{x} = \frac{\mathbf{i}}{\sqrt{2\pi}} \int_0^\infty dy \int_{-\infty}^\infty z e^{-z^2/2} e^{-\mathbf{i}xyz} dz$$

- It also holds for matrix:

$$\begin{aligned} A^{-1} &= \frac{\mathbf{i}}{\sqrt{2\pi}} \int_0^\infty dy \int_{-\infty}^\infty z e^{-z^2/2} e^{-\mathbf{i}yzA} dz \\ &\approx \frac{\mathbf{i}}{\sqrt{2\pi}} \int_0^Y dy \int_{-Z}^Z z e^{-z^2/2} e^{-\mathbf{i}yzA} dz \\ &\approx \frac{\mathbf{i}}{\sqrt{2\pi}} \sum_{j=0}^{J-1} \Delta_y \sum_{k=-K}^K \Delta_z Z_k e^{-z_k^2/2} e^{-\mathbf{i}y_j z_k A} \end{aligned}$$

$$\begin{aligned} Y &= \mathcal{O}\left(\kappa\sqrt{\log(\kappa/\epsilon)}\right), \\ Z &= \mathcal{O}\left(\sqrt{\log(\kappa/\epsilon)}\right) \end{aligned}$$

$$\begin{aligned} \text{LCU cost} &\approx \|c\|_1 \approx \int_0^Y dy \int_0^Z z e^{-z^2/2} dz \\ &= \mathcal{O}\left(\kappa\sqrt{\log(\kappa/\epsilon)}\right) \end{aligned}$$

QLSP via LCU (Fourier approach)

- It also holds for matrix:

$$A^{-1} \approx \frac{\mathbf{i}}{\sqrt{2\pi}} \sum_{j=0}^{J-1} \Delta_y \sum_{k=-K}^K \Delta_z z_k e^{-z_k^2/2} e^{-\mathbf{i}y_j z_k A}$$

$$Y = \mathcal{O}\left(\kappa\sqrt{\log(\kappa/\epsilon)}\right),$$

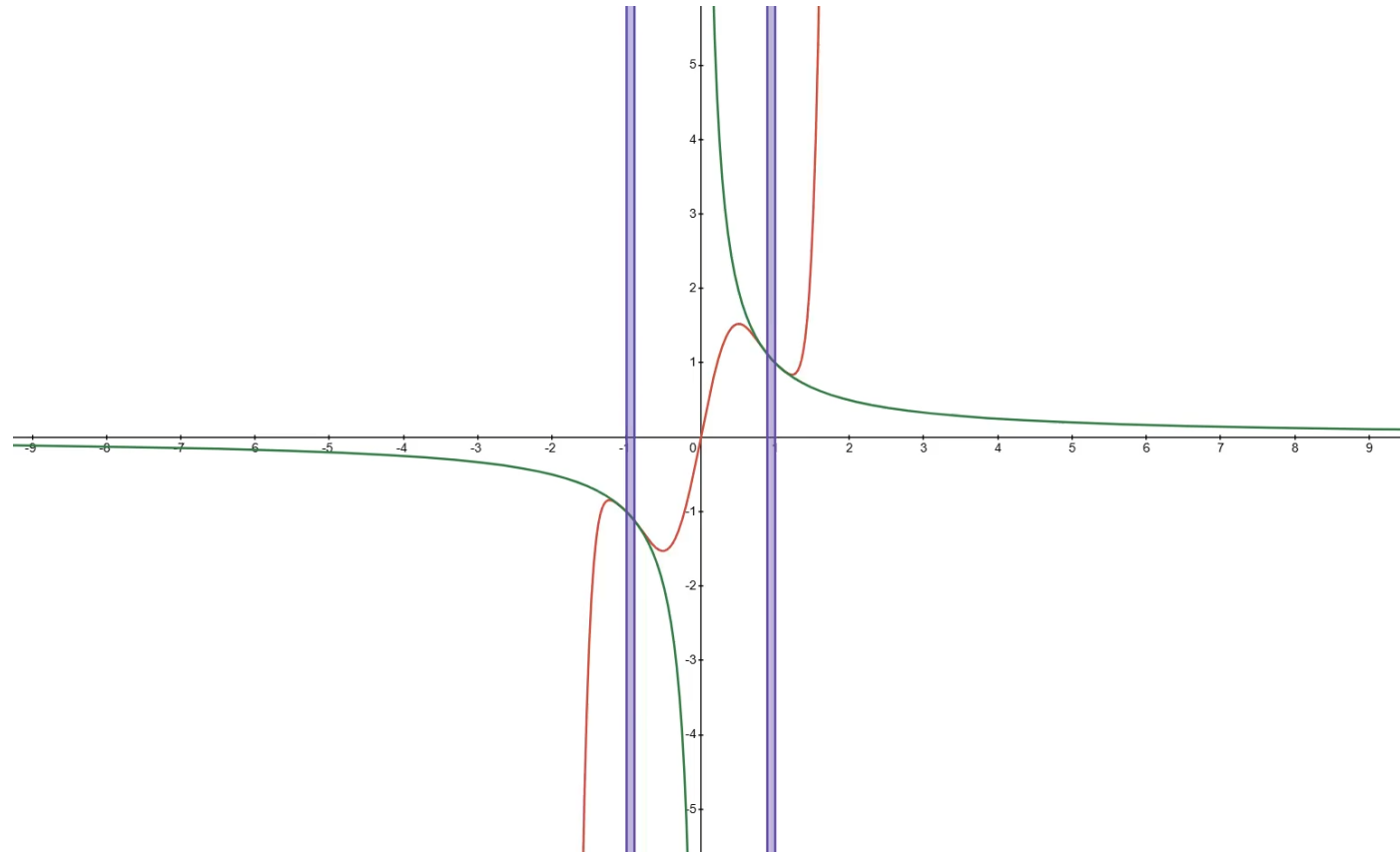
$$Z = \mathcal{O}\left(\sqrt{\log(\kappa/\epsilon)}\right)$$

- LCU cost: $\mathcal{O}\left(\kappa\sqrt{\log(\kappa/\epsilon)}\right)$
- Hamiltonian simulation $e^{-\mathbf{i}AT}$ cost: $T \text{polylog}(1/\epsilon) = \kappa \text{polylog}(\kappa/\epsilon)$
- Overall complexity:

$$\kappa\sqrt{\log(\kappa/\epsilon)} \times \kappa \text{polylog}(\kappa/\epsilon) = \kappa^2 \text{polylog}(\kappa/\epsilon)$$

QLSP via LCU (Chebyshev approach)

$$\frac{1}{x} \approx \frac{1 - (1 - x^2)^d}{x} \quad \forall x \in [-1, -\kappa] \cup [\kappa, 1] \quad d \sim \kappa^2 \log(\kappa/\epsilon)$$



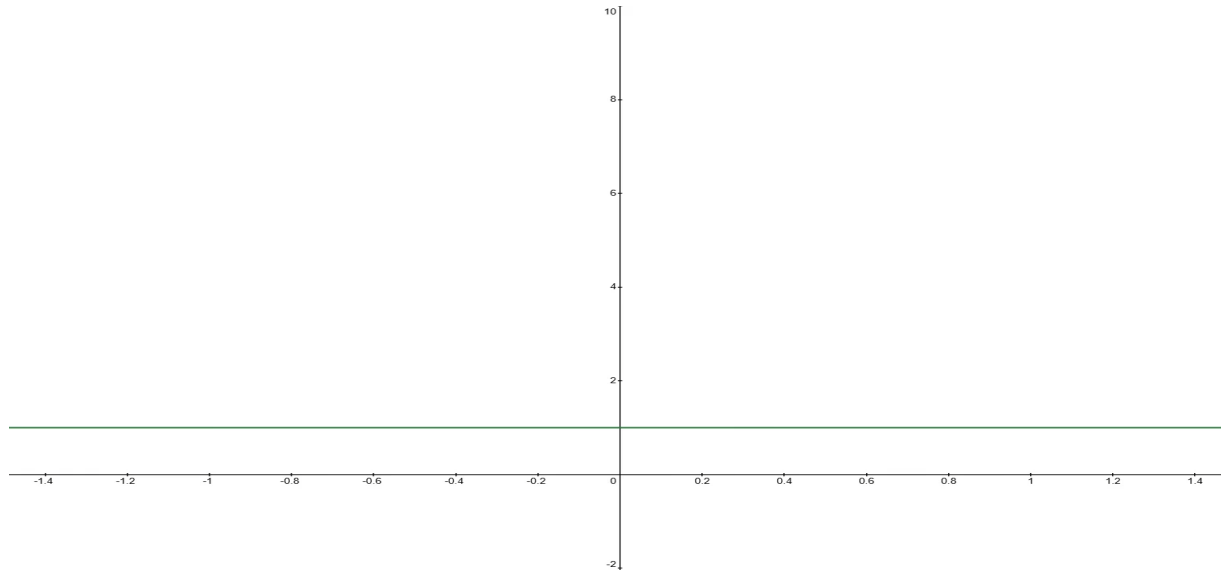
QLSP via LCU (Chebyshev approach)

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Chebyshev polynomials

$$T_n(\cos \theta) = \cos(n\theta)$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad T_0(x) = 1, T_1(x) = x$$



QLSP via LCU (Chebyshev approach)

$$\frac{1}{x} \approx \frac{1 - (1 - x^2)^d}{x} \quad \forall x \in [-1, -\kappa] \cup [\kappa, 1] \quad d \sim \kappa^2 \log(\kappa/\epsilon)$$

Chebyshev polynomials

$$T_n(\cos \theta) = \cos(n\theta)$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad T_0(x) = 1, T_1(x) = x$$

$$\begin{aligned} \frac{1 - (1 - x^2)^d}{x} &= 4 \sum_{j=0}^{d-1} (-1)^j \left(2^{-2d} \sum_{i=j+1}^d \binom{2d}{d+i} \right) T_{2j+1}(x) \\ &\approx 4 \sum_{j=0}^J (-1)^j \left(2^{-2d} \sum_{i=j+1}^d \binom{2d}{d+i} \right) T_{2j+1}(x) \quad J \sim \sqrt{d \log(d/\epsilon)} \end{aligned}$$

QLSP via LCU (Chebyshev approach)

$$A^{-1} \approx 4 \sum_{j=0}^{\kappa \text{polylog}(\kappa/\epsilon)} (-1)^j \left(2^{-2d} \sum_{i=j+1}^d \binom{2d}{d+i} \right) T_{2j+1}(A)$$

- The LCU cost $\approx \|c\|_1 = \mathcal{O}(\sqrt{d}) = \mathcal{O}(\kappa\sqrt{\log(\kappa/\epsilon)})$
- $\|T_{2j+1}(A)\| \leq 1$ but it is **non-unitary**, so we need to construct a block-encoding for it
 - Suppose it has a cost $\mathcal{O}(j) \leq \kappa \text{polylog}(\kappa/\epsilon)$
- Overall complexity:

$$\kappa\sqrt{\log(\kappa/\epsilon)} \times \kappa \text{polylog}(\kappa/\epsilon) = \kappa^2 \text{polylog}(\kappa/\epsilon)$$

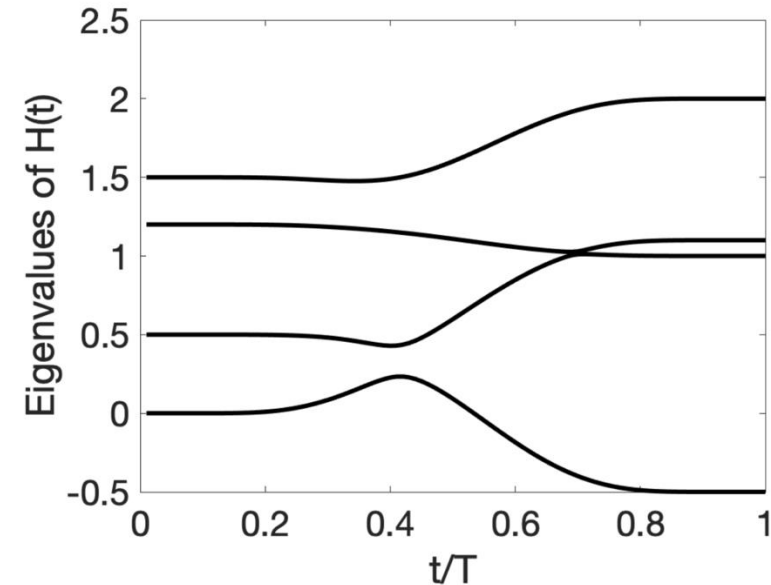
QLSP via Adiabatic quantum computation (AQC)

Schrödinger equation:

$$\begin{aligned}i\partial_t|\psi(t)\rangle &= H(t/T)|\psi(t)\rangle, & t \in [0, T] \\ H|\psi(0)\rangle &= \lambda|\psi_0\rangle\end{aligned}$$

Adiabatic evolution:

- Start from an eigenstate of the initial Hamiltonian $H(0)$
- $H(t/T)$ is changing slowly (i.e. T is large enough)
- Gap condition is satisfied
- The final state $|\psi(T)\rangle$ will approximate the eigenstate of $H(1)$



QLSP via Adiabatic quantum computation (AQC)

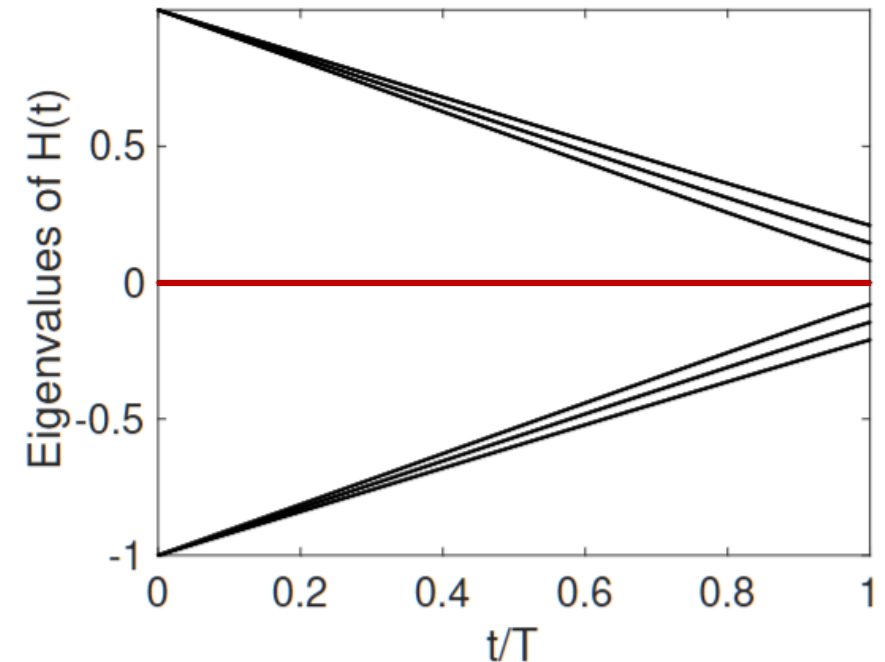
(Vanilla) AQC for QLSP:

$$H_0 = \begin{bmatrix} 0 & Q_b \\ Q_b & 0 \end{bmatrix}, \quad H_1 = \begin{bmatrix} 0 & AQ_b \\ Q_b A & 0 \end{bmatrix}$$

$$Q_b := I - |b\rangle\langle b|$$

$$H(s) = (1 - s)H_0 + sH_1$$

- H_0 has two eigenstates with eigenvalue 0: $\begin{bmatrix} b \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ b \end{bmatrix}$
- H_1 has two eigenstates with eigenvalue 0: $\begin{bmatrix} x \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ b \end{bmatrix}$
- If we start from $\begin{bmatrix} b \\ 0 \end{bmatrix}$, it will be evolved to $\begin{bmatrix} x \\ 0 \end{bmatrix}$
- QLSP \Rightarrow (Time-dependent) Hamiltonian simulation



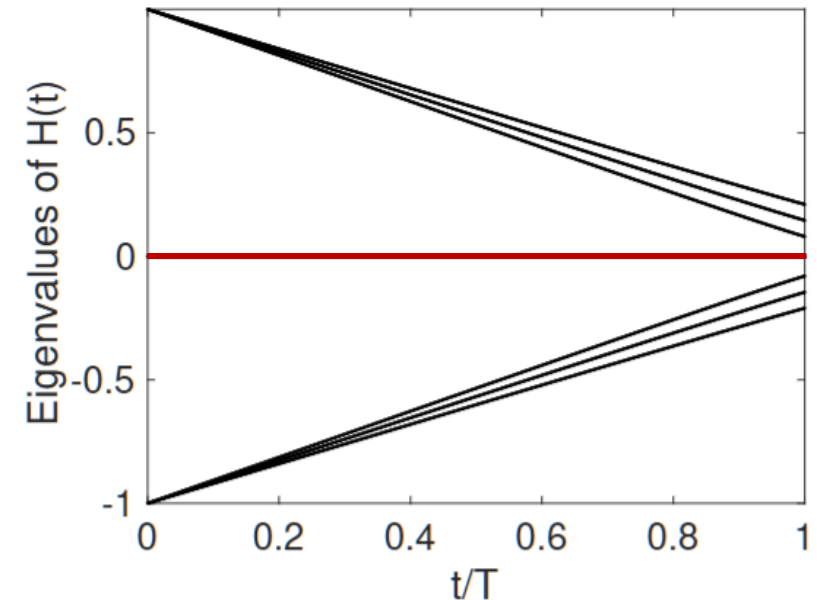
QLSP via Adiabatic quantum computation (AQC)

Quantum adiabatic theorem (Jansen-Ruskai-Seile '06).

Assume gap $\Delta(s)$, then the distance between the dynamics and the eigenvector can be bounded by

$$\eta(s) = \mathcal{O} \left(\frac{\|H'(0)\|}{T\Delta(0)^2} + \frac{\|H'(s)\|}{T\Delta(s)^2} + \frac{1}{T} \int_0^s \left(\frac{\|H''(\tau)\|}{\Delta(\tau)^2} + \frac{\|H'(\tau)\|^2}{\Delta(\tau)^3} \right) d\tau \right)$$

- To bound the error by ϵ , $T \sim \Delta_*^{-3} \epsilon^{-1}$
- In QLSP, $\Delta_* \sim \kappa^{-1}$
- Thus, $T \sim \kappa^3 \epsilon^{-1}$



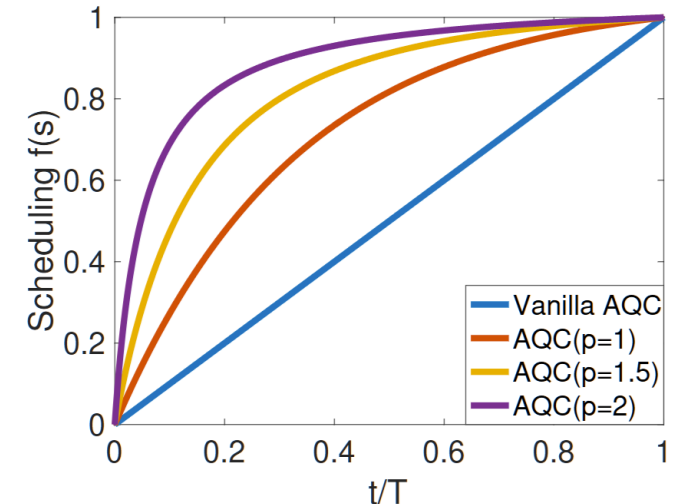
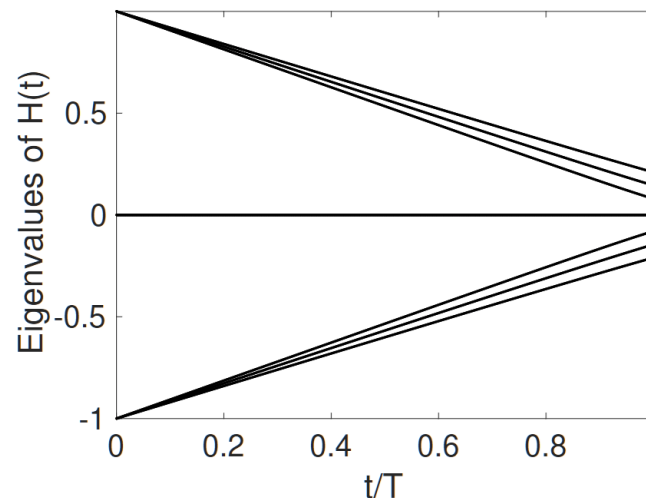
Time-optimal AQC for QLSP

$$i\partial_t|\psi(t)\rangle = H(t/T)|\psi(t)\rangle, \quad t \in [0, T]$$

- We can interpolate $H(s) = (1 - f(s))H_0 + f(s)H_1$ with a clever design of $f(s)$ such that $\|H'(s)\|$ is small when the gap $\Delta(s)$ is small
- An-Lin '19:

AQC(p): $\frac{df(s)}{ds} = c\Delta(f(s))^p \implies f(s) = \frac{\kappa}{\kappa - 1} \left(1 - (1 + s(\kappa^{p-1} - 1))^{\frac{1}{1-p}} \right)$

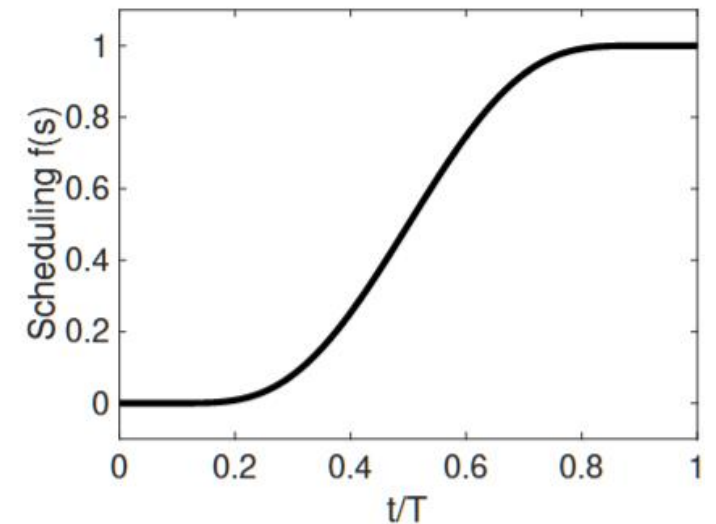
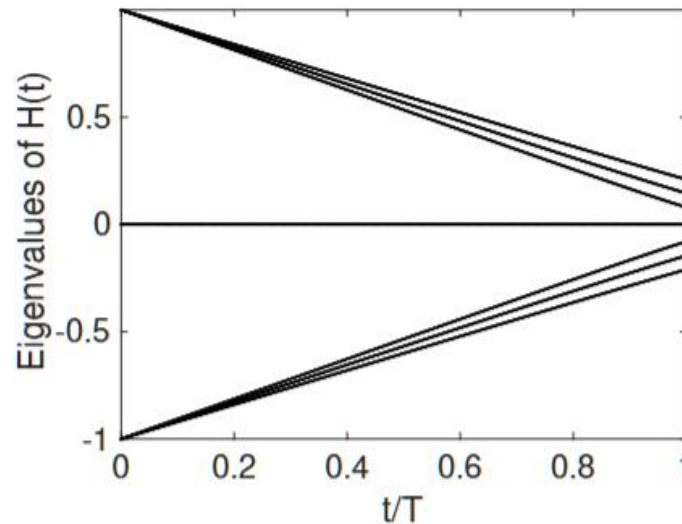
$$T = \mathcal{O}(\kappa/\epsilon)$$



- Quantum Adiabatic Theorem gives a **linear** rate error decaying
- To improve the ϵ -dependence, we need **higher-order** convergence, i.e. $\text{error} \sim T^{-k}$
- This is true if $f(s)$ satisfies the **boundary cancellation condition**: all derivatives of $H(f(s))$ vanishes at the boundary $s = 0$ and $s = 1$
- **An-Lin '19:**

AQC(exp):
$$f(s) = c' \int_0^s \exp\left(-\frac{1}{x(1-x)}\right) dx$$

- $T = \kappa \text{polylog}(\kappa/\epsilon)$
- Lower bound for QLSP:



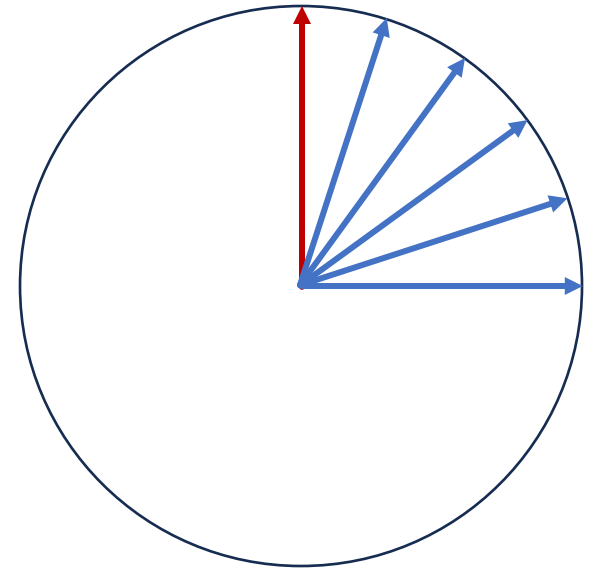
Quantum Zeno effect (QZE)

Projective measurement:

- Let P be a projector “implemented” in quantum
- We can apply P to a quantum state $|\psi\rangle$:
 - w.p. $\|P|\psi\rangle\|^2$, $|\psi\rangle \mapsto \frac{P|\psi\rangle}{\|P|\psi\rangle\|}$
 - w.p. $1 - \|P|\psi\rangle\|^2$, $|\psi\rangle \mapsto \frac{P^\perp|\psi\rangle}{\|P^\perp|\psi\rangle\|}$

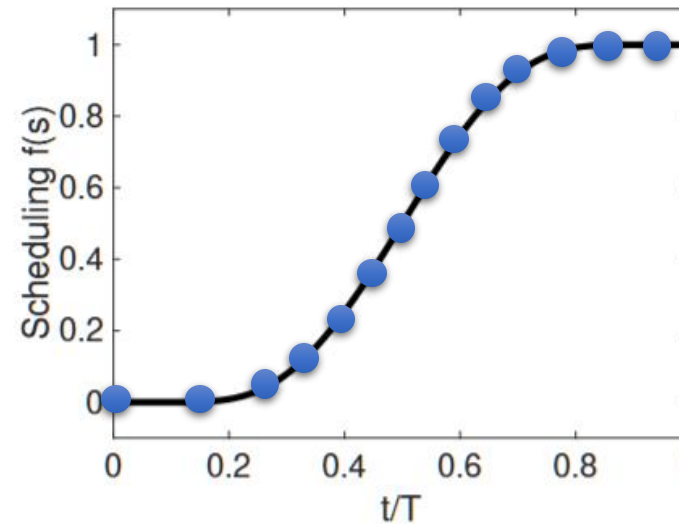
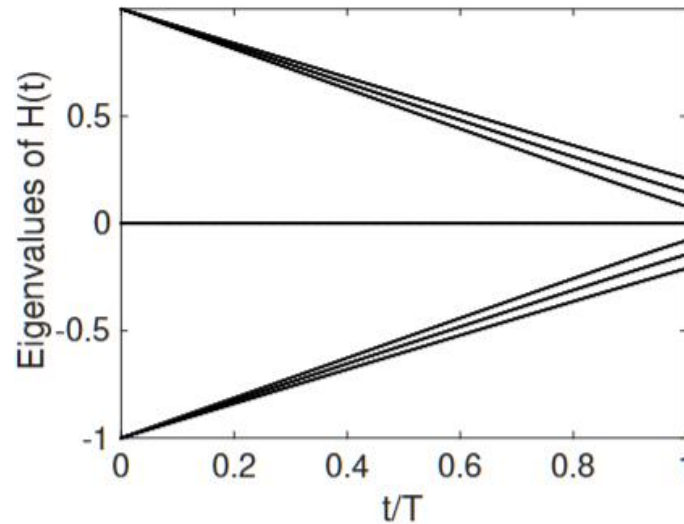
Quantum Zeno effect

- Suppose $|\psi_0\rangle, |\psi_1\rangle, \dots, |\psi_M\rangle$ s.t. $|\langle\psi_{i-1}|\psi_i\rangle|^2 \geq 1 - \mathcal{O}(M^{-1})$
- Let $P_i := |\psi_i\rangle\langle\psi_i|$ be the projector for each $i \in [M]$
- With $\mathcal{O}(1)$ success probability, we can convert $|\psi_0\rangle$ to $|\psi_M\rangle$ by applying projective measurements P_1, P_2, \dots, P_M to $|\psi_0\rangle$



QZE for adiabatic algorithms

Continuous AQC
path:



- Let $|x(t)\rangle$ be the ground state of $H(t)$
- Choose $0 = t_0 < t_1 < t_2 < \dots < t_M = 1$ such that $|\langle x(t-1) | x(t) \rangle|$ is sufficiently large
- Implement the projector $P_i := |x(t_i)\rangle\langle x(t_i)|$ (i.e. the ground state projector) in block-encoding
- By QZE, we can convert $|x(0)\rangle$ to $|x(t_M)\rangle = |x\rangle$ without **time-dependent** Hamiltonian simulation

Quantum linear algebra toolbox

- Basic linear algebra operations
 - Input models for vectors and matrices
 - Matrix-vector multiplication
 - Matrix/vector addition: linear combination of unitaries (LCU)
 - Matrix multiplication
- Linear systems of equations
 - HHL: κ^2/ϵ
 - LCU (Fourier and Chebyshev): $\kappa^2 \log(1/\epsilon)$ (Can be improved to $\kappa \log(1/\epsilon)$ via VTAA)
 - AQC: $\kappa \log(1/\epsilon)$ (optimal)
 - Recent survey: [arXiv:2411.02522v3](https://arxiv.org/abs/2411.02522v3)

Application of QLSP: quantum SVM

Classification:

- **Input:** training data $\{(\mathbf{x}_i, y_i)\}_{i \in [N]}$, where $y_i \in \{\pm 1\}$; kernel function $K(\cdot, \cdot)$
- **Goal:** learn a classifier

$$f(\mathbf{x}) = \text{sgn} \left(\sum_{i=1}^N \mathbf{w}_i K(\mathbf{x}_i, \mathbf{x}) \right)$$

Support vector machine (SVM)

- $K(\mathbf{x}, \mathbf{y}) := \phi(\mathbf{x})^\top \phi(\mathbf{y})$, where $\phi(\cdot)$ is a given feature map

$$\begin{aligned} \min_{\mathbf{w}, b, e} & \frac{1}{2} \mathbf{w}^\top \mathbf{w} + \frac{\gamma}{2} \sum_{i=1}^N e_i^2 \\ \text{s. t. } & y_i \mathbf{w}^\top \phi(\mathbf{x}_i) = 1 - e_i, \end{aligned}$$

$$\forall i \in [N]$$



$$(K + \gamma^{-1} I) \mathbf{w} = \mathbf{y}$$

$$K_{ij} := \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j)$$

QSVM

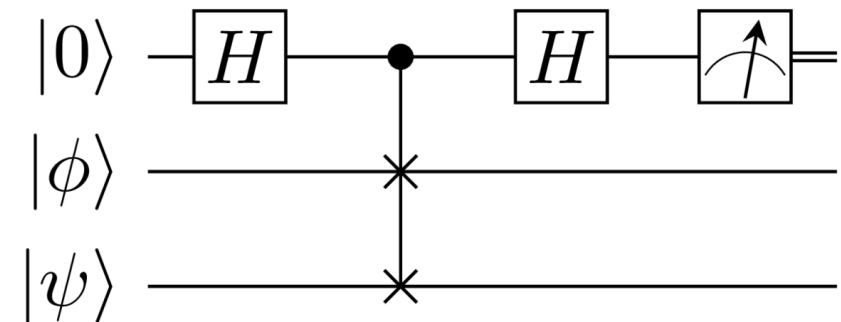
- Construct the block-encoding of the kernel matrix $K_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$
- Construct the block-encoding of the matrix $H = K + \gamma^{-1}I$
- Apply the QLS solver to prepare the state $|\mathbf{w}\rangle = H^{-1}|\mathbf{y}\rangle$
- For each test data \mathbf{x} :
 - Compute $f(\mathbf{x}) = \sum_{i=1}^N w_i K(\mathbf{x}_i, \mathbf{x})$
 - Output $\text{sgn}(f(\mathbf{x}))$

$$f(\mathbf{x}) = \langle \mathbf{w} | K(\cdot, \mathbf{x}) \rangle$$

We can prepare $|K(\cdot, \mathbf{x})\rangle$ and use the **swap test** to estimate the inner product

Complexity: $\tilde{O}(\kappa \alpha \text{polylog}(NM) \log(\epsilon^{-1}))$

- α : block-encoding normalization factor
- M : dim of feature space; N : number of data



Input model: matrices

Matrix as quantum gate (block-encoding):

Let A be a 2^n -by- 2^n matrix. A **block-encoding** of A is a 2^{n+a} -by- 2^{n+a} **unitary** U_A such that

$$A \approx \alpha(\langle 0^a | \otimes I) U_A (| 0^a \rangle \otimes I)$$

Or equivalently,

$$U_A \approx \begin{bmatrix} A/\alpha & * \\ * & * \end{bmatrix}$$

- α is called the block-encoding factor and should satisfy $\alpha \geq \|A\|$
- U_A is called an (α, a, ϵ) -block-encoding of A
- **Constructing U_A** is generally hard, but easy in special cases such as unitaries, sparse matrices, special structured matrices (Gilyen et al. '18; Camps et al. '22)

Construct block-encodings

Block-encoding always exists:

- Let A be a general matrix with $\|A\| \leq 1$
- Consider the SVD $A = W\Sigma V^\dagger$, where Σ 's diagonal entries are in $[0,1]$
- We have a $(1,1,0)$ -block-encoding for A :

$$\begin{aligned} U_A &:= \begin{bmatrix} W & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} \Sigma & \sqrt{I - \Sigma^2} \\ \sqrt{I - \Sigma^2} & -\Sigma \end{bmatrix} \begin{bmatrix} V^\dagger & 0 \\ 0 & I \end{bmatrix} \\ &= \begin{bmatrix} A & W\sqrt{I - \Sigma^2} \\ \sqrt{I - \Sigma^2}V^\dagger & -\Sigma \end{bmatrix} \end{aligned}$$

Construct block-encodings

Diagonal matrix:

- Let A be a diagonal matrix given by the quantum oracle:

$$O_A : |0\rangle|i\rangle \mapsto \left(A_{ii}|0\rangle + \sqrt{1 - |A_{ii}^2|}|1\rangle \right) |i\rangle$$

- $U_A := O_A$ is a $(1,1,0)$ -block-encoding for A :

$$\langle 0|\langle j|U_A|0\rangle|i\rangle = A_{ii}\delta_{ij} \quad \forall i, j \in [N]$$

Construct block-encodings

Sparse matrix:

- Let A be a sparse matrix such that each row/column has $\leq S = 2^s$ nonzero entries
- Three input oracles:

$$O_r|l\rangle|i\rangle = |r(i, l)\rangle|i\rangle$$

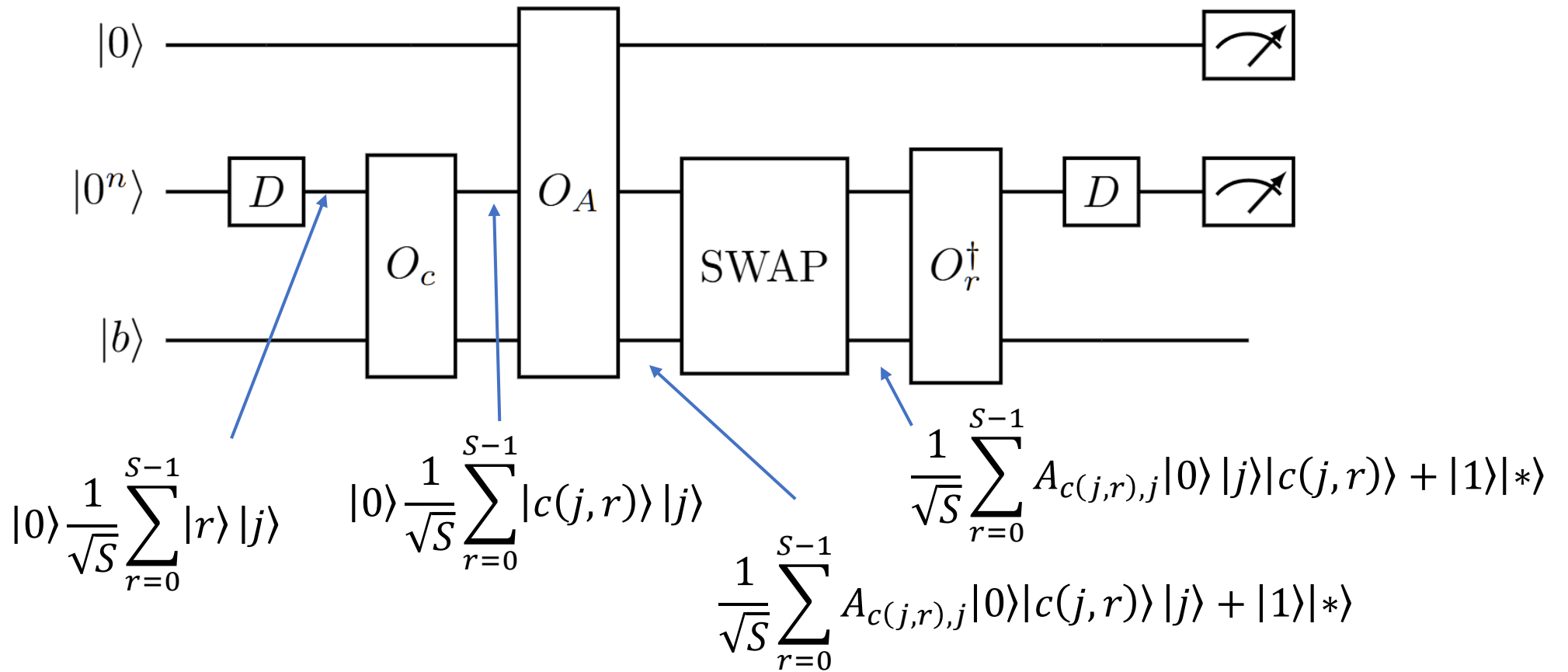
$$O_c|r\rangle|j\rangle = |c(j, r)\rangle|j\rangle$$

$$O_A|0\rangle|i\rangle|j\rangle = \left(A_{ii}|0\rangle + \sqrt{1 - |A_{ii}^2|}|1\rangle \right) |i\rangle|j\rangle$$

- $r(i, l)$ is the position of the l -th nonzero entry in the i -th row
- $c(j, r)$ is the position of the r -th nonzero entry in the j -th column

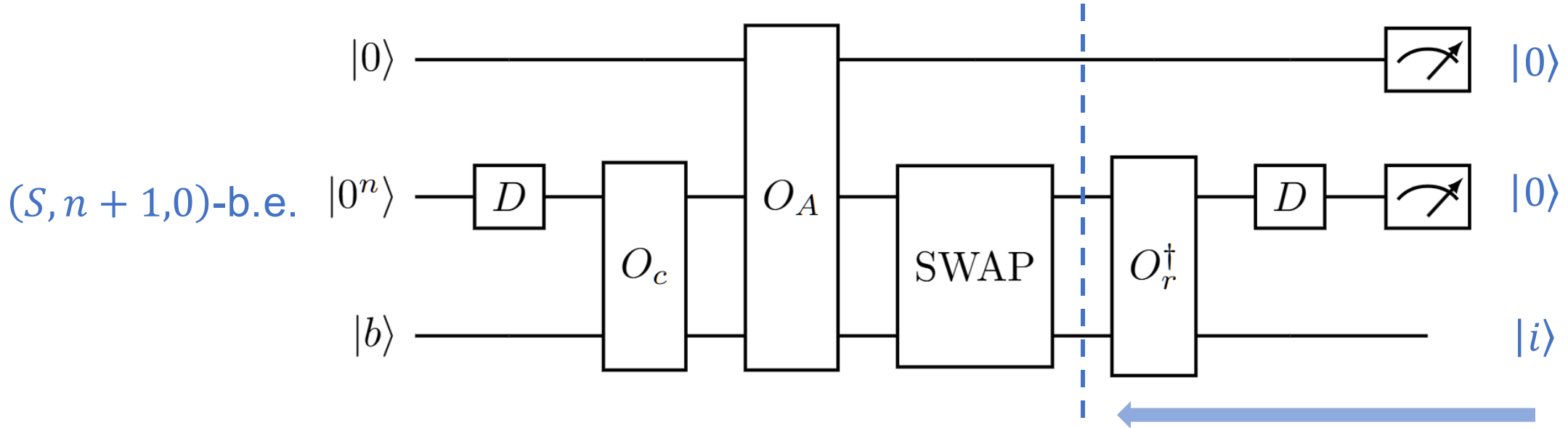
Construct block-encodings

Sparse matrix:



Construct block-encodings

Sparse matrix:



$$\frac{1}{\sqrt{S}} \sum_{r=0}^{S-1} A_{c(j,r),j} |0\rangle |j\rangle |c(j,r)\rangle + |1\rangle |*\rangle$$

$$\frac{1}{\sqrt{S}} \sum_{l=0}^{S-1} |0\rangle |r(i,l)\rangle |i\rangle$$

$$\langle 0 | \langle 0 | \langle i | U_A | 0 \rangle | 0 \rangle | j \rangle = \frac{1}{S} \sum_{l,r=0}^{S-1} A_{c(j,r),j} \delta_{i,c(j,r)} \delta_{j,r(i,l)} = \frac{1}{S} A_{ij}$$