Pasqal Defining the quantum reality

Q-KHAI Quantum Simulation

Part 3:
- 조합최적화: MIS, QUBO
- 양자 머신러닝: Quantum Evolution Kernel

Woojun Lee, Ph. D.
Technical Business Developer, Pasqal
Aug. 4, 2025

Contents

Pasqal

Part 1 (3, Mon) 1:30 pm

- 양자컴퓨팅 소개
- 중성원자 양자컴퓨터
- Pasqal 소프트웨어 스택
- Pulser Studio 실습

Part 2 (3, Mon) 2:30 pm

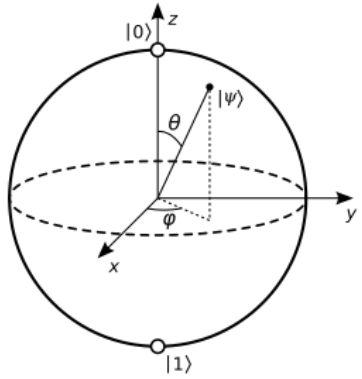
- 중성원자 양자 시뮬레이션 (Spin sytems, AFM states, Direct quantum simulation)
- 실습 (Pulser, 양자시뮬레이션)

Part 3 (4, Tue) 9 am

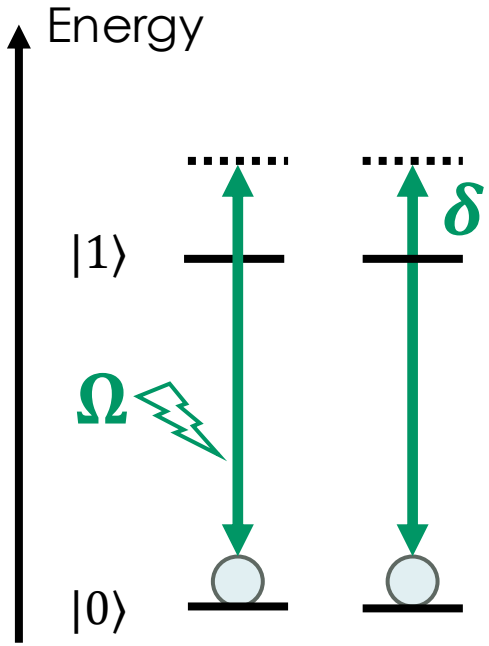
- MIS, QUBO theory, use cases, sdk
- QEK theory, use cases, sdk
- 실습 (QUBO, QEK)

Review: Hamiltonian and time evolution

Pasqal



Neutral atom system Hamiltonian



$$\hat{\mathcal{H}} = \hbar \sum_{i=1}^{N} \left(\frac{\Omega}{2} \hat{\sigma}_i^x - \delta\, \hat{n}_i \right) + \sum_{i<j} \frac{C_6}{|\mathbf{r}_i - \mathbf{r}_j|^6} \hat{n}_i \hat{n}_j$$

X-rotation | Z-rotation | Interaction

Ω: Rabi frequency (~ laser amplitude)

$\hat{n}_i$: 0=ground, 1=excited

δ: Detuning (~ laser frequency offset)

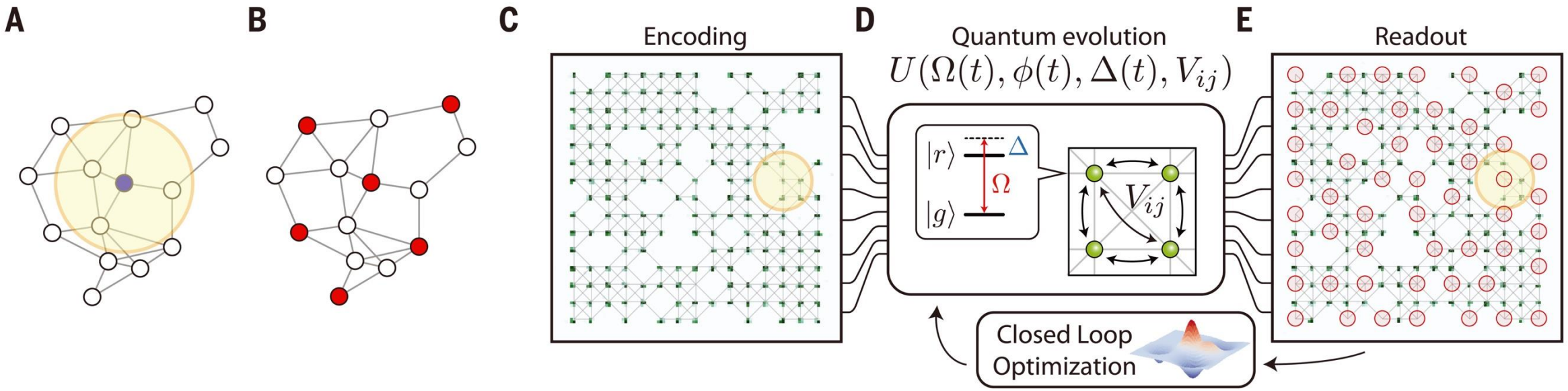
Maximum independent set (MIS) problem

Pasqal

Maximal independent set: subset of a graph with **no neighboring nodes**

Maximum independent set: **maximal indep. set with most number of nodes**

An **NP-hard** combinatorial optimization problem



S. Ebadi et al. (2022)

Pasqal Defining the quantum reality

Mission planning for Satellites

Quantum computing for earth observation

In collaboration with:

GENCI Le calcul intensif au service de la connaissance

THALES Building a future we can all trust

esa European Space Agency

Combinatorial optimization for satellites

Pasqal

Problem Introduction

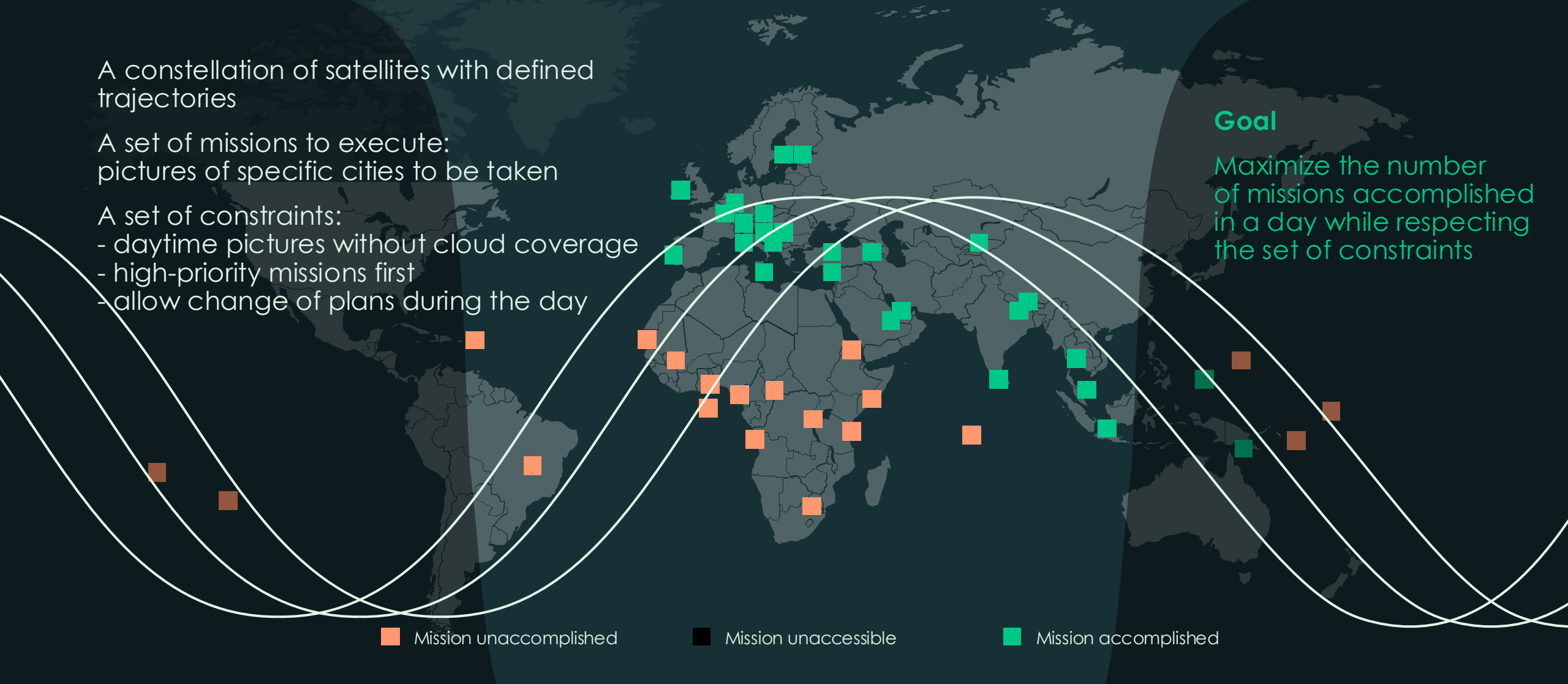
A constellation of satellites with defined trajectories

A set of missions to execute:
pictures of specific cities to be taken

A set of constraints:
- daytime pictures without cloud coverage
- high-priority missions first
- allow change of plans during the day

Goal

Maximize the number of missions accomplished in a day while respecting the set of constraints



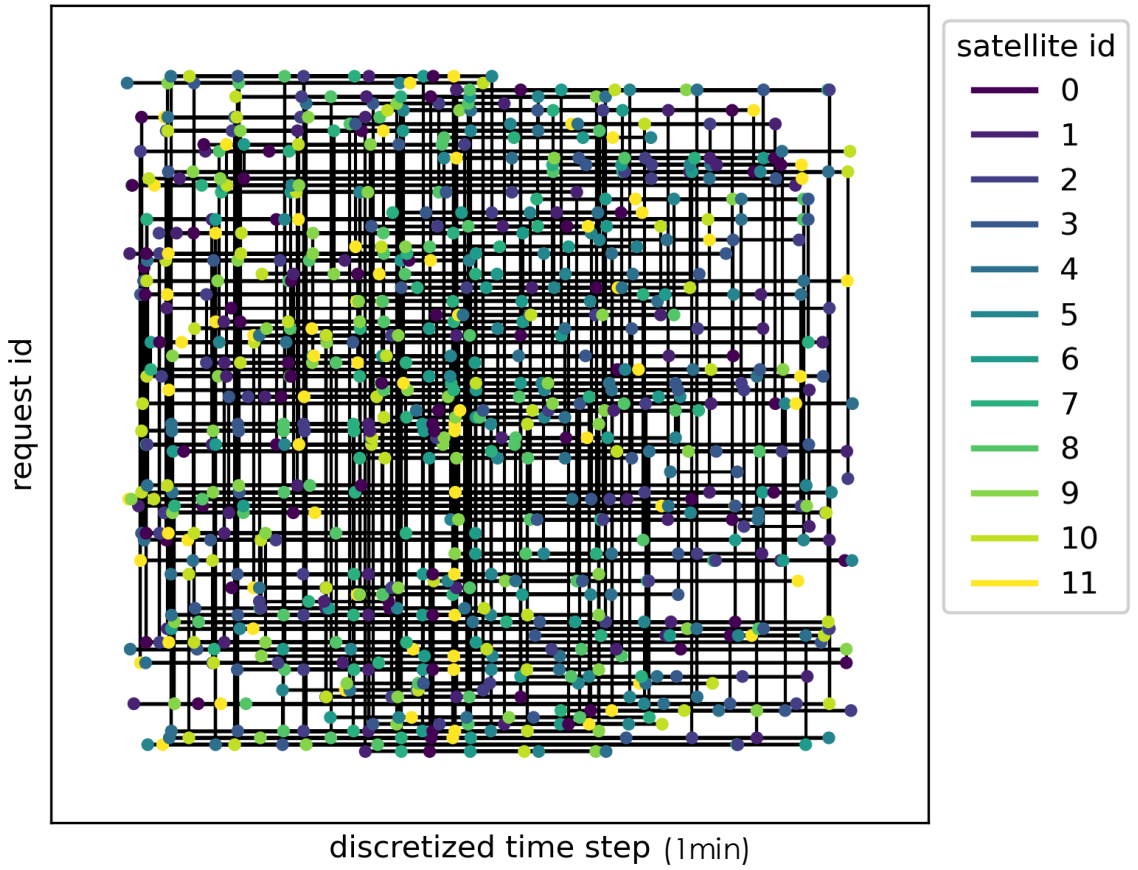
Encoding the problem in a Graph Structure

Pasqal

- Nodes are equivalent to mission slots
- Colors represent unique satellites of the c onstellation
- Edges are equivalent to incompatibilities of constrains
    1. Each request performed only once
    2. No overlapping time slots per satelli te

- To retrieve the solution we apply a Maximum Independent Set graph methodology [1,2]

Visiting capitals with 12 shifted ISS



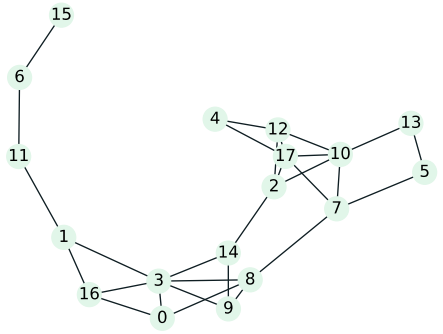
[1] D. Eddy et al. (2021)
[2] S. Ebadi et al. (2022)

Adiabatic state preparation of MIS configurations

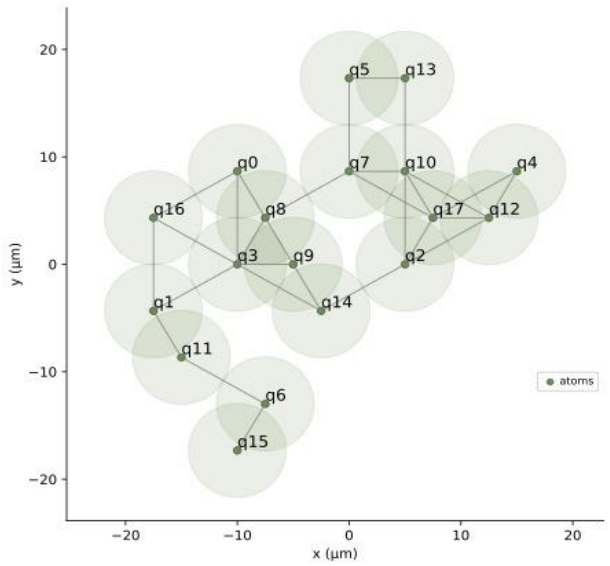
Pasqal

Maximum Independent Set (MIS) is a well-suited problem for Rydberg atoms

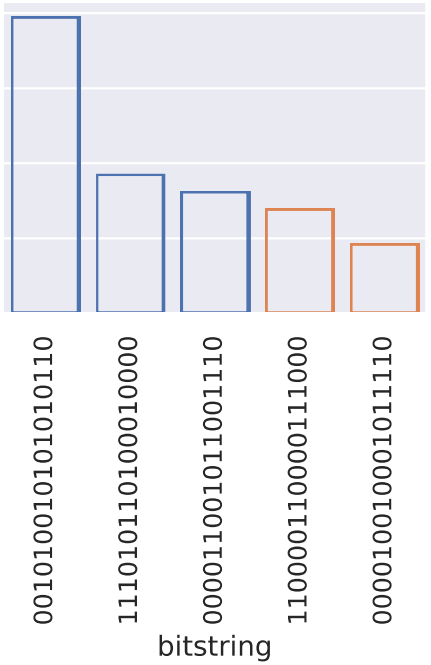
Original Graph



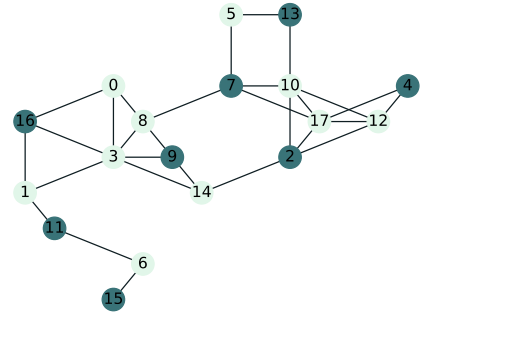
Embedding State preparation



Result Distribution



Maximum Independent Set



Quadratic unconstrained binary optimization (QUBO)

Pasqal

For a real matrix Q, find a binary vector $\boldsymbol{x}$ ($x_i \in \{0,1\}$) that minimizes $f_Q(\boldsymbol{x})$.

$$f_{\boldsymbol{Q}}(\boldsymbol{x}) = \boldsymbol{x}^{\mathsf{T}}\boldsymbol{Q}\boldsymbol{x} = \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{ij}x_i x_j.$$

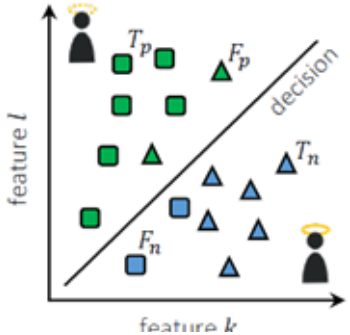
example of matrix Q

```
[-10.0, 19.7365809, 19.7365809, 5.42015853, 5.42015853],
[19.7365809, -10.0, 20.67626392, 0.17675796, 0.85604541],
[19.7365809, 20.67626392, -10.0, 0.85604541, 0.17675796],
[5.42015853, 0.17675796, 0.85604541, -10.0, 0.32306662],
[5.42015853, 0.85604541, 0.17675796, 0.32306662, -10.0],
```

Fallen Angel forecast (financial risk)

Pasqal

Will this company repay dept?

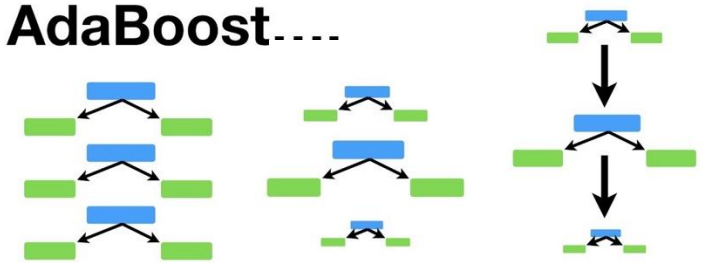


Decision = ML trained classifier

Data labels:

No Fallen Angel

Fallen Angel



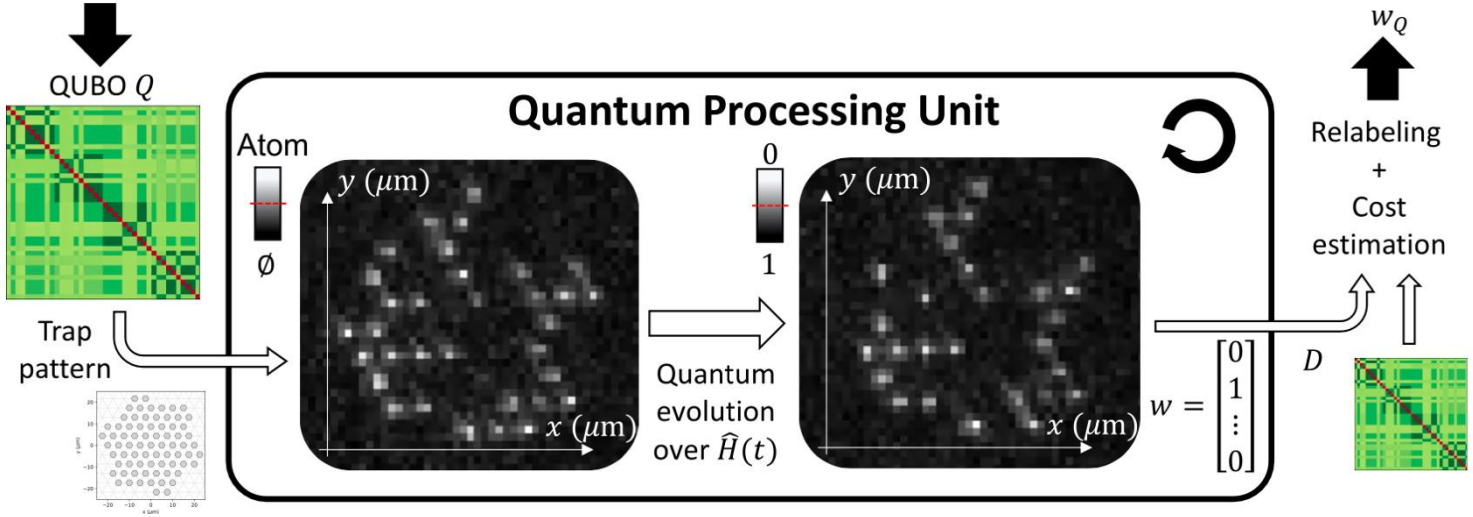
Weak learners $h_i(\vec{x}_s) \in \{-1,1\}$

- Strong classifier C (final decision)

$$C(\vec{x}) = \mathrm{sgn}\left(\frac{1}{N}\sum_{i}^{N} w_i^{\mathrm{opt}} h_i(\vec{x}) - T\right), \quad w_i \in \{0,1\}$$

Finding w_i^{opt} can be reformulated as a QUBO problem, so a QPU can efficiently solve.

$$\mathcal{H}_Q(w) = w^T Q w = \sum_{i,j}^{N} Q_{ij} w_i w_j, \quad Q_{ij} = \begin{cases} \mathrm{Corr}(h_i, h_j) & \text{if } i \neq j \\ \frac{S}{N^2} + \lambda - 2\mathrm{Corr}(h_i, y) & \text{otherwise.} \end{cases}$$



L. Leclerc *et al.* (2022)

StatQuest with Josh Starmer (2019) "AdaBoost, Clearly Explained" YouTube

QUBO use cases

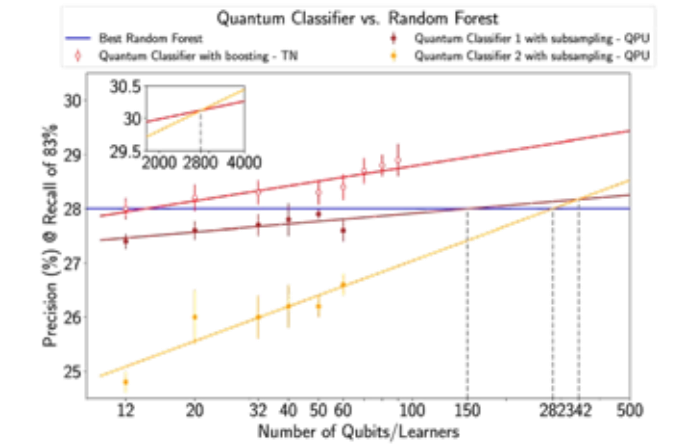
Pasqal

Finance

💳 Risk Management

Objective: Predicting "Fallen Angels" -credit rating downgrades- for early risk insights at **Crédit Agricole CIB**.

Metric	Classical	Quantum
# Trees	1200	**50**
Runtime	> 3 Hours	**50 Mins**

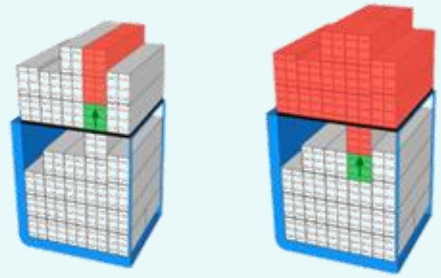


Logistics

🚢 Container Stowage

Objective: Optimally assign container slots during vessel loading to reduce berth time and fuel consumption.

- Minimize **Restows** & Port Time.
- Optimize **Stability** & Balance.
- Ensure **Damage Prevention**.



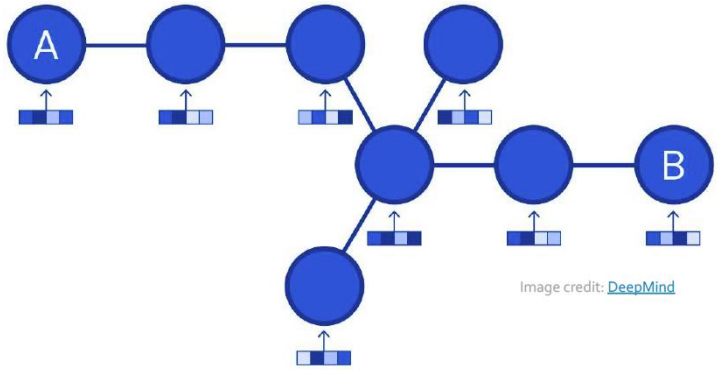
Sources: L. Leclerc et al. (2023) / Pasqal's project

Graph machine learning

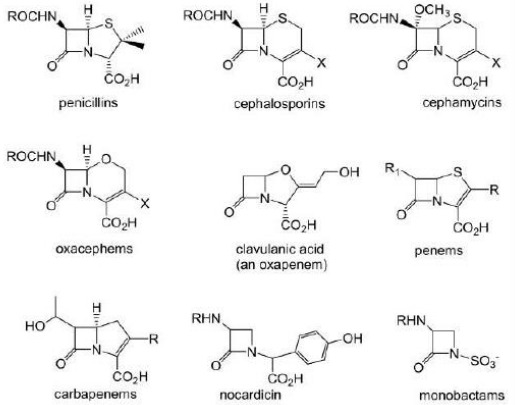
Pasqal

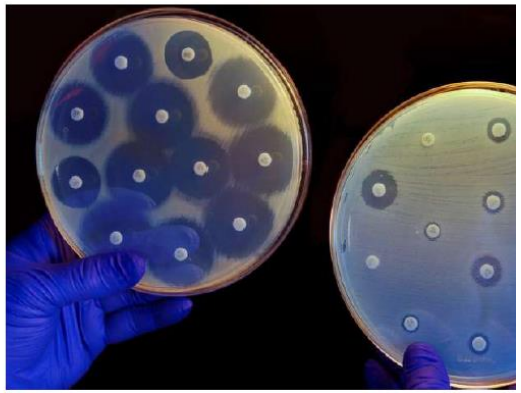
Traffic prediction

- **Nodes:** Road segments
- **Edges:** Connectivity between road segments



- **Antibiotics are small molecular graphs**
  - **Nodes:** Atoms
  - **Edges:** Chemical bonds

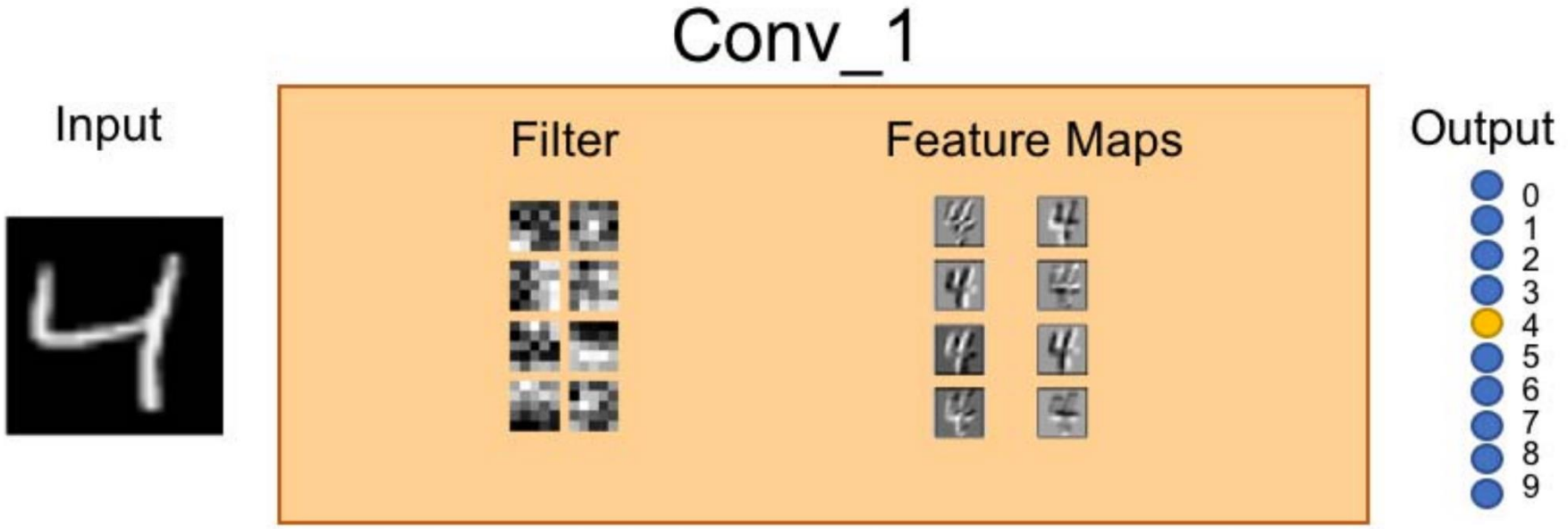




Yeeun Jang, "1. Machine Learning for Graphs" [Blog], GNN Tobigs, 25 Jul. 2021, https://velog.io/@tobigsgnn1415/Machine-Learning-for-Graphs

Feature maps in machine learning

Pasqal



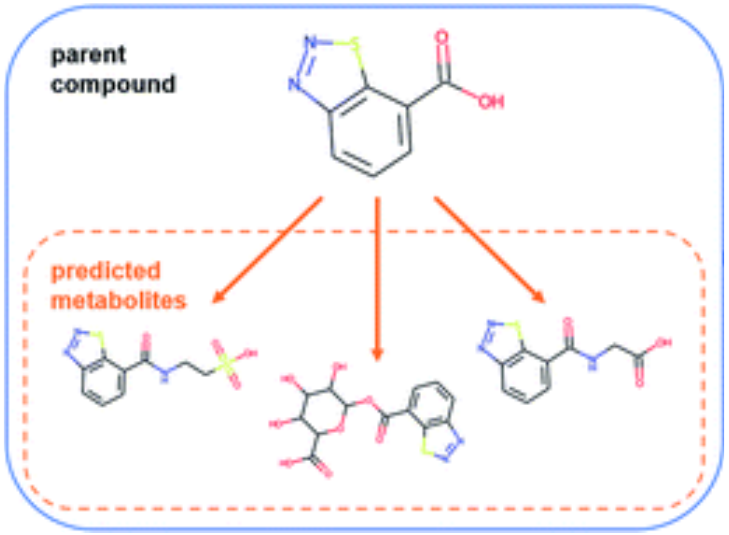
N. Meissler et al. *IEEE AIVR* (2019)

- Create kernel maps by filtering with filters (kernels)
- Classify the image using kernels

Toxicity prediction of molecules

Pasqal

Toxicity prediction through computational methods is crucial to help accelerate the identification of harmful substances, lowering costs significantly and reducing animal testing.



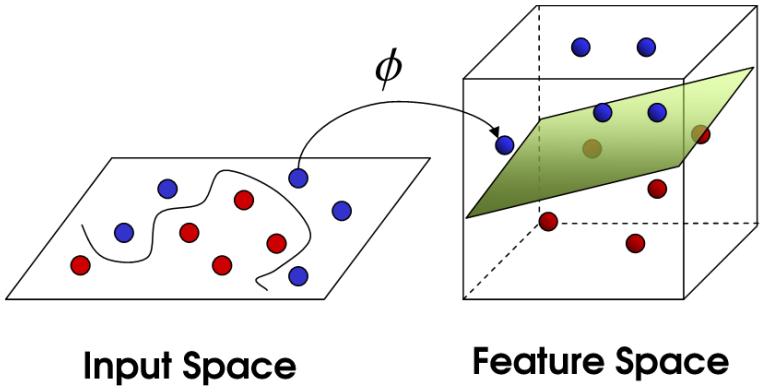
Objective:
tackle a binary classification task on a standard bio-chemistry data set

B. Albrecht et al. (2022)

Graph machine learning: Quantum Evolution Kernel (**QEK**)

Pasqal

Support Vector Machine (SVM) for classification



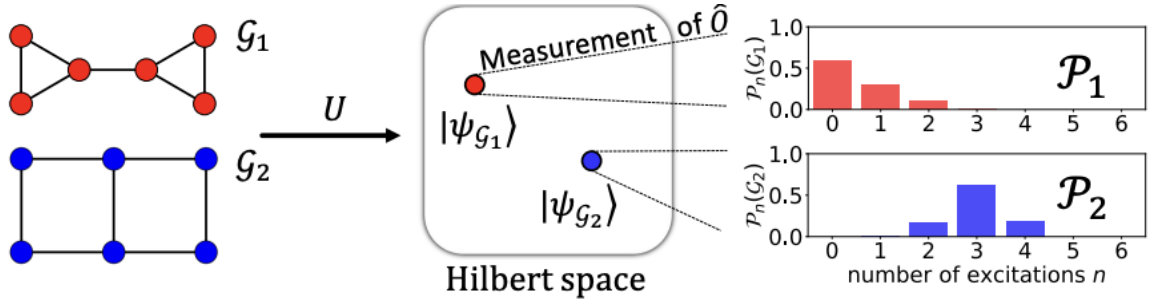
Kernel method $K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \phi(\boldsymbol{x}_i) \cdot \phi(\boldsymbol{x}_j)$

Some examples of (classical) kernels

- Polynomial (homogeneous): $k(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i \cdot \mathbf{x}_j)^d$
- Gaussian radial basis function: $k(\mathbf{x}_i, \mathbf{x}_j)$

$$= \exp\left(-\gamma \|\mathbf{x}_i - \mathbf{x}_j\|^2\right) \text{ for } \gamma > 0$$

Quantum kernel



$$K(\mathcal{G}, \mathcal{G}') = \exp[-\mu\, JS(\mathcal{P}_1, \mathcal{P}_2)]$$

(JS: Jansen-Shannon divergence)

B. Albrecht *et al.* (2023)

Quantum Evolution Kernel

Pasqal

With the right positioning of the atoms, and a reasonable approximation, this process encodes a graph.

Example of encoding: $\mathcal{P} = (p_1, \ldots p_{|\mathcal{G}|})$

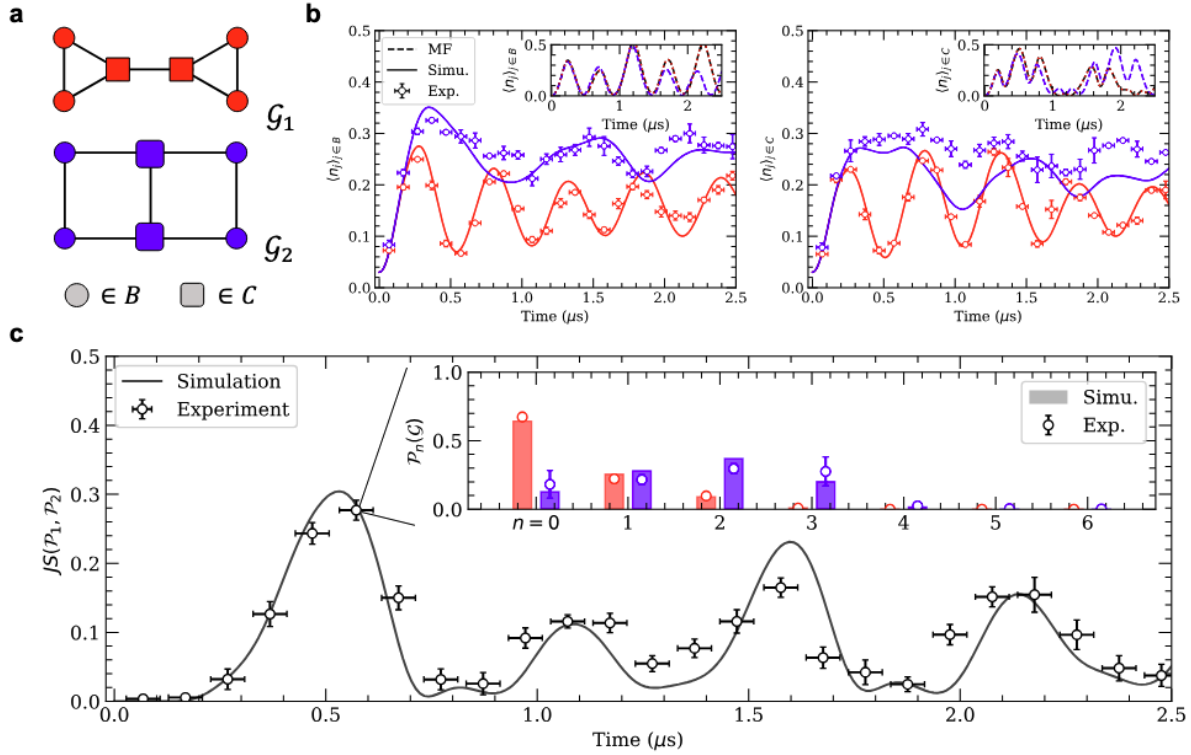
Histogram of graph

Jansen-Shannon divergence
(~distance in feature space)

$$JS(\mathcal{P}_1, \mathcal{P}_2) = H\left(\frac{\mathcal{P}_1 + \mathcal{P}_2}{2}\right) - \frac{H(\mathcal{P}_1) + H(\mathcal{P}_2)}{2}$$

where $H(\mathcal{P}) = -\sum_k p_k \log p_k$

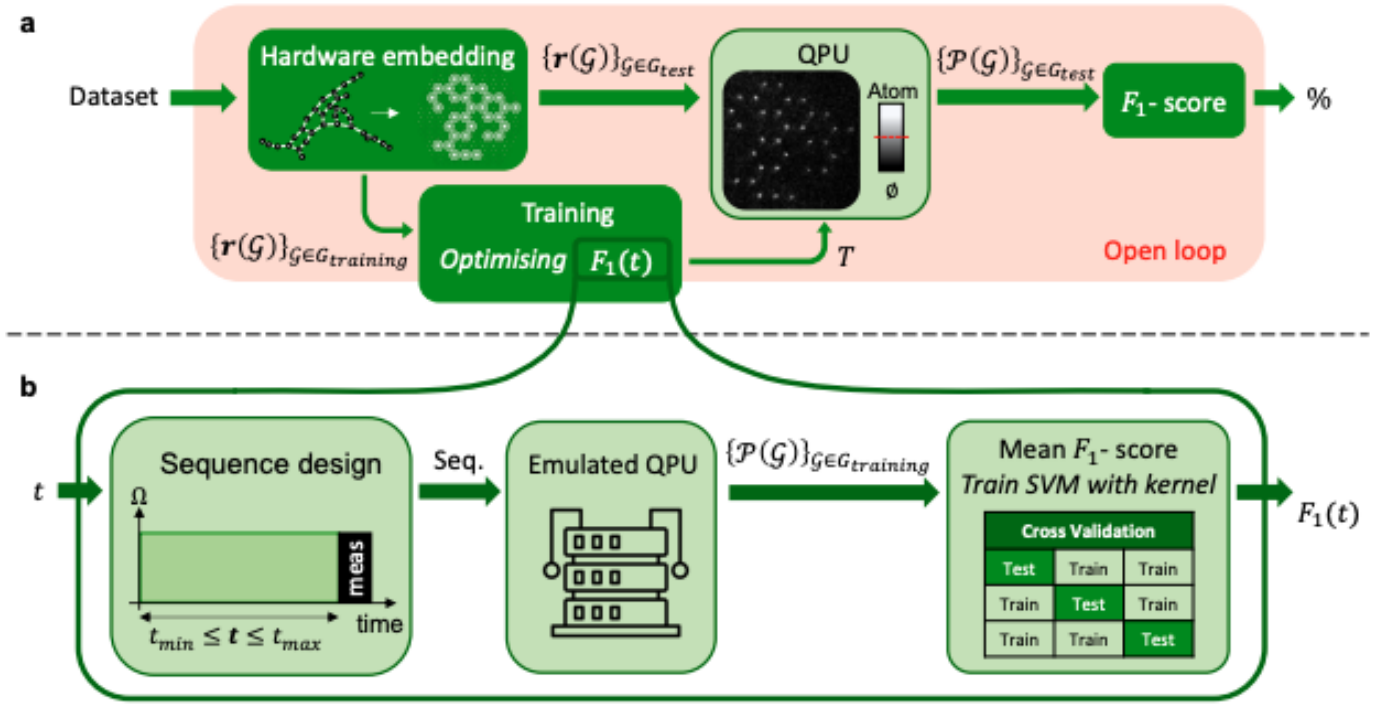
Shannon entropy



Quantum Evolution Kernel: $K(\mathcal{G}, \mathcal{G}') = \exp[-\mu\, JS(\mathcal{P}, \mathcal{P}')]$

Quantum Evolution Kernel

Pasqal



Kernel	F_1-score (%)
QEK	60.4 ± 5.1
QEK (size-compensated)	45.1 ± 3.7
SVM-ϑ	58.2 ± 5.5
Size	56.7 ± 5.6
Graphlet Sampling	56.9 ± 5.0
Random Walk	55.1 ± 6.9
Shortest Path	49.8 ± 6.0

F1-score reached experimentally on the PTC-FM (Predictive Toxicology Challenge) dataset

The optimization of the score function F1

- t, taken from the parameter space $[t_{min}, t_{max}]$ defines a laser sequence with Ω and δ fixed parameters followed by a measurement.

- QEK method shows competitive with standard classical kernels on PTC-FM dataset,
- and superior performance for some artificial dataset for exploiting the Hilbert (quantum) space

Pasqal

Other use cases

Telecom: Designing cellular networks in Paris

Pasqal

Context

Telecom operators are looking to optimize the distribution of wireless antennas and allocation of frequencies

Objective:
To save costs, minimize the no. of antennas and no. of frequencies used

Problem Definition

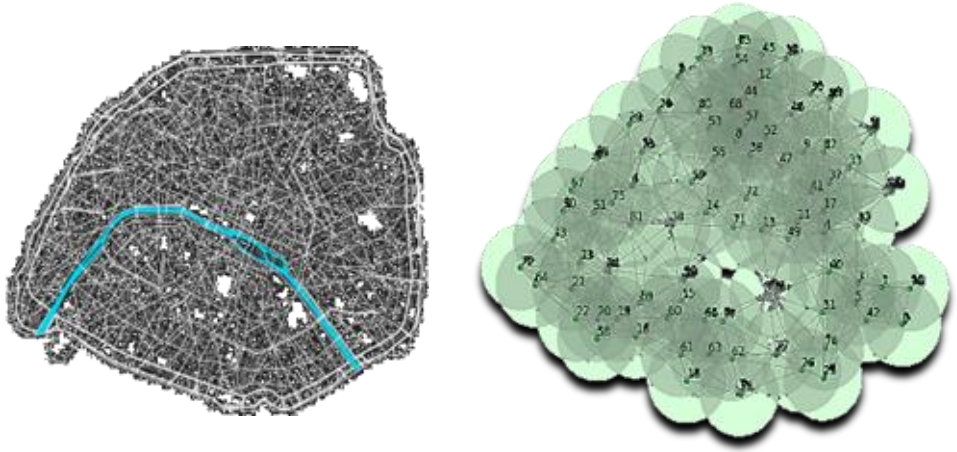
Combinatorial optimization problem: many possible combinations of no. antennas, distances in between, and frequencies

Each antenna is a vertex on a graph, vertices are connected if below a threshold distance or signals interfere, nodes are coloured for each frequency

Then, find minimum no. of independent sets with minimum no. of colours

Quantum solution

The novel hybrid algorithm called the *Quantum Graph Coloring method* was applied to the use case of assigning frequencies to 80 antennas for 5G networkin the centre of Paris and executed on Pasqal's quantum emulators



(1) Map of Paris and (2) Graph with antenna distribution

Source: https://journals.aps.org/pra/abstract/10.1103/PhysRevA.107.032426

Energy: Scheduling of Electric Vehicle (EV) charging with EDF

Pasqal x EDF

Context

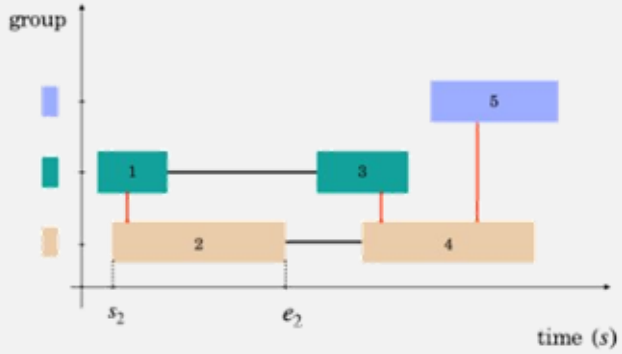
Charging of EVs presents both challenges and opportunities for grid electricity management

Objective:
Minimize the time of a number of charges, while no group (representing e.g. a vehicle fleet) is over-represented in the schedule

Problem definition

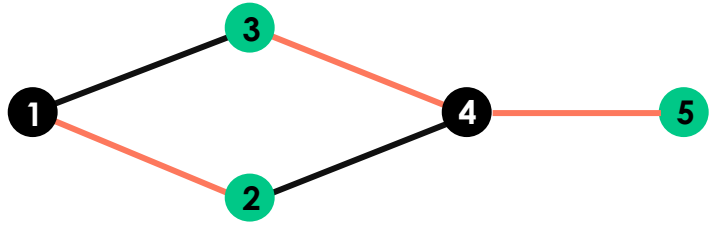
From a dataset of **2250 load tasks**, performed May '17 in Paris, randomly **N loads** were selected and grouped using a **uniform distribution**.

To embed this in **graphs**, nodes were assigned to each load (e.g. 1-5 below) and two nodes were connected by edges when either they belonged to the same group or their intervals overlapped (e.g. black/red lines).



Quantum solution

Reaching the objective equals finding the **Maximum Independent Sets (MIS)** of the graphs (e.g. nodes 2,3,5)



A so-called **quantum annealing algorithm** was proposed to solve this and implemented on a Pasqal QPU with **100 qubits**, allowing for graphs up to size 100.

Result: **an approximation ratio* of >98% with a strong diversity of solutions**

This diversity can be leveraged in hybrid classical/ quantum approaches for **1000 qubit** system size that promise energy performance gains vs. classical [1].

Pasqal achieved 1000 trapped atom in 2024.

*A measure of how close the solutions are to the optimal one

[1] Da Silva Coelho et al., Physical Review A 107.3 (2023): 032426
Source: Qualifying quantum approaches for hard industrial optimization problems, C. Dalyac et al
Implementing transferable annealing protocols for combinatorial optimisation, C. Dalyac et al

Pharma: Locating water molecules in proteins to aid drug design

Pasqal x Qubit Pharmaceuticals

Context

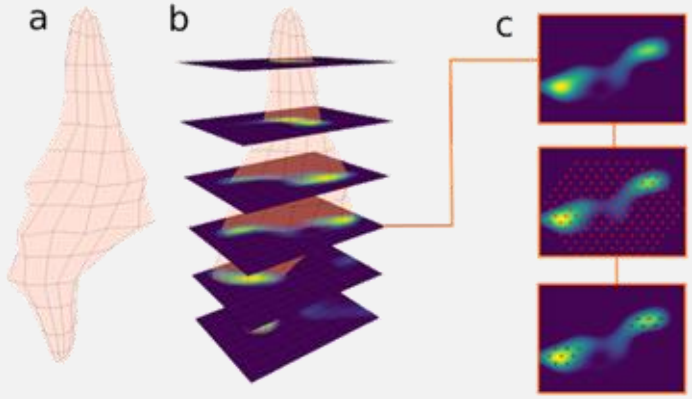
In medicine design, the presence of water molecules in cavities of harmful proteins can affect dramatically the binding strength of a drug

Objective:
Finding the number and location of water molecules in a specific protein's cavities

Classical methods

Molecular dynamics or Monte Carlo simulations provide accurate predictions but are time consuming and thus costly

A faster method called 3D-RISM* only delivers a probability distribution of water densities in a protein cavity

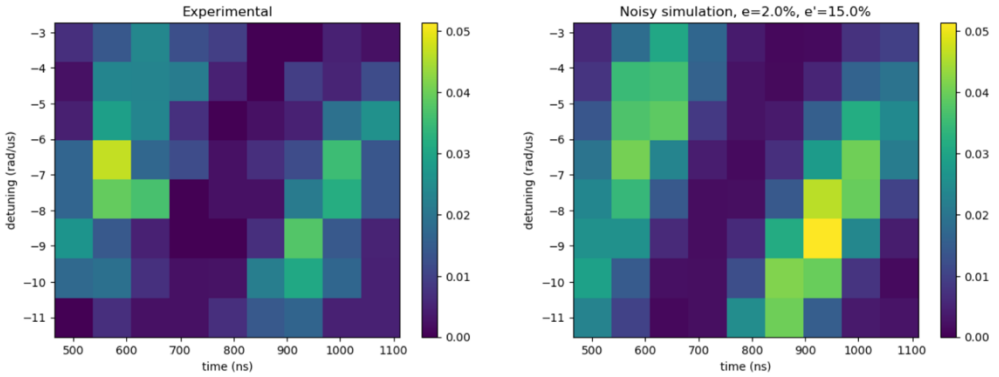


3D-RISM example result (a), sliced to 2D water density maps (b) and mapped to qubit registers (c)

Quantum solution

The result from a 3D-RISM simulation was used as an initial input for a quantum algorithm that can find the exact positions of the water molecules (centre figure)

Next, this algorithm was implemented on the Pasqal quantum simulator and tasked to minimize the difference between this guess, i.e. the water density distribution, and the quantum solution, i.e. the expected locations of the water molecules. Finally, it was checked to match experiments (below figure)



*3D-RISM = 3D-Reference Interaction Site Model
Source: Leveraging Analog Quantum Computing with Neutral Atoms for Solvent Configuration Prediction in Drug Discovery, M. D'Arcangelo et al, https://doi.org/10.1103/PhysRevResearch.6.043020

Structure-Activity

Pasqal

Efficient molecular similarity screening to determine structure-activity relationships like molecular toxicity or solubility

Industry relevance

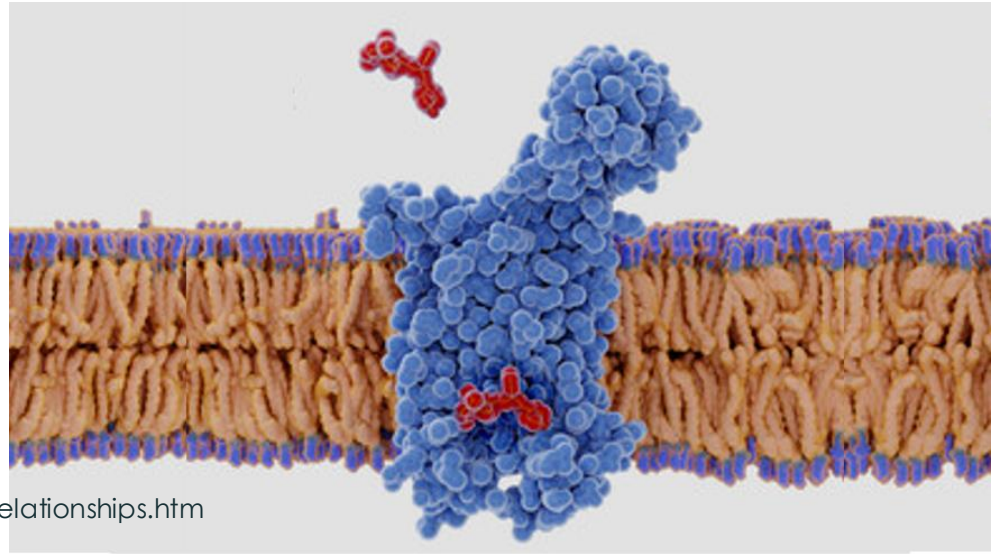
- Structure-Activity Relationship (SAR) analysis aims to find relationships between chemical structure and biological activity (e.g. solubility, toxicity) of molecules[1]
- SAR are derived from experimental data and their applicability can be broadened by assuming that similar molecular structures have similar activity[1]

Quantum solution

- PASQAL has developed a unique quantum kernel method to study graph similarity[2] and has tested this method on the SAR type problem of toxicity screening[3]
- Such graph kernel methods, implemented through the analog mode of PASQAL's quantum processors, are a prime candidate for quantum advantage as early as 2024

Computational challenge

- Existing SAR databases can be used to predict the activity of similar molecules, which requires an efficient method to compare the similarity of molecules
- Molecules are equal if their molecular graphs are isomorphic and the labels of the atoms and bonds are equal



1: https://www.oecd.org/chemicalsafety/risk-assessment/introductiontoquantitativestructureactivityrelationships.htm
2: DOI:10.1103/PhysRevA.104.032416
3: https://pasqal.io/2022/04/11/towards-quantum-advantage-with-efficient-graph-implementations/

Catalyst Design

Pasqal

Designing new catalysis for renewable energy feedstocks and green chemistry, through analysing and optimizing complex reaction pathways

Industry relevance

- Over 90% of industrial chemistry processes involve catalysts and transitioning to renewable (energy) feedstocks and green chemistry requires new generations of catalysts[1]

Computational challenge

- Because of the high dimensionality of the chemical PES[3], an exhaustive exploration of all possible pathways is generally unfeasible
- Alternatively, reaction networks[2], formulated as graph structures, can be solved with modern graph theoretical methods[4]. However these methods can become intractable at industry-relevant complexity

Quantum solution

- PASQAL's unique and proprietary quantum graph kernel learning methods[5] promises more accurate and faster solutions using highly efficient and feature-rich quantum kernels
- Such graph kernel methods, implemented through the analog mode of PASQAL's quantum processors, are a prime candidate for quantum advantage as early as 2025

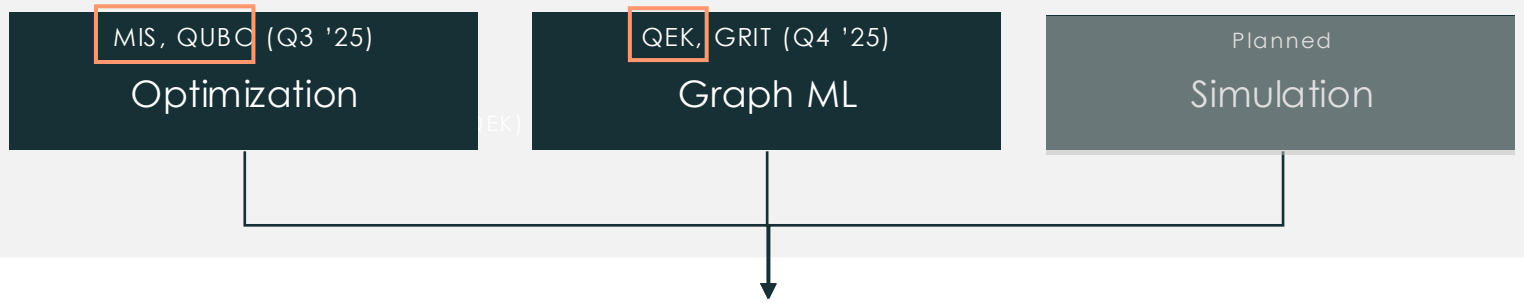
1: doi.org/10.1021/acs.jpca.8b10007;
2: reaction networks: reactants > intermediates > products
3: PES = potential energy surface;
4: for instance: https://doi.org/10.1039/C7SC03628K;
5: DOI:10.1103/PhysRevA.104.032416;
6: DOI:10.3389/fctls.2021.658965
7: for instance: DOI:10.1146/annurev-chembioeng-062011-081108 and DOI:10.1126/science.1106435

Software – an end-to-end stack to deliver solutions to users

Pasqal

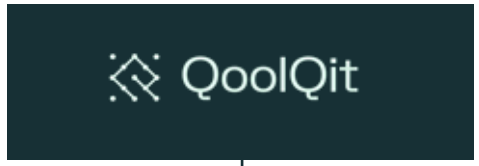
Quantum Applications

Ready-to-use quantum algorithms, designed to address specific computational challenges



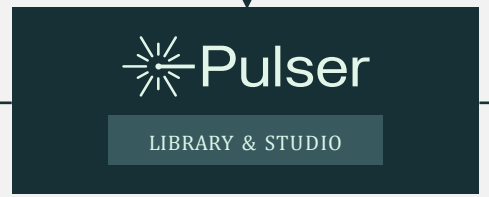
Quantum SDK

Create custom quantum applications with our intuitive, open-source SDK that simplifies algorithm development or use your favorite external SDK



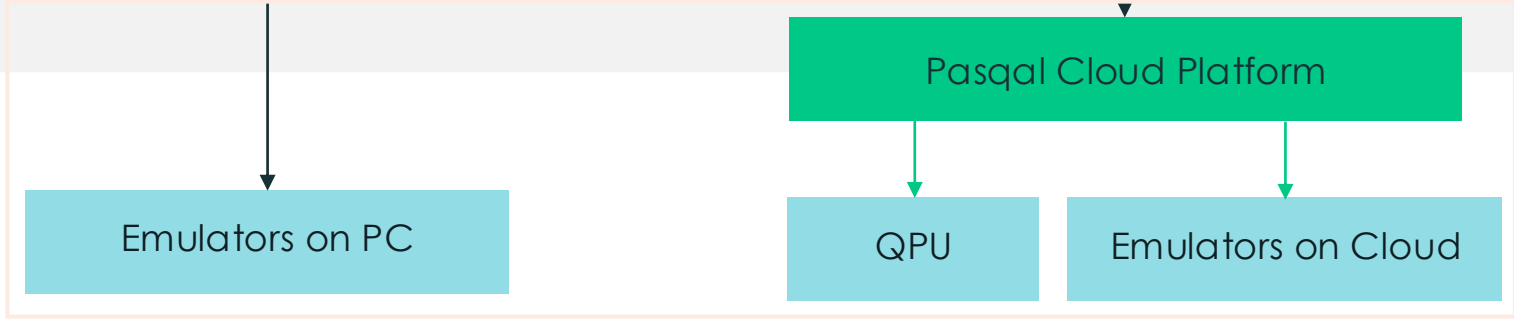
Neutral Atom Programming

Pulser (and Pulser Studio) provide a flexible ecosystem for programming neutral atom quantum processors, supporting users of all skill levels



Execution

Access Pasqal QPUs and quantum emulators via our cloud platform, and run your jobs



Pasqal Defining the quantum reality

실습: Solving QUBO with Pulser

Pasqal Defining the quantum reality

실습: Solving QUBO with Qubo-solver

Pasqal Defining the quantum reality

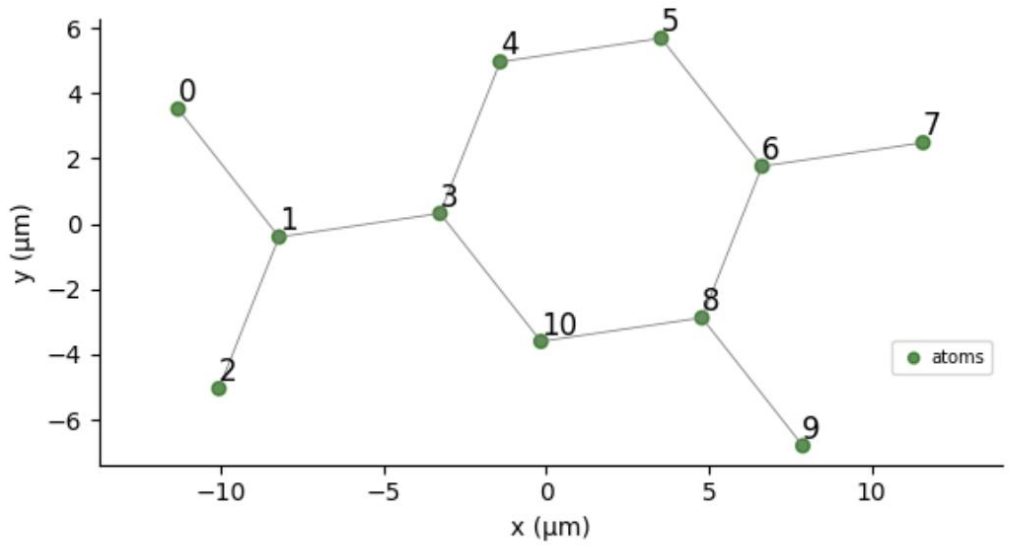
실습: QEK

Hands-on 1: Extracting machine-learning features (Tutorial 1)

Pasqal

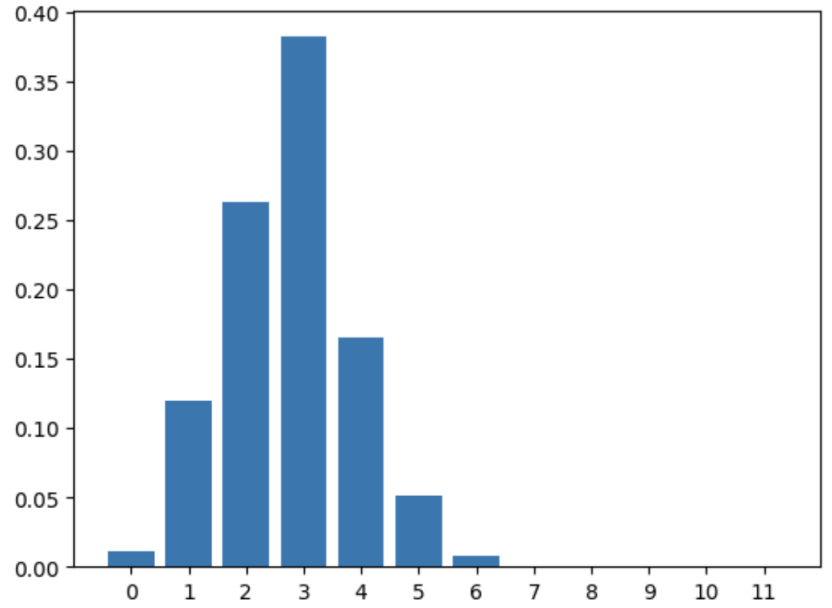
PTC-FM dataset: Predictive Toxicology Challenge, specifically the Female Mouse

In [8]:
```
dataset_example = processed_dataset[64]
dataset_example.draw_register()
```



In [11]:
```
dataset_example.draw_excitation()
```

```
Using categorical units to plot a list of strings that are all par
sable as floats or dates. If these strings should be plotted as nu
mbers, cast to the appropriate data type before plotting.
Using categorical units to plot a list of strings that are all par
sable as floats or dates. If these strings should be plotted as nu
mbers, cast to the appropriate data type before plotting.
```



Revisited: Quantum Evolution Kernel

Pasqal

With the right positioning of the atoms, and a reasonable approximation, this process encodes a graph.

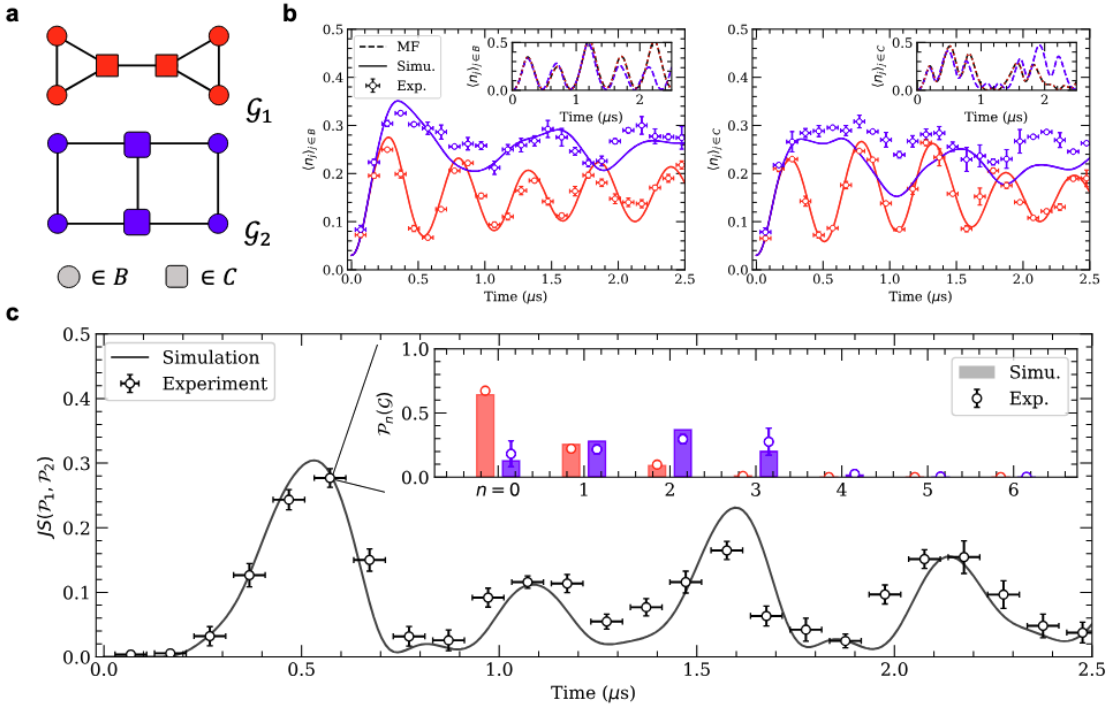
Measurement is mapped into a subgraph of G.

Jansen-Shannon divergence
(~distance in feature space)

$$JS(\mathcal{P}_1, \mathcal{P}_2) = H\left(\frac{\mathcal{P}_1 + \mathcal{P}_2}{2}\right) - \frac{H(\mathcal{P}_1) + H(\mathcal{P}_2)}{2}$$

where $H(\mathcal{P}) = -\sum_k p_k \log p_k$ Shannon entropy

$\mathcal{P} = (p_1, \ldots p_{|\mathcal{G}|})$ Histogram of graph

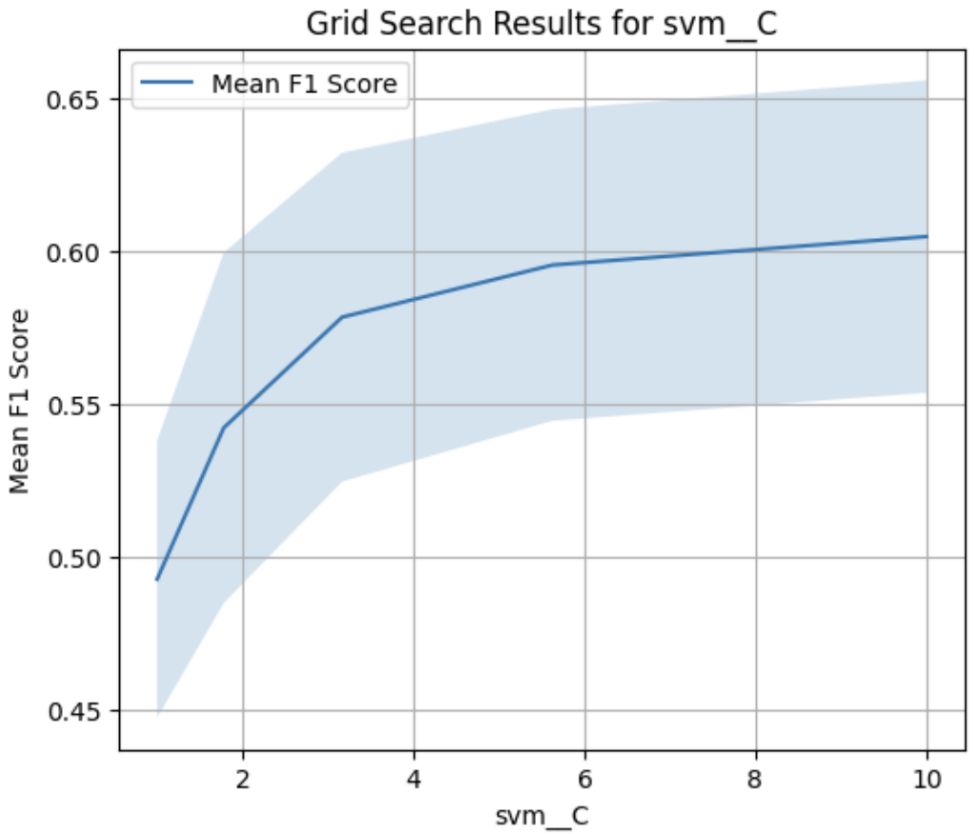


Quantum Evolution Kernel: $K(\mathcal{G}, \mathcal{G}') = \exp[-\mu\, JS(\mathcal{P}, \mathcal{P}')]$

Hands-on 2: Quantum Evolution Kernel-Based Machine Learning (Tutorial 2)

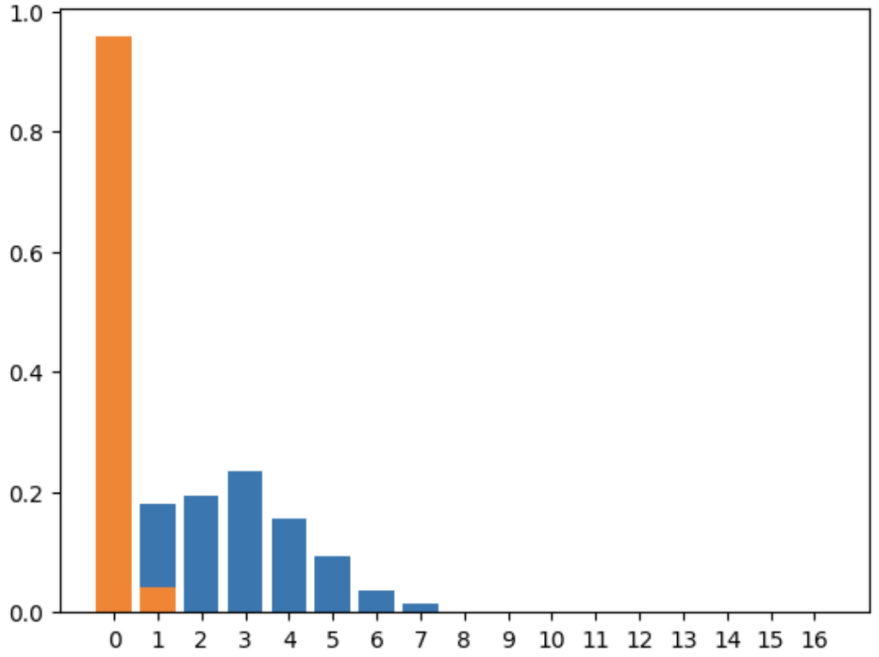
Pasqal

In [25]:
```
plot_grid_search_results(grid_search, 'svm__C')
```



In [11]:
```
graph_1.draw_excitation()
graph_2.draw_excitation()
```

```
Using categorical units to plot a list of strings that are all par
sable as floats or dates. If these strings should be plotted as nu
mbers, cast to the appropriate data type before plotting.
Using categorical units to plot a list of strings that are all par
sable as floats or dates. If these strings should be plotted as nu
mbers, cast to the appropriate data type before plotting.
Using categorical units to plot a list of strings that are all par
sable as floats or dates. If these strings should be plotted as nu
mbers, cast to the appropriate data type before plotting.
```



Any questions?

Pasqal

Woojun Lee
Technical Business Developer
woojun.lee@pasqal.com