Direct Estimation of the Derivative of Quadratic Mutual Information with Application in Supervised Dimension Reduction

Voot Tangkaratt, Hiroaki Sasaki, and Masashi Sugiyama

The University of Tokyo

Abstract

A typical goal of supervised dimension reduction is to find a low-dimensional subspace of the input space such that the projected input variables preserve maximal information about the output variables. The dependence maximization approach solves the supervised dimension reduction problem through maximizing a statistical dependence between projected input variables and output variables. A well-known statistical dependence measure is mutual information (MI) which is based on the Kullback-Leibler (KL) divergence. However, it is known that the KL divergence is sensitive to outliers. On the other hand, quadratic MI (QMI) is a variant of MI based on the L_2 distance which is more robust against outliers than the KL divergence, and a computationally efficient method to estimate QMI from data, called least-squares QMI (LSQMI), has been proposed recently. For these reasons, developing a supervised dimension reduction method based on LSQMI seems promising. However, not QMI itself, but the derivative of QMI is needed for subspace search in supervised dimension reduction, and the derivative of an accurate QMI estimator is not necessarily a good estimator of the derivative of QMI. In this paper, we propose to directly estimate the derivative of QMI without estimating QMI itself. We show that the direct estimation of the derivative of QMI is more accurate than the derivative of the estimated QMI. Finally, we develop a supervised dimension reduction algorithm which efficiently uses the proposed derivative estimator, and demonstrate through experiments that the proposed method is more robust against outliers than existing methods.

1 Introduction

Supervised learning is one of the central problems in machine learning which aims at learning an input-output relationship from given input-output paired data samples. Although many methods were proposed to perform supervised learning, they often work poorly when the input variables have high dimensionality. Such a situation is commonly referred to as the *curse of dimensionality* (Bishop, 2006), and a common approach to

mitigate the curse of dimensionality is to preprocess the input variables by *dimension reduction* (Burges, 2010).

A typical goal of dimension reduction in supervised learning is to find a lowdimensional subspace of the input space such that the projected input variables preserve maximal information about the output variables. Thus, a successive supervised learning method can use the low-dimensional projection of the input variables to learn the input-output relationship with a minimal loss of information. The purpose of this paper is to develop a novel supervised dimension reduction method.

The dependence maximization approach solves the supervised dimension reduction problem through maximizing a statistical dependence measure between projected input variables and output variables. *Mutual information* (MI) is a well-known tool for measuring statistical dependency between random variables (Cover and Thomas, 1991). MI is well-studied and many methods were proposed to estimate MI from data. A notable method is the *maximum likelihood MI* (MLMI) (Suzuki et al., 2008), which does not require any assumption on the data distribution and can perform model selection via cross-validation. For these reasons, MLMI seems to be an appealing tool for supervised dimension reduction. However, MI is defined based on the *Kullback-Leibler* divergence (Kullback and Leibler, 1951), which is known to be sensitive to outliers (Basu et al., 1998). Hence, MI is not an appropriate tool when it is applied on a dataset containing outliers.

Quadratic MI (QMI) is a variant of MI (Principe et al., 2000). Unlike MI, QMI is defined based on the L_2 distance. A notable advantage of the L_2 distance over the KL divergence is that the L_2 distance is more robust against outliers (Basu et al., 1998). Moreover, a computationally efficient method to estimate QMI from data, called *least-squares QMI* (LSQMI) (Sainui and Sugiyama, 2013), was proposed recently. LSQMI does not require any assumption on the data distribution and it can perform model selection via cross-validation. For these reasons, developing a supervised dimension reduction method based on LSQMI is more promising.

An approach to use LSQMI for supervised dimension reduction is to firstly estimate QMI between projected input variables and output variables by LSQMI, and then search for a subspace which maximizes the estimated QMI by a nonlinear optimization method such as gradient ascent. However, the essential quantity of the subspace search is the derivative of QMI w.r.t. the subspace, not QMI itself. Thus, LSQMI may not be an appropriate tool for developing supervised dimension reduction methods since the derivative of an accurate QMI estimator is not necessarily an accurate estimator of the derivative of QMI.

To cope with the above problem, in this paper, we propose a novel method to *directly* estimate the derivative of QMI without estimating QMI itself. The proposed method has the following advantageous properties: it does not require any assumption on the data distribution, the estimator can be computed analytically, and the tuning parameters can be objectively chosen by cross-validation. We show through experiments that the proposed direct estimator of the derivative of QMI is more accurate than the derivative of the estimated QMI. Then we develop a fixed-point iteration which efficiently uses the proposed estimator of the derivative of QMI to perform supervised dimension reduction. Finally, we demonstrate the usefulness of the proposed method is more robust against

outliers than existing methods.

The organization of this paper is as follows. We firstly formulate the supervised dimension reduction problem and review some of existing methods in Section 2, Then we give an overview of QMI and review some of QMI estimators in Section 3. The details of the proposed derivative estimator are given in Section 4. Then in Section 5 we develop a supervised dimension reduction algorithm based on the proposed derivative estimator. The experiment results are given in Section 6. The conclusion of this paper is given in Section 7.

2 Supervised Dimension Reduction

In this section, we firstly formulate the supervised dimension reduction problem. Then we briefly review existing supervised dimension reduction methods and discuss their problems.

2.1 **Problem Formulation**

Let $\mathcal{D}_{\mathbf{x}} \subset \mathbb{R}^{d_{\mathbf{x}}}$ and $\mathcal{D}_{\mathbf{y}} \subset \mathbb{R}^{d_{\mathbf{y}}}$ be the input domain and output domain with dimensionality $d_{\mathbf{x}}$ and $d_{\mathbf{y}}$, respectively, and $p(\mathbf{x}, \mathbf{y})$ be a joint probability density on $\mathcal{D}_{\mathbf{x}} \times \mathcal{D}_{\mathbf{y}}$. Firstly, assume that we are given an input-output paired data set $\mathcal{D} = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$, where each data sample is drawn independently from the joint density:

$$\{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^n \overset{i.i.d.}{\sim} p(\boldsymbol{x}, \boldsymbol{y}).$$

Next, let $W \in \{W \in \mathbb{R}^{d_z \times d_x} | WW^\top = I_{d_z}\}$ be an orthonormal matrix with a known constant $d_z \leq d_x$, where I_{d_z} denotes the d_z -by- d_z identity matrix and \top denotes the matrix transpose. Then assume that there exists a d_z -dimensional subspace in \mathbb{R}^{d_x} spanned by the rows of W such that the projection of x onto this subspace denoted by z = Wx preserves the maximal information about y of x. That is, we can substitute x by z with a minimal loss of information about y. We refer to the problem of estimating W from the given data as *supervised dimension reduction*. Below, we review some of the existing supervised dimension reduction methods.

2.2 Sliced Inverse Regression

Sliced inverse regression (SIR) (Li, 1991) is a well known supervised dimension reduction method. SIR formulates supervised dimension reduction as a problem of finding W which makes x and y conditionally independent given z:

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

The key principal of SIR lies on the following equality ¹

$$\mathbb{E}[\boldsymbol{c}^{\top}\boldsymbol{x}|\boldsymbol{W}\boldsymbol{x}] = a_0 + \sum_{i=1}^{d_z} a_i \boldsymbol{w}_i^{\top}\boldsymbol{x}, \qquad (2)$$

¹For simplicity, we assume that x is standardized so that $\mathbb{E}[x] = 0$ and $\mathbb{E}[xx^{\top}] = I_{d_{\mathbf{z}}}$

where \mathbb{E} denotes the conditional expectation and w_i denotes the *i*-th row of W. The importance of this equality is that if the equality holds for any $c \in \mathbb{R}^{d_x}$ and some constants $a_0, a_1, \ldots, a_{d_z}$, then the inverse regression curve $\mathbb{E}[\boldsymbol{x}|\boldsymbol{y}]$ lies on the space spanned by W which satisfies Eq.(1). Based on this fact, SIR estimates W as follows. First, the range of y is sliced into multiple slices. Then $\mathbb{E}[\boldsymbol{x}|\boldsymbol{y}]$ is estimated as the mean of \boldsymbol{x} for each slice of y. Finally, W is obtained as the d_z largest principal components of the covariance matrix of the means.

The significant advantages of SIR are its simplicity and scalability to large datasets. However, SIR relies on the equality in Eq.(2) which typically requires that p(x) is an elliptically symmetric distribution such as Gaussian. This is restrictive and thus the practical usefulness of SIR is limited.

2.3 Minimum Average Variance Estimation based on the Conditional Density Functions

The minimum average variance estimation based on the conditional density functions (dMAVE) (Xia, 2007) is a supervised dimension method which does not require any assumption on the data distribution and is more practical compared to SIR. Briefly speaking, dMAVE aims to find a matrix W which yields an accurate non-parametric estimation of the conditional density p(y|z).

The essential part of dMAVE is the following model:

$$H_b(\widetilde{y}-y) = m_b(\boldsymbol{z},y) + \varepsilon_b(y|\boldsymbol{z}),$$

where H_b denotes a symmetric kernel function with bandwidth b > 0, $m_b(z, y)$ denotes a conditional expectation of $H_b(\tilde{y} - y)$ given z, and $\varepsilon_b(y|z) = H_b(\tilde{y} - y) - \mathbb{E}[H_b(\tilde{y} - y)|z]$ with $\mathbb{E}[\varepsilon_b(y|z)] = 0$. An important property of this model is that $m_b(z, y) \rightarrow p(y|z)$ when $b \rightarrow 0$ as $n \rightarrow \infty$. Then, dMAVE estimates $m_b(z, y)$ by a local linear smoother (Fan et al., 1996). More specifically, a local linear smoother of $m_b(z_i, y_k)$ is given by

$$m_b(\boldsymbol{z}_i, y_k) \approx m_b(\boldsymbol{z}_j, y_k) + \frac{\partial m_b(\boldsymbol{z}_j, y_k)}{\partial \boldsymbol{z}} (\boldsymbol{z}_i - \boldsymbol{z}_j)$$

= $a_{jk} + \boldsymbol{b}_{jk}^{\top} \boldsymbol{W} (\boldsymbol{x}_i - \boldsymbol{x}_j),$ (3)

where z_j is an arbitrary point close to z_i , and $a_{jk} \in \mathbb{R}$ and $b_{jk} \in \mathbb{R}^{d_z}$ are parameters. Based on this local linear smoother, dMAVE solves the following minimization problem:

$$\min_{\boldsymbol{W}, a_{jk}, \boldsymbol{b}_{jk}} \frac{1}{n^3} \sum_{j,k=1}^n \rho(\boldsymbol{x}_j, y_k) \sum_{i=1}^n \left[H_b(y_i - y_k) - a_{jk} - \boldsymbol{b}_{jk}^\top \boldsymbol{W}(\boldsymbol{x}_i - \boldsymbol{x}_j) \right]^2 K_h(\boldsymbol{x}_i, \boldsymbol{x}_j),$$
(4)

where K_h is a symmetric kernel function with bandwidth h > 0. The function $\rho(x, y)$ is a trimming function which is evaluated as zero when the densities of x or y are lower than some threshold. A solution to this minimization problem is obtained by

alternatively solving quadratic programming problems for W, and (a_{jk}, b_{jk}) until convergence.

The main advantage of dMAVE is that it does not require any assumption on the data distribution. However, a significant disadvantage of dMAVE is that there is no systematic method to choose the kernel bandwidths and the trimming threshold. In practice, dMAVE uses a bandwidth selection method based on the *normal-reference* rule of the non-parametric conditional density estimation (Silverman, 1986; Fan et al., 1996), and a fixed trimming threshold. Although this model selection strategy works reasonably well in general, it does not always guarantee good performance on all kind of datasets.

Another disadvantage of dMAVE is that the optimization problem in Eq.(4) may have many local solutions. To cope with this problem, dMAVE proposed to use a supervised dimension reduction method called the *outer product of gradient based on conditional density functions* (dOPG) (Xia, 2007) to obtain a good initial solution. Thus, dMAVE may not perform well if dOPG fails to provide a good initial solution.

2.4 Kernel Dimension Reduction

Another supervised dimension reduction method which does not require any assumption on the data distribution is *kernel dimension reduction* (KDR) (Fukumizu et al., 2009). Unlike dMAVE which focuses on the conditional density, KDR aims to find a matrix W which satisfies the conditional independence in Eq.(1). The key idea of KDR is to evaluate the conditional independence through a conditional covariance operator over reproducing kernel Hilbert spaces (RKHSs) (Aronszajn, 1950).

Throughout this subsection, we use $(\mathcal{H}_{\mathbf{z}}, k_{\mathbf{z}})$ to denote an RKHS of functions on the domain $\mathcal{D}_{\mathbf{z}}$ equipped with reproducing kernel $k_{\mathbf{z}}$:

$$\langle f, k_{\mathbf{z}}(\cdot, \boldsymbol{z}) \rangle_{\mathcal{H}_{\mathbf{z}}} = f(\boldsymbol{z}),$$

for $f \in \mathcal{H}_{z}$ and $z \in \mathcal{D}_{z}$. The RKHSs of functions on domains \mathcal{D}_{x} and \mathcal{D}_{y} are also defined similarly as (\mathcal{H}_{x}, k_{x}) and (\mathcal{H}_{y}, k_{y}) , respectively. The *cross-covariance operator* $\Sigma_{YZ} : \mathcal{H}_{z} \to \mathcal{H}_{y}$ satisfies the following equality for all $f \in \mathcal{H}_{z}$ and $g \in \mathcal{H}_{y}$:

$$\langle g, \Sigma_{\boldsymbol{Y}\boldsymbol{Z}} f \rangle_{\mathcal{H}_{\boldsymbol{y}}} = \mathbb{E}_{\boldsymbol{z}\boldsymbol{y}} \left[f(\boldsymbol{z}) g(\boldsymbol{y}) \right] - \mathbb{E}_{\boldsymbol{z}} \left[f(\boldsymbol{z}) \right] \mathbb{E}_{\boldsymbol{y}} \left[g(\boldsymbol{y}) \right],$$

where \mathbb{E}_{zy} , \mathbb{E}_{z} , and \mathbb{E}_{y} denotes expectations over densities p(z, y), p(z), and p(y), respectively. Then, the *conditional covariance operator* can be defined using cross-covariance operators as

$$\Sigma_{\boldsymbol{Y}\boldsymbol{Y}|\boldsymbol{Z}} = \Sigma_{\boldsymbol{Y}\boldsymbol{Y}} - \Sigma_{\boldsymbol{Y}\boldsymbol{Z}} \Sigma_{\boldsymbol{Z}\boldsymbol{Z}}^{-1} \Sigma_{\boldsymbol{Z}\boldsymbol{Y}},$$
(5)

where it is assumed that Σ_{ZZ}^{-1} always exists. The importance of the conditional covariance operator in supervised dimension reduction lies in the following relations:

$$\Sigma_{\boldsymbol{Y}\boldsymbol{Y}|\boldsymbol{Z}} \ge \Sigma_{\boldsymbol{Y}\boldsymbol{Y}|\boldsymbol{X}},\tag{6}$$

where the inequality refers to the partial order of self-adjoint operators, and

$$\Sigma_{\boldsymbol{Y}\boldsymbol{Y}|\boldsymbol{Z}} = \Sigma_{\boldsymbol{Y}\boldsymbol{Y}|\boldsymbol{X}} \Longleftrightarrow (\boldsymbol{x} \perp \boldsymbol{y}) \mid \boldsymbol{z}.$$
(7)

These relations mean that the conditional independence can be achieved by finding a matrix W which minimizes $\Sigma_{YY|Z}$ in the partial order of self-adjoint operators. Based on this fact, KDR solves the following minimization problem:

$$\min_{\boldsymbol{W} \in \{\boldsymbol{W} | \boldsymbol{W} \boldsymbol{W}^{\top} = \boldsymbol{I}_{d_{\mathbf{Z}}}\}} \operatorname{Tr} \left[\boldsymbol{G}_{\mathbf{Y}} \left(\boldsymbol{G}_{\mathbf{Z}} + \lambda_n \boldsymbol{I}_n \right)^{-1} \right],$$
(8)

where λ_n denotes a regularization parameter, G_Z and G_Y denotes centered Gram matrices with the kernels k_z and k_y , respectively, and Tr [·] denotes the trace of an operator. A solution to this minimization problem is obtained by a gradient descent method.

KDR does not require any assumption on the data distribution and was shown to work well on various regression and classification tasks (Fukumizu et al., 2009). However, KDR has two disadvantages in practice. The first disadvantage of KDR is that even though the kernel parameters and the regularization parameter can heavily affect the performance, there seems to be no justifiable model selection method to choose these parameters so far. Although it is always possible to choose these tuning parameters based on a criterion of a successive supervised learning method with cross-validation, this approach results in a nested loop of model selection for both KDR itself and the successive supervised learning method. Moreover, this approach makes supervised dimension reduction depends on the successive supervised learning method which is unfavorable in practice.

The second disadvantage is that the optimization problem in Eq.(8) is non-convex and may have many local solutions. Thus, if the initial solution is not properly chosen, the performance of KDR may be unreliable. A simple approach to cope with this problem is to choose the best solution with cross-validation based on the successive supervised learning method, but this approach makes supervised dimension reduction depends on the successive supervised learning method and is unfavorable. A more sophisticated approach was considered in Fukumizu and Leng (2014) which proposed to use a solution of a supervised dimension reduction method called *gradient-based kernel dimension reduction* (gKDR) as an initial solution for KDR. However, it is not guarantee that gKDR always provide a good initial solution for KDR.

2.5 Least-Squares Dimension Reduction

The *least-squares dimension reduction* (LSDR) (Suzuki and Sugiyama, 2013) is another supervised dimension reduction method which does not require any assumption on the data distribution. Similarly to KDR, LSDR aims to find a matrix W which satisfies the conditional independence in Eq.(1). However, instead of the conditional covariance operators, LSDR evaluates the conditional independence through a statistical dependence measure.

LSDR utilizes a statistical dependence measure called *squared-loss mutual infor*mation (SMI). SMI between random variables z and y is defined as

$$SMI(Z,Y) = \frac{1}{2} \iint p(\boldsymbol{z})p(\boldsymbol{y}) \left(\frac{p(\boldsymbol{z},\boldsymbol{y})}{p(\boldsymbol{z})p(\boldsymbol{y})} - 1\right)^2 d\boldsymbol{z} d\boldsymbol{y}.$$
(9)

SMI(Z, Y) is always non-negative and equals to zero if and only if z and y are statistically independent, i.e., p(z, y) = p(z)p(y). The important properties of SMI in

supervised dimension reduction are the following relations:

$$SMI(Z, Y) \leq SMI(X, Y),$$

and

$$\mathrm{SMI}(Z,Y) = \mathrm{SMI}(X,Y) \iff (\boldsymbol{x} \perp \boldsymbol{y}) \mid \boldsymbol{z}$$

Thus, the conditional independence can be achieved by finding a matrix W which maximizes SMI(Z, Y). Since SMI(Z, Y) is typically unknown, it is estimated by the *least-squares mutual information* (Suzuki et al., 2009) method which directly estimates the density ratio $\frac{p(z,y)}{p(z)p(y)}$ without performing any density estimation. Then, LSDR solves the following maximization problem:

$$\max_{\boldsymbol{W} \in \{\boldsymbol{W} | \boldsymbol{W} \boldsymbol{W}^{\top} = \boldsymbol{I}_{d_{\mathbf{z}}}\}} \widehat{\mathrm{SMI}}(\boldsymbol{Z}, \boldsymbol{Y}), \tag{10}$$

where $\widehat{SMI}(Z, Y)$ denotes the estimated SMI. The solution to this maximization problem is obtained by a gradient ascent method. Note that this maximization problem is non-convex and may have many local solutions.

LSDR does not require any assumption on the data distribution, similarly to dMAVE and KDR. However, the significant advantage of LSDR over dMAVE and KDR is that LSDR can perform model selection via cross-validation and avoid a poor local solution without requiring any successive supervised learning method. This is a favorable property as a supervised dimension reduction method.

However, a disadvantage of LSDR is that the density ratio function $\frac{p(z,y)}{p(z)p(y)}$ can be highly fluctuated, especially when the data contains outliers. Since it is typically difficult to accurately estimate a highly fluctuated function, LSDR could be unreliable in the presence of outliers.

Next, we consider a supervised dimension reduction approach based on quadratic mutual information which can overcome the disadvantages of the existing methods.

3 Quadratic Mutual Information

In this section, we briefly introduce quadratic mutual information and discuss how it can be used to perform robust supervised dimension reduction.

3.1 Quadratic Mutual Information and Mutual Information

Quadratic mutual information (QMI) is a measure for statistical dependency between random variables (Principe et al., 2000), and is defined as

$$QMI(Z,Y) = \frac{1}{2} \iint (p(\boldsymbol{z},\boldsymbol{y}) - p(\boldsymbol{z})p(\boldsymbol{y}))^2 \, \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y}.$$
(11)

QMI(Z, Y) is always non-negative and equals to zero if and only if z and y are statistically independent, i.e., p(z, y) = p(z)p(y). Such a property of QMI is similar to that

of the ordinary mutual information (MI), which is defined as

$$MI(Z,Y) = \iint p(\boldsymbol{z},\boldsymbol{y}) \log\left(\frac{p(\boldsymbol{z},\boldsymbol{y})}{p(\boldsymbol{z})p(\boldsymbol{y})}\right) d\boldsymbol{z} d\boldsymbol{y}.$$
 (12)

The essential difference between QMI and MI is the discrepancy measure. QMI(Z, Y) is the L_2 distance between $p(\boldsymbol{z}, \boldsymbol{y})$ and $p(\boldsymbol{z})p(\boldsymbol{y})$, while MI(Z, Y) is the *Kullback-Leibler* (KL) divergence (Kullback and Leibler, 1951).

MI has been studied and applied to many data analysis tasks (Cover and Thomas, 1991). Moreover, an efficient method to estimate MI from data is also available (Suzuki et al., 2008). However, MI is not always the optimal choice for measuring statistical dependence because it is not robust against outliers. An intuitive explanation is that MI contains the log function and the density ratio: the value of logarithm can be highly sharp near zero, and density ratio can be highly fluctuated and diverge to infinity. Thus, the value of MI tends to be unstable and unreliable in the presence of outliers. In contrast, QMI does not contain the log function and the density ratio, and thus QMI should be more robust against outliers than MI.

Another explanation of the robustness of QMI and MI can be understood based on their discrepancy measures. Both L_2 distance (QMI) and KL divergence (MI) can be regarded as members of a more general divergence class called the *density power* divergence (Basu et al., 1998):

$$DP_{\alpha}(p||q) = \int \left(p(\boldsymbol{x})^{1+\alpha} - \left(1 + \frac{1}{\alpha}\right) p(\boldsymbol{x})q(\boldsymbol{x})^{\alpha} + \frac{1}{\alpha}q(\boldsymbol{x})^{1+\alpha} \right) d\boldsymbol{x}, \quad (13)$$

where $\alpha > 0$. Based on this divergence class, the L_2 distance and the KL divergence can be obtained by setting $\alpha = 1$ and $\alpha \rightarrow 0$, respectively. As discussed in Basu et al. (1998), the parameter α controls the robustness against outliers of the divergence, where a large value of α indicates high robustness. This means that the L_2 distance ($\alpha = 1$) is more robust against outliers than the KL divergence ($\alpha \rightarrow 0$).

In supervised dimension reduction, robustness against outliers is an important requirement because outliers often make supervised dimension reduction methods to work poorly. Thus, developing a supervised dimension reduction method based on QMI is an attractive approach since QMI is robust against outliers. This QMI-based supervised dimension reduction method is performed by finding a matrix W^* which maximizes QMI(Z, Y):

$$\boldsymbol{W}^* = \operatorname*{argmax}_{\boldsymbol{W} \in \{\boldsymbol{W} | \boldsymbol{W} \boldsymbol{W}^\top = \boldsymbol{I}_{d_{\mathbf{z}}}\}} \operatorname{QMI}(Z, Y).$$

The motivation is that, if QMI(Z, Y) is maximized then z and y are maximally dependent on each other, and thus we may disregard x with a minimal loss of information about y.

Since QMI(Z, Y) is typically unknown, it needs to be estimated from data. Below, we review existing QMI estimation methods and then discuss a weakness of performing supervised dimension reduction using these QMI estimation methods.

3.2 Existing QMI Estimation Methods

We review two QMI estimation methods which estimate QMI(Z, Y) from the given data. The first method estimates QMI through density estimation, and the second method estimates QMI through density difference estimation.

3.2.1 QMI Estimator based on Density Estimation

Expanding Eq.(11) allows us to express QMI(Z, Y) as

$$QMI(Z,Y) = \frac{1}{2} \iint \left(p(\boldsymbol{z},\boldsymbol{y})^2 - 2p(\boldsymbol{z},\boldsymbol{y})p(\boldsymbol{z})p(\boldsymbol{y}) + p(\boldsymbol{z})^2 p(\boldsymbol{y})^2 \right) d\boldsymbol{z} d\boldsymbol{y}.$$
(14)

A naive approach to estimate QMI(Z, Y) is to separately estimate the unknown densities p(z, y), p(z), and p(y) by density estimation methods such as *kernel density estimation* (KDE) (Silverman, 1986), and then plug the estimates into Eq.(14).

Following this approach, the KDE-based QMI estimator has been studied and applied to many problems such as *feature extraction for classification* (Torkkola, 2003; Principe et al., 2000), *blind source separation* (Principe et al., 2000), and *image registration* (Atif et al., 2003). Although this density estimation based approach was shown to work well, accurately estimating densities for high-dimensional data is known to be one of the most challenging tasks (Vapnik, 1998). Moreover, the densities contained in Eq.(14) are estimated independently without regarding the accuracy of the QMI estimator. Thus, even if each density is accurately estimated, the QMI estimator obtained from these density estimates does not necessarily give an accurate QMI. An approach to mitigate this problem is to consider density estimators which their combination minimizes the estimation error of QMI. Although this approach shows better performance than the independent density estimation approach, it still performs poorly in high-dimensional problems (Sugiyama et al., 2013).

3.2.2 Least-Squares QMI

To avoid the separate density estimation, an alternative method called *least-squares QMI* (LSQMI) (Sainui and Sugiyama, 2013) was proposed. Below, we briefly review the LSQMI method.

First, notice that QMI(Z, Y) can be expressed in term of the density difference as

$$QMI(Z,Y) = \frac{1}{2} \iint f(\boldsymbol{z},\boldsymbol{y})^2 d\boldsymbol{z} d\boldsymbol{y},$$
(15)

where

$$f(\boldsymbol{z}, \boldsymbol{y}) = p(\boldsymbol{z}, \boldsymbol{y}) - p(\boldsymbol{z})p(\boldsymbol{y}).$$

The key idea of LSQMI is to directly estimate the density difference f(z, y) without going through any density estimation by the procedure of the *least-squares density difference* (Sugiyama et al., 2013). Letting d(z, y) be a model of the density difference, LSQMI learns d(z, y) so that it is fitted to the true density difference under the squared loss:

$$\frac{1}{2} \iint \left(d(\boldsymbol{z}, \boldsymbol{y}) - f(\boldsymbol{z}, \boldsymbol{y}) \right)^2 \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y}.$$

By expanding the integrand, we obtain

$$\frac{1}{2} \iint d(\boldsymbol{z}, \boldsymbol{y})^2 \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y} - \iint d(\boldsymbol{z}, \boldsymbol{y}) f(\boldsymbol{z}, \boldsymbol{y}) \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y} + \frac{1}{2} \iint f(\boldsymbol{z}, \boldsymbol{y})^2 \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y}.$$

Since the last term is a constant w.r.t. the model d(z, y), we omit it and obtain the following criterion:

$$\frac{1}{2} \iint d(\boldsymbol{z}, \boldsymbol{y})^2 \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y} - \iint d(\boldsymbol{z}, \boldsymbol{y}) f(\boldsymbol{z}, \boldsymbol{y}) \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y}.$$
 (16)

Then, the density difference estimator $\hat{d}(z, y)$ is obtained as the solution of the following minimization problem:

$$\widehat{d} = \underset{d}{\operatorname{argmin}} \left[\frac{1}{2} \iint d(\boldsymbol{z}, \boldsymbol{y})^2 \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y} - \iint d(\boldsymbol{z}, \boldsymbol{y}) f(\boldsymbol{z}, \boldsymbol{y}) \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y} \right].$$
(17)

The solution of the minimization problem in Eq.(17) depends on the choice of the model d(z, y). LSQMI employs the following linear-in-parameter model

$$d(\boldsymbol{z},\boldsymbol{y}) = \boldsymbol{\alpha}^{\top} \boldsymbol{\psi}(\boldsymbol{z},\boldsymbol{y}),$$

where α is a parameter vector and $\psi(z, y)$ is a basis function vector. For this model, finding the solution of Eq.(17) is equivalent to solving

$$\min_{\boldsymbol{lpha}} \left[rac{1}{2} \boldsymbol{lpha}^{ op} \boldsymbol{D} \boldsymbol{lpha} - \boldsymbol{lpha}^{ op} \boldsymbol{q}
ight],$$

where

$$D = \iint \psi(z, y) \psi(z, y)^{\top} dz dy,$$
(18)

$$q = \iint \psi(z, y) f(z, y) dz dy$$
$$= \iint \psi(z, y) p(z, y) dz dy - \iint \psi(z, y) p(z) p(y) dz dy.$$
(19)

By approximating the expectation over the densities p(z, y), p(z), and p(y) with sample averages, we obtain the following empirical minimization problem

$$\min_{\boldsymbol{\alpha}} \left[\frac{1}{2} \boldsymbol{\alpha}^\top \boldsymbol{D} \boldsymbol{\alpha} - \boldsymbol{\alpha}^\top \widehat{\boldsymbol{q}} \right],$$

where \hat{q} is the sample approximation of Eq.(19):

$$\widehat{\boldsymbol{q}} = rac{1}{n}\sum_{i=1}^{n} \boldsymbol{\psi}(\boldsymbol{z}_i, \boldsymbol{y}_i) - rac{1}{n^2}\sum_{i,j=1}^{n} \boldsymbol{\psi}(\boldsymbol{z}_i, \boldsymbol{y}_j).$$

By including the L_2 regularization term, we obtain

$$\widehat{\boldsymbol{\alpha}} = \operatorname*{argmin}_{\boldsymbol{\alpha}} \left[\frac{1}{2} \boldsymbol{\alpha}^\top \boldsymbol{D} \boldsymbol{\alpha} - \boldsymbol{\alpha}^\top \widehat{\boldsymbol{q}} + \frac{\lambda}{2} \boldsymbol{\alpha}^\top \boldsymbol{\alpha} \right],$$

where $\lambda \ge 0$ is the regularization parameter. Then, the solution is obtained analytically as

$$\widehat{\boldsymbol{\alpha}} = (\boldsymbol{D} + \lambda \boldsymbol{I})^{-1} \, \widehat{\boldsymbol{q}}. \tag{20}$$

Therefore, the density difference estimator is obtained as

$$\widehat{d}(\boldsymbol{z}, \boldsymbol{y}) = \widehat{\boldsymbol{\alpha}}^{\top} \boldsymbol{\psi}(\boldsymbol{z}, \boldsymbol{y}).$$

Finally, QMI estimator is obtained by substituting the density difference estimator into Eq.(15). A direct substitution yields two possible QMI estimators:

$$\widehat{\text{QMI}}(Z,Y) = \frac{1}{2}\widehat{\boldsymbol{\alpha}}^{\top}\widehat{\boldsymbol{q}},\tag{21}$$

$$\widehat{\text{QMI}}(Z,Y) = \frac{1}{2}\widehat{\boldsymbol{\alpha}}^{\top} \boldsymbol{D}\widehat{\boldsymbol{\alpha}}.$$
(22)

However, it was shown in Sugiyama et al. (2013) that a linear combination of the two estimators defined as

$$\widehat{\text{QMI}}(Z,Y) = \widehat{\alpha}^{\top} \widehat{q} - \frac{1}{2} \widehat{\alpha}^{\top} D \widehat{\alpha}, \qquad (23)$$

provides smaller bias and is a more appropriate QMI estimator.

As shown above, LSQMI avoids multiple-step density estimation by directly estimating the density difference contained in QMI. It was shown that such direct estimation procedure tends to be more accurate than multiple-step estimation (Sugiyama et al., 2013). Moreover, LSQMI is able to objectively choose the tuning parameter contained in the basis function $\psi(z, y)$ and the regularization parameter λ based on cross-validation. This property allows LSQMI to solve challenging tasks such as *clustering* (Sainui and Sugiyama, 2013) and *unsupervised dimension reduction* (Sainui and Sugiyama, 2014) in an objective way.

3.3 Supervised Dimension Reduction via LSQMI

Given an efficient QMI estimation method such as LSQMI, supervised dimension reduction can be performed by finding a matrix W^* defined as

$$\boldsymbol{W}^* = \operatorname*{argmax}_{\boldsymbol{W} \in \{\boldsymbol{W} | \boldsymbol{W} \boldsymbol{W}^\top = \boldsymbol{I}_{d_{\mathbf{z}}}\}} \widehat{\mathrm{QMI}}(Z, Y).$$
(24)

A straightforward approach to solving Eq.(24) is to perform the gradient ascent:

$$\boldsymbol{W} \leftarrow \boldsymbol{W} + t \frac{\partial \widehat{\mathrm{QMI}}(Z,Y)}{\partial \boldsymbol{W}},$$

where t > 0 denotes the step size. The update formula means that the essential point of the QMI-based supervised dimension reduction method is not the accuracy of the QMI estimator, but the accuracy of the estimator of the derivative of the QMI. Thus, the existing LSQMI-based approach which first estimates QMI and then compute the derivatives of the QMI estimator is not necessarily appropriate since an accurate estimator of QMI does not necessarily mean that its derivative is an accurate estimator of the derivative of QMI. Next, we describe our proposed method which overcomes this problem.

4 Derivative of Quadratic Mutual Information

To cope with the weakness of the QMI estimation methods when performing supervised dimension reduction, we propose to *directly* estimate the derivative of QMI without estimating QMI itself.

4.1 Direct Estimation of the Derivative of Quadratic Mutual Information

From Eq.(15), the derivative of the QMI(Z, Y) w.r.t. the (ℓ, ℓ') -th element of W can be expressed by ²

$$\frac{\partial \text{QMI}(\boldsymbol{W})}{\partial W_{\ell,\ell'}} = \frac{\partial}{\partial W_{\ell,\ell'}} \left(\frac{1}{2} \iint f(\boldsymbol{z}, \boldsymbol{y})^2 d\boldsymbol{z} d\boldsymbol{y} \right)$$

$$= \iint f(\boldsymbol{z}, \boldsymbol{y}) \frac{\partial f(\boldsymbol{z}, \boldsymbol{y})}{\partial W_{\ell,\ell'}} d\boldsymbol{z} d\boldsymbol{y}$$

$$= \iint f(\boldsymbol{z}, \boldsymbol{y}) \frac{\partial f(\boldsymbol{z}, \boldsymbol{y})}{\partial \boldsymbol{z}}^{\top} \frac{\partial \boldsymbol{z}}{\partial W_{\ell,\ell'}} d\boldsymbol{z} d\boldsymbol{y}$$

$$= \iint p(\boldsymbol{z}, \boldsymbol{y}) \frac{\partial f(\boldsymbol{z}, \boldsymbol{y})}{\partial \boldsymbol{z}}^{\top} \frac{\partial \boldsymbol{z}}{\partial W_{\ell,\ell'}} d\boldsymbol{z} d\boldsymbol{y}$$

$$- \iint p(\boldsymbol{z}) p(\boldsymbol{y}) \frac{\partial f(\boldsymbol{z}, \boldsymbol{y})}{\partial \boldsymbol{z}}^{\top} \frac{\partial \boldsymbol{z}}{\partial W_{\ell,\ell'}} d\boldsymbol{z} d\boldsymbol{y},$$
(25)

where in the second line we assume that the order of the derivative and the integration is interchangeable. By approximating the expectations over the densities p(z, y), p(z), and p(y) with sample averages, we obtain an approximation of the derivative of QMI as

$$\frac{\widehat{\partial QMI}(\boldsymbol{W})}{\partial W_{\ell,\ell'}} = \sum_{i=1}^{n} \frac{\partial f(\boldsymbol{z}_i, \boldsymbol{y}_i)}{\partial \boldsymbol{z}}^{\top} \frac{\partial \boldsymbol{z}_i}{\partial W_{\ell,\ell'}} - \sum_{i,j=1}^{n} \frac{\partial f(\boldsymbol{z}_i, \boldsymbol{y}_j)}{\partial \boldsymbol{z}}^{\top} \frac{\partial \boldsymbol{z}_i}{\partial W_{\ell,\ell'}}.$$
 (26)

Note that since $z^{(\ell)} = \sum_{\ell'=1}^{d_{\mathbf{x}}} W_{\ell,\ell'} x^{(\ell')}$, we have that $\frac{\partial z}{\partial W_{\ell,\ell'}}$ is the $d_{\mathbf{z}}$ -dimensional vector with zero everywhere except at the ℓ -th dimension which has value $x^{(\ell')}$. Hence, Eq.(26)

²Throughout this section, we use QMI(W) instead of QMI(Z, Y) when we consider its derivative for notational convenience. However, they still represent the QMI between random variables z and y.

can be simplified as

$$\frac{\widehat{\partial QMI}(\boldsymbol{W})}{\partial W_{\ell,\ell'}} = \sum_{i=1}^{n} \frac{\partial f(\boldsymbol{z}_i, \boldsymbol{y}_i)}{\partial z^{(\ell)}} x_i^{(\ell')} - \sum_{i,j=1}^{n} \frac{\partial f(\boldsymbol{z}_i, \boldsymbol{y}_j)}{\partial z^{(\ell)}} x_i^{(\ell')}.$$
(27)

This means that the derivative of QMI(Z, Y) w.r.t. W can be obtained once we know the derivatives of the density difference w.r.t. $z^{(\ell)}$ for all $\ell \in \{1, \ldots, d_z\}$. However, these derivatives are often unknown and need to be estimated from data. Below, we first discuss existing approaches and their drawbacks. Then we propose our approach which can overcome the drawbacks.

4.2 Existing Approaches to Estimate the Derivative of the Density Difference

Our current goal is to obtain the derivative of the density difference w.r.t. $z^{(\ell)}$ which can be rewritten as

$$\frac{\partial f(\boldsymbol{z}, \boldsymbol{y})}{\partial z^{(\ell)}} = \frac{\partial p(\boldsymbol{z}, \boldsymbol{y})}{\partial z^{(\ell)}} - \frac{\partial p(\boldsymbol{z})}{\partial z^{(\ell)}} p(\boldsymbol{y}).$$
(28)

All terms in Eq.(28) are unknown in practice and need to be estimated from data. There are three existing approaches to estimate them.

(A) Density estimation

Separately estimate the densities p(z, y), p(z), and p(y) by, e.g., *kernel density estimation*. Then estimate the right-hand side of Eq.(28) as

$$rac{\partial \widehat{p}(oldsymbol{z},oldsymbol{y})}{\partial z^{(\ell)}} - rac{\partial \widehat{p}(oldsymbol{z})}{\partial z^{(\ell)}} \widehat{p}(oldsymbol{y}),$$

where $\widehat{p}(\boldsymbol{z}, \boldsymbol{y}), \widehat{p}(\boldsymbol{z})$, and $\widehat{p}(\boldsymbol{y})$ denote the estimated densities.

(B) Density derivative estimation

Estimate the density $p(\mathbf{y})$ by e.g., kernel density estimation. Next, separately estimate the densities derivative $\frac{\partial p(\mathbf{z}, \mathbf{y})}{\partial z^{(\ell)}}$ and $\frac{\partial p(\mathbf{z})}{\partial z^{(\ell)}}$ by, e.g., the method of *mean integrated square error for derivatives* (Sasaki et al., 2015), which can estimate the density derivative without estimating the density itself. Then estimate the right-hand side of Eq.(28) as

$$rac{\widehat{\partial p}(oldsymbol{z},oldsymbol{y})}{\partial z^{(\ell)}} - rac{\widehat{\partial p}(oldsymbol{z})}{\partial z^{(\ell)}}\widehat{p}(oldsymbol{y})$$

where $\hat{p}(\boldsymbol{y})$ denotes the estimated density, and $\frac{\partial \hat{p}(\boldsymbol{z},\boldsymbol{y})}{\partial z^{(\ell)}}$ and $\frac{\partial \hat{p}(\boldsymbol{z})}{\partial z^{(\ell)}}$ denote the (directly) estimated density derivatives.

(C) Density difference estimation

Estimate the density difference f(z, y) by e.g., *least-squares density difference*

(Sugiyama et al., 2013), which can estimate the density difference without estimating the densities themselves. Then estimate the left-hand side of Eq.(28) as

$$\frac{\partial \widehat{f}(\boldsymbol{z},\boldsymbol{y})}{\partial z^{(\ell)}},$$

where $\hat{f}(\boldsymbol{z}, \boldsymbol{y})$ denotes the (directly) estimated density difference.

The problem of approaches (A) and (B) is that they involve multiple estimation steps where some quantities are estimated first and then they are plugged into Eq.(28). Such multiple-step methods are not appropriate since each estimated quantity is obtained without regarding the others and the succeeding plug-in step using these estimates can magnify the estimation error contained in each estimated quantity.

On the other hand, approach (C) seems more promising than the previous two approaches since there is only one estimated quantity f(z, y). However, it is still not the optimal approach due to the fact that an accurate estimator of the density difference does not necessarily means that its derivative is an accurate estimator of the derivative of the density difference.

To avoid the above problems, we propose a new approach which directly estimates the derivative of the density difference.

4.3 Direct Estimation of the Derivative of the Density Difference

We propose to estimate the derivative of the density difference w.r.t. $z^{(\ell)}$ using a model $g_{\ell}(\boldsymbol{z}, \boldsymbol{y})$:

$$\frac{\partial f(\boldsymbol{z},\boldsymbol{y})}{\partial z^{(\ell)}} \approx g_{\ell}(\boldsymbol{z},\boldsymbol{y})$$

The model $g_{\ell}(\boldsymbol{z}, \boldsymbol{y})$ is learned so that it is fitted to its corresponding derivative under the square loss:

$$\frac{1}{2} \iint \left(g_{\ell}(\boldsymbol{z}, \boldsymbol{y}) - \frac{\partial f(\boldsymbol{z}, \boldsymbol{y})}{\partial z^{(\ell)}} \right)^2 \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y}.$$
(29)

By expanding the square, we obtain

$$\frac{1}{2}\iint g_{\ell}(\boldsymbol{z},\boldsymbol{y})^{2}\mathrm{d}\boldsymbol{z}\mathrm{d}\boldsymbol{y} - \iint g_{\ell}(\boldsymbol{z},\boldsymbol{y})\frac{\partial f(\boldsymbol{z},\boldsymbol{y})}{\partial z^{(\ell)}}\mathrm{d}\boldsymbol{z}\mathrm{d}\boldsymbol{y} + \frac{1}{2}\iint \left(\frac{\partial f(\boldsymbol{z},\boldsymbol{y})}{\partial z^{(\ell)}}\right)^{2}\mathrm{d}\boldsymbol{z}\mathrm{d}\boldsymbol{y}.$$

Since the last term is a constant w.r.t. the model $g_{\ell}(\boldsymbol{z}, \boldsymbol{y})$, we omit it and obtain the following criterion:

$$\frac{1}{2} \iint g_{\ell}(\boldsymbol{z}, \boldsymbol{y})^2 \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y} - \iint g_{\ell}(\boldsymbol{z}, \boldsymbol{y}) \frac{\partial f(\boldsymbol{z}, \boldsymbol{y})}{\partial z^{(\ell)}} \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y}.$$
(30)

The second term is intractable due to the unknown derivative of the density difference. To make this term tractable, we use *integration by parts* (Kasube, 1983) to obtain the following:

$$\iint [g_{\ell}(\boldsymbol{z}, \boldsymbol{y}) f(\boldsymbol{z}, \boldsymbol{y})]_{\boldsymbol{z}^{(\ell)} = -\infty}^{\boldsymbol{z}^{(\ell)} = -\infty} d\boldsymbol{z}_{\backslash \boldsymbol{z}^{(\ell)}} d\boldsymbol{y}$$
$$= \iint f(\boldsymbol{z}, \boldsymbol{y}) \frac{\partial g_{\ell}(\boldsymbol{z}, \boldsymbol{y})}{\partial \boldsymbol{z}^{(\ell)}} d\boldsymbol{z} d\boldsymbol{y} + \iint g_{\ell}(\boldsymbol{z}, \boldsymbol{y}) \frac{\partial f(\boldsymbol{z}, \boldsymbol{y})}{\partial \boldsymbol{z}^{(\ell)}} d\boldsymbol{z} d\boldsymbol{y}, \qquad (31)$$

where $\int \cdot dz_{\setminus z^{(\ell)}}$ denotes an integration over z except for the ℓ -th element. Here, we require

$$[g_{\ell}(\boldsymbol{z},\boldsymbol{y})f(\boldsymbol{z},\boldsymbol{y})]_{\boldsymbol{z}^{(\ell)}=-\infty}^{\boldsymbol{z}^{(\ell)}=\infty}=0, \qquad (32)$$

which is a mild assumption since the tails of the density difference p(z, y) - p(z)p(y) often vanish when $z^{(\ell)}$ approaches infinity. Applying the assumption to the left-hand side of Eq.(31) allows us to express Eq.(30) as

$$\frac{1}{2} \iint g_{\ell}(\boldsymbol{z}, \boldsymbol{y})^2 \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y} + \iint f(\boldsymbol{z}, \boldsymbol{y}) \frac{\partial g_{\ell}(\boldsymbol{z}, \boldsymbol{y})}{\partial z^{(\ell)}} \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y}$$

Then, the estimator $\widehat{g}_{\ell}(\boldsymbol{z}, \boldsymbol{y})$ is obtained as a solution of the following minimization problem:

$$\widehat{g}_{\ell} = \operatorname*{argmin}_{g_{\ell}} \left[\frac{1}{2} \iint g_{\ell}(\boldsymbol{z}, \boldsymbol{y})^2 \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y} + \iint f(\boldsymbol{z}, \boldsymbol{y}) \frac{\partial g_{\ell}(\boldsymbol{z}, \boldsymbol{y})}{\partial z^{(\ell)}} \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y} \right].$$
(33)

The solution of Eq.(33) depends on the choice of the model. Let us employ the following linear-in-parameter model as $g_{\ell}(\boldsymbol{z}, \boldsymbol{y})$:

$$g_{\ell}(\boldsymbol{z}, \boldsymbol{y}) = \boldsymbol{\theta}_{\ell}^{\top} \boldsymbol{\varphi}_{\ell}(\boldsymbol{z}, \boldsymbol{y}), \qquad (34)$$

where θ_{ℓ} is a parameter vector and $\varphi_{\ell}(z, y)$ is a basis function vector whose practical choice will be discussed later in detail. For this model, finding the solution of Eq.(33) is equivalent to solving

$$\min_{\boldsymbol{\theta}_{\ell}} \left[\frac{1}{2} \boldsymbol{\theta}_{\ell}^{\top} \boldsymbol{H}_{\ell} \boldsymbol{\theta}_{\ell} + \boldsymbol{\theta}_{\ell}^{\top} \boldsymbol{h}_{\ell} \right], \qquad (35)$$

where we define

$$\begin{aligned} \boldsymbol{H}_{\ell} &= \iint \boldsymbol{\varphi}_{\ell}(\boldsymbol{z}, \boldsymbol{y}) \boldsymbol{\varphi}_{\ell}(\boldsymbol{z}, \boldsymbol{y})^{\mathsf{T}} \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y}, \end{aligned} \tag{36} \\ \boldsymbol{h}_{\ell} &= \iint f(\boldsymbol{z}, \boldsymbol{y}) \frac{\partial \boldsymbol{\varphi}_{\ell}(\boldsymbol{z}, \boldsymbol{y})}{\partial \boldsymbol{z}^{(\ell)}} \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y} \\ &= \iint p(\boldsymbol{z}, \boldsymbol{y}) \frac{\partial \boldsymbol{\varphi}_{\ell}(\boldsymbol{z}, \boldsymbol{y})}{\partial \boldsymbol{z}^{(\ell)}} \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y} - \iint p(\boldsymbol{z}) p(\boldsymbol{y}) \frac{\partial \boldsymbol{\varphi}_{\ell}(\boldsymbol{z}, \boldsymbol{y})}{\partial \boldsymbol{z}^{(\ell)}} \mathrm{d}\boldsymbol{z} \mathrm{d}\boldsymbol{y}. \end{aligned} \tag{37}$$

By approximating the expectation over the densities p(z, y), p(z), and p(y) with sample averages, we obtain the following empirical minimization problem:

$$\min_{\boldsymbol{\theta}_{\ell}} \left[\frac{1}{2} \boldsymbol{\theta}_{\ell}^{\top} \boldsymbol{H}_{\ell} \boldsymbol{\theta}_{\ell} + \boldsymbol{\theta}_{\ell}^{\top} \widehat{\boldsymbol{h}}_{\ell} \right],$$
(38)

where \widehat{h}_{ℓ} is the sample approximation of Eq.(37):

$$\widehat{\boldsymbol{h}}_{\ell} = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial \varphi_{\ell}(\boldsymbol{z}_{i}, \boldsymbol{y}_{i})}{\partial z^{(\ell)}} - \frac{1}{n^{2}} \sum_{i,j=1}^{n} \frac{\partial \varphi_{\ell}(\boldsymbol{z}_{i}, \boldsymbol{y}_{j})}{\partial z^{(\ell)}}.$$
(39)

By including the L_2 regularization term to control the model complexity, we obtain

$$\widehat{\boldsymbol{\theta}}_{\ell} = \operatorname*{argmin}_{\boldsymbol{\theta}_{\ell}} \left[\frac{1}{2} \boldsymbol{\theta}_{\ell}^{\top} \boldsymbol{H}_{\ell} \boldsymbol{\theta}_{\ell} + \boldsymbol{\theta}_{\ell}^{\top} \widehat{\boldsymbol{h}}_{\ell} + \frac{\lambda_{\ell}}{2} \boldsymbol{\theta}_{\ell}^{\top} \boldsymbol{\theta}_{\ell} \right],$$
(40)

where $\lambda_{\ell} \geq 0$ denotes the regularization parameter. This minimization problem is convex w.r.t. the parameter θ_{ℓ} , and the solution can be obtained analytically as

$$\widehat{\boldsymbol{\theta}}_{\ell} = -\left(\boldsymbol{H}_{\ell} + \lambda_{\ell} \boldsymbol{I}\right)^{-1} \widehat{\boldsymbol{h}}_{\ell}, \qquad (41)$$

where I denotes the identity matrix. Finally, the estimator of the derivative of the density difference is obtained by substituting the solution into the model Eq.(34) as

$$\widehat{g}_{\ell}(\boldsymbol{z},\boldsymbol{y}) = \widehat{\boldsymbol{\theta}}_{\ell}^{\top} \boldsymbol{\varphi}_{\ell}(\boldsymbol{z},\boldsymbol{y}).$$
(42)

Using this solution, an estimator of the derivative of QMI can be directly obtained by substituting Eq.(42) into Eq.(27) as

$$\frac{\widehat{\partial QMI}(\boldsymbol{W})}{\partial W_{\ell,\ell'}} = \frac{1}{n} \sum_{i=1}^{n} \widehat{\boldsymbol{\theta}}_{\ell}^{\top} \boldsymbol{\varphi}_{\ell}(\boldsymbol{z}_{i}, \boldsymbol{y}_{i}) x_{i}^{(\ell')} - \frac{1}{n^{2}} \sum_{i,j=1}^{n} \widehat{\boldsymbol{\theta}}_{\ell}^{\top} \boldsymbol{\varphi}_{\ell}(\boldsymbol{z}_{i}, \boldsymbol{y}_{j}) x_{i}^{(\ell')}.$$
(43)

We call this method the *least-squares QMI derivative* (LSQMID).

4.4 Basis Function Design

As basis function $\varphi_{\ell}(\boldsymbol{z}, \boldsymbol{y})$, we propose to use

$$oldsymbol{arphi}_\ell(oldsymbol{z},oldsymbol{y}) = \left[arphi_\ell^{(1)}(oldsymbol{z},oldsymbol{y}),\cdots,arphi_\ell^{(b)}(oldsymbol{z},oldsymbol{y})
ight]^+,$$

where $b \leq n$. First, let us define the k-th Gaussian function as

$$\phi_{\ell}^{(k)}(\boldsymbol{z},\boldsymbol{y}) = \exp\left(-\frac{\|\boldsymbol{z}-\boldsymbol{u}_k\|^2 + \|\boldsymbol{y}-\boldsymbol{v}_k\|^2}{2\sigma_{\ell}^2}\right),\tag{44}$$

where u_k and v_k denote Gaussian centers chosen randomly from the data samples $\{z_i, y_i\}_{i=1}^n$, and σ_ℓ denotes the Gaussian width. We may use different Gaussian widths for z and y, but this approach significantly increases the computation time for model

selection which will be discussed in Section 4.5. In our implementation, we standardize each dimension of x and y to have unit variance and zero mean, and then use the common Gaussian width for both z and y. We also set $b = \min(n, 200)$ in the experiments.

Based on the above Gaussian function, we propose to use the following function as the *k*-th basis for the ℓ -th model of the derivative of the density difference:

$$\varphi_{\ell}^{(k)}(\boldsymbol{z}, \boldsymbol{y}) = \frac{\partial \phi_{\ell}^{(k)}(\boldsymbol{z}, \boldsymbol{y})}{\partial z^{(\ell)}}$$
$$= -\frac{1}{\sigma_{\ell}^{2}} (z^{(\ell)} - u_{k}^{(\ell)}) \phi_{\ell}^{(k)}(\boldsymbol{z}, \boldsymbol{y}).$$
(45)

This function is the derivative of the k-th Gaussian basis function w.r.t. $z^{(\ell)}$. A benefit of this basis function design is that the integral appeared in H_{ℓ} can be computed analytically. Through some simple calculation, we obtain the (k, k')-th element of H_{ℓ} as follows:

$$H_{\ell}^{(k,k')} = \frac{1}{\sigma_{\ell}^{4}} (\sqrt{\pi}\sigma_{\ell})^{d_{\mathbf{z}}+d_{\mathbf{y}}} \exp\left(-\frac{\|\boldsymbol{u}_{k}-\boldsymbol{u}_{k'}\|^{2}-\|\boldsymbol{v}_{k}-\boldsymbol{v}_{k'}\|^{2}}{4\sigma_{\ell}^{2}}\right) \times \left(u_{k}^{(\ell)}u_{k'}^{(\ell)} - \frac{(u_{k}^{(\ell)}+u_{k'}^{(\ell)})^{2}}{2} + (\frac{u_{k}^{(\ell)}+u_{k'}^{(\ell)}}{2})^{2} + \frac{\sigma_{\ell}^{2}}{2}\right).$$

As discussed in Section 5, this basis function choice has further benefits when we develop a supervised dimension reduction method.

4.5 Model Selection by Cross-Validation

The practical performance of the LSQMID method depends on the choice of the Gaussian width σ_{ℓ} and the regularization parameter λ_{ℓ} included in the estimator $\hat{g}_{\ell}(\boldsymbol{z}, \boldsymbol{y})$. These tuning parameters can be objectively chosen by the *K*-fold cross-validation (CV) procedure which is described below.

- 1. Divide the training data $\mathcal{D} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^n$ into K disjoint subsets $\{\mathcal{D}_j\}_{j=1}^K$ with approximately the same size. In the experiments, we choose K = 5.
- 2. For each candidate $M = (\tilde{\sigma}_{\ell}, \tilde{\lambda}_{\ell})$ and each subset \mathcal{D}_j , compute a solution $\hat{\theta}_{\ell,M,\setminus j}$ by Eq.(41) with the candidate M and samples from $\mathcal{D} \setminus \mathcal{D}_j$ (i.e., all data samples except samples in \mathcal{D}_j).
- 3. Compute the CV score of each candidate pair M by

$$CV_{\ell}(M) = \frac{1}{K} \sum_{j=1}^{K} \left[\frac{1}{2} \widehat{\boldsymbol{\theta}}_{\ell,M,\backslash j}^{\top} \boldsymbol{H}_{\ell,M} \widehat{\boldsymbol{\theta}}_{\ell,M,\backslash j} + \widehat{\boldsymbol{\theta}}_{\ell,M,\backslash j}^{\top} \widehat{\boldsymbol{h}}_{\ell,M,j} \right],$$

where $\hat{h}_{\ell,M,j}$ denotes \hat{h}_{ℓ} computed from the candidate M and samples in \mathcal{D}_{j} .

4. Choose the tuning parameter pair such that it minimizes the CV score as

$$(\widehat{\sigma}_{\ell}, \widehat{\lambda}_{\ell}) = \operatorname*{argmin}_{M} \operatorname{CV}_{\ell}(M).$$

5 Supervised Dimension Reduction via LSQMID

In this section, we propose a supervised dimension reduction method based on the proposed LSQMID estimator.

5.1 Gradient ascent via LSQMID

Recall that our goal in supervised dimension reduction is to find the matrix W^* :

$$\boldsymbol{W}^* = \operatorname*{argmax}_{\boldsymbol{W} \in \{\boldsymbol{W} | \boldsymbol{W} \boldsymbol{W}^\top = \boldsymbol{I}_{d_{\mathbf{z}}}\}} \operatorname{QMI}(Z, Y).$$
(46)

A straightforward approach to find a solution of Eq.(46) using the proposed method is to perform gradient ascent as

$$\boldsymbol{W} \leftarrow \boldsymbol{W} + t \frac{\partial \widehat{\mathrm{QMI}}(\boldsymbol{W})}{\partial \boldsymbol{W}},$$
 (47)

where t > 0 denotes the step size. It is known that choosing a good step size is a difficult task in practice (Nocedal and Wright, 2006). *Line search* is an algorithm to choose a good step size by finding a step size which satisfies certain conditions such as the *Armijo rule* (Armijo, 1966). However, these conditions often require access to the objective value QMI(W) which is unavailable in our current setup since the QMI derivative is directly estimated without estimating QMI. Thus, if we want to perform line search, QMI needs to be estimated separately. However, this is problematic since the estimation of the derivative of the QMI and the estimation of the QMI are performed independently without regard to the other, and thus they may not be consistent. For example, the gradient $\frac{\partial QMI(W)}{\partial W}$, which is supposed to be an ascent direction, may be regarded as a descent direction on the surface of the estimated QMI. For such a case, the step size chosen by any line search algorithm is unreliable and the resulting W may not be a good solution.

Below, we consider two approaches which can cope with this problem.

5.2 QMI Approximation via LSQMID

To avoid separate QMI estimation, we consider an approximated QMI which is obtained as a by-product of the proposed method. Recall that the proposed method models the derivative of the density difference as

$$egin{aligned} rac{\partial f(oldsymbol{z},oldsymbol{y})}{\partial z^{(\ell)}} &pprox g_\ell(oldsymbol{z},oldsymbol{y}) \ &= oldsymbol{ heta}_\ell^ op arphi_\ell(oldsymbol{z},oldsymbol{y}) \ &= oldsymbol{ heta}_\ell^ op rac{\partial \phi_\ell(oldsymbol{z},oldsymbol{y})}{\partial z^{(\ell)}} \ &= rac{\partial \left(oldsymbol{ heta}_\ell^ op \phi_\ell(oldsymbol{z},oldsymbol{y})
ight)}{\partial z^{(\ell)}} \end{aligned}$$

This means that the density difference can be approximated by

$$\widetilde{f}_{\ell}(\boldsymbol{z}, \boldsymbol{y}) = \widehat{\boldsymbol{\theta}}_{\ell}^{\top} \boldsymbol{\phi}_{\ell}(\boldsymbol{z}, \boldsymbol{y}) + c_{\ell},$$
(48)

where c_{ℓ} is an unknown quantity which is a constant w.r.t. $z^{(\ell)}$.

In a special case where $d_z = 1$, we can use Eq.(48) to obtain a proper approximator of QMI(Z, Y) in a similar fashion to the LSQMI method. To verify this, let us substitute Eq.(48) into one of the f(z, y) in Eq.(15) to obtain

$$\begin{split} \widetilde{\text{QMI}}(Z,Y) &= \frac{1}{2} \iint f(z,\boldsymbol{y}) \widetilde{f}(z,\boldsymbol{y}) \text{d}z \text{d}\boldsymbol{y} \\ &= \frac{1}{2} \iint f(z,\boldsymbol{y}) \left(\widehat{\boldsymbol{\theta}}^{\top} \boldsymbol{\phi}(z,\boldsymbol{y}) + c \right) \text{d}z \text{d}\boldsymbol{y} \\ &= \frac{1}{2} \iint f(z,\boldsymbol{y}) \widehat{\boldsymbol{\theta}}^{\top} \boldsymbol{\phi}(z,\boldsymbol{y}) \text{d}z \text{d}\boldsymbol{y} + \frac{1}{2} \iint f(z,\boldsymbol{y}) c \text{d}z \text{d}\boldsymbol{y} \\ &= \frac{1}{2} \iint f(z,\boldsymbol{y}) \widehat{\boldsymbol{\theta}}^{\top} \boldsymbol{\phi}(z,\boldsymbol{y}) \text{d}z \text{d}\boldsymbol{y}, \end{split}$$

where the last line follows from

$$\iint f(z, \boldsymbol{y}) c dz d\boldsymbol{y} = \iint p(z, \boldsymbol{y}) c dz d\boldsymbol{y} - \iint p(z) p(\boldsymbol{y}) c dz d\boldsymbol{y}$$
$$= 0.$$

By approximating the expectation with sample averages, we obtain a QMI approximator as

$$\widetilde{\text{QMI}}(Z,Y) = \frac{1}{2n} \sum_{i=1}^{n} \widehat{\boldsymbol{\theta}}^{\top} \boldsymbol{\phi}(z_i, \boldsymbol{y}_i) - \frac{1}{2n^2} \sum_{i,j=1}^{n} \widehat{\boldsymbol{\theta}}^{\top} \boldsymbol{\phi}(z_i, \boldsymbol{y}_j).$$
(49)

The main advantage of using $\widetilde{\text{QMI}}(Z, Y)$ is that it is obtained from the derivative estimation, and thus should be consistent with the estimated derivative. This allows us to perform line search for the gradient ascent in a consistent manner. We may further improve the optimization procedure by considering an optimization problem over the *Grassmann manifold*:

$$\boldsymbol{W}^{*} = \operatorname*{argmax}_{\boldsymbol{W} \in \operatorname{Gr}_{d\mathbf{z}}^{d\mathbf{x}}} \widetilde{\operatorname{QMI}}(Z, Y),$$
(50)

where $\operatorname{Gr}_{d_{\mathbf{z}}}^{d_{\mathbf{x}}}$ is defined as

$$\operatorname{Gr}_{d_{\mathbf{z}}}^{d_{\mathbf{x}}} := \{ \boldsymbol{W} \in \mathbb{R}^{d_{\mathbf{z}} \times d_{\mathbf{x}}} \mid \boldsymbol{W} \boldsymbol{W}^{T} = \boldsymbol{I}_{d_{\mathbf{z}}} \} / \sim$$

That is, $\operatorname{Gr}_{d_{\mathbf{z}}}^{d_{\mathbf{x}}}$ is a set of $d_{\mathbf{z}}$ -by- $d_{\mathbf{x}}$ orthonormal matrices whose rows span the same subspace. This manifold optimization is more efficient than the original optimization since every step of the optimization always satisfies the orthonormal constraint, and we no longer need to perform orthonormalization. More details of manifold optimization can be found in Absil et al. (2008).

Although the QMI approximation in Eq.(49) allows us to choose step size by line search in a consistent manner, such an approximation is unavailable when $d_z > 1$. Next, we consider an alternative optimization strategy which does not require an access to the QMI value.

5.3 Fixed-Point Iteration

To avoid the problem of choosing the step size which requires an access to the QMI value, we propose to use a fixed-point iteration for finding a solution of Eq.(46). Note that from the first order optimality condition, a solution W^* is a stationary point which satisfies

$$rac{\partial \mathrm{QMI}(oldsymbol{W}^*)}{\partial oldsymbol{W}} = oldsymbol{0}_{d_{\mathbf{z}},d_{\mathbf{x}}}$$

where $\mathbf{0}_{d_z,d_x}$ denotes d_z -by- d_x zero matrix. By using the proposed basis function in Eq.(45), Eq.(43) can be expressed as

$$\frac{\partial \mathrm{QMI}(\boldsymbol{W})}{\partial W_{\ell,\ell'}} = F_1^{(\ell,\ell')} - F_2^{(\ell,\ell')} - W_{\ell,\ell'}F_3^{(\ell,\ell')},\tag{51}$$

where we define

$$\begin{split} F_{1}^{(\ell,\ell')} &= \widehat{\boldsymbol{\theta}}_{\ell}^{\top} \left(\boldsymbol{u}^{(\ell)} \odot \left(\frac{1}{n} \sum_{i=1}^{n} \phi_{\ell}(\boldsymbol{z}_{i}, \boldsymbol{y}_{i}) x_{i}^{(\ell')} - \frac{1}{n^{2}} \sum_{i,j=1}^{n} \phi_{\ell}(\boldsymbol{z}_{i}, \boldsymbol{y}_{j}) x_{i}^{(\ell')} \right) \right) \sigma_{\ell}^{-2}, \\ F_{2}^{(\ell,\ell')} &= \sum_{m \neq \ell'}^{d_{\mathbf{x}}} W_{\ell,m} \widehat{\boldsymbol{\theta}}_{\ell}^{\top} \left(\frac{1}{n} \sum_{i=1}^{n} \phi_{\ell}(\boldsymbol{z}_{i}, \boldsymbol{y}_{i}) x_{i}^{(m)} x_{i}^{(\ell')} - \frac{1}{n^{2}} \sum_{i,j=1}^{n} \phi_{\ell}(\boldsymbol{z}_{i}, \boldsymbol{y}_{j}) x_{i}^{(m)} x_{i}^{(\ell')} \right) \sigma_{\ell}^{-2}, \\ F_{3}^{(\ell,\ell')} &= \widehat{\boldsymbol{\theta}}_{\ell}^{\top} \left(\frac{1}{n} \sum_{i=1}^{n} \phi_{\ell}(\boldsymbol{z}_{i}, \boldsymbol{y}_{i}) x_{i}^{(\ell')} x_{i}^{(\ell')} - \frac{1}{n^{2}} \sum_{i,j=1}^{n} \phi_{\ell}(\boldsymbol{z}_{i}, \boldsymbol{y}_{j}) x_{i}^{(\ell')} x_{i}^{(\ell')} \right) \sigma_{\ell}^{-2}, \end{split}$$

with $u^{(\ell)}$ be the column vector of length b consisting of the ℓ -th dimension over all u_k and the symbol \odot represents the element-wise vector product. Then, an approximated solution may be obtained by finding $W_{\ell,\ell'}$ for all (ℓ, ℓ') such that the left-hand side of Eq.(51) is zero. This optimization strategy results in a fixed-point iteration for each dimension of W:

$$W_{\ell,\ell'} \leftarrow \frac{F_1^{(\ell,\ell')} - F_2^{(\ell,\ell')}}{F_3^{(\ell,\ell')}}.$$

Finally, we orthonormalize the solution after each iteration as

$$oldsymbol{W} \leftarrow ig(oldsymbol{W}oldsymbol{W}^{ op}ig)^{-rac{1}{2}}oldsymbol{W}$$

In practice, we perform this orthonormalization only every several iterations for computational efficiency.

Note that the optimization problem in Eq.(46) is non-convex and may have many local solutions. To avoid obtaining a poor local optimal solution, we perform the optimization starting from several initial guesses and choose the solution which gives the maximum estimated QMI as the final solution.

6 Experiments

In this section, we demonstrate the usefulness of the proposed method through experiments.

6.1 Illustrative Experiment

Firstly, we perform the following experiment to illustrate the usefulness of the proposed method in term of the QMI derivative estimation. Let $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ denotes the Gaussian distribution with mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$. Then, for $\epsilon \sim \mathcal{N}(0, 0.15^2)$, we generate a dataset $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ and a matrix \boldsymbol{W} as follows:

$$\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{0}_2, \boldsymbol{I}_2),$$
$$\boldsymbol{y} = (x^{(1)})^2 + \epsilon,$$
$$\boldsymbol{W} = \begin{bmatrix} \cos\theta & \sin\theta \end{bmatrix}$$

where $\mathbf{0}_2$ denotes a zero vector of length 2. Thus we have $z = x^{(1)} \cos \theta + x^{(2)} \sin \theta$. The goal is to estimate

$$\frac{\partial \text{QMI}(Z,Y)}{\partial \theta} = \frac{\partial \text{QMI}(Z,Y)}{\partial \boldsymbol{W}} \frac{\partial \boldsymbol{W}}{\partial \theta}$$

at different value of θ . Note that QMI(Z, Y) is maximized at $\theta = 0$, i.e., $W = \begin{bmatrix} 1 & 0 \end{bmatrix}$.

Figure 1(a) shows the averaged value over 20 experiment trials of the estimated QMI(Z, Y) by LSQMI. The vertical axis indicates the value of the estimated QMI and the horizontal axis indicates value of $\theta \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$. We use n = 3000 and n = 100 for estimating QMI and denote the results by LSQMI(3000) and LSQMI(100), respectively. We perform cross validation at $\theta = 0$ and use the chosen tuning parameters for all values of θ . The result shows that LSQMI accurately estimates QMI(Z, Y) when the sample size is large. However, when the sample size is small, the estimated QMI(Z, Y) has high fluctuation.

Figure 1(b) shows the averaged value over 20 experiment trials of the derivative of QMI(Z, Y) w.r.t. θ computed by LSQMI(3000), LSQMI(100), and the proposed method with n = 100 which is denoted by LSQMID(100). For the proposed method, we perform cross validation at $\theta = 0$ and use the chosen tuning parameters for all values of θ . The result shows that LSQMID(100) gives a smoother estimate than LSQMI(100) which has high fluctuation. To further explain the cause of the fluctuation of LSQMI(100), we plot experiment results of 4 trials in Figure 2, where the left column corresponds to the value of the estimated QMI(Z, Y) while the right column corresponds to the value of the estimated derivative of QMI(Z, Y) w.r.t. θ . These results show that for LSQMI(100), a small fluctuation in the estimated QMI can cause a large fluctuation in the estimated derivative of QMI. On the other hand, LSQMID directly estimates the derivative of QMI and thus does not suffer from this problem.

6.2 Artificial Datasets

Next, we evaluate the usefulness of the proposed method in supervised dimension reduction using artificial datasets. Firstly, let U(a, b) denote the uniform distribution over an interval [a, b], $\Gamma(a, b)$ denote the gamma distribution with shape parameter a and scale parameter b, and Laplace(a, b) denote the Laplace distribution with mean a and scale parameter b. Then we consider the input x with $d_x = 5$, the output y with $d_y = 1$, and the optimal matrix W_{opt} (including their rotations) as follows:



Figure 1: The mean and standard error of the estimated QMI(Z, Y) and the estimated derivative of QMI(Z, Y) w.r.t. θ over 20 experiment trials.

Dataset A: For $\epsilon \sim \Gamma(0.25, 0.25)$, we use

$$\begin{aligned} \boldsymbol{x} &\sim \mathcal{N}(\boldsymbol{0}_{5}, \boldsymbol{I}_{5}), \\ y &= \exp(-\frac{(x^{(1)} + x^{(2)})^{2}}{0.5}) + \epsilon, \\ \boldsymbol{W}_{\text{opt}} &= \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \end{bmatrix}. \end{aligned}$$

Dataset B: For $\epsilon \sim \Gamma(0.25, 0.5)$ and $i \in \{1, \dots, 5\}$, we use

$$x^{(i)} \sim U(-1, 1),$$

$$z = \frac{1}{\sqrt{5}} (x^{(1)} + 2x^{(2)}),$$

$$y = z \sin(z) - \epsilon,$$

$$W_{\text{opt}} = \begin{bmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} & 0 & 0 & 0 \end{bmatrix}$$

Dataset C: For $\epsilon \sim \Gamma(0.25, 0.5)$ and $i \in \{1, \ldots, 5\}$, we use

$$\begin{aligned} x^{(i)} &\sim \mathrm{U}(-1,1), \\ y &= \frac{1}{\sqrt{2}} x^{(1)} x^{(2)} - \epsilon, \\ \mathbf{W}_{\mathrm{opt}} &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} \end{aligned}$$

Dataset D: For $\epsilon \sim \mathcal{N}(0, 0.25)$ and $i \in \{1, \dots, 5\}$, we use

$$\begin{aligned} x^{(i)} &\sim \text{Laplace}(0, 0.5), \\ y &= \text{sinc}(\frac{x^{(1)}\pi}{2}) + x^{(2)}\epsilon \\ \mathbf{W}_{\text{opt}} &= \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix}. \end{aligned}$$



Figure 2: Examples of the estimated QMI and the estimated derivative of QMI. The left column shows the estimated QMI(Z, Y), and the right column shows the estimated derivative of QMI(Z, Y) w.r.t. θ . Each row indicates each experiment trial.



Figure 3: Artificial datasets.

For the datasets **A**, **B**, and **C**, ϵ is an additive gamma noise, while for the datasets **D**, ϵ is a multiplicative Gaussian noise. Figure 3 shows the plot of these datasets (after standardization). Note the presence of outliers in the datasets.

To estimate W from $\{(x_i, y_i)\}_{i=1}^n$, we execute the following methods:

- **LSQMID:** The proposed method. Supervised dimension reduction is performed by maximizing QMI(Z, Y) where the derivative of QMI(Z, Y) is estimated by the proposed method. The solution \widehat{W} is obtained by fixed-point iteration.
- **LSQMI:** Supervised dimension reduction is performed by maximizing QMI(Z, Y) where QMI(Z, Y) is estimated by LSQMI and the derivative of QMI(Z, Y) w.r.t. W is computed from the QMI estimator. The solution \widehat{W} is obtained by gradient ascent with linesearch over the Grassmann manifold ³.
- **LSDR** (Suzuki and Sugiyama, 2013): Supervised dimension reduction is performed by maximizing SMI(Z, Y). The solution \widehat{W} is obtained by gradient ascent with

³We use the manifold optimization toolbox (Boumal et al., 2014) to perform the optimization.

linesearch over the Grassmann manifold ⁴.

- **dMAVE** (Xia, 2007): Supervised dimension reduction is performed by minimizing an error of the local linear smoother of the conditional density p(y|z). The solution \widehat{W} is obtained by alternatively solving quadratic programming problems ⁵.
- **KDR** (Fukumizu et al., 2009): Supervised dimension reduction is performed by minimizing the trace of the conditional covariance operator $\Sigma_{YY|Z}$. The solution \widehat{W} is obtained by gradient descent with linesearch over the Stiefel manifold ⁶.

For methods which require initial solutions, i.e., LSQMID, LSQMI, and LSDR, we randomly generate 10 orthonormal matrices and use them as the initial solutions. For dMAVE and KDR, we use a solution obtained by dOPG and gKDR, respectively, as the initial solution. Finally, the obtained solution \widehat{W} is evaluated by the dimension reduction error defined as

$$\operatorname{Error}_{\mathrm{DR}} = \| \boldsymbol{W}_{\mathrm{opt}}^{\top} \boldsymbol{W}_{\mathrm{opt}} - \widehat{\boldsymbol{W}}^{\top} \widehat{\boldsymbol{W}} \|_{\mathrm{Frobenius}},$$

where $\|\cdot\|_{\text{Frobenius}}$ denotes the Frobenius norm of a matrix.

Table 1 shows the mean and standard error over 30 experiment trials of the dimension reduction error on the artificial datasets with different sample size. The results show that the proposed method works well overall. LSDR performs well especially for dataset **A** and **B**. KDR also performs well overall. However, its performance is quite unstable for dataset **B**, which can be seen by relatively large standard errors. This is because gKDR might provide a poor initial solution to KDR in some experiment trials, which makes KDR fails to find a good solution.

On the other hand, both LSQMI and dMAVE do not perform well overall. LSQMI tends to be unstable and works very poorly especially when the sample size is small, except for dataset **D**. The cause of this failure could be the high fluctuation of the derivative of QMI by LSQMI, as shown previously in the illustrative experiment. Although the solution of dMAVE is quite stable, its performance is not overall comparable to the other methods. This is because the model selection strategy in dMAVE did not perform well for these datasets.

6.3 Benchmark Datasets

Finally, we evaluate the proposed method in supervised dimension reduction on UCI benchmark datasets (Bache and Lichman, 2013). For all datasets, we append the original input \boldsymbol{x} with noise features of dimensionality 5. More specifically, for the original input \boldsymbol{x} with dimensionality $d_{\mathbf{x}}$, we consider the augmented input $\tilde{\boldsymbol{x}}$ with dimensionality $d_{\tilde{\mathbf{x}}} = d_{\mathbf{x}} + 5$ as

$$\widetilde{\boldsymbol{x}} = \left[\boldsymbol{x}^{ op}, \gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5
ight]^{ op},$$

⁴We use the program code: http://www.ms.k.u-tokyo.ac.jp/software.html#LSDR

⁵We use the program code: http://www.stat.nus.edu.sg/~staxyc/

⁶We use the program code: http://www.ism.ac.jp/~fukumizu/software.html

Table 1: Mean and standard error of the dimension reduction error over 30 trials for artificial datasets. The best method in term of the mean error and comparable methods according to the paired *t-test* at the significance level 5% are specified by bold face.

		1.001/00		1 0 0 0		
Dataset	n	LSQMID	LSQMI	LSDR	dMAVE	KDR
А	100	0.126(0.039)	0.394(0.094)	0.073(0.007)	0.123(0.009)	0.077(0.008)
	200	0.046(0.006)	0.077(0.035)	0.046(0.005)	0.082(0.007)	0.048(0.006)
В	100	0.079(0.009)	0.488(0.097)	0.072(0.006)	0.128(0.010)	0.306(0.088)
	200	0.041(0.004)	0.174(0.064)	0.038(0.003)	0.078(0.006)	0.099(0.045)
С	200	0.192(0.026)	0.633(0.100)	0.203(0.011)	0.146(0.010)	0.155(0.010)
	400	0.084(0.005)	0.108(0.011)	0.128(0.006)	0.105(0.006)	0.090(0.007)
D	300	0.245(0.050)	0.301(0.054)	0.286(0.032)	0.370(0.046)	0.257(0.025)
	500	0.128(0.017)	0.129(0.013)	0.185(0.015)	0.263(0.038)	0.198(0.013)

Table 2: Mean and standard error of the root mean squared error over 30 trials for benchmark datasets. The best method in term of the mean error and comparable methods according to the paired *t-test* at the significance level 5% are specified by bold face.

Dataset	n_{tr}	$d_{\widetilde{\mathbf{x}}}$	$d_{\mathbf{z}}$	LSQMID	LSQMI	LSDR	dMAVE	KDR
Fertility	50	14	1	1.215(0.049)	1.092(0.043)	1.315(0.043)	1.321(0.063)	1.116(0.050)
			2	1.051(0.045)	1.029(0.043)	1.199(0.031)	1.340(0.052)	1.104(0.044)
			3	1.052(0.044)	1.038(0.047)	1.104(0.044)	1.288(0.048)	1.121(0.043)
			4	1.046(0.042)	1.026(0.042)	1.092(0.039)	1.271(0.033)	1.146(0.044)
Yacht	100	11	1	0.120(0.005)	0.546(0.042)	0.180(0.012)	0.213(0.017)	0.124(0.007)
			2	0.154(0.011)	0.675(0.047)	0.344(0.023)	0.224(0.014)	0.278(0.033)
			3	0.314(0.024)	0.690(0.037)	0.425(0.018)	0.265(0.013)	0.353(0.028)
			4	0.413(0.021)	0.732(0.043)	0.494(0.015)	0.352(0.017)	0.399(0.012)
	200	13	1	0.621(0.013)	0.606(0.014)	0.606(0.008)	0.582(0.006)	0.791(0.030)
Concrete			2	0.568(0.010)	0.591(0.009)	0.568(0.010)	0.529(0.009)	0.614(0.025)
Concrete			3	0.557(0.009)	0.579(0.011)	0.576(0.012)	0.539(0.007)	0.579(0.016)
			4	0.545(0.012)	0.667(0.025)	0.568(0.010)	0.540(0.008)	0.571(0.014)
	200	15	1	0.447(0.011)	0.523(0.018)	0.442(0.010)	0.375(0.007)	0.447(0.012)
Droost concor			2	0.435(0.010)	0.473(0.012)	0.437(0.009)	0.420(0.012)	0.454(0.014)
breast-cancer			3	0.376(0.004)	0.462(0.010)	0.431(0.007)	0.426(0.008)	0.430(0.007)
			4	0.377(0.005)	0.419(0.008)	0.436(0.007)	0.426(0.011)	0.433(0.007)
	300	19	1	0.043(0.011)	0.070(0.019)	0.016(0.001)	0.139(0.051)	0.513(0.059)
Pilco			2	0.036(0.005)	0.035(0.003)	0.049(0.002)	0.081(0.007)	0.291(0.050)
DIKe			3	0.037(0.005)	0.032(0.003)	0.065(0.002)	0.086(0.008)	0.243(0.037)
			4	0.060(0.006)	0.051(0.007)	0.077(0.002)	0.071(0.005)	0.213(0.029)

where $\gamma_i \sim \Gamma(1,2)$ for $i \in \{1,\ldots,5\}$. Then we use the paired data $\{(\tilde{\boldsymbol{x}}_i, y_i)\}_{i=1}^n$ to perform experiments. We randomly choose n_{tr} samples for training purposes, and use the rest $n_{te} = n - n_{tr}$ for testing purposes. We execute the supervised dimension reduction methods with target dimensionality $d_z \in \{1, 2, 3, 4\}$ to obtain solutions $\widehat{\boldsymbol{W}}$. Then we train a kernel ridge regressor $\widehat{\boldsymbol{y}} = f(\widehat{\boldsymbol{W}}\widehat{\boldsymbol{x}})$ with the Gaussian kernel where the tuning parameters are chosen by 5-fold cross-validation. Finally, we evaluate the regressor by the *root mean squared error* (RMSE):

RMSE =
$$\sqrt{\frac{1}{n_{\text{te}}} \sum_{i=1}^{n_{\text{te}}} (y_i - f(\widehat{\boldsymbol{W}}\widetilde{\boldsymbol{x}}_i))^2}.$$

Table 2 shows the RMSE averaged over 30 trials for the benchmark experiments. It shows that the proposed method performs well overall on all datasets. LSQMI performs very well for the 'Fertility' and 'Bike' datasets, but its performance is quite poor for the other datasets. In contrast, dMAVE performs very well especially for the 'Concrete' dataset where it gives the best solutions for all value of d_z . However, its performance is quite poor for the 'Fertility' and 'Bike' datasets. Both LSDR and KDR do not perform well on these datasets.

7 Conclusion

We proposed a novel supervised dimension reduction method based on efficient maximization of quadratic mutual information (QMI). Our key idea was to *directly* estimate the derivative of QMI without estimating QMI itself. We firstly developed a method to directly estimate the derivative of QMI, and then developed fixed-point iteration which efficiently uses the derivative estimator to find a maximizer of QMI. In addition to the robustness against outliers thanks to the property of QMI, the proposed method is widely applicable because it does not require any assumption on the data distribution and tuning parameters can be objectively chosen via cross-validation. The experiment results on artificial and benchmark datasets showed that the proposed method is promising.

References

- Absil, P.-A., Mahony, R., and Sepulchre, R. (2008). *Optimization Algorithms on Matrix Manifolds*. Princeton University Press, Princeton, NJ.
- Armijo, L. (1966). Minimization of functions having lipschitz continuous first partial derivatives. *Pacific Journal of Mathematics*, 16(1):1–3.
- Aronszajn, N. (1950). Theory of reproducing kernels. *Transactions of the American Mathematical Society*, 68(3):337–404.
- Atif, J., Ripoche, X., Coussinet, C., and Osorio, A. (2003). Non rigid medical image registration based on the maximization of quadratic mutual information. In *Proceedings of Bioengineering Conference, 2003 IEEE 29th Annual*, pages 71–72.

Bache, K. and Lichman, M. (2013). UCI machine learning repository.

- Basu, A., Harris, I. R., Hjort, N. L., and Jones, M. C. (1998). Robust and efficient estimation by minimising a density power divergence. *Biometrika*, 85(3):549–559.
- Bishop, C. M. (2006). *Pattern Recognition and Machine Learning (Information Science and Statistics)*. Springer-Verlag New York, Inc., Secaucus, NJ, USA.
- Boumal, N., Mishra, B., Absil, P.-A., and Sepulchre, R. (2014). Manopt, a Matlab toolbox for optimization on manifolds. *Journal of Machine Learning Research*, 15:1455– 1459.
- Burges, C. J. C. (2010). Dimension reduction: A guided tour. *Foundations and Trends in Machine Learning*, 2(4).
- Cover, T. M. and Thomas, J. A. (1991). *Elements of Information Theory*. Wiley-Interscience, New York, NY, USA.
- Fan, J., Yao, Q., and Tong, H. (1996). Estimation of conditional densities and sensitivity measures in nonlinear dynamical systems. *Biometrika*, 83(1):189–206.
- Fukumizu, K., Bach, F. R., and Jordan, M. I. (2009). Kernel dimension reduction in regression. *The Annals of Statistics*, 37(4):1871–1905.
- Fukumizu, K. and Leng, C. (2014). Gradient-based kernel dimension reduction for regression. *Journal of the American Statistical Association*, 109(505):359–370.
- Kasube, H. E. (1983). A technique for integration by parts. *The American Mathematical Monthly*, 90(3):210–211.
- Kullback, S. and Leibler, R. A. (1951). On information and sufficiency. *The Annals of Mathematical Statistics*, 22(1):79–86.
- Li, K.-C. (1991). Sliced inverse regression for dimension reduction. *Journal of the American Statistical Association*, 86(414):316–342.
- Nocedal, J. and Wright, S. J. (2006). *Numerical Optimization, second edition*. World Scientific.
- Principe, J. C., Xu, D., Zhao, Q., and Fisher, J. W. (2000). Learning from examples with information theoretic criteria. *VLSI Signal Processing*, 26(1-2):61–77.
- Sainui, J. and Sugiyama, M. (2013). Direct approximation of quadratic mutual information and its application to dependence-maximization clustering. *IEICE Transactions*, 96-D(10):2282–2285.
- Sainui, J. and Sugiyama, M. (2014). Unsupervised dimension reduction via least-squares quadratic mutual information. *IEICE Transactions*, 97-D(10):2806–2809.

- Sasaki, H., Noh, Y., and Sugiyama, M. (2015). Direct density-derivative estimation and its application in kl-divergence approximation. In *Proceedings of the Eighteenth International Conference on Artificial Intelligence and Statistics, AISTATS 2015, San Diego, California, USA, May 9-12, 2015.*
- Silverman, B. W. (1986). *Density Estimation for Statistics and Data Analysis*. Chapman & Hall, London.
- Sugiyama, M., Kanamori, T., Suzuki, T., du Plessis, M. C., Liu, S., and Takeuchi, I. (2013). Density-difference estimation. *Neural Computation*, 25(10):2734–2775.
- Suzuki, T. and Sugiyama, M. (2013). Sufficient dimension reduction via squared-loss mutual information estimation. *Neural Computation*, 25(3):725–758.
- Suzuki, T., Sugiyama, M., Kanamori, T., and Sese, J. (2009). Mutual information estimation reveals global associations between stimuli and biological processes. *BMC Bioinformatics*, 10(S-1).
- Suzuki, T., Sugiyama, M., Sese, J., and Kanamori, T. (2008). Approximating mutual information by maximum likelihood density ratio estimation. In *Third Workshop on New Challenges for Feature Selection in Data Mining and Knowledge Discovery, FSDM 2008, held at ECML-PKDD 2008, Antwerp, Belgium, September 15, 2008,* pages 5–20.
- Torkkola, K. (2003). Feature extraction by non-parametric mutual information maximization. *Journal of Machine Learning Research*, 3:1415–1438.

Vapnik, V. (1998). Statistical learning theory. Wiley.

Xia, Y. (2007). A constructive approach to the estimation of dimension reduction directions. *The Annals of Statistics*, 35(6):2654–2690.