An Introduction to Quantum Computing

Lecture 19:

Variational Quantum Algorithms

Paolo Zuliani

Dipartimento di Informatica
Università di Roma “La Sapienza”, Rome, Italy

Agenda

- Variational Algorithms and the NISQ Era
- Variational Quantum Eigensolver and Optimization

Variational Algorithms

The quantum circuits seen so far (Grover's, Shor's, *etc.*) depended on the input size:

- the same circuit is used for inputs of some maximum length;
- if the input gets larger, one needs a different, larger circuit;

Variational Algorithms

The quantum circuits seen so far (Grover's, Shor's, *etc.*) depended on the input size:

- the same circuit is used for inputs of some maximum length;
- if the input gets larger, one needs a different, larger circuit;

Variational Quantum Algorithms:

- quantum circuits are updated as a way to solve an optimization problem;
- the circuits are usually small and not exceedingly deep;
- the circuits can be run on NISQ (Noisy Intermediate-Scale Quantum) computers.

Extremal Eigenvalue Problem

Definition (Extremal Eigenvalue Problem)

Given an Hermitian matrix, find its <u>extremal</u> eigenvalues.

Extremal Eigenvalue Problem

Definition (Extremal Eigenvalue Problem)

Given an Hermitian matrix, find its extremal eigenvalues.

Given a generic optimization problem where $C(\cdot)$ is a real cost function and S is a set representing some constraints

$$\max / \min C(x)$$
$$\text{subject to } x \in S$$

can be reduced to an extremal eigenvalue problem.

Optimization as an Extremal Eigenvalue Problem

Assume that the set of solutions Y is finite, so can use finite bit-strings to encode the solutions.

Optimization as an Extremal Eigenvalue Problem

Assume that the set of solutions Y is finite, so can use finite bit-strings to encode the solutions.

We build the Hermitian operator

$$H_C = \sum_{y \in Y} C(y) \, |y\rangle\langle y|$$

which implies that $H_C \, |x\rangle = C(x) \, |x\rangle$ for any $x \in Y$.

Optimization as an Extremal Eigenvalue Problem

Assume that the set of solutions Y is finite, so can use finite bit-strings to encode the solutions.

We build the Hermitian operator

$$H_C = \sum_{y \in Y} C(y) \left|y\right\rangle\!\left\langle y\right|$$

which implies that $H_C \left|x\right\rangle = C(x) \left|x\right\rangle$ for any $x \in Y$.

Therefore:

- $\min_x C(x) =$ minimal eigenvalue of H_C;
- $\max_x C(x) =$ maximal eigenvalue of $H_C =$ minimal eigenvalue of $-H_C$

Variational Quantum Eigensolver

How to find the minimal eigenvalue of an Hermitian operator?

Theorem

Let A be an Hermitian operator/matrix on an Hilbert space $\mathcal{H}$ and λ_{min} its least eigenvalue. Then:

$$\forall \left|\psi\right\rangle \in \mathcal{H} \quad \left\langle\psi\middle|A\psi\right\rangle \geqslant \lambda_{\text{min}}$$

with equality iff $\left|\psi\right\rangle = \left|\psi\right\rangle_{\text{min}}$ (an eigenvector associated to λ_{min}).

Variational Quantum Eigensolver

How to find the minimal eigenvalue of an Hermitian operator?

Theorem

Let A be an Hermitian operator/matrix on an Hilbert space $\mathcal{H}$ and λ_{min} its least eigenvalue. Then:

$$\forall\, |\psi\rangle \in \mathcal{H} \quad \langle\psi|A\psi\rangle \geqslant \lambda_{\text{min}}$$

with equality iff $|\psi\rangle = |\psi\rangle_{\text{min}}$ (an eigenvector associated to λ_{min}).

Therefore, we can solve our extremal eigenvalue problem by <u>minimizing</u> the function $f : \mathcal{H} \to \mathbb{R}$ defined as:

$$f(|\psi\rangle) = \langle\psi|A\psi\rangle$$

Variational Quantum Eigensolver

How to find the minimal eigenvalue of an Hermitian operator?

Theorem

Let A be an Hermitian operator/matrix on an Hilbert space $\mathcal{H}$ and λ_{min} its least eigenvalue. Then:

$$\forall\, |\psi\rangle \in \mathcal{H} \quad \langle\psi|A\psi\rangle \geqslant \lambda_{\text{min}}$$

with equality iff $|\psi\rangle = |\psi\rangle_{\text{min}}$ (an eigenvector associated to λ_{min}).

Therefore, we can solve our extremal eigenvalue problem by <u>minimizing</u> the function $f : \mathcal{H} \to \mathbb{R}$ defined as:

$$f(|\psi\rangle) = \langle\psi|A\psi\rangle$$

Note that f is a well-behaved function. Only problem: the state space is usually huge!

Variational Quantum Eigensolver: The Main Idea

To generate a *sequence* of quantum circuits whose output is close to $\langle \psi_{\mathsf{min}} | A \psi_{\mathsf{min}} \rangle$.

The quantum circuits are parameterized by a number (say p) of real parameters.

Variational Quantum Eigensolver: The Main Idea

To generate a *sequence* of quantum circuits whose output is close to $\langle \psi_{\mathsf{min}} | A \psi_{\mathsf{min}} \rangle$.

The quantum circuits are parameterized by a number (say p) of real parameters.

$$\text{parameters } \theta \in \mathbb{R}^p \xrightarrow{\text{circuit } Q_\theta} \text{evaluate circuit} \xrightarrow{|\psi_\theta\rangle} \text{estimate } \langle \psi_\theta | A \psi_\theta \rangle$$

Variational Quantum Eigensolver: The Main Idea

To generate a *sequence* of quantum circuits whose output is close to $\langle \psi_{\mathsf{min}} | A \psi_{\mathsf{min}} \rangle$.

The quantum circuits are parameterized by a number (say p) of <u>real parameters</u>.

$$\text{parameters } \theta \in \mathbb{R}^p \xrightarrow{\text{circuit } Q_\theta} \text{evaluate circuit} \xrightarrow{|\psi_\theta\rangle} \text{estimate } \langle \psi_\theta | A \psi_\theta \rangle$$

How to estimate $\langle \psi_\theta | A \psi_\theta \rangle$? (Remember: huge state spaces!)

Variational Quantum Eigensolver: The Main Idea

To generate a *sequence* of quantum circuits whose output is close to $\langle \psi_{\min} | A \psi_{\min} \rangle$.

The quantum circuits are parameterized by a number (say p) of <u>real parameters</u>.

$$\text{parameters } \theta \in \mathbb{R}^p \xrightarrow{\text{circuit } Q_\theta} \text{evaluate circuit} \xrightarrow{|\psi_\theta\rangle} \text{estimate } \langle \psi_\theta | A \psi_\theta \rangle$$

How to estimate $\langle \psi_\theta | A \psi_\theta \rangle$? (Remember: huge state spaces!)

We "simply" measure A (it is an Hermitian operator, hence a valid observable) multiple times in order to estimate the amplitudes of the basis states.

Recall that given a cost function $C(\cdot)$ we have

$$\langle \psi | H_C \psi \rangle = \sum_y |\alpha_y|^2 C(y) \quad \text{where } |\psi\rangle = \sum_y \alpha_y |y\rangle$$

Variational Quantum Eigensolver: The Main Idea

The quantum circuits are built from an **ansatz** (a ‘template’ or ‘educated guess’) circuit containing single-qubit parameterized rotations and 2-qubit gates.

An example of ansatz on two qubits:

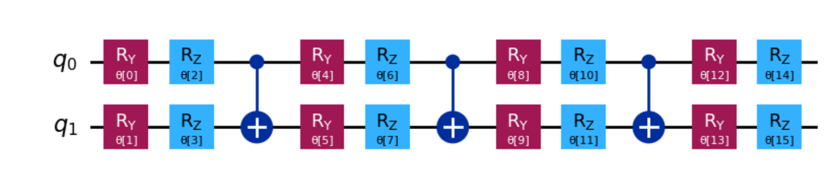

Figure: from `https://learning.quantum.ibm.com/tutorial/variational-quantum-eigensolver`

The ansatz should be able to reach much of the Hilbert space by an appropriate choice of parameters. Choosing the right ansatz is quite an art.

Variational Quantum Optimization

Now that we can estimate $f(|\psi_\theta\rangle) = \langle\psi_\theta|A\psi_\theta\rangle$, and since $f : \mathbb{R}^p \to \mathbb{R}$ is a classical function, we can use any standard (classical) optimization technique to minimize f.

Variational Quantum Optimization

Now that we can estimate $f(|\psi_\theta\rangle) = \langle\psi_\theta|A\psi_\theta\rangle$, and since $f : \mathbb{R}^p \to \mathbb{R}$ is a classical function, we can use any standard (classical) optimization technique to minimize f.

Algorithm 2: Optimization by VQE

Input: Cost function C, number of circuit evaluations N

Output: An approximation of min C

$\theta = \theta_0$
done = **false**
while not *done* **do**
    generate circuit Q_θ from ansatz with parameters θ
    for N *times* **do**
        $|\psi_\theta\rangle = Q_\theta\,|00\ldots0\rangle$
        measure H_C on $|\psi_\theta\rangle$
    I_θ = estimate $\langle\psi_\theta|A\psi_\theta\rangle$ from measurements
    if classical optimization algorithm decides I_θ is OK **then**
        done = **true**
    else
        update θ