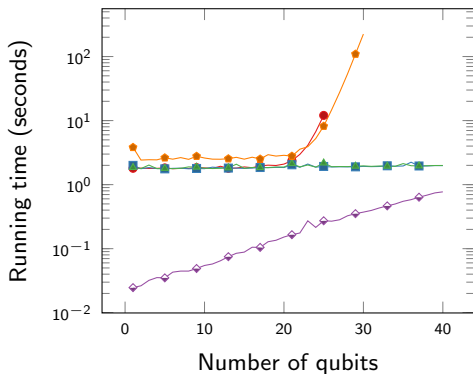


Simulating Quantum Computation Using Probabilistic Programming

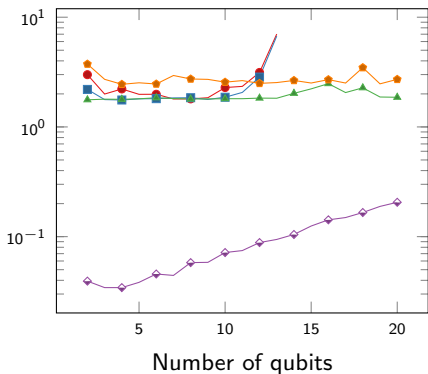
Yafei Yang and Chung-chieh Shan, Indiana University

December 2025

Hadamard to the last qubit



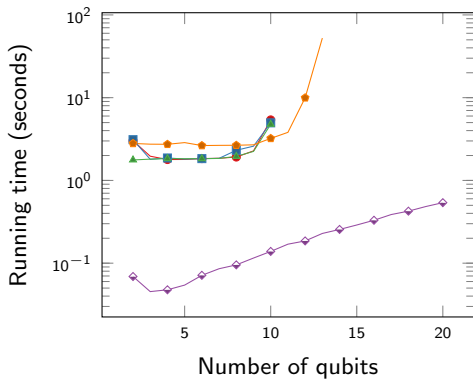
Deutsch-Jozsa with the 0 oracle



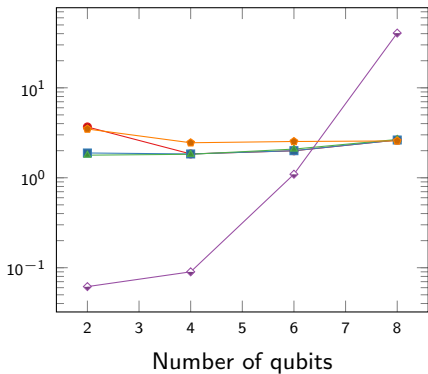
- FGG with scatter opt
- FGG with scatter, expand opts
- ▲ FGG with scatter, expand, $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ opts

- ◆ Compiling quantum to probabilistic
- ◆ Qiskit

Deutsch-Jozsa with the even oracle



Simon's



- FGG with scatter opt
- FGG with scatter, expand opts
- ▲ FGG with scatter, expand, $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ opts

- ◆ Compiling quantum to probabilistic
- ◆ Qiskit

Motivations

Higher-level quantum programming

- ▶ Capture nondeterministic intuition
- ▶ Scale up from qubit tyranny
- ▶ Compose quantum computations

Simulation using probabilistic programming

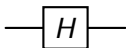
- ▶ Reveal shared techniques
- ▶ Reuse existing implementation
- ▶ Relate quantum and probabilistic programming

Source language: Symmetric pattern matching

Iso	$\omega ::= \{ v \leftrightarrow e \cdots v \leftrightarrow e \}$
Extended value	$e ::= v \mid e + e \mid \alpha e \mid \text{let } p = \omega p \text{ in } e$
Pure value	$v ::= \langle \rangle \mid x \mid \langle v, v \rangle \mid \text{inl } v \mid \text{inr } v$
Pattern	$p ::= \langle \rangle \mid x \mid \langle p, p \rangle$
Variable	x
Weight	$\alpha \in \mathbb{C}$

$$\text{Hadamard} :: \mathbb{1} \oplus \mathbb{1} \leftrightarrow \mathbb{1} \oplus \mathbb{1}$$

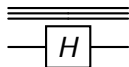
$$\left\{ \begin{array}{l} | \text{inl} \rangle \leftrightarrow \frac{1}{\sqrt{2}}(\text{inl} \rangle) + \frac{1}{\sqrt{2}}(\text{inr} \rangle) \\ | \text{inr} \rangle \leftrightarrow \frac{1}{\sqrt{2}}(\text{inl} \rangle) - \frac{1}{\sqrt{2}}(\text{inr} \rangle) \end{array} \right\} \quad \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$



Source language: Symmetric pattern matching

Iso	$\omega ::= \{ v \leftrightarrow e \cdots v \leftrightarrow e \}$
Extended value	$e ::= v \mid e + e \mid \alpha e \mid \text{let } p = \omega p \text{ in } e$
Pure value	$v ::= \langle \rangle \mid x \mid \langle v, v \rangle \mid \text{inl } v \mid \text{inr } v$
Pattern	$p ::= \langle \rangle \mid x \mid \langle p, p \rangle$
Variable	x
Weight	$\alpha \in \mathbb{C}$

$\text{sndHadamard} :: a \otimes (\mathbb{1} \oplus \mathbb{1}) \leftrightarrow a \otimes (\mathbb{1} \oplus \mathbb{1})$
 $\{ | \langle x, y \rangle \leftrightarrow \text{let } z = \text{Hadamard } y \text{ in } \langle x, z \rangle \}$



$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & & & & \\ 1 & -1 & & & & \\ & & 1 & 1 & & \\ & & 1 & -1 & & \\ & & & & \ddots & \\ & & & & & 1 & 1 \\ & & & & & 1 & -1 \end{bmatrix}$$

Source language: Symmetric pattern matching

Iso	$\omega ::= \{ v \leftrightarrow e \cdots v \leftrightarrow e \}$
Extended value	$e ::= v \mid e + e \mid \alpha e \mid \text{let } p = \omega p \text{ in } e$
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Pattern	$p ::= \langle \rangle \mid x \mid \langle p, p \rangle$
Variable	x
Weight	$\alpha \in \mathbb{C}$

Hadamard* $:: a \oplus a \leftrightarrow a \oplus a$

$$\left\{ \begin{array}{l} | \text{inl } x \leftrightarrow \frac{1}{\sqrt{2}}(\text{inl } x) + \frac{1}{\sqrt{2}}(\text{inr } x) \\ | \text{inr } x \leftrightarrow \frac{1}{\sqrt{2}}(\text{inl } x) - \frac{1}{\sqrt{2}}(\text{inl } x) \end{array} \right\}$$

$$\frac{1}{\sqrt{2}} \left[\underbrace{\begin{matrix} 1 & & & \\ & \ddots & & \\ & & 1 & \\ & 1 & & \ddots & \\ & & & & 1 \end{matrix}}_{|a|} \quad \underbrace{\begin{matrix} 1 & & & \\ & \ddots & & \\ & & -1 & \\ & -1 & & \ddots & \\ & & & & -1 \end{matrix}}_{|a|} \right] \left\{ \begin{array}{l} |a| \\ |a| \end{array} \right\}$$

Source language: Symmetric pattern matching

Iso	$\omega ::= \{ \mid v \leftrightarrow e \cdots \mid v \leftrightarrow e \}$
Extended value	$e ::= v \mid e + e \mid \alpha e \mid \text{let } p = \omega p \text{ in } e$
Pure value	$v ::= \langle \rangle \mid x \mid \langle v, v \rangle \mid \text{inl } v \mid \text{inr } v$
Pattern	$p ::= \langle \rangle \mid x \mid \langle p, p \rangle$
Variable	x
Weight	$\alpha \in \mathbb{C}$

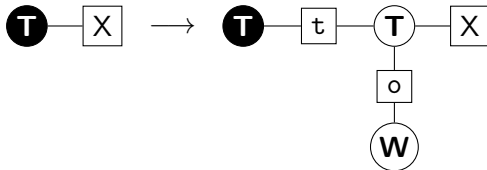
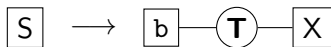
$$\text{swap} :: a \oplus b \leftrightarrow b \oplus a$$

$$\left\{ \begin{array}{l} \mid \text{inl } x \leftrightarrow \text{inr } x \\ \mid \text{inr } y \leftrightarrow \text{inl } y \end{array} \right\}$$

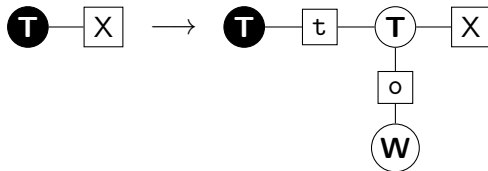
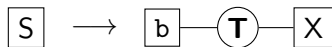
$$\left[\begin{array}{cc} & \begin{matrix} 1 & \cdots & 1 \end{matrix} \\ \begin{matrix} 1 & \cdots & 1 \end{matrix} & \end{array} \right] \left\{ \begin{array}{l} |a| \\ |b| \end{array} \right\}$$

$\underbrace{\hspace{10em}}_{|b|} \quad \underbrace{\hspace{10em}}_{|a|}$

Target language: Factor graph grammar

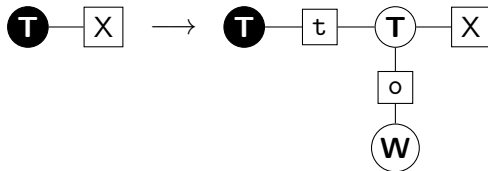
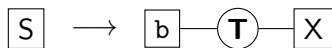


Target language: Factor graph grammar

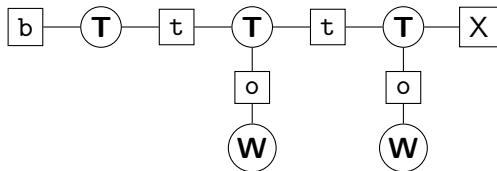
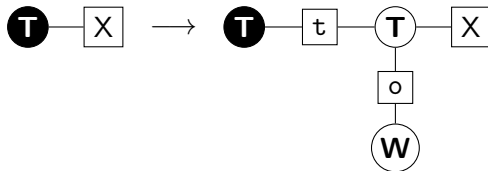
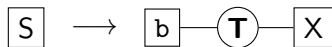


$\boxed{S}$

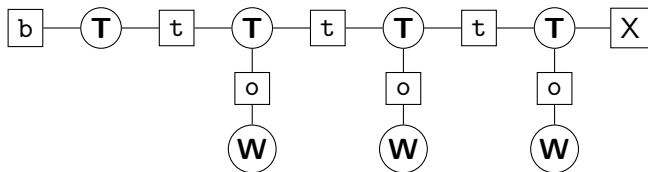
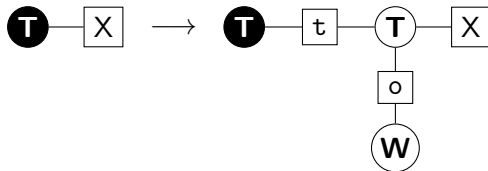
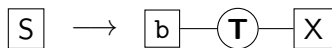
Target language: Factor graph grammar



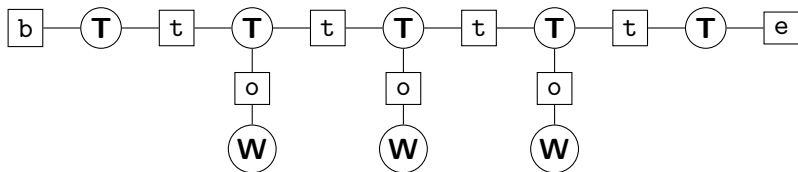
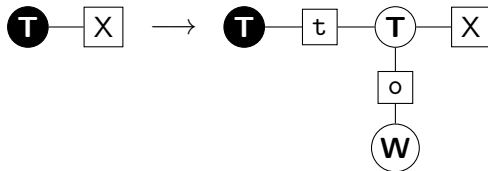
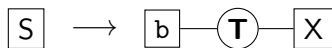
Target language: Factor graph grammar



Target language: Factor graph grammar



Target language: Factor graph grammar



Target language: Factor graph grammar

Factor graph grammar	$fgg ::= (r = E) \dots$
Tensor expression	$E, F ::= r \mid \alpha \mid E + E \mid 0^{(s, \dots)}$ $\mid \text{expand}(E[\vec{x}] \rightarrow \vec{z})$ $\mid \text{einsum}(E[\vec{x}], \dots \rightarrow \vec{z})$ $\mid \text{scatter}(E[\vec{x}] \rightarrow e \dots)$
Tensor variable	r
Weight	$\alpha \in \mathbb{C}$
Upper bound	$s \in \mathbb{N}$

$$\text{coin} = \frac{2}{3} \cdot \begin{bmatrix} 1 & 0 \end{bmatrix} + \frac{1}{3} \cdot \begin{bmatrix} 0 & 1 \end{bmatrix}$$

$$\text{same} = \text{coin} \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \cdot \text{coin}^t$$

Target language: Factor graph grammar

Factor graph grammar	$fgg ::= (r = E) \dots$
Tensor expression	$E, F ::= r \mid \alpha \mid E + E \mid 0^{(s, \dots)}$ $\mid \text{expand}(E[\vec{x}] \rightarrow \vec{z})$ $\mid \text{einsum}(E[\vec{x}], \dots \rightarrow \vec{z})$ $\mid \text{scatter}(E[\vec{x}] \rightarrow e \dots)$
Index variable sequence	$\vec{x}, \vec{y}, \vec{z} ::= x^{(s)} \dots$
Index variable	$x^{(s)}, y^{(s)}, z^{(s)}, t^{(s)}$
Upper bound	$s \in \mathbb{N}$

$$\text{expand}([6 \ 7] [x^{(2)}] \rightarrow x^{(2)} y^{(3)}) = \begin{bmatrix} 6 & 6 & 6 \\ 7 & 7 & 7 \end{bmatrix}$$

$$\text{einsum}(E_1[xy], E_2[yz] \rightarrow xz) = \text{matrix multiplication}$$

Target language: Factor graph grammar

Factor graph grammar $fgg ::= (r = E) \dots$

Tensor expression $E, F ::= r \mid \alpha \mid E + E \mid 0^{(s, \dots)}$
 $\mid \text{expand}(E[\vec{x}] \rightarrow \vec{z})$
 $\mid \text{einsum}(E[\vec{x}], \dots \rightarrow \vec{z})$
 $\mid \text{scatter}(E[\vec{x}] \rightarrow e \dots)$

Index variable sequence $\vec{x}, \vec{y}, \vec{z} ::= x^{(s)} \dots$

Index variable $x^{(s)}, y^{(s)}, z^{(s)}, t^{(s)}$

Axis expression $e ::= x^{(s)} \mid \mathbb{1} \mid e \otimes e \mid s \oplus e \oplus s$

$$\text{scatter}([6 \ 7] [x] \rightarrow xx) = \begin{bmatrix} 6 & 0 \\ 0 & 7 \end{bmatrix}$$

$$\text{scatter}\left(\begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} [xy] \rightarrow (x \otimes y)\right) = [5 \ 6 \ 7 \ 8]$$

$$\text{scatter}([6 \ 7] [x] \rightarrow (2 \oplus x \oplus 3)) = [0 \ 0 \ 6 \ 7 \ 0 \ 0 \ 0]$$

Compilation preserves denotational semantics

$$\begin{aligned} \llbracket \Delta \vdash_t t : a \rrbracket (\delta, v) &= \llbracket \text{comp}(\Delta \vdash_t t : a) \rrbracket_\gamma \\ &\quad \left[(\text{comp}_\delta(\Delta, \delta), \text{comp}_v(a, v)) \right] \end{aligned}$$

$$\begin{aligned} \llbracket \vdash_i \omega : a \leftrightarrow b \rrbracket (v_1, v_2) &= \llbracket \text{comp}(\vdash_i \omega : a \leftrightarrow b) \rrbracket_\gamma \\ &\quad \left[(\text{comp}_v(a, v_1), \text{comp}_v(b, v_2)) \right] \end{aligned}$$

Three optimizations

$$\begin{aligned} & \llbracket \text{einsum}(\text{scatter}(E[x] \rightarrow xx)[xy], F[yz] \rightarrow xz) \rrbracket \\ &= \llbracket \text{einsum}(E[y], F[yz] \rightarrow yz) \rrbracket \end{aligned}$$

$$\begin{aligned} & \llbracket \text{einsum}(\text{expand}(E[xy] \rightarrow xyt)[xyt], F[yz] \rightarrow xyz) \rrbracket \\ &= \llbracket \text{expand}(\text{einsum}(E[xy], F[yz] \rightarrow xyz)[xyz] \rightarrow xyz) \rrbracket \end{aligned}$$

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \llbracket \text{scatter}(\text{expand}(1[] \rightarrow x)[x] \rightarrow xx) \rrbracket$$

Conclusion

- ▶ Compile quantum to probabilistic (proven correct)
- ▶ Get quantum simulator for free
- ▶ Optimize summation-free einsum-expand (proven correct)

Future work

- ▶ Optimize non-summation-free einsum-expand
- ▶ Higher-order isos and recursion
- ▶ Polymorphism; partial evaluation
- ▶ More benchmarks of expressivity and performance