Exercises for Introduction to Quantum Computing

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1. Trotter Formula

The general Trotter formula for two Hermitian operators A, B is given by

$$\lim_{n\to\infty}\left(e^{iAt/n}e^{iBt/n}\right)^n = e^{i(A+B)t}$$

a) We shall attempt to prove this. Let's start from the fact that the exponential function can be written as Taylor expansion of the form,

$$e^x = \sum_{n=0}^{\infty}\frac{x^n}{n!}$$

Thus, we have,

$$e^{i\hat{A}\frac{t}{n}} = \hat{I} + \frac{1}{n}i\hat{A}t + \mathcal{O}\left(\frac{1}{n^2}\right)$$

We can thus write down the terms inside the bracket as,

$$e^{i\hat{A}\frac{t}{n}}e^{i\hat{B}\frac{t}{n}} = \hat{I} + \frac{1}{n}i(\hat{A}+\hat{B})t + \mathcal{O}\left(\frac{1}{n^2}\right)$$

Now to raise it to the n^{th} power, we can use the Binomial formula,

$$(x+y)^n = \sum_{k=0}^{n}\frac{n!}{k!(n-k)!}x^{n-k}y^k$$

we get,

$$\left(e^{i\hat{A}\frac{t}{n}}e^{i\hat{B}\frac{t}{n}}\right)^n = \sum_{k=0}^{n}\frac{n!}{k!(n-k)!}\frac{1}{n^k}(i(\hat{A}+\hat{B})t)^k$$

if we take k to be constant, we can then take the limit,

$$\lim_{n\to\infty}\left(e^{i\hat{A}\frac{t}{n}}e^{i\hat{B}\frac{t}{n}}\right)^n = \lim_{n\to\infty}\sum_{k=0}^{n}\frac{n!}{k!(n-k)!}\frac{1}{n^k}(i(\hat{A}+\hat{B})t)^k$$

Taking this limit, we get

$$\left(e^{i\hat{A}\frac{t}{n}}e^{i\hat{B}\frac{t}{n}}\right)^n \simeq \sum_{k=0}^{n}\frac{(i(\hat{A}+\hat{B})t)^k}{k!} + \mathcal{O}\left(\frac{1}{n}\right) \simeq e^{i(\hat{A}+\hat{B})t}$$

The RHS can be written down as an exponential as we saw earlier, thus we have,

$$\left(e^{i\hat{A}\frac{t}{n}}e^{i\hat{B}\frac{t}{n}}\right)^n \simeq e^{i(\hat{A}+\hat{B})t}$$

b) We are to prove,

$$S_1(\delta t) = e^{iA\delta t}\cdot e^{iB\delta t} = e^{i(A+B)\delta t} + \mathcal{O}\left(\delta t^2\right)$$

for this we simply Taylor expand the LHS upto first-order,

$$e^{iA\delta t}\cdot e^{iB\delta t} = (\mathbb{I} + A\delta t)(\mathbb{I} + B\delta t)$$
$$e^{iA\delta t}\cdot e^{iB\delta t} = \mathbb{I} + (A+B)\delta t + \mathcal{O}(\delta t^2)$$

and compare it with the first order Taylor expansion of the RHS,

$$e^{i(A+B)\delta t} = \mathbb{I} + (A+B)\delta t + \mathcal{O}(\delta t^2)$$

Thus,

$$S_1(\delta t) = e^{iA\delta t}\cdot e^{iB\delta t} = e^{i(A+B)\delta t} + \mathcal{O}\left(\delta t^2\right)$$

Q.E.D

c) To prove the second order Suzuki-Trotter approximation, we simply need to expand the exponentials upto second order,

$$S_2(\delta t) = e^{iA\delta t/2} \cdot e^{iB\delta t} \cdot e^{iA\delta t/2}$$

$$S_2(\delta t) = \left(\mathbb{I} + \frac{i\delta t}{2}A - \frac{\delta t^2}{2!.4}A^2\right)\left(\mathbb{I} + i\delta t B - \frac{\delta t^2}{2}B^2\right)\left(\mathbb{I} + \frac{i\delta t}{2}A - \frac{\delta t^2}{2!.4}A^2\right)$$

Ignoring terms of order $\mathcal{O}(\delta t^4)$, we have

$$S_2(\delta t) = \mathbb{I} + i\delta t A + i\delta t B + \frac{1}{2}\delta t^2(A^2 + B^2 + AB + BA) + \mathcal{O}(\delta t^3)$$

The RHS looks like the Taylor expansion of an exponential upto second order, thus, we have,

$$S_2(\delta t) = e^{i(A+B)\delta t} + \mathcal{O}(\delta t^3)$$

Q.E.D

d) We are to compute s in,

$$S_4(\delta t) = S_2(s\delta t)S_2((1-2s)\delta t)S_2(s\delta t) = e^{i(A+B)\delta t} + \mathcal{O}\left(\delta t^5\right)$$

We know what $S_2(\delta t)$ is can be written as

$$S_2(\delta t) = e^{i(A+B)\delta t + R_3\delta t^3 + \mathcal{O}\left(\delta t^4\right)} = e^{i(A+B)\delta t}e^{R_3\delta t^3} + \mathcal{O}\left(\delta t^4\right)$$

for an operator R_3. Thus, we first expand out $S_4(\delta t)$,

$$S_4(\delta t) = e^{i(A+B)\delta t}e^{iR_3[2s^3+(1-2s)^3]\delta t^3} + \mathcal{O}(\delta t^5)$$

Comparing it with the RHS of first equation we have,

$$2s^3 + (1-2s)^3 = 1$$

Thus,

$$S = [0, -1]$$

2. Quantum simulation

We have the operator

$$H = \alpha Z + \beta X$$

a) The Hamiltonian has the eigenvalues,

$$\lambda = \pm\sqrt{\alpha^2 + \beta^2}$$

b) For the Hamiltonian to be unitary,it must satisfy the condition,

$$HH^\dagger = \mathbb{I}$$

The Pauli matrices are Hermitian,

$$Z = Z^\dagger$$
$$X = X^\dagger$$

thus we have

$$(\alpha Z + \beta X)(\alpha^* Z + \beta^* X) = \mathbb{I}$$

$$\alpha^2\mathbb{I} + \beta^2\mathbb{I} - i\beta\alpha Y + i\alpha\beta Y = \mathbb{I}$$

$$\alpha^2\mathbb{I} + \beta^2\mathbb{I} = \mathbb{I}$$

in matrix form, this can be written as,

$$\begin{pmatrix} \alpha^2 + \beta^2 & 0 \\ 0 & \alpha^2 + \beta^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Thus, equating the individual matrix entries we have,

$$\alpha^2 + \beta^2 = 1$$

Since $\alpha, \beta \in \mathbb{R}$, thus we can have the following values for α and β

$$\alpha = \frac{1}{\sqrt{2}}, \beta = \frac{1}{\sqrt{2}}$$

c) We wish to write down exact implementation of the operator

$$U = e^{iHt}$$

$$U = e^{it(\alpha Z+\beta X)} = e^{it\alpha Z} e^{it\beta X}$$

We know that the exponentials of Pauli matrices can be written as,

$$e^{ik\sigma_n} = \mathbb{I}\cdot\cos(k) + i\sigma_n\cdot\sin(k)$$

where σ_n is a Pauli matrix and k is some real number. This holds as we can simply Taylor expand the exponential, and since the Pauli matrices square to $\mathbb{I}$, we have,

$$e^{ik\sigma_n} = \mathbb{I} + ik\sigma_n - \frac{k^2}{2!}\mathbb{I} - i\frac{k^3}{3!}\sigma_n + \frac{k^4}{4!}\mathbb{I} + i\frac{k^5}{5!}\sigma_n \ldots = \mathbb{I}\cdot\left(1 - \frac{k^2}{2!} + \frac{k^4}{4!} - \cdots\right) + i\sigma_n\left(k - \frac{k^3}{3!} + \frac{k^5}{5!} - \cdots\right)$$

this we can see are simply is,

$$e^{ik\sigma_n} = \mathbb{I}\cdot\cos(k) + i\sigma_n\cdot\sin(k)$$

Thus, for our operator U, we have

$$U = (\mathbb{I}\cdot\cos(\alpha t) + iZ\cdot\sin(\alpha t))(\mathbb{I}\cdot\cos(\beta t) + iX\cdot\sin(\beta t))$$

This can be multiplied out to give,

$$U = \cos(\alpha t)\cos(\beta t)\mathbb{I} + i\sin(\alpha t)\cos(\beta t)Z + i\sin(\beta t)\cos(\alpha t)X - i\sin(\alpha t)\sin(\beta t)Y$$

This is the exact implementation of the unitary operator.