Selecting the rank of truncated SVD by Maximum Approximation Capacity

Mario Frank and Joachim M. Buhmann
mario.frank@inf.ethz.ch, j buhmann@inf.ethz.ch
Department of Computer Science, ETH Zurich; Universitätsstrasse 6, CH-8006 Zürich, Switzerland

Abstract—Truncated Singular Value Decomposition (SVD) calculates the closest rank-$k$ approximation of a given input matrix. Selecting the appropriate rank $k$ defines a critical model order choice in most applications of SVD. To obtain a principled cut-off criterion for the spectrum, we convert the underlying optimization problem into a noisy channel coding problem. The optimal approximation capacity of this channel controls the appropriate strength of regularization to suppress noise. In simulation experiments, this information theoretic method to determine the optimal rank competes with state-of-the-art model selection techniques.

I. INTRODUCTION

Singular Value Decomposition (SVD) is a widely used technique for exploratory data analysis. It decomposes a given input matrix into a product of three matrices such that $X = USV^T$. Thereby, $U$ and $V$ are unitary matrices and they essentially induce a rotation of the input data. $S$ is a diagonal matrix (inducing a scaling) with the singular values as entries. Quite often, one is rather interested in an approximation of $X$ instead of the exact decomposition such as, for instance, in Principal Components Analysis (PCA). For SVD, this approximation technically requires to set all but the first $k$ diagonal entries in $S$ to 0. The resulting reconstruction $US_kV^T$ has rank $k$. Neglecting all but the first $k$ components is justified since the noise in the data perturbs the small eigenvalues, whereas the first $k$ components supposedly capture the underlying structure or the signal of the data. Selecting the cutoff value $k$ defines the central model-order selection problem of truncated SVD.

In this paper we propose a novel method for selecting $k$ which is based on the framework of approximation set coding (ASC) [1]. ASC defines the maximum approximation capacity (maxAC) principle for model-order selection. For a given model order and a given noisy dataset, ASC theory enables us to compute the capacity of a hypothetical channel. MaxAC selects the model that achieves highest capacity, i.e., the model of highest complexity that can still be robustly optimized in the presence of noise. Originally, maxAC was derived for discrete optimization problems. So far, it was applied to decoding for the binary channel [1] and for selecting the number of clusters in clustering problems [2]. In this contribution, we adopt it, for the first time, to a continuous optimization problem, namely for selecting the cut-off rank of truncated SVD. Thereby, we investigate the challenges of the continuous solution space. Moreover, we provide an experimental comparison with other model-selection methods indicating that our maxAC adaption to SVD can compete with state-of-the-art methods. In the remainder of the paper we will first introduce the main concepts of ASC in Section II. In Section III we then derive the approximation capacity for SVD, point to problems and solutions and report our numerical findings.

II. APPROXIMATION SET CODING

In this section we briefly recapitulate the principle of maximum approximation capacity (maxAC). Due to the page limit, we must refer to the original paper [1] for a more detailed description.

Consider a generic optimization problem with the input $X = \{x_1, \ldots, x_N\} \in \mathcal{X}$ consisting of $N$ measurements. The vector $x_i \in \mathbb{R}^D$ identifies the $i^{th}$ measurement. Let the output of the optimization problem be the solution or hypothesis $c \in \mathcal{C}$ where $\mathcal{C}$ is the set of all hypotheses satisfying the constraints of the problem, the hypothesis space. An optimization problem involves a cost function $R : \mathcal{C} \times \mathcal{X} \rightarrow \mathbb{R}_{\geq 0}$ that maps a hypothesis $c$ to a real value $R(c, X)$. Finally, let $c^* = \arg \min_c R(c, X)$ be the hypothesis that minimizes costs. In order to rank all solutions of the optimizer, we introduce approximation weights

$$w : \mathcal{C} \times \mathcal{X} \times \mathbb{R}_+ \rightarrow [0, 1],$$

$$(c, X, \beta) \mapsto w_{\beta}(c, X) = \exp(-\beta R(c, X)).$$

These weights, parameterized by the inverse computational temperature $\beta$, define the two weight sums $Z_1, Z_2$, and the joint weight sum $Z_{12}$

$$Z_{\nu} := \sum_{c \in \mathcal{C}} \exp\left(-\beta R(c, X^{(\nu)})\right), \nu = 1, 2$$

$$Z_{12} := \sum_{c \in \mathcal{C}} \exp\left(-\beta (R(c, X^{(1)}) + R(c, X^{(2)}))\right),$$

where $X^{(1)}$ and $X^{(2)}$ are two random subsets of the input $X$ and $\exp(-\beta (R(c, X^{(1)}) + R(c, X^{(2)})))$ measures how well a single solution $c$ minimizes costs on both datasets. The sums (2) play a central role in ASC. If $\beta = 0$, all weights $w_{\beta}(c, X) = 1$ are independent of the costs. In this case, $Z_\nu = |\mathcal{C}|$ indicates the size of the hypothesis space, and $Z_{12} = Z_1 = Z_2$. For intermediate $\beta$, $Z(\cdot)$ takes a value between 0 and $|\mathcal{C}|$, giving rise to the interpretation of $Z(\cdot)$ as the effective number of hypotheses that approximately fit
the dataset $X^{(\nu)}$, whereas $\beta$ defines the precision of this approximation.

ASC constructs a hypothetical coding scenario where sender and receiver have to communicate problem solutions via transformations $\tau \in \mathcal{T}$ of noisy datasets $X^{(1)}$ and $X^{(2)}$. As derived in [11], an asymptotically vanishing error rate for such a channel is achievable for rates

$$\rho \leq I_\beta(\tau_s, \hat{\tau}) = \frac{1}{N} \log \left( \frac{|\{\tau_s\}| \cdot Z_{12}}{Z_1 \cdot Z_2} \right). \tag{4}$$

Eq. (4) denotes the mutual information between the encoded transformation $\tau_s$ of the dataset and the decoded transformation $\hat{\tau}$. A higher approximation precision $\beta$ has two effects. First, the hypothesis space is covered by more patches of approximate solutions leading to more available codewords and a higher codeword entropy $|\{\tau_s\}|$. Second, these patches have a higher overlap such that, in the decoding step, codewords are possibly confused. The maximum of $I_\beta(\tau_s, \hat{\tau})$ with respect to $\beta$ is called the approximation capacity.

III. APPROXIMATION CAPACITY OF SVD

To select the cut-off rank for SVD, we have to find the rank $k^*$ with maximal approximation capacity. This search involves maximizing Eq. (4) for all ranks that we investigate. By going through the list of all quantities introduced in the last section, we relate them to truncated SVD. The input of the problem is a matrix $X \in \mathbb{R}^{N \times D}$. The cost function is the Frobenius norm:

$$R(X, U, S, V) = \sum_{i,j} \left( x_{ij} - \sum_{t=1}^{k} u_{it} s_{tt} v_{tj} \right)^2 \tag{5}$$

An optimizer for this problem outputs a decomposition $c^*(X^{(\nu)}) = U^{(\nu)} S^{(\nu)} V^{(\nu)}$, whereas all but the first $k \leq \min(N, D)$ diagonal entries of $S^{(\nu)}$ are zero due to truncation (we will denote the third matrix by $V$ instead of $V^T$ for convenience). The solution $c^*(X^{(\nu)})$ gives the closest rank-$k$ approximation of $X^{(\nu)}$ with respect to the Frobenius norm. In the case of SVD, a hypothesis $c = (U, S, V)$ is a particular decomposition of the input matrix (in clustering, for instance, $c$ is a relation that assigns objects to clusters). The $k \times D$ matrix with the entries $w_{tj} := s_{it} v_{tj}$ is a new basis and $U$ provides the linear weights needed to represent the data $X$ in this basis. When the empirical mean of $X$ is the origin, this representation corresponds to PCA.

We define the hypothesis space for truncated SVD with cut-off rank $k$ as follows. For a fixed basis $W$, the hypothesis space is spanned by all $N \times k$ matrices $U$. For a given dataset $X^{(\nu)}$, $U^{(\nu)}$ is the cost-minimizing solution. We parameterize the different transformations $\tau \in \mathcal{T}$ for encoding messages in datasets by $\tau \circ X^{(\nu)} = X^{(\nu)} + U\tau W^{(\nu)}$. The identity transformation is $U_{id} = 0$.

The mutual information Eq. (4) was originally derived for finite hypothesis spaces, such as for clustering solutions or binary message strings. The challenges of computing the weight sums (2) and (3) are twofold. First, in a small volume of a continuous hypothesis space, there are infinitely many transformations. Second, transformations can have infinite distance to each other such that the receiver can always distinguish an infinite subset of $\mathcal{T}$ even when the datasets are noisy. This makes the union bound in the derivation of the error-probability in [11], Eq. (7) inadequate. For these reasons, calculating the capacity under the assumption that $U$ can be any real $N \times k$ matrix fails. In the following, we will first demonstrate the effect of this assumption by providing the naïve analytical calculation of the mutual information in Eq. (4). Then we introduce constraints on the transformations $\mathcal{T}$ such that Eq. (4) can be computed.

A. Unconstraint Hypothesis Space

We abbreviate $R_\nu = R(X^{(\nu)}, U, S^{(\nu)}, V^{(\nu)})$ and $R_\Delta = 1/2 \left( R(X^{(1)}, U, S^{(1)}, V^{(1)}) + R(X^{(2)}, U, S^{(1)}, V^{(1)}) \right)$ and use the short-hand notation of $m_{i\nu}$, as the $i$th row of a matrix M. By integrating over the space of all linear combinations $U$, we obtain the weight sums:

$$Z_\nu = \int_{-\infty}^{\infty} \exp \left[ -\beta R_\nu \right] dU, \quad \nu \in \{1, 2\} \tag{6}$$

$$= \prod_{i,j} e^{-\beta x_{ij}^2} \int_{-\infty}^{\infty} \exp \left[ -\beta \left( \sum_k u_{it} w_{ik} \right)^2 - 2 \sum_k u_{it} w_{ik} x_{ij} \right] d^k u_{it}. \tag{7}$$

The solution of Gaussian integrals yields

$$\int_{-\infty}^{\infty} e^{-1/2 \sum_{i,j} \sum_k b_{ij} w_{ij} + \sum_k b_{ij}} = \sqrt{\frac{2\pi}{\det(A)}} e^{1/2 b^T A^{-1} b},$$

wheras in our case

$$A_{(ij)} = 2\beta w_{ij}^T w_{ij}, \quad b_{(ij)} = 2\beta x_{ij} w_{ij}^T, \quad A_{(\Delta)} = A_{(ij)}^{\nu}, \quad b_{(\Delta)} = 2\beta (x_{ij}^2 + x_{ij}^2) w_{ij}^T. \tag{8}$$

The weight sums are

$$Z_{12} = \prod_{i,j} e^{-\beta x_{ij}^2} \left[ 1 - \beta \sum_j x_{ij} w_{ij}^T (1 - w_{ij}^T w_{ij})^{-1} w_{ij}^T \right]. \tag{9}$$

We abbreviated $D^{(\nu)}_{ij} := \det(w_{ij}^T w_{ij}^T)$. In step (i), we used that for a $n \times n$ matrix $M$ and a scalar $p$, it holds that $\det(pM) = p^n \det(M)$. In step (ii), we used that
In the regime where $\tau_1$ we write $\sigma$ on the capacity. We create data $X$ on an equispaced grid in a hypercube of finite size. Second, we experimentally investigate the influence of these parameters: an infinitely large capacity due to i) an infinitely large transformation space $\mathbb{R}^{N \times k}$ (or a negative one if we disregard the infinitely many possible codewords) and ii) due to the existence of infinitely many transformations in an arbitrary small volume of this space. For a practical implementation of the maxAC criterion for SVD we have to i) bound the hypothesis space and ii) constraint the density of transformations to a finite number. This renders the integrals for computing the weight sums to finite sums which must be explicitly computed. In our experiments, we use two ways of summing over the hypothesis space. First, we experimentally populate the hypothesis space on an equispaced grid in a hypercube of finite size. Second, we randomly sample transformations from an isotropic Gaussian. In both cases the set of transformations is centered around the cost minimizing solution $U^{(1)}$ (the identity transformation $U_{id}$). For both ways, one must choose the boundaries (the size of the grid or the variance of the Gaussian) as well as the number of transformations.

We experimentally investigate the influence of these parameters. First, we study the influence of the integration range on the capacity. We create data $X^{(\nu)}$ from a mixture of 4 Gaussians with isotropic noise, leading to an optimal rank 4. We compute the approximation capacity by sampling transformations from a Gaussian sphere around the cost-minimizing SVD solution $U^{(\nu)}$ with standard deviation $\sigma$. Our experimental findings for various magnitudes of $\sigma$ are illustrated in Fig. 2. We write $\sigma$ in units of $\Delta = 1/N \sum_{i=1}^N \|u^{(1)}_{i} - u^{(2)}_{i}\|$, whereas $U^{(1,2)}$ is the matrix that satisfies $X^{(2)} = U^{(1,2)}W^{(1)}$. In the regime where $1/N \|U_{\nu}\| \approx \Delta$, a transformed dataset $\tau_j \circ X^{(2)}$ could possibly be confused with $X^{(1)}$. When the transformations are smaller than $\Delta$, none of the transformations could possibly be used in a codebook as they are all indistinguishable from the identity transformation. As a result, the obtained capacity is too low. On the contrary, for a too high integration range, the capacity converges to the naive analytical solution because infinitely many transformations could serve as distinguishable codewords.

The second experiment studies the influence of the number of transformations on the mutual information. This time, we use a grid of fixed size and vary the density of grid points. In order to sufficiently cover the hypothesis space, we increase the number of transformations by a factor of 2 when increasing $k$. While this increment is still too low to preserve the transformation density, it already imposes a computational challenge. In our experiments with larger datasets, we sample the hypothesis space more sparsely. The influence of the number of transformations is illustrated in Fig. 3. The results demonstrate that this number only affects the stability of the computation and not the maximum of the capacity.

### Continuous and bounded hypothesis space

The numerical experiment on the influence of the number of transformations suggests that for a defined transformation density, the analytical solution should provide the desired result if only the integration range is properly defined. We calculate the mutual information as in Section III-A but, this time, we weight the integrand with an isotropic Gaussian around the identity $u^{(1)}_{it}, \forall i, t$ to suppress the contribution of heavy transformations.

$$Z_{\nu} = \int_{-\infty}^{\infty} e^{-\beta R_{\nu}} e^{-\frac{1}{2} \sigma \sum_{i,t} (u_{it} - u^{(1)}_{it})^2} dU, \quad \nu \in \{1, 2\}$$

$$Z_{12} = \int_{-\infty}^{\infty} e^{-\beta R_{\Delta}} e^{-\frac{1}{2} \sum_{i,t} (u_{it} - u^{(1)}_{it})^2} dU$$

The derivation of the mutual information is provided in Appendix B. The simulations depicted in Fig. 3 illustrate that for an analytically computed mutual information (see Eq. 40), the width $\sigma$ influences the capacity much more than in the numerical computation (compare with Fig. 2). However, if a maximum exists (square markers in Fig. 3), it is at the correct rank.
approximation capacity against rank for various numbers of sample points. The optimal rank is \( k = 4 \). Even though the individual trends still vary a lot for very few sample points, the optimal model-order is already found. With increasing number of transformations the calculations are stabilized.

![Fig. 1](image)

Fig. 1. Approximation capacity against rank for various numbers of sample points. The optimal rank is \( k = 4 \). Even though the individual trends still vary a lot for very few sample points, the optimal model-order is already found. With increasing number of transformations the calculations are stabilized.

D. Comparison with other model-selection techniques

We study how well maxAC and other model-order selection methods select the appropriate rank for approximating a noisy dataset via rank-limited SVD. A comparison with the following methods is performed: ‘Laplace’ and ‘BIC’ approximate the marginal likelihood (the evidence) for probabilistic PCA [3]. The first method applies Laplace approximation to the involved integral. The well-known BIC score [4] further simplifies that the likelihood exhibits the same sensitivity to all model parameters. A third method, the minimum transfer cost principle (‘MTC’) [5], mimics cross-validation. It learns a rank-limited SVD on one random subset of the data and then computes the costs when applying it to another one. Thereby, the model parameters are transferred by a mapping function \( \psi \) which maps each object in the first dataset to its nearest neighbor in the second dataset.

We create objects from a number of centroids with a defined separation from each other and add Gaussian noise. The difficulty of the problem is controlled by altering the variance relative to the separation of the centroids. When going to a higher number of centroids, the dimensionality must also be increased to preserve their separation. To enable a comparison with the PCA methods, the data mean is shifted to the origin. For a given true number of generating components and a given noise level relative to the centroid separation, there exists one SVD rank that yields the reconstruction with the minimal deviation from the noise-free matrix. For very noisy data or a high number of components and dimensions, this optimally denoising rank is smaller than the true number of generating components. Inspecting Fig. 4 one can see that all methods select a rank between the best denoising rank and the true rank. For low noise (Fig. 4(a)) learning the rank is easy. For a high noise level, the learning problem becomes hard when the number of generating components and the dimensionality increase. There exists a transitional regime where all methods start selecting a lower rank than the true one (Fig. 4(b)). For very high noise levels, all methods select \( k = 1 \) (Fig. 4(c)).

IV. CONCLUSION

We proposed a novel technique for selecting the cut-off rank of truncated SVD. Our criterion selects the rank that maximizes the approximation capacity (maxAC) and, thereby, captures the maximum amount of information in the data that can be reliably inferred from random subsets of the input dataset. We demonstrated, for the first time, how to apply maxAC to an optimization problem with a continuous solution space like SVD. The Euclidean geometry of the parameter space renders the computation of the approximation capacity more difficult than in the clustering case with random permutations [2]. We discussed the challenges with such problem domains and proposed solutions. Finally, we demonstrated in comparative experiments that the model-order selection of our technique conforms with established methods. Future work will address the application of the maxAC criterion to other continuous optimization problems such as, for instance, sparse linear regression.

ACKNOWLEDGMENTS

This work was partially supported by the Zurich Information Security Center and by the FP7 EU project SIMBAD.

REFERENCES

[1] J. M. Buhmann, “Information theoretic model validation for clustering,” in ISIT, 2010.
[2] J. M. Buhmann, M. H. Chehreghani, M. Frank, and A. P. Streich, “Information theoretic model selection for pattern analysis,” in JMLR: Workshop and Conference Proceedings 7, 1-8, 2011.
[3] T. P. Minka, “Automatic choice of dimensionality for PCA,” in NIPS, 2000, p. 514.
[4] G. Schwarz, “Estimating the dimension of a model,” The Annals of Statistics, vol. 6, no. 2, pp. 461-464, 1978.
[5] M. Frank, M. H. Chehreghani, and J. M. Buhmann, “The minimum transfer cost principle for model-order selection,” in ECML, 2011.
APPENDIX A: ATTAINING CAPACITY

There are several ways of numerically maximizing the mutual information in Eq. [3] with respect to the temperature. The simplest way is to compute \( I_\beta \) for several values of \( \beta \) and pick the maximum. This creates a quantization error of the optimum that depends on the step-size of the temperature scale. Moderate step-sizes already lead to good results as \( I_\beta \) is usually flat around its maximum.

Using a gradient-descent method like Newton iterations provide more precise results. In the following, we report the first and the second derivation of \( I_\beta \) which are needed for the Newton updates. The derivation of the mutual information \( I_\beta \) (Eq. [4]) with respect to the inverse temperature \( \beta \) is

\[
\frac{\partial I(\beta)}{\partial \beta} = 1/N \frac{\partial}{\partial \beta} \left[ \log \left( |C_\gamma| \right) - \sum_{\nu=1}^{2} \log \left( \left| \mathcal{C}^{(\nu)}_\gamma \right| \right) \right]
\]

(15)

\[
= \frac{1}{N} \left( \frac{\partial}{\partial \beta} |\Delta C_\gamma| - \sum_{\nu=1}^{2} \frac{\partial}{\partial \beta} \left| \mathcal{C}^{(\nu)}_\gamma \right| \right)
\]

(16)

\[
\frac{\partial^2 I(\beta)}{\partial \beta^2} = \frac{1}{N} \sum_{\nu=1}^{2} \left( \frac{\partial}{\partial \beta} \frac{\partial}{\partial \beta} \left| \mathcal{C}^{(\nu)}_\gamma \right| \right)
\]

(17)

Where \( p_{C}(R_\Delta) = Z^{-1} \exp(-\beta R_\Delta) \) is the Gibbs distribution with normalization constant \( Z = \int_{-\infty}^{\infty} \exp(-\beta R_\Delta) dU \). These expectations can easily be computed either for a finite set of transformations or with a continuous integral.

Accordingly, the second derivative is:

\[
\frac{\partial^2 I(\beta)}{\partial \beta^2} = \frac{1}{N} \sum_{\nu=1}^{2} \left( \frac{\partial}{\partial \beta} \frac{\partial}{\partial \beta} \left| \mathcal{C}^{(\nu)}_\gamma \right| \right)
\]

(18)

\[
= \frac{1}{N} \left( \frac{\partial}{\partial \beta} \left[ \left| \mathcal{C}^{(1)}_\gamma \right| \right] + \frac{\partial}{\partial \beta} \left| \mathcal{C}^{(2)}_\gamma \right| \right)
\]

(19)

APPENDIX B: ANALYTICAL CALCULATION WITH BOUNDED INTEGRATION RANGE

We derive the mutual information Eq. [40] when the transformations are weighted with a Gaussian centered around the identity transformation \( u_{it}^{(1)} \). Except for this modification the derivation is analog to the derivation of the unconstraint mutual information in Eq. [11]. The approximation sets and the joint approximation set are

\[
\left| \mathcal{C}^{(\nu)}_\gamma \right| = \int_{-\infty}^{\infty} \exp \left( -\beta R(X^{(\nu)} , U, S^{(\nu)} , V^{(\nu)}) \right) \exp \left( -\frac{1}{2\sigma} \sum_{t} u_{it} - u_{it}^{(1)} \right) dU \quad \nu \in \{1, 2\}
\]

(20)

\[
= \prod_{ij} \exp \left( -\beta x_{ij}^{(\nu)^2} \right) \exp \left( -\frac{1}{2\sigma D} \sum_{t} u_{it}^2 \right)
\]

(21)

\[
\cdot \int_{-\infty}^{\infty} \exp \left( -\beta \sum_{t} \sum_{t'} u_{it} \left( \frac{1}{\sigma D} u_{it}^{(1)} - 2w_{ij}^{(\nu)} u_{ij}^{(\nu)} \right) \right)
\]

\[
\cdot \exp \left( -2\beta \sum_{t} \sum_{t'} \sum_{t''} u_{it}^{(\nu)^2} u_{it'} u_{it''} + \frac{1}{2\sigma D} \sum_{t} u_{it} \right) d^4 u_{i}.
\]

and

\[
|\Delta C_\gamma| = \int_{-\infty}^{\infty} \exp \left( -\beta/2 \left( R(X^{(1)} , U, S^{(1)} , V^{(1)}) + R(X^{(2)} , U, S^{(1)} , V^{(1)}) \right) \right) \exp \left( -\frac{1}{2\sigma} \sum_{t} u_{it} - u_{it}^{(1)} \right) dU
\]

(22)

\[
= \prod_{ij} \exp \left( -\beta/2 \left( x_{ij}^{(1)^2} + x_{ij}^{(2)^2} \right) \right) \exp \left( -\frac{1}{2\sigma D} \sum_{t} u_{it}^2 \right)
\]

(23)

\[
\cdot \int_{-\infty}^{\infty} \exp \left( -\beta \sum_{t} \sum_{t'} u_{it} \left( \frac{1}{\sigma D} u_{it}^{(1)} - 2w_{ij}^{(1)} u_{ij}^{(1)} \right) + \frac{1}{2\sigma D} \sum_{t} u_{it} \right) d^4 u_{i}.
\]
The characteristic terms of the integrals are

\[ A^{(\nu)}_{ij} = 2\beta a^{(\nu)}_{ij}, \]
\[ b^{(\nu)}_{(i,j)} = 2\beta x^{(\nu)}_{ij} w^{(\nu)}_{ij}^T - \frac{1}{\sigma D} u^{(1)}_{i}, \]
\[ A^{(\Delta)}_{ij} = A^{(1)}_{ij}, \]
\[ b^{(\Delta)}_{(i,j)} = \beta \left( x_{ij}^{(1)} + x_{ij}^{(2)} \right) w_{ij}^{(1)} - \frac{1}{\sigma D} u_{i}^{(1)}, \]

with

\[ a^{(\nu)}_{ij} := w_{ij}^{(\nu)^T} w_{ij}^{(\nu)} + \frac{1}{2\sigma \beta D} I. \]

These terms determine the cardinalities of the approximation sets:

\[
\left| C^{(\nu)}_{\gamma} \right| = \prod_{i,j} \frac{1}{\sqrt{2\pi}} \exp \left( -\beta x^{(\nu)^2}_{ij} \right) \exp \left( -\frac{1}{2\sigma D} u^{(1)}_{i} u^{(1)^T}_{i} \right) \sqrt{\frac{(2\pi)^k}{\det \left( 2\beta a^{(\nu)}_{ij} \right)}} EXP \left( \frac{1}{2} b^{(\nu)}_{(i,j)} A^{(\nu)}_{ij}^{-1} b^{(\nu)}_{(i,j)} \right) \]  

\[
= \left( \frac{\pi}{\beta} \right)^{\frac{N D k}{2}} \prod_{i,j} \det \left( a^{(\nu)}_{ij} \right)^{-1/2} \exp \left( -\beta x^{(\nu)^2}_{ij} - \frac{1}{2\sigma D} u^{(1)}_{i} u^{(1)^T}_{i} \right) + \frac{1}{4\beta} \left( 2\beta \right)^{\nu} x^{(\nu)^T}_{ij} w^{(\nu)}_{ij} - \frac{1}{\alpha D} u^{(1)}_{i} \left( a^{(\nu)}_{ij} - \frac{1}{2\beta} \right) w^{(\nu)}_{ij} - \frac{1}{\sigma D} u^{(1)}_{i} \right) \]  

\[
= \left( \frac{\pi}{\beta} \right)^{\frac{N D k}{2}} \prod_{i,j} \det \left( a^{(\nu)}_{ij} \right)^{-\frac{N}{2}} \prod_{i,j} \exp \left( -\beta x^{(\nu)^2}_{ij} \right) \left( 1 - w^{(\nu)}_{ij} a^{(\nu)}_{ij}^{-1} w^{(\nu)}_{ij} \right) - \frac{1}{2\sigma D} u^{(1)}_{i} u^{(1)^T}_{i} \left( a_{ij}^{(1)} - \frac{1}{2\beta} \right) w^{(1)}_{ij} - \frac{1}{4\beta \sigma^2 D^2} u^{(1)}_{i} a^{(1)}_{ij}^{-1} u^{(1)^T}_{i} \right) \]  

and

\[
\left| \Delta C_{\gamma} \right| = \prod_{i,j} \frac{1}{\sqrt{2\pi}} \exp \left( -\beta \left( x^{(1)^2}_{ij} + x^{(2)^2}_{ij} \right) \right) \exp \left( -\frac{1}{2\sigma D} u^{(1)}_{i} u^{(1)^T}_{i} \right) \sqrt{\frac{(2\pi)^k}{\det \left( 2\beta a^{(1)}_{ij} \right)}} EXP \left( \frac{1}{2} b^{(\Delta)}_{(i,j)} A^{(1)}_{ij}^{-1} b^{(\Delta)}_{(i,j)} \right) \]  

\[
= \left( \frac{\pi}{\beta} \right)^{\frac{N D k}{2}} \prod_{i,j} \det \left( a^{(1)}_{ij} \right)^{-\frac{N}{2}} \prod_{i,j} \exp \left( -\beta \left( x^{(1)^2}_{ij} + x^{(2)^2}_{ij} - \frac{1}{2} \left( x^{(1)}_{ij} + x^{(2)}_{ij} \right)^2 \right) \right) \left( 1 - w^{(1)}_{ij} a^{(1)}_{ij}^{-1} w^{(1)}_{ij} \right) - \frac{1}{2\sigma D} u^{(1)}_{i} u^{(1)^T}_{i} \left( a_{ij}^{(1)} - \frac{1}{2\beta} \right) w^{(1)}_{ij} - \frac{1}{4\beta \sigma^2 D^2} u^{(1)}_{i} a^{(1)}_{ij}^{-1} u^{(1)^T}_{i} \right) \]
The number of random transformations depends on the size of the Gaussian sphere $b$:

\[
 b = \int_{-\infty}^{\infty} \exp \left( -\frac{1}{2\sigma} \sum_{i,t} (u_{it} - u_{it}^{(1)})^2 \right) dU
\]

\[
 = \prod_i \sqrt{\frac{(2\pi)^k}{\det (\sigma^{-1}\Pi)}}
\]

\[
 = (2\pi\sigma)^{\frac{nk}{2}}.
\]

Define the auxiliary variables $F^{(\nu)}_{(j)} := w^{(\nu)}_{ij} a^{(\nu)}_j^{-1} w^{(\nu)^T}_{ij}$. Then, the mutual information is

\[
 I(\beta) = 1/N \left( |\{\tau_j\}| + \log (|\Delta C_\gamma|) - \frac{1}{2} \sum_{\nu=1}^2 \log \left( |C_\gamma^{(\nu)}| \right) \right)
\]

\[
 = k/2 \log(2\pi\sigma) + \frac{Dk}{2} (\log (\beta) - \log (\pi)) + \frac{1}{2} \sum_j \log \left( \det \left( a^{(2)}_{(j)} \right) \right)
\]

\[
 + \frac{1}{N} \sum_{ij} \left[ \frac{\beta}{2} \left( x_{ij}^{(1)2} + x_{ij}^{(2)2} - \frac{1}{2} \left( x_{ij}^{(1)} + x_{ij}^{(2)} \right)^2 \right) F^{(1)}_{(j)} + \frac{1}{2\sigma D} u^{(1)}_{ij} u^{(2)}_{ji} + \frac{1}{4\beta\sigma^2 D^2} u^{(1)}_{ij} a^{(2)}_j u^{(2)}_{ji} \right]
\]

\[
 + \frac{1}{N} \sum_{ij} \left[ \frac{\beta}{2} \left( x_{ij}^{(1)2} + x_{ij}^{(2)2} - \frac{1}{2} \left( x_{ij}^{(1)} + x_{ij}^{(2)} \right)^2 \right) F^{(2)}_{(j)} + \frac{1}{2\sigma D} u^{(1)}_{ij} u^{(2)}_{ji} + \frac{1}{4\beta\sigma^2 D^2} u^{(1)}_{ij} a^{(2)}_j u^{(2)}_{ji} \right]
\]

\[
 = k/2 \log(2\pi\sigma) + \frac{kD}{2} \log \left( \frac{\beta}{\pi} \right) + \frac{1}{2} \sum_j \log \left( \det \left( a^{(2)}_{(j)} \right) \right)
\]

\[
 + \frac{1}{2\sigma N} \sum_i u^{(1)}_{i} u^{(2)}_{ji} + \frac{1}{4\beta\sigma^2 D^2 N} \sum_{ij} u^{(1)}_{ij} a^{(2)}_j u^{(1)}_{ij}
\]

\[
 + \frac{\beta}{2N} \sum_{ij} \left[ x_{ij}^{(1)2} \left( 1 - \frac{3}{2} F^{(1)}_{(j)} \right) + x_{ij}^{(2)2} \left( 1 - 2F^{(2)}_{(j)} + \frac{1}{2} F^{(1)}_{(j)} \right) + x_{ij}^{(1)} x_{ij}^{(2)} F^{(1)}_{(j)} \right].
\]