Quantum Fourier transform beyond Shor's algorithm

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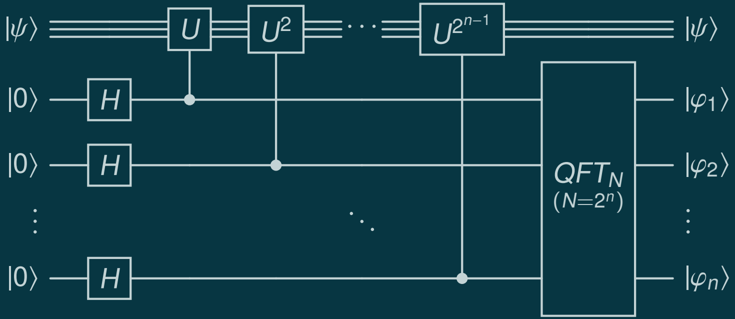
Day 2 – Quantum Phase Estimation & Connecting Discrete and Continuous Fourier Transforms

Quantum Phase Estimation

Given a (black-box) unitary U and one of its eigenvectors $|\psi\rangle$ with unknown eigenvalue $e^{2\pi i\varphi}$ we would like to learn the phase $\varphi \in [0,1)$ by implementing a map $|\psi\rangle|0\rangle \to |\psi\rangle|\varphi\rangle$.

Phase estimation circuit when $\varphi = 0.\varphi_1\varphi_2\ldots\varphi_n$ has (at most) n-bits



$$|\psi\rangle|0\rangle^{\otimes n} \xrightarrow{H^{\otimes n}} \frac{1}{\sqrt{N}}\sum_{t=0}^{N-1}|\psi\rangle|t\rangle \xrightarrow{\sum_{t=0}^{N-1} U^t\otimes|t\rangle\langle t|} \frac{1}{\sqrt{N}}\sum_{t=0}^{N-1} U^t|\psi\rangle|t\rangle = |\psi\rangle\underbrace{\frac{1}{\sqrt{N}}\sum_{t=0}^{N-1} e^{2\pi i\varphi t}|t\rangle}_{QFT_N^{-1}|N\cdot\varphi\rangle}$$

Quantum Phase Estimation – arbitrary phases

Computing the amplitudes for general φ

$$\frac{1}{\sqrt{N}}\sum_{t=0}^{N-1} e^{2\pi i\varphi t}|t\rangle \quad \overset{QFT_N}{\rightarrow} \quad \frac{1}{N}\sum_{t=0}^{N-1}\sum_{k=0}^{N-1} e^{2\pi i\varphi t}e^{-2\pi i k t/N}|k\rangle$$

$$= \quad \frac{1}{N}\sum_{k=0}^{N-1}\sum_{t=0}^{N-1} e^{2\pi i(\varphi-0.k_1k_2\ldots k_n)t}|k\rangle$$

$$= \quad \frac{1}{N}\sum_{k=0}^{N-1} \frac{e^{2\pi i(\varphi-0.k_1k_2\ldots k_n)N}-1}{e^{2\pi i(\varphi-0.k_1k_2\ldots k_n)}-1}|k\rangle \qquad \text{(by geometric summation)}$$

The output distribution in terms of $\Delta := \varphi - 0.k_1k_2\ldots k_n$

$$\left|\frac{1}{N}\frac{e^{2\pi i(\varphi-0.k_1k_2\ldots k_n)N}-1}{e^{2\pi i(\varphi-0.k_1k_2\ldots k_n)}-1}\right|^2 = \left|\frac{1}{N}\frac{e^{\pi N i\Delta}-e^{-\pi N i\Delta}}{e^{\pi i\Delta}-e^{-\pi i\Delta}}\right|^2 \qquad \left(\text{multiply by } \frac{e^{-\pi N i\Delta}}{e^{-\pi i\Delta}} \text{ under } |\cdot|\right)$$

$$= \left|\frac{1}{N}\frac{\sin(\pi N\Delta)}{\sin(\pi\Delta)}\right|^2 \qquad (e^{ix}-e^{-ix}=2\sin(x))$$

$$= \left|\frac{\mathrm{sinc}(\pi N\Delta)}{\mathrm{sinc}(\pi\Delta)}\right|^2 \qquad (\mathrm{sinc}(x)=\sin(x)/x)$$

Heavy tail

Although, we get the best two estimates with high probability, the distribution has a heavy tail:

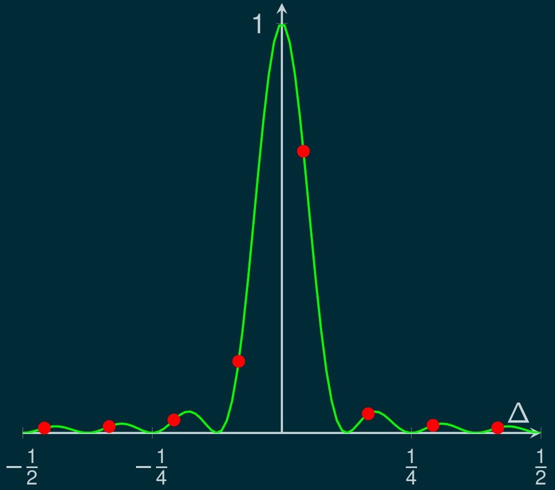


Figure: Plot of $\frac{\text{sinc}^2(\pi N \Delta)}{\text{sinc}^2(\pi \Delta)}$ for $N = 8$ and true phase $1/24$.

Quantum Phase Estimation – error probabilities

The probability of obtaining estimate off by Δ

We just computed it for $\Delta \in [-\frac{1}{2}, \frac{1}{2})$:

$$\frac{\mathrm{sinc}^2(\pi N \Delta)}{\mathrm{sinc}^2(\pi \Delta)}$$

- The probability of obtaining the best n-bit estimate is when $|\Delta \mod 1|$ is the smallest. The worst case is when $\Delta_{\min} = \frac{1}{2N}$:

$$\frac{\mathrm{sinc}^2(\pi N \Delta_{\min})}{\mathrm{sinc}^2(\pi \Delta_{\min})} \geq \frac{\mathrm{sinc}^2(\pi N \frac{1}{2N})}{\mathrm{sinc}^2(\pi \frac{1}{2N})} \geq \mathrm{sinc}^2(\pi/2) = (\frac{1}{\pi/2})^2 = \frac{4}{\pi^2} > 40\%$$

- The probability of obtaining one of the two best n-bit estimates corresponds to $\Delta_{\min}$, $\frac{1}{N} - \Delta_{\min}$. The worst case is once again when $\Delta_{\min} = \frac{1}{2N}$:

$$\frac{\mathrm{sinc}^2(\pi N \Delta_{\min})}{\mathrm{sinc}^2(\pi \Delta_{\min})} + \frac{\mathrm{sinc}^2(\pi N (\frac{1}{N} - \Delta_{\min}))}{\mathrm{sinc}^2(\pi (\frac{1}{N} - \Delta_{\min}))} \geq 2 \frac{\mathrm{sinc}^2(\pi N \frac{1}{2N})}{\mathrm{sinc}^2(\pi \frac{1}{2N})} \geq 2(\frac{1}{\pi/2})^2 = \frac{8}{\pi^2} > 80\%$$

Boosting

The median trick

Suppose our estimator outputs an ε-precise estimate with probability at least 80%.

- Take s independent estimates, and compute their median.
- The expected number of estimates within ε-precision is at least 80%.
- It is exponentially unlikely in s that at least 50% of estimates are farther than ε. (See the Chernoff bound.)
- When more than 50% of estimates are ε-precise their median is also ε-precise!

Median on the cycle?

- Output the most frequently seen element (in case of a tie, choose one randomly).
- It is exponentially unlikely that the most frequently seen estimate is not one of the two best n-bit estimates (as they have jointly probability $\geq$ 80%).
- The output distribution is exponentially concentrated on the two best estimates!

Unfortunately, we cannot ensure that that we get a unique estimate with high probability!

Unbiased (symmetric) estimator

The random shift trick

Input: $\left|\psi(\phi)\right\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{i\phi k}|k\rangle$ (for unknown ϕ), and a parameter $n \in \mathbb{N}$

1: Sample a uniformly random n-digit binary number $u \in [0, 1)$ and define $\xi := \frac{2\pi u}{N}$

2: Apply multi-phase gate $\sum_{k=0}^{N-1} e^{-i\xi k}|k\rangle\langle k|$ to $\left|\psi(\phi)\right\rangle$

3: Perform inverse Fourier transform over $\mathbb{Z}_N$ and measure the state, yielding outcome j

4: **Return** $\varphi := \frac{2\pi j}{N} + \xi = \frac{2\pi}{N}(j + u)$

Median on the cycle?

Theorem (Unbiased Phase Estimation – Apeldoorn, Cornelissen, G, Nannicini (2022))

If we run the above Algorithm with $n = \infty$ in Line 1, then it returns a random phase $\varphi \in [0, 2\pi)$ with probability density function

$$f(\varphi) := \frac{N}{2\pi} \frac{\operatorname{sinc}^2\left(\frac{N}{2}|\phi - \varphi|_{2\pi}\right)}{\operatorname{sinc}^2\left(\frac{1}{2}|\phi - \varphi|_{2\pi}\right)}.$$

Applications: (almost) optimal coherent tomography, improved estimation algorithms for partition functions, low-depth amplitude estimation, etc.

The continuous probability density function of estimates

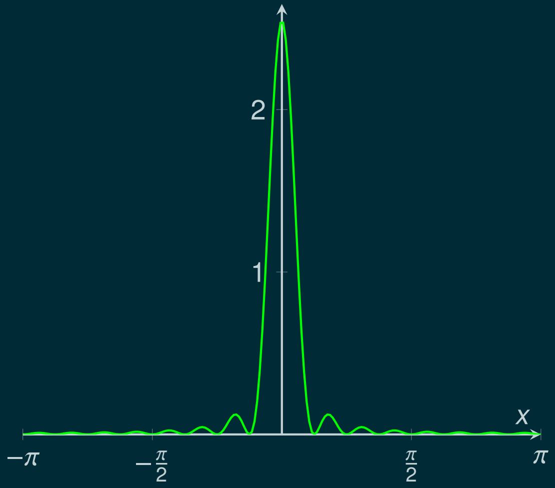


Figure: Plot of $f(\varphi)$ for $x = \phi - \varphi$ and $M = 16$.

Can you boost it while keeping the distribution symmetric?

Connecting Discrete and Continuous Fourier Transforms

Discrete vs. Continuous Fourier Transform

The Continuous Fourier Transform $\mathcal{F}$

$$\hat{f}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} f(t) dt$$

$\mathcal{F} : \mathcal{L}_2 \to \mathcal{L}_2$ is a unitary transformation (on the Hilbert space of square integrable functions)

Periodic Wrapping of Continuous Functions

Let $f : \mathbb{R} \to \mathbb{C}$, and $r \in \mathbb{R}_+$ be a “period”. We define its wrapping as a function $[0, r] \to \mathbb{C}$

$$f^{(r)}(x) := \lim_{\mathbb{N} \ni K \to \infty} \sum_{k=-K}^{K} f(x + kr).$$

Similarly we define discretized wrapping for $N \in \mathbb{N}$ as a vector in $\mathbb{C}^N$ defined as

$$f_j^{(r,N)} := \lim_{\mathbb{N} \ni K \to \infty} \sum_{k=-K}^{K} f(\frac{j}{N} r + kr).$$

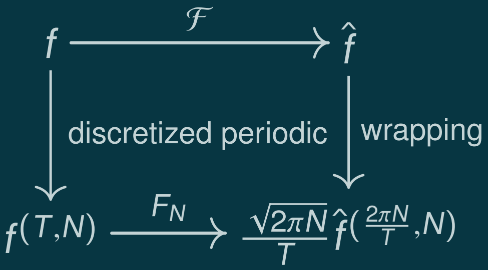
Discrete vs. Continuous Fourier Transform

Connection between Discrete and Continuous Fourier transform

$$\widehat{f^{(T,N)}} = \frac{\sqrt{2\pi N}}{T}\hat{f}^{(\frac{2\pi N}{T},N)}$$

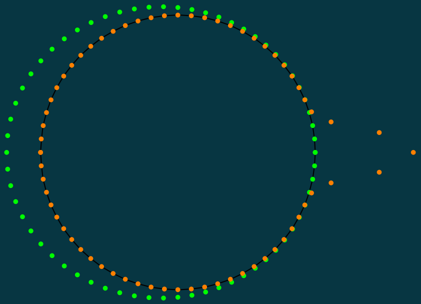
Terms and conditions apply, but certainly holds for smooth rapidly decaying functions. For more details see Chen, Kastoryano, Brandão, G (2023).

A Commutative Diagram Representation (ignoring the scalar factor)



Continuous Fourier Transform: shift ↔ point-wise phase multipl.

Set $T = N = 64$ and $\varphi = 6/37$ – absolute amplitude plot on the circle

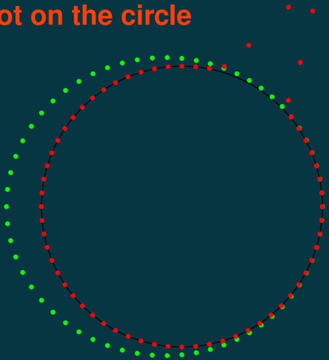


Shifted (discretized) Gaussian

$$f(t) \propto \exp(-(t-32)^2/256),$$

and its Fourier Transform

$$|\widehat{f^{(N,N)}}_j| \propto \exp(-(2\pi j)^2/96).$$



Shifted, phase kicked Gaussian

$$f(t) \propto \exp(\frac{12\pi}{37} it - (t-32)^2/256),$$

and its Fourier Transform

$$|\widehat{f^{(N,N)}}_j| \propto \exp(-(2\pi j)^2/96).$$

The key observation

In the Gaussian case due to the rapid decay of the tail we have:

$$f^{(T,N)}_{|[0,T)} \approx f^{(T,N)} \qquad \widehat{f^{(T,N)}} = \frac{\sqrt{2\pi N}}{T}\hat{f}^{(\frac{2\pi N}{T},N)} \qquad \hat{f}^{(\frac{2\pi N}{T},N)} \approx \hat{f}^{(\frac{2\pi N}{T},N)}_{|[-\pi,\pi)}$$

With phase shift

Let us introduce

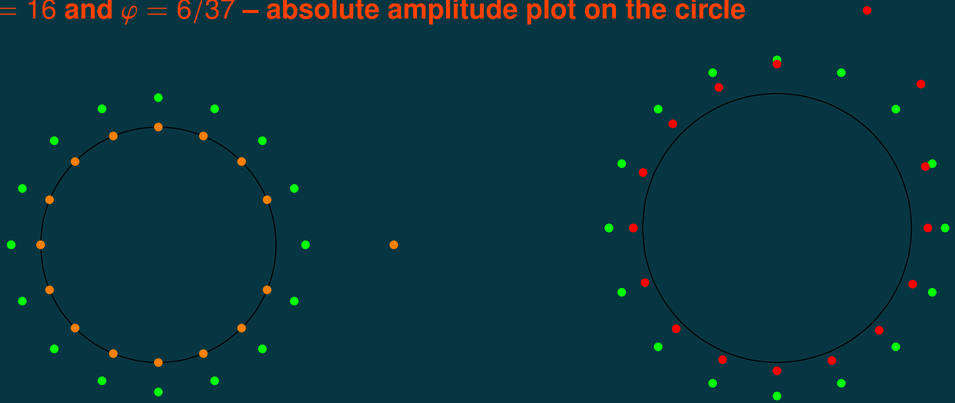
$$f_\varphi(t) := f(t) \cdot e^{2\pi i \cdot \varphi t}$$

$$f^{(T,N)}_{\varphi\,|[0,T)} \approx f^{(T,N)} \qquad \widehat{f^{(T,N)}_\varphi} = \frac{\sqrt{2\pi N}}{T}\hat{f}_\varphi^{(\frac{2\pi N}{T},N)} \qquad \hat{f}_\varphi^{(\frac{2\pi N}{T},N)} \approx \hat{f}^{(\frac{2\pi N}{T},N)}_{\varphi\,|[2\pi(\varphi-\frac{1}{2}),2\pi(\varphi+\frac{1}{2}))}$$

Note that changing $\varphi \pm 1$ does not change anything due to periodic wrapping!

Compare to vanilla phase estimation

Set $N = 16$ and $\varphi = 6/37$ – absolute amplitude plot on the circle



No phase shift, i.e., $\varphi = 0$

Phase shift: $\varphi = 6/37$

Bonus in the Gaussian case: we can increase the resolution cheaply!
Increase N, keep $T = N$ and do not change the Gaussian function just its wrapping.
This does not change the “query” complexity just requires a larger *QFT*.

Gaussian parameters

Let $\sigma \approx \sqrt{\log(1/\delta)}/\varepsilon$ and $f(t) \propto \exp(-t^2/(2\sigma^2))$. Then

$$\hat{f}(\omega) \propto \exp(-\sigma^2\omega^2/2).$$

Implying that the absolute amplitude of $|j\rangle$ in $\widehat{f^{(N,N)}}$ is roughly proportional to $(\omega \leftarrow \frac{2\pi j}{N})$

$$\exp(-\sigma^2(2\pi j/N)^2/2).$$

Gaussian tail bound

$$\int_x^\infty \frac{1}{\sigma} e^{-t^2/(2\sigma^2)} dt \leq \frac{1}{\sigma}\int_x^\infty \frac{t}{x} e^{-t^2/(2\sigma^2)} dt = \frac{\sigma}{x}\int_x^\infty \frac{t}{\sigma^2} e^{-t^2/(2\sigma^2)} dt = \frac{\sigma}{x} e^{-x^2/(2\sigma^2)}$$

To get δ accuracy we need about $\sqrt{\log(1/\delta)}\sigma \approx \log(1/\delta)/\varepsilon$ uses of U.

If $N = \Omega(\sqrt{\log(1/\delta)}\sigma) = \Omega(\log(1/\delta)/\varepsilon)$, then due to the above tail bound the truncated and the wrapped (discrete) Gaussians are $\mathcal{O}(\delta)$ close to each other.

High accuracy phase estimation in a single run

Idea: use Gaussian amplitudes

- Wrapped Gaussian is almost the same as truncated Gaussian due to rapid decay.
- Fourier transform of a Gaussian is Gaussian, so we get Gaussian noise!
- Choosing parameters appropriately we get an estimator with standard deviation about $1/N$ (up to logarithmic factors) in a single run without garbage ancilla states.
- Initial Gaussian amplitudes can be efficiently prepared – see McArdle, G, Berta (2022)
- Further optimized initial weights can give potential constant improvements: use Kaiser window function from signal processing. See Berry et al. (2022).

Application to Energy Estimation

Hamiltonian Simulation Using Block Encodings

- Suppose we are given a unitary V block encoding of a Hamiltonian H

$$H = (\langle\bar{0}| \otimes I)V(|\bar{0}\rangle \otimes I)$$

- Quantum signal processing efficiently implements e^{itH} by $\mathcal{O}\left(t + \log(1/\varepsilon)\right)$ uses of V.
- For more details see next week Ewin's lectures.

Using phase estimation we get an ε-precise energy estimate using $\widetilde{\mathcal{O}}\left(1/\varepsilon\right)$ uses of U.

Application to Singular Value Estimation

Block Encoding of an arbitrary matrix

- Suppose we are given a unitary V block encoding a (rectangular) matrix A

$$A = (\langle 0|^{\otimes a} \otimes I) V (|0\rangle^{\otimes b} \otimes I)$$

Singular vector estimation

- Consider the singular value decomposition

$$A = \sum_j \sigma_j |u_j\rangle\langle v_j|,$$

  where $\sigma_j \geq 0$ are the singular values and $|u_j\rangle, |v_j\rangle$ are the left and right singular vectors.
- Similarly to phase estimation we wish to estimate the singular value of a given (right) singular vector $|v_j\rangle$
- Similar performance to phase estimation, except we get estimates of $\pm\sigma_j$. See Kerenidis and Prakash (2016), Chakraborty, G, Jeffery (2018), Cornelissen and Hamoudi (2022).