Quantum Causal Algebra for Data Representation: A New Operator-Theoretic Framework Beyond Correlation

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Abstract

This paper proposes a new algebraic foundation for data representation and dimensionality reduction based on quantum causal influence, rather than classical correlation. While classical machine learning relies heavily on covariance matrices and symmetric similarity measures, classical causality is fundamentally asymmetric and therefore incompatible with the eigen-operator framework required by PCA and SVD. We show that quantum causality, especially in the forms of entanglement, indefinite causal order, and process-matrix formalisms, naturally provides symmetric (Hermitian) operators that generalize correlation. We introduce the Quantum Causal Matrix (QCM), Quantum Causal Tensor (QCT), and Quantum Causal Principal Components (QC-PCA). This work lays the theoretical groundwork for a new operator-based causal linear algebra.

1 Introduction

The foundations of modern data analysis and machine learning rely heavily on *correlation* as the primary mathematical tool for describing relationships among variables. Correlation, covariance matrices, and their spectral decompositions—such as Principal Component Analysis (PCA)—form the backbone of linear representation learning and dimensionality reduction [8]. From the perspective of linear algebra, correlation acts as a symmetric bilinear form, enabling the construction of Hermitian operators whose eigenvectors define optimal bases for data representation.

However, correlation captures only *association*, not *causation*. Classical causality, as formalized by Pearl's do-calculus [13], is intrinsically *directional* and therefore *asymmetric*. This fundamental asymmetry prevents the construction of a causal matrix suitable for spectral decomposition, because a non-symmetric operator generally does not admit an orthonormal eigenbasis. Thus, classical causality and classical linear algebra are misaligned at a structural level.

Quantum theory suggests a radically different view. In quantum mechanics, systems may exhibit correlations that go beyond classical expectations, such as entanglement, which is symmetric and nonlocal [6]. Furthermore, recent developments show that the very *order* of causal events need not be fixed: quantum processes can exist in a superposition of different causal orders [1, 11]. This framework, known as *indefinite causal order*, generalizes classical causality and introduces operator structures that remain Hermitian or completely positive, making them suitable for spectral analysis.

This raises a fundamental question:

Can quantum causal influence replace correlation as the algebraic foundation for data representation?

If so, all classical concepts—covariance, similarity matrices, PCA, SVD, kernel methods—could be generalized using a new operator: the *Quantum Causal Matrix* (QCM). Such an operator would encode not merely statistical association, but directional and potentially time-symmetric causal structures compatible with quantum theory. In this sense, quantum causal influence may provide the missing algebraic symmetry that classical causality lacks.

The purpose of this work is therefore threefold:

1. To formally define the Quantum Causal Matrix (QCM) as a Hermitian operator derived from quantum causal influence.

2. To introduce the Quantum Causal Tensor (QCT) as a multilinear extension suitable for higher-order interactions.

3. To develop Quantum Causal Principal Component Analysis (QC-PCA), a generalization of PCA in which eigenvectors represent principal directions of quantum causal influence.

This paper lays foundational definitions and theoretical motivations for a new operator-theoretic framework for causal representation learning. A companion paper (not included here) develops a classical analogue based on Shannon information flow and entropy-based causal matrices.

2 Related Works

This section reviews the three scientific foundations that intersect in our proposed Quantum Causal Algebra: (1) classical correlation-based linear algebra used in data analysis, (2) classical causal inference and its incompatibility with spectral methods, and (3) quantum causal structures that motivate a new operator-theoretic framework.

2.1 Correlation-Based Linear Algebra in Machine Learning

Conventional machine learning relies heavily on symmetric similarity measures, particularly covariance and correlation matrices. Principal Component Analysis (PCA), Singular Value Decomposition (SVD), kernel PCA, and many spectral methods assume data relationships can be encoded in Hermitian or symmetric positive semidefinite operators [4, 8]. These operators admit orthonormal eigenbases, enabling geometric interpretations and efficient dimensionality reduction.

However, since correlation does not capture causal direction, correlation-based linear algebra cannot distinguish between spurious association and true causal influence. This limitation motivates investigating algebraic structures that encode directional relationships.

2.2 Classical Causality and Its Structural Asymmetry

Classical causal inference, especially in Pearl's structural causal models (SCM), represents causal relations through directed acyclic graphs (DAGs), structural equations, and the *do*-operator [13, 16]. These models produce asymmetric causal effects: $X \to Y$ is fundamentally different from $Y \to X$.

This asymmetry makes classical causality incompatible with spectral decomposition of linear operators. Non-symmetric matrices may have complex eigenvalues, non-orthogonal eigenvectors, or may not be diagonalizable at all. Thus, classical causal graphs cannot directly form the basis for PCA-like representation learning.

Prior work attempted to quantify causal strength numerically (e.g., causal influence, interventional mutual information, or average causal effects) [7], but these quantities still inherit directional asymmetry.

Therefore, a direct extension of PCA or operator-based learning to classical causality is mathematically limited.

2.3 Quantum Correlations and Entanglement

Quantum information theory introduces correlations that cannot be explained by classical causal models. Quantum entanglement produces symmetric and nonlocal dependencies that violate Bell inequalities [6]. Unlike classical causation, quantum correlations arise from joint states in Hilbert space and are represented by density matrices and Hermitian operators.

These operators naturally support eigen-decomposition, making them compatible with the algebraic requirements of PCA and spectral methods.

2.4 Indefinite Causal Order and Process Matrices

Recent breakthroughs show that the causal order between two events need not be fixed in quantum mechanics. In the *process matrix* formalism, a quantum system can exhibit superpositions of different causal orders [1,2,11].

The *quantum switch*, for example, allows operations A and B to be applied in a coherent superposition of $A \prec B$ and $B \prec A$ [2]. These structures enable causality to become symmetric or partially symmetric, making it suitable for algebraic frameworks requiring Hermitian operators.

This paper leverages these properties to construct a *Quantum Causal Matrix (QCM)*: a Hermitian operator encoding quantum causal influence among data attributes.

2.5 Position of This Work

To the best of our knowledge, no prior work has:

- formalized a Hermitian *causal operator* suitable for eigen-decomposition and PCA-like representation learning;
- extended dimensionality reduction into the domain of quantum causal structures;
- or proposed a multilinear extension in the form of a Quantum Causal Tensor (QCT).

Thus, this paper aims to open a new research direction connecting causal reasoning, operator theory, and quantum information into a unified framework for data representation.

3 Quantum Causal Matrix: Formal Definitions

This section introduces the formal mathematical definition of the *Quantum Causal Matrix* (QCM), which serves as the central operator in our proposed framework. The key idea is to represent data features not merely as numerical variables but as quantum states embedded in a Hilbert space. Causal influence between features is then encoded through completely positive (CP) maps, process matrices, or entanglement-based influence operators.

3.1 Hilbert Space Representation of Data Attributes

Let the dataset consist of d attributes. We embed each attribute X_i into a Hilbert space $\mathcal{H}$, typically $\mathcal{H} \cong \mathbb{C}^m$ for m samples or via a feature map $\phi : X_i \mapsto |\phi_i\rangle \in \mathcal{H}$.

The inner product

$$\langle \phi_i, \phi_j \rangle$$

generalizes classical correlation to the quantum domain. A density-operator representation is obtained by

$$\rho_i = \frac{|\phi_i\rangle \langle\phi_i|}{\langle\phi_i, \phi_i\rangle},$$

analogous to pure-state representations in quantum mechanics [10].

3.2 Quantum Causal Influence Operators

In quantum causal theory, the relationship between two systems A and B can be formalized through a process matrix W or a completely positive (CP) map $\mathcal{E}_{A\to B}$ [2, 11].

We define the *quantum causal influence* of attribute X_i on X_j as:

$$\mathcal{C}_{i\to j} = \mathrm{Tr}_i \left[W_{ij} \left(\rho_i \otimes I_j \right) \right],$$

where:

- W_{ij} is a two-party process matrix,
- ρ_i is the quantum state associated with attribute X_i, and
- I_j is the identity on subsystem j.

This operator represents the causal effect of i on j in the sense of quantum process theory, which allows for coexistence of $i \prec j$, $j \prec i$, or a superposition thereof.

3.3 Symmetrized Quantum Causal Operator

Classical causality is asymmetric, but quantum causality admits a symmetric bilinear structure due to the Hermitian nature of process matrices and CP maps. We define the *quantum causal interaction* between i and j as:

$$H_{ij} = \frac{1}{2} \left(\mathcal{C}_{i\to j} + \mathcal{C}_{j\to i}^{\dagger} \right).$$

This symmetrization is natural because:

1. Hermitian operators correspond to observables in quantum mechanics.

2. Spectral decomposition requires Hermiticity.

3. Entanglement-induced causal correlations are inherently symmetric.

It follows that H_{ij} satisfies:

$$H_{ij} = H_{ij}^{\dagger},$$

ensuring real eigenvalues and orthonormal eigenvectors.

3.4 Definition of the Quantum Causal Matrix (QCM)

We now define the Quantum Causal Matrix:

$$\boxed{\text{QCM} = [H_{ij}]_{i,j=1}^{d}}$$

where each H_{ij} is the Hermitian quantum causal interaction operator between features i and j.

The QCM generalizes the classical correlation matrix in three ways:

1. It incorporates directional causal influence through quantum process matrices.

2. It supports symmetric Hermitian structure necessary for operator-based learning.

3. It encodes both classical and nonclassical (quantum) dependencies, including entanglement and indefinite causal order.

3.5 Properties of QCM

The QCM satisfies the following:

- **Hermitian:** $\text{QCM}^{\dagger} = \text{QCM}$.

- **Positive semidefinite:** $\langle v | \text{QCM} | v \rangle \geq 0$ for all vectors v.

- **Diagonalizable:** Admits a decomposition

  $$\text{QCM} = U \Lambda U^{\dagger},$$

  where Λ contains eigenvalues and U contains quantum causal principal directions.

- **Classical limit:** If causal influence reduces to classical correlation,

$$H_{ij} \to \mathrm{Corr}(X_i, X_j),$$

  then QCM reduces to the classical correlation matrix.

This establishes QCM as a valid algebraic object for spectral learning methods, generalizing classical PCA.

4 Quantum Causal PCA (QC-PCA)

Given the Quantum Causal Matrix (QCM) defined in the previous section, we now develop the corresponding spectral method: *Quantum Causal Principal Component Analysis* (QC-PCA). This section shows how QCM can be diagonalized, how quantum causal principal components are defined, and how dimensionality reduction is performed in the quantum causal setting.

4.1 Spectral Decomposition of QCM

Since the QCM is Hermitian by construction, it admits a spectral decomposition of the form

$$\mathrm{QCM} = U \Lambda U^\dagger,$$

where:

- $U = [\,|u_1\rangle\,, |u_2\rangle\,, \ldots, |u_d\rangle\,]$ is a unitary matrix whose columns are orthonormal eigenvectors,
- $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d)$ contains real eigenvalues in descending order $\lambda_1 \geq \lambda_2 \geq \cdots \geq 0$.

Each eigenpair $(\lambda_k, |u_k\rangle)$ represents a principal direction of quantum causal influence in the dataset. This generalizes classical PCA, where eigenvalues represent variance and eigenvectors represent orthogonal modes of correlation [8].

4.2 Quantum Causal Principal Components

Let the feature vector in Hilbert space be

$$\Phi = \begin{bmatrix} |\phi_1\rangle \\ |\phi_2\rangle \\ \vdots \\ |\phi_d\rangle \end{bmatrix}.$$

The k-th *quantum causal principal component* (QC-PC) is defined as:

$$|\psi_k\rangle = U_k^\dagger \Phi,$$

where $U_k^\dagger$ denotes the conjugate transpose of the k-th row of U.

Thus, QC-PCs represent projections of the quantum-embedded data onto principal causal directions determined by the QCM.

4.3 Interpretation of QC-PCA

QC-PCA encodes not only statistical association but also quantum causal influence, including entanglement and indefinite causal order. The eigenvalue λ_k measures the *magnitude of quantum causal influence* along the direction $|u_k\rangle$.

Unlike classical PCA:

- principal components reflect both directional and nondirectional quantum dependencies,
- eigenvectors may correspond to coherent superpositions of causal pathways,
- QC-PCs can represent mixtures of $i \prec j$ and $j \prec i$ causal structures.

This creates a richer representation of relationships among data attributes.

4.4 Dimensionality Reduction via QC-PCA

Given $r < d$, the reduced representation is:

$$\Phi_r = U_r^\dagger \Phi,$$

where U_r contains the top r eigenvectors of QCM.

The projection preserves the largest quantum causal influences in the dataset:

$$\sum_{k=1}^{r} \lambda_k \quad \text{maximized subject to } r.$$

Thus, QC-PCA solves the optimization problem:

$$U_r = \arg \max_{U:U^\dagger U = I_r} \operatorname{Tr}\left(U^\dagger \mathrm{QCM}\, U\right).$$

This is the natural quantum causal analogue of classical PCA.

4.5 Classical Limit of QC-PCA

If the quantum causal operator H_{ij} reduces to classical correlation $\mathrm{Corr}(X_i, X_j)$, then

$$\mathrm{QCM} \to R,$$

the correlation matrix, and QC-PCA reduces to classical PCA.

If H_{ij} reduces to covariance,

$$\mathrm{QCM} \to \Sigma,$$

then QC-PCA reduces to covariance-based PCA.

Therefore, QC-PCA strictly generalizes classical PCA while retaining compatibility with classical interpretations.

4.6 Quantum Advantage in QC-PCA

Quantum causal structures allow QC-PCA to capture phenomena that classical PCA cannot represent, including:

- nonclassical correlations quantified by quantum mutual information [10],
- coherent superpositions of causal orders [2, 11],
- entanglement-induced causal effects,
- causal influence without definite temporal order.

These properties provide QC-PCA with the ability to represent highly structured dependencies in complex datasets.

5 Quantum Causal Tensor (QCT)

The Quantum Causal Matrix (QCM) introduced earlier captures pairwise quantum causal influence between attributes. However, many causal interactions in real systems involve more than two variables. Examples include synergistic causal mechanisms, mediated causal pathways, three-way entanglement, and higher-order quantum processes such as GHZ or W states [3,5].

To model these phenomena, we extend QCM to a *Quantum Causal Tensor* (QCT), which encodes multilinear causal interactions among any number of variables.

5.1 Motivation for Higher-Order Causal Operators

Classical causality typically focuses on pairwise effects (e.g., $X \to Y$), but higher-order structures arise naturally in:

- mediated causal chains ($X \to Z \to Y$),
- synergistic causal interactions (X_1 and X_2 jointly cause Y),
- quantum entanglement among three or more qubits,
- process matrices with multipartite causal influence [1, 11],
- tensor-network representations of quantum correlations [12].

Thus, a multilinear representation is required.

5.2 Definition of QCT

Let $\rho_i = |\phi_i\rangle \langle\phi_i|$ denote the quantum state associated with feature i. Let $W_{i_1 i_2 \cdots i_k}$ denote a k-partite quantum process matrix.

We define the *Quantum Causal Tensor* of order k:

$$T_{i_1 i_2 \cdots i_k} = \mathrm{Tr}_{\setminus\{i_1,\ldots,i_k\}} \left[W_{i_1 i_2 \cdots i_k} \left(\rho_{i_1} \otimes \rho_{i_2} \otimes \cdots \otimes \rho_{i_k} \otimes I_{\mathrm{rest}} \right) \right].$$

Interpretation of $T_{i_1 i_2 \cdots i_k}$:

- It measures the joint quantum causal influence among variables $\{i_1, i_2, \ldots, i_k\}$.

- It captures entanglement or causal correlations that cannot be decomposed into pairwise components.

- It generalizes covariance tensors used in multilinear PCA [9].

5.3 Tensor Symmetry

Although classical causal tensors are not symmetric, quantum process matrices are Hermitian and obey cyclic symmetry under partial trace.

Thus, for QCT:

$$T^{\dagger}_{i_1 i_2 \cdots i_k} = T_{i_1 i_2 \cdots i_k}.$$

This allows decomposition via:

- Higher-Order SVD (HOSVD),

- Tucker decomposition,

- Tensor-train decomposition,

- or spectral unfolding methods.

These methods produce multilinear causal principal components.

5.4 Mode-n Unfolding and Projection to QC-PCA

QCT can be reduced to a QCM through mode-n unfolding:

$$\mathrm{QCM}^{(n)} = \mathrm{unfold}_n(T).$$

In this way:

- QCT serves as the full causal model,

- QCM provides pairwise projections,

- QC-PCA extracts principal causal directions.

5.5 Quantum Causal Tensor Networks

QCT naturally leads to quantum causal tensor networks:

$$\mathcal{N} = \bigotimes_{\alpha} T^{(\alpha)},$$

where each $T^{(\alpha)}$ is a local causal tensor. This structure parallels:

- matrix product states (MPS),
- projected entangled pair states (PEPS),
- MERA networks,

which have been used extensively in quantum information and many-body physics [12].

5.6 Classical Limit of QCT

If quantum causal influence reduces to classical joint correlation:

$$T_{i_1 i_2 \cdots i_k} \to \mathbb{E}[X_{i_1} X_{i_2} \cdots X_{i_k}],$$

then QCT reduces to classical high-order covariance tensors.

Thus QCT generalizes both:

- classical higher-order statistics,
- quantum multipartite causal influence.

This establishes QCT as a foundational object for multilinear causal learning.

6 Geometric Interpretation of QCM, QC-PCA, and QCT

Classical PCA is built on Euclidean geometry, where correlation defines a symmetric inner product between feature vectors. In contrast, the Quantum Causal Matrix (QCM) and Quantum Causal Tensor (QCT) define a new geometry on feature space derived from quantum causal influence. This section provides the geometric interpretation corresponding to the operator structures introduced earlier.

6.1 From Euclidean Geometry to Quantum Causal Geometry

Let X_i, X_j be classical feature vectors. In PCA, their geometric relationship is encoded in the Euclidean inner product:

$$\langle X_i, X_j \rangle = \sum_{k=1}^{m} X_{ik} X_{jk}.$$

Correlation-based PCA interprets this as the cosine of an angle between vectors, producing a geometry where data relationships are purely based on symmetric statistical association.

QCM modifies this foundation by embedding features into a Hilbert space $\mathcal{H}$:

$$X_i \mapsto |\phi_i\rangle \in \mathcal{H}.$$

The geometric structure is now induced by a *quantum causal bilinear form*:

$$\langle \phi_i, \phi_j \rangle_{\text{QCM}} = \langle \phi_i | \, H_{ij} \, | \phi_j \rangle \, .$$

Thus, the inner product is deformed by the causal influence operator H_{ij}.

6.2 Quantum Causal Geometry as an Operator-Weighted Space

For QCM, the geometry is defined by the metric:

$$g_{ij} = H_{ij}.$$

Since H_{ij} is Hermitian and positive semidefinite, it defines a valid quantum generalization of the classical metric tensor. Distances in this geometry satisfy:

$$d^2(\phi_i, \phi_j) = \langle \phi_i - \phi_j | \; H \; | \phi_i - \phi_j \rangle \, .$$

This is analogous to:

- Mahalanobis distance using covariance,
- quantum Fisher information metric,
- Bures metric on density matrices.

Thus, QCM induces a *quantum causal information geometry.*

6.3 Eigenvectors as Principal Quantum Causal Directions

In classical PCA, eigenvectors of the covariance matrix represent orthogonal directions of maximal variance. In QC-PCA, eigenvectors of QCM represent:

principal directions of quantum causal influence.

Geometrically:

- They define orthogonal axes in a Hilbert space deformed by causal operators.
- Each axis corresponds to a coherent mixture of causal pathways.
- These axes may represent superpositions of temporal orders $i \prec j$ and $j \prec i$.

Thus, QC-PCA identifies "causal eigen-directions" in feature space.

6.4 Geometric Structure of QCT (Multilinear Causal Geometry)

QCT extends pairwise geometry to multilinear geometry. A QCT of order k:

$$T_{i_1 i_2 \cdots i_k}$$

defines a multilinear form:

$$\mathcal{T}(|v_1\rangle, \ldots, |v_k\rangle) = \sum_{i_1,\ldots,i_k} v_{1,i_1} \cdots v_{k,i_k} T_{i_1 \cdots i_k}.$$

This generalizes:

- bilinear forms (matrices),
- quadratic forms,
- covariance tensors,
- entanglement tensors (e.g., GHZ/W states),

- tensor networks in quantum physics.

Geometrically:

- QCT encodes higher-order curvature of the causal manifold,
- mode-n components represent directional slices of the causal geometry,
- tensor decompositions identify multilinear causal principal modes.

QCT therefore induces a *multipartite quantum causal manifold*.

6.5 Interpretation via Quantum Information Geometry

Quantum information theory defines a family of metrics derived from distinguishability of quantum states, including:

- Bures metric,
- Quantum Fisher Information (QFI) metric,
- Fubini-Study metric.

QCM is compatible with these metrics because it is Hermitian and positive. Thus, the geometric structure of QCM naturally integrates with quantum information geometry [14, 15].

6.6 Classical Limit of the Geometry

When H_{ij} reduces to classical correlation:

$$\langle \phi_i, \phi_j \rangle_{\mathrm{QCM}} \to \langle X_i, X_j \rangle,$$

the geometry reduces to Euclidean geometry.

When H_{ij} reduces to covariance:

$$d^2(\phi_i, \phi_j) \to (\phi_i - \phi_j)^\top \Sigma^{-1} (\phi_i - \phi_j),$$

the geometry reduces to Mahalanobis geometry.

Thus, quantum causal geometry strictly generalizes classical geometries.

7 Algorithms: Constructing and Using QCM / QCT

This section provides concrete algorithmic recipes for:

1. Constructing a Quantum Causal Matrix (QCM) from data;
2. Performing Quantum Causal PCA (QC-PCA);
3. Constructing and decomposing Quantum Causal Tensors (QCT) and projecting them to QCM;
4. Practical classical or hybrid approximations when full quantum estimation is infeasible.

We present pseudocode, complexity notes, and implementation remarks for each stage.

7.1 Overview of the full pipeline

High-level pipeline (idealized):

1. **Embed** each attribute X_i into a quantum state ρ_i (feature map / encoding).
2. **Estimate** pairwise (and higher-order) process matrices $W_{i_1 \dots i_k}$ via quantum process tomography or model-based inference.
3. **Compute** causal interaction operators $\mathcal{C}_{i \to j}$ and symmetrize to obtain H_{ij}.
4. **Assemble** QCM $= [H_{ij}]$ and QCT $= [T_{i_1 \dots i_k}]$.
5. **Perform** spectral decomposition (QC-PCA) or tensor decompositions (HOSVD, Tucker) and extract reduced representations.

7.2 Pseudocode: Construct QCM (ideal quantum procedure)

Inputs:

- Raw dataset $X \in \mathbb{R}^{m\times d}$ (or samples from joint distribution).
- Quantum encoding map $\phi : X_i \mapsto \rho_i$.
- Max interaction order $k_{\max}$ (typically 2 for QCM).

Output: QCM $\in \mathbb{C}^{d\times d}$ (operator-valued entries reduced to scalars/expectations or matrix blocks depending on representation).

Algorithm 1 (Construct-QCM-Quantum):

1. **For** each feature $i = 1 \ldots d$:
   (a) Encode empirical samples of X_i into quantum state(s) $\rho_i = \phi(X_i)$.
   (b) (Optional) perform state tomography to obtain explicit density matrix ρ_i.
2. **For** each ordered pair (i, j):
   (a) Estimate/obtain the two-party process matrix W_{ij} (via process tomography or theoretical model).
   (b) Compute causal effect operator:
   $$\mathcal{C}_{i\to j} \leftarrow \mathrm{Tr}_i\,[\,W_{ij}(\rho_i \otimes I_j)\,]\,.$$
   (c) Compute the Hermitian interaction:
   $$H_{ij} \leftarrow \tfrac{1}{2}\big(\mathcal{C}_{i\to j} + \mathcal{C}^\dagger_{j\to i}\big).$$
3. Assemble QCM $\leftarrow [H_{ij}]_{i,j=1}^{d}$.
4. (Optional) Normalize / regularize QCM to ensure positive semidefiniteness (e.g., project onto PSD cone).

Notes:

- Estimating W_{ij} exactly requires quantum process tomography; resources grow quickly with subsystem dimension.
- In practice $\mathcal{C}_{i\to j}$ can be represented by expectation values (scalars) if one contracts with an observable O_j:
  $$c_{i\to j} = \mathrm{Tr}\big[O_j\,\mathcal{C}_{i\to j}\big],$$
  yielding a scalar causal weight for entry (i, j). This yields a numerical QCM (matrix of scalars) suitable for spectral decomposition.

7.3 Pseudocode: QC-PCA (spectral reduction)

Inputs: QCM (scalar or block-matrix form), target rank r.
Output: reduced representation Φ_r (quantum or classical coefficients).

Algorithm 2 (QC-PCA):

1. Compute spectral decomposition:

$$\mathrm{QCM} = U \Lambda U^{\dagger}.$$

2. Select top-r eigenvectors U_r and eigenvalues Λ_r.

3. Project feature embeddings:

$$\Phi_r \leftarrow U_r^{\dagger} \Phi.$$

4. (Optional) If QCM entries are operator blocks, perform block-wise contractions to produce scalar feature coefficients.

Notes:

- If QCM is real/complex PSD matrix of scalars, QC-PCA reduces to a standard eigen-decomposition (classical linear algebra).
- If QCM has block-operators (e.g., each entry is a small matrix), one can perform a generalized eigen-decomposition via vectorization or an operator basis.

7.4 Pseudocode: Construct and Decompose QCT (multilinear)

Inputs: order k QCT entries estimation routine, T.
Outputs: multilinear principal components (via HOSVD/Tucker/TT).

Algorithm 3 (Construct-and-Decompose-QCT):

1. For each index tuple $(i_1, \ldots, i_k)$ estimate

$$T_{i_1 \ldots i_k} = \mathrm{Tr}_{\setminus \{i_1, \ldots, i_k\}} \big[W_{i_1 \ldots i_k} \left(\rho_{i_1} \otimes \cdots \otimes \rho_{i_k} \otimes I \right) \big].$$

2. Form the k-way tensor T with dimensions $(d, \ldots, d)$.

3. Choose decomposition method:
   - HOSVD: unfold T along each mode and compute SVDs.
   - Tucker: alternating least squares for core tensor and factor matrices.
   - Tensor-Train (TT): perform sequential SVDs for large k.
4. Extract top-r_n factors per mode to obtain reduced multilinear representation.

Notes:

- Mode-n unfolding can produce pairwise QCM proxies $\text{unfold}_n(T)$ for QC-PCA.
- Decomposition algorithms have well-known numerical libraries (e.g., TensorLy) that can be used with estimated numeric tensor T.

7.5 Complexity and Measurement Requirements

Quantum tomography / process estimation

- State tomography for a subsystem of dimension d_s scales as $O(d_s^2)$ parameters to estimate; full tomography via measurements typically requires $O(d_s^2)$ observables and $O(\text{poly}(1/\epsilon))$ samples to accuracy ϵ.
- Process tomography (for W_{ij}) scales as $O(d_s^4)$ parameters for two d_s-dimensional subsystems (Choi representation). Hence full estimation is expensive and does not scale to large d without structural assumptions.

Classical spectral steps

- If QCM is an $d \times d$ numeric matrix, eigen-decomposition costs $O(d^3)$ (dense) or less with sparse methods.
- HOSVD of an order-k tensor with dimension d per mode is dominated by SVDs on unfolded matrices of size $d \times d^{k-1}$; complexity grows exponentially in k unless structure exploited.

7.6 Practical / Hybrid Implementations

Because exact quantum process estimation is resource-heavy, we outline practical alternatives:

(A) Classical surrogate via information-theoretic measures

- Compute directed information measures (transfer entropy, conditional mutual information) to form scalar causal weights:

$$c_{i\to j} \approx \mathrm{TE}(X_i \to X_j).$$

- Symmetrize (or Hermitize via complex lift) to obtain numeric QCM proxy:

$$H_{ij} \leftarrow \tfrac{1}{2}(c_{i\to j} + c_{j\to i}).$$

- This produces a *Shannon-based Causal Matrix* suitable for spectral methods (see companion paper).

(B) Model-based / parametric estimation

- Assume process matrices come from a parametric family (e.g., low-rank CP maps, Gaussian channels), then fit parameters by maximum likelihood from measurement statistics.
- Far fewer parameters $\rightarrow$ feasible estimation.

(C) Variational hybrid quantum-classical method

- Use parameterized quantum circuits (PQCs) to represent feature embeddings and/or process ansätze.
- Define a loss function that encourages capture of causal influence (e.g., maximize $\mathrm{Tr}[O\,\mathcal{C}_{i\to j}]$ for chosen observables).
- Optimize circuit parameters on a quantum backend with classical optimizer (VQE-like).
- This approach avoids full tomography by directly optimizing the downstream criterion for QC-PCA.

7.7 Numerical Stability and Regularization

When assembling QCM from empirical estimates:

- Estimates are noisy — regularize by adding ϵI to ensure PSD.
- If block-operators are used, rescale blocks to comparable operator norms before spectral decomposition.
- Use truncated SVD/HOSVD to remove small eigenvalue directions dominated by estimation noise.

7.8 Algorithmic Summary Table

Stage	**Method / Complexity**
State encoding	$\rho_i = \phi(X_i)$ (circuit depth depends on encoding)
Process estimation	Process tomography $O(d_s^4)$ params (expensive)
QCM assembly	d^2 operator computations; numeric matrix eigen $O(d^3)$
QCT construction	$O(d^k)$ entries (infeasible for large k)
HOSVD / Tucker	dominated by SVD on unfoldings (costly in k)
Hybrid variational	depends on PQC size and optimization budget

7.9 Implementation suggestions and tooling

- Classical prototyping: Python (NumPy/SciPy), TensorLy for tensors, scikit-learn for PCA baselines.
- Quantum simulation / PQC: Qiskit, Cirq, PennyLane (supports hybrid VQAs).
- Tomography & process estimation: use libraries in Qiskit Ignis, or custom maximum-likelihood tomography routines.

7.10 Remarks on Identifiability and Causal Interpretation

- Estimating causal influence from observational data remains fundamentally ill-posed without interventions or strong assumptions; quantum process formalism alleviates some classical constraints but does not eliminate identifiability issues.

- Practical QCM entries obtained from measurements must be interpreted carefully: they combine information about encoding, measurement choices, and underlying causal physics.

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