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Quantum-probabilistic SVD: complex-valued factorization of matrix data

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Abstract
The paper reports a method for compressed representation of matrix data on the principles of quantum theory. The method is formalized as complex-valued matrix factorization based on standard singular value decomposition. The developed approach establishes a bridge between standard methods of semantic data analysis and quantum models of cognition and decision. According to the quantum theory, real-valued observable quantities are generated by wavefunctions being complex-valued vectors in multidimensional Hilbert-space. Wavefunctions are defined as superpositions of basis vectors encoding composition of semantic factors. Basis vectors are found by singular value decomposition of the initial data matrix transformed to a real-valued amplitude form. Phase-dependent superposition amplitudes are found to optimize approximation of the source data. The resulting model represents the observed real-valued data as generated from a small number of basis wavefunctions superposed with complex-valued coefficients. The method is tested for random matrices of sizes from 3 × 3 to 12 × 12 and dimensionality of latent Hilbert-space from 2 to 4. The best approximation is achieved by encoding latent factors in normalized complex-valued amplitude vectors interpreted as wavefunctions generating the data. In terms of approximation fitness, the developed method surpasses standard truncated SVD of the same dimensionality. The mean advantage over the considered range of parameters is 22 %. The method permits cognitive interpretation in accord with the existing quantum models of cognition and decision. The method can be integrated in the algorithms of semantic data analysis including natural language processing. In these tasks, the obtained improvement of approximation translates to the increased precision of similarity measures, principal component analysis, advantage in classification, and document ranking methods. Integration with quantum models of cognition and decision is expected to boost methods of artificial intelligence and machine learning improving imitation of natural thinking.

Keywords
quantum probability, cognitive modeling, semantic analysis, wavefunction, matrix decomposition

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УДК 004.82

Комплекснозначное разложение матричных данных на принципах квантовой теории

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Аннотация
Предмет исследования. Представлен метод сжатого представления матричных данных на принципах квантовой теории. Данные имеют вид таблицы численных значений набора величин в ряде экспериментов. Метод формализован в виде факторизации данных на основе сингулярного разложения, обобщенного на

поле комплексных чисел. Рассмотрена возможность интерпретации разработанного метода в соответствии с принципами квантовой когнитивистики. **Метод.** В соответствии с квантовой теорией, действительные величины в исходных данных порождаются волновыми функциями в виде комплекснозначных векторов в многомерном гильбертовом пространстве. Волновые функции определяются суперпозициями базисных векторов, представляющими композицию семантических факторов. Базисные вектора рассчитываются с помощью сингулярного разложения матрицы исходных данных, приведенной к амплитудной форме. Комплекснозначные коэффициенты разложения определяются по условию наилучшей аппроксимации исходных данных. **Основные результаты.** Метод апробирован на случайно сгенерированных матрицах размером от 3 × 3 до 12 × 12 и размерностях сжатого гильбертова пространства от 2 до 4. Наилучшая точность приближения достигается при использовании в качестве элементов разложения нормированных комплекснозначных векторов, выполняющих роль порождающих волновых функций. Полученная точность во всех случаях превосходит точность приближения стандартным методом усеченного сингулярного разложения. Среднее повышение точности на исследованном интервале параметров составило 22 %. Метод допускает когнитивную интерпретацию, совместимую с квантовыми моделями поведения и принятия решений. **Практическая значимость.** Представленный метод применим в задачах семантического анализа данных, включая задачи обработки естественного языка. В этих приложениях полученный результат может быть использован для повышения точности выделения главных смысловых компонент, совершенствования методов классификации и ранжирования текстовых документов. Возможность когнитивной интерпретации и формализация в форме матричного разложения открывает подходы к дальнейшему использованию моделей квантовой когнитивистики в задачах анализа данных. Ожидается, что встраивание квантовой логики на основе комплекснозначного вероятностного исчисления в алгоритмы машинного обучения и искусственного интеллекта позволит имитировать работу естественных когнитивных систем.

Ключевые слова

квантовая вероятность, волновая функция, когнитивное моделирование, семантический анализ, матричное разложение

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Introduction

Most of the existing methods of data science represent features of the analyzed data by real numbers. Recent progress in cognitive-behavioral modeling, however, calls into question the appropriateness of this choice. Namely, quantum models of human behavior show the advantage of encoding cognitive factors by complex-valued amplitudes related to the observable quantities by quantum-theoretic Born's rule. The resulting probabilistic structure captures regularities of human behavior better than classical probability, making progress in problems challenging classical approaches [1–5]. When data originate from human behavior (e.g., for texts in natural language, social and economic statistics), complex-valued quantum-probabilistic structure is then expected to improve performance of the existing methods of analysis.

In this paper we focus on a Singular Value Decomposition (SVD) used to approximate a two-dimensional array of data as a product of smaller size matrices encoding "semantic" structure behind the observed data. Using real-valued calculus by default, this procedure is a mathematical core of latent semantic analysis of natural language [6–8]. As motivated above, we turn SVD from classical to complex-valued structure, while keeping its basic matrix-factorization idea.

Stage 1: real-valued amplitude-wise SVD

Source data have a form of a real-valued matrix $\mathbf{P}$ with M rows and N columns. Rows of matrix $\mathbf{P}$ stand for M target features that can have two outcomes, say 0 and 1. Columns are $N > M$ experiments in which these features are observed. Real positive element $\mathbf{P}[i, j] = p_{ij}$ is the probability of observing feature i in experiment j, normalized such that total probability of all features in each experiment is unity:

$$\|\mathbf{p}_j\|_1 = \sum_{i=1}^{M} p_{ij} = 1. \quad (1)$$

Vector $\mathbf{p}_j$ can be interpreted as a probabilistic profile of the observed features in experiment j. Normalized matrix $\mathbf{P}$ is then converted to the *amplitude* matrix $\mathbf{A}$ by element-wise square root

$$a_{ij} = \sqrt{p_{ij}},\ a_{ij} \in R^+ \quad (2)$$

so that the probability vectors $\mathbf{p}_j$ are transformed to the real-valued amplitude column forming matrix $\mathbf{A}$.

Next, matrix $\mathbf{A}$ is approximated by a product

$$\tilde{\mathbf{A}} = \mathbf{U_t} \times \mathbf{\Lambda_t} \times \mathbf{V_t}, \quad (3)$$

where $\mathbf{U_t}$, $\mathbf{\Lambda_t}$ and $\mathbf{V_t}$ are truncated versions of the real-valued matrices obtained from standard SVD shown in Fig. 1. Namely, matrix $\mathbf{U_t}$ consists of $K \le M$ orthogonal columns, $\mathbf{V_t}$ consists of K orthogonal rows, and λ_i are the corresponding eigenvalues. Decomposition (3) approximates initial amplitude matrix $\mathbf{A}$ optimally in the least-squares sense [6, 9].

Return to the probabilities is realized by element-wise squaring of the approximated amplitudes $\tilde{\mathbf{A}}^2$ inverting the relation (2). The result is different from the approximation $\tilde{\mathbf{P}}$ obtained from standard SVD applied directly to the

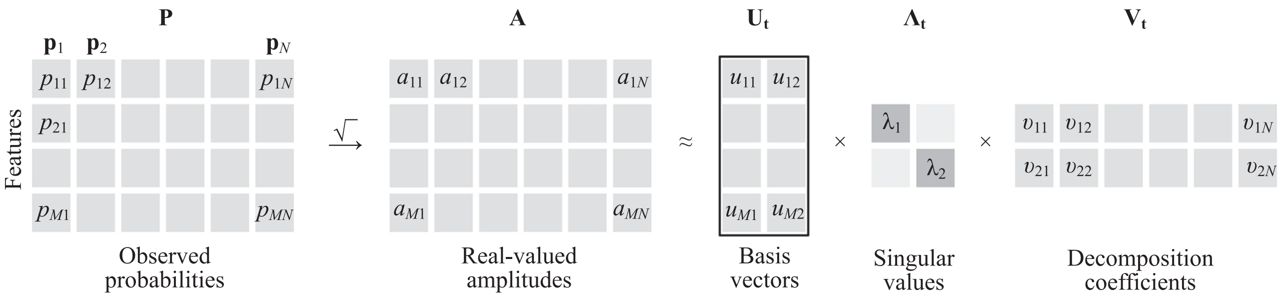

Fig. 1. Amplitude-wise singular value decomposition. First, normalized source probability data **P** (1) are converted by element-wise square root (2) to positive real amplitudes **A**. This matrix is approximated by standard SVD truncated to K largest eigenvalues (3). Shown is the case $N = 6$, $M = 4$, $K = 2$

source data and truncated to the same dimension K. The latter approximates the source data more accurately, as measured by the Frobenius norm $||\cdot||$:

$$d_{\text{SVD}} = ||\mathbf{P} - \tilde{\mathbf{P}}|| < ||\mathbf{P} - \tilde{\mathbf{A}}^2||. \quad (4)$$

This measure is used to estimate the advantage of the developed method in section "Testing".

Stage 2: Complex-valued factorization

Advantage over the standard SVD (4) is achieved by extending the domain of the amplitude matrix **A** to complex numbers. Observable probabilities are then generated from a complex-valued matrix **Ψ** by element-wise application of the Born's rule generalizing square-root relation (2)

$$\mathbf{P}_{\text{exp}} = |\mathbf{\Psi}|^2, \qquad p_{ij} = |\psi_{ij}|^2. \quad (5)$$

Matrix **Ψ** is factorized in the product

$$\mathbf{\Psi} = \mathbf{U_t} \times \mathbf{C}, \quad (6)$$

where $\mathbf{U_t}$ is the same as in (3), while matrix **C** consists of N complex-valued column vectors $|\mathbf{c}_j\rangle$ of length K as shown in Fig. 2.

Column vectors of **Ψ** are superpositions

$$|\mathbf{\Psi}_j\rangle = \mathbf{U}_\text{t}|\mathbf{c}_j\rangle = \sum_{i=1}^{K} c_{ij}|\mathbf{u}_i\rangle. \quad (7)$$

As required by (1), these vectors are normalized as

$$\langle\boldsymbol{\psi}_j|\boldsymbol{\psi}_j\rangle = \langle\mathbf{c}_j|\mathbf{c}_j\rangle = 1, \quad (8)$$

where row vector $\langle\cdot|$ is conjugate (Hermitian) transpose of $|\cdot\rangle$ in quantum-theoretic bra-ket notation. Accordingly, vectors $|\boldsymbol{\psi}_j\rangle$ play the role of *wavefunctions* generating probabilistic profiles $\mathbf{p}_j$ in each of N experiments.

As in quantum physics [10], K mutually orthogonal real-valued columns $|\mathbf{u}_i\rangle$ of matrix $\mathbf{U_t}$ are interpreted as *stationary* cognitive states of the (behavioral) system that generated the data. They function as an incomplete set of basis vectors in M-dimensional Hilbert-space H_M accommodating wavefunctions $|\boldsymbol{\psi}_j\rangle$. K-dimensional subspace H_K they span is a complex-valued version of a low-dimensional semantic space used in latent semantic analysis [6–8]. Normalized vectors $|\mathbf{c}_j\rangle$ in this space are cognitive wavefunctions representing behavioral data in compressed "semantic" form.

Stage 3: Finding the coefficients

Coefficient matrix **C** in (6) is sought to obtain the wavefunction matrix **Ψ** that would reproduce source data **P** in the best possible way. Namely,

$$\mathbf{C} = \text{argmin}||\mathbf{P} - \mathbf{P}_{\text{exp}}||, \quad (9)$$

where $\mathbf{P}_{\text{exp}}$ is the matrix of explained probabilities generated by element-wise Born's rule (5), and $||\cdot||$ is the Frobenius (Hilbert-Schmidt) matrix norm. Definition (9)

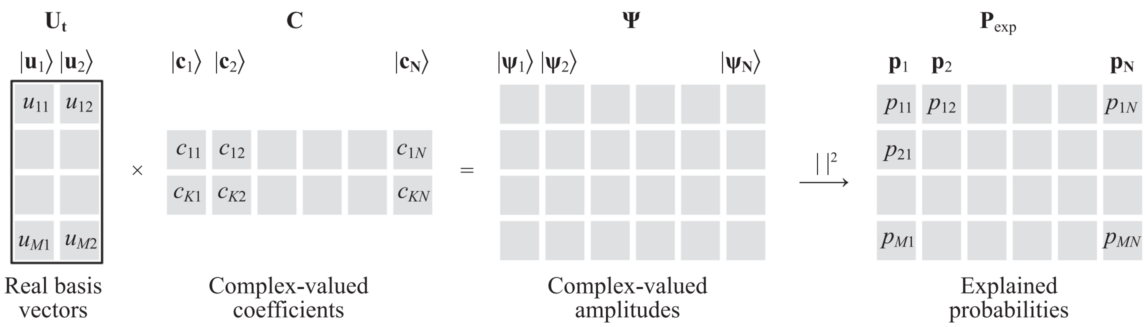

Fig. 2. Scheme of the complex-valued matrix factorization (6). Real-valued basis vectors $|\mathbf{u}_i\rangle$ obtained from amplitude-wise truncated SVD (Fig. 1) are superposed with N complex-valued coefficient vectors $|\mathbf{c}_j\rangle$ forming the matrix **C** of shape $K \times N$. This produces N wavefunctions $|\boldsymbol{\psi}_j\rangle$ (7) generating the explained probabilities $\mathbf{P}_{\text{exp}}$ via the Born's rule (5). Coefficients **C** are set to minimize the Frobenius distance between explained and actual probability matrices. As in Fig. 1, shown is the case $N = 6$, $M = 4$, $K = 2$

prescribes to find N complex-valued vectors $|\mathbf{c}_j\rangle$ of length K satisfying normalization (8). Each component c_{ij} is encoded by magnitude r and phase φ, both being real numbers, whereas phase of one c_{ij} in every $|\mathbf{c}_j\rangle$ is set to zero due to insensitivity of the observable probabilities to the global phase factor. In total, this results in

$$2N(K-1) \tag{10}$$

real-valued parameters sought to minimize distance between the explained and actual data (9). This problem is addressed by standard numerical optimization methods. We used the Nelder-Mead algorithm from SciPy library [11] applied for N independent optimization problems of $2(K-1)$ dimensions for each vector $|\mathbf{c}_j\rangle$.

Testing

This section summarizes approbation of the developed algorithm. The first test validates normalization of the complex-valued vectors in (7) and (8), supporting their interpretation as wavefunctions of data. Tests 2 and 3 quantify improvement of the data approximation achieved by the developed method relative to its real-valued version and the standard SVD.

Test 1: normalization

Normalization of coefficients c_{ij} in (7) is due to interpretation of vectors $|\mathbf{c}_j\rangle$ as wavefunctions of experimental data in K-dimensional latent space. This choice is verified by lifting restriction (8) and allowing vectors $|\mathbf{c}_j\rangle$ to have arbitrary lengths

$$r_j = \sqrt{\langle c_j|c_j\rangle}. \tag{11}$$

Compared to (10), this adds one additional parameter for each of N vectors $|\mathbf{c}_j\rangle$, so that the total number of optimization variables becomes $N(2K-1)$. Histogram of the resulting values (11) from 2000 optimized vectors is shown in Fig. 3. The mean and standard deviation of this statistics

$$r_j = 1.002 + 0.016 \tag{12}$$

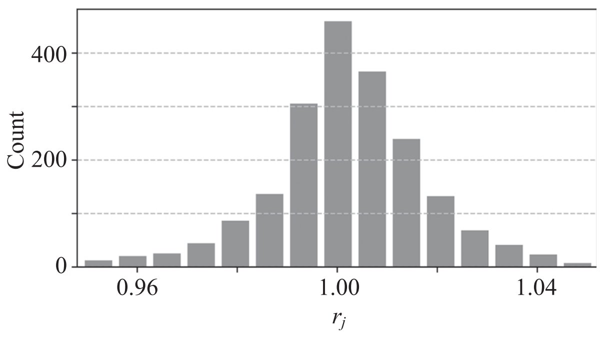

Fig. 3. Distribution of 2000 coefficient vector lengths (11) obtained in complex-valued decomposition of random data with shape $N = 6$, $M = 4$, and truncation to $K = 2$ basis dimensions. Heights of the bars show the number of the values falling in the corresponding bins. The mean value is sharply peaked at unity (12) in agreement with normalization (8)

indicate that in agreement with quantum-theoretic reason normalization (8) simplifies representation without degrading its accuracy.

Test 2: real-complex difference for the same algorithm

This test quantifies how generalization to complex numbers improves quality of the approximation obtained from the same form of matrix decomposition. Namely, complex-valued algorithm shown in Fig. 2 is compared with its performance when the coefficient matrix $\mathbf{C}$ in optimization (9) is limited to real numbers. In this latter case, real-valued amplitude matrix $\mathbf{\Psi}_R$ approximates the source data with Frobenius distance

$$d_{\text{real}} = ||\mathbf{P} - \mathbf{\Psi}_R^2||$$

analogous to (4). This value is compared with the distance obtained from the complex-valued version of an algorithm

$$d_{\text{complex}} = ||\mathbf{P} - |\mathbf{\Psi}|^2|| \tag{13}$$

by relative improvement

$$R_1 = \frac{d_{\text{real}} - d_{\text{complex}}}{d_{\text{real}}}. \tag{14}$$

This quantity is measured for truncation numbers K ranging from 2 to 4 and sizes N and M of the source data matrix $\mathbf{P}$ ranging from $K + 1$ to $K + 8$. In each set (K, N, M), independent optimizations producing d_{real} and d_{complex} were performed for 100 randomly generated matrices $\mathbf{P}$.

The resulting values (14) are shown in Fig. 4. The largest improvements are achieved for the smallest N and M close to K. For each K, decreasing of R_1 as a function of M is due to an increasing number of features addressed by the same number of the optimized phase factors. Averaging of R_1 over all N and M for $K = 2, 3, 4$ produces mean relative improvements of 41 %, 56 %, and 75 %, respectively. To compare, the mean difference between the sides of inequality (4) over the same range of parameters is 6 %.

Test 3: quantum-probabilistic decomposition and standard truncated SVD

In this test, the quantum-probabilistic scheme shown in Fig. 2 is compared with the standard truncated SVD. The corresponding distances (13) and (4) are compared by relative improvement

$$R_2 = \frac{d_{\text{SVD}} - d_{\text{complex}}}{d_{\text{SVD}}}. \tag{15}$$

Identically to the previous one, this test is performed for $K = 2, 3, 4$ and sizes of source data N and M ranging from $K + 1$ to $K + 8$. The obtained color maps, analogous to shown in Fig. 4, indicate that improvement (15) is largely independent on N. Therefore, these data are shown in Fig. 5 as functions of M for each K. As in the test 2, the largest improvements are observed for the number of features $M = K + 1$ reaching ≈80 % for $K = 4$. Average improvement over all $K = 2, 3, 4$ is $\langle R_2\rangle = 22$ %.

Test 3 is significant in two aspects. First, it shows the advantage over widely used baseline method of semantic data analysis. Test 2, in contrast, compares the developed

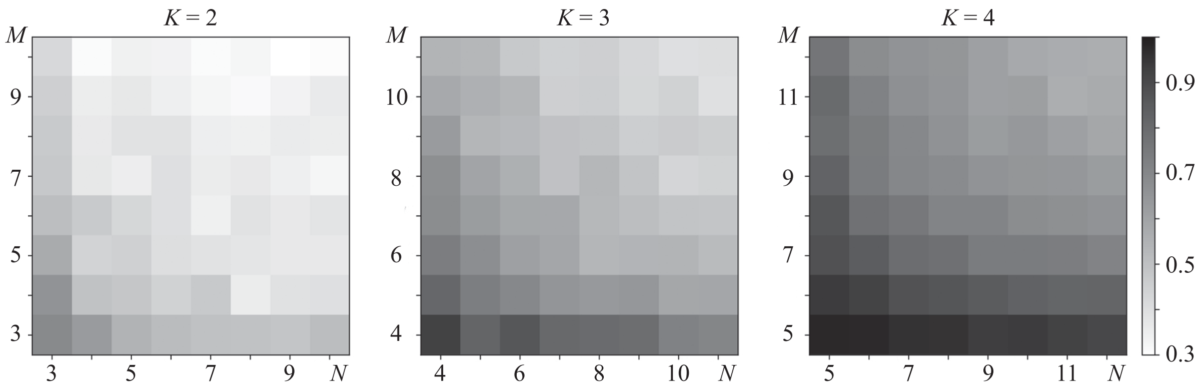

Fig. 4. Advantage in approximation fitness achieved by complex-valued decomposition (Fig. 2) over its real-valued version. Color maps show relative improvement (14) for $K = 2, 3, 4$ with the number of experiments N (horizontal axis) and the number of features M (vertical axis) ranging from $K + 1$ to $K + 8$ in each case

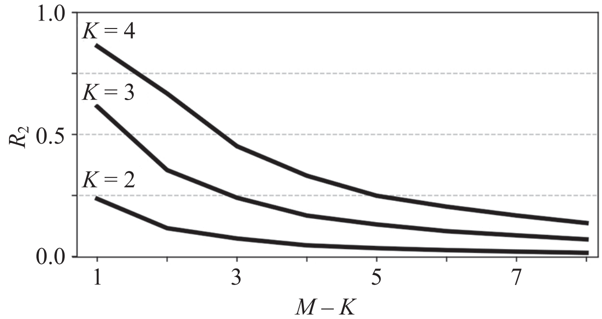

Fig. 5. Relative improvement (15) quantifying the advantage of the developed algorithm over the standard SVD approximation truncated to the same number of latent factors K

algorithm with its real-valued version realized specifically to explicate the difference brought in by using complex numbers. The resulting improvement shown in Fig. 4 is then explainable by the larger number of parameters in the complex-valued version, adding the new (phase) degrees of freedom.

Results of test 3 are not explained by this argument. For $K = 2$, for example, the total numbers of parameters in both algorithms are equal: matrix **C** (Fig. 2) and the product $\mathbf{\Lambda_t} \times \mathbf{V_t}$ in standard SVD (Fig. 1) have the same number of parameters $2N$ (10). Higher approximation fitness in this case is then due to more efficient use of these parameters by the developed algorithm. Analogous advantage of the quantum-probabilistic approach is observed for the Hilbert-space model of semantics of natural language [12].

Discussion

Although the quantum-probabilistic structure was previously used mostly to model of human-generated (behavioral) data, the obtained result shows its advantage even for the pseudo-random matrices taken for testing above. In this case, the obtained model works in “as if” mode, suggesting a cognitive structure of a living agent that might generate the considered data. This process is the essence of an “intentional stance”, virtually endowing behavior with human-like subjectness [13].

Formally, the obtained improvement in accuracy is due to phase degrees of freedom allowing account of non-linear composition of probabilistic factors by linear superposition of the basis wavefunctions. Analogous to similar method [14], this aligns with previous results showing that this “interference effect” is necessary for modeling of data not restricted to rational Boolean logic [15]. Within the intentional stance, interference accounts for regularities of semantic composition, central in modeling of natural language, information retrieval, and artificial intelligence in general [16–23]. The obtained result connects these methods to classical LSA and its successors [24, 25]. In this perspective, phase degrees of freedom account for subjectivity of meaning non-predetermined by the input data, thereby allowing modeling of alternative interpretations of the same factuality.

Conclusion

The obtained result shows the benefit of turning from real- to complex-valued calculus in the baseline method of data analysis. Better approximation of data with the same number of parameters reveals fundamental advantage of quantum-theoretic calculus for compressed representation of information. This advantage can be projected to other methods of data analysis, processing of natural language, and algorithms of artificial intelligence. Analogous to LSA and SVD considered here, these areas can harness the advantage of the Hilbert-space probability structure.

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