Computationally Efficient Sufficient Dimension Reduction via Squared-Loss Mutual Information

Makoto Yamada   YAMADA@SG.CS.TITECH.AC.JP
Gang Niu   GANG@SG.CS.TITECH.AC.JP
Jun Takagi   TAKAGI@SG.CS.TITECH.AC.JP
Masashi Sugiyama   SUGI@CS.TITECH.AC.JP
Department of Computer Science, Tokyo Institute of Technology

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Abstract

The purpose of sufficient dimension reduction (SDR) is to find a low-dimensional expression of input features that is sufficient for predicting output values. In this paper, we propose a novel *distribution-free* SDR method called *sufficient component analysis* (SCA), which is computationally more efficient than existing methods. In our method, a solution is computed by iteratively performing dependence estimation and maximization: Dependence estimation is analytically carried out by recently-proposed *least-squares mutual information* (LSMI), and dependence maximization is also analytically carried out by utilizing the *Epanechnikov kernel*. Through large-scale experiments on real-world image classification and audio tagging problems, the proposed method is shown to compare favorably with existing dimension reduction approaches.

Keywords: Sufficient dimension reduction, squared-loss mutual information, Epanechnikov kernel, image classification, audio tagging.

1. Introduction

The goal of *sufficient dimension reduction* (SDR) is to learn a transformation matrix $\boldsymbol{W}$ from input feature $\boldsymbol{x}$ to its low-dimensional representation $\boldsymbol{z}\ (=\boldsymbol{W}\boldsymbol{x})$ which has 'sufficient' information for predicting output value $\boldsymbol{y}$. Mathematically, SDR can be formulated as the problem of finding $\boldsymbol{z}$ such that $\boldsymbol{x}$ and $\boldsymbol{y}$ are conditionally independent given $\boldsymbol{z}$ (Cook, 1998; Fukumizu et al., 2009).

Earlier SDR methods developed in statistics community, such as *sliced inverse regression* (Li, 1991), *principal Hessian direction* (Li, 1992), and *sliced average variance estimation* (Cook, 2000), rely on the elliptic assumption (e.g., Gaussian) of the data, which may not be fulfilled in practice.

To overcome the limitations of these approaches, *kernel dimension reduction* (KDR) was proposed (Fukumizu et al., 2009). KDR employs a kernel-based dependence measure, which does not require the elliptic assumption (i.e., distribution-free), and the solution $\boldsymbol{W}$ is computed by a gradient method. Although KDR is a highly flexible SDR method, its critical weakness is the kernel function choice—the performance of KDR depends on the choice of kernel functions and the regularization parameter, but there is no systematic model

selection method available[1]. Furthermore, KDR scales poorly to massive datasets since the gradient-based optimization is computationally demanding. Another important limitation of KDR in practice is that there is no good way to set an initial solution—many random restarts may be needed for finding a good local optimum, which makes the entire procedure even slower and the performance of dimension reduction unreliable.

To overcome the limitations of KDR, a novel SDR method called *least-squares dimension reduction* (LSDR) was proposed recent (Suzuki and Sugiyama, 2010). LSDR adopts a squared-loss variant of mutual information (SMI) as a dependency measure, which is efficiently estimated by a method called *least-squares mutual information* (LSMI) (Suzuki et al., 2009). A notable advantage of LSDR over KDR is that kernel functions and its tuning parameters such as the kernel width and the regularization parameter can be naturally optimized based on cross-validation, which is independent of succeeding predictors. However, LSDR still relies on a computationally expensive gradient method and there is no good initialization scheme.

In this paper, we propose a novel SDR method called *sufficient component analysis* (SCA), which can overcome the computational inefficiency of LSDR. In SCA, the solution $\boldsymbol{W}$ in each iteration is obtained *analytically* by just solving an eigenvalue problem, which highly contributes to improving the computational efficiency. Moreover, based on the above analytic-form solution, we develop a method to design a useful initial value for optimization, which further reduces the computational cost and helps to obtain a good solution.

Through large-scale experiments using the *PASCAL Visual Object Classes (VOC) 2010* dataset (Everingham et al., 2010) and the *Freesound* dataset (The Freesound Project, 2011), we demonstrate the usefulness of the proposed method.

2. Sufficient Dimension Reduction with Squared-Loss Mutual Information

In this section, we formulate the problem of *sufficient dimension reduction* (SDR) based on *squared-loss mutual information* (SMI).

2.1. Problem Formulation

Let $\mathcal{X}$ ($\subset \mathbb{R}^d$) be the domain of input feature $\boldsymbol{x}$ and $\mathcal{Y}$ be the domain of output data[2] $\boldsymbol{y}$. Suppose we are given n independent and identically distributed (i.i.d.) paired samples,

$$D^n = \{(\boldsymbol{x}_i, \boldsymbol{y}_i) \mid \boldsymbol{x}_i \in \mathcal{X}, \ \boldsymbol{y}_i \in \mathcal{Y}, \ i = 1, \ldots, n\},$$

drawn from a joint distribution with density $p_{\mathrm{xy}}(\boldsymbol{x}, \boldsymbol{y})$.

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1. In principle, it is possible to choose the Gaussian width and the regularization parameter by cross-validation over a succeeding predictor. However, this results in a deeply nested cross-validation procedure and therefore this is computationally very expensive. Furthermore, features extracted based on cross-validation are no longer independent of predictors. Thus, a merit of sufficient dimension reduction (i.e., the obtained features are independent of the choice of predictors and thus reliable) is lost.

2. $\mathcal{Y}$ could be either continuous (i.e., regression) or categorical (i.e., classification). Multi-dimensional outputs (e.g., multi-task regression and multi-label classification) and structured outputs (such as sequences, trees, and graphs) can also be handled in the proposed framework.

The goal of SDR is to find a low-dimensional representation $\boldsymbol{z}$ ($\in \mathbb{R}^m$, $m \le d$) of input $\boldsymbol{x}$ that is sufficient to describe output $\boldsymbol{y}$. More precisely, we find $\boldsymbol{z}$ such that

$$\boldsymbol{y} \perp\!\!\!\perp \boldsymbol{x} \mid \boldsymbol{z}. \tag{1}$$

This means that, given projected feature $\boldsymbol{z}$, feature $\boldsymbol{x}$ is conditionally independent of output $\boldsymbol{y}$.

In this paper, we focus on linear dimension reduction scenarios:

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x},$$

where $\boldsymbol{W}$ ($\in \mathbb{R}^{m \times d}$) is a transformation matrix. $\boldsymbol{W}$ is assumed to belong to the *Stiefel manifold* $\mathbb{S}_m^d(\mathbb{R})$:

$$\mathbb{S}_m^d(\mathbb{R}) := \{\boldsymbol{W} \in \mathbb{R}^{m \times d} \mid \boldsymbol{W}\boldsymbol{W}^\top = \boldsymbol{I}_m\},$$

where $^\top$ denotes the transpose and $\boldsymbol{I}_m$ is the m-dimensional identity matrix. Below, we assume that the reduced dimension m is known.

2.2. Dependence Estimation-Maximization Framework

It was showed that the optimal transformation matrix $\boldsymbol{W}^*$ that leads to Eq.(1) can be characterized as follows (Suzuki and Sugiyama, 2010):

$$\boldsymbol{W}^* = \operatorname*{argmax}_{\boldsymbol{W} \in \mathbb{R}^{m \times d}} \operatorname{SMI}(Z, Y) \ \ \text{s.t.} \ \boldsymbol{W}\boldsymbol{W}^\top = \boldsymbol{I}_m, \tag{2}$$

where $\operatorname{SMI}(Z, Y)$ is the *squared-loss mutual information* (SMI) defined by

$$\operatorname{SMI}(Z, Y) := \frac{1}{2} \mathbb{E}_{p_z, p_y} \left[\left(\frac{p_{zy}(\boldsymbol{z}, \boldsymbol{y})}{p_y(\boldsymbol{y}) p_z(\boldsymbol{z})} - 1 \right)^2 \right].$$

In the above, $\mathbb{E}_{p_z, p_y}$ denotes the expectation over the marginals $p_z(\boldsymbol{z})$ and $p_y(\boldsymbol{y})$. Note that SMI is the *Pearson divergence* (Pearson, 1900) from $p_{zy}(\boldsymbol{z}, \boldsymbol{y})$ to $p_z(\boldsymbol{z}) p_y(\boldsymbol{y})$, whereas ordinary mutual information is the *Kullback-Leibler divergence* (Kullback and Leibler, 1951) from $p_{zy}(\boldsymbol{z}, \boldsymbol{y})$ to $p_z(\boldsymbol{z}) p_y(\boldsymbol{y})$. The Pearson divergence and the Kullback-Leibler divergence both belong to the class of f-*divergences* (Ali and Silvey, 1966; Csiszár, 1967), and thus they share similar theoretical properties. For example, SMI is non-negative and takes zero if and only if Z and Y are statistically independent, as ordinary mutual information.

Based on Eq.(2), we develop the following iterative algorithm for learning $\boldsymbol{W}$:

(i) Initialization: Initialize the transformation matrix $\boldsymbol{W}$ (see Section 3.3).

(ii) Dependence estimation: For current $\boldsymbol{W}$, an SMI estimator $\widehat{\operatorname{SMI}}$ is obtained (see Section 3.1).

(iii) Dependence maximization: Given an SMI estimator $\widehat{\operatorname{SMI}}$, its maximizer with respect to $\boldsymbol{W}$ is obtained (see Section 3.2).

(iv) Convergence check: The above (ii) and (iii) are repeated until $\boldsymbol{W}$ fulfills some convergence criterion[3].

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3. In experiments, we used the criterion that the improvement of $\widehat{\operatorname{SMI}}$ is less than 10^{-6}.

3. Proposed Method: Sufficient Component Analysis

In this section, we describe our proposed method called the *sufficient component analysis* (SCA).

3.1. Dependence Estimation

In SCA, we utilize a non-parametric SMI estimator called *least-squares mutual information* (LSMI) (Suzuki et al., 2009), which was shown to possess a desirable convergence property (Suzuki and Sugiyama, 2010). Here, we briefly review LSMI.

3.1.1. BASIC IDEA

The key idea of LSMI is to directly estimate the *density ratio* (Sugiyama et al., 2012),

$$w(\boldsymbol{z}, \boldsymbol{y}) = \frac{p_{\mathrm{zy}}(\boldsymbol{z}, \boldsymbol{y})}{p_{\mathrm{z}}(\boldsymbol{z}) p_{\mathrm{y}}(\boldsymbol{y})},$$

without going through density estimation of $p_{\mathrm{zy}}(\boldsymbol{z}, \boldsymbol{y})$, $p_{\mathrm{z}}(\boldsymbol{z})$, and $p_{\mathrm{y}}(\boldsymbol{y})$. Here, the density ratio function $w(\boldsymbol{z}, \boldsymbol{y})$ is directly modeled as

$$w_{\boldsymbol{\alpha}}(\boldsymbol{z}, \boldsymbol{y}) = \sum_{\ell=1}^{n} \alpha_\ell K(\boldsymbol{z}, \boldsymbol{z}_\ell) L(\boldsymbol{y}, \boldsymbol{y}_\ell), \tag{3}$$

where $\boldsymbol{z}_\ell = \boldsymbol{W} \boldsymbol{x}_\ell$, and $K(\boldsymbol{z}, \boldsymbol{z}')$ and $L(\boldsymbol{y}, \boldsymbol{y}')$ are kernel functions for $\boldsymbol{z}$ and $\boldsymbol{y}$, respectively.

Then, the parameter $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)^\top$ is learned so that the following squared error is minimized:

$$J_0(\boldsymbol{\alpha}) := \frac{1}{2} \mathbb{E}_{p_{\mathrm{z}}, p_{\mathrm{y}}} \left[(w_{\boldsymbol{\alpha}}(\boldsymbol{z}, \boldsymbol{y}) - w(\boldsymbol{z}, \boldsymbol{y}))^2 \right].$$

After a few lines of calculation, we can see that J_0 is expressed as

$$J_0(\boldsymbol{\alpha}) = J(\boldsymbol{\alpha}) + \mathrm{SMI}(Z, Y) + \frac{1}{2},$$

where

$$J(\boldsymbol{\alpha}) := \frac{1}{2} \boldsymbol{\alpha}^\top \boldsymbol{H} \boldsymbol{\alpha} - \boldsymbol{h}^\top \boldsymbol{\alpha},$$

$$H_{\ell, \ell'} := \mathbb{E}_{p_{\mathrm{z}}, p_{\mathrm{y}}} \left[K(\boldsymbol{z}, \boldsymbol{z}_\ell) L(\boldsymbol{y}, \boldsymbol{y}_\ell) K(\boldsymbol{z}, \boldsymbol{z}_{\ell'}) L(\boldsymbol{y}, \boldsymbol{y}_{\ell'}) \right],$$

$$h_\ell := \mathbb{E}_{p_{\mathrm{zy}}} \left[K(\boldsymbol{z}, \boldsymbol{z}_\ell) L(\boldsymbol{y}, \boldsymbol{y}_\ell) \right].$$

Since $\mathrm{SMI}(Z, Y)$ is constant with respect to $\boldsymbol{\alpha}$, minimizing J_0 is equivalent to minimizing J.

3.1.2. COMPUTING THE SOLUTION

Approximating the expectations in $\boldsymbol{H}$ and $\boldsymbol{h}$ included in J by empirical averages, we arrive at the following optimization problem:

$$\min_{\boldsymbol{\alpha}} \left[\frac{1}{2} \boldsymbol{\alpha}^\top \widehat{\boldsymbol{H}} \boldsymbol{\alpha} - \widehat{\boldsymbol{h}}^\top \boldsymbol{\alpha} + \frac{\lambda}{2} \boldsymbol{\alpha}^\top \boldsymbol{R} \boldsymbol{\alpha} \right],$$

where a regularization term $\lambda \boldsymbol{\alpha}^\top \boldsymbol{R} \boldsymbol{\alpha}/2$ is included for avoiding overfitting, $\lambda\ (\geq 0)$ is a regularization parameter, $\boldsymbol{R}\ (\in \mathbb{R}^{n \times n})$ is a positive semi-definite regularization matrix, and

$$\widehat{H}_{\ell,\ell'} := \frac{1}{n^2} \sum_{i,j=1}^{n} K(\boldsymbol{z}_i, \boldsymbol{z}_\ell) L(\boldsymbol{y}_j, \boldsymbol{y}_\ell) K(\boldsymbol{z}_i, \boldsymbol{z}_{\ell'}) L(\boldsymbol{y}_j, \boldsymbol{y}_{\ell'}),$$

$$\widehat{h}_\ell := \frac{1}{n} \sum_{i=1}^{n} K(\boldsymbol{z}_i, \boldsymbol{z}_\ell) L(\boldsymbol{y}_i, \boldsymbol{y}_\ell).$$

Differentiating the above objective function with respect to $\boldsymbol{\alpha}$ and equating it to zero, we can obtain the optimal solution $\widehat{\boldsymbol{\alpha}}$ analytically as

$$\widehat{\boldsymbol{\alpha}} = (\widehat{\boldsymbol{H}} + \lambda \boldsymbol{R})^{-1} \widehat{\boldsymbol{h}}. \tag{4}$$

Then, based on the fact that $\mathrm{SMI}(Z, Y)$ is expressed as

$$\mathrm{SMI}(Z, Y) = \frac{1}{2} \mathbb{E}_{p_{\mathrm{zy}}} \left[w(\boldsymbol{z}, \boldsymbol{y}) \right] - \frac{1}{2},$$

the following SMI estimator can be obtained:

$$\widehat{\mathrm{SMI}} = \frac{1}{2} \widehat{\boldsymbol{h}}^\top \widehat{\boldsymbol{\alpha}} - \frac{1}{2}. \tag{5}$$

3.1.3. MODEL SELECTION

Hyper-parameters included in the kernel functions and the regularization parameter can be optimized by cross-validation with respect to J (Suzuki et al., 2009), which is described below.

First, samples $\mathcal{Z} = \{(\boldsymbol{z}_i, \boldsymbol{y}_i)\}_{i=1}^{n}$ are divided into K disjoint subsets $\{\mathcal{Z}_k\}_{k=1}^{K}$ of (approximately) the same size. Then, an estimator $\widehat{\boldsymbol{\alpha}}_{\mathcal{Z}_k}$ is obtained using $\mathcal{Z} \backslash \mathcal{Z}_k$ (i.e., all samples without $\mathcal{Z}_k$), and the approximation error for hold-out samples $\mathcal{Z}_k$ is computed as

$$J_{\mathcal{Z}_k}^{(K\text{-CV})} := \frac{1}{2} \widehat{\boldsymbol{\alpha}}_{\mathcal{Z}_k}^\top \widehat{\boldsymbol{H}}_{\mathcal{Z}_k} \widehat{\boldsymbol{\alpha}}_{\mathcal{Z}_k} - \widehat{\boldsymbol{h}}_{\mathcal{Z}_k}^\top \widehat{\boldsymbol{\alpha}}_{\mathcal{Z}_k},$$

where, for $|\mathcal{Z}_k|$ being the number of samples in subset $\mathcal{Z}_k$,

$$[\widehat{H}_{\mathcal{Z}_k}]_{\ell,\ell'} := \frac{1}{|\mathcal{Z}_k|^2} \sum_{\boldsymbol{z} \in \mathcal{Z}_k} \sum_{\boldsymbol{y} \in \mathcal{Z}_k} K(\boldsymbol{z}, \boldsymbol{z}_\ell) L(\boldsymbol{y}, \boldsymbol{y}_\ell) K(\boldsymbol{z}, \boldsymbol{z}_{\ell'}) L(\boldsymbol{y}, \boldsymbol{y}_{\ell'}),$$

$$[\widehat{h}_{\mathcal{Z}_k}]_\ell := \frac{1}{|\mathcal{Z}_k|} \sum_{(\boldsymbol{z}, \boldsymbol{y}) \in \mathcal{Z}_k} K(\boldsymbol{z}, \boldsymbol{z}_\ell) L(\boldsymbol{y}, \boldsymbol{y}_\ell).$$

This procedure is repeated for $k = 1, \ldots, K$, and its average $J^{(K\text{-CV})}$ is outputted as

$$J^{(K\text{-CV})} := \frac{1}{K} \sum_{k=1}^{K} J_{\mathcal{Z}_k}^{(K\text{-CV})}.$$

Finally, we compute $J^{(K\text{-CV})}$ for all model candidates, and choose the model that minimizes $J^{(K\text{-CV})}$.

3.2. Dependence Maximization

Given an SMI estimator $\widehat{\text{SMI}}$ (5), we next show how $\widehat{\text{SMI}}$ can be efficiently maximized with respect to $\boldsymbol{W}$:

$$\max_{\boldsymbol{W} \in \mathbb{R}^{m \times d}} \widehat{\text{SMI}} \quad \text{s.t. } \boldsymbol{W}\boldsymbol{W}^{\top} = \boldsymbol{I}_m.$$

We propose to use a truncated negative quadratic function called the *Epanechnikov kernel* (Epanechnikov, 1969) as a kernel for $\boldsymbol{z}$:

$$K(\boldsymbol{z}, \boldsymbol{z}_\ell) = \max \left(0, 1 - \frac{\|\boldsymbol{z} - \boldsymbol{z}_\ell\|^2}{2\sigma_{\mathrm{z}}^2} \right).$$

Let $I(c)$ be the indicator function, i.e., $I(c) = 1$ if c is true and zero otherwise. Then, for the above kernel function, $\widehat{\text{SMI}}$ can be expressed as

$$\widehat{\text{SMI}} = \frac{1}{2} \text{tr} \left(\boldsymbol{W}\boldsymbol{D}\boldsymbol{W}^{\top} \right) - \frac{1}{2},$$

where $\text{tr}(\cdot)$ is the trace of a matrix and

$$\boldsymbol{D} = \frac{1}{n} \sum_{i=1}^{n} \sum_{\ell=1}^{n} \widehat{\alpha}_\ell(\boldsymbol{W}) I \left(\frac{\|\boldsymbol{W}\boldsymbol{x}_i - \boldsymbol{W}\boldsymbol{x}_\ell\|^2}{2\sigma_{\mathrm{z}}^2} < 1 \right)$$
$$\times L(\boldsymbol{y}_i, \boldsymbol{y}_\ell) \left[\frac{1}{m} \boldsymbol{I}_d - \frac{1}{2\sigma_{\mathrm{z}}^2} (\boldsymbol{x}_i - \boldsymbol{x}_\ell)(\boldsymbol{x}_i - \boldsymbol{x}_\ell)^{\top} \right].$$

Here, by $\widehat{\alpha}_\ell(\boldsymbol{W})$, we explicitly indicated the fact that $\widehat{\alpha}_\ell$ depends on $\boldsymbol{W}$.

Let $\boldsymbol{D}'$ be $\boldsymbol{D}$ with $\boldsymbol{W}$ replaced by $\boldsymbol{W}'$, where $\boldsymbol{W}'$ is a transformation matrix obtained in the previous iteration. Thus, $\boldsymbol{D}'$ no longer depends on $\boldsymbol{W}$. Here we replace $\boldsymbol{D}$ in $\widehat{\text{SMI}}$ by $\boldsymbol{D}'$, which gives the following simplified SMI estimate:

$$\frac{1}{2} \text{tr} \left(\boldsymbol{W}\boldsymbol{D}'\boldsymbol{W}^{\top} \right) - \frac{1}{2}. \tag{6}$$

A maximizer of Eq.(6) can be analytically obtained by $(\boldsymbol{w}_1 | \cdots | \boldsymbol{w}_m)^{\top}$, where $\{\boldsymbol{w}_i\}_{i=1}^{m}$ are the m principal components of $\boldsymbol{D}'$.

3.3. Initialization

In the dependence estimation-maximization framework described in Section 2.2, initialization of the transformation matrix $\boldsymbol{W}$ is important. Here we propose to initialize it based on dependence maximization without dimensionality reduction.

More specifically, we determine the initial transformation matrix as $(\boldsymbol{w}_1^{(0)}|\cdots|\boldsymbol{w}_m^{(0)})^\top$, where $\{\boldsymbol{w}_i^{(0)}\}_{i=1}^m$ are the m principal components of $\boldsymbol{D}^{(0)}$:

$$\boldsymbol{D}^{(0)} = \frac{1}{n}\sum_{i=1}^n\sum_{\ell=1}^n \widehat{\alpha}_\ell^{(0)} I\left(\frac{\|\boldsymbol{x}_i - \boldsymbol{x}_\ell\|^2}{2\sigma_{\mathrm{x}}^2} < 1\right) L(\boldsymbol{y}_i, \boldsymbol{y}_\ell)$$

$$\times\left[\frac{1}{m}\boldsymbol{I}_d - \frac{1}{2\sigma_{\mathrm{x}}^2}(\boldsymbol{x}_i - \boldsymbol{x}_\ell)(\boldsymbol{x}_i - \boldsymbol{x}_\ell)^\top\right],$$

$$\widehat{\boldsymbol{\alpha}}^{(0)} = (\widehat{\boldsymbol{H}}^{(0)} + \lambda\boldsymbol{R})^{-1}\widehat{\boldsymbol{h}}^{(0)},$$

$$\widehat{H}_{\ell,\ell'}^{(0)} = \frac{1}{n^2}\sum_{i,j=1}^n K'(\boldsymbol{x}_i, \boldsymbol{x}_\ell)L(\boldsymbol{y}_i, \boldsymbol{y}_\ell)K'(\boldsymbol{x}_j, \boldsymbol{x}_{\ell'})L(\boldsymbol{y}_j, \boldsymbol{y}_{\ell'}),$$

$$\widehat{h}_\ell^{(0)} = \frac{1}{n}\sum_{i=1}^n K'(\boldsymbol{x}_i, \boldsymbol{x}_\ell)L(\boldsymbol{y}_i, \boldsymbol{y}_\ell),$$

$$K'(\boldsymbol{x}, \boldsymbol{x}_\ell) = \max\left(0, 1 - \frac{\|\boldsymbol{x} - \boldsymbol{x}_\ell\|^2}{2\sigma_{\mathrm{x}}^2}\right).$$

σ_{x} is the kernel width and is chosen by cross-validation (see Section 3.1.3).

4. Relation to Existing Methods

Here, we review existing SDR methods and discuss the relation to the proposed SCA method.

4.1. Kernel Dimension Reduction

Kernel dimension reduction (KDR) (Fukumizu et al., 2009) tries to directly maximize the conditional independence of $\boldsymbol{x}$ and $\boldsymbol{y}$ given $\boldsymbol{z}$ based on a kernel-based independence measure.

The KDR learning criterion is given by

$$\max_{\boldsymbol{W}\in\mathbb{R}^{m\times d}} \mathrm{tr}\left[\widetilde{\boldsymbol{L}}(\widetilde{\boldsymbol{K}} + n\epsilon\boldsymbol{I}_n)^{-1}\right] \text{ s.t. } \boldsymbol{W}\boldsymbol{W}^\top = \boldsymbol{I}_m, \tag{7}$$

where $\widetilde{\boldsymbol{L}} = \boldsymbol{\Gamma}\boldsymbol{L}\boldsymbol{\Gamma}$, $\boldsymbol{\Gamma} = \boldsymbol{I} - \frac{1}{n}\boldsymbol{1}_n\boldsymbol{1}_n^\top$, $L_{i,j} = L(\boldsymbol{y}_i, \boldsymbol{y}_j)$, $\widetilde{\boldsymbol{K}} = \boldsymbol{\Gamma}\boldsymbol{K}\boldsymbol{\Gamma}$, $K_{i,j} = K(\boldsymbol{z}_i, \boldsymbol{z}_j)$, and ϵ is a regularization parameter.

Solving the above optimization problem is cumbersome since the objective function is non-convex. In the original KDR paper (Fukumizu et al., 2009), a gradient method is employed for finding a local optimal solution. However, the gradient-based optimization is computationally demanding due to its slow convergence and it requires many restarts for finding a good local optima. Thus, KDR scales poorly to massive datasets.

Another critical weakness of KDR is the kernel function choice. The performance of KDR depends on the choice of kernel functions and the regularization parameter, but there

is no systematic model selection method for KDR available. Using the Gaussian kernel with its width set to the median distance between samples is a standard heuristic in practice, but this does not always work well.

Furthermore, KDR lacks a good way to set an initial solution in the gradient procedure. Then, in practice, we need to run the algorithm many times with random initial points for finding a good solution. However, this makes the entire procedure even slower and the performance of dimension reduction unreliable.

The proposed SCA method can successfully overcome the above weaknesses of KDR—SCA is equipped with cross-validation for model selection (Section 3.1.3), its solution can be computed analytically (see Section 3.2), and a systematic initialization scheme is available (see Section 3.3).

4.2. Least-Squares Dimensionality Reduction

Least-squares dimension reduction (LSDR) is a recently proposed SDR method that can overcome the limitations of KDR (Suzuki and Sugiyama, 2010). That is, LSDR is equipped with a natural model selection procedure based on cross-validation.

The proposed SCA can actually be regarded as a computationally efficient alternative to LSDR. Indeed, LSDR can also be interpreted as a dependence estimation-maximization algorithm (see Section 2.2): the dependence estimation procedure is essentially the same as the proposed SCA, i.e., LSMI is used. However, the dependence maximization procedure is different from SCA—LSDR uses a *natural gradient* method (Amari, 1998) over the Stiefel manifold (Nishimori and Akaho, 2005).

In LSDR, the following SMI estimator is used:

$$\widetilde{\mathrm{SMI}} = \widehat{\boldsymbol{\alpha}}^\top \widehat{\boldsymbol{h}} - \frac{1}{2}\widehat{\boldsymbol{\alpha}}^\top \widehat{\boldsymbol{H}}\widehat{\boldsymbol{\alpha}} - \frac{1}{2},$$

where $\widehat{\boldsymbol{\alpha}}$, $\widehat{\boldsymbol{h}}$, and $\widehat{\boldsymbol{H}}$ are defined in Section 3.1. Then the gradient of $\widetilde{\mathrm{SMI}}$ is given by

$$\frac{\partial \widetilde{\mathrm{SMI}}}{\partial W_{\ell,\ell'}} = \frac{\partial \widehat{\boldsymbol{h}}^\top}{\partial W_{\ell,\ell'}}(2\widehat{\boldsymbol{\alpha}} - \widehat{\boldsymbol{\beta}}) - \widehat{\boldsymbol{\alpha}}^\top \frac{\partial \widehat{\boldsymbol{H}}}{\partial W_{\ell,\ell'}}(\frac{3}{2}\widehat{\boldsymbol{\alpha}} - \widehat{\boldsymbol{\beta}}) + \lambda\widehat{\boldsymbol{\alpha}}^\top \frac{\partial \boldsymbol{R}}{\partial W_{\ell,\ell'}}(\widehat{\boldsymbol{\beta}} - \widehat{\boldsymbol{\alpha}}),$$

where $\widehat{\boldsymbol{\beta}} = (\widehat{\boldsymbol{H}} + \lambda\boldsymbol{R})^{-1}\widehat{\boldsymbol{H}}\widehat{\boldsymbol{\alpha}}$. The *natural gradient* update of $\boldsymbol{W}$, which takes into account the structure of the Stiefel manifold (Amari, 1998), is given by

$$\boldsymbol{W} \leftarrow \boldsymbol{W}\exp\left(\eta\left(\boldsymbol{W}^\top\frac{\partial \widetilde{\mathrm{SMI}}}{\partial \boldsymbol{W}} - \frac{\partial \widetilde{\mathrm{SMI}}}{\partial \boldsymbol{W}}^\top\boldsymbol{W}\right)\right),$$

where 'exp' for a matrix denotes the *matrix exponential*. $\eta \geq 0$ is a step size, which may be optimized by a line-search method such as *Armijo's rule* (Patriksson, 1999).

Since cross-validation in terms of the density-ratio approximation error is available for model selection of LSMI (see Section 3.1.3), LSDR is more favorable than KDR. However, its optimization still relies on a gradient-based method and thus it is computationally expensive.

Furthermore, there seems no good initialization scheme of the transformation matrix $\boldsymbol{W}$. In the original paper (Suzuki and Sugiyama, 2010), initial values were chosen randomly and the gradient method was run many times for finding a better solution.

The proposed SCA method can successfully overcome the above weaknesses of LSDR, by providing an analytic-form solution (see Section 3.2) and a systematic initialization scheme (see Section 3.3).

5. Experiments

In this section, we experimentally investigate the performance of the proposed and existing SDR methods using artificial and real-world datasets.

5.1. Artificial Datasets

We compare the performance and computation time of the proposed SCA, LSDR[4] (Suzuki and Sugiyama, 2010), KDR[5] (Fukumizu et al., 2009), sliced inverse regression (SIR)[6] (Li, 1991), and sliced average variance estimation (SAVE)[6] (Cook, 2000).

We use the following four datasets (see Figure 1):

(a) Data1:

$$Y = X_2 + 0.5E,$$

where $(X_1, \ldots, X_4)^\top \sim U([-1\ 1]^4)$ and $E \sim N(0, 1)$. Here, $U(\mathcal{S})$ denotes the uniform distribution on $\mathcal{S}$, and $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ is the Gaussian distribution with mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$.

(b) Data2:

$$Y = (X_3)^2 + 0.1E,$$

where $(X_1, \ldots, X_{10})^\top \sim N(\mathbf{0}_{10}, \boldsymbol{I}_{10})$ and $E \sim N(0, 1)$.

(c) Data3:

$$Y = \frac{(X_1)^2 + X_2}{0.5 + (X_2 + 1.5)^2} + (1 + X_2)^2 + 0.1E,$$

where $(X_1, \ldots, X_4)^\top \sim N(\mathbf{0}_4, \boldsymbol{I}_4)$ and $E \sim N(0, 1)$.

(d) Data4:

$$Y|X_2 \sim \begin{cases} N(0, 0.2) & \text{if } X_2 \leq |1/6| \\ 0.5N(1, 0.2) + 0.5N(-1, 0.2) & \text{otherwise} \end{cases}$$

where $(X_1, \ldots, X_5)^\top \sim U([-0.5\ 0.5]^5)$ and $E \sim N(0, 1)$.

In SCA, we use the Gaussian kernel for y:

$$L(y, y_\ell) = \exp\left(-\frac{(y - y_\ell)^2}{2\sigma_y^2}\right).$$

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4. We used the program code available from
'http://sugiyama-www.cs.titech.ac.jp/~sugi/software/LSDR/'.
5. We used the program code provided by one of the authors of (Fukumizu et al., 2009), which 'anneals' the Gaussian kernel width over gradient iterations.
6. We used the program code available from
'http://mirrors.dotsrc.org/cran/web/packages/dr/index.html'.
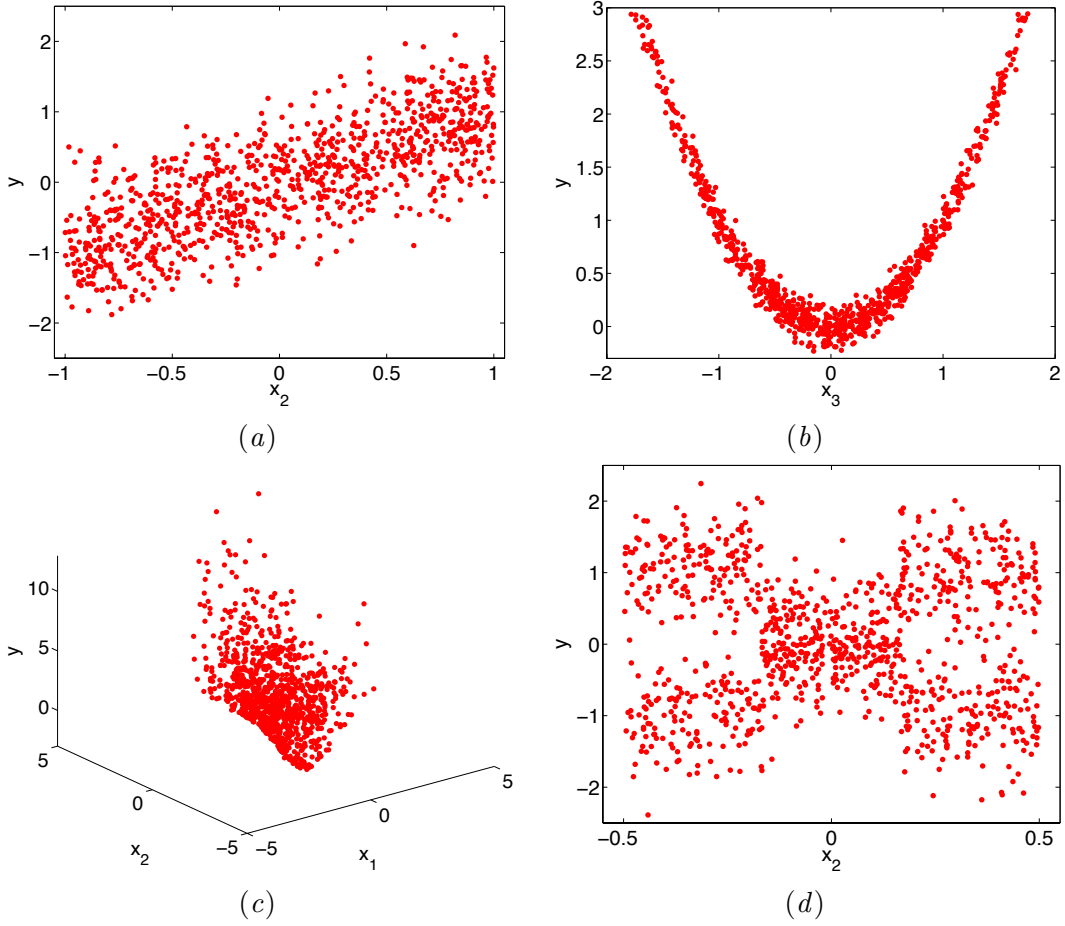
Figure 1: Artificial datasets.

The identity matrix is used as regularization matrix $\boldsymbol{R}$, and kernel widths σ_{x}, σ_{y}, and σ_{z} as well as the regularization parameter λ are chosen based on 5-fold cross-validation from

$$\sigma_{\mathrm{x}} \in \{0.25 m_{\mathrm{x}}, 0.5 m_{\mathrm{x}}, 0.75 m_{\mathrm{x}}, m_{\mathrm{x}}\},$$
$$\sigma_{\mathrm{y}} \in \{0.25 m_{\mathrm{y}}, 0.5 m_{\mathrm{y}}, 0.75 m_{\mathrm{y}}, m_{\mathrm{y}}\},$$
$$\sigma_{\mathrm{z}} \in \{0.25 m_{\mathrm{z}}, 0.5 m_{\mathrm{z}}, 0.75 m_{\mathrm{z}}, m_{\mathrm{z}}\},$$
$$\lambda \in \{10^{-3}, 10^{-2}\},$$

where

$$m_{\mathrm{x}} = \mathrm{median}(\{\|\boldsymbol{x}_i - \boldsymbol{x}_j\|\}_{i,j=1}^{n}),$$
$$m_{\mathrm{y}} = \mathrm{median}(\{|y_i - y_j|\}_{i,j=1}^{n}),$$
$$m_{\mathrm{z}} = \mathrm{median}(\{\|\boldsymbol{z}_i - \boldsymbol{z}_j\|\}_{i,j=1}^{n}).$$

The performance of each method is measured by

$$\frac{1}{\sqrt{2m}} \|\widehat{\boldsymbol{W}}^{\top} \widehat{\boldsymbol{W}} - \boldsymbol{W}^{*\top} \boldsymbol{W}^*\|_{\mathrm{Frobenius}},$$

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Table 1: Mean of Frobenius-norm error (with standard deviations in parentheses) and mean CPU time over 100 trials. Computation time is normalized so that LSDR is one. LSDR was repeated 5 times with random initialization and the transformation matrix with the minimum CV score was chosen as the final solution. 'SCA(0)' indicates the performance of the initial transformation matrix obtained by the method described in Section 3.3. The best method achieving the smallest mean Frobenius-norm error and comparable methods according to the *t-test* at the significance level 1% are specified by bold face.

Datasets	d	m	SCA(0)	SCA	LSDR	KDR	SIR	SAVE
Data1	4	1	.089(.042)	**.048(.031)**	**.056(.021)**	**.048(.019)**	.257(.168)	.339(.218)
Data2	10	1	.078(.019)	**.007(.002)**	.039 (.023)	.024 (.007)	.431(.281)	.348(.206)
Data3	4	2	.065(.035)	**.018(.010)**	.090 (.069)	**.029(.119)**	.362(.182)	.343(.213)
Data4	5	1	.118(.046)	**.042(.030)**	.151 (.296)	.118 (.238)	.421(.268)	.356(.197)
Average time			0.03	0.49	1.0	0.96	<0.01	<0.01

where $\| \cdot \|_{\text{Frobenius}}$ denotes the Frobenius norm, $\widehat{\boldsymbol{W}}$ is an estimated transformation matrix, and $\boldsymbol{W}^*$ is the optimal transformation matrix. Note that the above error measure takes its value in $[0, 1]$.

The performance of each method is summarized in Table 1, which depicts the mean and standard deviation of the Frobenius-norm error over 100 trials when the number of samples is $n = 1000$. As can be observed, the proposed SCA overall performs well. 'SCA(0)' in the table indicates the performance of the initial transformation matrix obtained by the method described in Section 3.3. The result shows that SCA(0) already gives a reasonably good transformation matrix with a tiny computational cost. Note that KDR and LSDR have high standard deviation for Data3 and Data4, meaning that KDR and LSDR sometimes perform poorly.

5.2. IDA Benchmark Datasets

Next, we compare the performance of SDR methods using the *IDA benchmark datasets* (Rätsch et al., 2001), which consist of binary classification tasks (i.e., the output y takes either $+1$ or -1). We apply SCA, LSDR, and KDR to obtaining projections onto low-dimension subspaces with dimension $m = \lfloor d/4 \rfloor$ or $m = \lfloor d/2 \rfloor$. Then we train kernel logistic regression models (Hastie et al., 2001) on the projected training samples. The kernel width and the regularization parameter in kernel logistic regression are chosen based on 5-fold cross-validation in terms of the misclassification error. In SCA, we use the linear kernel for y, i.e., $L(y, y_\ell) = yy_\ell$.

Table 2 summarizes the mean misclassification rates (and their standard deviation in parentheses) over 20 trials. The results show that SCA overall compares favorably with LSDR and KDR in terms of the misclassification rate, and moreover the computational cost of SCA is much smaller than those of LSDR and KDR.

Table 2: Mean misclassification rates (and their standard deviation in parentheses) over 20 trials for the IDA benchmark datasets. Computation time is normalized so that LSDR is one. The best method achieving the smallest mean misclassification rate and comparable methods according to the *t-test* at the significance level 1% are specified by bold face.

Datasets	m	SCA		LSDR		KDR	
brestcancer	2	**.293**	**(.041)**	**.283**	**(.060)**	**.281**	**(.049)**
	4	**.275**	**(.040)**	**.277**	**(.039)**	**.281**	**(.025)**
diabetes	2	**.258**	**(.023)**	**.246**	**(.014)**	**.244**	**(.019)**
	4	**.249**	**(.022)**	**.257**	**(.023)**	**.259**	**(.020)**
flaresolar	2	**.347**	**(.033)**	**.345**	**(.019)**	**.352**	**(.018)**
	4	**.346**	**(.023)**	**.348**	**(.024)**	**.345**	**(.027)**
german	5	**.239**	**(.020)**	.271	(.024)	**.251**	**(.019)**
	10	**.235**	**(.018)**	**.250**	**(.023)**	.256	(.027)
heart	3	**.192**	**(.034)**	.236	(.035)	.219	(.025)
	6	**.189**	**(.029)**	.227	(.036)	**.210**	**(.035)**
ringnorm	5	.151	(.007)	**.137**	**(.008)**	**.136**	**(.009)**
	10	.091	(.010)	**.075**	**(.008)**	**.075**	**(.007)**
thyroid	1	**.044**	**(.027)**	**.039**	**(.025)**	**.035**	**(.023)**
	2	**.041**	**(.020)**	**.049**	**(.022)**	**.038**	**(.018)**
twonorm	5	**.028**	**(.005)**	.032	(.004)	.037	(.005)
	10	**.028**	**(.003)**	.036	(.007)	.033	(.005)
waveform	5	.133	(.010)	**.120**	**(.011)**	**.117**	**(.009)**
	10	.135	(.011)	**.112**	**(.008)**	**.112**	**(.006)**
Average time	–	0.03	—	1.0	—	0.78	—

5.3. Multi-label Classification for Real-world Datasets

Finally, we evaluate the performance of the proposed method in real-world multi-label classification problems.

5.3.1. SETUP

Below, we compare SCA, *multi-label dimensionality reduction via dependence maximization* (MDDM)[7] (Zhang and Zhou, 2010), *canonical correlation analysis* (CCA)[8] (Hotelling, 1936), and *principal component analysis* (PCA)[9] (Bishop, 2006). We use a real-world image classification dataset called the *PASCAL visual object classes (VOC) 2010* dataset (Everingham et al., 2010) and a real-world automatic audio-tagging dataset called the *Freesound*

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7. We used the program code available from
   'http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/MDDM.htm'.
8. We used the MATLAB implementation;
   see 'http://www.mathworks.com/help/toolbox/stats/canoncorr.html'.
9. We used the MATLAB implementation;
   see 'http://www.mathworks.com/help/toolbox/stats/princomp.html'.

dataset (The Freesound Project, 2011). Since the computational costs of KDR and LSDR were unbearably large, we decided not to include them in the comparison.

We employ the misclassification rate by the one-nearest-neighbor classifier as a performance measure:

$$\text{err} = \frac{1}{nc} \sum_{i=1}^{n} \sum_{k=1}^{c} I(\widehat{y}_{i,k} \neq y_{i,k}),$$

where c is the number of classes, $\widehat{y}$ and y are the estimated and true labels, and $I(\cdot)$ is the indicator function. For SCA and MDDM, we use the following kernel function (Sarwar et al., 2001) for $\boldsymbol{y}$:

$$L(\boldsymbol{y}, \boldsymbol{y}') = \frac{(\boldsymbol{y} - \overline{\boldsymbol{y}})^{\top}(\boldsymbol{y}' - \overline{\boldsymbol{y}})}{\|\boldsymbol{y} - \overline{\boldsymbol{y}}\|\|\boldsymbol{y}' - \overline{\boldsymbol{y}}'\|},$$

where $\overline{\boldsymbol{y}}$ is the sample mean: $\overline{\boldsymbol{y}} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{y}_i$.

5.3.2. PASCAL VOC 2010 Dataset

The VOC 2010 dataset consists of 20 binary classification tasks of identifying the existence of a person, aeroplane, etc. in each image. The total number of images in the dataset is 11319, and we used 1000 randomly chosen images for training and the rest for testing.

In this experiment, we first extracted visual features from each image using the *speed up robust features* (SURF) algorithm (Bay et al., 2008), and obtained 500 *visual words* as the cluster centers in the SURF space. Then, we computed a 500-dimensional *bag-of-feature* vector by counting the number of visual words in each image. We randomly sampled training and test data 100 times, and computed the means and standard deviations of the misclassification error.

The results are plotted in Figure 2(a), showing that SCA outperforms the existing methods, and SCA is the only method that outperforms 'ORI' (no dimension reduction)—SCA achieves almost the same error rate as 'ORI' with only a 10-dimensional subspace. Note that, MDDM, CCA, and PCA capture only linear dependency, whereas the proposed SCA can identify general non-linear dependency. This would be the reason why SCA performed well in this experiment. To the best of our knowledge, SCA is the only method that can capture non-linear dependency and scale to large-sized problems.

5.3.3. Freesound Dataset

The *Freesound* dataset (The Freesound Project, 2011) consists of various audio files annotated with word tags such as 'people', 'noisy', and 'restaurant'. We used 230 tags in this experiment. The total number of audio files in the dataset is 5905, and we used 1000 randomly chosen audio files for training and the rest for testing.

We first extracted *mel-frequency cepstrum coefficients* (MFCC) (Rabiner and Juang, 1993) from each audio file, and obtained 1024 *audio features* as the cluster centers in the MFCC space. Then, we computed a 1024-dimensional *bag-of-feature* vector by counting the number of audio features in each audio file. We randomly chose training and test samples 100 times, and computed the means and standard deviations of the misclassification error.

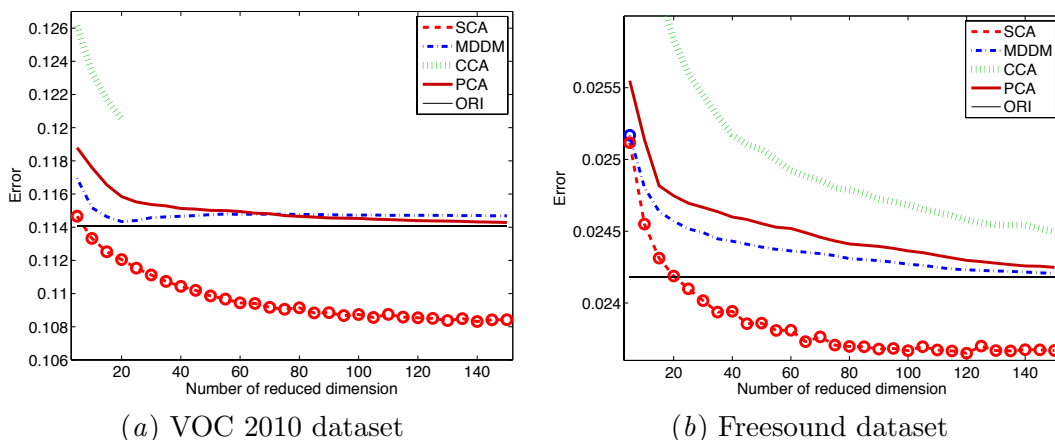(a) VOC 2010 dataset   (b) Freesound dataset

Figure 2: Results on image classification with VOC 2010 dataset and audio classification with Freesound datasets. Misclassification rates when the one-nearest-neighbor classifier is used as a classifier are reported. The best dimension reduction method achieving the smallest mean error and comparable methods according to the t-test at the significance level 1% are specified by '○'. CCA can be applied to dimension reduction up to c dimensions, where c is the number of classes ($c = 20$ in VOC 2010 and $c = 230$ in Freesound). 'ORI' denotes the original data without dimension reduction.

The results plotted in Figure 2(b) show that, similarly to the image classification task, the proposed SCA outperforms the existing methods, and SCA is the only method that outperforms 'ORI'.

6. Conclusion

In this paper, we proposed a novel *sufficient dimension reduction* (SDR) method called *sufficient component analysis* (SCA), which is computationally more efficient than existing SDR methods. In SCA, a transformation matrix was estimated by iteratively performing dependence estimation and maximization, both of which are *analytically* carried out. Moreover, we developed a systematic method to design an initial transformation matrix, which highly contributes to further reducing the computational cost and helps to obtain a good solution. We applied the proposed SCA to real-world image classification and audio tagging tasks, and experimentally showed that the proposed method is promising.

Acknowledgments

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