Linear and Non-linear Relational Analyses for Quantum Program Optimization

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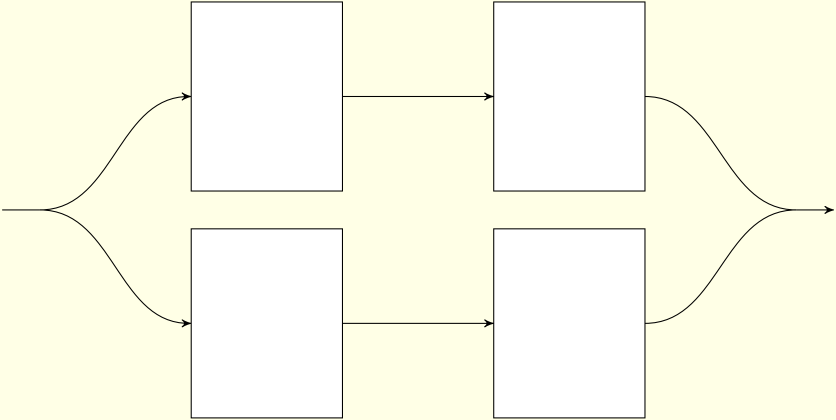
POPL
Denver, January 22nd, 2025

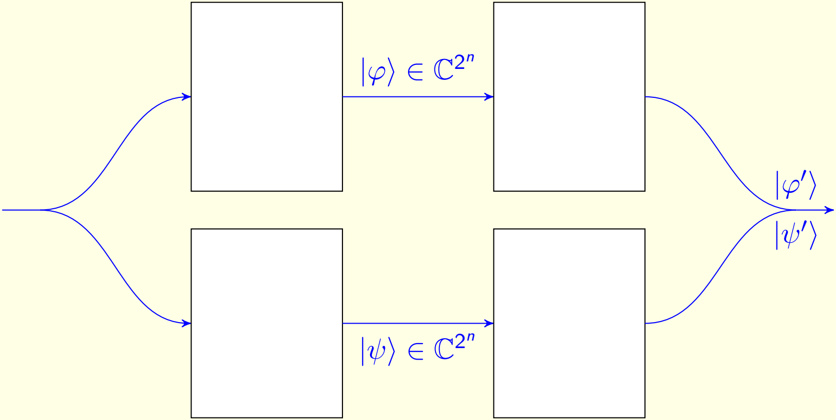
What is this talk about?

- Integration of circuit optimizations in hybrid quantum-classical toolchains
- The interaction between classical control & quantum data
  - Quantum (data flow) vs (quantum data) flow!

Quantum code + classical control

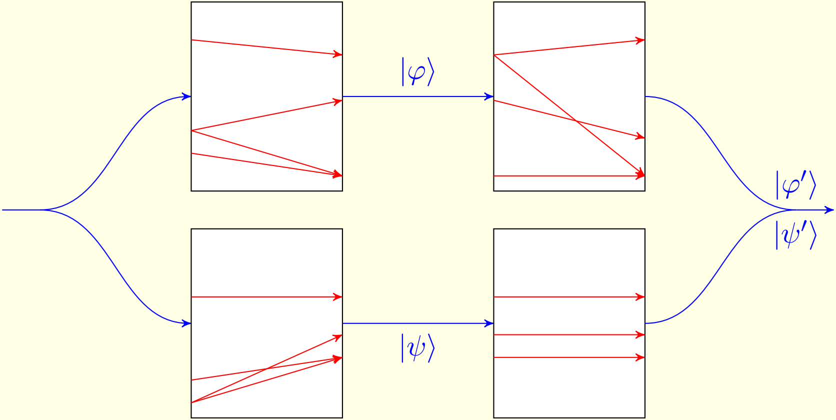


(Quantum data) flow



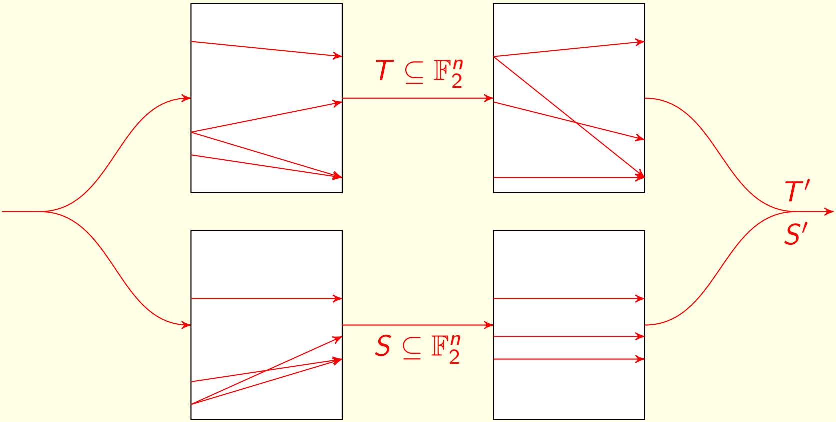
$|\psi'\rangle$ & $|\varphi'\rangle$ have exponential size, so can't do much analysis...

What's in the box?????????



Quantum (data flow)!

= classical data in (& out) of superposition



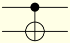
S' and T' are classical so can use classical methods!

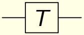
The quantum circuit model

n-qubit quantum state = superposition of classical *n*-bit states

$$|\psi\rangle = \sum_{\mathbf{x}\in\mathbb{F}_2^n} \alpha_{\mathbf{x}} |\mathbf{x}\rangle \in \mathbb{C}^{2^n}$$

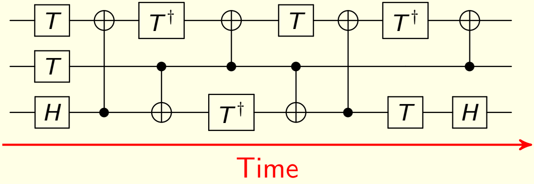
n-qubit quantum gate = unitary (linear, invertible) operator on $\mathbb{C}^{2^n}$

CNOT =  $= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

T = 

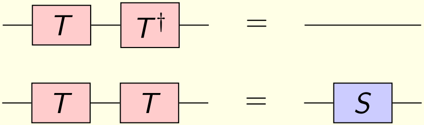
$= \begin{bmatrix} 1 & 0 \\ 0 & \omega := e^{i\frac{\pi}{4}} \end{bmatrix}$

Quantum program = sequence of gates



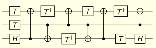
Quantum circuit optimizations

Rewrite-based:

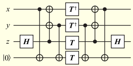


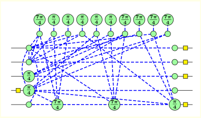
Semantics-based:

$$\sum_{\mathbf{y}} e^{iP(\mathbf{x},\mathbf{y})} |A(\mathbf{x},\mathbf{y})\rangle$$



$$R(P_1)R(P_2)\cdots R(P_k)$$





The quantum phase folding optimization

Merge + cancel diagonal gates where possible

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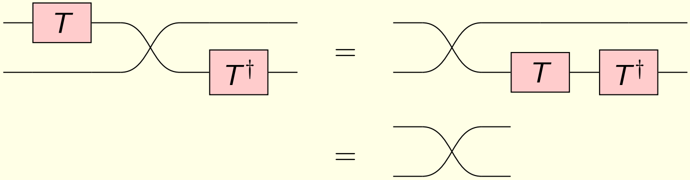

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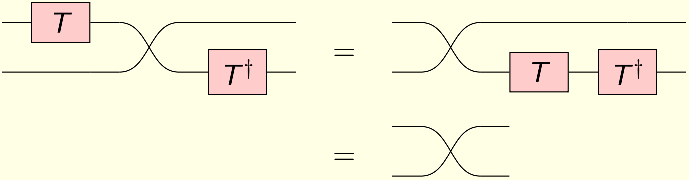
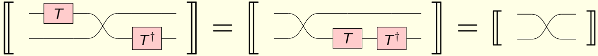


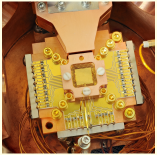
Semantics-based mod out by these commutations:



Welcome to the real-world™

A quantum program isn't just a circuit

sequence of gates



measurement results

Welcome to the real-world^{TM}

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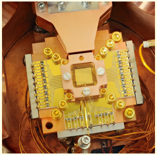
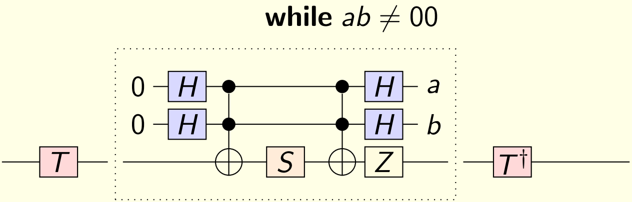


measurement results

Problem for semantics-based approaches:
two distinctly different semantics!

A real-world^{TM} program



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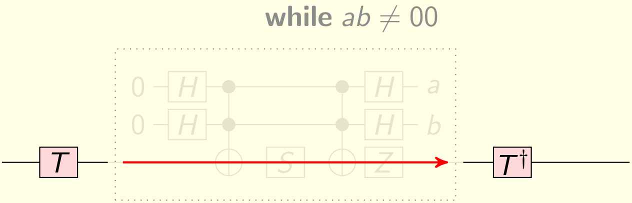
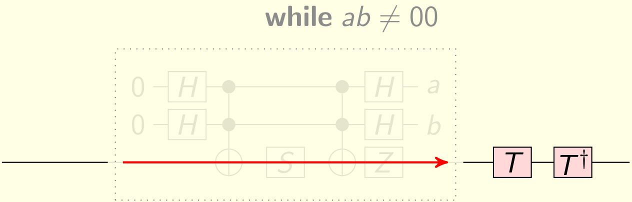


A real-world$^{\mathrm{TM}}$ program



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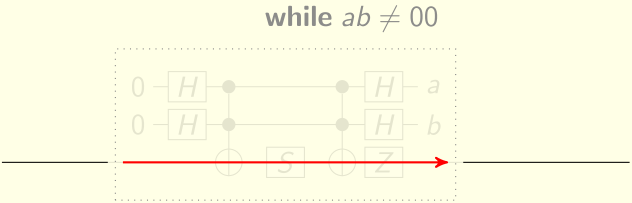


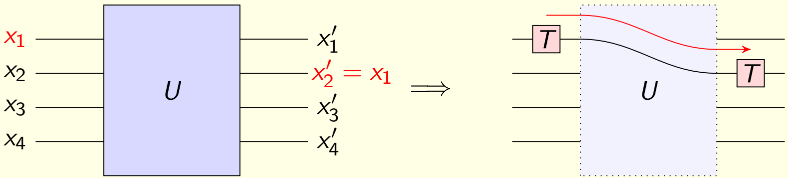
How can we formalize these optimizations?

A relational approach to phase folding

Proposition

Let $R \subseteq \mathbb{F}_2^n \times \mathbb{F}_2^n$ a relation on length n bit strings such that $\langle \mathbf{x}' | U | \mathbf{x} \rangle \neq 0 \implies (\mathbf{x}, \mathbf{x}') \in R$. Then if for all $(\mathbf{x}, \mathbf{x}') \in R$, $x'_j = x_i$,

$$T_{q_i} U = U T_{q_j}.$$



Extending to programs

Program model (non-deterministic quantum WHILE)

$$\Sigma ::= \textbf{skip} \mid q := |0\rangle \mid U\mathbf{q} \mid \textbf{meas } q \mid \textbf{call } p(\mathbf{q})$$
$$T ::= R \mid T_1;\ T_2 \mid \textbf{if} \star \textbf{then } T_1 \textbf{ else } T_2 \mid \textbf{while} \star \textbf{do } T$$

Classical semantics is the union of non-zero transitions $\langle \mathbf{x}'|\pi|\mathbf{x}\rangle \neq 0$ over all executions $\pi \in \Sigma^*$:

$$\begin{aligned}
\mathcal{C}\,[\![E \in \Sigma]\!] &= \{(\mathbf{x}, \mathbf{x}') \mid \langle \mathbf{x}'|E|\mathbf{x}\rangle \neq 0\} \\
\mathcal{C}\,[\![T_1;\ T_2]\!] &= \mathcal{C}\,[\![T_2]\!] \circ \mathcal{C}\,[\![T_1]\!] \\
\mathcal{C}\,[\![T_1 + T_2]\!] &= \mathcal{C}\,[\![T_1]\!] \cup \mathcal{C}\,[\![T_2]\!] \\
\mathcal{C}\,[\![T^*]\!] &= \cup_{k=0}^{\infty} \mathcal{C}\left[\!\!\left[T^k\right]\!\!\right]
\end{aligned}$$

How can we approximate the classical semantics?

Affine subspaces

Standard gates implement affine classical transformations + branching (in superposition)

$$T : |x\rangle \mapsto \omega^x |x\rangle$$
$$X : |x\rangle \mapsto |1 + x\rangle$$
$$\mathrm{CNOT} : |x, y\rangle \mapsto |x, x + y\rangle$$
$$H : |x\rangle \mapsto \frac{1}{\sqrt{2}} \sum_{y \in \mathbb{F}_2} (-1)^{xy} |y\rangle$$

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Abstract gates as affine subspaces of the pre and post state!

$$\begin{aligned} \mathcal{A}[\![T]\!] &= \langle x' = x \rangle & &= \{(x, x) \mid x \in \mathbb{F}_2\} \\ \mathcal{A}[\![X]\!] &= \langle x' = 1 + x \rangle & &= \{(x, 1 + x) \mid x \in \mathbb{F}_2\} \\ \mathcal{A}[\![CNOT]\!] &= \langle x' = x, y' = x + y \rangle & &= \{(x, y, x, x + y) \mid x, y \in \mathbb{F}_2\} \\ \mathcal{A}[\![H]\!] &= \top & &= \{(x, x') \mid x, x' \in \mathbb{F}_2\} \end{aligned}$$

Quantum affine relation analysis

Spoiler: it's just classical affine relation analysis

Proposition (Karr 1976, paraphrased heavily)

Given a flowchart program with affine assignments, a sound affine relation on program variables can be calculated in polynomial-time.

- Composition = relational composition
- Replace union with affine hull
- No infinite ascending chains, so Kleene closure terminates

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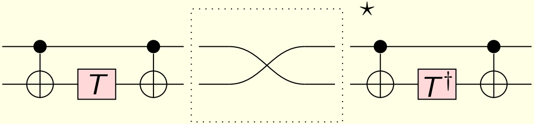
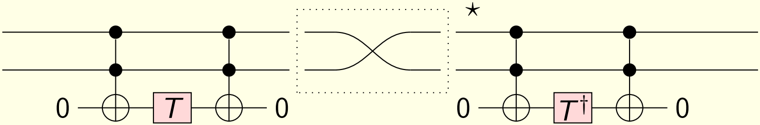


Loop invariant $\langle x' + y' = x + y \rangle$ allows canceling the T gates!

What if we need more precision?



- The non-linear loop invariant $x'y' = xy$ allows eliminating both T gates
- The strongest affine loop invariant $\langle x' + y' = x + y\rangle$ is unable to prove the relation $x'y' = xy$

  $\implies$ need non-linear relations for this optimization!

From affine subspaces to varieties

Replace affine subspaces with affine varieties and affine relations with polynomial ideals

$$I = \mathbb{I}(V) = \{f \in \mathbb{F}_2[\mathbf{X}, \mathbf{X}'] \mid f(\mathbf{x}, \mathbf{x}') = 0 \ \forall(\mathbf{x}, \mathbf{x}') \in V\}.$$

Gröbner basis methods suffice to compute compositions & (infinite) unions

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Gröbner basis methods suffice to compute compositions & (infinite) unions

Do we get all polynomial relations now? Yes(-ish)!

Proposition (Hilbert's strong Nullstellensatz for $\mathbb{F}_2$)

$$\mathbb{I}(\mathbb{V}(I)) = I + \langle X_i^2 - X_i \mid X_i \in \mathbf{X} \rangle$$

The catch

Sequential composition is not precise!

$$\mathcal{A}\,[\![H]\!] \circ \mathcal{A}\,[\![H]\!] = \top \circ \top = \top$$

$$\mathcal{A}\,[\![HH]\!] = \mathcal{A}\,[\![I]\!] = \langle x, x' \rangle$$

Problem is interference, which is used in quantum programs to implement non-linear classical transitions

The catch

Sequential composition is not precise!

$$\mathcal{A}\llbracket H \rrbracket \circ \mathcal{A}\llbracket H \rrbracket = \top \circ \top = \top$$

$$\mathcal{A}\llbracket HH \rrbracket = \mathcal{A}\llbracket I \rrbracket = \langle x, x' \rangle$$

Problem is interference, which is used in quantum programs to implement non-linear classical transitions

Idea: treat circuits precisely and then extract precise transition relations for circuit blocks

Symbolic path integrals

Path integral = classical transitions + amplitudes

$$(\!|C|\!) = |\mathbf{x}\rangle \mapsto \sum_{\mathbf{y}\in\mathbb{F}_2^k} \Phi(\mathbf{x},\mathbf{y})|f_1(\mathbf{x},\mathbf{y})\rangle \otimes \cdots \otimes |f_n(\mathbf{x},\mathbf{y})\rangle$$

The ideal $\exists \mathbf{Y}.\langle X_1' = f_1(\mathbf{X},\mathbf{Y}), \ldots, X_n' = f_n(\mathbf{X},\mathbf{Y})\rangle$ hence (over-)approximates the classical transitions of C

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Knowing the amplitudes allows re-writing to eliminate infeasible transitions!

$$\begin{aligned} (\!|H|\!) \circ (\!|H|\!) &= |x\rangle \mapsto \frac{1}{\sqrt{2}} \sum_{y,z\in\mathbb{F}_2} (-1)^{y(x+z)}|z\rangle & \implies \exists Y, Z\langle X' + Z\rangle = \top \\ &\equiv |x\rangle \mapsto |x\rangle & \implies \langle X' + X\rangle \end{aligned}$$

Implementation

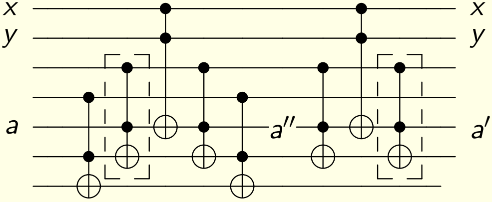
- Implemented affine & polynomial analyses on openQASM 3.0 in Feynman[1]
- Finds non-trivial optimizations based on loop invariants
- Easy + deep integration of phase folding in compilers for hybrid workflows

Benchmark	n	Original	$\mathbf{PF}_{\mathrm{Aff}}$		$\mathbf{PF}_{\mathrm{Pol}}$		Loop invariant
		$\#\ T$	$\#\ T$	time (s)	$\#\ T$	time (s)	
RUS	3	16	10	0.30	8	0.35	$\langle z' + z \rangle$
Grover	129	$1736e9$	$1470e9$	1.98	TIMEOUT		–
Reset-simple	2	2	1	0.15	1	0.23	–
If-simple	2	2	0	0.18	0	0.16	–
Loop-simple	2	2	0	0.17	0	0.16	$\langle x' + x, y + y' + xy + xy' \rangle$
Loop-h	2	2	0	0.16	0	0.16	$\langle y' + y \rangle$
Loop-nested	2	3	2	0.17	2	0.18	$\langle x' + x \rangle$, $\langle x' + x \rangle$
Loop-swap	2	2	0	0.30	0	0.20	$\langle x' + y' + x + y, x' + xy + xx' + yx' \rangle$
Loop-nonlinear	3	30	18	0.44	0	0.26	$\langle x' + x, z' + z, y' + y + xy + xy' \rangle$
Loop-null	2	4	1	0.18	1	0.17	$\langle x' + x, y' + y \rangle$

[1] https://github.com/meamy/feynman

Circuit optimization

With the relational approach, phase folding is strictly better than previous approaches due to the use of non-linear reasoning



- The relation $a' = a$ allows removing 2 T gates
- Proving $a' = a$ requires deriving the non-linear relations

$$a'' = a + xy \qquad a' = a'' + xy$$

- No previous circuit optimizer has achieved this

Conclusion

In this talk...

- Reframed a standard circuit optimization as a relational analysis of the classical semantics
- Used classical techniques in this framing to extend to quantum program optimization
- Gave a method of increasing the precision by temporarily using a more precise "quantum" domain of path integrals

Take-aways

- Quantum (data flow) = classical data flowing in superposition
  - So you can re-use your classical techniques!

Thank you!