

Quantum Krylov Algorithm for Szegő Quadrature

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1. Goal

Approximate

$$\langle \psi_a | f(U) | \psi_b \rangle$$

$f(U)$ = function of unitary operator

$|\psi_a\rangle, |\psi_b\rangle$ = quantum states

Cast as expectation value

$$\langle \psi_0 | f(U) | \psi_0 \rangle,$$

by combining results with $|\psi_0\rangle = |\psi_a\rangle \pm |\psi_b\rangle, |\psi_a\rangle \pm i|\psi_b\rangle$

Example applications

1. Gibbs states (for $U = e^{-iH\Delta t}$):

$$f(U) = U^{-i\beta/\Delta t} = e^{-\beta H}$$

2. Green's functions:

$$f(U) = [i \log(U)/\Delta t - \omega - i\eta]^{-1}$$

3. Polynomials of U

2. Unitary Krylov Algorithm

$$1. |\psi_0\rangle \Rightarrow U|\psi_0\rangle \Rightarrow \dots \Rightarrow U^{D-1}|\psi_0\rangle$$

$$2. (\mathbf{U}, \mathbf{S}) = \text{project } U \text{ onto } \underbrace{\text{span}[|\psi_0\rangle, U|\psi_0\rangle, U^2|\psi_0\rangle, \dots, U^{D-1}|\psi_0\rangle]}_V$$

$$\begin{bmatrix} V^\dagger \end{bmatrix} \begin{bmatrix} U \end{bmatrix} \begin{bmatrix} V \end{bmatrix} = \begin{bmatrix} \mathbf{U} \end{bmatrix}, \quad \begin{bmatrix} V^\dagger \end{bmatrix} \begin{bmatrix} V \end{bmatrix} = \begin{bmatrix} \mathbf{S} \end{bmatrix}$$

$$3. \text{Orthogonalize: } \widetilde{U} = \mathbf{S}^{-1/2} \mathbf{U} \mathbf{S}^{-1/2} \text{ (in practice, regularize here)}$$

3. Quadrature Rules

For measure $d\mu$, quadrature rule is defined by nodes and weights (λ_k, ω_k) s.t.

$$\int_R f(x) d\mu(x) \approx \sum_k \omega_k f(\lambda_k)$$

Gauss rule: optimal for real line — d -node rule exact for degree $2d - 1$ poly

Szegő rule: optimal for $\mathbb{T}$ (unit circle in $\mathbb{C}$) — exact for degree $d - 1$ Laurent poly

4. Quantum Szegő Quadrature

$$\langle \psi_0 | f(U) | \psi_0 \rangle = \int_{\mathbb{T}} f(z) d\mu(z) \text{ for } d\mu(z) = \sum_{j=0}^{N-1} |\gamma_j|^2 \delta(z - \zeta_j)$$

ζ_j $\downarrow$ U eigenvalues
 γ_j $\downarrow$

Require one further classical step: project $\widetilde{U}$ to nearest unitary.

$$\widetilde{U} \leftarrow V^\dagger W \text{ for SVD } \widetilde{U} = V^\dagger D W$$

Main result:

Nodes λ_k of Szegő quadrature rule for $d\mu$ are eigenvalues of $\widetilde{U}$.

Weights ω_k are

$$\omega_k = |v_{k,0}|^2,$$

$v_{k,0}$ = zeroth entry of normalized eigenvector v_k of $\widetilde{U}^T$.

$$\text{Corollary: } \langle \psi_0 | f(U) | \psi_0 \rangle \approx \sum_{k=0}^{d-1} \omega_k f(\lambda_k)$$

Key facts:

- Once rule (λ_k, ω_k) is calculated for given $U, |\psi_0\rangle$, can use for any f
- No direct approximation of f required (e.g. series expansion)
- Error at least as good as optimal degree $d - 1$ Laurent polynomial approximation of f

7. Examples (U = Heisenberg model dynamics)

