A simple coding for cross-domain matching with dimension reduction via spectral graph embedding

Hidetoshi Shimodaira*

Division of Mathematical Science
Graduate School of Engineering Science
Osaka University
1-3 Machikaneyama-cho
Toyonaka, Osaka, Japan
e-mail: shimo@sigmath.es.osaka-u.ac.jp

Abstract:
Data vectors are obtained from multiple domains. They are feature vectors of images or vector representations of words. Domains may have different numbers of data vectors with different dimensions. These data vectors from multiple domains are projected to a common space by linear transformations in order to search closely related vectors across domains. We would like to find projection matrices to minimize distances between closely related data vectors. This formulation of cross-domain matching is regarded as an extension of the spectral graph embedding to multi-domain setting, and it includes several multivariate analysis methods of statistics such as multiset canonical correlation analysis, correspondence analysis, and principal component analysis. Similar approaches are very popular recently in pattern recognition and vision. In this paper, instead of proposing a novel method, we will introduce an embarrassingly simple idea of coding the data vectors for explaining all the above mentioned approaches. A data vector is concatenated with zero vectors from all other domains to make an augmented vector. The cross-domain matching is solved by applying the single-domain version of spectral graph embedding to these augmented vectors of all the domains. An interesting connection to the classical associative memory model of neural networks is also discussed by noticing a coding for association. A cross-validation method for choosing the dimension of the common space and a regularization parameter will be discussed in an illustrative numerical example.

Keywords and phrases: multiple domains, common space, matching weight, multivariate analysis, canonical correlation analysis, spectral graph embedding, associative memory, sparse coding.

1. Introduction

We consider multiple domains for getting data vectors. Let $D$ be the number of domains, and $d = 1, \ldots, D$ denote each domain. For example, $d = 1$ may be for images, and $d = 2$ for words. From domain $d$, we get data vectors $\mathbf{x}_d^i \in \mathbb{R}^{p_d}$, $i = 1, \ldots, n_d$, where $n_d$ is the number of data vectors, and $p_d$ is the dimension of the data vector. They may be image feature vectors for $d = 1$, and word vectors computed by word2vec (Mikolov et al., 2013) from texts for $d = 2$. Typically, $p_d$ is hundreds, and $n_d$ is thousands to millions. We would like to retrieve relevant words from an image query, and alternatively retrieve images from a word query.

We specify the strength of association between two data vectors $\mathbf{x}_d^i$ and $\mathbf{x}_e^j$ by a matching weight $w_{de}^{ij} \in \mathbb{R}$ for $d, e = 1, \ldots, D$, $i = 1, \ldots, n_d$, $j = 1, \ldots, n_e$. (Note that “matching” here

* Supported in part by Grant KAKENHI (24300106, 26120523) from MEXT of Japan.
is nothing related to that of graph theory.) We assume the weight is symmetric $w_{ij}^{de} = w_{ji}^{ed}$. For example, $w_{12}^{12} = 3$ for the association between an image “apple” ($x_1^1$) and word “apple” ($x_2^2$), and $w_{12}^{12} = 1$ for the association between the image “apple” and word “red” ($x_2^2$). However, it could be the case that the image apple is unlabeled and $w_{12}^{12} = 0$, while the color may be automatically classified as red and $w_{12}^{12} = 1$ remains. Let $w_{ij}^{de}$ be the matching weight representing the underlying true associations, and $w_{ij}^{de}$ be observed ones sampled from the true associations. We assume $w_{ij}^{de} = w_{ij}^{de}$ with a small probability, and $w_{ij}^{de} = 0$ otherwise, so that $W^{de} = (w_{ij}^{de}) \in \mathbb{R}^{n_a \times n_e}$ would be a sparse matrix.

The data vectors from all the domains will be projected to a single common space of $\mathbb{R}^K$ for some $K > 0$. Using a matrix $A^d \in \mathbb{R}^{p_d \times K}$, we define a linear transformation by

$$y_i^d = (A^d)^T x_i^d, \quad i = 1, \ldots, n_d; \quad d = 1, \ldots, D.$$  

(1)

Here $T$ denotes matrix transpose. Later we use matrix notation such as $\text{tr}()$ for the matrix trace, $\text{diag}()$ for a diagonal matrix, and $\text{Diag}()$ for a block diagonal matrix. Each element of $y_i^d \in \mathbb{R}^K$ is

$$(y_i^d)_k = (a_k^d)^T x_i^1, \quad k = 1, \ldots, K,$$

where $a_k^d \in \mathbb{R}^{p_d}$ are defined as $A^d = (a_1^d, \ldots, a_K^d)$. The error function of cross-domain matching is

$$\phi(A^1, \ldots, A^D) = \frac{1}{2} \sum_{d=1}^D \sum_{i=1}^{n_d} \sum_{j=1}^{n_e} w_{ij}^{de} \|y_i^d - y_j^e\|^2,$$  

(2)

and we would like to find $A^1, \ldots, A^D$ that minimize (2) subject to certain constraints. This is a supervised learning with the matching weights as training data. It handles the problem of semi-supervised learning and missing observation by simply letting unobserved weights zero. For a new query image, say, the data vector $x_i^1 \in \mathbb{R}^{p_1}$ is transformed to $y_i^1 = (A^1)^T x_i^1$. Then look for points close to $y_i^1$ in the collection $\{y_i^d\}$. By working on the common space in this way, we will perform data retrieval across domains and data fusion from multiple domains.

This formulation of cross-domain matching is regarded as an extension of the spectral graph embedding of Yan et al. (2007) to the multi-domain setting, and similar approaches are very popular recently in pattern recognition and vision (Correa et al., 2010; Yuan et al., 2011; Kan et al., 2012; Huang et al., 2013; Shi et al., 2013; Wang et al., 2013; Gong et al., 2014; Yuan and Sun, 2014). In particular, the formulation reduces to a classical multivariate analysis of statistics, known as the multiset canonical correlation analysis (MCCA) (Kettenring, 1971; Takane, Hwang and Abdi, 2008; Tenenhaus and Tenenhaus, 2011) by letting $n_1 = n_2 = \cdots = n_D$ and connecting all vectors across domains with the same index as $w_{ii}^{de} \neq 0$ and $w_{ij}^{de} = 0$ for $i \neq j$. Class labels are coded by indicator variables (called dummy variables in statistics), and treated as domains; they appear in canonical discriminant analysis and correspondence analysis. The formulation becomes the classical canonical correlation analysis (CCA) of Hotelling (1936) by further letting $D = 2$, or it becomes principal component analysis (PCA) by letting $p_1 = p_2 = \cdots = p_D = 1$.

In this paper, we do not intend to propose a novel method. Instead, we will introduce an embarrassingly simple idea of coding the data vectors for explaining all the above mentioned approaches. This coding is similar to that of Daumé III (2009). Let $P = \sum_{d=1}^D p_d$ and $N = \sum_{d=1}^D n_d$. The data vector $x_i^d$ is coded as an augmented vector $	ilde{x}_i^d \in \mathbb{R}^P$ defined as

$$(\tilde{x}_i^d)^T = (0_{p_1})^T, \ldots, (0_{p_{d-1}})^T, (x_i^d)^T, (0_{p_d+1})^T, \ldots, (0_{p_D})^T.$$  

(3)
Here, $0_p \in \mathbb{R}^p$ is the vector with zero elements. This is a sparse coding (Olshausen and Field, 2004) in the sense that nonzero elements for domains do not overlap each other. All the $N$ vectors of all domains are now represented as points in the same $\mathbb{R}^P$. We will get the solution of the optimization problem of (2) by applying the single-domain version of the spectral graph embedding of Yan et al. (2007) to these $\tilde{x}_d^i$ vectors.

In Section 2, we will review the spectral graph embedding methods. In Section 3, we will show that the coding (3) solves the minimization of (2). An interesting connection to the classical associative memory model of neural networks (Kohonen, 1972; Nakano, 1972) is also discussed there by noticing that coding $\tilde{x}_d^i + \tilde{x}_e^j$ corresponds to the matching $w_{de}^{ij}$. In Section 4, the relations to the multivariate analysis methods are explained. In Section 5, we show an illustrative numerical example of cross-domain matching. In particular, we discuss a cross-validation method for choosing the dimension $K$ of the common space and a regularization parameter; we resample the matching weights $w_{de}^{ij}$ instead of data vectors $x_d^i$ there.

2. A brief review of the spectral graph embedding

2.1. The spectral graph theory

Before discussing the cross-domain matching, here we review the spectral graph theory (Chung, 1997). We then consider extra constraints in Section 2.2. This result will be used for the cross-domain matching in Section 3. The following argument is based on the spectral clustering, in particular the normalized graph Laplacian (Shi and Malik, 2000; Ng et al., 2002; Von Luxburg, 2007) and the spectral embedding (Belkin and Niyogi, 2003).

Let $N > 0$ be the number of vertices of a graph, and these vertices are represented by vectors $y_i \in \mathbb{R}^K$, $i = 1, \ldots, N$ of dimension $K \leq N$. The weighted adjacency matrix is $W = (w_{ij}) \in \mathbb{R}^{N \times N}$ with symmetric weights $w_{ij} = w_{ji} \geq 0$, $i, j = 1, \ldots, N$. Let $M = \text{diag}(W1_N) \in \mathbb{R}^{N \times N}$ be the diagonal matrix with elements $\sum_{j=1}^N w_{ij}$, $i = 1, \ldots, N$. Here $1_N \in \mathbb{R}^N$ denotes the vector with all elements being 1. The graph Laplacian is $M - W$.

For a given $W$, we would like to find $y_1, \ldots, y_N$ that minimize the error function

$$\phi(y_1, \ldots, y_N) = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N w_{ij} \|y_i - y_j\|^2$$

subject to certain constraints. For avoiding the trivial solution of all zero vectors, we assume the constraints

$$Y^TMY = I_K,$$

where $Y \in \mathbb{R}^{N \times K}$ is defined by $Y^T = (y_1, \ldots, y_N)$, and $I_K \in \mathbb{R}^{K \times K}$ is the identity matrix. By simple rearrangement of the formula, we get

$$\text{tr}(Y^TMY) = \sum_{i=1}^N \sum_{j=1}^N w_{ij} y_i^T y_j, \quad \text{tr}(Y^TMY) = \sum_{i=1}^N \left( \sum_{j=1}^N w_{ij} \right) \|y_i\|^2.$$

Thus the error function is rewritten as

$$\phi(y_1, \ldots, y_N) = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N w_{ij} \left( \|y_i\|^2 + \|y_j\|^2 - 2y_i^T y_j \right)$$

$$= \text{tr}(Y^T(M - W)Y)$$

$$= K - \text{tr}(Y^T(WY)).$$
Therefore, minimization of (4) is equivalent to maximization of \( \text{tr}(Y^T W Y) \).

Let \( M^{-1/2} \in \mathbb{R}^{N \times N} \) be the diagonal matrix with elements \((\sum_{j=1}^{N} u_{ij})^{-1/2}, i = 1, \ldots, N\). The eigenvalues of \( M^{-1/2} WM^{-1/2} \) are \( \rho_1 \geq \rho_2 \geq \cdots \geq \rho_N \) and the corresponding normalized eigenvectors are \( u_1, \ldots, u_N \in \mathbb{R}^N \). The solution of minimizing (4) subject to (5) is given by \( Y = M^{-1/2}(u_1, \ldots, u_K) \).

### 2.2. The spectral graph embedding for dimensionality reduction

In addition to the constraints (5), Yan et al. (2007) introduced extra constraints that the column vectors of \( Y \) are included in a specified linear subspace. Let us specify \( x_i \in \mathbb{R}^P, i = 1, \ldots, N \) with some \( K \leq P \leq N \). Define the data matrix \( X \in \mathbb{R}^{N \times P} \) by \( X^T = (x_1, \ldots, x_N) \). We assume that \( Y \) is expressed in the form

\[
Y = XA
\]

(6)

using an arbitrary matrix \( A \in \mathbb{R}^{P \times K} \). Therefore, minimization of (4) is equivalent to finding \( A \) that maximizes \( \text{tr}(A^T X^T W X A) \) subject to the constraints \( A^T X^T M X A = I_K \).

For numerical stability, we introduce quadratic regularization terms similar to those of Takane, Hwang and Abdi (2008). First, we define two \( P \times P \) matrices by

\[
G = X^T M X + \gamma_M L_M, \quad H = X^T W X + \gamma_W L_W.
\]

Here \( \gamma_M, \gamma_W \in \mathbb{R} \) are regularization parameters, and \( L_M, L_W \in \mathbb{R}^{P \times P} \) are non-negative definite, typically \( L_M = L_W = I_P \). Then, we consider the optimization problem:

Maximize \( \text{tr}(A^T H A) \) with respect to \( A \in \mathbb{R}^{P \times K} \)

(7)

subject to \( A^T G A = I_K \).

(8)

This reduces to the problem of Section 2.1 by letting \( X = I_N, \gamma_M = \gamma_W = 0 \). For the solution of the optimization problem, we denote \( G^{1/2} \in \mathbb{R}^{P \times P} \) be one of the matrices satisfying \( (G^{1/2})^T G^{1/2} = G \). The inverse matrix is denoted by \( G^{-1/2} = (G^{1/2})^{-1} \). These are easily computed by, say, Cholesky decomposition or spectral decomposition of symmetric matrix. The eigenvalues of \( (G^{-1/2})^T H G^{-1/2} \) are \( \rho_1 \geq \rho_2 \geq \cdots \rho_P \), and the corresponding normalized eigenvectors are \( u_1, u_2, \ldots, u_P \in \mathbb{R}^P \). The solution of our optimization problem is

\[
A = G^{-1/2}(u_1, \ldots, u_K).
\]

(9)

To see what we are actually solving, let us rewrite the error function (4) with respect to \( A \) under the constraints (6) and (8).

\[
\phi(A) = \text{tr}(Y^T(M - W)Y)
= \text{tr}(A^T X^T (M - W) X A)
= \text{tr}(A^T (G - H - \gamma_M L_M + \gamma_W L_W) A)
= K - \text{tr}(A^T H A) - \text{tr}(A^T (\gamma_M L_M - \gamma_W L_W) A)
\]

Thus, maximization of (7) subject to (8) is equivalent to minimization of

\[
\phi(A) + \text{tr}(A^T (\gamma_M L_M - \gamma_W L_W) A).
\]

(10)

For the second term working as a regularization term properly, \( \gamma_M L_M - \gamma_W L_W \) should be nonnegative definite.
3. Cross-domain matching correlation analysis

Now we are back to the cross-domain matching. We define several matrices for rewriting (1) and (2) in a simple form. The data matrices $\mathbf{X}^d \in \mathbb{R}^{n_d \times p_d}$ for domains $d = 1, \ldots, D$ are defined by $(\mathbf{X}^d)^T = (x^d_1, \ldots, x^d_{n_d})$. We put these $D$ matrices in the block diagonal positions of a $N \times P$ matrix to define a large data matrix $\mathbf{X} = \text{Diag}((\mathbf{X}^1, \ldots, \mathbf{X}^D)) \in \mathbb{R}^{N \times P}$. We concatenate the transformation matrices to define $\mathbf{A} \in \mathbb{R}^{P \times K}$ as $\mathbf{A}^T = ((\mathbf{A}^1)^T, \ldots, (\mathbf{A}^D)^T)$. The vectors in the common space are also concatenated to define $\mathbf{Y}^d \in \mathbb{R}^{n_d \times K}$. Using the Kronecker delta, the correlation matrix $\mathbf{R}$ is that the large data matrix $\mathbf{X}$ is solved by the single-domain version of the spectral graph embedding. An important point is that the large data matrix $\mathbf{X}$ is expressed as

$$\mathbf{X}^T = (\mathbf{x}^1_1, \ldots, \mathbf{x}^{n_1}_1, \ldots, \mathbf{x}^D_{n_d}),$$

meaning $\mathbf{X}$ is the data matrix consists of the augmented vectors. What we have done is, therefore, interpreted as simply applying the spectral graph embedding of Yan et al. (2007) to the $N$ augmented vectors in $\mathbb{R}^P$.

It would be better to rewrite the constraints (8) in terms of $\mathbf{A}^1, \ldots, \mathbf{A}^D$ for cross-domain matching. Notice $\mathbf{M} = \text{Diag}((\mathbf{M}^1, \ldots, \mathbf{M}^D))$ with $\mathbf{M}^d = \text{diag}((\mathbf{W}^d_1, \ldots, \mathbf{W}^d_{n_d}))$, and so $\mathbf{X}^T \mathbf{M} \mathbf{X} = \text{Diag}((\mathbf{X}^1)^T \mathbf{M}^1 (\mathbf{X}^1)^T, \ldots, (\mathbf{X}^D)^T \mathbf{M}^D (\mathbf{X}^D)^T)$. For simplicity, we assume that the regularization matrix is written as a block diagonal matrix as $\mathbf{L}_M = \text{Diag}(\mathbf{L}_M^1, \ldots, \mathbf{L}_M^D)$. Then we have

$$\mathbf{A}^T \mathbf{G} \mathbf{A} = \sum_{d=1}^D (\mathbf{A}^d)^T ((\mathbf{X}^d)^T \mathbf{M}^d \mathbf{X}^d + \gamma_M \mathbf{L}_M^d) \mathbf{A}^d = \mathbf{I}_K.$$

This is expressed for the vectors in $\mathbf{A}^d$ as

$$\sum_{d=1}^D (a^d_k)^T ((\mathbf{X}^d)^T \mathbf{M}^d \mathbf{X}^d + \gamma_M \mathbf{L}_M^d) a^d_l = \delta_{kl}, \quad k, l = 1, \ldots, K \quad (11)$$

using the Kronecker delta.

As a final remark of this section, we discuss a coding of matching for further implications. Let $E$ be the number of nonzero elements in the lower triangular part of $\mathbf{W}$. In other words, $E$ is the number of edges in the graph. We define a diagonal matrix $\mathbf{W} \in \mathbb{R}^E \times E$ with elements of these nonzero $\{w^d_{ij}\}$. Instead of working on the vertices of the graph, here we work on the edges of the graph for data analysis. So, the data vector is now coded as $\mathbf{x}^d_1 + \mathbf{x}^d_2$ for the matching weight $w^d_{ij}$. We define the data matrix $\mathbf{X} \in \mathbb{R}^E \times P$ by concatenating $\mathbf{x}^d_1 + \mathbf{x}^d_2$ in the same order as $\mathbf{W}$. Since $\mathbf{X}^T \mathbf{W} \mathbf{X} = \mathbf{X}^T \mathbf{M} \mathbf{X} + \mathbf{X}^T \mathbf{W} \mathbf{X}$, minimization of (10) is equivalent to maximization of $\text{tr}(\mathbf{A}^T \mathbf{X}^T \mathbf{W} \mathbf{X} + \gamma_M \mathbf{L}_M + \gamma_W \mathbf{L}_W) \mathbf{A}$). Therefore, the cross-domain matching is interpreted as a kind of PCA for input patterns coded as $\mathbf{x}^d_1 + \mathbf{x}^d_2$. Interestingly, this idea is found in one of the classical neural network models. Any part of the memorized vector can be used as a key for recalling the whole vector in the auto-associative correlation matrix memory (Kohonen, 1972; Nakano, 1972). This associative memory may recall $\mathbf{x}^d_1 + \mathbf{x}^d_2$ for input key either $\mathbf{x}^d_1$ or $\mathbf{x}^d_2$. It would be a subject of future research to work on $\mathbf{x}^d_1 + \mathbf{x}^d_2 + \mathbf{x}^d_3 + \cdots$ for joint associations of three or more vectors.
4. Relations to multiset canonical correlation analysis

In this section, we assume that the numbers of vectors are the same for all domains. Then the cross-domain matching reduces to a classical multivariate analysis of statistics. Let \( n_1 = \cdots = n_D = n \), and \( N = nD \). We assume that the weight matrix is specified as \( W^{de} = c_{de} I_n \) using a coefficient \( c_{de} \geq 0 \) for all \( d, e = 1, \ldots, D \). In this case, the cross-domain matching becomes a version of MCCA, where connections between sets of variables are specified by the coefficients \( c_{de} \) (Tenenhaus and Tenenhaus, 2011). Another version of MCCA with all \( c_{de} = 1 \) is discussed extensively in Takane, Hwang and Abdi (2008).

Here we show how the objective function (7) and the constraints (8) are expressed in the case of MCCA. Noting that \( X^T W X \) is an array of \( (X^d)^TW^{de}X^e = c_{de}(X^d)^TX^e \), \( d, e = 1, \ldots, D \), we have

\[
\text{tr}(A^T HA) = \sum_{d=1}^{D} \sum_{e=1}^{D} c_{de} \text{tr}((A^d)^T (X^d)^TX^e A^e) + \gamma_W \sum_{d=1}^{D} \text{tr}((A^d)^T L_W^d A^d)
\]

\[
= \sum_{k=1}^{K} \left( \sum_{d=1}^{D} \sum_{e=1}^{D} c_{de} (a_k^d)^T (X^d)^TX^e a_k^e \right) + \sum_{d=1}^{D} \gamma_W (a_k^d)^T L_W^d a_k^d \tag{12}
\]

For simplicity, we assumed that the regularization matrix is written as a block diagonal matrix as \( L_W = \text{Diag}(L_W^1, \ldots, L_W^D) \). The constraints (8) are expressed as (11) with \( M^d = (\sum_{e=1}^{D} c_{de}) I_n \). The constraints correspond to eq. (31) of Takane, Hwang and Abdi (2008) except for a difference in scaling, when \( c_{de} = 1 \), \( L_M = L_W \), and \( \gamma_M = D\gamma_W \).

Further assume that \( p_1 = \cdots = p_D = 1 \) and \( P = D \). Each \( X^d \in \mathbb{R}^{n \times 1} \) is a vector now. \( (G^{-1/2})^T H G^{-1/2} \) becomes the sample correlation matrix scaled by the factor \( D^{-1} \). Thus, the cross-domain matching is equivalent to PCA.

5. An illustrative numerical example

5.1. Data generation

We look at a very simple example to see how the methods work. We randomly generated a data with \( D = 3, p_1 = 10, p_2 = 30, p_3 = 100, n_1 = 125, n_2 = 250, n_3 = 500 \) in the following steps.

1. We placed points on a \( 5 \times 5 \) grid in \( R^2 \) as \((1, 1), (1, 2), (1, 3), (1, 4), (1, 5), (2, 1), \ldots, (5, 5)\). They are \((x_{0}^{d})^T, \ldots, (x_{25}^{d})^T\), where \( d = 0 \) is treated as a special domain for data generation. These 25 values are repeatedly used to define \( x_i^d \) for \( i = 26, 27, \ldots \).

2. We made random matrices \( B^d \in \mathbb{R}^{p_d \times 2}, d = 1, 2, 3 \), with all elements distributed as \( N(0, 1) \) independently. Then, we generated data vectors \( x_i^d = B^d x_i^0 + \epsilon_i^d, i = 1, \ldots, n_d \). Elements of \( \epsilon_i^d \) are distributed as \( N(0, 0.5^2) \) independently. Each column of \( X^d \) is standardized to mean zero and variance one.

3. The numbers of data vectors \( x_i^d \) generated from each grid point are 5, 10, 20, respectively, for \( d = 1, 2, 3 \). For defining underlying true associations, we linked these 35 vectors to each other, except for those within a same domain. The true weights for these 35 vectors are \( \bar{w}_{ij}^{de} = 1 \) for \( d \neq e \). All other weights across grid points are zero. The numbers of nonzero elements (lower triangular) are 1250, 2500, 5000 (total 8750), respectively, for \( \bar{W}^{21}, \bar{W}^{31}, \bar{W}^{32} \).

4. We made weight matrices \( W^{de} \) by randomly sampling 2% of links from \( \bar{W}^{de} \). The numbers of nonzero elements (lower triangular) became 28, 50, 97 (total 175), respectively, for \( W^{21}, W^{31}, W^{32} \).
5.2. Finding the common space

We applied the cross-domain matching with $\gamma_W = 0$, $\gamma_M = 0.1$ to the generated data. The regularization matrix is block diagonal $L_M = \text{Diag}(L_{A1}^M, L_{A2}^M, L_{A3}^M)$ with $L_{A_d}^M = \alpha_d I_{p_d}$ and $\alpha_d = \text{tr}((X^d)^T M^d X^d)/p_d$. The results are shown in Fig. 1 and Fig. 2.

Like PCA, we denote $PC_k$ for the $k$-th component of the common space ($y^d_k$). Scatter plots of data vectors in the common space are shown in Fig. 1(a) and Fig. 1(b). The $5 \times 5$ structure is clearly observed in (PC1, PC2), while PC3 looks almost noise. Looking at plots of data vectors in the common space are shown in Fig. 1(c), they are almost 1 for PC1 and PC2, and decrease rapidly for $k \geq 3$, indicating $K = 2$ is a good choice. The number of positive $\rho_k$ is 40 ($= p_1 + p_2$ in this example). We only look at these 40 PC’s, because negative $\rho_k$ are due to change of the sign of axes.

Picking a data vector ($d = 2, i = 1$) as a query, and look for vectors close to it in the common space. In Fig. 1(d), distances to other vectors $\|y^d_i - y^d_j\|, i = 1, \ldots, n_d, d = 1, \ldots, D$ are computed with $K = 2$. The “true” distances are computed as $\|x^0_i - x^0_j\|$. They agree very well, meaning that we will find closely related vectors.

What happens if we use a wrong $K$? Results are shown in Fig. 2. The observed distances in the common space are disturbed by PC3 in Fig. 2(a). The situation becomes worse in Fig. 2(b), and it is not possible to make a reasonable data-retrieval any more. It is very important to choose an appropriate $K$.

5.3. Choosing $K$ and $\gamma_M$ by cross-validation

We write $A = A(W, \gamma_M)$ for (9) and $\phi(A, W)$ for (2) by omitting $X$ from the notation. The error function is decomposed into each PC$k$ as $\phi(A, W) = \sum_{k=1}^K \phi_k(A, W)$ with

$$\phi_k(A, W) = \frac{1}{2} \sum_{d=1}^D \sum_{e=1}^D n_e \sum_{i=1}^{n_e} \sum_{j=1}^{n_e} w^{de}_{ij} \left( (y^d_i)_k - (y^d_j)_k \right)^2.$$  

For verifying an appropriate value for $K$ and $\gamma_M$, the error $\phi_k(A(W, \gamma_M), \hat{W})$ with respect to the true weights $\hat{w}^{de}_{ij}$ is computed for $\gamma_M = 0, 0.01, 0.1, 1.0$ in Fig. 3(a). The error is small for $k = 1, 2$, and it rapidly increases for $k \geq 3$, confirming $K = 2$ is the right choice. Also, we confirm that the errors in PC1 and PC2 are minimized when $\gamma_M = 0.1$.

The values of $\hat{w}^{de}_{ij}$ are unknown in reality, and we have to compute the error only from the observed $w^{de}_{ij}$. We performed cross-validation analysis as follows. 95% of nonzero elements (lower triangular) of $W$ are resampled to make $W^*$. In other words, the elements of $W^*$ are defined as $w_{ij}^{de*} = w_{ij}^{de} z_{ij}^{de}; z_{ij}^{de}$ are generated by the Bernoulli trial with $P(z_{ij}^{de} = 1) = 0.95$ and $P(z_{ij}^{de} = 0) = 0.05$. The number of nonzero elements (lower triangular) of $W^*$ was 165, and that of the remaining matrix $W - W^*$ was 10, from which we computed $\phi_k(A(W^*, \gamma_M), W - W^*)$. By repeating this process 50 times, we computed the average error. This cross-validation error is shown in Fig. 3(b). The plot is very similar to Fig. 3(a), and we choose $K = 2$, $\gamma_M = 0.1$.

Acknowledgments

I would like to thank Kazuki Fukui and Haruhisa Nagata for helpful discussions.
References

BELKIN, M. and NIYOGI, P. (2003). Laplacian eigenmaps for dimensionality reduction and data representation. \textit{Neural computation} \textbf{15} 1373–1396.

CHUNG, F. R. (1997). \textit{Spectral graph theory} 92. American Mathematical Soc.

CORREA, N. M., EICHELE, T., ADALI, T., LI, Y.-O. and CALHOUN, V. D. (2010). Multi-set canonical correlation analysis for the fusion of concurrent single trial ERP and functional MRI. \textit{Neuroimage} \textbf{50} 1438–1445.

DAUMÉ III, H. (2009). Frustratingly easy domain adaptation. In \textit{Proceedings of the 45th Annual Meeting of the Association of Computational Linguistics} 256–263.

GONG, Y., KE, Q., ISARD, M. and LAZEBNIK, S. (2014). A multi-view embedding space for modeling internet images, tags, and their semantics. \textit{International Journal of Computer Vision} \textbf{106} 210–233.

HOTELLING, H. (1936). Relations between two sets of variates. \textit{Biometrika} 321–377.

HUANG, Z., SHAN, S., ZHANG, H., LAO, S. and CHEN, X. (2013). Cross-view graph embedding. In \textit{Computer Vision–ACCV 2012} 770–781. Springer.

KAN, M., SHAN, S., ZHANG, H., LAO, S. and CHEN, X. (2012). Multi-view discriminant analysis. In \textit{Computer Vision–ECCV 2012} 808–821. Springer.

KETTNERING, J. R. (1971). Canonical analysis of several sets of variables. \textit{Biometrika} \textbf{58} 433–451.

KOHONEN, T. (1972). Correlation matrix memories. \textit{Computers, IEEE Transactions on} \textbf{100} 353–359.

MIKOLOV, T., SUTSKEVER, I., CHEN, K., CORRADO, G. S. and DEAN, J. (2013). Distributed representations of words and phrases and their compositionality. In \textit{Advances in Neural Information Processing Systems} 3111–3119.

NAKANO, K. (1972). Associatron – A model of associative memory. \textit{Systems, Man and Cybernetics, IEEE Transactions on} \textbf{3} 380–388.

NG, A. Y., JORDAN, M. I., WEISS, Y. et al. (2002). On spectral clustering: Analysis and an algorithm. \textit{Advances in neural information processing systems} \textbf{2} 849–856.

OLSHAUSEN, B. A. and FIELD, D. J. (2004). Sparse coding of sensory inputs. \textit{Current opinion in neurobiology} \textbf{14} 481–487.

SHI, J. and MALIK, J. (2000). Normalized cuts and image segmentation. \textit{Pattern Analysis and Machine Intelligence, IEEE Transactions on} \textbf{22} 888–905.

SHI, X., LIU, Q., FAN, W. and YU, P. S. (2013). Transfer across completely different feature spaces via spectral embedding. \textit{Knowledge and Data Engineering, IEEE Transactions on} \textbf{25} 906–918.

TAKANE, Y., HWANG, H. and ABDI, H. (2008). Regularized multiple-set canonical correlation analysis. \textit{Psychometrika} \textbf{73} 753–775.

TENENHAUS, A. and TENENHAUS, M. (2011). Regularized generalized canonical correlation analysis. \textit{Psychometrika} \textbf{76} 257–284.

VON LUXBURG, U. (2007). A tutorial on spectral clustering. \textit{Statistics and computing} \textbf{17} 395–416.

WANG, K., HE, R., WANG, W., WANG, L. and TAN, T. (2013). Learning coupled feature spaces for cross-modal matching. In \textit{Computer Vision (ICCV), 2013 IEEE International Conference on} 2088–2095. IEEE.

YAN, S., XU, D., ZHANG, B., ZHANG, H.-J., YANG, Q. and LIN, S. (2007). Graph embedding and extensions: a general framework for dimensionality reduction. \textit{Pattern Analysis and Machine Intelligence, IEEE Transactions on} \textbf{29} 40–51.
Yuan, Y.-H. and Sun, Q.-S. (2014). Graph regularized multiset canonical correlations with applications to joint feature extraction. *Pattern Recognition* **47** 3907–3919.

Yuan, Y.-H., Sun, Q.-S., Zhou, Q. and Xia, D.-S. (2011). A novel multiset integrated canonical correlation analysis framework and its application in feature fusion. *Pattern Recognition* **44** 1031–1040.
(a) (PC1, PC2)

(b) (PC1, PC3)

(c) Canonical correlations

(d) Distances from $y_t^2 (K = 2)$

Fig 1. Cross-domain matching of Section 5.2 ($\gamma_M = 0.1$)
(a) Distances from $y_i^2$ ($K = 3$)  
(b) Distances from $y_i^2$ ($K = 20$)

Fig 2. Using larger $K$ ($\gamma_M = 0.1$)

(a) True error of each PC  
(b) Cross-validation error of each PC

Fig 3. Cross-validation analysis of Section 5.3