i) multi basis graph encodings   ii) non-linear activation.

Multi Basis encoding introduces additional constraints that are beneficial to the algorithms performance, reducing its susceptibility to local minima in training landscape. MBEs halve the number of qubits required, also by utilizing single-qubit measurements, these algorithms yield up to a quadratic reduction in runtime.

VQE Framework and Tensor Network Formalism

For a graph of n-vertices, the problem reduces to finding the n-qubit wave function $|\psi\rangle$ that minimizes the energy expectation value $E = \langle\psi|H|\psi\rangle$ of the classical Ising Model Hamiltonian:

$$H = \sum_{j<i}^{n} w_{ij}^{ZZ} \sigma_i^{Z} \sigma_j^{Z} \qquad (1)$$

As 'H' contains only terms in the z-basis, its eigenvectors are classical, such that $|\psi_i\rangle = \otimes_s |s\rangle$ where $|s\rangle = \{|0\rangle, |1\rangle\}$

As Eq. (1) has Z_2 symmetry, the ground state $|\psi_g\rangle$ is degenerate with the state $X^{\otimes n}|\psi_g\rangle$

Z_2 symmetry means, it commutes with an operator that squares to the identity.

$$[H, X^{\otimes n}] = 0$$

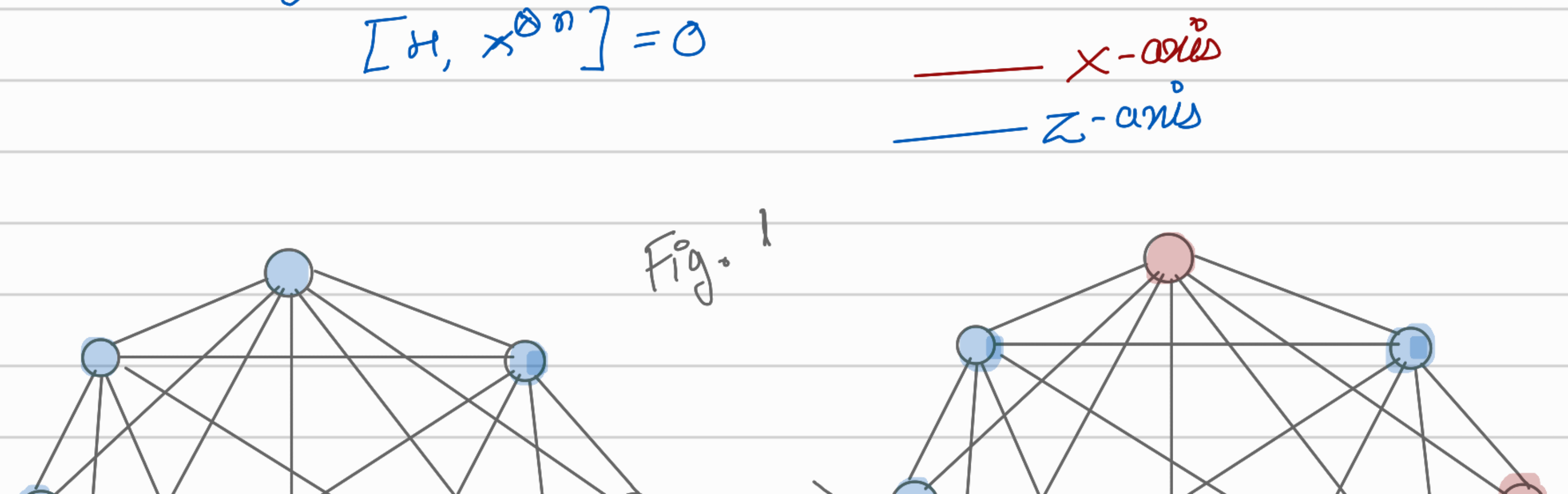
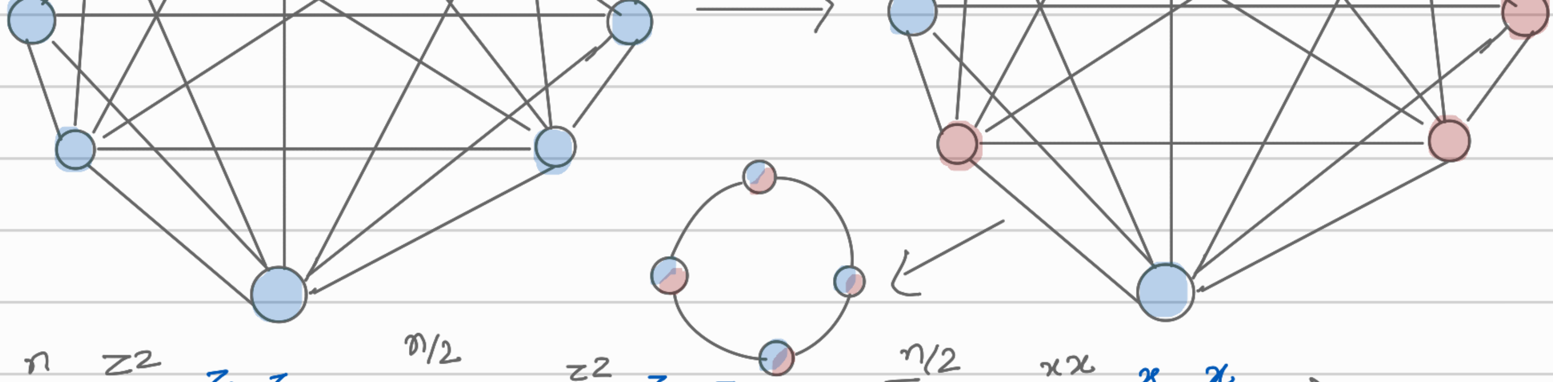


Fig. 1



$$\sum_{j<i}^{n} w_{ij}^{zz}\sigma_i^z\sigma_j^z \longrightarrow \sum_{j<i}^{n/2} w_{ij}^{zz}\sigma_i^z\sigma_j^z + \sum_{j<i}^{n/2} w_{ij}^{xx}\sigma_i^x\sigma_j^x \longrightarrow L_{MBE}$$

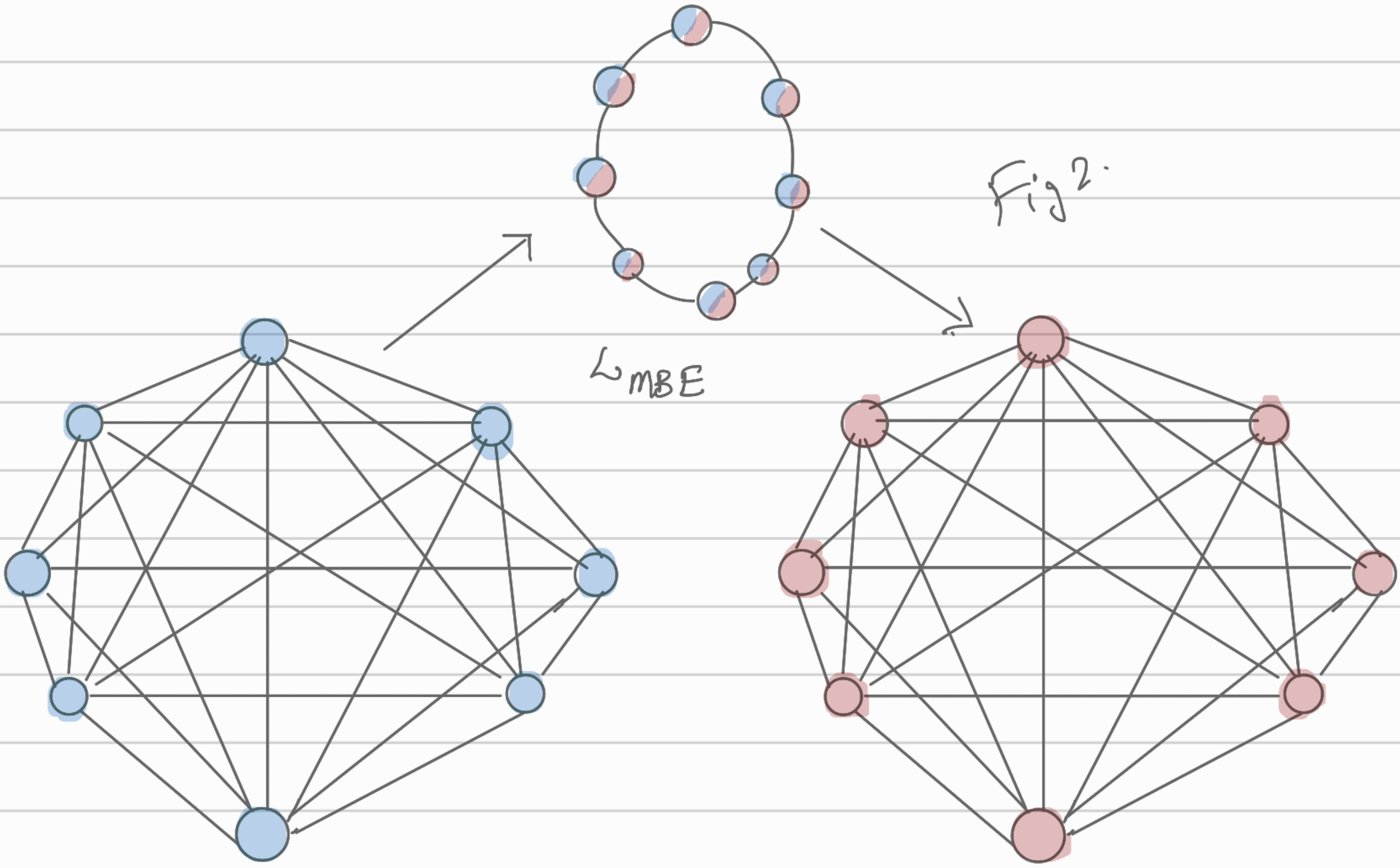


Fig 2.

$$\sum_{j<i} w_{ij}^{zz}\sigma_i^z\sigma_j^z \qquad\qquad \sum_{j<i} w_{ij}^{xx}\sigma_i^x\sigma_j^x.$$

In Fig 1. Multi-Basis Encoding of a graph : we reassign $n/2$ vertices from σ^z to σ^x operators, allowing us to map the graph to just $n/2$ qubits. The Max-Cut is obtained by optimizing this state via single-qubit measurement.

Fig 2: Multi Basis Encoding with two distinct n-qubit graphs.

$\mathbb{Z}_2$ symmetry : a symmetry operation that yields the identity if applied twice.

we define the input state as the n-qubit zero state

$$|0\rangle = \otimes_n |0\rangle$$

$$|\psi\rangle = U(\hat{\theta})\,|0\rangle$$

$\hookrightarrow$ our parameterized unitary

then this unitary U is decomposed as $\wedge$ subunitaries

$$U(\hat{\theta}) = \prod_k^{\wedge} U_k(\hat{\theta}_k)$$

where

$$U_k(\hat{\theta}_k) = \prod_{j=1}^{n} \exp(-i\hat{\theta}_j\, w_j)\, M_k$$

thus the gradient $g_t(\hat{O}) = \dfrac{\partial \langle \hat{O} \rangle}{\partial \theta_t}$ w.r.t any parameter θ_t

$$\boxed{g_t(\hat{O}) = i\langle 0|\, U_R^{\dagger}\left[w_\ell,\, U_L^{\dagger}\hat{O}\,U_L\right] U_R|0\rangle}$$

where U_L and U_R are the compositions of unitaries U_k with $k \geq \ell$ and $k < \ell$

$$H = \sum_{j<i}^{n} \omega_{ij}^{zz}\, \sigma_i^z \sigma_j^z$$

Matrix Product operator $H^{\{\beta,\gamma\}}$

Energy $L = E$

$$L = \langle \psi | H | \psi \rangle$$

$$E = \sum_{\{\beta,\gamma,\delta,\epsilon\}} \psi^{\{\beta\}}\, U^{\{\beta,\gamma\}}\, H^{\{\gamma,\delta\}}\, U^{\{\delta,\epsilon\}}\, \psi^{\{\epsilon\}}$$

$$\psi^{\{\beta\}} = \psi^{\beta_0 \cdots \beta_{m-1}}$$

$$U^{\{B,\gamma\}} = U^{\beta_0, \gamma_0, \ldots \beta_{m-1}, \gamma_{m-1}}$$

Max cut objective

$$\max \frac{1}{2} \sum_{j<i} w_{ij} (1 - v_i v_j)$$

$$E = \langle \psi | H | \psi \rangle$$

$$H = \sum_{j<i}^{n} w_{ij} \sigma_i^z \sigma_j^z$$

substituting vertices v_i for the Pauli-Z spin operators σ_i^z

All the terms are in Z-basis

Eigenvectors and eigenvalues

Each of the (Hermitian) Pauli matrices has two eigenvalues, +1 and −1. The corresponding normalized eigenvectors are:

$$\psi_{x+} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \psi_{x-} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix},$$

$$\psi_{y+} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}, \quad \psi_{y-} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix},$$

$$\psi_{z+} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \psi_{z-} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

classical (zero-entanglement product states)

Now $H = \sum_{j<i}^{n} w_{ij} \sigma_i^z \sigma_j^z$ has $\mathbb{Z}_2$ symmetry, and the lowest eigenvalue "ground state" is $|\psi_g\rangle$

$|\psi_g\rangle$ is degenerate with the state $X^{\otimes n} |\psi_g\rangle$

$$[H, X^{\otimes n}] = H X^{\otimes n} - X^{\otimes n} H$$

$$\Rightarrow \left(\sum_{j<i}^{n} w_{ij} \sigma_i^z \sigma_j^z \right) (X^{\otimes n}) - (X^{\otimes n}) \left(\sum_{j<i}^{n} w_{ij} \sigma_i^z \sigma_j^z \right)$$

$$\Rightarrow \sum_{j<i}^{n} w_{ij} \left(\sigma_i^z \sigma_j^z X^{\otimes n} - X^{\otimes n} \sigma_i^z \sigma_j^z \right)$$

Since σ_i^z and σ_j^z act on different qubits and commute with each other, we can rearrange the terms.

$$\Rightarrow \sum_{j<i} w_{ij} \left(\sigma_i^z X \sigma_j^z X \ldots X - X\sigma_i^z X \sigma_j^z \ldots X \right)$$

$$\Rightarrow \sum_{j<i}^{n} w_{ij} \left(\sigma_i^z X^2 \sigma_j^z - X\sigma_i^z X \sigma_j^z \right)$$

and $X^2 = \mathbb{1}$

$$\Rightarrow \sum_{j<i}^{n} w_{ij} \left(\sigma_i^z \sigma_j^z - X\sigma_i^z X\sigma_j^z \right)$$

$$\Rightarrow \sum_{j<i}^{n} w_{ij} \left(\sigma_i^z \sigma_j^z - \sigma_i^z \sigma_j^z \right)$$

$\Rightarrow 0$ Hence $[H, X^{\otimes n}] = 0$

this means

$$\boxed{\begin{aligned} H|\psi_g\rangle &= |\psi_g\rangle \\ X^{\otimes n}|\psi_g\rangle &= |\psi_g\rangle \end{aligned}}$$

Variational Quantum Eigensolver part.

start with the input state $|0\rangle = \otimes_n |0\rangle$

$$|\psi\rangle = U(\hat{\theta})\,|0\rangle$$

$\hookrightarrow$ the variational circuit whose parameters $\hat{\theta}$ will be varied.

This Unitary U, will be decomposed into $\wedge$ sub unitaries

$$U(\hat{\theta}) = \Pi_k^{\wedge} U_k(\hat{\theta}_k)$$

and

$$U_k(\hat{\theta}_k) = \Pi_{j=1}^{n} \exp(-i\theta_j w_j) M_k$$

and ... these evolve

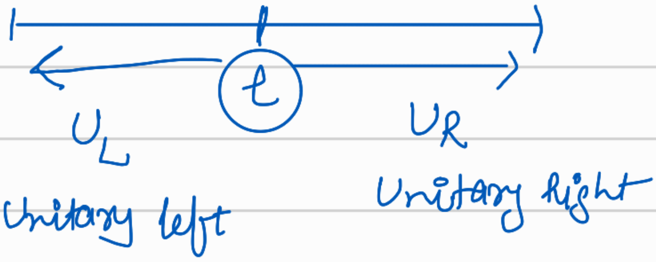
gradient

$$\underline{g_\ell}(\hat{O}) = i\langle 0| U_R^\dagger [W_\ell, U_L^\dagger \hat{O} U_L] U_R |0\rangle$$

with θ_i

computational basis states

W_ℓ is the Hermitian corresponding to the ℓ-th parameter



i) $U_L^\dagger O U_L$ → transformed operator O under the action of unitaries U_L.

ii) $[W_\ell, U_L^\dagger O U_L]$ → commutator between the Hermitian operator W_ℓ and transformed $U_L^\dagger O U_L$

iii) $U_R^\dagger [W_\ell, U_L^\dagger O U_L] U_R$ → transformed commutator under the action of unitaries U_R.

iv) $\langle 0| \cdots |0\rangle$ ~ expectation value of the transformed commutator in quantum state $|0\rangle$.

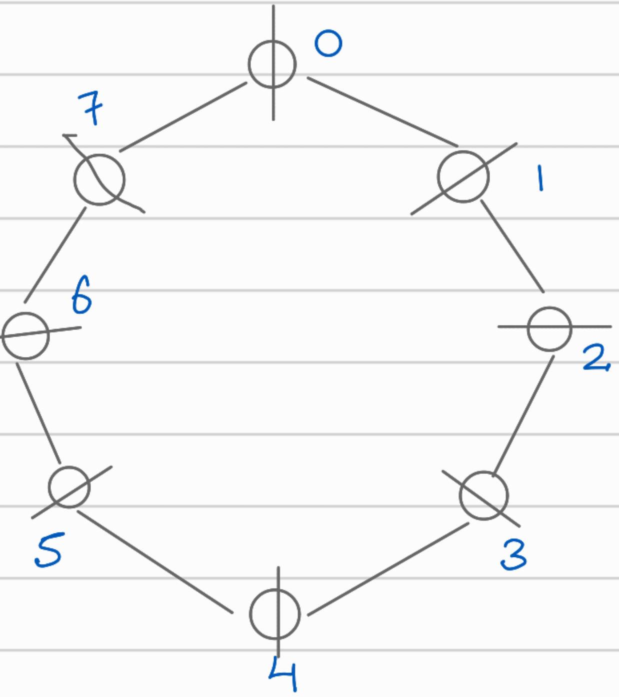
The composition of the subunitaries $U(\hat{\theta}) = \prod_k U_k(\hat{\theta}_k)$ is denoted as U_L and U_R which captures the cumulative effect of these transformations up to an index ℓ.

By breaking the evolution into left and right composition, we can isolate the contributions of different parameter to the overall transformation.

The commutator $[W_\ell, U_L^\dagger O U_L]$ captures the non-commutativity between the Hermitian W_ℓ (corresponding to the parameter θ_ℓ). This quantifies how the parameter θ_e affects the evolution of the system and the operator O. The expectation value essentially represents the sensitivity of the operator O to changes in θ_e

In summary, the expression enables the calculation of gradients by decomposing the evolution of the quantum system into individual parameterized transformations and quantify the effects of these transformations on the operator of interest.

1-D tensor ring



instead of using extensively connected circuits, we'll make use of 1-D tensor ring circuit of 'n' qubits.

Here $n = 8$

qubit 0 is connected with qubit $n-1$.

Multi-Basis Encoding

$$H_{zx} = \sum_{j<i} w_{ij}^{zz} \sigma_i^z \sigma_j^z + \sum_{j<i} w_{ij}^{xx} \sigma_i^x \sigma_j^x + \sum_{i,j} w_{ij}^{zx} \sigma_i^z \sigma_j^x$$

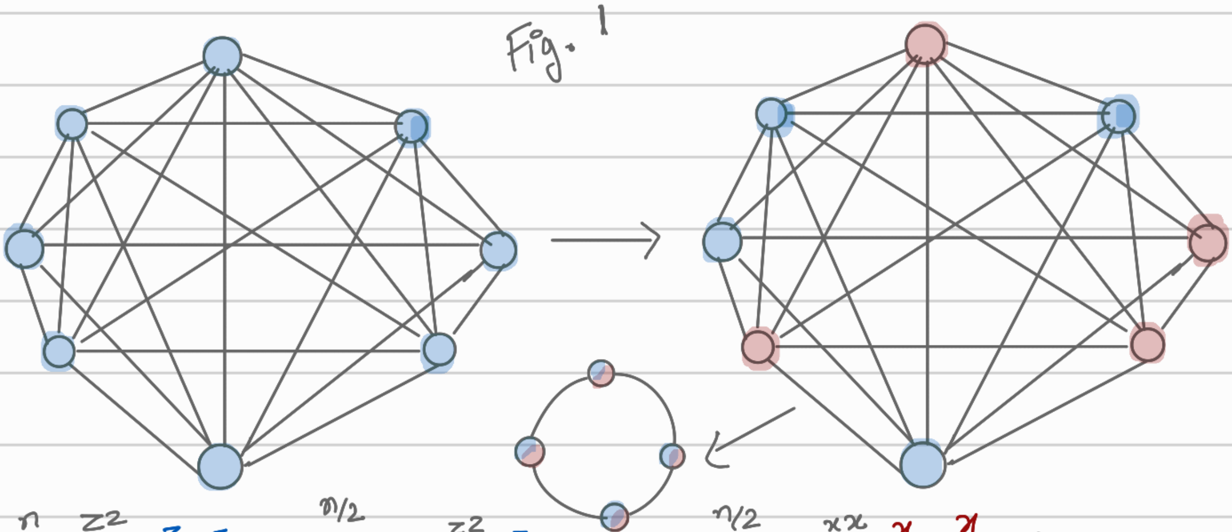
The key difference between this equation and Multi-Basis Encoding is that MBE utilizes the product of single-qubit measurements and non linear activation functions to encode separate vertices into the z and x- basis.

x-axis

z-axis

Algorithm

Fig. 1



$$\sum_{j<i}^{n} w_{ij}^{zz}\sigma_i^z\sigma_j^z \longrightarrow \sum_{j<i}^{n/2} w_{ij}^{zz}\sigma_i^z\sigma_j^z + \sum_{j<i}^{n/2} w_{ij}^{xx}\sigma_i^x\sigma_j^x \longrightarrow L_{MBE}$$

first $\lceil \frac{n}{2} \rceil$ on z   second $\lfloor \frac{n}{2} \rfloor$ on x-axis

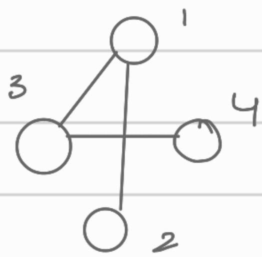
thus enabling 'n' vertices to be encoded into only $\lceil \frac{n}{2} \rceil$ qubits.
If 'n' is odd, then the x-axis of the n^{th} qubit is unneeded.

The MBE loss function

$$L_{MBE} = \sum_{j<i}^{n/2} w_{ij}^{zz} \tanh(\langle\sigma_i^z\rangle)\tanh(\langle\sigma_j^z\rangle) + \sum_{j<i}^{n/2} w_{ij}^{xx}\tanh(\langle\sigma_i^x\rangle)\tanh(\langle\sigma_j^x\rangle) + \sum_{i,j} w_{ij}^{zx}\tanh(\langle\sigma_i^z\rangle)\tanh(\langle\sigma_i^x\rangle)$$

Ex.

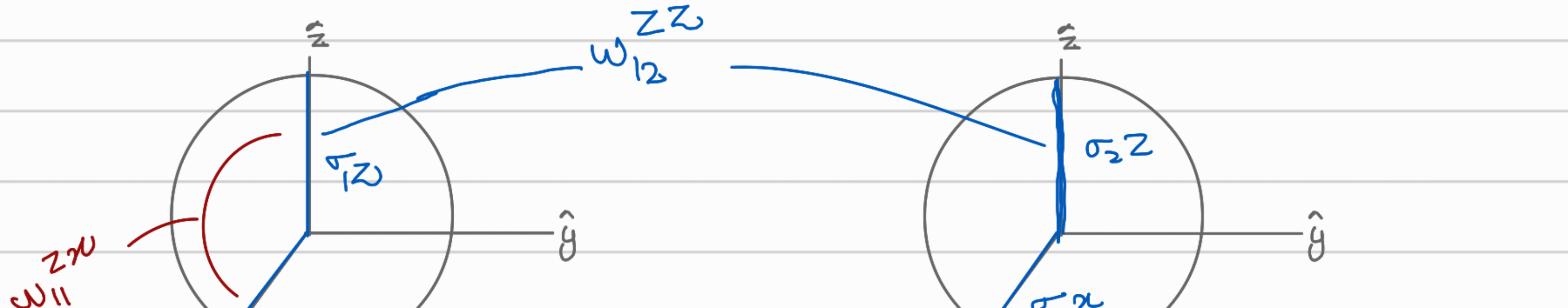
Four-vertex graph with four qubit Ising model.

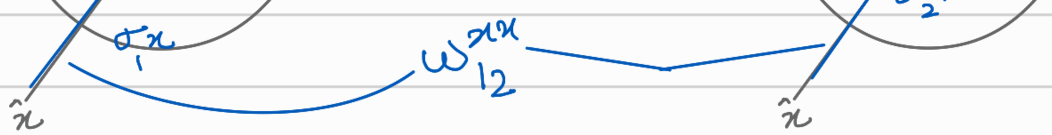


$$H = w_{12}\sigma_1^z\sigma_2^z + w_{34}\sigma_3^z\sigma_4^z + w_{13}\sigma_1^z\sigma_3^z$$

would be optimized with two-qubit MBE

$$L_{MBE} = w_{12}^{zz}\tanh(\langle\sigma_1^z\rangle)\tanh(\langle\sigma_2^z\rangle) + w_{12}^{xx}\tanh(\langle\sigma_1^x\rangle)\tanh(\langle\sigma_2^x\rangle) + w_{11}^{zx}\tanh(\langle\sigma_1^z\rangle)\tanh(\langle\sigma_1^x\rangle)$$





Hence three are distinct Pauli strings that are independently measured on separate circuit preparations, the uncertainty principle is not violated for w_{ij}^{zx} with $j = i$.

MBE is a dual-axis quantum analog to linear programming relaxations.

We are minimizing

$$\mathcal{L}_{MBE} = \sum_{j<i}^{n/2} w_{ij}^{zz} \tanh(\langle\sigma_i^z\rangle)\tanh(\langle\sigma_j^z\rangle) + \sum_{j<i}^{n/2} w_{ij}^{xx} \tanh(\langle\sigma_i^x\rangle)\tanh(\langle\sigma_j^x\rangle) + \sum_{i,j}^{n/2} w_{ij}^{zx} \tanh(\langle\sigma_i^z\rangle)\tanh(\langle\sigma_j^x\rangle)$$

under the constraint

$$\langle\sigma_i^z\rangle^2 + \langle\sigma_i^x\rangle^2 \leq 1$$

hence it doesn't yield classical solutions to

$$\frac{1}{2}\sum_{j<i} w_{ij}(1 - v_i v_j)$$

hence a rounding procedure for the classification and scoring of a cut C for a graph G:

$$C_{MBE}(\theta; G) = \sum_{j<i}^{n/2} \frac{w_{ij}^{zz}}{2}\left[1 - R(\langle\sigma_i^z\rangle)R(\langle\sigma_j^z\rangle)\right] + \sum_{j<i}^{n/2} \frac{w_{ij}^{xx}}{2}\left[1 - R(\langle\sigma_i^x\rangle)R(\langle\sigma_j^x\rangle)\right] + \sum_{i,j}^{n/2} \frac{w_{ij}^{zx}}{2}\left[1 - R(\langle\sigma_i^z\rangle)R(\langle\sigma_j^x\rangle)\right]$$

where classically implemented function R rounds the measured expectation values to ± 1.

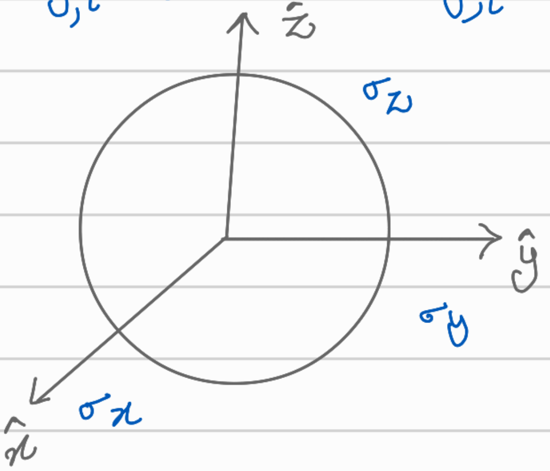
can it be extended to a 3-in-1?

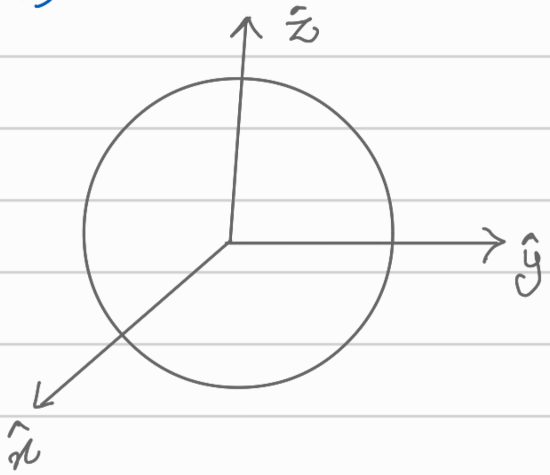
Maxcut : maximize $\frac{1}{2}\sum_{j<i} w_{ij}(1-v_i v_j)$

Multi Basis Encoding

$$H_{zxy} = \sum_{j<i} w_{ij}^{zz}\sigma_i^z\sigma_j^z + \sum_{j<i} w_{ij}^{xx}\sigma_i^x\sigma_j^x + \sum_{j<i} w_{ij}^{yy}\sigma_i^y\sigma_j^y +$$

$$\sum_{j,i} w_{ij}^{zx}\sigma_i^z\sigma_j^x + \sum_{j,i} w_{ij}^{zy}\sigma_i^z\sigma_j^y + \sum_{j,i} w_{ij}^{xy}\sigma_i^x\sigma_j^y$$





Constraint $\langle\sigma_i^x\rangle^2 + \langle\sigma_i^y\rangle^2 + \langle\sigma_i^z\rangle^2 \leq 1$

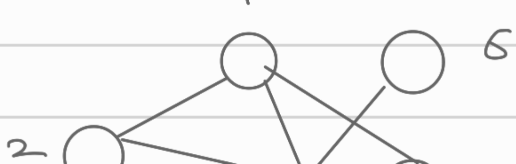
$$\mathcal{L}_{MBE} = \sum_{j<i}^{n/3} w_{ij}^{zz}\tanh(\langle\sigma_i^z\rangle)\tanh(\langle\sigma_j^z\rangle) + \sum_{j<i}^{n/3} w_{ij}^{xx}\tanh(\langle\sigma_i^x\rangle)\tanh(\langle\sigma_j^x\rangle)$$

$$+ \sum_{j<i}^{n/3} w_{ij}^{yy}\tanh(\langle\sigma_i^y\rangle)\tanh(\langle\sigma_j^y\rangle) +$$

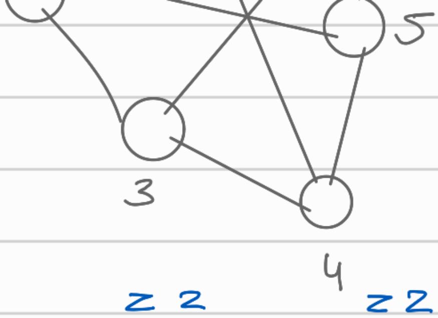
$$\sum_{i,j}^{n/3} w_{ij}^{zx}\tanh(\langle\sigma_i^z\rangle)\tanh(\langle\sigma_j^x\rangle) + \sum_{i,j}^{n/3} w_{ij}^{zy}\tanh(\langle\sigma_i^z\rangle)\tanh(\langle\sigma_j^y\rangle)$$

$$+ \sum_{i,j}^{n/3} w_{ij}^{xy}\tanh(\langle\sigma_i^x\rangle)\tanh(\langle\sigma_j^y\rangle)$$

Ex: 12 14 15



23 25
34 36
45



$$\omega_{12}\sigma_1^z\sigma_2^z + \omega_{14}\sigma_1^z\sigma_2^z + \omega_{15}\sigma_1^z\sigma_2^z + \omega_{23}\sigma_1^z\sigma_2^z + \omega_{25}\sigma_1^z\sigma_2^z + \omega_{34}\sigma_1^z\sigma_2^z + \omega_{36}\sigma_1^z\sigma_2^z + \omega_{45}\sigma_1^z\sigma_2^z$$

would be optimized with the three-qubit MBE IOA function

Tensor Train Representation

It is a way of representing a quantum state in a many-body system, such as system of spins.

Computational Basis Product Space $\{|0\rangle, |1\rangle\}$

$$|s_1\rangle \otimes |s_2\rangle \otimes |s_3\rangle \cdots \otimes |s_n\rangle$$

Tensor Train Representation : the quantum state is represented as a structured tensor network, where each tensor correspond to grouping of spins

Tensor = multi dimensional array

$$A = [A(i_1, \ldots, i_d)] \qquad i_k \in \{1, \ldots n_k\}$$

dimensionality = d (number of indices)

sizes $= n_1 \times \cdots \times n_d$ (number of nodes along each axis)

$d=1$ vector | $d=2$ matrix

number of elements = n^d (exponential in d)

So when $n = 2$, $d = 100$

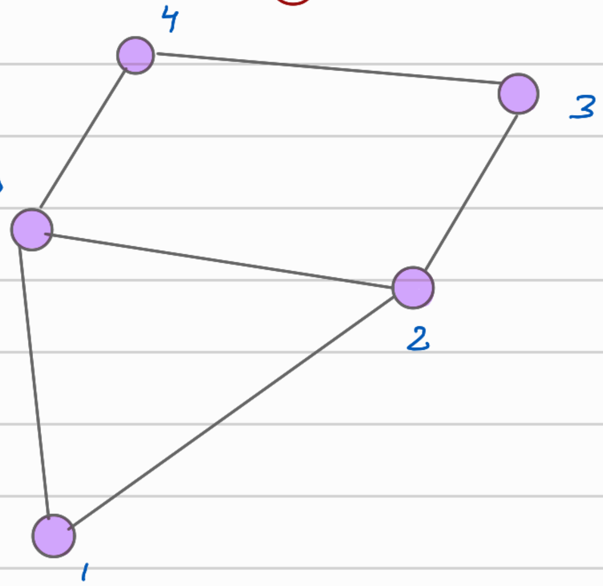
$$2^{100} > 10^{30} \quad [\simeq 10^{18} \text{ PB of memory.}]$$

we cannot work with tensors using standard methods.

Example

Five vertices

$\{[0, 1, 2, 3, 4]\}$



Edges

$[(0,1), (0,4), (0,2),$
$(1,2), (2,3), (3,4)]$

The vertices are divided into two groups

$\{[0,1,2]\}$ and $[3,4]$

$/$ $\qquad\qquad$ $/$

$Z_0 Z_1 Z_2$ $\qquad\qquad$ $X_0 X_1$

When using QAOA, the loss function is directly the $\langle H \rangle$

$$H = \sum Z_i Z_j$$

Now H forms is

$$H = Z_0 Z_1 + Z_0 Z_4 + Z_0 Z_2 + Z_1 Z_2 + Z_2 Z_3 + Z_3 Z_4$$

but using MBE, loss function become

$\hookrightarrow$ MBE

A non-linear activation function tanh is also applied to each measurement value.

$$[Z_0, Z_1, Z_2, X_0, X_1]$$

apply tanh and then express the loss function accor to apply tanh and then express the loss function across the connection

$$\mathcal{L}^{q} = \tanh\langle z_0 \rangle \tanh\langle z_1 \rangle + \tanh\langle z_0 \rangle \tanh\langle x_1 \rangle + \cdots$$

CODE

We do have the Expectation value, and we have to alter the parameters for the variational circuit and then the rounding method.

i) get_expectation_with_grad

Calculates the expectation value and a gradient of a quantum circuit with respect to a given Hamiltonian

i) Ensure hams is a list of Hamiltonians

ii) Ensure the data type of Hamiltonian matches the simulator.

iii) Validate each Hamiltonian and checks that they match the number of qubits in simulator.