VQA Summer Internship 2023

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OPTIMIZING ANSATZ DESIGN IN QAOA FOR MAX-CUT

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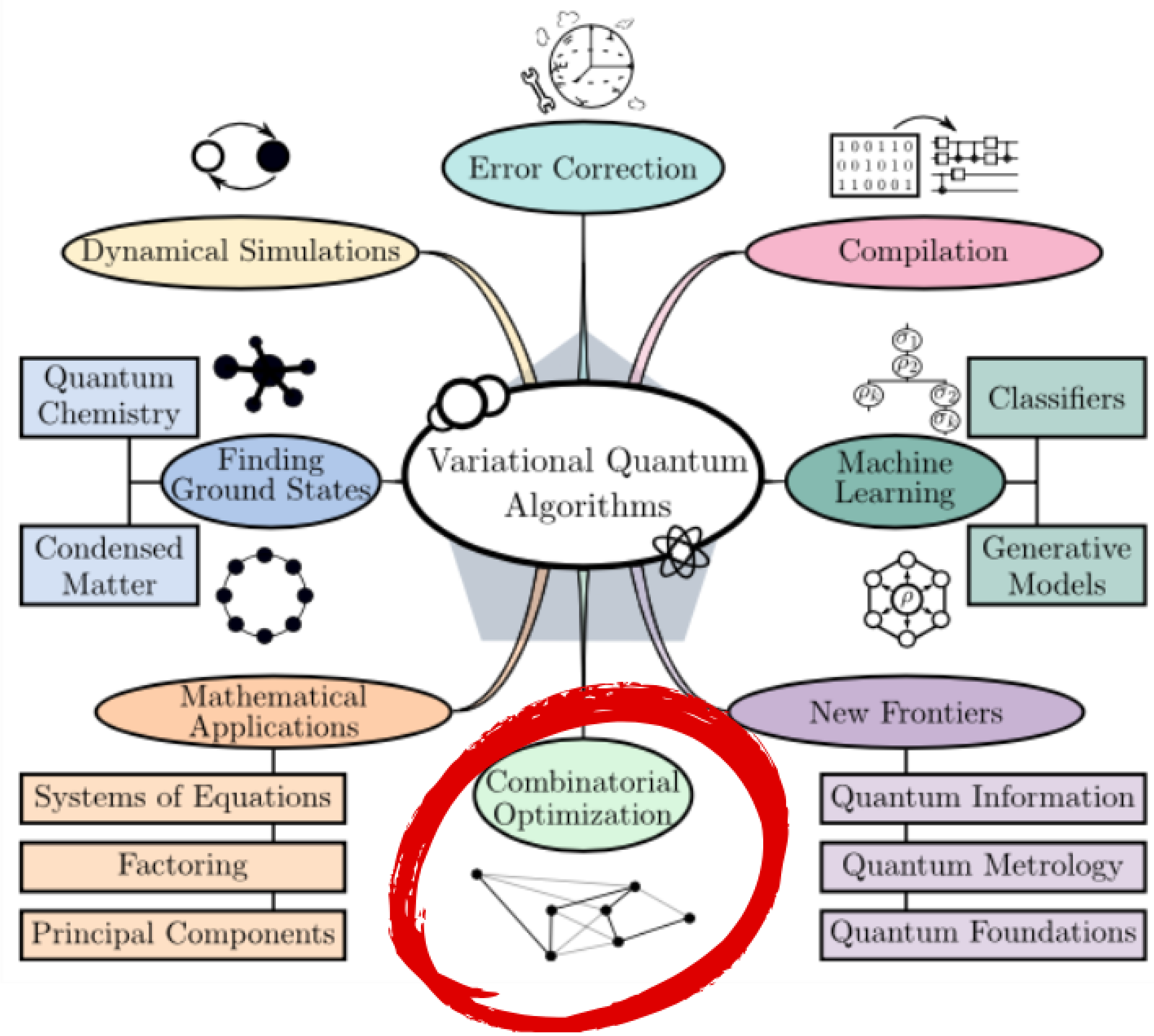
CONTENTS

01. QAOA



QAOA 정의

A type of VQA that focuses on finding good approximate solutions to combinatorial optimization problems.

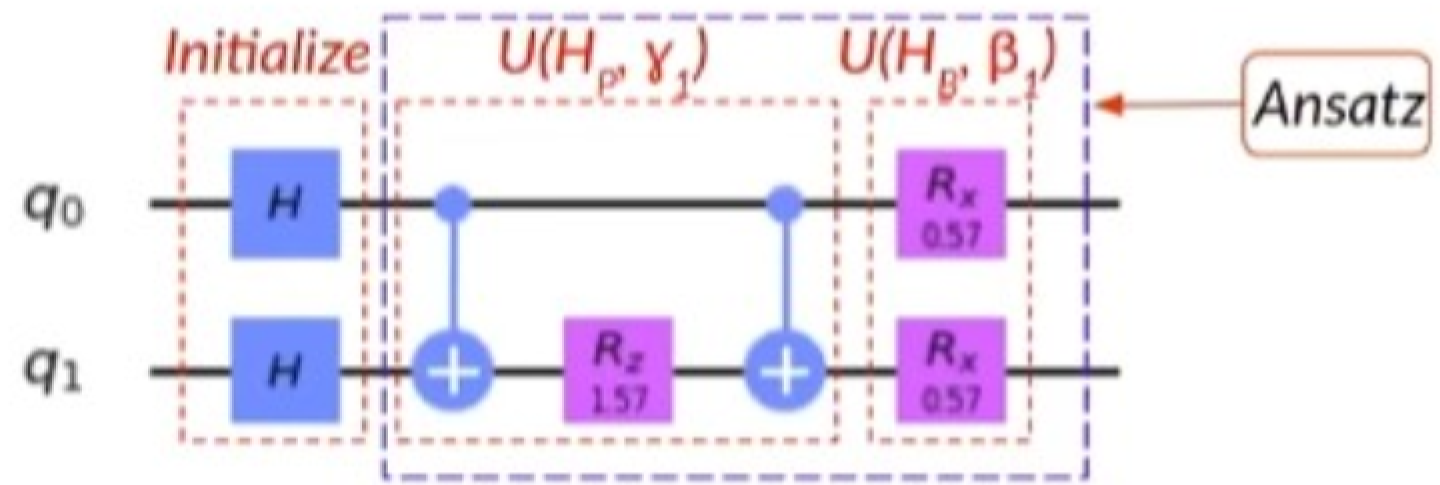
QAOA 연구

Most widely for finding the maximum cut of a grdph (Called the Max-cut problem)

01. QAOA

Quantum Approximate Optimization Algorithm (QAOA)

1. (Classical) Initialize 2p parameters: $\beta = \beta_1\beta_2 \dots \beta_p$ and $\gamma = \gamma_1\gamma_2 \dots \gamma_p$
2. (Quantum) Initial state $|\psi\rangle = \frac{1}{\sqrt{2^n}} \sum_{i=1}^{2^n} |i\rangle$
3. (Quantum) Construct the state $|\gamma\beta\rangle = U(H_B, \beta_p)U(H_P, \gamma_p)\dots U(H_B, \beta_1)U(H_P, \gamma_1)\,|\psi\rangle$



4. (Quantum) Measure the state and calculate the expectation value $\langle\gamma\beta \mid H_p \mid \gamma\beta\rangle$
5. (Classical) Optimize β and γ such that the expectation value is maximized.
6. Repeat steps 2-5 with the new set of parameters β and γ.

Example Graph

01. QAOA

Promises and limitations of QAOA

Promises

1. The expectation value is a non-decreasing function of the depth p.
2. At $p \to \infty$ QAOA produces the optimal solution.
3. For $p = 1$, QAOA provides an approximation ratio of 0.692 for 3 - regular graphs.
4. The probability distribution generated by QAOA at $p = 1$ cannot be efficiently sampled in a classical computer unless P = NP.
5. QAOA requires only 2 parameters per layer - lower complexity for classical optimizer.

Limitations

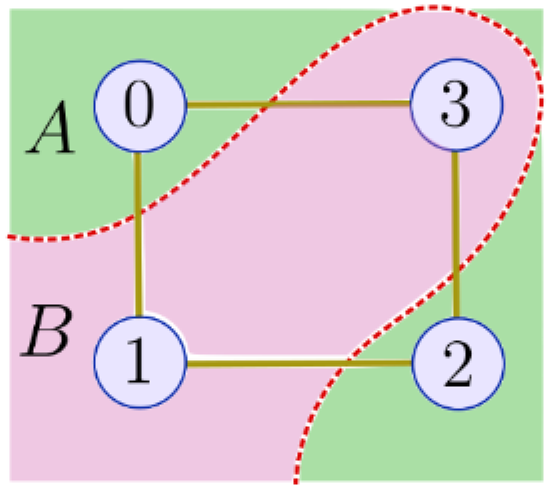
1. Recent results show that for $p < O(\log n)$, QAOA cannot outperform the best known classical algorithm for Max-cut.
2. Experiments from Google show that the performance of QAOA decreases beyond $p = 3$.

Noise is the culprit

Solutions

1. Make better (less noisy) devices.
2. Incorporate error mitigation techniques.
3. Tweak the ansatz to reduce noise.

01. MAX-CUT



MAX-CUT

주어진 무방향 그래프의 노드를 두 집합으로 나누어 색상 노드와 다른 색상 노드를 연결하는 에지의 수와 가중치를 최대화해야 하는 최적화 문제(색은 한 노드 집합과 다른 노드 집합을 구분하는 것)

Max-cut problem

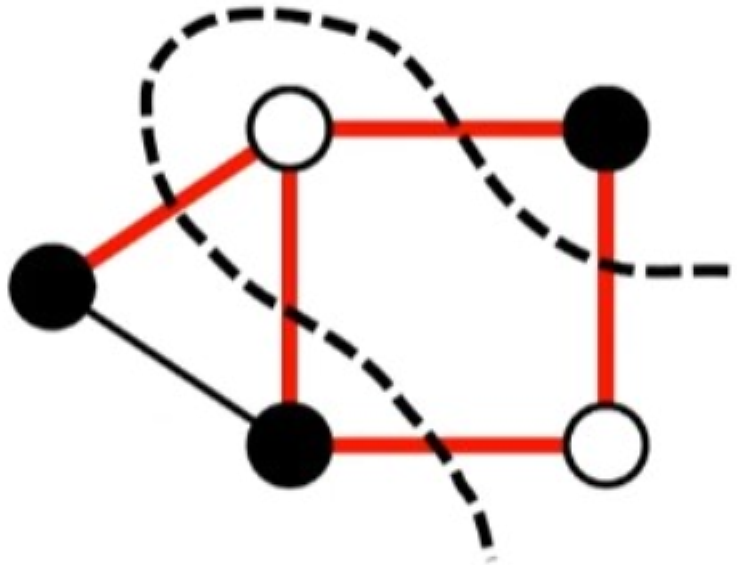


Image: wikipedia/maximum_cut

Problem statement: Given a graph G = (V,E) partition V into two disjoint sets such that the number of edges crossing from one set to another is maximized.

- This is an NP-Hard problem.
- This is an APX-Hard problem. There exists no Polynomial Time Approximation Scheme (PTAS) that can find a cut which is arbitrarily close to the best solution.
- Best known classical algorithm is the Goeman Williamson algorithm that has an approximation ratio of 0.878.
- It is not possible to approximate better than 0.941 unless P = NP.
- If the Unique Game Conjecture is true, then it is not possible to find an approximation ratio better than 0.878.

02. 논문의 주제

=> Primarily on reducing the number of CNOT gates in the design of QAOA ansatz for Max-cut

First, we present a method based on Edge Coloring of the input graph that minimizes the the number of cycles (termed as depth of the circuit), and reduces upto n/2 CNOT gates.

Next, we depict another method based on Depth First Search (DFS) on the input graph that reduces n − 1 CNOT gates, but increases depth of the circuit moderately.

+ CNOT gates are 100 times more prone to error compared to the other gates in the ansatz.

03. EDGE COLORING BASED ANSATZ OPTIMIZATION

=> minimize the depth of the circuit
=> reduction in CNOT gates in the depth optimized circuit

objective function of a depth-p QAOA for Max-cut

$$\max_{\psi(\gamma,\beta)} \langle\psi(\gamma,\beta)|H_P|\psi(\gamma,\beta)\rangle$$

can potentially contribute a lot to depth since the edge operators do not act on disjoint vertice

$$exp(-i\gamma_l H_P) = \Pi_{(i,j)\in E} exp\left(-i\gamma_l\left(\frac{I - Z_j Z_k}{2}\right)\right)$$

=> the minimun depth of the circuit will correspond to the minimum value k

=> partition the set of edges E as a disjoint union ∪iEi where each subset Ei consists of a vertex disjoint collection of edges

03. EDGE COLORING BASED ANSATZ OPTIMIZATION

=> 모서리 색상 문제는 최소 색상 수 k를 사용하여 모서리를 색상으로 칠하는 것으로 구성

=> 1. 색 지수라고 불리는 최적의 색상의 수는 회로의 최소 깊이에 해당

2. 동일한 색상의 에지는 동시에 실행할 수 있는 연산자 $exp\left(-i\gamma_l\left(\frac{I - Z_j Z_k}{2}\right)\right)$ 에 해당

Algorithm 1 Edge Coloring based Ansatz Optimization

Input: A graph $G = (V, E)$.

Output: Largest set S_{max} of edges having the same color.

Use the Misra and Gries algorithm to color the edges of the graph G.

$S_i \leftarrow$ set of edges having the same color i, $1 \leq i \leq \chi'$.

$S_{max} \leftarrow max\{S_1, S_2, \ldots, S_{\chi'}\}$.

Return S_{max}.

=> 이 에지 컬러링 접근 방식은 다항식 시간 전처리를 사용하여 QAOA ansatz에 대해 달성할 수 있는 최소 깊이를 제공합니다.

=> 최대 θ + 1 색상을 사용한 다항식 시간 색상입니다. 여기서 θ 는 그래프의
대 차수입니다.

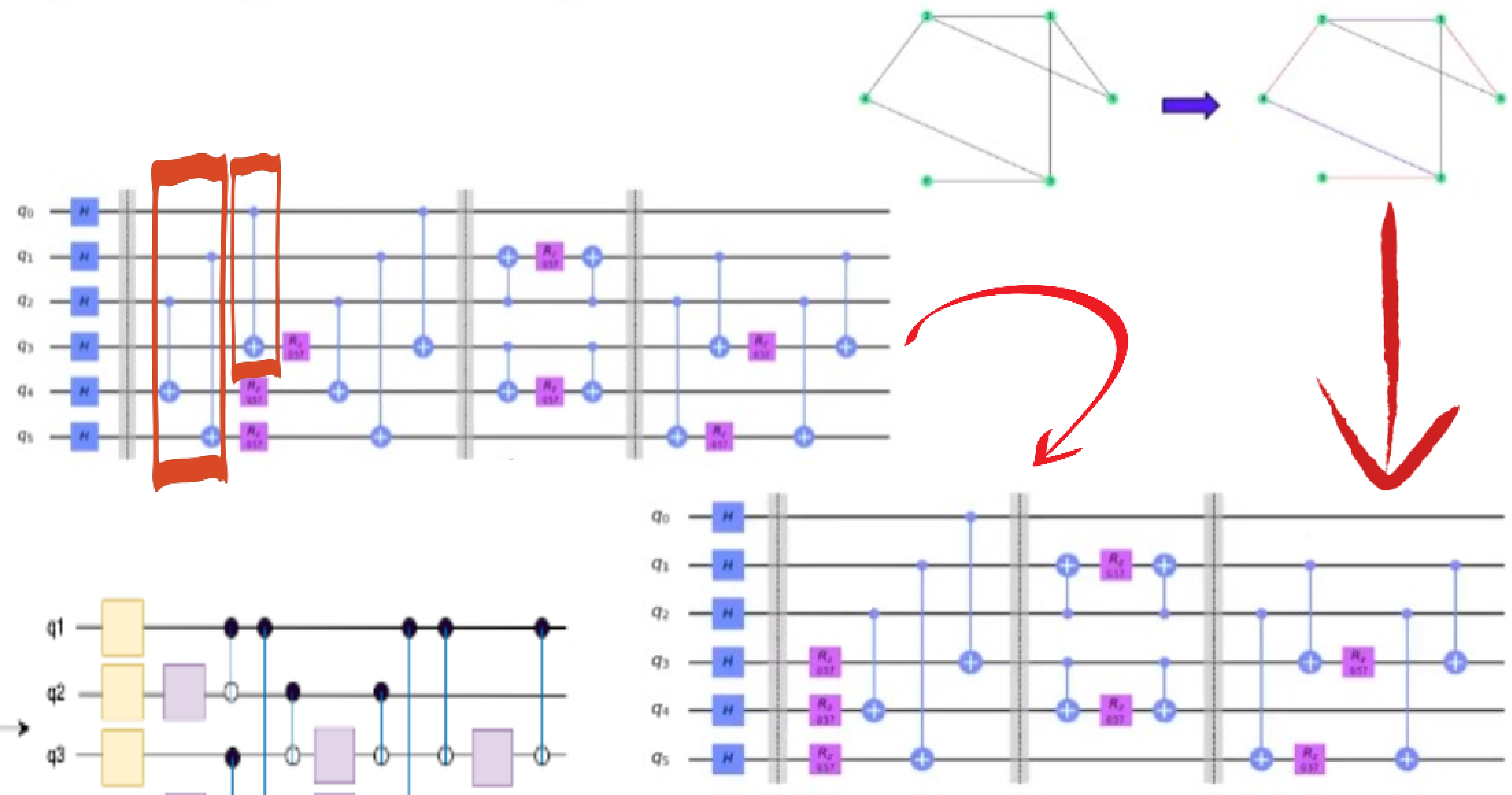
=> On an average, $\lceil \frac{m}{\Delta + 1} \rceil$ edges have the same color.

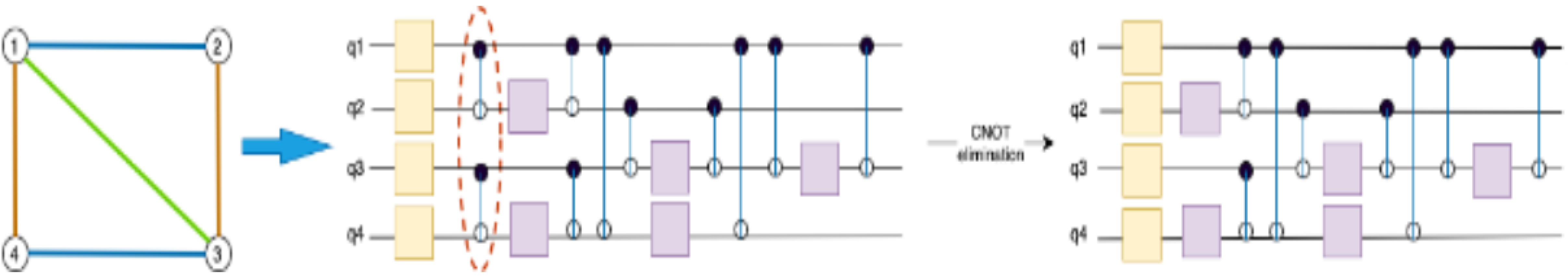
$$\lceil \frac{m}{\Delta + 1} \rceil \leq \# \, Optimized \; Edges \leq \lfloor \frac{n}{2} \rfloor.$$

The dominant color can be used at most on n/2 edges, where n= |V|.

03. EDGE COLORING BASED ANSATZ OPTIMIZATION

Edge Coloring based Ansatz Optimization

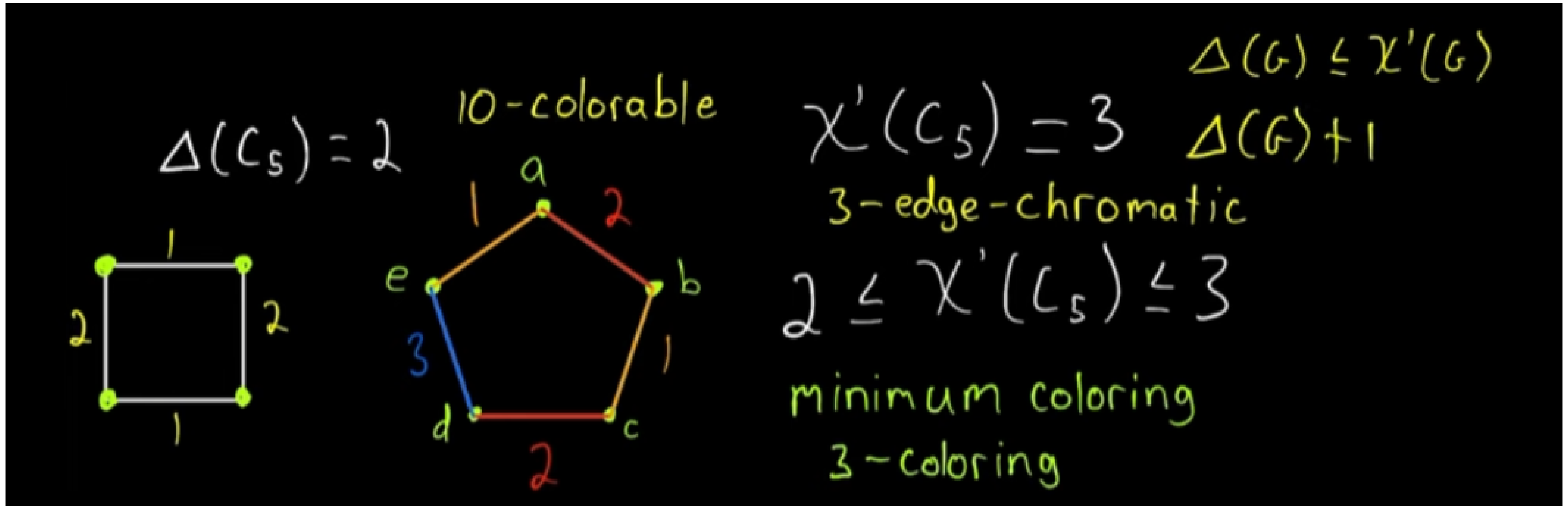


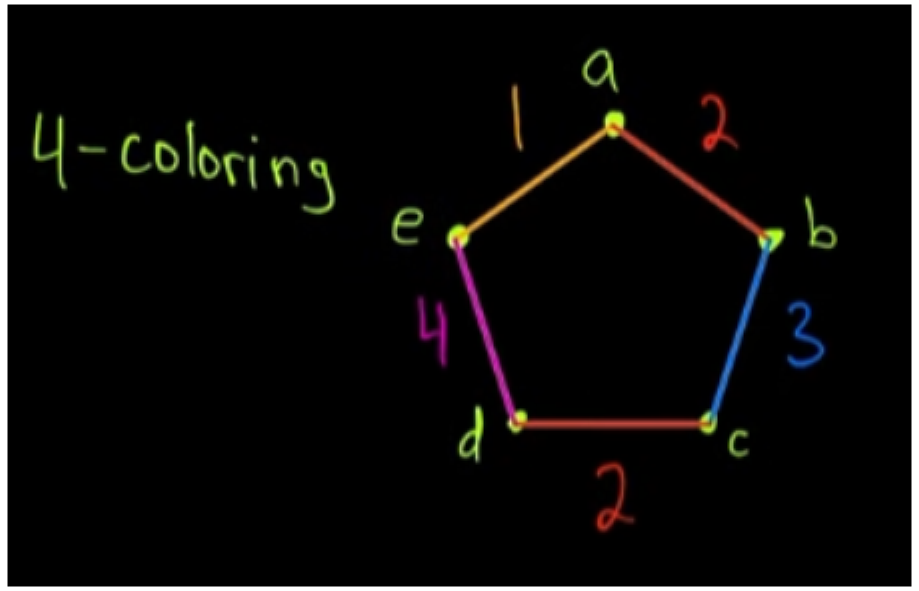


+ WHAT IS EDGE COLORING?

=> 그래프의 G의 엣지 컬러링은 G 엣지에 색상을 할당해 인접한 에지가 다르게 컬러링되도록 하는 것

=> 그래프의 가장자리를 색칠하는데 사용할 수 있는 최소 색상수는
색 지수 또는 가장자리 색 수
+ 짝수의 주기정도는 2, 홀수의 주기정도는 3 <= Δ + 1 최대 degree: Δ(G) + 1





=> 만약 k 색이 그래프 G를 색칠하기에 충분한다면, 그래프는 k 색이라고 합니다.
만약 k=x'(G)이면 G는 k-edge-chromatic.

=>Vizing's Theorem: Every no empty graph G, Δ(G) <= X'(G) <= Δ(G)+1

04. DEPTH FIRST SEARCH(DFS)

=> DFS based optimization procedure which can optimize n−1 edges.

A reduction in the number of CNOT gates by n−1.

Algorithm 2 DFS based Ansatz Optimization

Input: A graph $G = (V, E)$.
Output: A list E_{dfs} of $n-1$ edges.

1: $E_{dfs} = \{\}$
2: $u \leftarrow$ randomly selected vertex from V.
3: Start DFS from the vertex u. For every vertex v discovered from its predecessor v', $E_{dfs} = E_{dfs} \cup (v', v)$.
4: Return E_{dfs}.

DFS 트리의 모든 엣지 e = (u,v)에 대해 정점 u가 컨트롤이 되고 v는 해당 엣지에 해당하는 CNOT 게이트의 대상이 됨.

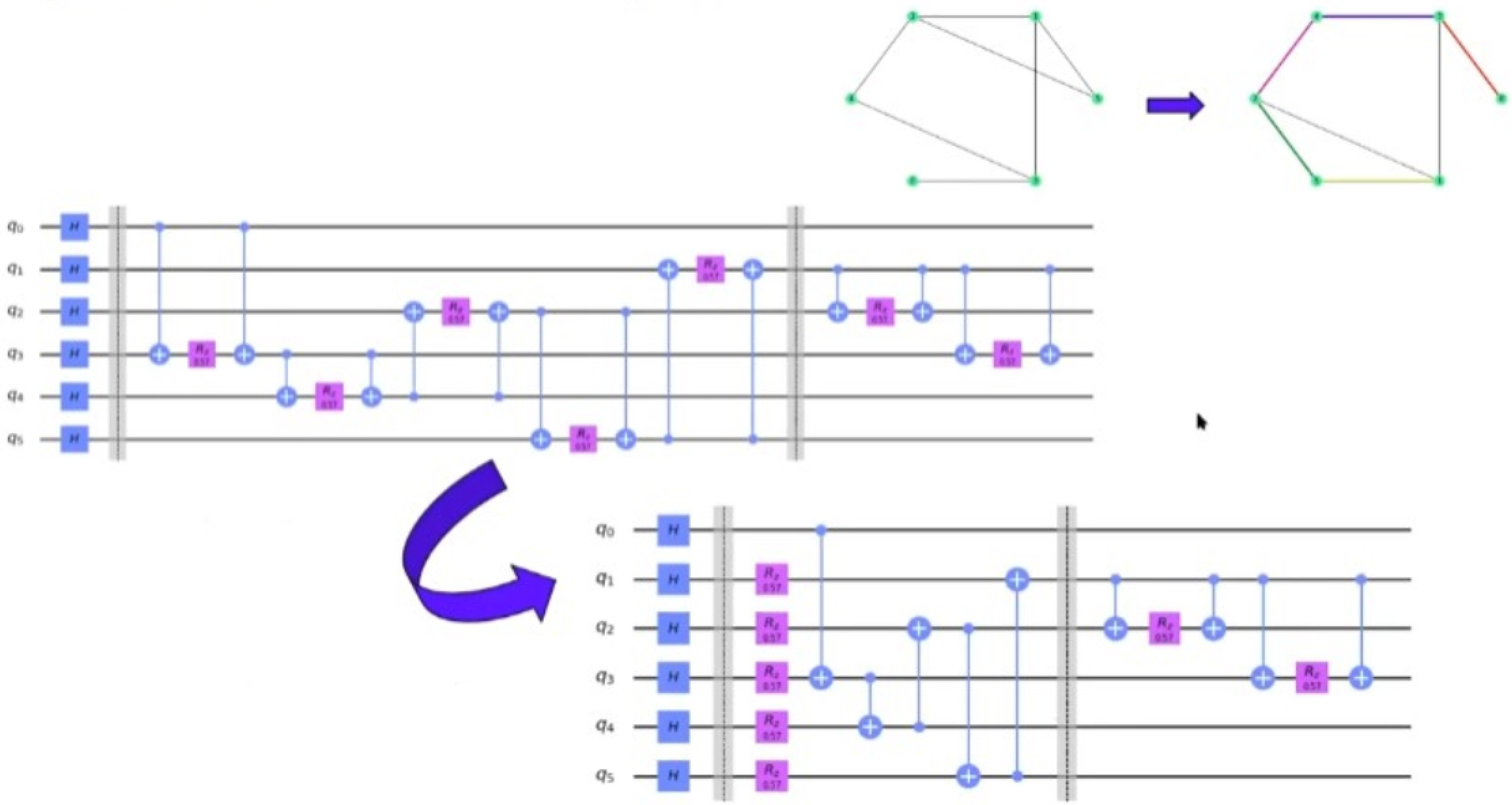
04. DEPTH FIRST SEARCH(DFS)

=> 최적화된 엣지 수는 DFS 방식이 최적

=> DFS는 회로의 깊이를 증가시킬 수 있음.

==> CNOT 게이트에서 최적의 감소를 가져오는 DFS의 단점은 회로의 깊이를 증가 시킴

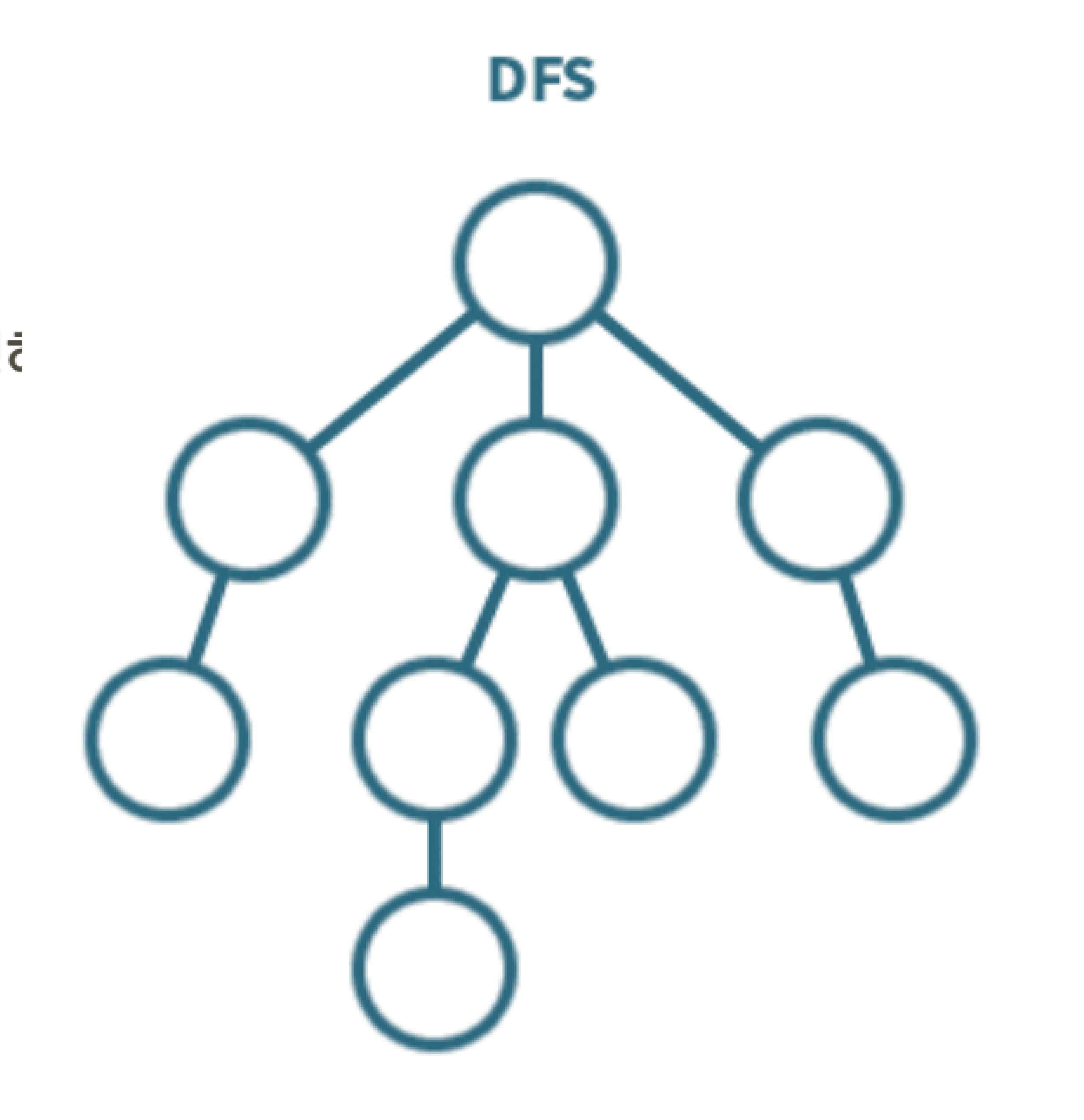
Depth First Search based Ansatz Optimization



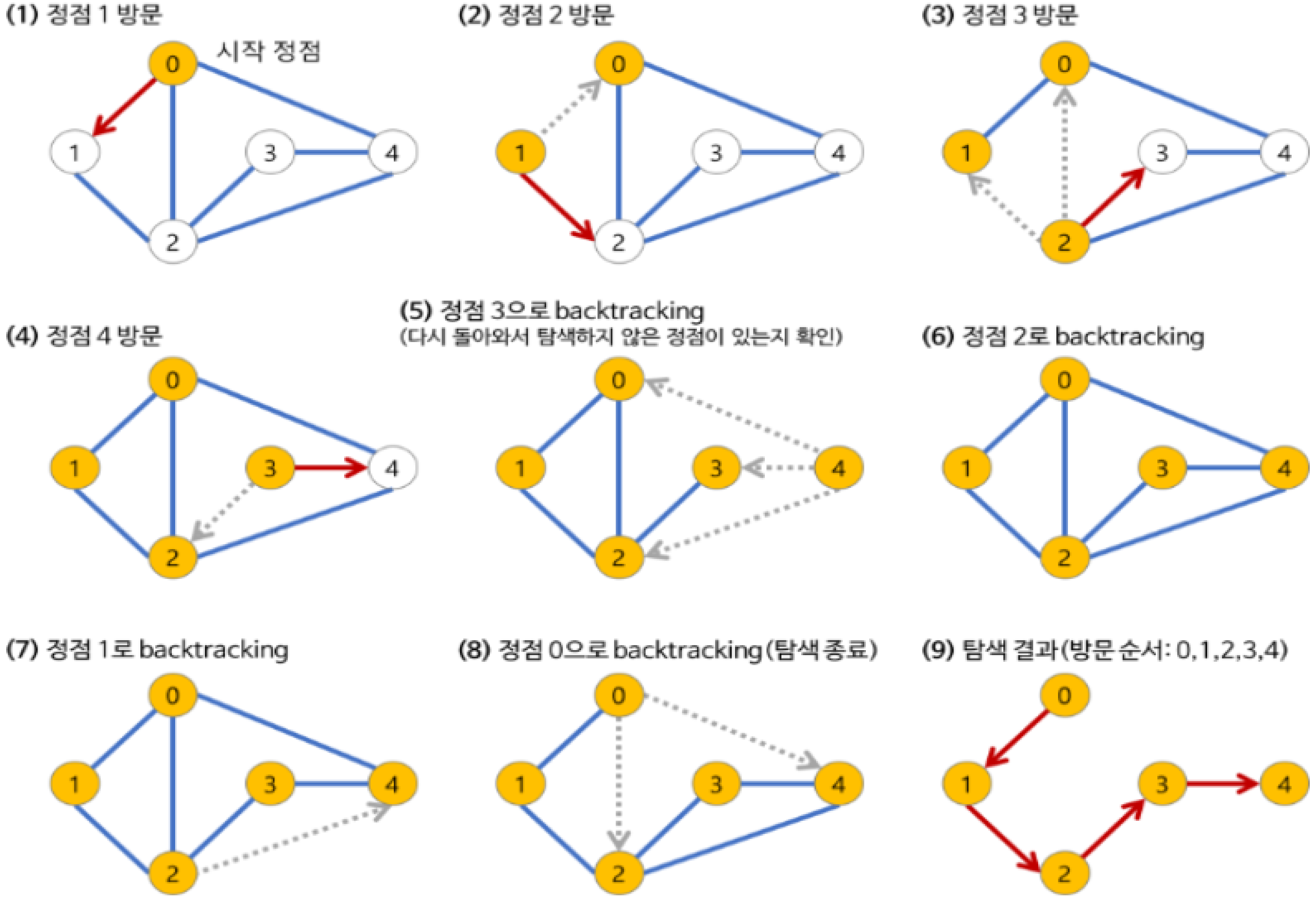
+ WHAT IS DFS?

=> 깊게 탐색하는 것
=> 사용하는 경우: 모든 노드를 방문하고자 하는 경우에 이 방법 선택

=> 탐색 시작 노드를 스택에 방문 처리 - 스택의 최상단 노드에 방문 X
- 인접한 노드가 하나라도 있아면 그 노드를 스택에 넣고 방문 처리
&방문하지 않은 인접 노드 없을시 스택에서 최상단 노드 꺼냄 - 더이상 2번 과정을 수행ㅎ
않을 때까지 반복
==> 기본 원리는 갈 수 있는 만큼 최대한 깊이가고, 더이상 갈곳이 없으면 이전 정점으로 돌아간다는 것



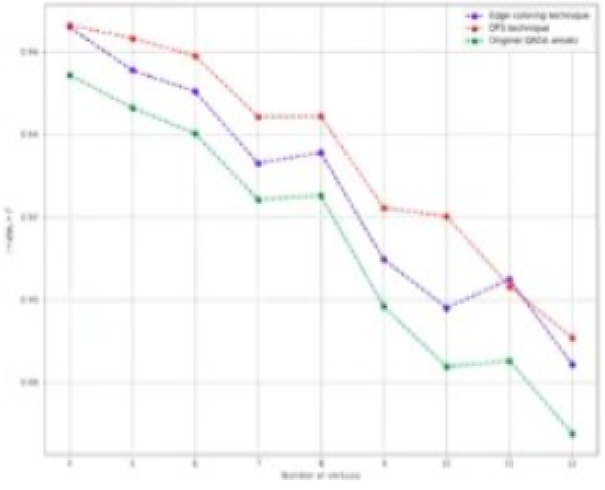
<DFS 탐색 과정>



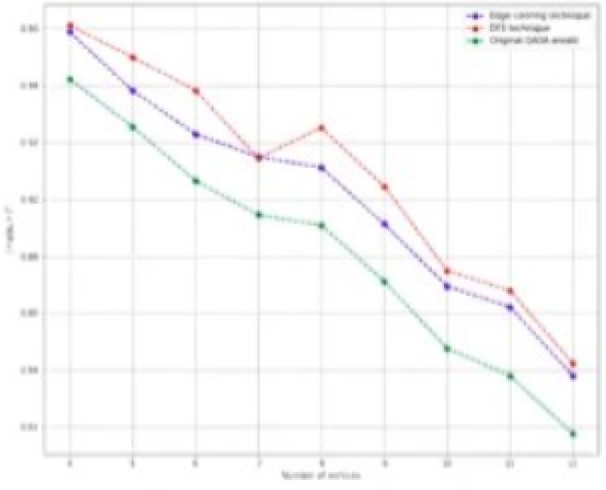
05 코드 구현

1. DFS
2. Edge coloring
3. Traditional QAOA

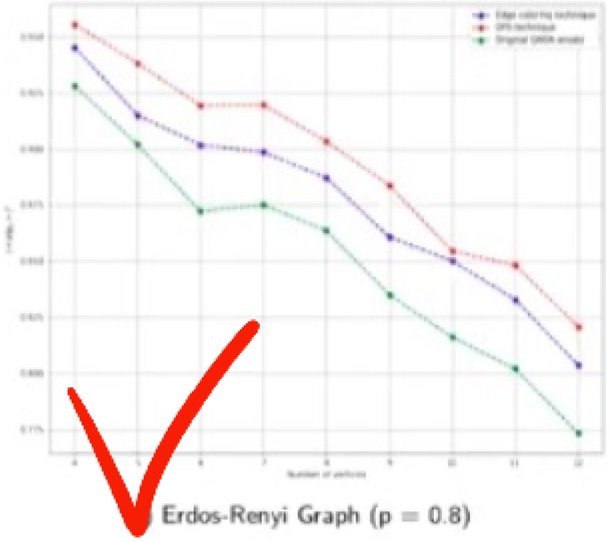
Lowering the probability of error



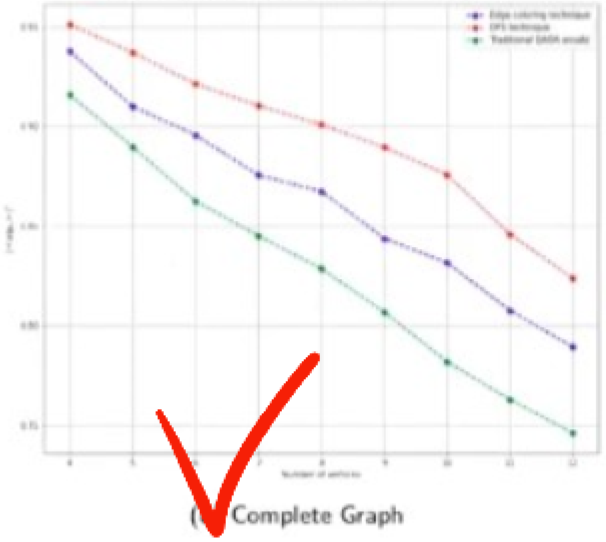
(a) Erdos-Renyi Graph (p = 0.4)



(b) Erdos-Renyi Graph (p = 0.6)



Erdos-Renyi Graph (p = 0.8)



(Complete Graph

<코드 구현>

1.CNOT 개수, 회로 깊이 개수 비교
2. Hellinger_fidelity로 회로 비교후 결과물 비교

<Hellinger_fidelity>
Computes the Hellinger fidelity between two counts distributions.
The fidelity is defined as 1-H where H is the Hellinger distance. This value is bounded in the range [0, 1].

=> returns: Fidlity

Erdos-Renyi Graph p=0.8일때
Complete Graph일 때
=> 그래프의 순대로 결과가 잘 나왔는지

Graph Family	# qubits	# CNOT gates in Max-Cut QAOA ansatz circuit		
		Traditional	Edge coloring	DFS
Complete graph	10	90	85	81
	20	380	370	361
	30	870	855	841
	40	1560	1540	1521
	50	2450	2425	2401
	60	3540	3510	3481
Erdos-Renyi (p_{edge} = 0.8)	10	70	66	61
	20	302	292	283
	30	698	683	669
	40	1216	1197	1177
	50	1956	1931	1907
	60	2822	2792	2763
Erdos-Renyi (p_{edge} = 0.6)	10	50	46	41
	20	234	225	215
	30	504	491	475
	40	960	940	921
	50	1504	1479	1455
	60	2114	2085	2055
Erdos-Renyi (p_{edge} = 0.4)	10	36	31	27
	20	164	154	145
	30	362	348	333
	40	586	566	547
	50	950	925	901
	60	1468	1440	1409

<Qubit 기준으로 계산>

Edge coloring: n/2 만큼 감소
DFS: n-1 만큼 감소

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양자 근사 최적화 알고리즘을 사용한 자원 할당 기법
Pennylane, QAOA for max-cut

https://youtu.be/3MWbGkjMu-w?feature=shared
https://www.techiedelight.com/ko/greedy-coloring-graph/
https://excelsior-cjh.tistory.com/197
https://www.qmunity.tech/tutorials/quantum-approximate-optimization-algorithm-maxcut
https://gmlwjd9405.github.io/2018/08/14/algorithm-dfs.html
https://currygamedev.tistory.com/10
https://www.youtube.com/watch?v=X2B_J1ajsIY

THANK YOU

덕성여자대학교 김민지