Unitary tools for non-unitary tasks

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or, modern methods in quantum numerical linear algebra

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👉 Linear combinations of unitary transformations ...

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👉 Today

A taxonomy for quantum numerical linear algebra

Walking through recently developed algorithmic families[1]

Ultimate bounds on unitary techniques

Numerical tips & tricks in practice

Applications & open problems

[1]Bits & pieces of LCHS, QET, LCHM, G-QSP, ...

Trends in quantum numerical linear algebra

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Maps for singular values & eigenvalues [GSLW19, LS26, MW24], general matrix decompositions [QR22], generalized product formulas [CST+21], randomized techniques [MR25], widely applied to to simulation, linear systems, PCA, statistical inference ... [MRTC21]

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Less addressed: compilation for real instances

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Inflexible compilation: when scheduling these families of algorithms to hardware, our choices are limited

Simulating dynamics

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In parallel, the perfect excuse to communicate clearly and effectively with diverse adjacent subfields …

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Parameters include t, ε, α, κ, and cost is sensitive to properties of A!

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Given kernel function $\hat{f}$ whose FT decays rapidly, for[1] $A = L + iH$, we can use sums of unitaries to approximate non-unitary transforms [ALL23, ACL26]

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Even in homogenous, time-independent case, R and $\|\hat{f}\|_{L^1}$ introduces nonideal polylog ε^{-1} dependence, and expensive quadrature

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$$\forall x \geq 0, \quad |e^{-x} - f(x)| \leq \varepsilon \quad \Longrightarrow \tag{6}$$

$$\forall t \geq 0, \quad e^{-(L+iH)t} \approx \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(k)\, e^{-i(kL+H)t}\, dk. \tag{7}$$

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Contributions of [LS25]: a good choice of contour, simple quadrature, and block encoding to greatly reduce costs!

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Finally, almost all of complex analysis lifts from statements on scalar functions to normed (Banach) spaces — perfect for matrix functions

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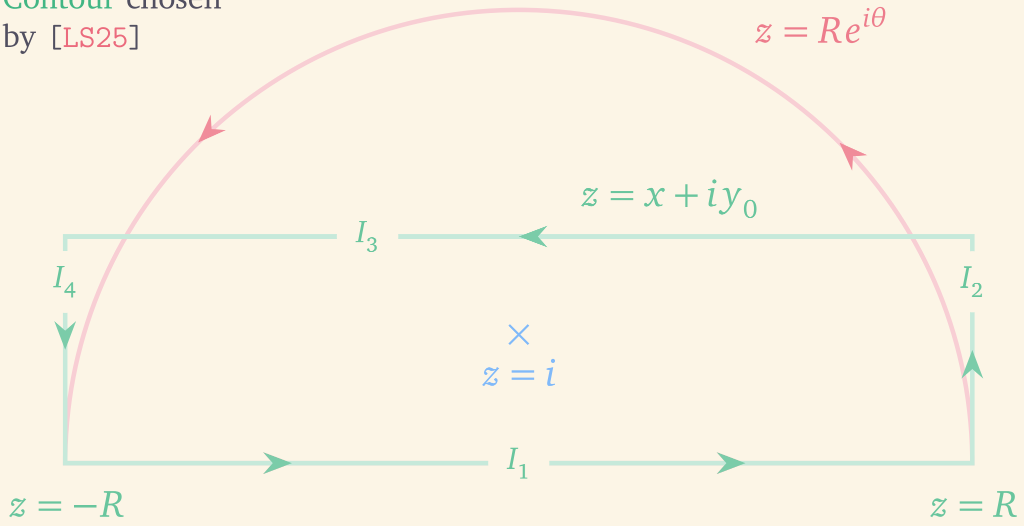
Contour chosen
by [LS25]



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$$O_R(t) \equiv \frac{1}{\sqrt{2\pi}} \int_{-R}^{R} \hat{f}(k) U(t;k)\, dk,$$
$$U_0(t) \equiv \frac{1}{\sqrt{2\pi}} \oint_{\Gamma} \hat{f}(z) U(t;z)\, dz = -U(t;i) = \mathcal{T}\left\{ e^{-\int_0^t L(s') + iH(s')\, ds'} \right\}.$$

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Then we argue properties of each piece of the difference

$$U_0(t) = \oint_\Gamma g(z)\,dz = I_1 + I_2 + I_3 + I_4 \tag{8}$$

$$\|O_R(t) - U_0(t)\| \leq \left\| \int_{\mathbb{R}\setminus[-R,R]} g(k)\,dk \right\| + \left\| \int_{\mathbb{R}} g(k+iy_0)\,dk \right\| \tag{9}$$

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Crucially, I_3 will no longer have to converge to 0 as $y_0 \to \infty$

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Note $\alpha_{\hat{f}_2} = e^c \mathrm{erfc}(1/2\gamma)$; appearing in integral of $e^{-t^2/\gamma^2}/(1+t^2)\, dt$

Choosing kernels and contours

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We can choose f to be *entire*[1], e.g., the convolution:

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Note pole at $k = -i$, and lack of decay over lower half-plane

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Let $A = L + iH$ for L, H finite L_1 norm

Choosing ε, R, γ, and c, one can argue a sufficient *uniform step-size* of $h \le \mathcal{O}([\|L\|_{L^1} + \log(1/\varepsilon')]^{-1})$ allows us to bound error:

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where I' is the uniform h-discretization of $O_R(t)$.

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While technical, convergence of this simple discretization is established by [TW14] for functions analytic in finite strip[1]

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Optimal LCHS: formal theorem breakdown

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Thm 1: Let $t \geq 0$, $A = L + iH$ for $\|L\|_{L^1}, \|H\|_{L^1} < \infty$, and[1] $L \succeq 0$. *On strip* assume $\hat{f}(z) \to 0$ for $|z| \to \infty$, and $(z+i)\hat{f}(z)$ analytic with residue $i/\sqrt{2\pi}$. Then finite integral error bound holds!

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Thms 3 & 4: Fix ε' and parameters above; then choice of h-discretization $h \leq \mathcal{O}([\|L\|_1 + \log(1/\varepsilon')]^{-1})$ bounds error to $\varepsilon + \varepsilon'$.

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Moreover, we can block encode $U_0(t)$ to precision ε'' using LCU PREP and SEL with two-qubit gate cost $\mathcal{O}(\log(||L||_{L^1} + \log \varepsilon^{-1}) \log^{5/2} \varepsilon^{-1})$ and $\mathcal{O}(Q \log(||L||_{L^1} + \log \varepsilon^{-1}))$ respectively[2]

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[2]Here meaning more than the full $\pm R$ integration.

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⚠️ Statements of optimality are made in time-independent case, while for time-dependent we get logarithmic overhead [LW19]

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Notably: choice of quadrature means $\alpha_{\hat{f},R,h} \approx \alpha_{\hat{f}}$, where the former is the LCU-subnormalization for our discretized integral, and the latter the L^1 norm of our kernel function

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👉 *Reasonable structure, cheap block encodings, flexible precision, and device characteristics affect method deeply!*

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Extensions, insights, and related work

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👉 *Relaxing circuit forms, hybridizing methods, and applying classical numerical tools exposes weakly formulated lower bounds*

Building bridges to higher-order methods

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Q1: *What can we do given access to non-unitary dynamics?*

Q2: *What can we do with near-unitary dynamics?*

Q3: *What is the irrep-label equivalent to eigenvalue processing?*

Q4: *Which methods can furnish more fine-grained lower bounds?*

Further reading on new techniques

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Sum-of-squares decomposition techniques for low-energy Hamiltonian simulation [KLB+26], simulating RLC circuit networks [DCTK26], adapted matrix inversion [DLS26]

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Properties of initial state,

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Simpler instances [SLBB25] often admit more realistic versions [SBS26]...

🏠 To take home

Simulation lower bounds are over-generic and experimentally un-generous

Adapted simulation methods are still limited: e.g., low-energy, time-independent [KLB+26, ZAH26]

Matrix equations, algebraically constrained dynamics, and operator approximation techniques are still only cursorily applied [DCTK26, SBS26]

👉 *Functional analytic techniques are flexible, well-understood, numerically friendly, and apply to settings well beyond spectral maps*

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