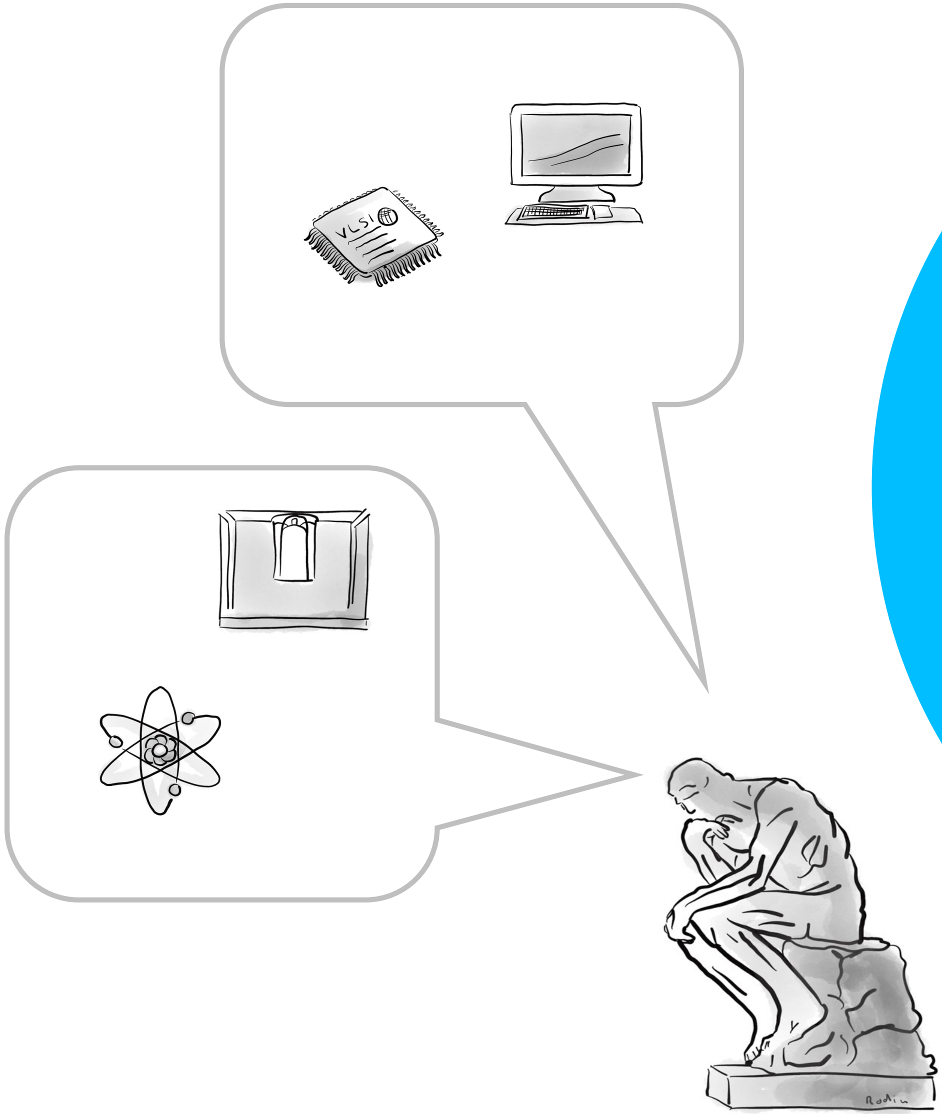
Universität Stuttgart
Institute of Architecture of Application Systems (IAAS)



Crete

4.7.2022

Quantum Patterns & QHAna

Johanna Barzen

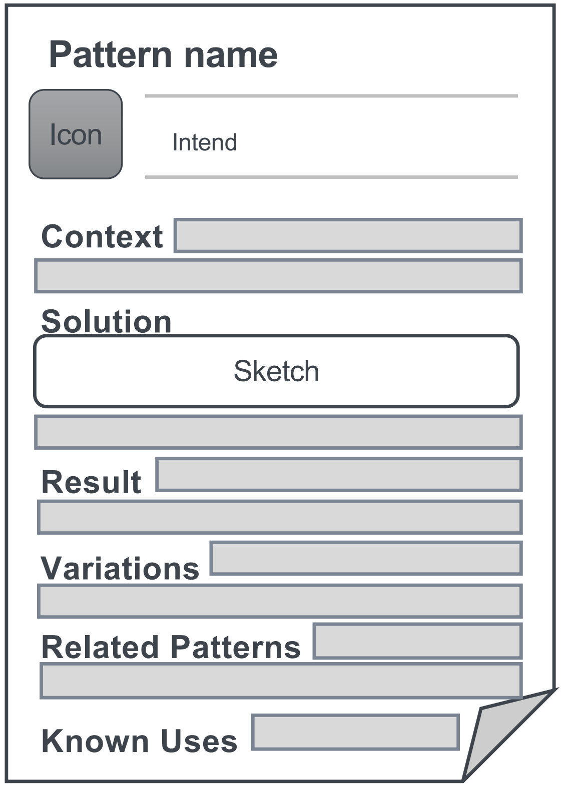
Quantum Patterns

Why Quantum Computing Patterns?

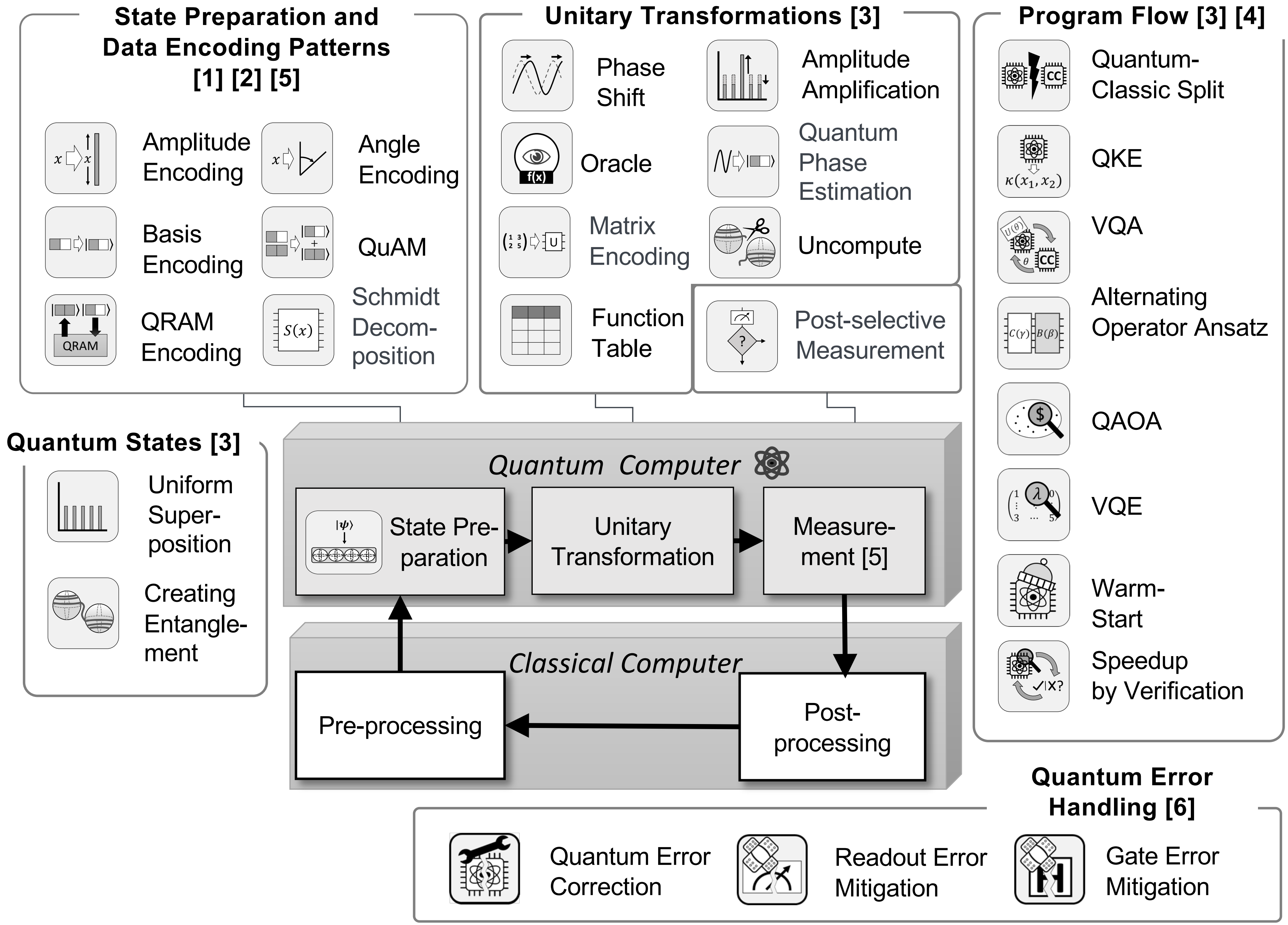
- Upcoming technology:
  - Rapid developments in recent years
  - Access available to the public
  - Potential impact in several application areas:
    - Combinatorial optimization (Graph problems, scheduling problems)
    - Chemistry (Design of materials & drugs)
    - Machine learning (Quantum neural networks, classification, clustering)
- Involving heterogenous disciplines
- Huge demand of education for industry

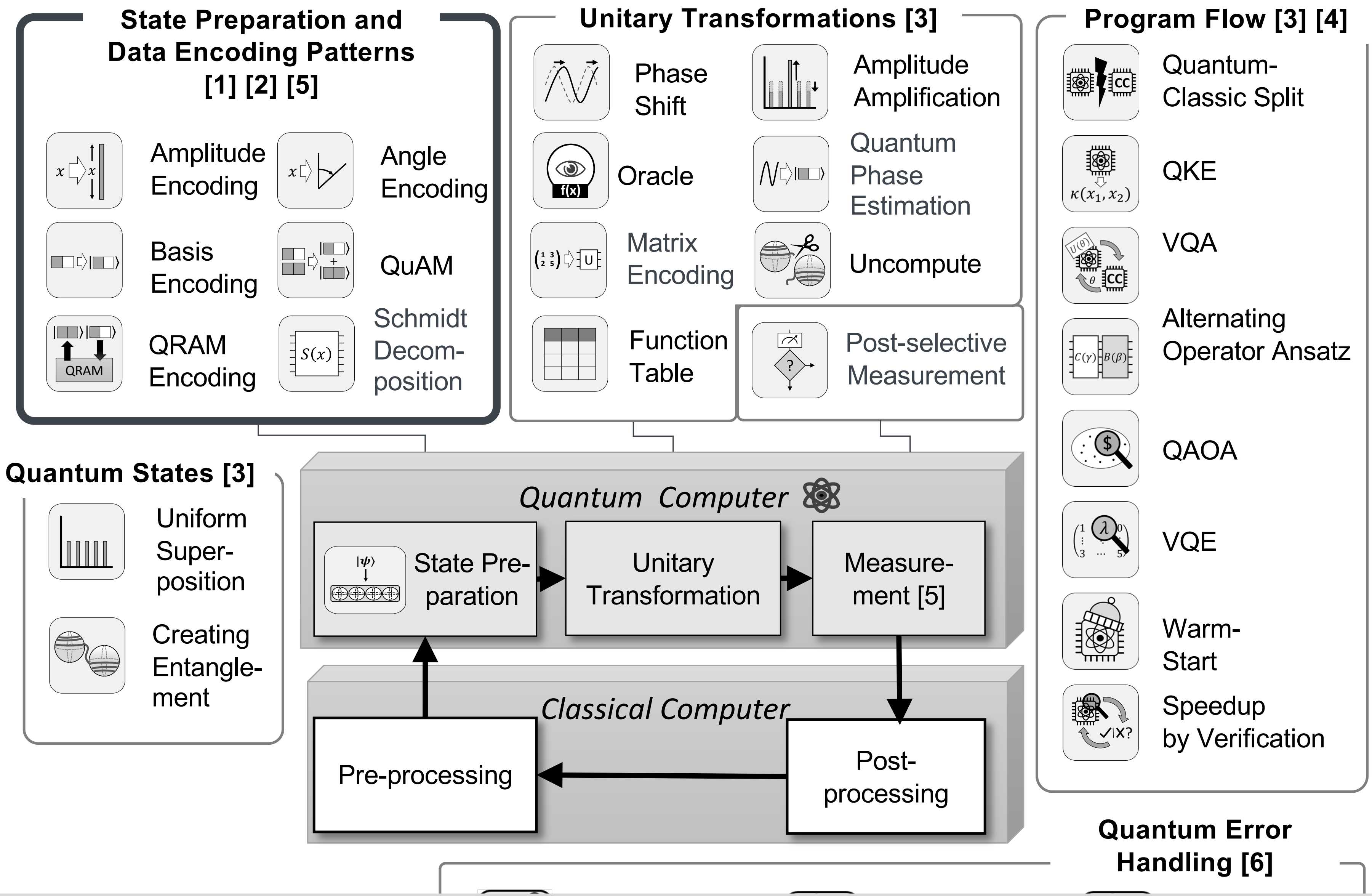
Quantum Computing Patterns: Format

- Make proven solutions explicit
- Introduce non-experts (e.g., software developers) to an interdisciplinary and complex domain

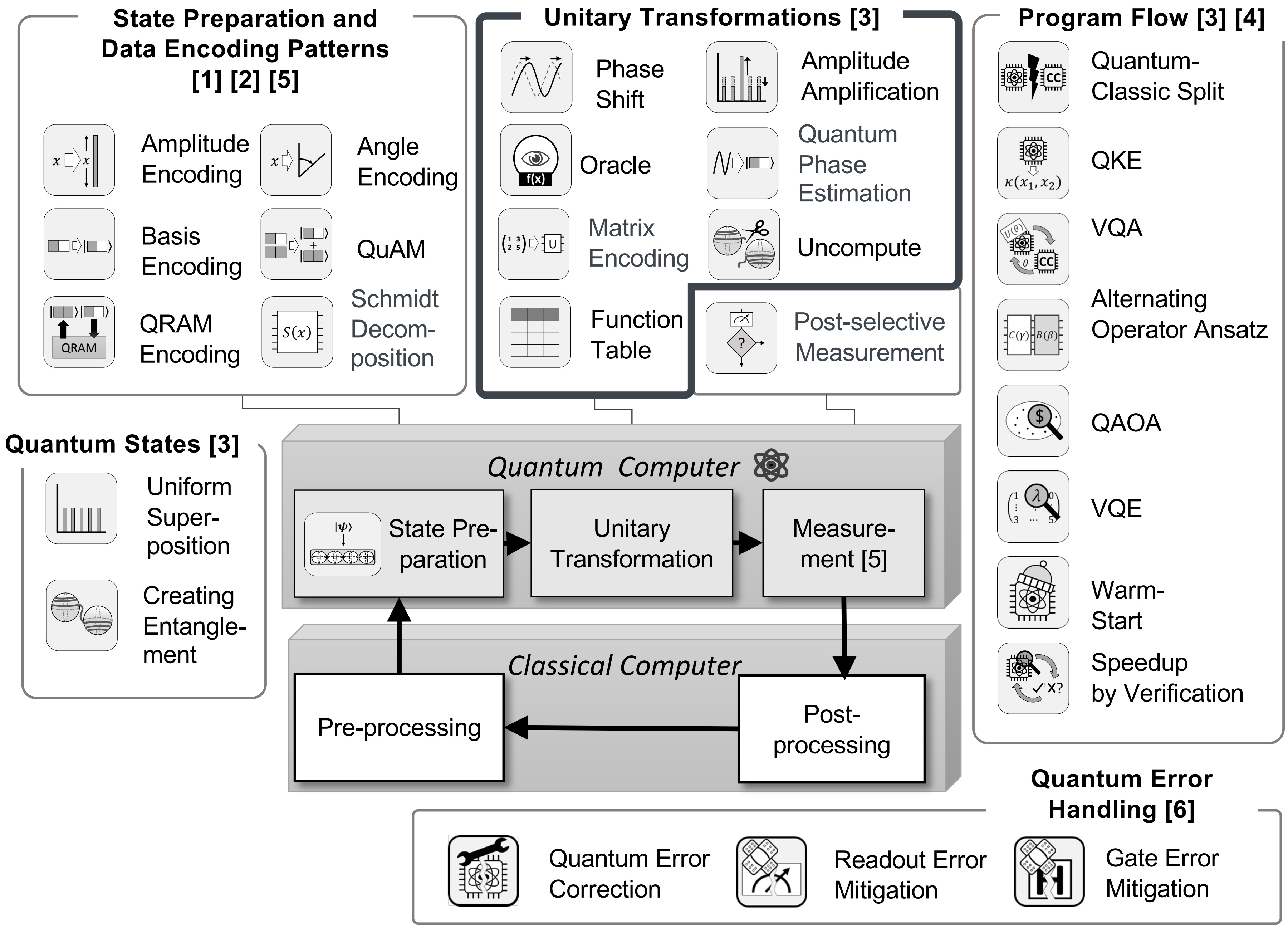


- Abstracted from concrete solutions
  (in our case: quantum algorithms)
- Patterns build on each other composing a patter language

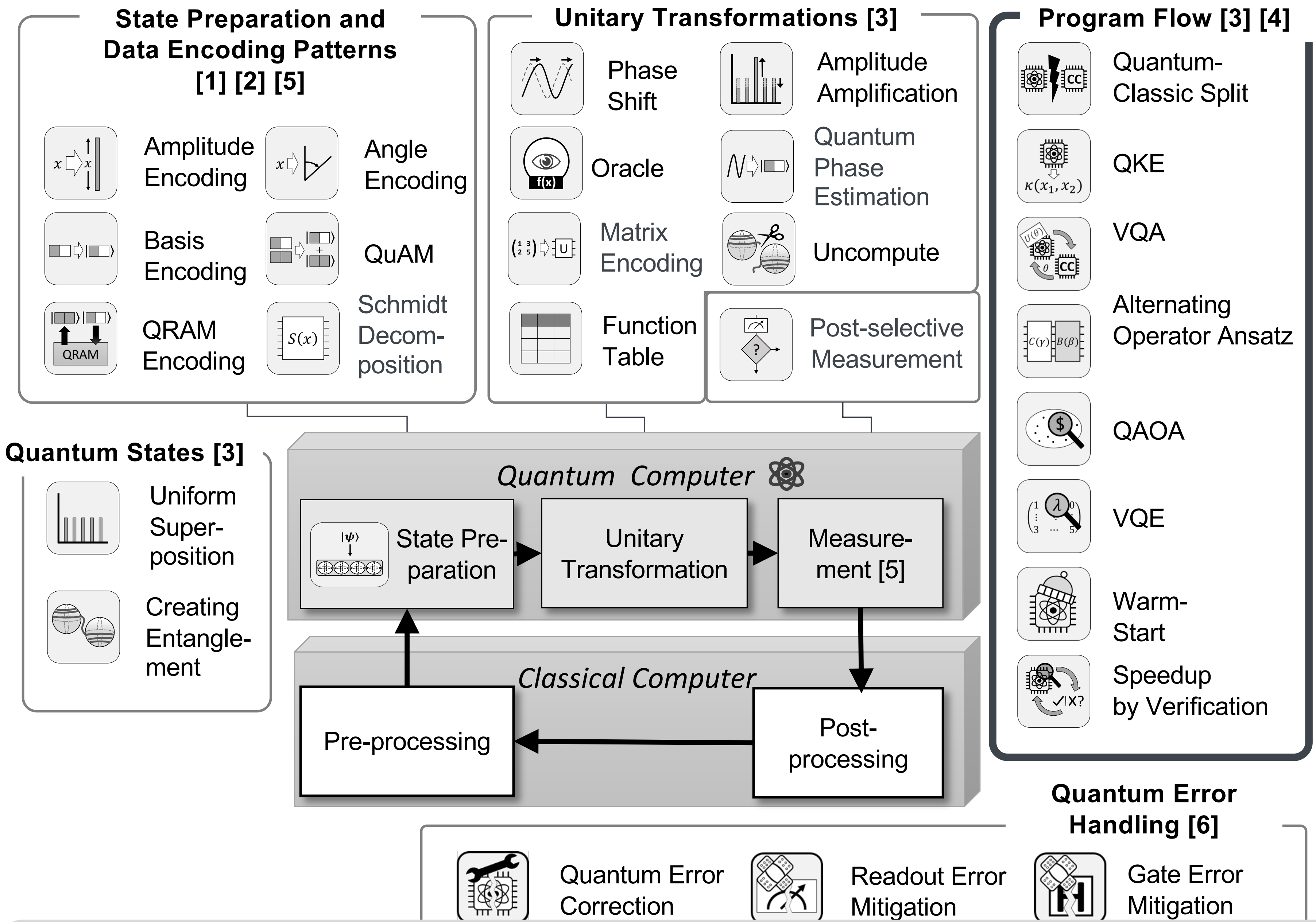

State Preparation and Data Encoding Patterns [1] [2] [5]
Amplitude Encoding
Angle Encoding
Basis Encoding
QuAM
QRAM Encoding
QRAM
Schmidt Decom-position
Unitary Transformations [3]
Phase Shift
Amplitude Amplification
Oracle
f(x)
Quantum Phase Estimation
Matrix Encoding
Uncompute
Function Table
Post-selective Measurement
Program Flow [3] [4]
Quantum-Classic Split
QKE
VQA
Alternating Operator Ansatz
QAOA
VQE
Warm-Start
Speedup by Verification
Quantum States [3]
Uniform Super-position
Creating Entangle-ment
Quantum Computer
State Pre-paration
Unitary Transformation
Measure-ment [5]
Classical Computer
Pre-processing
Post-processing
Quantum Error Handling [6]
Quantum Error Correction
Readout Error Mitigation
Gate Error Mitigation



[1] Weigold, Manuela; Barzen, Johanna; Leymann, Frank; Salm, Marie: Data Encoding Patterns for Quantum Algorithms. In: The Hillside Group (Hrsg): Proceedings of the 27th Conference on Pattern Languages of Programs (PLoP '20), 2021 (to appear)
[2] Weigold, Manuela; Barzen, Johanna; Leymann, Frank; Salm, Marie: Expanding Data Encoding Patterns For Quantum Algorithms In: 2021 IEEE 18th International Conference on Software Architecture Companion (ICSA-C), IEEE, 2021
[5] Weigold, Manuela; Barzen, Johanna; Leymann, Frank; Salm, Marie: Encoding Patterns For Quantum Algorithms In: IET Quantum Communications, Wiley, 2021

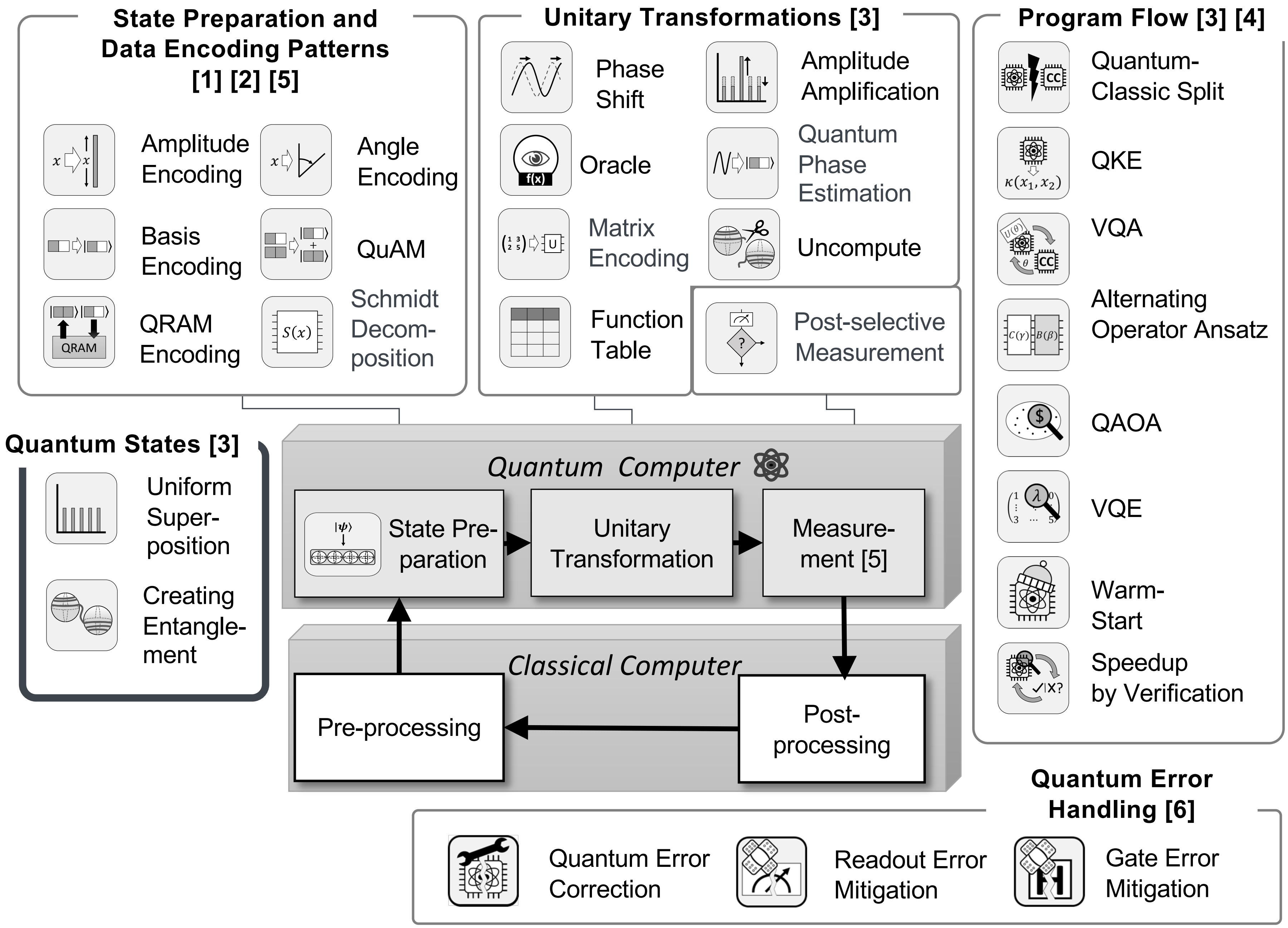


[3] Leymann, Frank: Towards a Pattern Language for Quantum Algorithms. In: First International Workshop, QTOP 2019, Munich, Germany, March 18, 2019, Proceedings, Springer, 2019

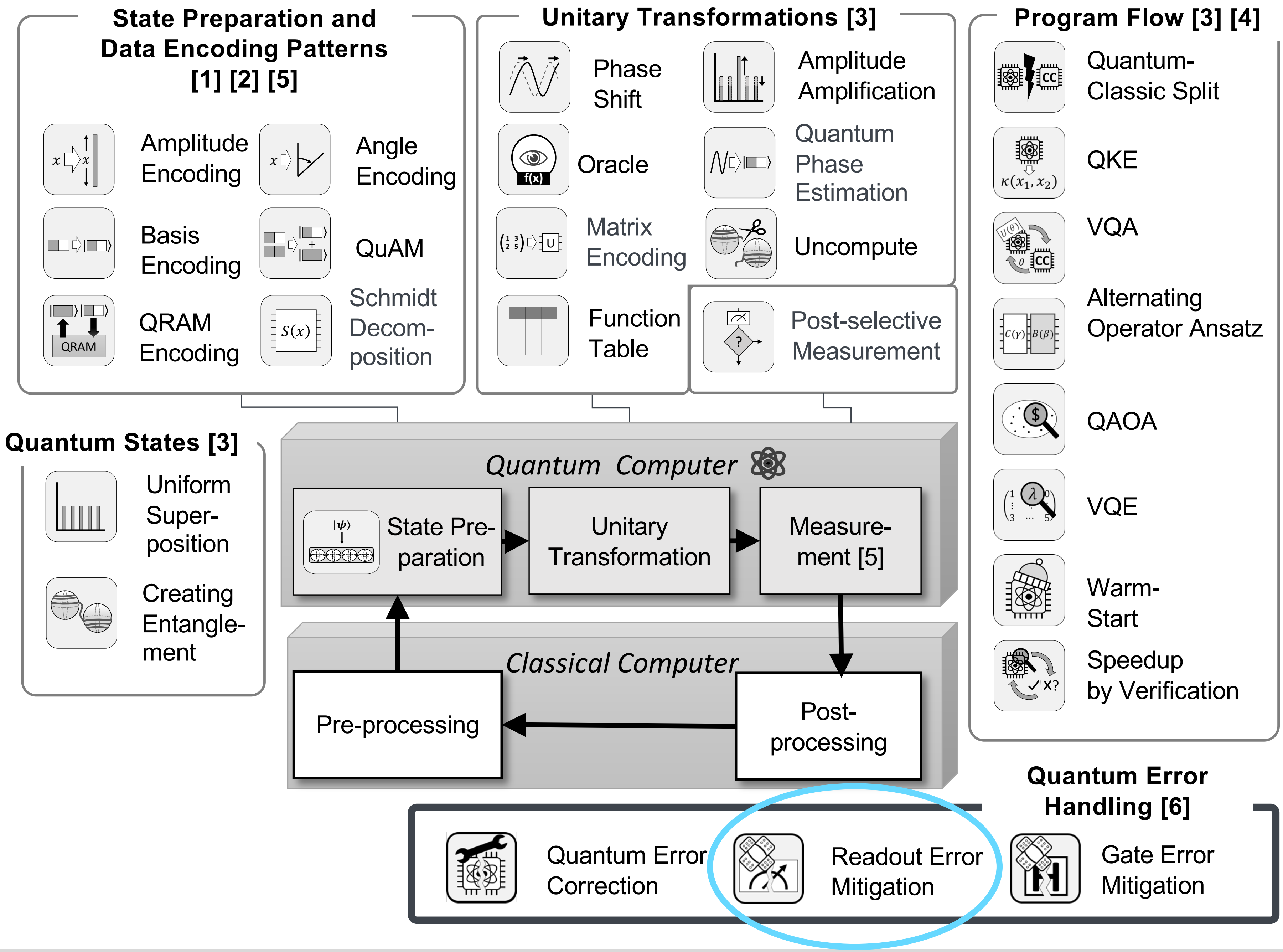


[3] Leymann, Frank: Towards a Pattern Language for Quantum Algorithms. In: First International Workshop, QTOP 2019, Munich, Germany, March 18, 2019, Proceedings, Springer, 2019

[4] Weigold, M., Barzen, J., Leymann, F., Vietz, D.: Patterns for Hybrid QuantumAlgorithms. In: Proceedings of the 15th Symposium and Summer School on Service-Oriented Computing (SummerSOC 2021). pp. 34–51. Springer International Publishing (Sep 2021).



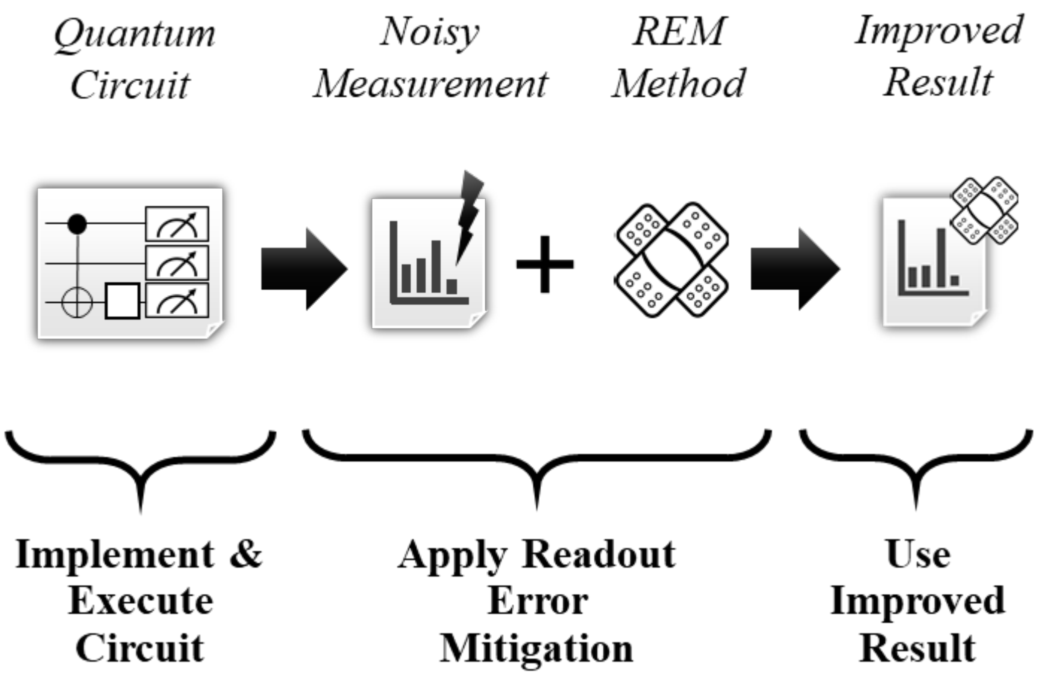
[3] Leymann, Frank: Towards a Pattern Language for Quantum Algorithms. In: First International Workshop, QTOP 2019, Munich, Germany, March 18, 2019, Proceedings, Springer, 2019



[6] Beisel, Martin; Barzen, Johanna; Leymann, Frank; Truger, Felix; Weder, Benjamin; Yussupov, Vladimir: Patterns for Quantum Error Handling. In: Proceedings of the 14th International Conference on Pervasive Patterns and Applications (PATTERNS 2022), Xpert Publishing Services (XPS), 2022

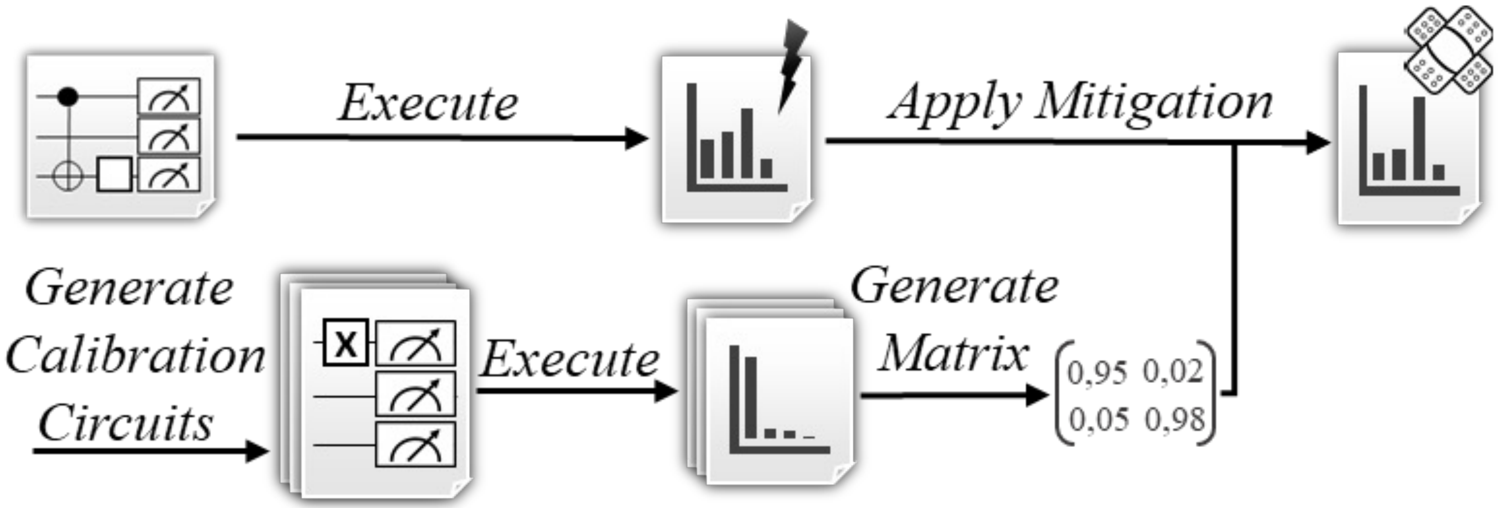
Pattern: Readout Error Mitigation (REM)

- **Intent**: How to reduce the impact of measurement errors?
- **Forces**: Low decoherence times, inaccurate measurements, small number of qubits
- **Solution**: Apply REM method, which improves the result quality based on observed measurement characteristics



Pattern: Readout Error Mitigation (REM)

- **Result**: More precise probability distribution at the cost of classical post-processing
- **Example**:



Quantum Computing Patterns

This is the start of a collection of patterns for quantum computing.
The icons of the patterns are licensed under a [Creative Commons Attribution 4.0 International License] and can be downloaded at [Resources].

- Basis Encoding
- Quantum Associative Memory
- Amplitude Encoding
- Angle Encoding
- QRAM Encoding
- Quantum Kernel Estimator (QKE)
- Variational Quantum Algorithm
- Variational Quantum Eigensolver
- Alternating Operator Ansatz
- Quantum Approximate Optimization Algorithm
- Warmstart
- Matrix Encoding
- Schmidt Decomposition
- Quantum Phase Estimation
- Post-Selective Measurement

More patterns for the categories *Quantum States, Unitary Transformation* and *Program Flow* can be found in this publication:

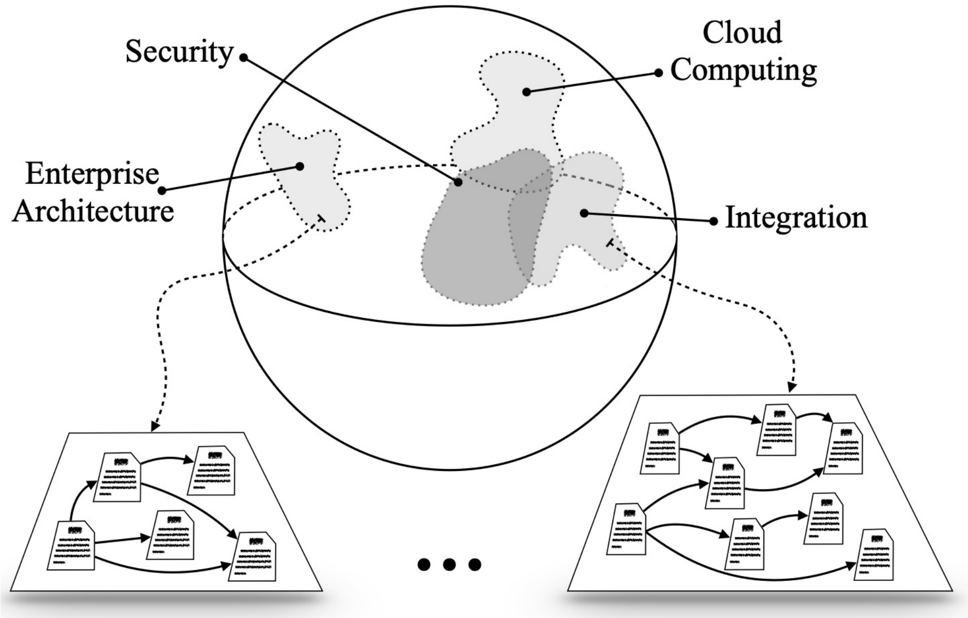
- Initialization aka State Preparation
- Uniform Superposition
- Creating Entanglement
- Function Table
- Oracle
- Uncompute
- Phase Shift
- Amplitude Amplification
- Speedup by Verification
- Quantum-Classic Split

https://quantumcomputingpatterns.org

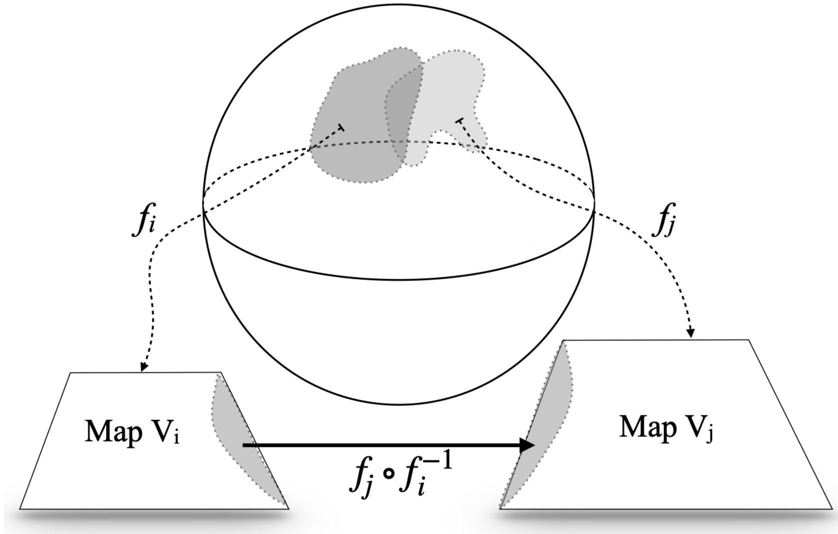
Pattern Atlas

„PatternPedia 2.0“

Patterns	Cartography
Pattern Languages	Maps of geographic regions
Links	Arrangements of maps
Views	Special representations of regions
Solutions	Concrete renderings of a map
Entries	Index



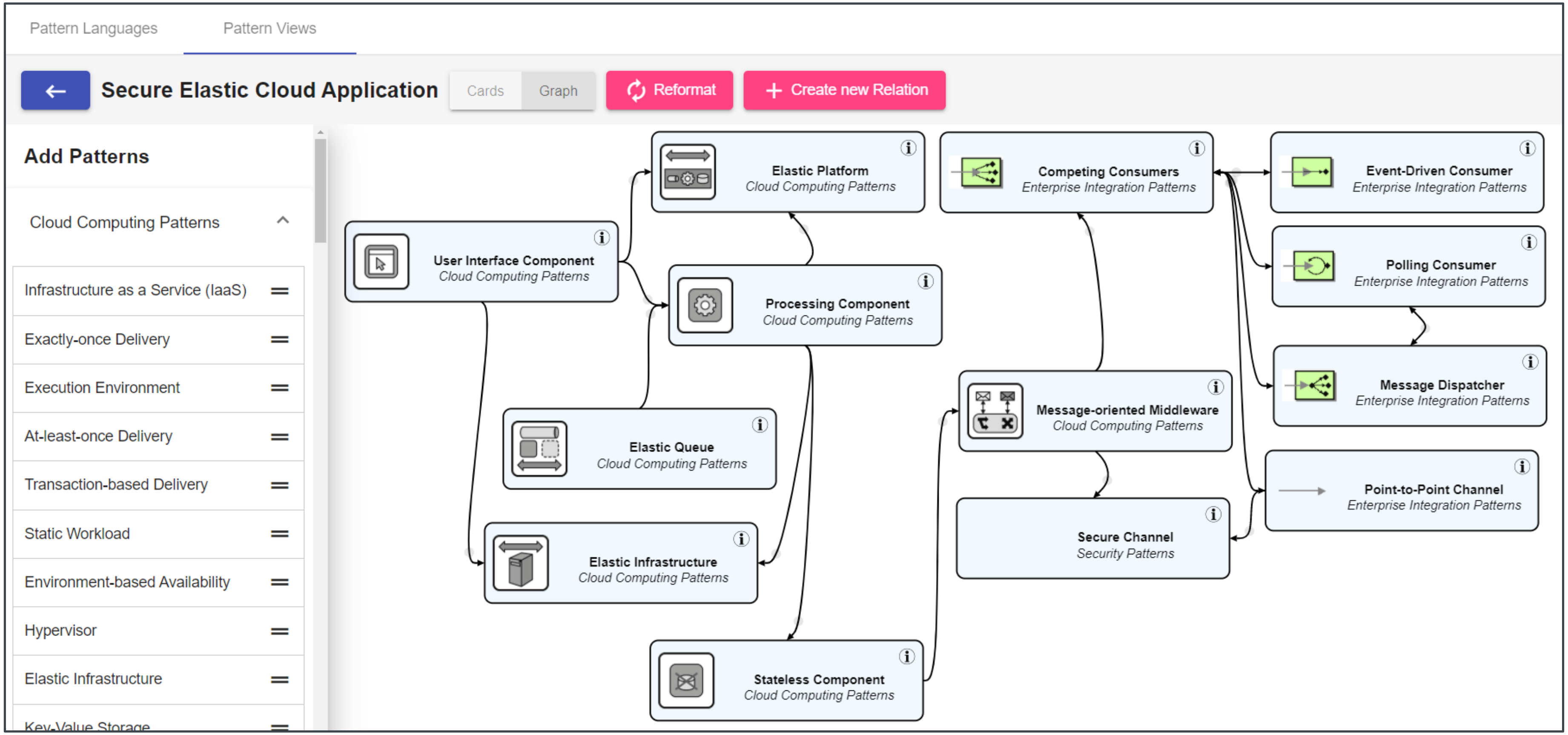
Pattern languages as maps of IT domains



Glueing maps together

Leymann, Frank; Barzen, Johanna: Pattern Atlas. In: Next-Gen Digital Services. A Retrospective and Roadmap for Service Computing of the Future, Springer International Publishing, 2021

Pattern Atlas: Tooling for Interconnected Pattern Languages



QHAna

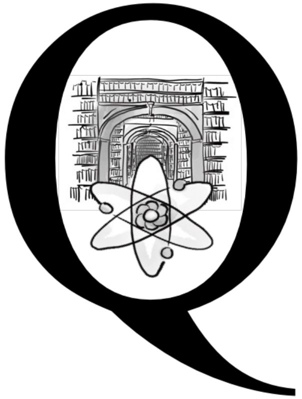
Quantum Humanities Analysis Tool

Barzen, J.: From Digital Humanities to Quantum Humanities: Potentials and Applications. In: E. R. Miranda (Ed.): An Introduction to Core Concepts, Theory and Applications, Cham: Springer, 2022.

Starting points

- Establishment of the Digital Humanities (DH)
- Quantum computers (QC) are becoming real

Digital Gipfel 2019
IBM QC, 53 Qubits



uantum Humanities

A Vision for Quantum Computing in the Digital Humanities

Barzen, J., Leymann, F.: Quantum humanities: a vision for quantum computing in digital humanities. In: SICS Software-Intensive Cyber-Physical Systems, Heidelberg: Springer Berlin Heidelberg, 2019.

Barzen, J., Leymann, F.: Quantum Humanities: A First Use Case for Quantum-ML in Media Science. In: ISAAI'19 Proceedings — Artificial Intelligence, Digitale Welt. Vol. 4(1), 2020

Reasons for using an (ideal) QC in the DH

(1) ... they solve certain types of problems much faster

(2) ...they enable the processing of large amounts of data in a single step

(3) ...their results promise a much higher degree of accuracy

(4) ...they solve problem classes, which are practically not solvable so far

(5) ...there are problems that can only be solved on a quantum computer

(6) ...their use promises to be significantly cheaper than that of a supercomputer

(7) ...they are much more energy efficient

→ NISQ
(Noisy Intermediate-Scale Quantum)

Challenges

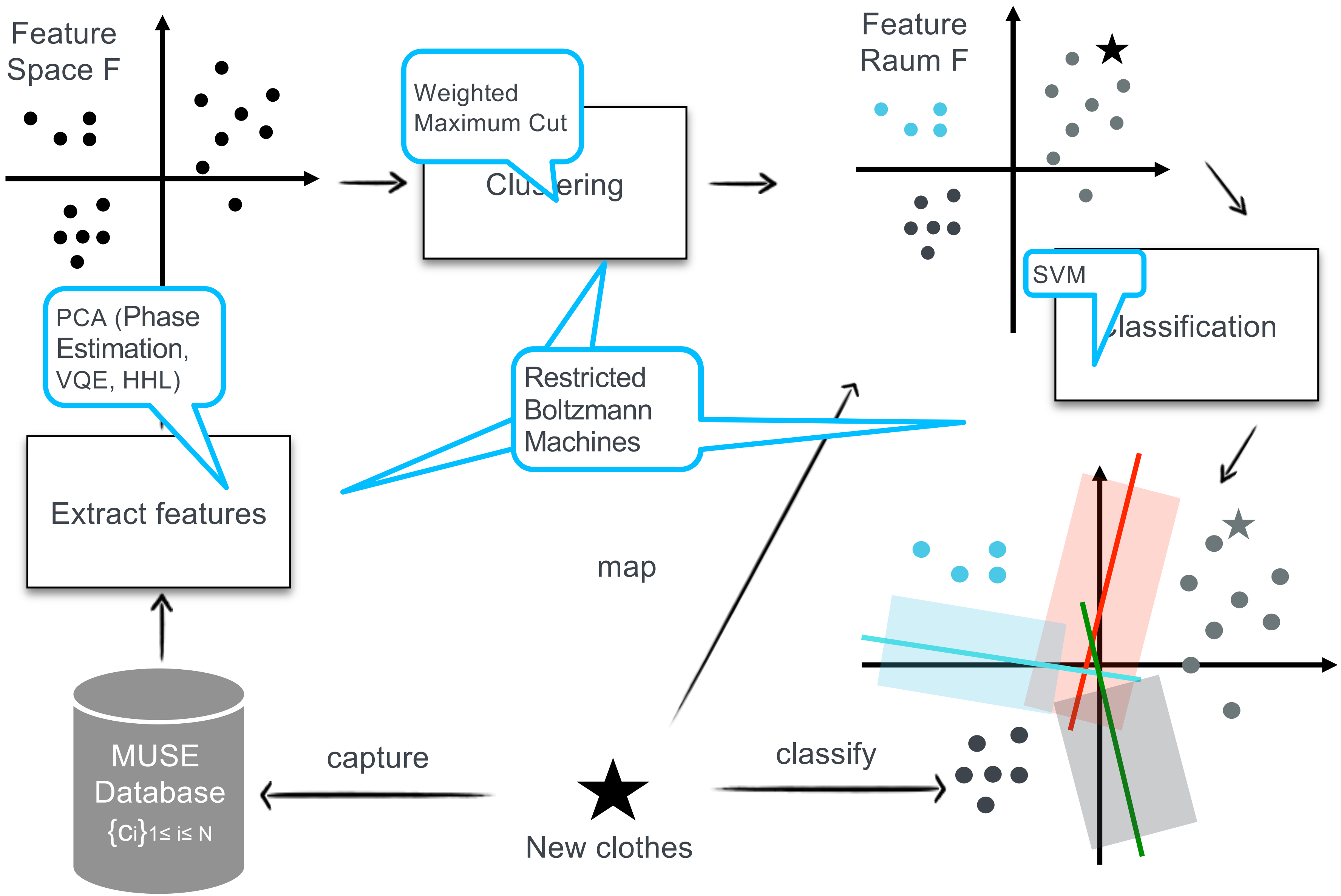
- From the application side:
  - Define suitable problem
  - Finding a common language
  - Selection of algorithms
  - Categorical data.....
- From QC side
  - Data preparation
  - Oracle expansion
  - Connectivity
  - Readout errors
  - ….

Leymann, F. et al.: Quantum in the Cloud: Application Potentials and Research Opportunities. In: Proceedings of the 10th International Conference on Cloud Computing and Services Science (CLOSER), 2020

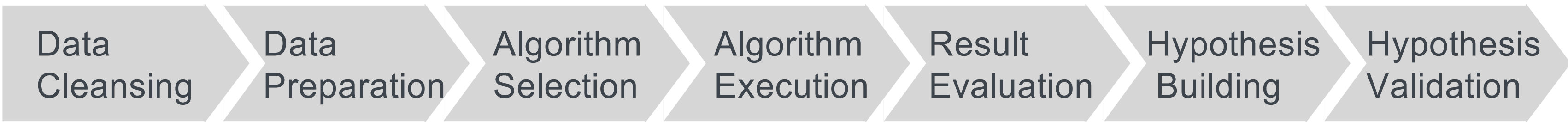
Barzen, J. et al. : Relevance of Near-Term Quantum Computing in the Cloud: A Humanities Perspective. In: Cloud Computing and Services Science. Vol. 1399, Springer International Publishing, 2021

Leymann, F., Barzen, J.: The bitter truth about gate-based quantum algorithms in the NISQ era. In: Quantum Science and Technology, IOP Publishing Ltd, 2020)

Use Case: MUSE Analysis



Data Analysis Pipeline



Data Analysis Pipeline

Data
Cleansing

Data cleansing:

- data acquisition
- format conversion
- missing value treatment
- data repair

Data Analysis Pipeline

Data Cleansing → Data Preparation

Data preparation:

- categorical data (nominal or ordinal) / numerical data?
- the proper encoding (e.g. one-hot encoding) needs to be determined
- features of the data must be engineered
  - e.g. feature selection or feature extraction are performed
  - possible dimension reduction (e.g. via proper embeddings) is determined

Data Analysis Pipeline

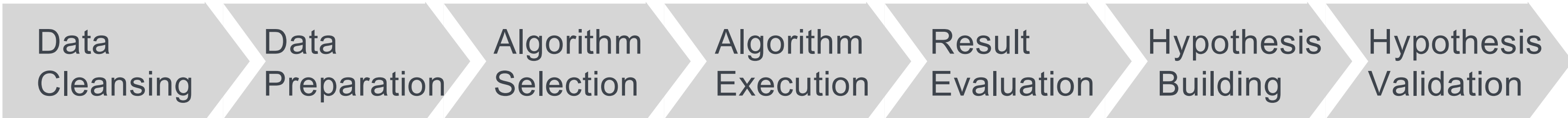
Algorithm selection

- determines the family of algorithms (e.g. classification, clustering, regression)
- selects a proper member of the family
- makes choices for the hyperparameters of the selected algorithm

Algorithm Execution

→ *several algorithms, even several algorithms of the same family of algorithms, are typically applied within an overall data analysis project.*

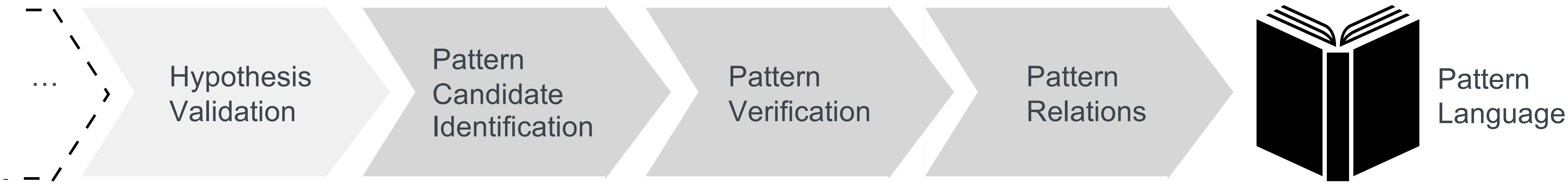
Data Analysis Pipeline



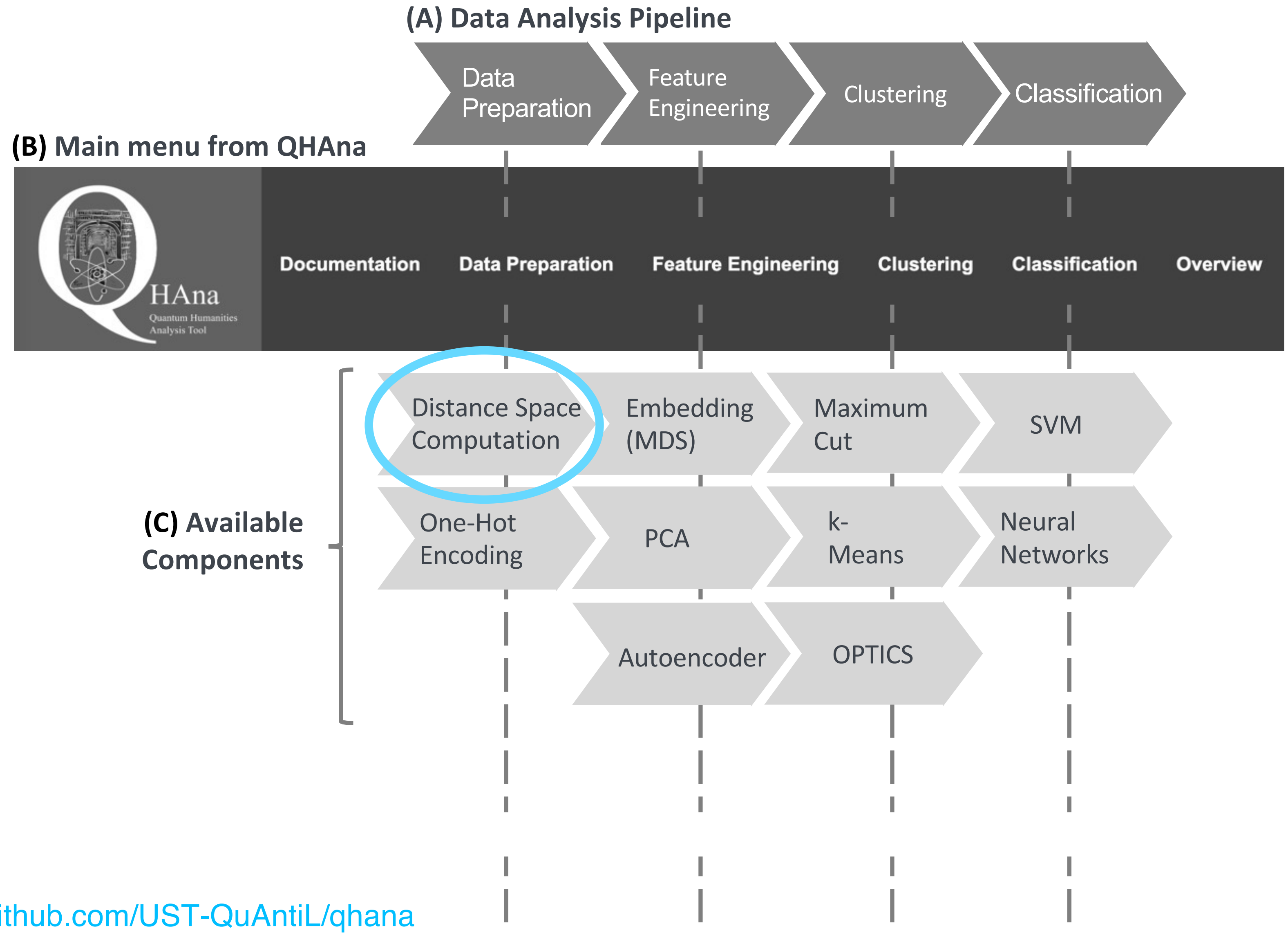
- Result evaluation is often based on visualizing the results
- It includes the creation of hypotheses based on the results
- Each hypothesis must be validated

→ *If no hypothesis can be build or none of the hypotheses can be successfully validated, other algorithms may be tried out to finally succeed with at least one proper hypothesis.*

Pattern Identification

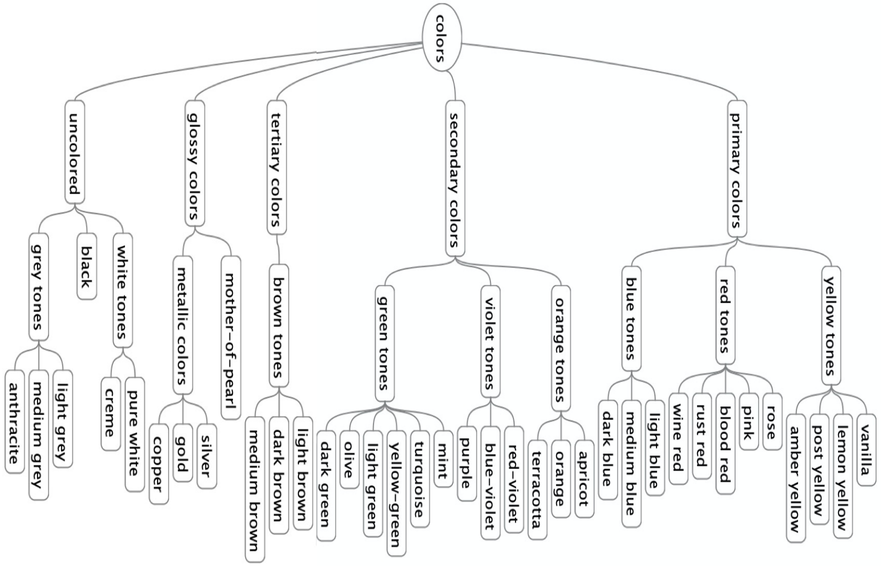


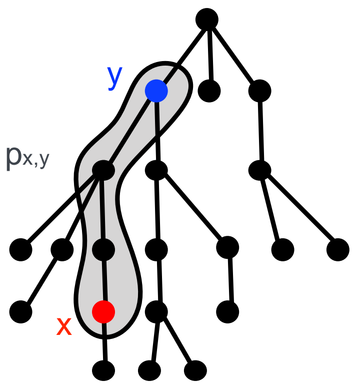
QHAna

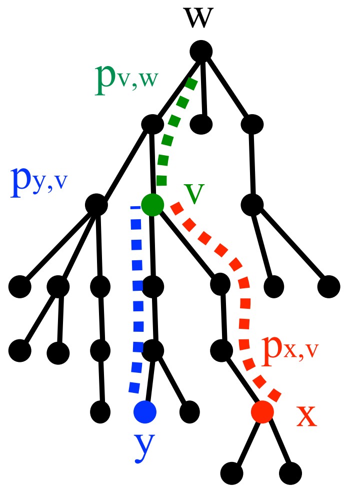


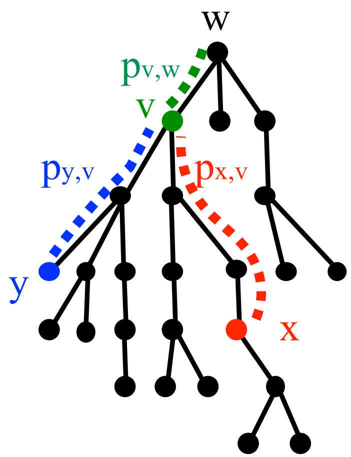
QHAna:
https://github.com/UST-QuAntiL/qhana

Wu-Palmer similarity









$$\omega(x,y) = 2 \cdot \frac{1}{3+2+2\cdot 1} = \frac{2}{7}$$

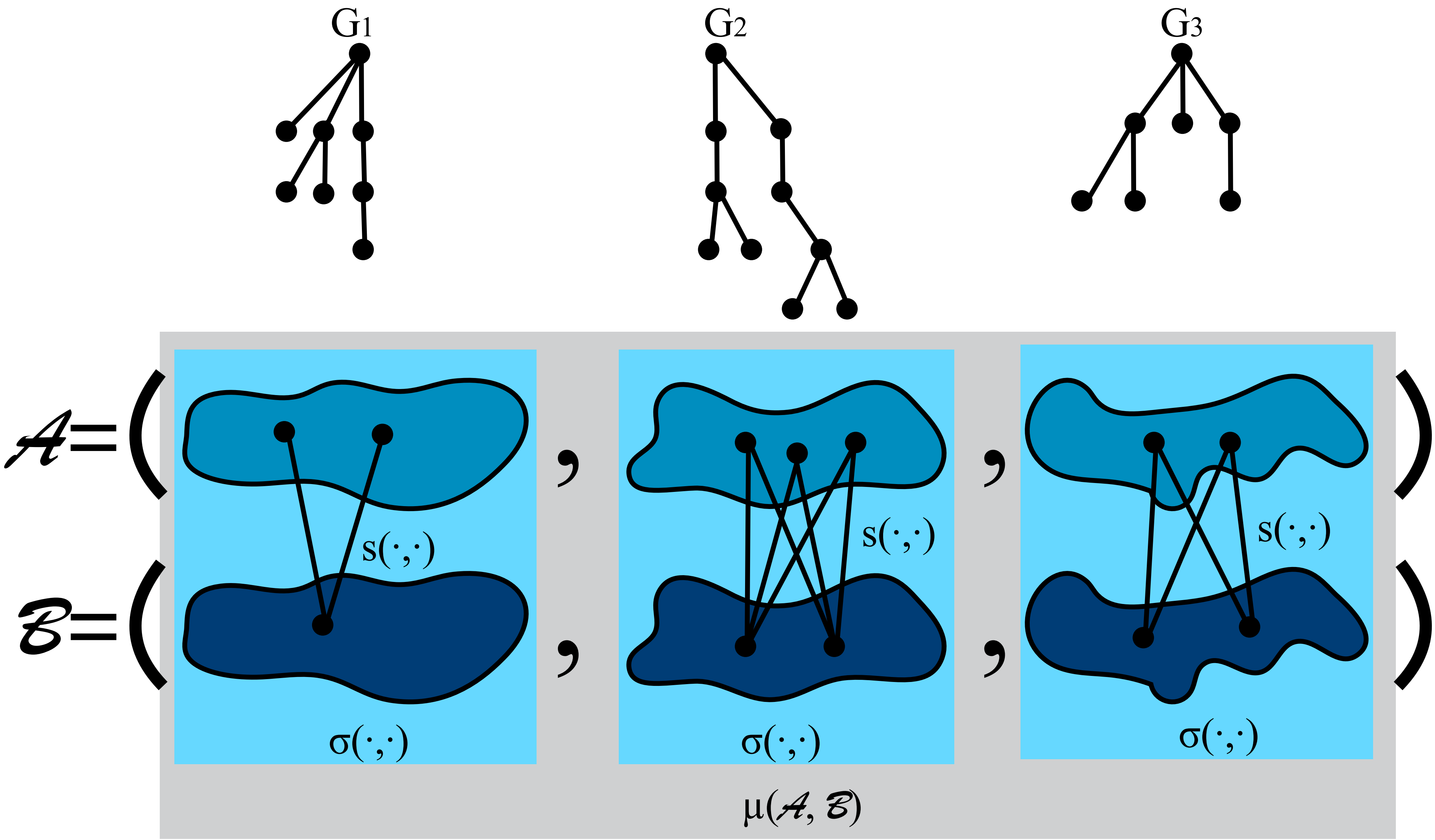
Let x, y ∈ N. Then

$$\omega(x,y) = \frac{2 \cdot L(p_{v,w})}{L(p_{x,v}) + L(p_{y,v}) + 2 \cdot L(p_{v,w})}$$

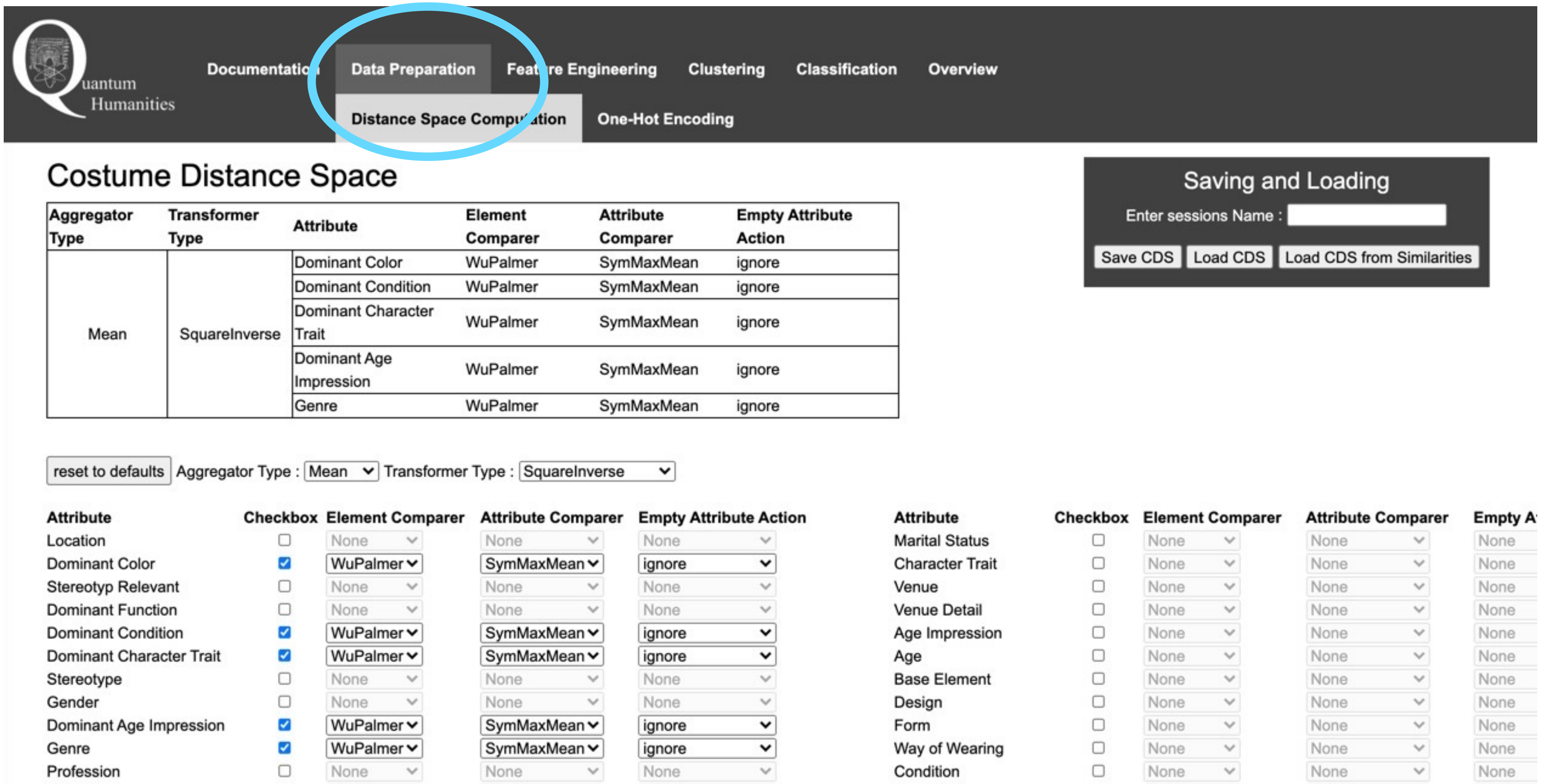
is the (Wu-Palmer) similarity of x and y.

Similarity calculation

Thus, tuples whose components are sets whose elements are each structured by a taxonomy can be given a similarity measure (thus a distance measure).

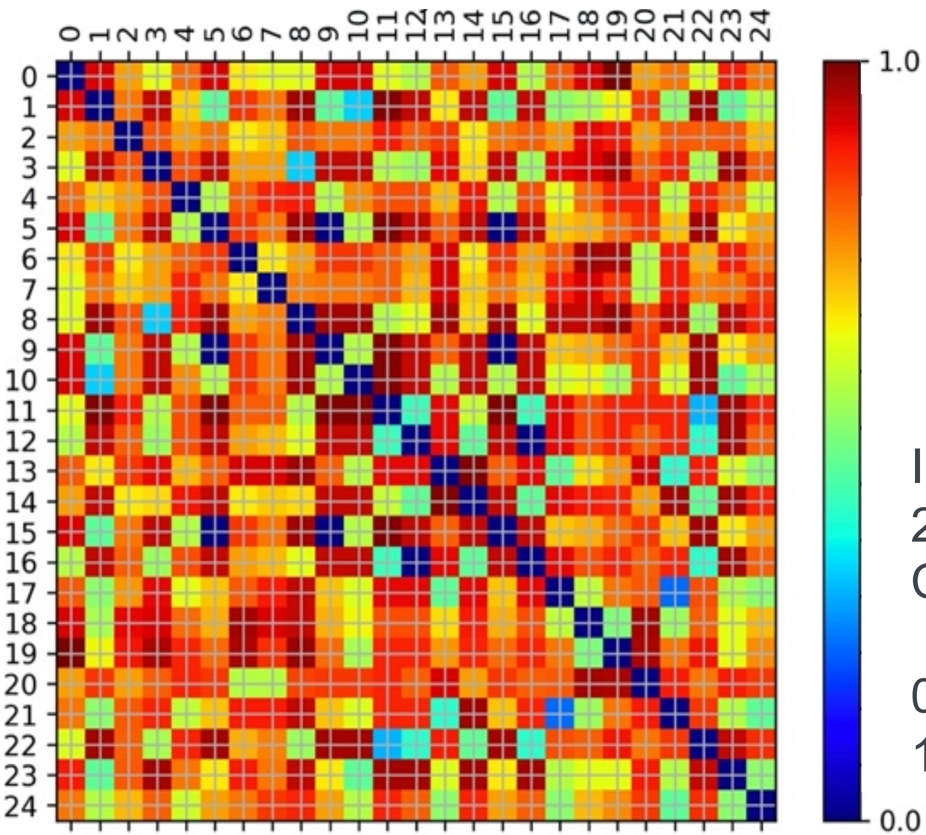


QHAna



Quantum Humanities
Documentation
Data Preparation
Feature Engineering
Clustering
Classification
Overview
Distance Space Computation
One-Hot Encoding
Costume Distance Space
Aggregator Type | Transformer Type | Attribute | Element Comparer | Attribute Comparer | Empty Attribute Action
Mean | SquareInverse | Dominant Color | WuPalmer | SymMaxMean | ignore
Dominant Condition | WuPalmer | SymMaxMean | ignore
Dominant Character Trait | WuPalmer | SymMaxMean | ignore
Dominant Age Impression | WuPalmer | SymMaxMean | ignore
Genre | WuPalmer | SymMaxMean | ignore
Saving and Loading
Enter sessions Name :
Save CDS
Load CDS
Load CDS from Similarities
reset to defaults
Aggregator Type : Mean
Transformer Type : SquareInverse
Attribute | Checkbox | Element Comparer | Attribute Comparer | Empty Attribute Action
Location | None | None | None
Dominant Color | WuPalmer | SymMaxMean | ignore
Stereotyp Relevant | None | None | None
Dominant Function | None | None | None
Dominant Condition | WuPalmer | SymMaxMean | ignore
Dominant Character Trait | WuPalmer | SymMaxMean | ignore
Stereotype | None | None | None
Gender | None | None | None
Dominant Age Impression | WuPalmer | SymMaxMean | ignore
Genre | WuPalmer | SymMaxMean | ignore
Profession | None | None | None
Attribute | Checkbox | Element Comparer | Attribute Comparer | Empty A
Marital Status | None | None | None
Character Trait | None | None | None
Venue | None | None | None
Venue Detail | None | None | None
Age Impression | None | None | None
Age | None | None | None
Base Element | None | None | None
Design | None | None | None
Form | None | None | None
Way of Wearing | None | None | None
Condition | None | None | None

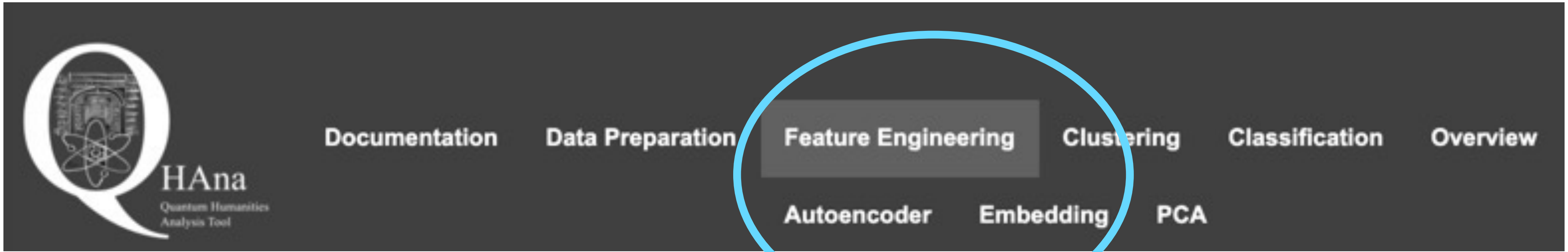
Distance matrix



Input:
25 costumes
Color and genre values

0 = max. similar
1 = max. dissimilar

Multi-Dimensional Scaling (MDS) in QHAna



Initialize Embedding

Enter Embedding Type [mds] [initialize]

Saving and Loading

Enter sessions Name : [ ]

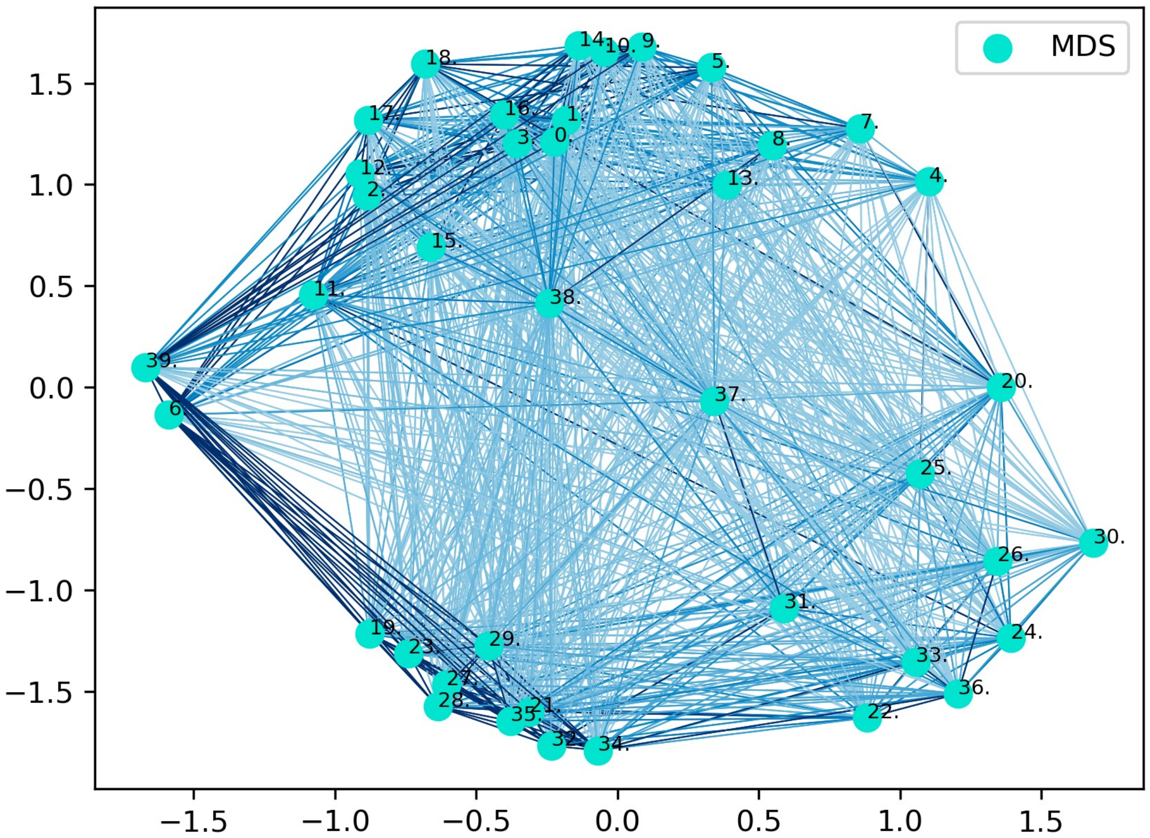
[Save Embedding] [Load Embedding]

Initialized Embedding

[set parameters]

Parameter	Input	Description
ScalingTyp	Multidimensional Scaling	choosen Scaling Type
Dimensions	2	(int, optional, default: 2) Number of dimensions in which to immerse the dissimilarities.
repeat SMACOF Algorithm	4	(int, optional, default: 4) Number of times the SMACOF algorithm will be run with different initializations. The final results will be the best output of the runs, determined by the run with the smallest final stress.
Number Iterations	300	(int, optional, default: 300) Maximum number of iterations of the SMACOF algorithm for a single run.
Dissimilarity	euclidean	('euclidean' | 'precomputed', optional, default: 'euclidean') Dissimilarity measure to use: 'euclidean': Pairwise Euclidean distances between points in the dataset. 'precomputed': Pre-computed dissimilarities are passed directly to fit and fit_transform.
Epsilon	0,001	(float, optional, default: 1e-3) Relative tolerance with respect to stress at which to declare convergence.
Static Eulidean Coordinates	☐	bool, optional (default=False) If the parameter is True the Object do not calculate new Euclidean Coordinates for the same similarity matrix.

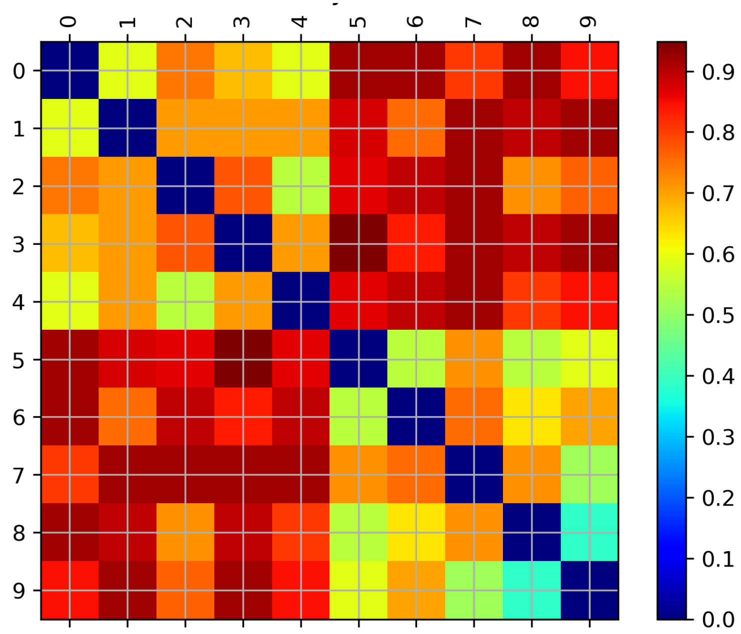
Multi-Dimensional Scaling (MDS)



Input:

- 40 costumes
- Color and genre values
- 2 dimensions

Distance matrix (2)

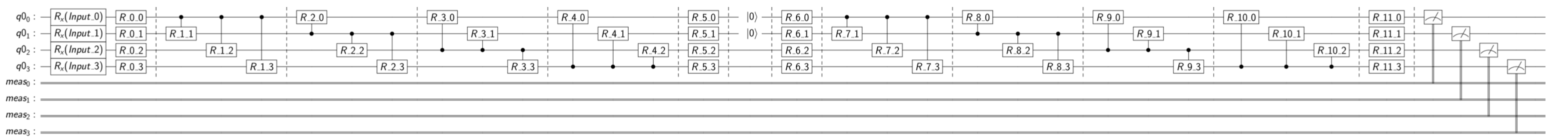


calculated about the Wu and Palmer similarity

Quantum Autoencoder

2. Encoder

4. Decoder

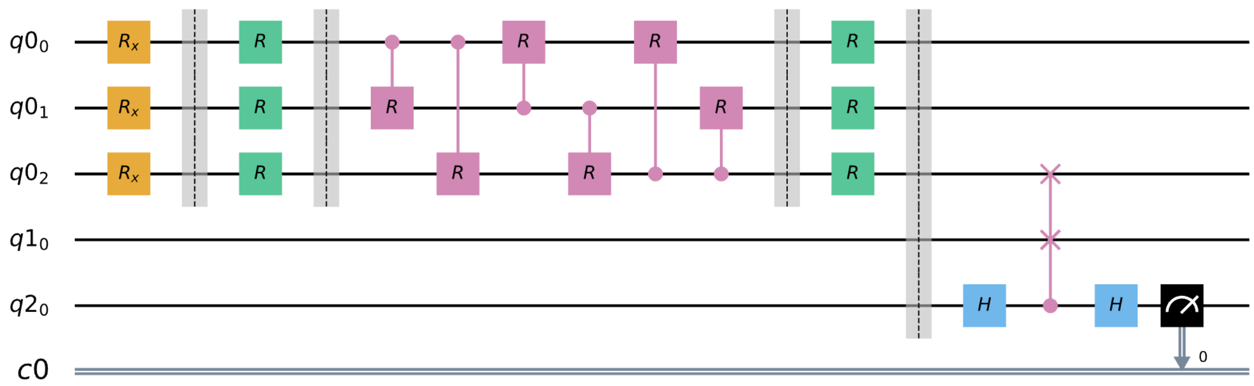


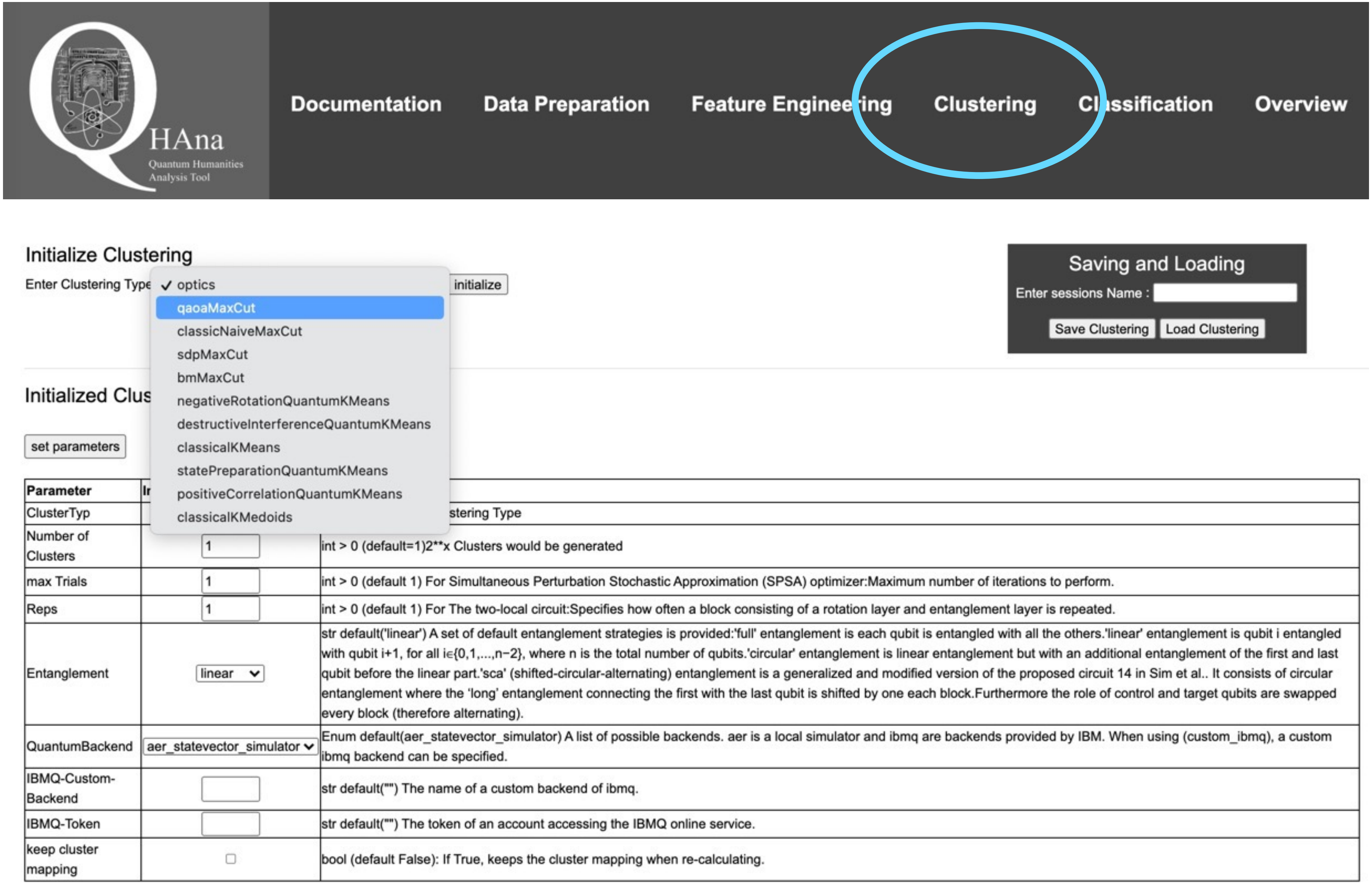
1. Input Preperation

3. Resetting the qubits to |0 ⟩

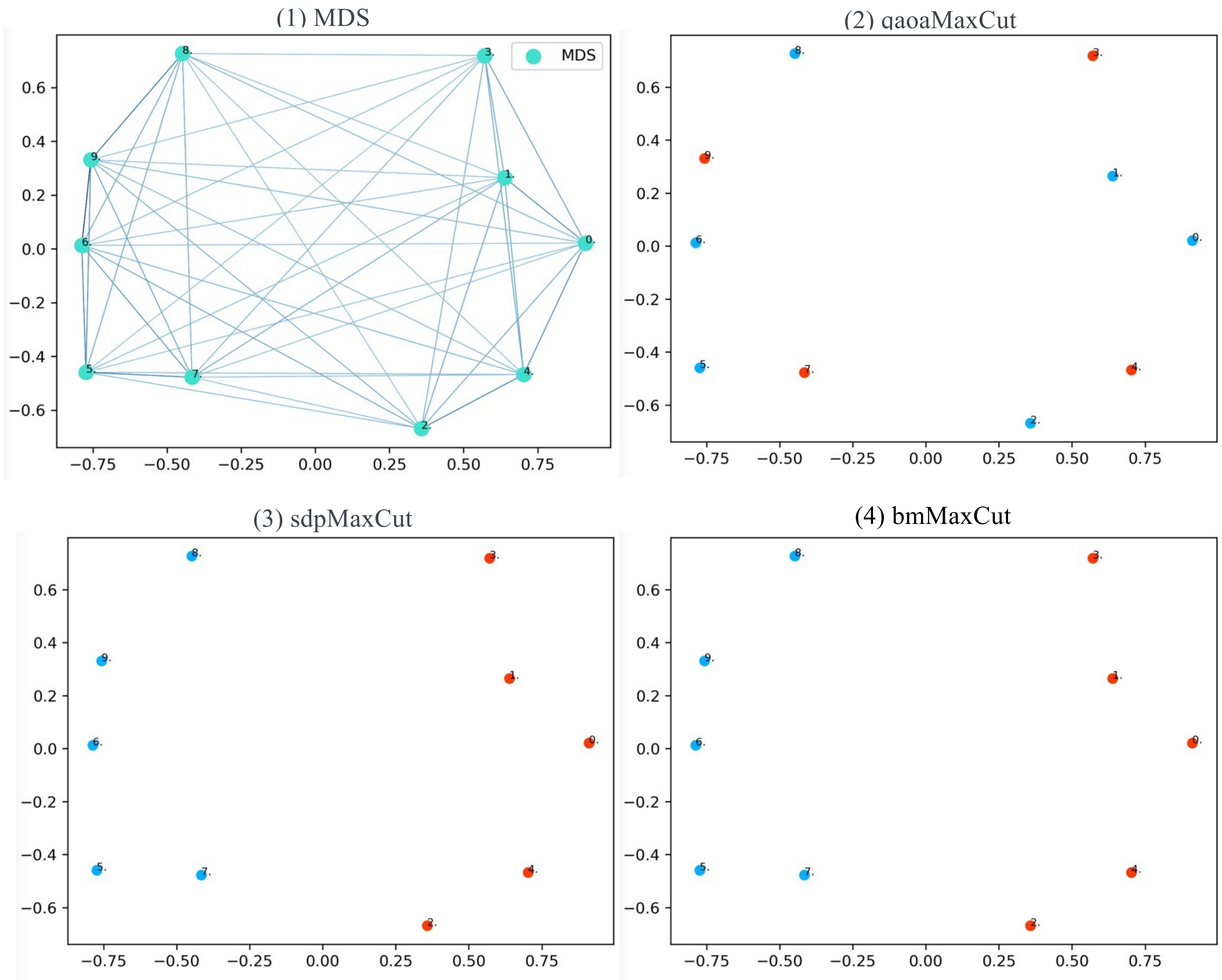
5. Messen

Training




HAna
Quantum Humanities Analysis Tool
Documentation
Data Preparation
Feature Engineering
Clustering
Classification
Overview
Initialize Clustering
Enter Clustering Type
✓ optics
qaoaMaxCut
classicNaiveMaxCut
sdpMaxCut
bmMaxCut
negativeRotationQuantumKMeans
destructiveInterferenceQuantumKMeans
classicalKMeans
statePreparationQuantumKMeans
positiveCorrelationQuantumKMeans
classicalKMedoids
initialize
Saving and Loading
Enter sessions Name :
Save Clustering
Load Clustering
Initialized Clus
set parameters
Parameter
Ir
ClusterTyp
stering Type
Number of Clusters
1
int > 0 (default=1)2**x Clusters would be generated
max Trials
1
int > 0 (default 1) For Simultaneous Perturbation Stochastic Approximation (SPSA) optimizer:Maximum number of iterations to perform.
Reps
1
int > 0 (default 1) For The two-local circuit:Specifies how often a block consisting of a rotation layer and entanglement layer is repeated.
Entanglement
linear
str default('linear') A set of default entanglement strategies is provided:'full' entanglement is each qubit is entangled with all the others.'linear' entanglement is qubit i entangled with qubit i+1, for all i∈{0,1,...,n−2}, where n is the total number of qubits.'circular' entanglement is linear entanglement but with an additional entanglement of the first and last qubit before the linear part.'sca' (shifted-circular-alternating) entanglement is a generalized and modified version of the proposed circuit 14 in Sim et al.. It consists of circular entanglement where the 'long' entanglement connecting the first with the last qubit is shifted by one each block.Furthermore the role of control and target qubits are swapped every block (therefore alternating).
QuantumBackend
aer_statevector_simulator
Enum default(aer_statevector_simulator) A list of possible backends. aer is a local simulator and ibmq are backends provided by IBM. When using (custom_ibmq), a custom ibmq backend can be specified.
IBMQ-Custom-Backend
str default("") The name of a custom backend of ibmq.
IBMQ-Token
str default("") The token of an account accessing the IBMQ online service.
keep cluster mapping
bool (default False): If True, keeps the cluster mapping when re-calculating.

Clustering (1)



Values of 10 costumes embedded via MDS (1) and their clustering results of different maximum cut implementations (2-4)

HAna
Quantum Humanities Analysis Tool

Documentation | Data Preparation | Feature Engineering | Clustering | Classification | Overview

Initialize Clustering

Enter Clustering Type

✓ optics
qaoaMaxCut
classicNaiveMaxCut
sdpMaxCut
bmMaxCut
negativeRotationQuantumKMeans
destructiveInterferenceQuantumKMeans
classicalKMeans
statePreparationQuantumKMeans
positiveCorrelationQuantumKMeans
classicalKMedoids

initialize

Saving and Loading

Enter sessions Name :

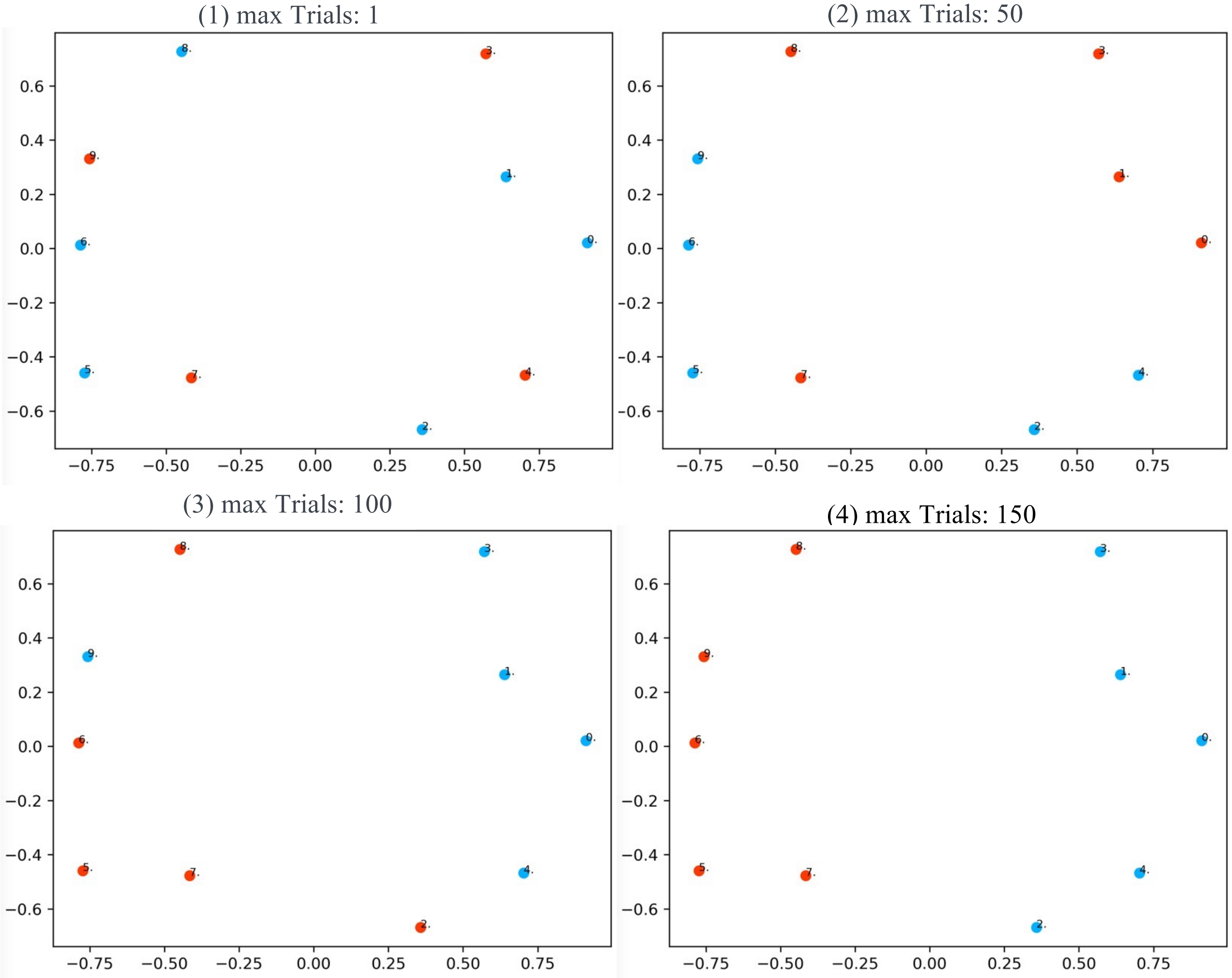
Save Clustering | Load Clustering

Initialized Clus

set parameters

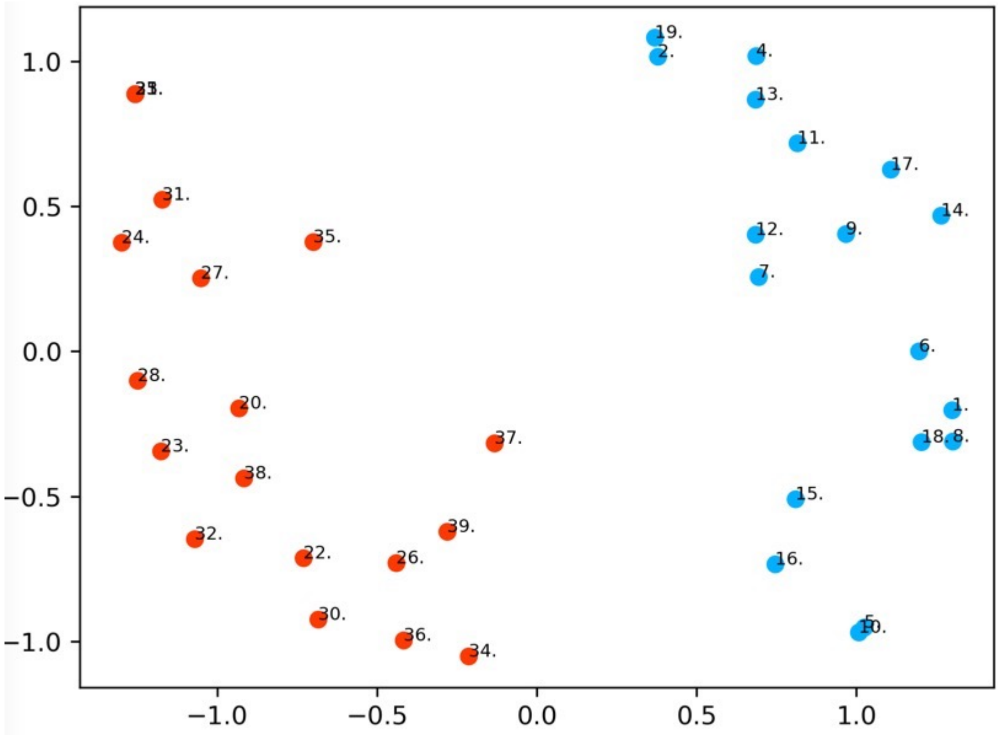
Parameter	Ir	
ClusterTyp		stering Type
Number of Clusters	1	int > 0 (default=1)2**x Clusters would be generated
max Trials	1	int > 0 (default 1) For Simultaneous Perturbation Stochastic Approximation (SPSA) optimizer:Maximum number of iterations to perform.
Reps	1	int > 0 (default 1) For The two-local circuit:Specifies how often a block consisting of a rotation layer and entanglement layer is repeated.
Entanglement	linear	str default('linear') A set of default entanglement strategies is provided:'full' entanglement is each qubit is entangled with all the others.'linear' entanglement is qubit i entangled with qubit i+1, for all i∈{0,1,...,n−2}, where n is the total number of qubits.'circular' entanglement is linear entanglement but with an additional entanglement of the first and last qubit before the linear part.'sca' (shifted-circular-alternating) entanglement is a generalized and modified version of the proposed circuit 14 in Sim et al.. It consists of circular entanglement where the 'long' entanglement connecting the first with the last qubit is shifted by one each block.Furthermore the role of control and target qubits are swapped every block (therefore alternating).
QuantumBackend	aer_statevector_simulator	Enum default(aer_statevector_simulator) A list of possible backends. aer is a local simulator and ibmq are backends provided by IBM. When using (custom_ibmq), a custom ibmq backend can be specified.
IBMQ-Custom-Backend		str default("") The name of a custom backend of ibmq.
IBMQ-Token		str default("") The token of an account accessing the IBMQ online service.
keep cluster mapping	☐	bool (default False): If True, keeps the cluster mapping when re-calculating.

Clustering (2)

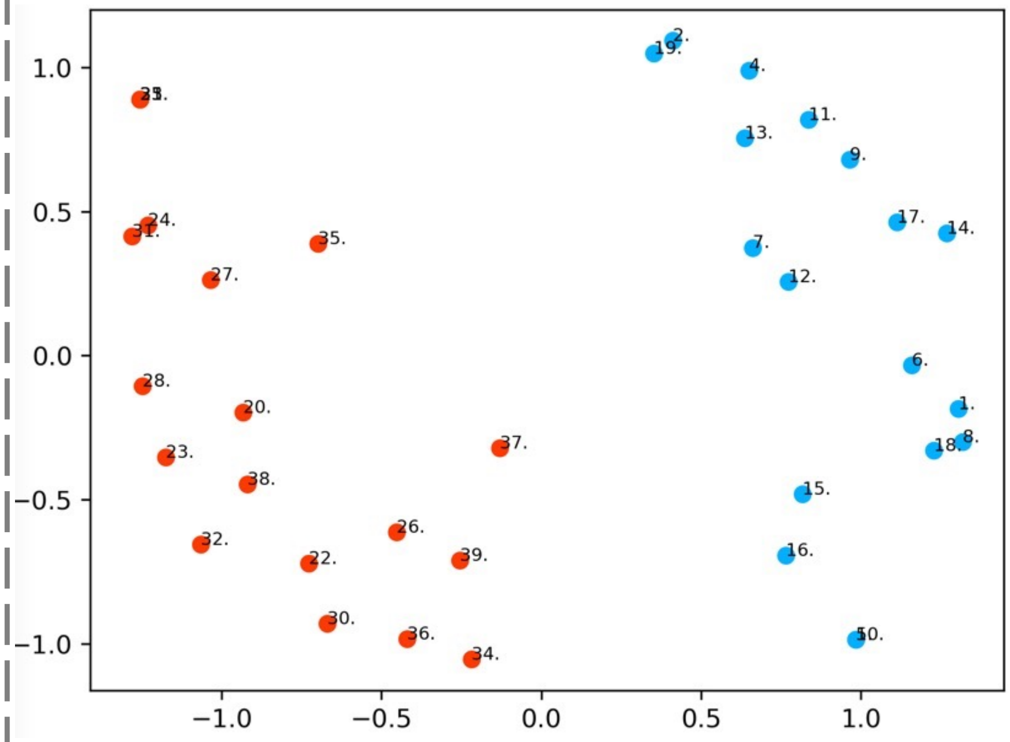


Clustering results of the quantum-classical maximum cut implementations when changing the number of maximum iterations performed

Clustering (3)

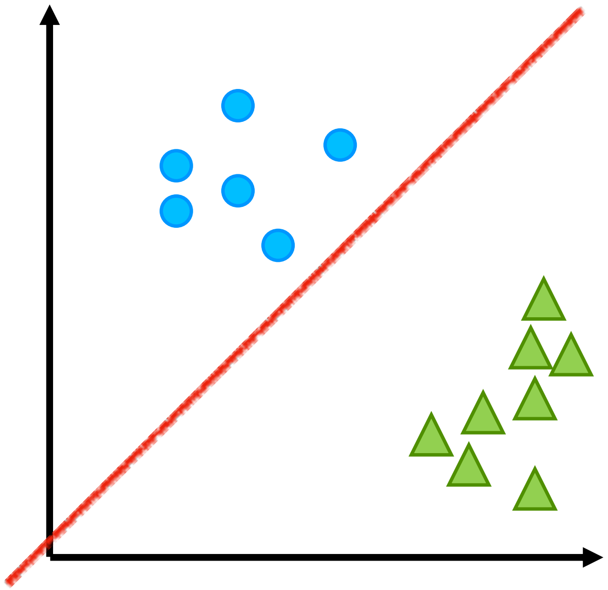


A) Cluster results with classical k-Means



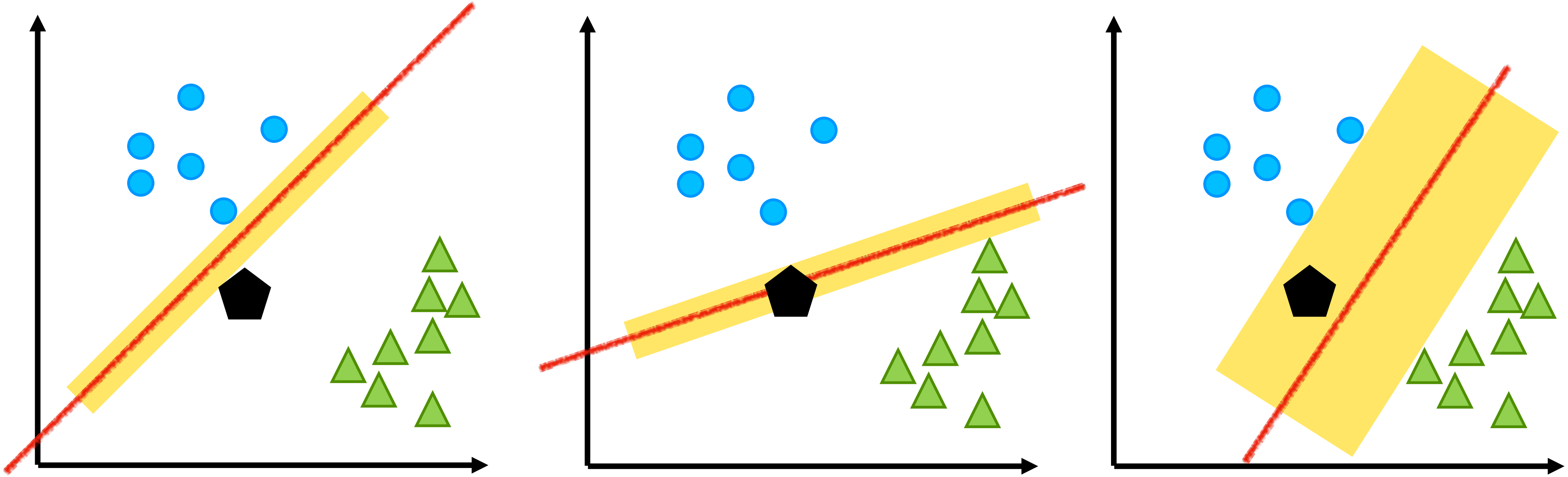
B) Cluster results with quantum-based k-Means.

Classification



- Two classes (blue circles, green triangles).
- Finding a dividing line (hyperplane in general) that distinguishes between these classes.
- New objects are classified by being to the left or right of the line.

Selection of the ”best” hyperplane

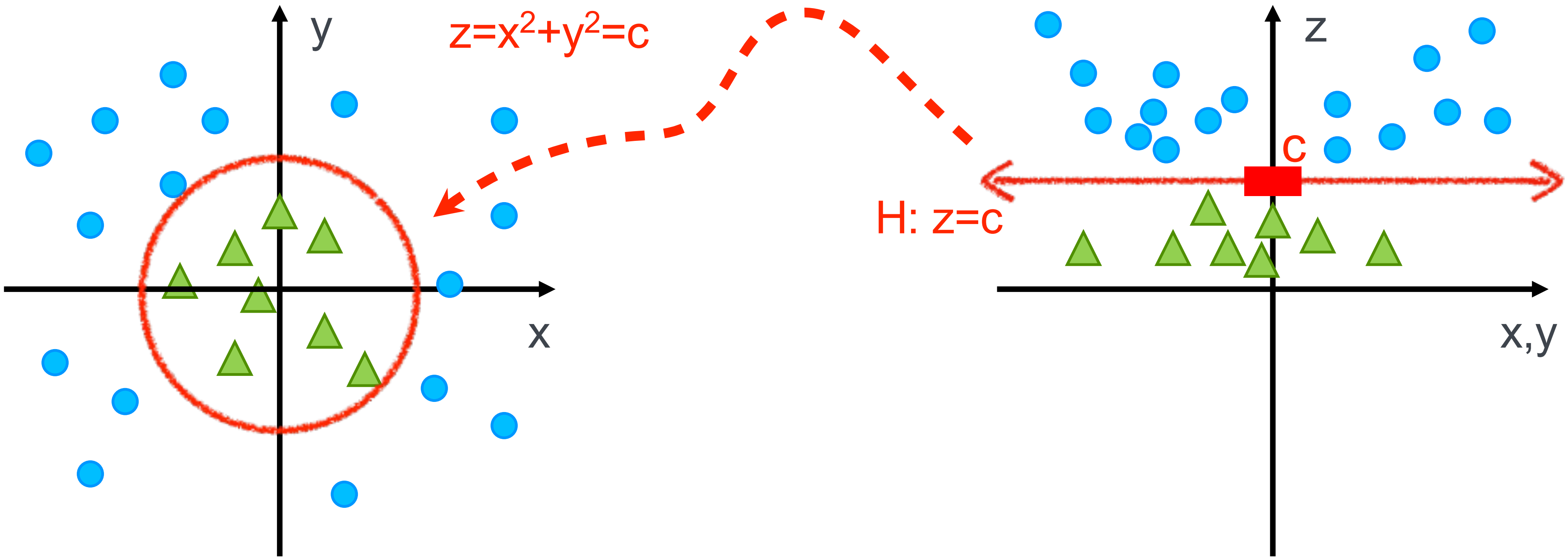


Seems to be a green triangle.

Cannot be classified.

It is clearly a blue circle.

Nonlinear separability



That's what quantum computers are really good at!

HAna
Quantum Humanities Analysis Tool

Documentation | Data Preparation | Feature Engineering | Clustering | Classification | Overview

Initialize Classification

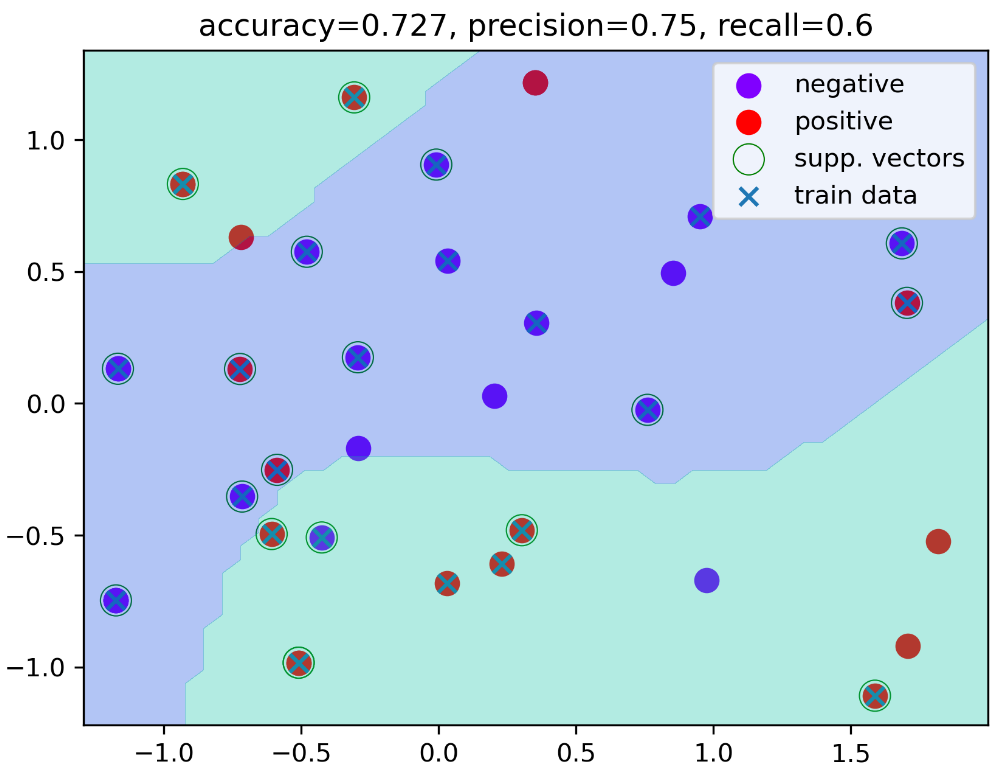
Enter Classification Type: ✓ classicSklearnSVM | qiskitQSVC | qiskitVQC | classicSklearnNN | HybridQNN [initialize]

Initialized Classi

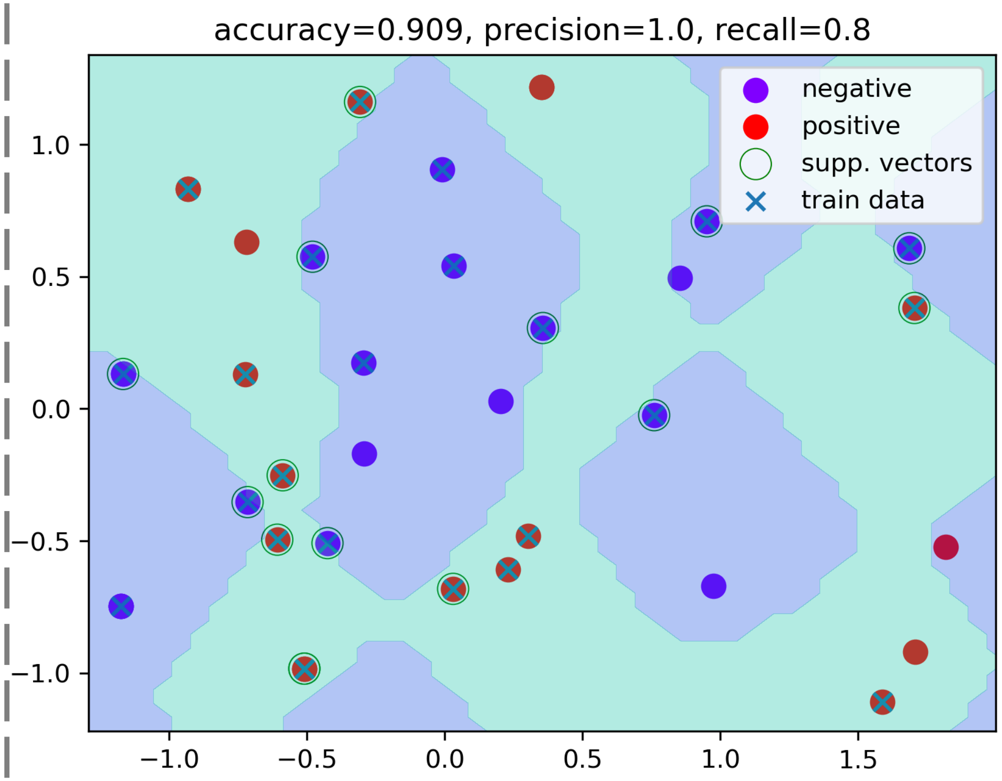
[set parameters]

Parameter	Input	Description
ClassificationType	qiskit Quantum Support Vector Classifier (QSVC; using quantum kernel)	Name of choosen classification type
Feature Map	ZFeatureMap	Feature Map : {'ZFeatureMap', 'ZZFeatureMap', 'PauliFeatureMap'}, (default='ZFeatureMap') Feature map module used to transform data.
Entanglement	linear	Entanglement : {'full', 'linear'}, (default='full') Specifies the entanglement structure.
Repetitions	2	reps : int, (default=2) The number of repeated circuits.
Shots	1024	Shots : int, (default=1024) Number of repetitions of each circuit, for sampling.
QuantumBackend	aer_statevector_simulator	Backend : Enum default(aer_statevector_simulator) A list of possible backends. aer is a local simulator and ibmq are backends provided by IBM.
IBMQ-Custom-Backend		str default("") The name of a custom backend of ibmq.
IBMQ-Token		IBMQ-Token : str, (default='') IBMQ-Token for access to IBMQ online service

Classifier

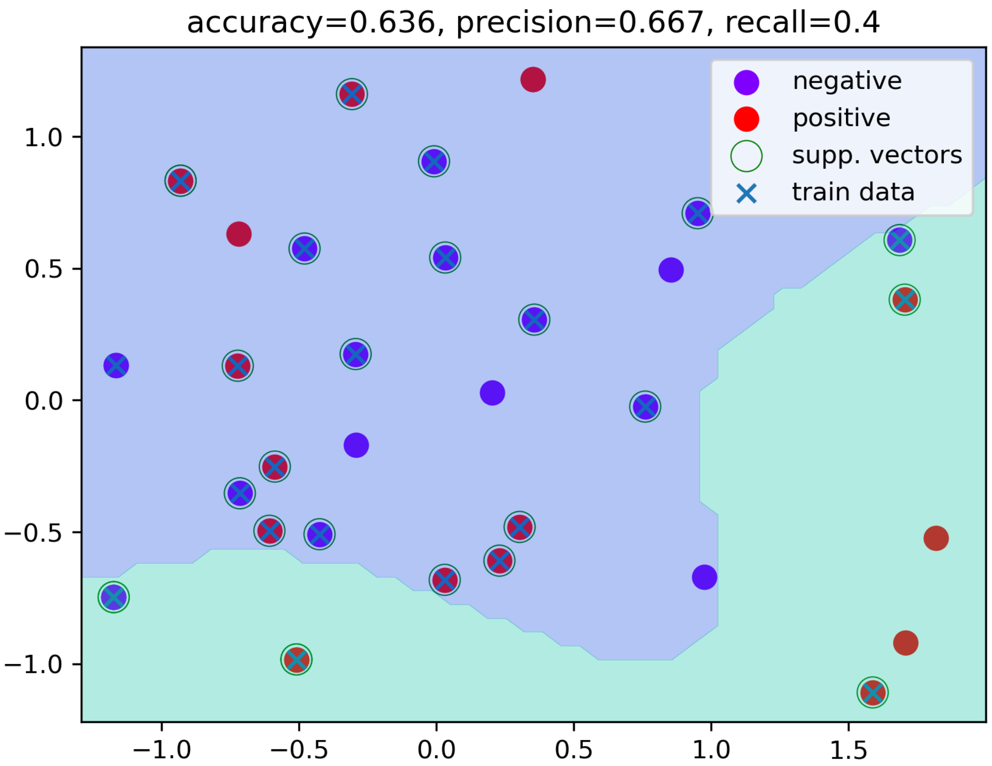


Classification result with classical SVM
(Radial Basis Function (RBF) Kernel)

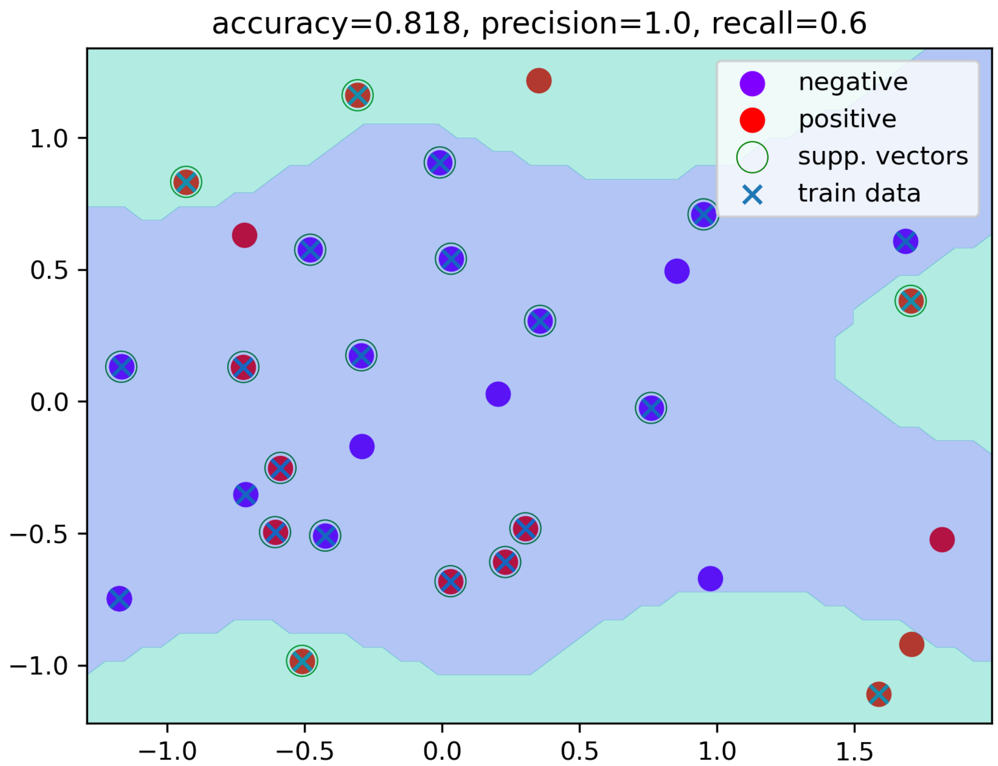


Classification result with quantum-based SVM
(Quantum Kernel Estimation (QKE))

Classifier (2)



Classification result with classic SVM
(Polynomial Kernel Function: Degree 3)



Classification result with classic SVM
(Polynomial Kernel Function: Degree 6)

Goals QHAna

- Identifying patterns candidates in the use case from MUSE
  -> but: Tool independent of presented use case
- Comparing the results of classical and quantum based analysis algorithm
  -> as well as: different values of hyperparameters, different backends.
- Providing easy access for mathematically and physically inexperienced users
- Support of heterogeneous tools in a single analysis pipeline
- Evaluating potentials for further quantum humanities

In future work

- QC Patterns:
  - Integrate patterns in the PlanQK pattern repository
  - Constantly re-evaluate state-of-the-art as quantum computing is growing rapidly
  - Develop a corresponding solution language containing concrete implementations

- QHAna
  - Integration of further algorithms
  - Workflow will be supported
  - Rendering of all algorithms as REST APIs (Invocable from workflows)

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Thank you!

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