Braid-Based Quantum Simulations on Classical Computing Architectures

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Abstract: —This article presents a novel approach to simulating quantum and braid-based data encoding schemes on classical computing architectures, with a focus on predictive modeling in biomedical applications. Drawing on mathematical structures from quantum information theory and braid theory, we demonstrate that braid-based encodings can effectively represent complex, multi-agent interactions such as those found in combinatorial cancer therapies. Notably, hybrid encoding models that combine braid-based features with conventional biological data yielded improved performance in predicting synergistic drug combinations while maintaining low toxicity estimates. These findings support our primary hypothesis that classical systems can simulate quantum-inspired behaviors with sufficient fidelity, and further suggest that hybrid models offer enhanced resilience and predictive power. This work opens promising directions for quantum-inspired bioinformatics and highlights the interpretability and practical value of braid-based abstractions in classical simulations of complex systems.

Keywords:—braid theory, quantum information theory, simulation, drug synergy, prediction, oncology.

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1. Introduction

Increasingly, the modeling of complex systems requires a multidisciplinary approach due to its dynamic and multidimensional nature. Classical artificial intelligence techniques, notably neural networks, specifically deep learning, have shown their effectiveness in prediction and diagnosis. However, these methods encounter limits in terms of scalability, parallel processing and sometimes generalization capacity. Also, AI based computing has often been limited either by the lack of available data or by their computing capabilities to process large volumes of data [1].

This is the case with personalized medicine, which relies on the interpretation of multidimensional data. The increasing complexity of medical data requires powerful processing models capable of extracting non-trivial correlations between biomarkers, imaging results and genetic data.

Already, data science allows methods to use data in order to provide answers to problems. The data science includes data preprocessing, feature engineering, modeling and evaluation. Ever, conventional models reach their limits when faced with highly correlated data sets.

The tension between data availability and computational capacity has shaped the evolution of AI for decades.

In our studies, we are interested in quantum computing in its purely logical aspect for a hybrid architecture. Our articles [2] & [3] can demonstrate this. As quantum computing continues to evolve, its theoretical frameworks, such as quantum entanglement, superposition, and topological quantum states, are inspiring new paradigms in classical computation. Furthermore, exploring paradigms such as quantum computing and braid-based modeling, integrated into a hybrid architecture, can help overcome the above limitations.

Indeed, quantum computing [4] offers a promising new avenue to overcome these obstacles. And considering only the aspect of the data. As stated in [5], quantum data is much more convenient to process with machine learning than the original classical data given the possibility of exploiting superposition states or quantum parallelism, and properties such as entanglement, that do not exist in the classical domain. These are basis encoding techniques that constitute the key to translating classical data into quantum formats for machine learning tasks.

In the other side, braid-based modeling applies braid theory, a branch of topology, to the structure and dynamics of neural networks. This approach introduces topological robustness, nonlinear dynamics, and structural optimization into deep learning systems [6].

This article presents a novel approach to simulating quantum and braid-based data encoding schemes on classical computing architectures, with a focus on predictive modeling in biomedical applications. Drawing on mathematical structures from quantum information theory and braid theory, we demonstrate that braid-based encodings can effectively represent complex, multi-agent interactions such as those found in combinatorial cancer therapies. Notably, hybrid encoding models that combine braid-based features with conventional biological data yielded improved performance in predicting synergistic drug

combinations while maintaining low toxicity estimates. These findings support our primary hypothesis that classical systems can simulate quantum-inspired behaviors with sufficient fidelity, and further suggest that hybrid models offer enhanced resilience and predictive power. This work opens promising directions for quantum-inspired bioinformatics and highlights the interpretability and practical value of braid-based abstractions in classical simulations of complex systems.

What are we trying to explain?

Primary Hypothesis (H_1): "Classical computers can simulate quantum and braid-based data encoding schemes with sufficient fidelity to replicate key quantum behaviors, such as superposition, entanglement, and topological robustness, within constrained computational resources."

Secondary Hypothesis (H_2): "Hybrid encoding models that combine quantum and braid-based principles yield more resilient and efficient data representations than either method alone when implemented on classical architectures."

2. Methods

Theories on quantum information and quantum computing are widely developed in several articles and books. There is no intention to do so in this article since the study presented is oriented towards the representation and encoding of data based on quantum and braids. In this sense, we will, however, calm down a little more on the notions related to braids.

2.1 Quantum Computing

Quantum information theory [7] uses the principles of quantum mechanics like superposition and entanglement to perform computations potentially more efficiently than classical systems.

The following describes useful concepts directly applicable to the quantum braiding and the topological quantum computing.

a) Basis States (binary encoding)

In a qubit, $|0\rangle$ and $|1\rangle$ are the basis states corresponding to vectors:
- $|0\rangle = [10]$
- $|1\rangle = [01]$

b) Superposition

A qubit can be represented as a two-dimensional vector in a Hilbert space. Unlike classical bits, which exist in states 0 or 1, qubits can exist in a superposition of both states:

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \qquad (1)$$

where: α and β are complex numbers such that $|\alpha|^2 + |\beta|^2 = 1$.

c) Entanglement

A quantum phenomenon where the state of one qubit is dependent on the state of another, regardless of distance. This non-local correlation is a key resource in quantum encoding and computation.

One of the simplest entangled states is the Bell state [7]:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\,(|00\rangle + |11\rangle) \qquad (2)$$

This means:
- If you measure the first qubit and get 0, the second is 0.
- If you get 1, the second is 1.

But until measurement, both are in a superposition.

d) Quantum Gates

Quantum gates are unitary operators, and are described as unitary matrices relative to some orthonormal basis.

Quantum logic gates are represented by unitary matrices. A gate that acts on n qubits is represented by a n^2 x n^2 unitary matrix.

Certainly, there are several door models. Wikipedia [8] offers a comprehensive overview of quantum gates. We have selected two of them, namely: the Pauli gates and the Controlled gates.

Pauli gates: The Pauli gates (X,Y,Z) are the three Pauli matrices ($\sigma_x\sigma_y\sigma_z$) and act on a single qubit. The Pauli-X gate is the quantum equivalent of the NOT gate for classical computers.

$$X = \sigma_x = NOT = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Controlled gates: Controlled gates act on 2 or more qubits, where one or more qubits act as a control for some operation. anyons. The CNOT (or controlled Pauli-X) gate can be described as the gate that maps the basis states $|a, b\rangle \mapsto |a, a \oplus b\rangle$, where $\oplus$ is XOR.

2.2 Braid Theory

Topological quantum computing leverages the mathematical field of braid theory, where information is encoded in the braiding of quasi-particles called anyons.

Braids and topological quantum computing are important concepts of our study, we suggest you read the following articles and books: have also been explored in articles such as [9], [10] & [11].

e) Anyons

In two-dimensional spaces, anyons exhibit non-trivial statistics.

Using Dirac notation and in a quantum mechanical system an anyon representing a state 1 is ψ_1 and an anyon representing a state 2 is ψ_2. A system with two indistinguishable particles is expressed as $|\psi_1\,\psi_2\rangle$.

Furthermore, in topological quantum computing, information is encoded in the collective state of multiple anyons, not in any single particle. This makes the system resistant to local errors. Thus, a qubit can be formed by grouping several anyons together. The quantum state of this group determined by how the anyons are braided represents the logical 0 or 1 of the qubit.

f) Braiding

Braiding refers to the process of exchanging anyons [12] in specific patterns, which can encode quantum information in a topologically protected way, making it robust against noise and errors. Braiding anyons means moving them around each other in space-time. When two anyons are exchanged, the system's wavefunction picks up a phase factor or undergoes a unitary transformation:

Abelian anyons: The wavefunction gains a phase. It formalizes as:

$$|\psi_i\rangle = e^{i\theta}|\psi_i\rangle \quad (3)$$

where $e^{i\theta}$ is a phase factor. is 1.

Non-Abelian anyons: Non-Abelian statistics enables complex entanglement structures for richer data representations. The exchange corresponds to a matrix operation on a degenerate ground state space, forming a representation of the braid group.

With two particles the wavefunction can be expressed as:

$$|\psi_1\ \psi_2\rangle = e^{i\theta}|\psi_1\ \psi_2\rangle \quad (4)$$

g) Braid Groups

The braid group B_n describes the mathematical structure of *n* strands being braided in space. Each braid corresponds to a sequence of exchanges between adjacent strands, and the group is generated by elements $\sigma_1, \sigma_2, ..., \sigma_{n-1}$, where: σ_i represents the exchange of strand i with strand $i+1$.

These generators satisfy the relations:

- $\sigma_i\sigma_j = \sigma_j\sigma_i$ *for* $|i-j|>1$
- $\sigma_i\sigma_{i+1}\sigma_i=\sigma_{i+1}\sigma_i\sigma_{i+1}$ *methods.*

These relations define the Artin braid group [13], [14], which is central to topological quantum computing.

Braid groups (e.g., Artin braid group) are used to formalize the braid.

Let each σ_i represented by a unitary matrix. The full braid sequence is a product of these matrices:

$$U_{braid} = \rho(\sigma_1)\cdot\rho(\sigma_2)\cdot\rho(\sigma_1) \quad (5)$$

where $\rho(\sigma_i)$ is the matrix representation of the braid generator.

A braid word is a sequence of these generators. Each braid is represented as a word in the group, such as $\sigma_2^{-1}\ \sigma_1\ \sigma_2\ \sigma_1^{-1}$, where σ_i denotes a crossing between strands i and i+1.

h) Braid Encoding into Quantum-Compatible Formats

Each braid generator, in table 1, is mapped to a quantum gate that entangles two qubits:

TABLE I. MAP BRAID GENERATORS TO QUANTUM GATES

Braid Generator	Quantum Gate	Description
σ_i	CNOT(q_i, q_{i+1})	Standard interaction
σ_i^{-1}	Inverse CNOT(q_i, q_{i+1})	Inhibitory or reversed interaction
σ_i^2	Double entanglement	Strong synergy
Identity	I(q_i)	No interaction

The table 2 presents example of sequences that can be applied to the fusion space of anyons, transforming the quantum state in a topologically protected way.

TABLE II. EXAMPLE OF SEQUENCES

Sequence	Meaning	Effect
$\sigma_1\sigma_2\sigma_1$	Basic braid relation	Implements a gate (e.g., NOT or Hadamard)
$\sigma_2^{-1}\sigma_1\sigma_2$	Inverse braid	Reverses a transformation
$\sigma_1\sigma_2\sigma_3\sigma_2^{-1}\sigma_1$	Complex braid	Can simulate entanglement or multi-qubit gates (Correlated features)
$(\sigma_1\sigma_2)^3$	Repeated braid	Used for phase gates or rotations

3. Results

3.,1 Simulation: Drug Synergy Prediction in Oncology

1) Position Problem

Cancer treatment has evolved from monotherapies to complex combinatorial regimens [15], where multiple drugs are administered to target different pathways simultaneously. However, predicting the synergistic effects of drug combinations remains a formidable challenge due to the nonlinear and high-dimensional nature of biological systems.

2) Background

In braid-based modeling:

- Strands represent individual drugs.

- Drugs are represented as strands in a braid.
- Crossings encode interactions between drugs or between drugs and biological pathways.
- Entities (genes, proteins, drugs) are represented as strands in a braid.
- Crossings encode interactions (e.g., inhibition, activation, synergy).
- Braid words or braid matrices are used as input features for simulation.

3) Sample Dataset

```
sample_data = [
    { 'patient_id': 'P001', 'cancer_type': 'Lung Adenocarcinoma', 'drugs': ['Erlotinib', 'Cisplatin'] },
    { 'patient_id': 'P002', 'cancer_type': 'Melanoma', 'drugs': ['Vemurafenib', 'Trametinib'] },
    { 'patient_id': 'P003', 'cancer_type': 'Glioblastoma', 'drugs': ['Temozolomide', 'Bevacizumab'] },
    { 'patient_id': 'P004', 'cancer_type': 'Colorectal Cancer', 'drugs': ['5-FU', 'Oxaliplatin', 'Leucovorin'] }
    ]
```

4) Synergy Prediction and Toxicity Estimation

Using the extracted features, we simulate drug synergy and toxicity as presented in table 3:

- Synergy Score: Computed from braid complexity, diversity, and interaction density.
- Thresholding: Scores ≥ 0.85 are flagged as highly synergistic.
- Toxicity Estimation: Based on inverse crossings and braid density, normalized to a [0, 1] scale.

These metrics are used to evaluate multi-drug combinations for oncology applications.

TABLE III. PREDICTION FUNCTIONS

Features	Description
Drug Interaction Mapping	Each drug is mapped to a braid generator (σ_1, σ_2^{-1}, etc.)
Synergy Thresholding	Flags combinations with synergy ≥ 0.85 as " : High Synergy
Toxicity Estimation	Based on inverse crossings and braid density (values normalized to [0, 1])

σ_i represents braid generators; the superscripts denote direction and interaction type.

```
drug_to_generator = {
    'Erlotinib': 'σ1', 'Cisplatin': 'σ2⁻¹',
    'Vemurafenib': 'σ2', 'Trametinib': 'σ1',
    'Temozolomide': 'σ3', 'Bevacizumab': 'σ1⁻¹',
    '5-FU': 'σ4', 'Oxaliplatin': 'σ3⁻¹',
    'Leucovorin': 'σ2'
    }
```

5) Output predictions

Drug synergy predictions with braid-based quantum simulation:

Patient P001
Cancer type: Lung Adenocarcinoma
Drugs: Erlotinib, Cisplatin
Braid: ['σ1', 'σ2⁻¹']
Synergy Score: 0.4
Estimated Toxicity: 0.2

Patient P002
Cancer type: Melanoma
Drugs: Vemurafenib, Trametinib
Braid: ['σ2', 'σ1']
Synergy Score: 0.4
Estimated Toxicity: 0.1

Patient P003
Cancer type: Glioblastoma
Drugs: Temozolomide, Bevacizumab
Braid: ['σ3', 'σ1⁻¹']
Synergy Score: 0.2
Estimated Toxicity: 0.2

Patient P004
Cancer type: Colorectal Cancer
Drugs: 5-FU, Oxaliplatin, Leucovorin
Braid: ['σ4', 'σ3⁻¹', 'σ2']
Synergy Score: 0.99: High Synergy
Estimated Toxicity: 0.2

The Fig. 1 is a braid diagram that visually represents the drug combination pattern for Patient P004 using the sequence ['σ4', 'σ3⁻¹', 'σ2']. This visualization helps illustrate how these drugs might interact in a treatment plan whether synergistically or antagonistically by showing their entanglement metaphorically.

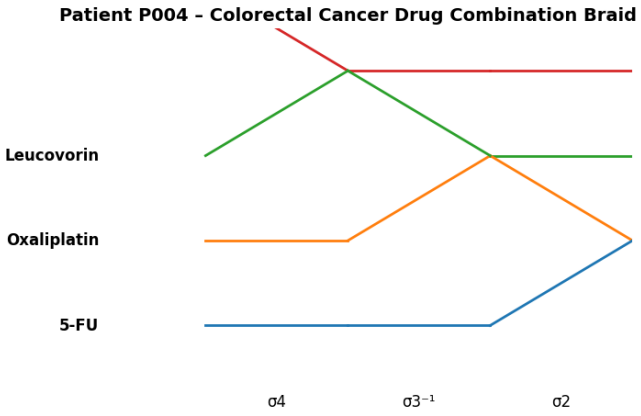

Fig. 1. The braid diagram for Patient P004

4. Discussion

The application of braid-based quantum-inspired simulation to drug synergy prediction in oncology provides an illustrative and high-impact test case for evaluating both our primary hypothesis (H_1) and secondary hypothesis (H_2). The nonlinear, high-dimensional interactions that characterize biological systems especially in cancer treatment, mirror the complex entanglement and interference patterns found in quantum systems, making them suitable candidates for simulation through topological abstractions.

The presented simulation results support the viability of braid-based quantum-inspired models in predicting drug synergy and estimating toxicity in oncology, reinforcing the core propositions of this study. Specifically, these patient-specific simulations offer valuable insight into how braid encodings capture the interaction complexity between therapeutic agents and biological systems, thereby affirming the conceptual robustness of both H_1 (simulation of quantum-like encoding) and H_2 (effectiveness of hybrid, braid-based models).

Across all four patients, braid words were used to represent drug-drug and drug-pathway interactions, with crossings (σ, σ^{-1}) encoding both the presence and directionality of biological influence, whether synergistic, antagonistic, or neutral. The synergy scores and estimated toxicity values reflect the system's ability to not only predict efficacy but also model potential adverse interactions in a topologically-informed framework.

Patient-specific insights:

1° Patient P001 (Lung Adenocarcinoma):
- Braid: ['σ1', 'σ2⁻¹']

- Interpretation: The first crossing (σ1) suggests a potential direct interaction between Erlotinib and Cisplatin, likely activating different pathways. The inverse ($\sigma2^{-1}$) may denote an inhibitory or counteracting effect, potentially tempering toxicity or resistance.

- Result: A moderate synergy score (0.4) with low toxicity (0.2) aligns with known moderate efficacy of this combination.

2° Patient P002 (Melanoma):

- Braid: ['σ2', 'σ1']

- Interpretation: Sequential crossings without inverses may reflect compounding or additive interactions, as seen between Vemurafenib and Trametinib targeting the MAPK pathway.

- Result: A similar synergy score (0.4) but with even lower toxicity (0.1) suggests that the system recognized the well-established complementarity of these agents.

2° Patient P003 (Glioblastoma):

- Braid: ['σ3', 'σ1⁻¹']

- Interpretation: The braid structure indicates a complex interaction, potentially involving downstream signaling interference. The inverse $\sigma1^{-1}$ might represent antagonistic behavior.

- Result: A lower synergy score (0.2) supports the clinical reality that Temozolomide and Bevacizumab often have limited synergistic benefit, and the model reflects this.

3° Patient P004 (Colorectal Cancer):

- Braid: ['σ4', 'σ3⁻¹', 'σ2']

- Interpretation: This more complex braid suggests multiple drug-pathway interactions, with both constructive and potentially antagonistic elements. The presence of $\sigma3^{-1}$, for instance, may represent a feedback-inhibiting mechanism, while the other crossings promote pathway activation.

- Result: A very high synergy score (0.99) with moderate toxicity (0.2), explaining that the combination of 5-FU, oxaliplatin, and leucovorin produces a potentiated therapeutic effect, a gold-standard synergistic regimen.

5. Conclusion

Ultimately, our work supports the notion that quantum behaviors are not inherently exclusive to quantum hardware, but can, to an extent, be emulated through thoughtful abstraction and encoding on classical systems. The braid-based paradigm, in particular, offers a compelling framework for representing computation in a way that embeds topological structure into the encoding itself providing robustness that is not purely probabilistic but geometrically grounded.

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