

Valeria Repetto, Tutor: Romina D'Aurizio, PhD



THE ITALIAN
EDUCATION
& RESEARCH
NETWORK

Quantum Machine Learning per l'identificazione di marker nei tumori rari

“A Quantum enhanced Machine Learning tool for drug repurposing in Rare Cancer”



BORSISTI DAY

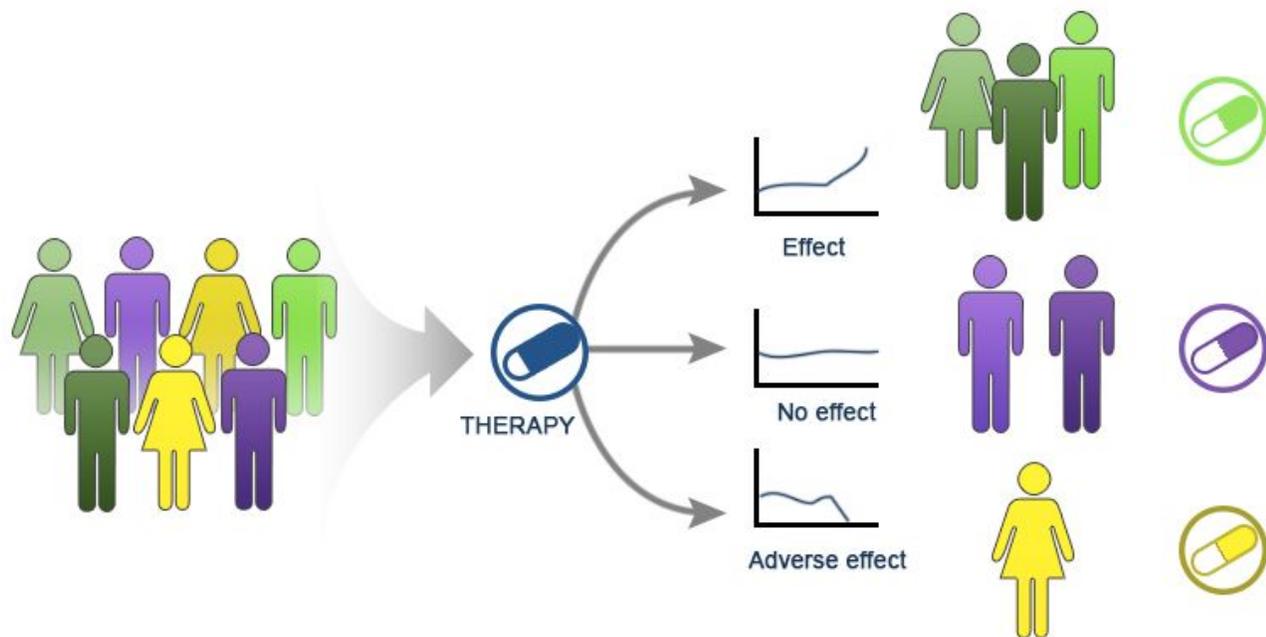
lunedì 27 febbraio 2023

Host institution: IIT-CNR





Medicina di precisione



Necessita di tanti dati

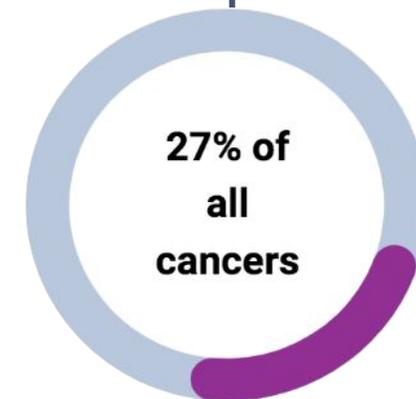


Tumori rari

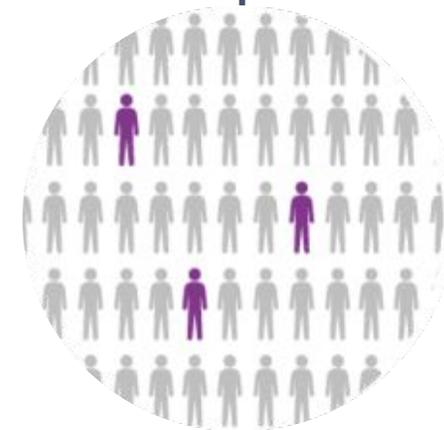
Sono tumori che colpiscono **meno di 6 persone** ogni **100 000 abitanti** ogni anno



COLLETTIVAMENTE I
TUMORI RARI
RAPPRESENTANO

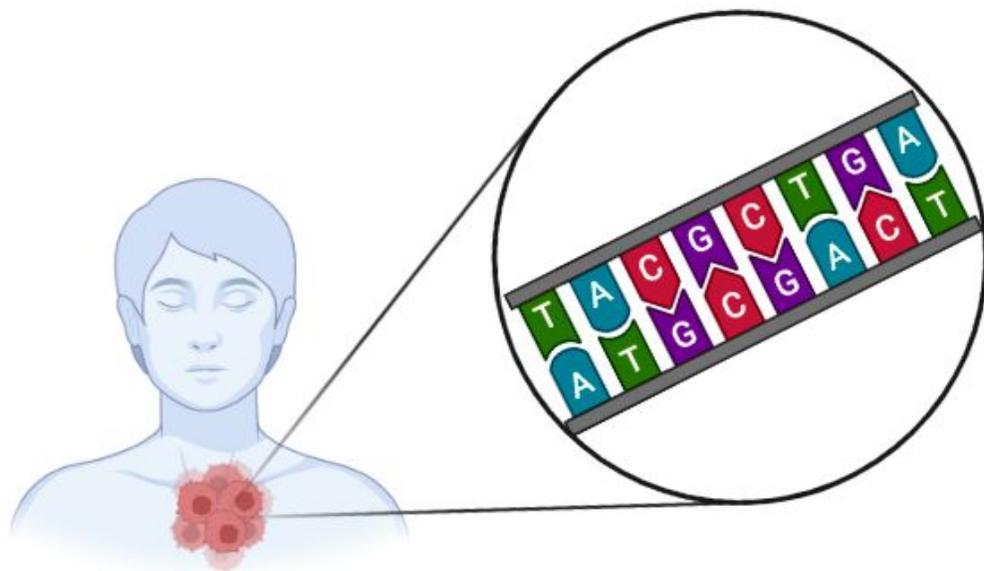


MENO DATI SIGNIFICA
CHE SONO PIÙ **DIFFICILI**
DA STUDIARE

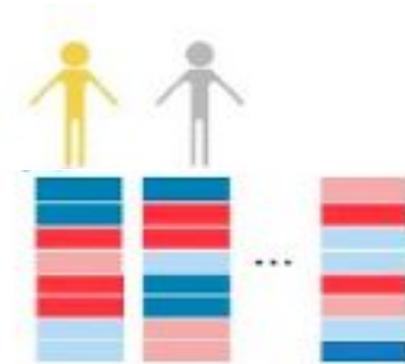




Il Problema



Pochi dati e molto
eterogenei



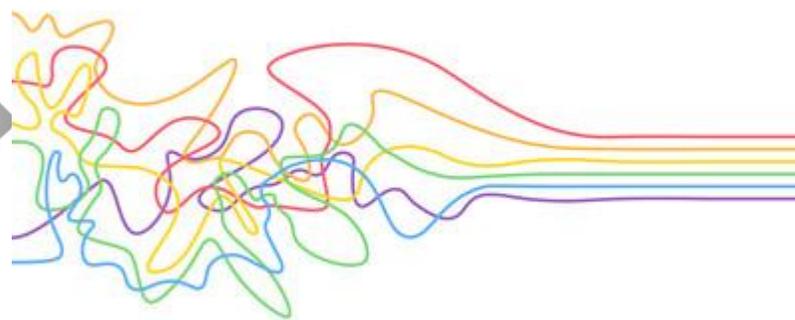
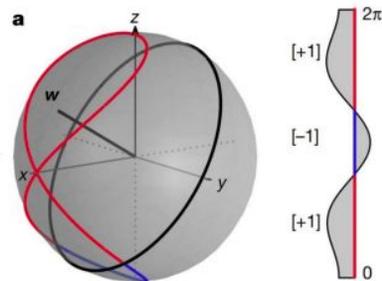
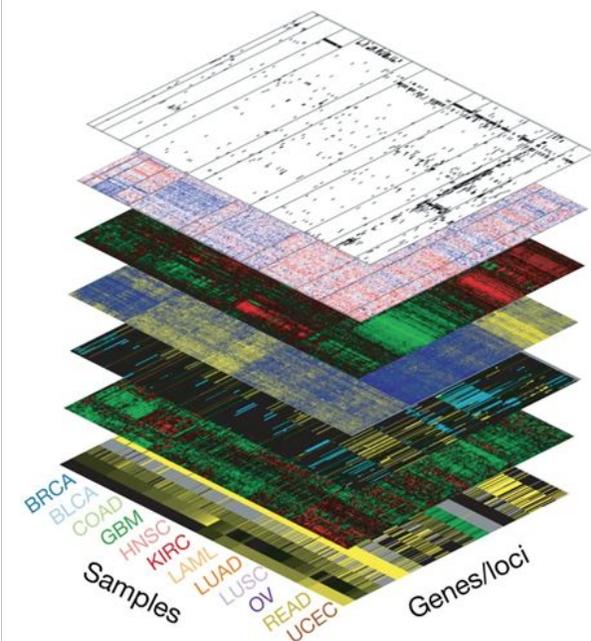
**Identificare
biomarcatori per
ogni paziente**

Approcci classici falliscono



Usare la **computazione quantistica** per lo studio di **Sistemi complessi biologici reali**?

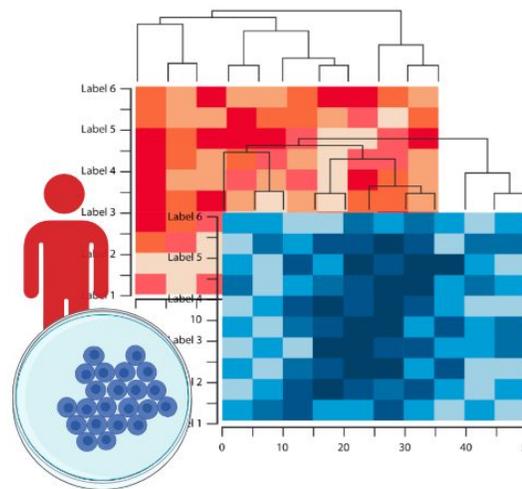
Omics characterizations



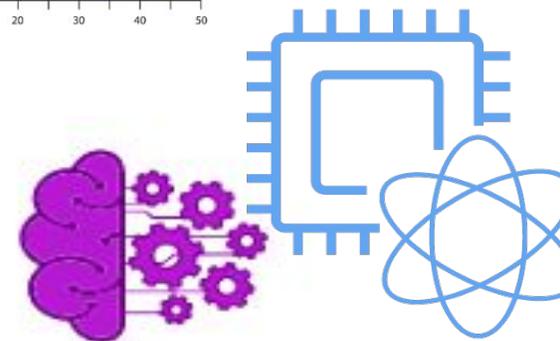


Scopo del progetto

I modelli **classici** spesso non riescono a catturare la **complessità** dei **dati oncologici** specialmente nel caso dei **tumori rari**



Sfruttare il Quantum Machine Learning per identificare **biomarcatori** per **tumori rari**

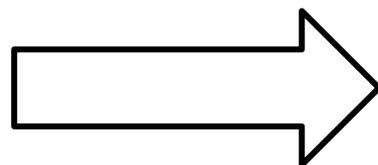




Quantum Computing

La computazione quantistica **cambia il paradigma** computazionale classico sfruttando i principi della **meccanica quantistica**

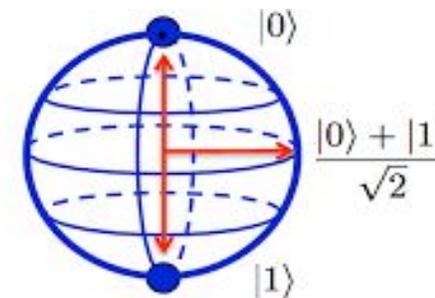
$$\frac{1}{\sqrt{2}}|\text{cat}\rangle + \frac{1}{\sqrt{2}}|\text{dog}\rangle$$



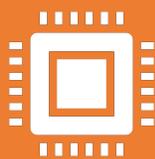
● 0

● 1

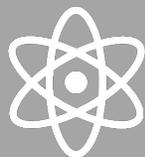
Classical Bit



Qubit



La comunità scientifica è concorde sul riconoscere come questa tecnologia possa superare quella classica in specifiche applicazioni



- Velocità • Problemi di ottimizzazione • Crittografia

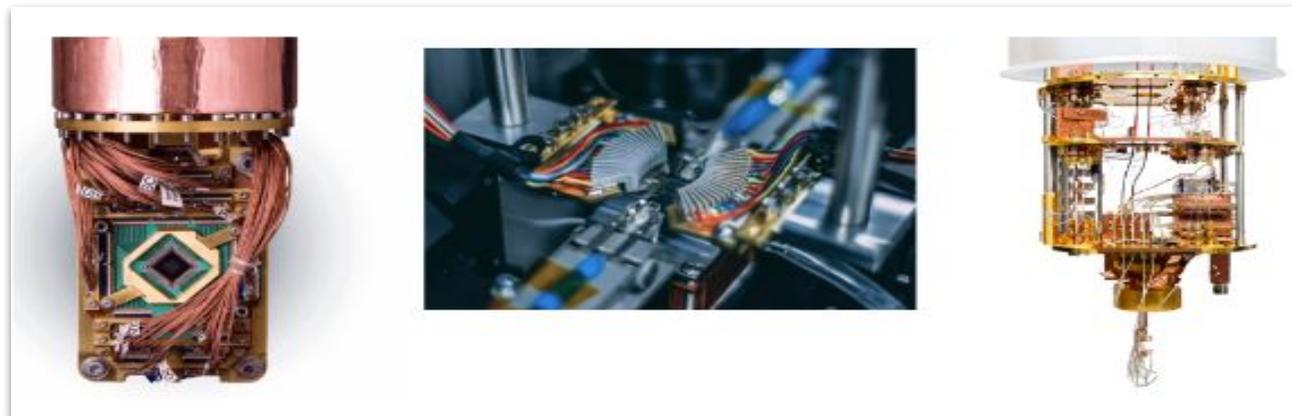


La Computazione Quantistica

IBM Quantum
System One



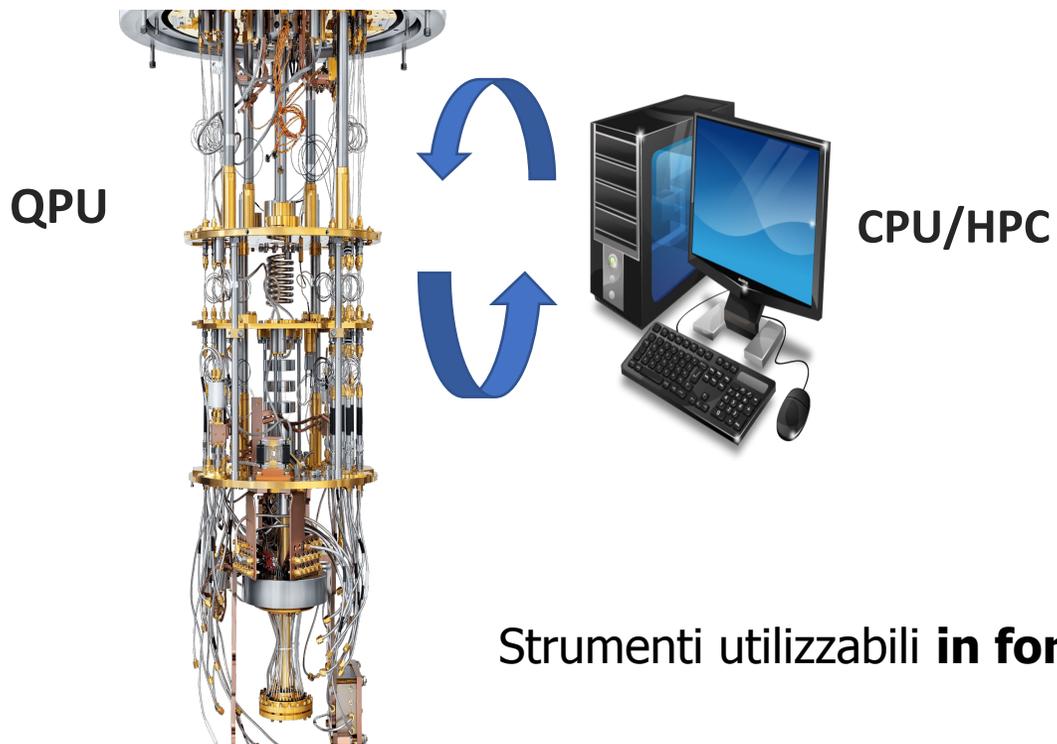
Dove siamo oggi? L'era dei NISQ



NISQ = **Noisy Intermediate-Scale Quantum**
with no error correction



Possiamo usarli in ogni caso?

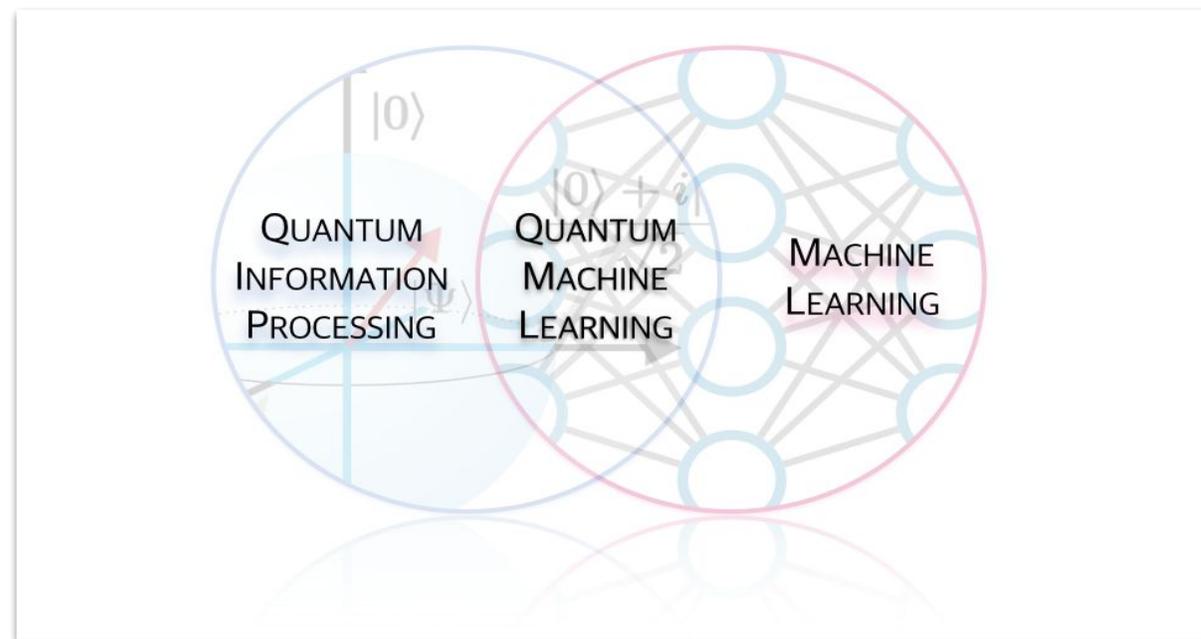


Strumenti utilizzabili **in forma ibrida**



Quantum Enhanced Machine Learning

Algoritmi di **Machine Learning** che possono essere potenziati attraverso l'integrazione con il **dominio quantistico**



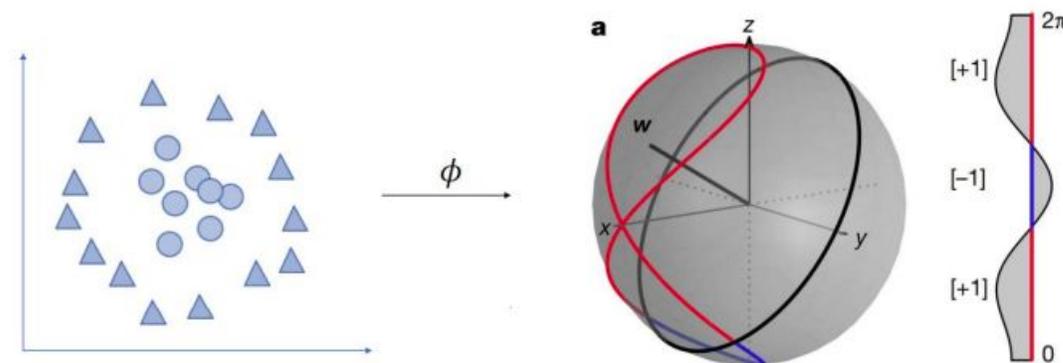


Feature Map:

Codifica input classico in uno stato quantistico

$$\vec{x} \mapsto |\Phi(\vec{x})\rangle = \mathcal{U}_{\Phi(\vec{x})} |0\rangle^{\otimes n}$$

Qual è il limite?



N features = N Qubits



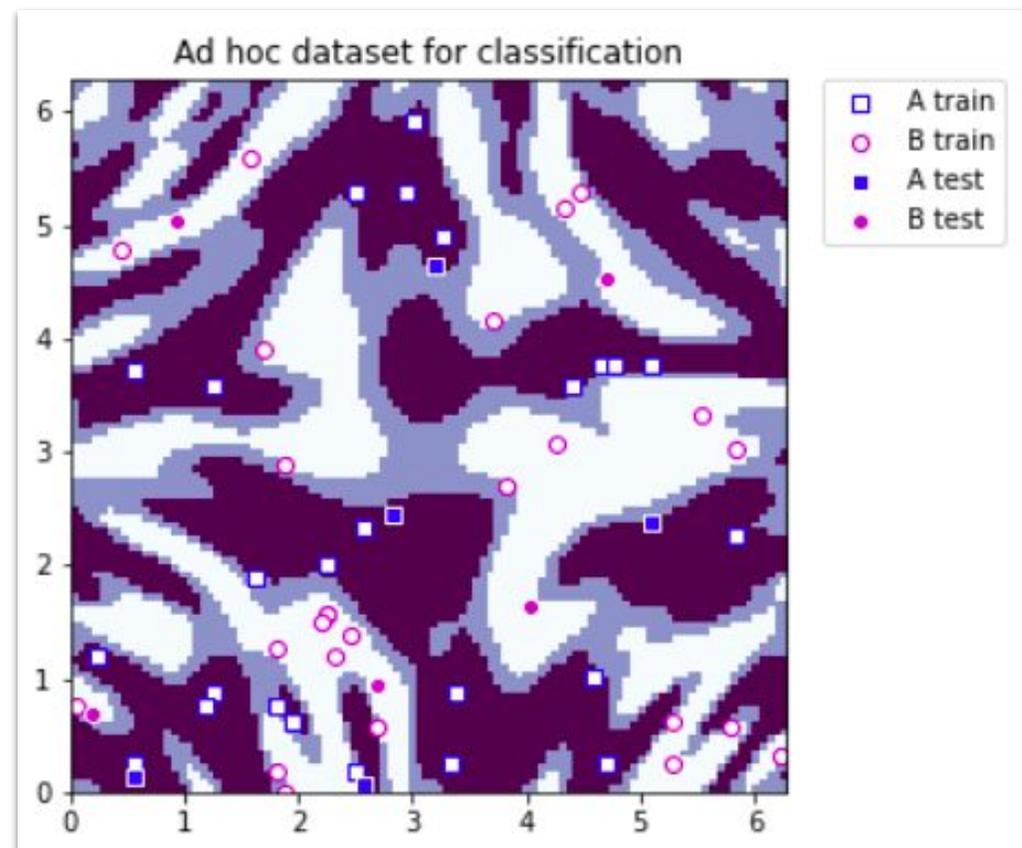
*Image taken from Havlicek et al., 2018



Qual è il vantaggio?

Meno dati ...

**Complessità classicamente
inaccessibile**





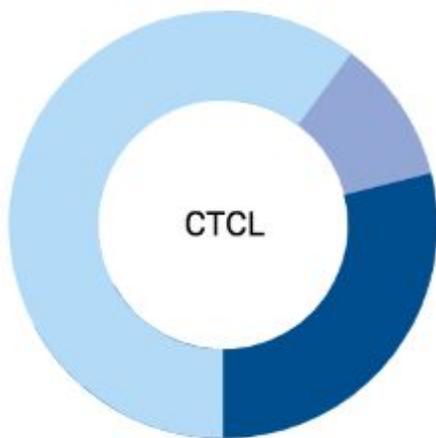
Progetto & sviluppo



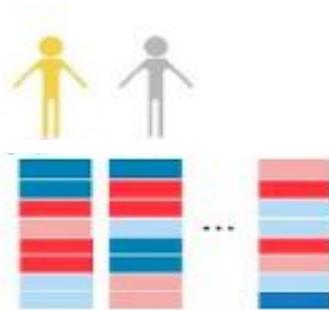
Linfoma Cutaneo delle Cellule T

Due sottotipi principali
particolarmente **aggressivi**

- 60% Mycosis Fungoidea
- 5% Sezary syndrome
- 35% other T-cell lymphomas



Coorti **piccole e eterogenee**

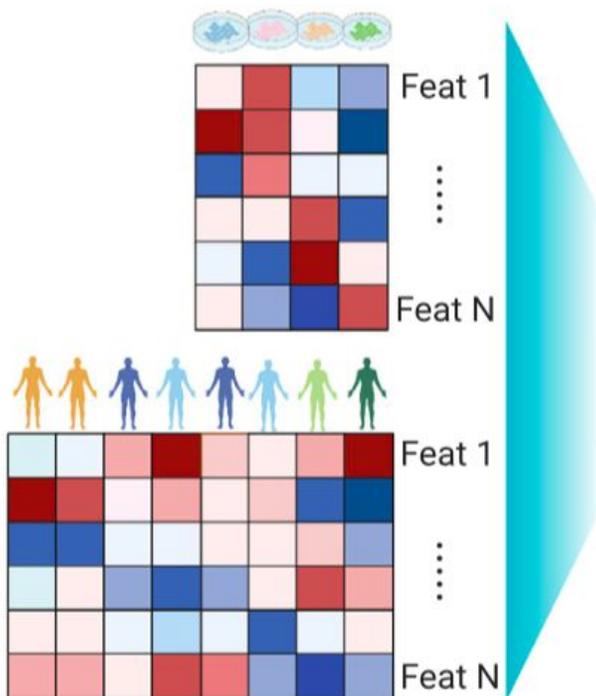


Assenza di **biomarcatori universali**

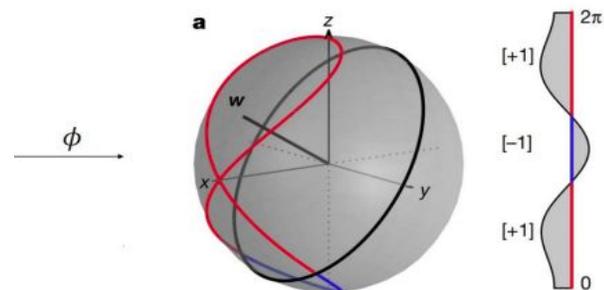




Linee cellulari tumorali e campioni tumorali

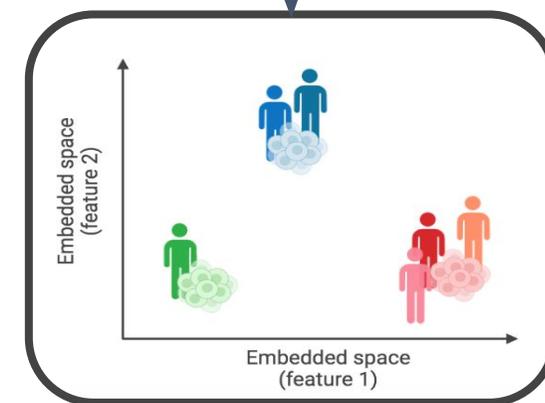
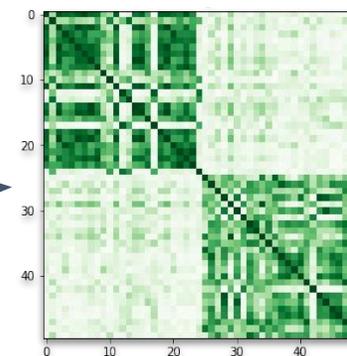


Il progetto



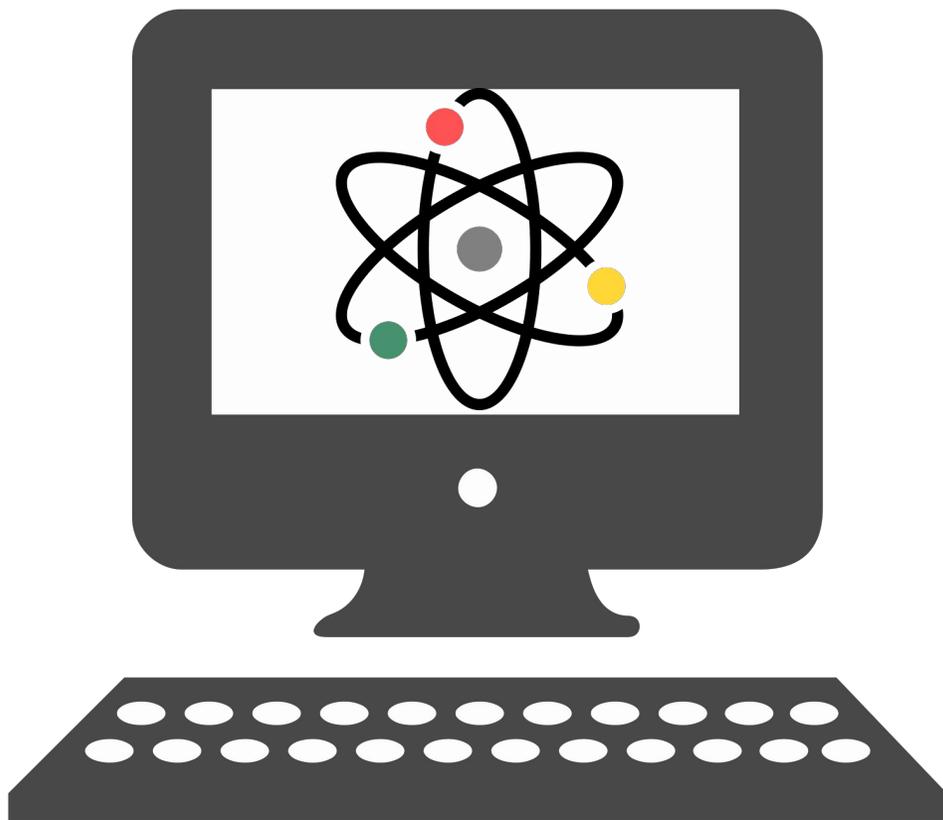
Quantum Machine Learning non-supervisionato

Kernel dati

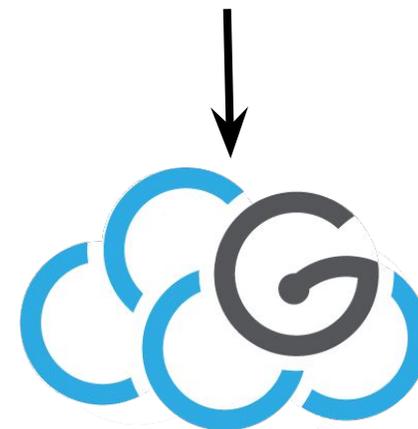




Simulazioni Computer Quantistici



Simulazioni per testare
configurazione ottimale



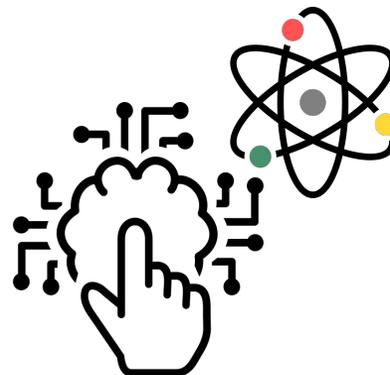
Servizi GARR



Sviluppo

Raccolta , elaborazione dei
dati e riduzione della
dimensionalità

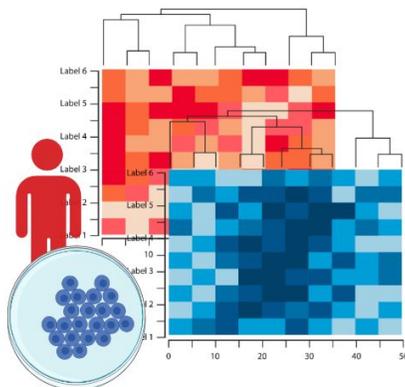
1



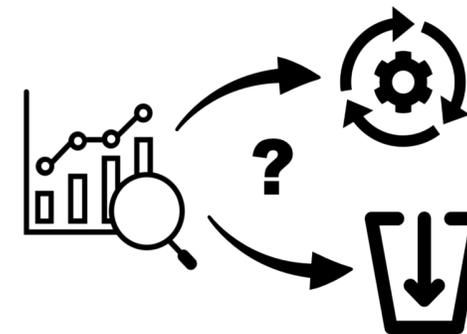
Valutazione e
integrazione risultati

3

2



Codifica quantistica
delle features e calcolo
del kernel

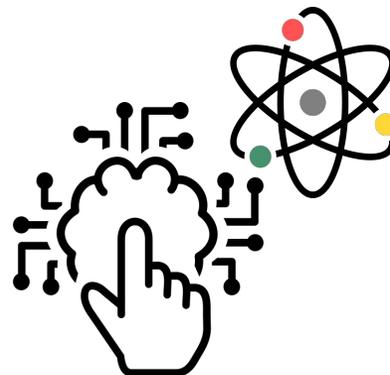
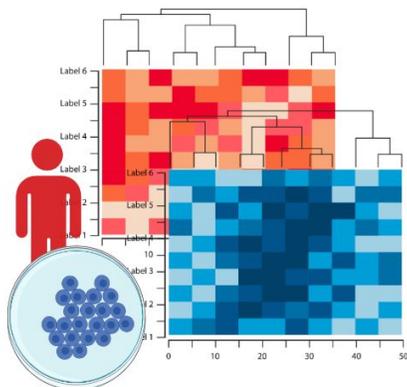




Sviluppo

Raccolta , elaborazione dei
dati e riduzione della
dimensionalità

1

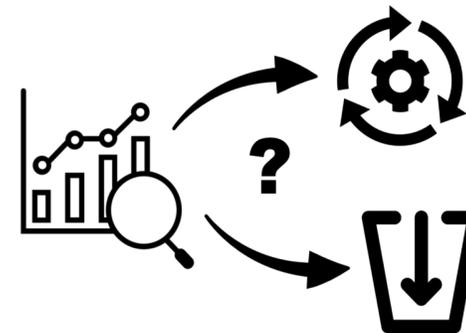


2

Codifica quantistica
delle features e calcolo
del kernel

Valutazione e
integrazione risultati

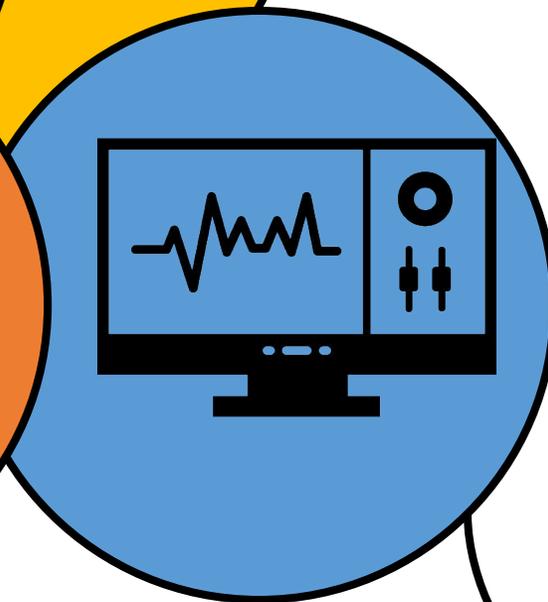
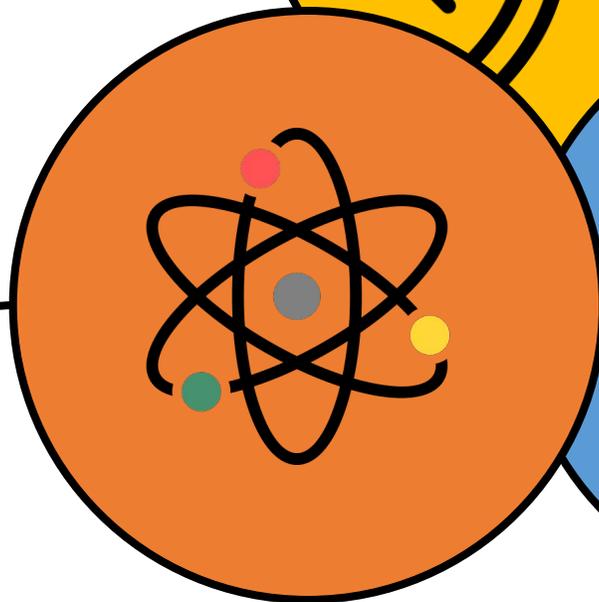
3





Risultati attesi

**Applicazione
Quantum
Machine
Learning**



**Nuovi
Marker**

**Risorsa
esplorazione
Risultati**



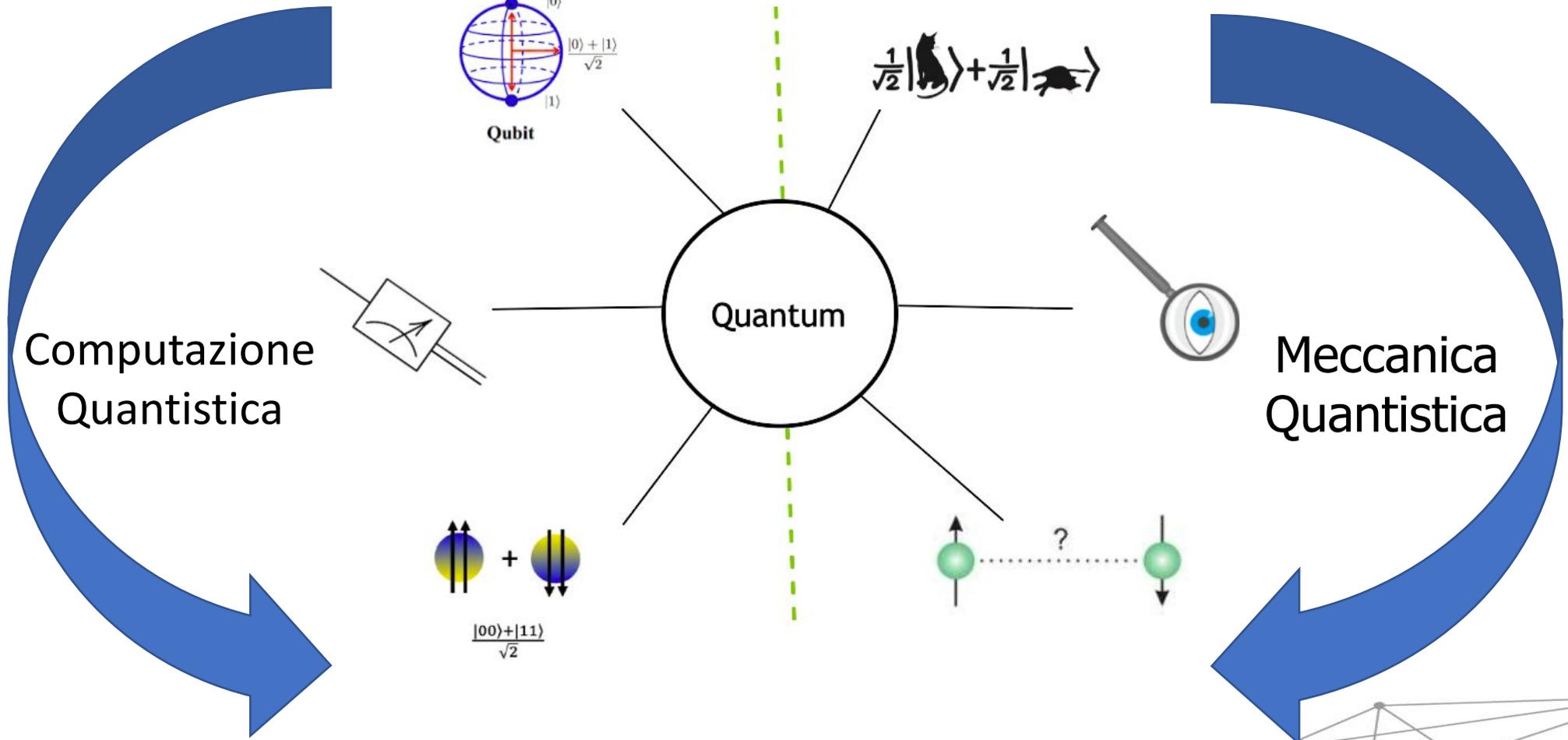
Grazie per l'attenzione



Slides di supporto

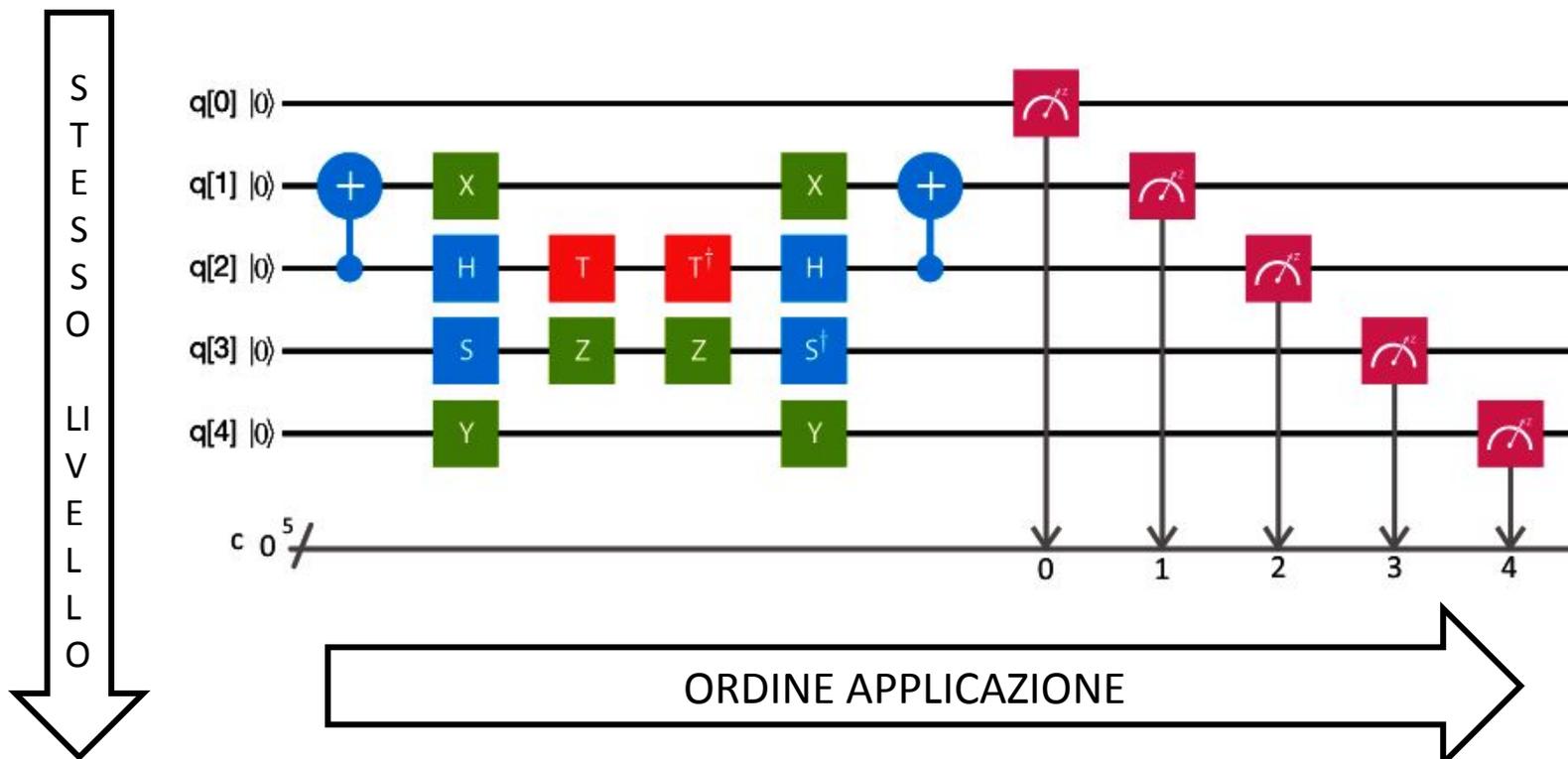


Quantum Computing





Gate Model

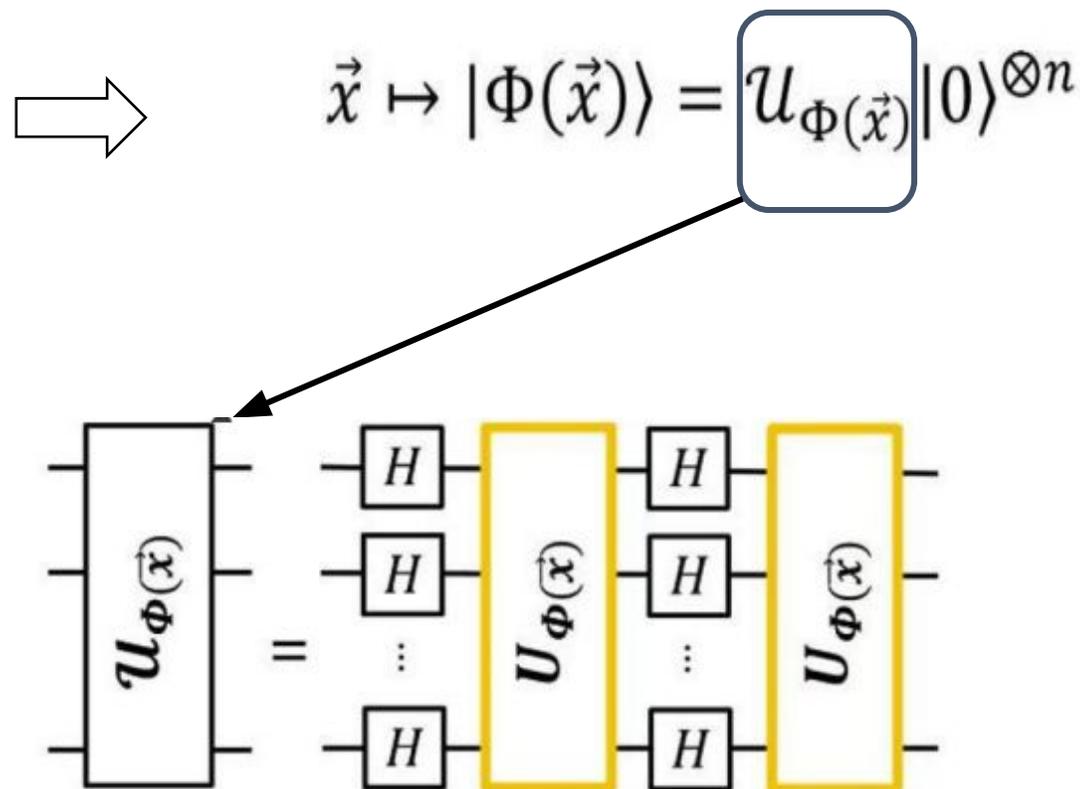
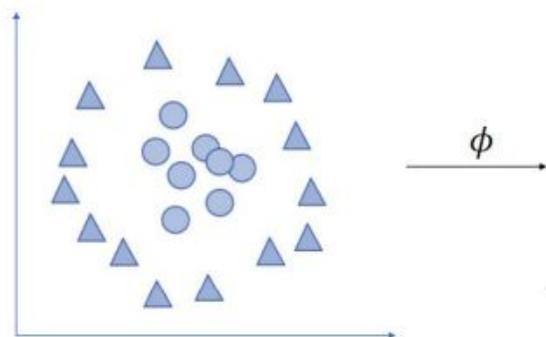




Circuit implementation

Feature Map: Encodes classical input data into a quantum state.

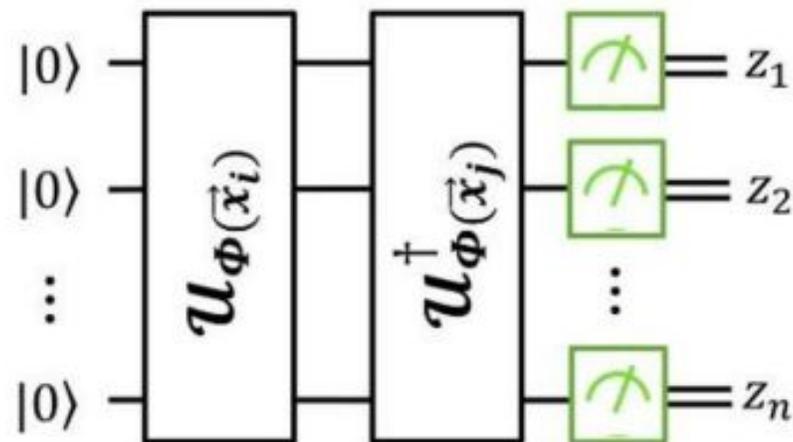
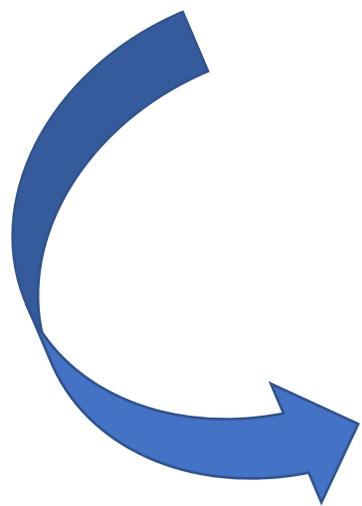
Different feature maps lead to different kernels and accordingly influence on the classification accuracy





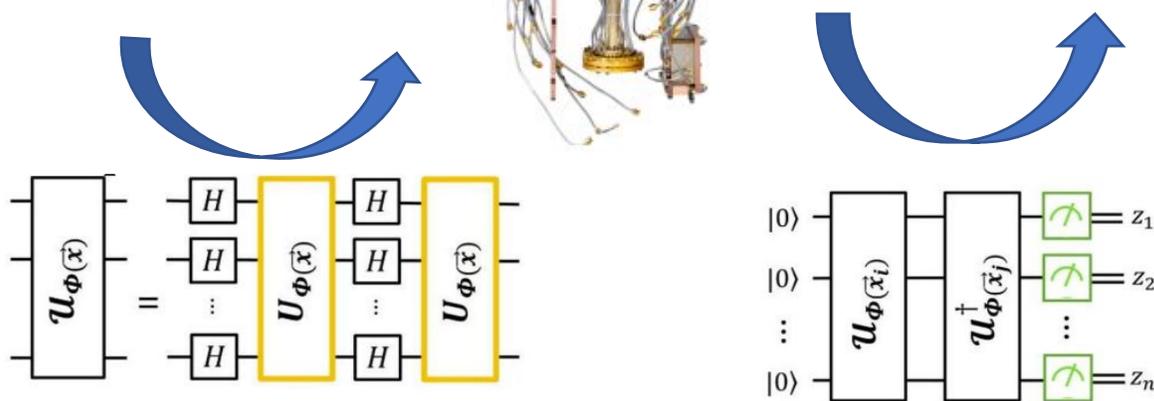
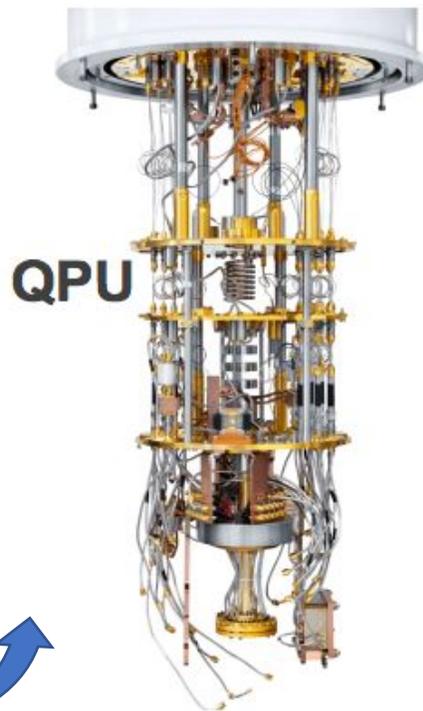
Quantum Kernel: Entries are Inner products between two states. The exact evaluation is obtained by a similar circuit

$$K(\vec{x}_i, \vec{x}_j) = |\langle \Phi(\vec{x}_i) | \Phi(\vec{x}_j) \rangle|^2 = \left| \langle 0 | \mathcal{U}_{\Phi(\vec{x}_j)}^\dagger \mathcal{U}_{\Phi(\vec{x}_i)} | 0 \rangle^{\otimes n} \right|^2$$



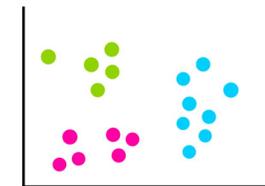
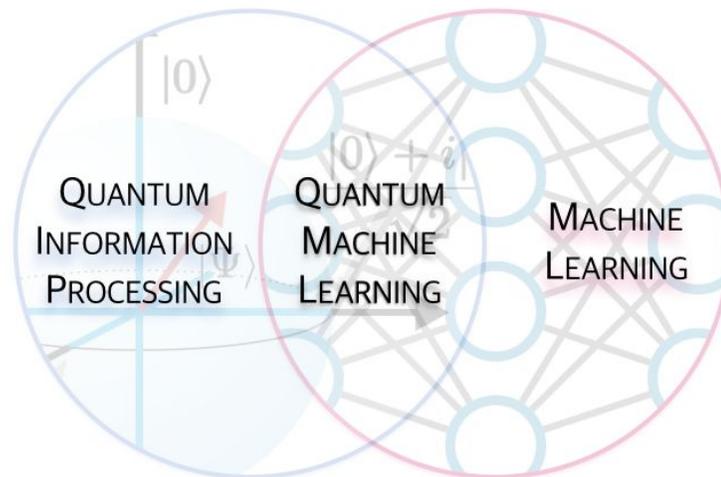
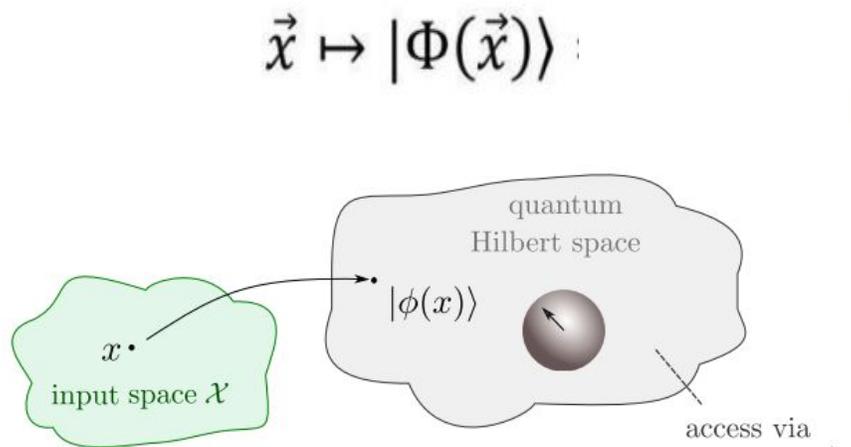


GIORNATA DI INCONTRO BORSE DI STUDIO GARR "ORIO CARLINI"
BORSISTI DAY 2023

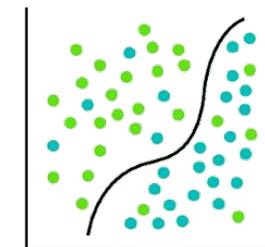




Metodi di kernel Quantistici



Clustering



Classification

Quantum Enhanced Machine Learning

$$K(\vec{x}_i, \vec{x}_j) = |\langle \Phi(\vec{x}_i) | \Phi(\vec{x}_j) \rangle|^2$$

Quantum kernels



Linee cellulari tumorali

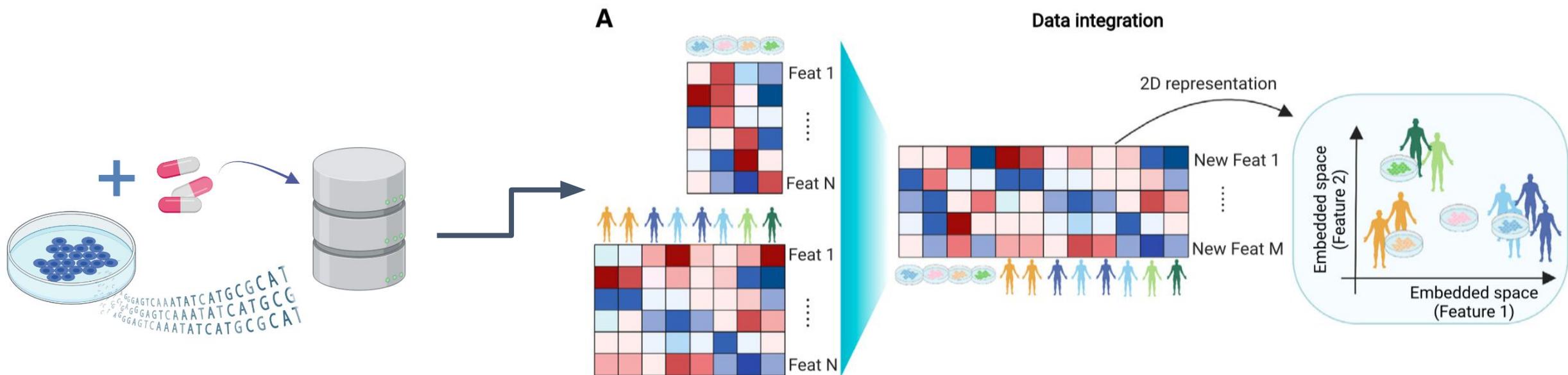


Image from: Computational estimation of quality and clinical relevance of cancer cell lines; Lucia Trastulla et al; Molecular Systems Biology, 2022



ibmq_montreal

Details

27 Qubits	Status: ● Online	Avg. CNOT Error: 1.331e-2
128 QV	Total pending jobs: 164 jobs	Avg. Readout Error: 3.301e-2
2K CLOPS	Processor type ⓘ: Falcon r4	Avg. T1: 117.79 us
	Version: 1.11.14	Avg. T2: 103.56 us
	Basis gates: CX, ID, RZ, SX, X	Providers with access: 1 Providers ↓
	Your usage: 1293 jobs (3 pending)	Supports Qiskit Runtime: Yes

Your upcoming reservations 0

Calibration data Last calibrated: 12 minutes ago ↓

Map view | Graph view | Table view

Qubit: Frequency (GHz)
 Avg 4.998
 min 4.835 max 5.105

Connection: CNOT error
 Avg 1.331e-2
 min 6.020e-3 max 3.545e-2

Implementazione pratica

Libreria python QISKIT

QISKIT



Qiskit

Most used quantum SDK with access of quantum devices

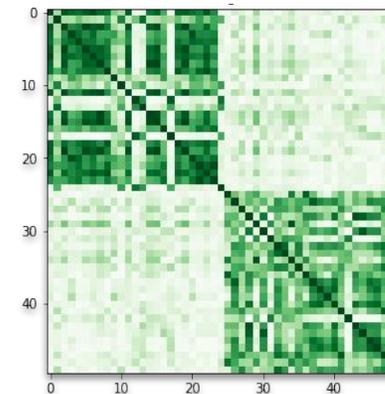
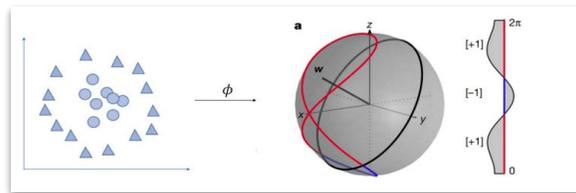
Machine learning modules



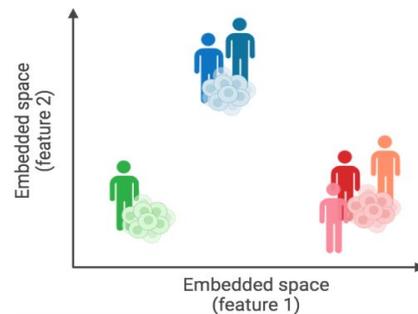
QML non-supervisionato
per mappare CCL e CTCL

Quantum Machine learning :

Quantum encoding



Valutazione risultati:

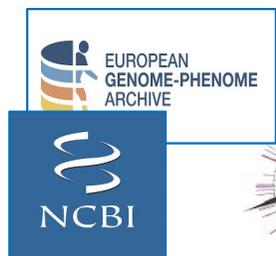


Integrazione risultati per la
visualizzazione e determinazione
terapie personalizzate

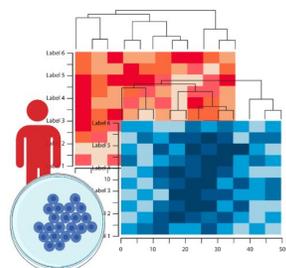


Valutazione **cluster pazienti** e
estrazione **fattori determinanti**

Raccolta e elaborazione dati:



Raccolta **datasets pubblici** di **omiche** e
elaborazione **standard**

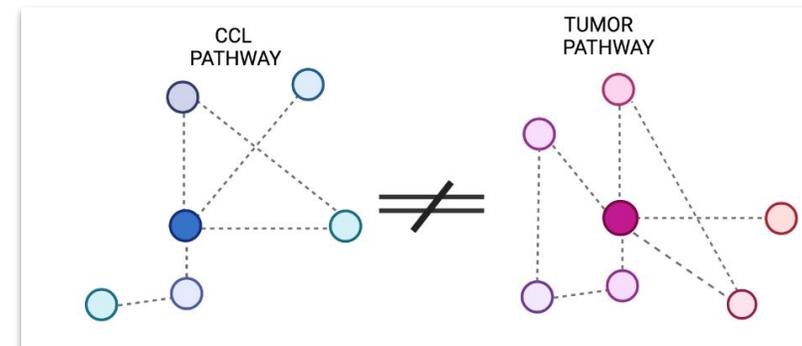




Exploiting Cancer Cell Lines(CCLs)

Fundamental tools for tumours research as they are **experimentally easy** to manipulate and suitable for **high-throughput screens**

(a) **Systematic** differences solvable with **computational tools**



Main issues:

(b) **Lack of CCLs** for most **rare tumors**





Data collection and Preprocessing

RACCOLTA DATI



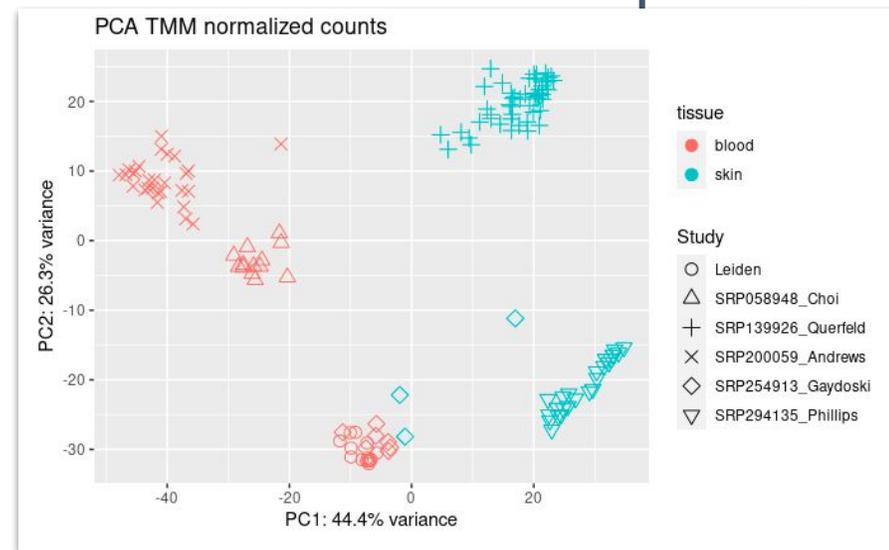
Data-set
Pubblici
RNA-seq

CTCL DATA

ESTRAZIONE MATRICE DELLE CONTE

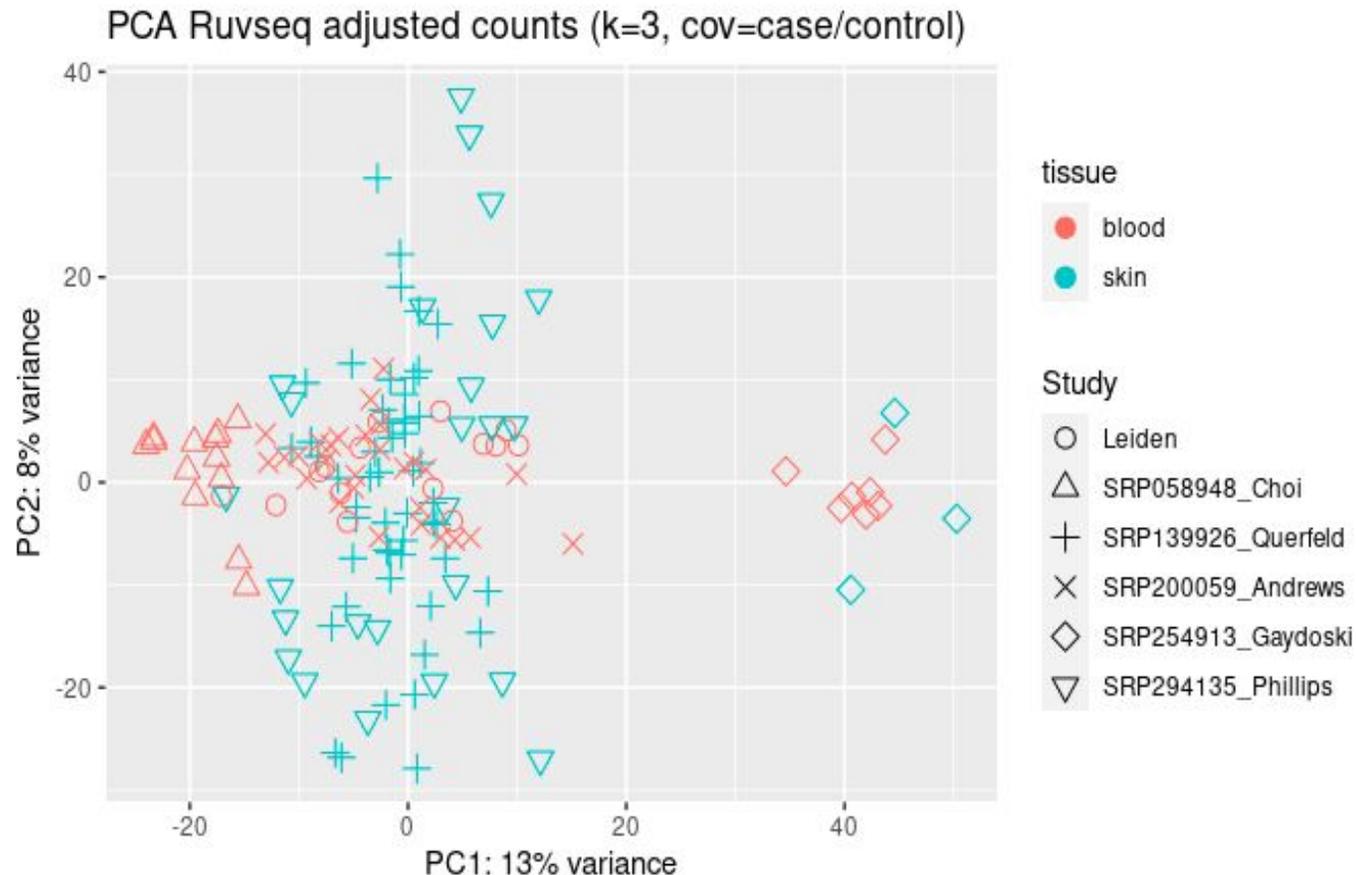
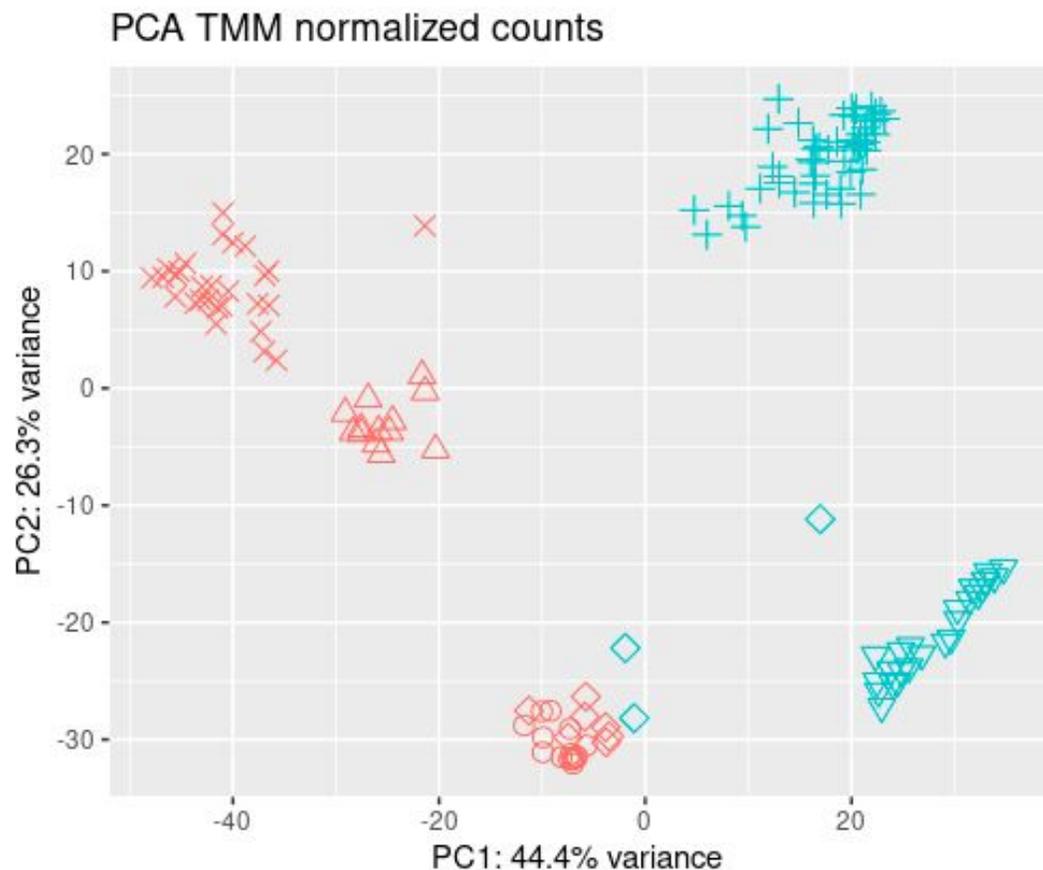


143
Campioni
Provenienti da
6 studi





Correzione di Batch





Future steps

Comparazione dati **linee cellulari tumorali** e **CTCL**

Applicazione **Quantum Machine Learning**

Valutazione e integrazione risultati

Rimozione **differenze sistematiche**

Manipolazione del dato nel **dominio quantistico**

Estrazione **cluster pazienti** e **pattern informativi**