科学计算中的量子算法：量子傅立叶变换

安冬

北京大学北京国际数学研究中心（BICMR）

andong@bicmr.pku.edu.cn

25-26 学年第 2 学期

量子傅立叶变换

定义：

$$U_{\text{QFT}}|j\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} e^{i2\pi jk/N}|k\rangle, \quad U_{\text{QFT}} = \frac{1}{\sqrt{N}}(e^{i2\pi jk/N})_{j\in[N],k\in[N]}$$

$$U_{\text{QFT}}^{\dagger}|j\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} e^{-i2\pi jk/N}|k\rangle$$

$$U_{\text{QFT}}|0\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}|k\rangle = H^{\otimes n}|0\rangle$$

- 传统意义上的逆傅立叶变换
- 传统快速傅立叶变换（FFT）：$\mathcal{O}(N\log(N))$

量子傅立叶变换（QFT）

$$U_{\mathrm{QFT}} |j\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{i2\pi jk/N} |k\rangle$$

核心思想：U_{QFT} 具有“类似于张量积”的形式

QFT：记号

$$N = 2^n$$

$$k = (k_{n-1} \cdots k_1 k_0)_2 = \sum_{l=0}^{n-1} k_l 2^l$$

$$j = (j_{n-1} \cdots j_1 j_0)_2 = \sum_{l=0}^{n-1} j_l 2^l$$

QFT：分解

$$\begin{aligned}\frac{jk}{N} &= \frac{j}{2^n}\sum_{l=0}^{n-1} k_l 2^l = \sum_{l=0}^{n-1} k_l \frac{j}{2^{n-l}} \\ &= k_0(.j_{n-1}j_{n-2}\cdots j_1 j_0)_2 + k_1(j_{n-1}.j_{n-2}\cdots j_1 j_0)_2 + \cdots + k_{n-1}(j_{n-1}j_{n-2}\cdots j_1.j_0)_2\end{aligned}$$

$$\begin{aligned}e^{i2\pi jk/N} &= e^{i2\pi k_0(.j_{n-1}\cdots j_0)_2} e^{i2\pi k_1(j_{n-1}.j_{n-2}\cdots j_0)_2} \ldots e^{i2\pi k_{n-2}(j_{n-1}\cdots j_2.j_1 j_0)_2} e^{i2\pi k_{n-1}(j_{n-1}\cdots j_1.j_0)_2} \\ &= e^{i2\pi k_0(.j_{n-1}\cdots j_0)_2} e^{i2\pi k_1(.j_{n-2}\cdots j_0)_2} \ldots e^{i2\pi k_{n-2}(.j_1 j_0)_2} e^{i2\pi k_{n-1}(.j_0)_2}\end{aligned}$$

QFT：分解

$$
\begin{aligned}
U_{\text{QFT}}\left|j\right\rangle &= \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} e^{i2\pi jk/N}\left|k\right\rangle \\
&= \frac{1}{\sqrt{2^n}}\sum_{k_{n-1},\cdots,k_0} e^{i2\pi k_0(.j_{n-1}\cdots j_0)_2}\, e^{i2\pi k_1(.j_{n-2}\cdots j_0)_2}\cdots e^{i2\pi k_{n-2}(.j_1 j_0)_2}\, e^{i2\pi k_{n-1}(.j_0)_2}\left|k_{n-1}\cdots k_1 k_0\right\rangle \\
&= \frac{1}{\sqrt{2^n}}\left(\sum_{k_{n-1}} e^{i2\pi k_{n-1}(.j_0)_2}\left|k_{n-1}\right\rangle\right)\otimes\left(\sum_{k_{n-2}} e^{i2\pi k_{n-2}(.j_1 j_0)_2}\left|k_{n-2}\right\rangle\right) \\
&\quad \otimes\cdots\otimes\left(\sum_{k_0} e^{i2\pi k_0(.j_{n-1}\cdots j_1 j_0)_2}\left|k_0\right\rangle\right) \\
&= \frac{1}{\sqrt{2^n}}\left(\left|0\right\rangle + e^{i2\pi(.j_0)_2}\left|1\right\rangle\right)\otimes\left(\left|0\right\rangle + e^{i2\pi(.j_1 j_0)_2}\left|1\right\rangle\right)\otimes\cdots\otimes\left(\left|0\right\rangle + e^{i2\pi(.j_{n-1}\cdots j_0)_2}\left|1\right\rangle\right)
\end{aligned}
$$

QFT：分解

$$
\begin{aligned}
& |j_{n-1}\rangle \otimes |j_{n-2}\rangle \otimes \cdots \otimes |j_1\rangle \otimes |j_0\rangle \\
\mapsto & \frac{1}{\sqrt{2^n}} \left(|0\rangle + e^{i2\pi(.j_0)_2}|1\rangle\right) \otimes \left(|0\rangle + e^{i2\pi(.j_1 j_0)_2}|1\rangle\right) \otimes \cdots \otimes \left(|0\rangle + e^{i2\pi(.j_{n-1}\cdots j_0)_2}|1\rangle\right)
\end{aligned}
$$

我们先暂时交换输出量子比特的顺序，并考虑：

$$
\begin{aligned}
& |j_{n-1}\rangle \otimes \cdots \otimes |j_1\rangle \otimes |j_0\rangle \\
\mapsto & \frac{1}{\sqrt{2^n}} \left(|0\rangle + e^{i2\pi(.j_{n-1}\cdots j_0)_2}|1\rangle\right) \otimes \cdots \otimes \left(|0\rangle + e^{i2\pi(.j_1 j_0)_2}|1\rangle\right) \otimes \left(|0\rangle + e^{i2\pi(.j_0)_2}|1\rangle\right)
\end{aligned}
$$

QFT：算法

0: Hadamard

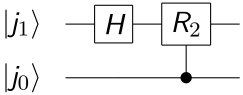
$$|j_0\rangle \mapsto \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2\pi(.j_0)_2}|1\rangle\right)$$

1:

$$|j_1\rangle \mapsto \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2\pi(.j_1j_0)_2}|1\rangle\right) = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2\pi(.0j_0)_2}e^{i2\pi(.j_1)_2}|1\rangle\right)$$

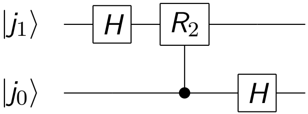
$$|j_1\rangle \mapsto \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2\pi(.j_1)_2}|1\rangle\right) \mapsto \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2\pi(.0j_0)_2}e^{i2\pi(.j_1)_2}|1\rangle\right)$$

QFT：算法



$$R_2 = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2} \end{pmatrix}$$

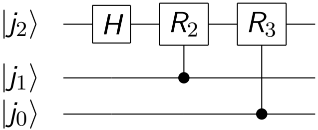
总的运算： $|j_1\rangle |j_0\rangle \mapsto \frac{1}{\sqrt{2}} \left(|0\rangle + e^{i2\pi(.j_1 j_0)_2} |1\rangle\right) \otimes \frac{1}{\sqrt{2}} \left(|0\rangle + e^{i2\pi(.j_0)_2} |1\rangle\right)$



QFT：算法

2:

$$|j_2\rangle \mapsto \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2\pi(.j_2j_1j_0)_2}\,|1\rangle\right) = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2\pi(.00j_0)_2}\,e^{i2\pi(.0j_1)_2}\,e^{i2\pi(.j_2)_2}\,|1\rangle\right)$$

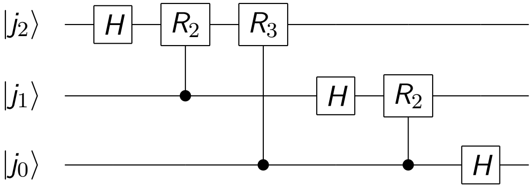


$$R_2 = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2} \end{pmatrix}, \quad R_3 = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2^2} \end{pmatrix}$$

QFT：算法

总的运算：

$$
\begin{aligned}
&|j_2\rangle\,|j_1\rangle\,|j_0\rangle \\
\mapsto\ & \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2\pi(.j_2j_1j_0)_2}\,|1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2\pi(.j_1j_0)_2}\,|1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2\pi(.j_0)_2}\,|1\rangle\right)
\end{aligned}
$$

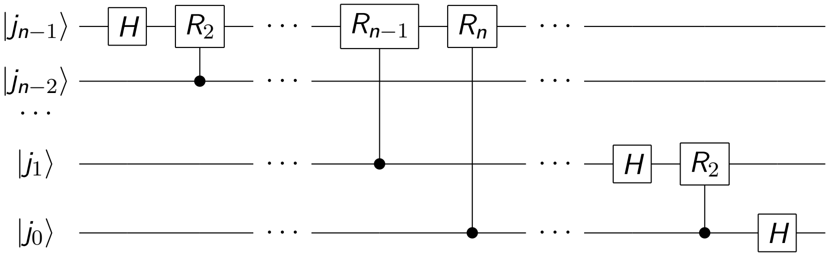


$$
R_l = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2^{l-1}} \end{pmatrix}
$$

QFT：算法

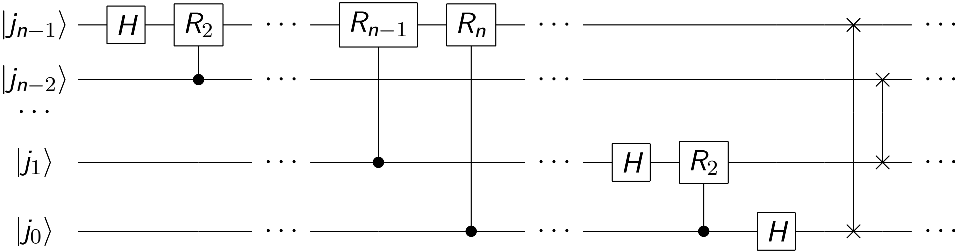
一般情况（注意此时输出比特的顺序是反的）：

$$
\begin{aligned}
&|j_{n-1}\rangle \otimes \cdots \otimes |j_1\rangle \otimes |j_0\rangle \\
\mapsto &\frac{1}{\sqrt{2^n}} \left(|0\rangle + e^{i2\pi(.j_{n-1}\cdots j_0)_2}|1\rangle\right) \otimes \cdots \otimes \left(|0\rangle + e^{i2\pi(.j_1 j_0)_2}|1\rangle\right) \otimes \left(|0\rangle + e^{i2\pi(.j_0)_2}|1\rangle\right)
\end{aligned}
$$



QFT：算法

QFT 最终算法：



$$R_l = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2^{l-1}} \end{pmatrix}$$

量子门复杂度：$\mathcal{O}((\log(N))^2)$ （对比经典 FFT：$\mathcal{O}(N\log(N))$）

QFT：小结

$$U_{\mathrm{QFT}}|j\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1} e^{i2\pi jk/N}|k\rangle$$

量子门复杂度：$\mathcal{O}(n^2) = \mathcal{O}((\log(N))^2)$

拓展：

- 近似量子傅立叶变换（Approximate Quantum Fourier Transform）
- 量子余弦/正弦变换（Quantum Cosine/Sine Transform）
- 量子拉普拉斯变换（Quantum Laplace Transform）

阅读：

- LL: Chapter 3.3