Conditional Manifold Learning

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This paper addresses a problem called “conditional manifold learning”, which aims to learn a low-dimensional manifold embedding of high-dimensional data, conditioning on auxiliary manifold information. This auxiliary manifold information is from controllable or measurable conditions, which are ubiquitous in many science and engineering applications. A broad class of solutions for this problem, conditional multidimensional scaling (including a conditional ISOMAP variant), is proposed. A conditional version of the SMACOF algorithm is introduced to optimize the objective function of conditional multidimensional scaling.

Keywords: dimension reduction, distance scaling, ISOMAP, multidimensional scaling, SMACOF.

1. Introduction

The “curse of dimensionality” refers to the challenges of learning from high-dimensional data. The “manifold hypothesis” is commonly assumed in machine learning to address these challenges. Given a dataset of \( N \) observations in an \( n \)-dimensional space \( \{ \mathbf{y}_i = [y_{i,1}, y_{i,2}, \ldots, y_{i,n}]^T \in \mathbb{R}^n: i = 1, 2, \ldots, N \} \), the manifold hypothesis states that the high-dimensional data \( \mathbf{y}_i \)'s approximately lie on some low \( p \)-dimensional manifold embedded in their \( n \)-dimensional space. In mathematical form, this hypothesis implies that

\[
\mathbf{y}_i = \mathbf{g}(\mathbf{u}_i) + \mathbf{e}_i, \tag{1}
\]

where \( \mathbf{u}_i = [u_{i,1}, u_{i,2}, \ldots, u_{i,p}]^T \in \mathbb{R}^p \) is the manifold coordinates of observation \( i \), \( \mathbf{g}(\mathbf{u}_i) = [g_1(\mathbf{u}_i), g_2(\mathbf{u}_i), \ldots, g_n(\mathbf{u}_i)]^T \in \mathbb{R}^n \) is some unknown function that maps the \( p \)-vector \( \mathbf{u}_i \) to the \( n \)-vector \( \mathbf{y}_i \), and \( \mathbf{e}_i \) is a zero-mean noise.
The manifold hypothesis allows performing dimension reduction for \( \{ \mathbf{y}_i : i = 1, 2, ..., N \} \) to simplify learning tasks. Manifold learning algorithms do this precisely, by learning from \( \{ \mathbf{y}_i : i = 1, 2, ..., N \} \) an embedding in a \( p \)-dimensional space \( \{ \mathbf{u}_i : i = 1, 2, ..., N \} \), which provides an implicit representation of the manifold of the \( \mathbf{y}_i \)'s. Manifold learning is usually known with two seminal approaches: isometric feature mapping (ISOMAP; Tenenbaum et al., 2000) and local linear embedding (Roweis and Saul, 2000). Other notable manifold learning algorithms include Laplacian eigenmap (Belkin and Niyogi, 2002), Hessian eigenmaps (Donoho and Grimes, 2003), t-distributed stochastic neighbor embedding (van der Maaten and Hinton, 2008), and more recently, uniform manifold approximation and projection (McInnes et al., 2018).

In fact, earlier methods such as classical multidimensional scaling (Torgerson, 1952), Sammon mapping (Sammon, 1969), and curvilinear component analysis (Demartines and Hérault, 1997) also seek for a low-dimensional embedding of high-dimensional data. These methods belong to a broad class of multidimensional scaling (MDS) techniques, which solves for \( \mathbf{u}_i \) by minimizing the stress function

\[
\min_{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_N} \sum_{i < j} w_{ij} (\tilde{\delta}_{ij} - ||\mathbf{u}_i - \mathbf{u}_j||)^2,
\]

where \( w_{ij} \) is the weight of the observations \( i \) and \( j \), and \( \tilde{\delta}_{ij} \) is some monotone transformation of the dissimilarity between observations \( i \) and \( j \). Classical multidimensional scaling fixes \( w_{ij} = 1 (\forall i, j = 1, 2, ..., N) \); Sammon mapping uses \( w_{ij} = \delta_{ij}^{-1} (\forall i, j = 1, 2, ..., N) \); and curvilinear component analysis sets \( w_{ij} \) as some decreasing function of \( ||\mathbf{u}_i - \mathbf{u}_j|| \) (\( \forall i, j = 1, 2, ..., N \)). Note that Sammon mapping and curvilinear component analysis emphasize local behavior through the weights \( w_{ij} \)'s, and hence, can learn nonlinear manifolds. In contrast, classical multidimensional scaling is mainly for learning close to linear manifold, as it focuses on global behavior. ISOMAP is indeed a direct extension of classical multidimensional scaling to handle highly nonlinear manifolds by applying classical multidimensional scaling to “geodesic” distances, instead of the original distances/dissimilarities. The geodesic distance between two points is the shortest distance between them along their manifold.
In many applications, one has a set of auxiliary information \( \{v_i = [v_{i,1}, v_{i,2}, \ldots, v_{i,q}]^T \in \mathbb{R}^q : i = 1, 2, \ldots, N \} \), which together with \( \{u_i: i = 1, 2, \ldots, N \} \) constitute the observations on the manifold. In other words, the manifold parameters include both \( u \) (which is unknown) and \( v \) (which is known). For example, in the kinship terms example in Section 3, auxiliary information such as gender or kinship degree can be derived directly from the kinship terms (see Section 3 for more details). Such situations are indeed common in practice, as there are often controllable/measurable conditions in most science or engineering domains. In such situations, we can mathematically represent each observation by:

\[
\mathbf{y}_i = f(\mathbf{u}_i, \mathbf{v}_i) + \mathbf{e}_i,
\]

where \( f(\mathbf{u}_i, \mathbf{v}_i) = [f_1(\mathbf{u}_i, \mathbf{v}_i), f_2(\mathbf{u}_i, \mathbf{v}_i), \ldots, h_n(\mathbf{u}_i, \mathbf{v}_i)]^T \) is some unknown function that maps the effects of both unknown manifold coordinates \( \mathbf{u}_i \) and known manifold coordinates \( \mathbf{v}_i \) onto observation \( i \). Here, the goal is to learn the unknown manifold coordinates \( \{\mathbf{u}_i: i = 1, 2, \ldots, N \} \) from \( \{\mathbf{y}_i: i = 1, 2, \ldots, N \} \) and \( \{\mathbf{v}_i: i = 1, 2, \ldots, N \} \). In this paper, this problem is referred to as “conditional manifold learning”, and a conditional MDS approach is proposed to solve this problem. A conditional ISOMAP extension to handle highly nonlinear manifold is straightforward from conditional MDS.

It is important to note that the problem and algorithms in this paper are fundamentally different from those in the “supervised manifold learning”. Supervised manifold learning methods literature (see, e.g., the review paper of Chao et al., 2019) largely focus on classification contexts, in which one has class labels \( \{C_i: i = 1, 2, \ldots, N \} \) of the observations and the main goal is to build a model to predict the class labels of \( \{\mathbf{y}_i: i = 1, 2, \ldots, N \} \). These methods map the high-dimensional \( \mathbf{y}_i \)’s to some low-dimensional \( \mathbf{u}_i \)’s to mitigate the curse of dimensionality. Essentially, these methods assume there exists a function that maps the \( \mathbf{u}_i \)’s to the class labels \( C_i \)’s. However in our context, the \( \mathbf{v}_i \)’s can be independent of the \( \mathbf{u}_i \)’s, i.e., there exists no such functional relationship between the \( \mathbf{u}_i \)’s and the \( \mathbf{v}_i \)’s. In addition, the \( \mathbf{v}_i \)’s can be multivariate with both numerical or categorical values, unlike the univariate categorical class variable in supervised manifold learning. Some
supervised manifold learning methods are also for data visualization, but their visualization is mainly for separating well observations from different classes (i.e., observations from different classes generally have different \( u \) values). In contrast, in our conditional manifold learning settings, observations with the same class labels (say, corresponding to the \( v_{1} \) variable) can have similar \( u \) values, as \( u \) and \( v \) can be independent. For example, kinship terms Father and Mother are in the same generation (say, a variable \( u \)) even that they clearly have different gender classes, as shown in Figure 2 in Section 3.1.

2. Proposed Solutions for Conditional Manifold Learning

This section proposes a broad class of conditional multidimensional scaling (conditional MDS) solutions for the conditional manifold learning problem, including the conditional ISOMAP variant. An algorithm called conditional SMACOF will also be developed to optimize the objective function of conditional MDS (hereafter, condMDS). For simplicity, let denote \( \mathbf{U}^T = [u_1, u_2, ..., u_N] \in \mathbb{R}^{p \times N} \) and \( \mathbf{V}^T = [v_1, v_2, ..., v_N] \in \mathbb{R}^{q \times N} \). Let \( \Delta = \left[ \delta_{ij} \right]_{i,j=1}^{N} \) be the Euclidean distance matrix of the \( N \) observations \( \{\mathbf{y}_i: i = 1, 2, ..., N\} \). In general, \( \Delta \) can be any given dissimilarity matrix of \( N \) entities when \( \{\mathbf{y}_i: i = 1, 2, ..., N\} \) are not available. Let \( [\mathbf{U} \ \mathbf{B}] \in \mathbb{R}^{N \times (p+q)} \) be all the manifold coordinates of \( \{\mathbf{y}_i: i = 1, 2, ..., N\} \), where \( \mathbf{B} \in \mathbb{R}^{q \times q} \) is a \( q \times q \) matrix to be estimated (simultaneously with \( \mathbf{U} \)). The affine transformation \( \mathbf{VB} \) is needed to control the scales of the elements in \( \mathbf{v} \), with respect to the given dissimilarity matrix \( \Delta \). In addition, let \( d_{ij}(\mathbf{U}) = \|u_i - u_j\| \) denote the Euclidean distance between \( u_i \) and \( u_j \). Note that \( d_{ij}(\mathbf{V} \mathbf{B}) = \|\mathbf{B}^T(v_i - v_j)\| \) and \( d_{ij}(\mathbf{U}, \mathbf{B}) = \sqrt{\|u_i - u_j\|^2 + \|\mathbf{B}^T(v_i - v_j)\|^2} \).

The objective function of condMDS is the conditional stress function, defined as follows:

\[
\sigma(\mathbf{U}, \mathbf{B}) = \sum_{i<j} w_{ij} \left( \tilde{\delta}_{ij} - d_{ij}(\mathbf{U}, \mathbf{B}) \right)^2
\]

(4)

where as defined in (2), \( w_{ij} \) denotes the given weight of the pair of observations \( i \) and \( j \), and \( \tilde{\delta}_{ij} \) is some monotone transformation of \( \delta_{ij} \). The learning task of condMDS is to find:

\[
(\mathbf{U}^*, \mathbf{B}^*) = \arg\min_{\mathbf{U} \in \mathbb{R}^{N \times p}, \mathbf{B} \in \mathbb{R}^{q \times q}} \sigma(\mathbf{U}, \mathbf{B})
\]

(5)
To solve the optimization problem in (5), this paper proposes the conditional SMACOF algorithm. This algorithm is based on the SMACOF algorithm of de Leeuw (1977) for solving the optimization of the conventional MDS approach based on majorization (see Borg and Groenen (2005) for a detailed presentation of the SMACOF algorithm). Without loss of generality, an identity transformation \( \delta_{ij} = \delta_{ij} (\forall i, j) \) will be used in this paper. Then, (4) is equivalent with:

\[
\sigma(U, B) = \sum_{i<j} w_{ij} \delta_{ij}^2 + \sum_{i<j} w_{ij} d_{ij}^2(U, B) - 2 \sum_{i<j} w_{ij} \delta_{ij} d_{ij}(U, B)
\]

\[= \eta_\delta^2 + \eta^2(U, B) - 2 \rho(U, B),
\]

where \( \eta_\delta^2 = \sum_{i<j} w_{ij} \delta_{ij}^2 \) is a constant, \( \eta^2(U, B) = \sum_{i<j} w_{ij} d_{ij}^2(U, B) \), and \( \rho(U, B) = \sum_{i<j} w_{ij} \delta_{ij} d_{ij}(U, B) \).

For now we focus on the second summand \( \eta^2(U, B) = \sum_{i<j} w_{ij} d_{ij}^2(U, B) \) in the conditional stress \( \sigma(U, B) \). First, note that:

\[
d_{ij}^2(U, B) = \|u_i - u_j\|^2 + \|B^T(v_i - v_j)\|^2 = d_{ij}^2(U) + d_{ij}^2(VB)
\]

It can be shown that:

\[
\sum_{i<j} w_{ij} d_{ij}^2(U) = \text{tr}(U^T H U),
\]

where

\[
H = [h_{ij}]_{i,j=1}^N \in \mathbb{R}^{N \times N} \text{ with } h_{ij} = -w_{ij} \text{ if } i \neq j \text{ and } h_{ii} = \sum_{j=1, j \neq i}^N w_{ij}.
\]

Similarly, we can show that:

\[
\sum_{i<j} w_{ij} d_{ij}^2(VB) = \text{tr}((VB)^T H V B) = \text{tr}(B^T G B),
\]

where \( G = V^T H V \in \mathbb{R}^{q \times q} \). Thus, we have:

\[
\eta^2(U, B) = \sum_{i<j} w_{ij} d_{ij}^2(U, B)
\]

\[= \sum_{i<j} w_{ij} d_{ij}^2(U) + \sum_{i<j} w_{ij} d_{ij}^2(VB) \quad \text{(from Eq. 7)}
\]

\[= \text{tr}(U^T H U) + \text{tr}(B^T G B), \quad \text{(from Eq. 8 and Eq. 10)}
\]

which is quadratic in \( U \) and \( B \).
Now, consider the third summand \(-2\rho(U,B) = -2\sum_{i<j} w_{ij} d_{ij}(U, B)\) in the conditional stress \(\sigma(U,B)\). We will construct a majorizing function of \(-\rho(U,B)\), which is convenient for optimization. Let \(Z_u \in \mathbb{R}^{N \times p}\) and \(Z_b \in \mathbb{R}^{q \times q}\) be two matrices having the same shapes with \(U\) and \(B\), respectively. Using the Cauchy-Schwarz inequality, it can be shown that:

\[
-\rho(U,B) = -\sum_{i<j} w_{ij} \delta_{ij} d_{ij}(U, B) \\
\leq -\text{tr}([U VB]^T C(U,B)[Z_u \ VZ_b]) \\
= -\text{tr}(U^T C(U,B)Z_u) - \text{tr}(B^T V^T C(U,B)VZ_b),
\]

where \(C(U,B) = \begin{bmatrix} c_{ij} \end{bmatrix}_{i,j=1}^N\) with

\[
c_{ij} = \begin{cases} \frac{w_{ij} \delta_{ij}}{d_{ij}(U, B)} & \text{if } i \neq j \text{ and } d_{ij}(U, B) \neq 0 \\ 0 & \text{if } i \neq j \text{ and } d_{ij}(U, B) = 0 \end{cases}
\text{ and } c_{ii} = \sum_{j=1, j \neq i}^N c_{ij}.
\]

(13)

Note that \(\rho(U,B)\) is linear in \(U\) and \(B\) and the equality occurs when \(Z_u = U\) and \(Z_b = B\).

Combining (4), (11), and (12), we have:

\[
\sigma(U,B) \leq \eta_0^2 + \text{tr} U^T H U + \text{tr} B^T G B - 2\text{tr}(U^T C(U,B)Z_u) - 2\text{tr}(B^T V^T C(U,B)VZ_b) \\
= \tau(U,B,Z_u,Z_b),
\]

(14)

which is a majorizing function of the conditional stress \(\sigma(U,B)\). This function has a nice quadratic form in \(U\) and \(B\). Hence, we can minimize \(\sigma(U,B)\) via minimizing \(\tau(U,B,Z_u,Z_b)\), by setting the derivatives of \(\tau(U,B,Z_u,Z_b)\) w.r.t. \(U\) and \(B\) to zero:

\[
\begin{align*}
0 &= \frac{\partial \tau(U,B,Z_u,Z_b)}{\partial U} = 2HU - 2C(U,B)Z_u \\
0 &= \frac{\partial \tau(U,B,Z_u,Z_b)}{\partial B} = 2GB - 2V^T C(U,B)VZ_b
\end{align*}
\]

\[
\Rightarrow \begin{cases} 
HU = C(U,B)Z_u \\
GB = V^T C(U,B)VZ_b
\end{cases}
\]

(15)

As a result, the update formulas for \(U\) and \(B\) are:

\[
U = H^+ C(U,B)Z_u
\]

(16)

\[
B = G^+ V^T C(U,B)VZ_b,
\]

where \(H^+\) and \(G^+\) are the Moore-Penrose inverse of \(H\) and \(G = V^T H V\), respectively. Note that there is a simpler expression for the former case: \(H^+ = (H + 1_{N\times N})^{-1} - N^{-2} 1_{N\times N}\), where \(1_{N\times N}\) is an \(N\times N\) matrix with all elements equal 1.
Remark: If \( w_{ij} = 1 \) (\( \forall i, j = 1, 2, \ldots, N \)), then from (9) we have \( H = N(I - N^{-1}1_{N \times N}) \). Note that \( (I - N^{-1}1_{N \times N}) \) is a centering matrix, and it can be shown that \( H^+ = N^{-1} \). The update formula for \( U \) is then:

\[
U = N^{-1}C(U, B)Z_u,
\]

which the avoids having to invert an \( N \times N \) matrix as in the update formula in (15), and therefore, is more computationally efficient, especially for large \( N \) cases.

Algorithm 1 summarizes the main steps of the condMDS algorithm, based on conditional SMACOF. The required inputs include the given \( N \times N \) dissimilarity matrix \( \Delta = [\delta_{ij}]_{i,j=1}^N \) (or if \( Y \) is given, the Euclidean distance matrix of \( Y \)), the auxiliary manifold information \( V \), the weights \( w_{ij} \)'s, the min improvement of the conditional stress \( \gamma \) for each iteration, and the max number of iterations \( l_{max} \). Step 1 of the algorithm initializes and pre-compute necessary quantities for the iterations in Step 2. Note that \( B \) can be initialized by an identity matrix, and \( U \) can be initialized by random values. In Step 2, \( U \) and \( B \) are iteratively updated based on (15), until the number of iterations reaches \( l_{max} \) or the reduction of the conditional stress \( \sigma(U, B) \) from the previous iteration is not greater than \( \gamma \) anymore.

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**Algorithm 1: condMDS**

**Inputs:** \( \Delta, V, w_{ij} \)'s, \( \gamma \), and \( l_{max} \).

**Step 1:**
- a) Initialize \( U[0] \) and \( B[0] \)
- b) Compute \( H^+ \) and \( \bar{G}^+ = G^+VT \)
- c) Compute \( \sigma[0] = \sigma(0)(U[0], B[0]) \)
- d) Set \( \sigma[-1] = \infty \) and \( l = 0 \)

**Step 2:** While \( (l < l_{max}) \) or \( (\sigma[l-1] - \sigma[l] > \gamma) \) do:
- a) \( l = l + 1 \)
- b) Compute transformations
  \[
  U[l] = H^+C(U[l-1], B[l-1])U[l-1] \\
  B[l] = \bar{G}^+C(U[l-1], B[l-1])VB[l-1]
  \]
- c) Compute the conditional stress
  \[
  \sigma[l] = \sigma(U[l], B[l])
  \]

**Outputs:** \( U[l] \) and \( B[l] \)
Remark: When \( q \) is large, we can speed up condMDS by imposing a diagonal structure for \( \mathbf{B} = \text{diag}(\mathbf{b}) \), where \( \mathbf{b} = [b_1, b_2, ..., b_q]^T \in \mathbb{R}^q \). Then, (11) reduces to

\[
\eta^2(\mathbf{U}, \mathbf{B}) = \text{tr}(\mathbf{U}^T \mathbf{H} \mathbf{U}) + \text{tr}(\mathbf{B}^T \mathbf{G} \mathbf{B}) = \text{tr}(\mathbf{U}^T \mathbf{H} \mathbf{U}) + \sum_l b_l^2 g_{ll}.
\] (18)

In addition, let \( \mathbf{T}(\mathbf{U}, \mathbf{B}) = [t_1 \ t_2 \ ... \ t_q] = \mathbf{V}^T \mathbf{C}(\mathbf{U}, \mathbf{B}) \mathbf{V} \), then

\[
\text{tr}(\mathbf{B} \mathbf{V}^T \mathbf{C}(\mathbf{U}, \mathbf{B}) \mathbf{V} \mathbf{Z}_b) = \text{tr}(\mathbf{B} \mathbf{T}(\mathbf{U}, \mathbf{B}) \mathbf{Z}_b) = \sum_l b_l t_{ll} z_{bl}.
\] (19)

Plugging (18) and (19) into (14), the conditional stress is

\[
\tau(\mathbf{U}, \mathbf{b}, \mathbf{Z}_w, \mathbf{Z}_b) = \eta^2 + \text{tr}(\mathbf{U}^T \mathbf{H} \mathbf{U}) + \sum_l b_l^2 g_{ll} - 2\text{tr}(\mathbf{U}^T \mathbf{C}(\mathbf{U}, \mathbf{B}) \mathbf{Z}_u) - 2 \sum_l b_l t_{ll} z_{bl}.
\] (20)

Setting \( \frac{\partial \tau(\mathbf{U}, \mathbf{b}, \mathbf{Z}_w, \mathbf{Z}_b)}{\partial \mathbf{b}} = \mathbf{0} \), we obtain

\[
2[b_1 g_{11} \ b_2 g_{22} \ ... \ b_q g_{qq}]^T - 2[t_{11} z_{b1} \ t_{22} z_{b2} \ ... \ t_{qq} z_{bq}]^T = \mathbf{0}.
\]

As a result, the update formula for \( \mathbf{b} \) is:

\[
b_i = \frac{t_{ii}}{g_{ii}} z_{bi} \ (i = 1, 2, ..., q).
\] (21)

A conditional ISOMAP (condISOMAP) extension of condMDS can be derived in the same manner as ISOMAP extended classical multidimensional scaling. Algorithm 2 summarizes the steps of condISOMAP. The required inputs are the same as in Algorithm 1 and an extra neighborhood parameter (either \( k \) nearest neighbors or \( \epsilon \)-radius hypersphere). In Step 1, an weighted neighborhood graph \( \mathcal{G} \) is constructed from the given \( N \times N \) dissimilarity matrix \( \Delta = [\delta_{ij}]_{i,j=1}^N \) and the neighborhood parameter \( k \) or \( \epsilon \). This graph has \( N \) nodes, and the weight of the edge between a node \( i \) and a node \( j \) is \( \delta_{ij} \). Step 2 computes a graph distance matrix \( \Delta^g = [\delta_{ij}^g]_{i,j=1}^N \), where \( \delta_{ij}^g \) is the shortest path distance between a point \( i \) and a point \( j \) on \( \mathcal{G} \). Note that \( \Delta^g \) is an estimate of the geodesic distance between all pairs of points on the manifold. Step 3 calls the conditional SMACOF algorithm to find an optimal embedding \( \mathbf{U}^* \) for the graph distance matrix \( \Delta^g \) obtained in Step 2.
Algorithm 2: CondISOMAP

**Inputs:** $k$ (or $\varepsilon$), $\Delta$, $V$, $w_{ij}$’s, $\gamma$, and $l_{\text{max}}$.

**Step 1:** Construct an weighted neighborhood graph $G$.

**Step 2:** Compute a graph distance matrix $\Delta^g = [\delta^g_{ij}]_{i,j=1}^N$.

**Step 3:** Find $(U^*, B^*) = \text{condMDS}(\Delta^g, V, w_{ij}$’s, $\gamma, k_{\text{max}})$.

**Outputs:** $U^*$ and $B^*$

3. Kinship Terms Example

In this section, the proposed conditional manifold learning methods are illustrated with a kinship terms example. The kinship terms dataset (Rosenberg and Kim, 1975) contains percentages of college students in a study who did not group together 15 kinship terms (14 of which are listed in Table 1, and the other is “Cousin”). The percentages (shown in Table 2) can be regarded as pairwise dissimilarities between the kinship terms. It is not difficult to conjecture that “Gender” and “Kinship Degree” (the values of which are defined in Table 1) contribute to these pairwise dissimilarities. In other words, they could be used as the auxiliary manifold information.

For the sake of illustration, the term “Cousin” will be excluded in this example because “Gender” is not defined for this term.

Table 1. Fourteen kinship terms with auxiliary “Gender” and “Kinship Degree” information.

| Kinship terms   | Gender | Kinship Degree |       | Kinship terms   | Gender | Kinship Degree |
|----------------|--------|----------------|-------|----------------|--------|----------------|
| Aunt           | 2      | 3              |       | Grandson       | 1      | 2              |
| Brother        | 1      | 2              |       | Mother         | 2      | 1              |
| Daughter       | 2      | 1              |       | Nephew         | 1      | 3              |
| Father         | 1      | 1              |       | Niece          | 2      | 3              |
| Granddaughter  | 2      | 2              |       | Sister         | 2      | 2              |
| Grandfather    | 1      | 2              |       | Son            | 1      | 1              |
| Grandmother    | 2      | 2              |       | Uncle          | 1      | 3              |

Figure 1 plots two embedding coordinates of the 14 kinship terms in Table 1 from MDS, using the smacof R package of (Leeuw and Mair, 2009) and $w_{ij} = 1(\forall i,j)$. Up to some rotation, one MDS embedding dimension apparently corresponds to Gender. While this is correct, we lose an
embedding dimension for this finding, which can be expected (or was already discovered from a previous analysis). Hence, it is helpful to marginalize out Gender from the embedding result, which is the motivation for conditional manifold learning. Besides, the interpretation for the other embedding dimension in Figure 1 is not obvious.

Table 2. Percentages of college students who did not group together the kinship terms in Table 1.

|     | Aunt | Brother | Daughter | Father | Granddaughter | Grandfather | Grandmother | Grandson | Mother | Nephew | Niece | Sister | Son | Uncle |
|-----|------|---------|----------|--------|---------------|-------------|-------------|----------|--------|--------|-------|-------|-----|-------|
| Aunt | 0    | 79      | 59       | 73     | 57            | 77          | 55          | 79       | 51     | 56     | 32    | 58    | 80  | 27   |
| Brother | 79  | 0       | 62       | 38     | 75            | 57          | 80          | 51       | 63     | 53     | 76    | 28    | 38  | 57   |
| Daughter | 59  | 62      | 0        | 57     | 46            | 77          | 54          | 72       | 31     | 74     | 52    | 37    | 29  | 80   |
| Father | 73   | 38      | 57       | 0      | 79            | 51          | 70          | 54       | 29     | 59     | 81    | 63    | 32  | 51   |
| Granddaughter | 57  | 75     | 46       | 79     | 0             | 57          | 32          | 29       | 56     | 74     | 51    | 50    | 72  | 80   |
| Grandfather | 77  | 57     | 77       | 51     | 57            | 0           | 29          | 31       | 75     | 58     | 79    | 79    | 55  | 55   |
| Grandmother | 55  | 80     | 54       | 70     | 32            | 29          | 0           | 57       | 50     | 79     | 58    | 57    | 78  | 77   |
| Grandson | 79   | 51     | 72       | 54     | 29            | 31          | 57          | 0        | 79     | 51     | 74    | 75   | 47  | 58   |
| Mother | 51   | 63     | 31       | 29     | 56            | 75          | 50          | 79       | 0      | 81     | 60    | 39    | 57  | 73   |
| Nephew | 56   | 53     | 74       | 59     | 74            | 58          | 79          | 51       | 81     | 0      | 27    | 76   | 52  | 33   |
| Niece | 32   | 76     | 52       | 81     | 51            | 79          | 58          | 74       | 60     | 27     | 0     | 53   | 74  | 56   |
| Sister | 58   | 28     | 37       | 63     | 50            | 79          | 57          | 75       | 39     | 76     | 53    | 0     | 62  | 79   |
| Son | 80   | 38     | 29       | 32     | 72            | 55          | 78          | 47       | 57     | 52     | 74    | 62   | 0   | 59   |
| Uncle | 27   | 57     | 80       | 51     | 80            | 55          | 77          | 58       | 73     | 33     | 56    | 79   | 59  | 0    |

Figure 2 shows a similar plot to Figure 1, but for the embedding result of condMDS, conditioning on Gender with $w_{ij} = 1(\forall i, j)$. Interestingly, we can see in Figure 2 seven pairs of highly similar kinship terms: Sister/Brother (i.e., Sibling), Mother/Father (i.e., Parent), Daughter/Son (i.e., Child), Grandmother/Grandfather (i.e., Grandparent), Granddaughter/Grandson (i.e., Grandchild), Niece/Nephew (i.e., Nibling), and Aunt/Uncle (i.e., Pibling). With Gender marginalized out, it can be seen more clearly that the direction from the top right corner to the bottom left corner of Figure 2 seems to correspond to Kinship Degree (defined in Table 1).
Figure 1. 2D embedding plot of conventional MDS, using $w_{ij} = 1 (\forall i, j)$.

Figure 2. 2D embedding plot of condMDS, conditioning on Gender, with $w_{ij} = 1 (\forall i, j)$. 
Let us now use condMDS, conditioning on both Gender and Kinship Degree, to marginalize them out of the embedding result. The weights \( w_{ij} \)'s remain \( w_{ij} = 1(\forall i, j) \). The 2D embedding result in this case is shown in Figure 3. Same as in Figure 2, we also see seven pairs of gender-neutral kinship terms. Unlike Figure 2 however, the pairs Pibling and Nibling (which have the largest Kinship Degree level) are now mixed with the pairs Parent, Child (which have the smallest Kinship Degree level) in Figure 3. After both Gender and Kinship Degree are marginalized out, the horizontal axis of the embedding in Figure 3 looks corresponding to the generation differences implied by the kinship terms. Specifically, from left to right of Figure 3, the pair Sibling implies a generation difference of 0; the pairs Nibling, Child, Parent, or Pibling imply a generation difference of 1; and the pairs Grandchild or Grandparent imply a generation difference of 2. Note that this finding is not inferable from the embedding of the conventional MDS method shown in Figure 1. This demonstrates the benefit of conditional manifold learning for marginalizing out known manifold parameters to reveal other unknown or unanticipated manifold parameters.

![Figure 3. 2D embedding plot of condMDS, conditioning on Gender and Kinship Degree, with \( w_{ij} = 1(\forall i, j) \).](image)
We can continue this process, and add the newly discovered manifold parameter “Generation Difference” to the conditioning list for condMDS. Figure 4 shows the 2D embedding result of condMDS, conditioning on Gender, Kinship Degree, and Generation Difference, and $w_{ij} = 1(\forall i, j)$. We can see that the direction from the upper right to the lower left of Figure 4 corresponds to a transition from older generations (Grandparent, Parent, and Pibling), to same generation (Sibling), to younger generations (Child, Nibling, and Grandchild). This observation is totally hidden from the embedding result of conventional MDS in Figure 1. In fact, Grandparent and Grandchild are very close in Figure 1, due to their small dissimilarities in the data in comparison with other kinship terms. Because condMDS take into account the effect of Generation Difference in the dissimilarities, it can separate Grandparent and Grandchild to reveal the generation transition in Figure 4. This again shows the benefit of conditional manifold learning.

Figure 4. 2D embedding plot of condMDS, conditioning on Gender, Kinship Degree, and Generation Difference, with $w_{ij} = 1(\forall i, j)$. 
If we define a Generation variable with values of -2 for Grandparent, -1 for Parent and Pibling, 0 for Sibling, 1 for Child and Nibling, and 2 for Grandchild, then Generation Difference is the absolute value (and thus not a linear function) of Generation. Hence, we theoretically can discover Generation alone, using a nonlinear conditional manifold learning approach. To verify this, condMDS conditioning on Gender and Kinship Degree is tried again, but with Sammon map weights $w_{ij} = \left( \delta_{ij} \sum_{i<j} \delta_{ij} \right)^{-1} (\forall i, j)$ to focus on local behavior of the dissimilarities. Figure 5 shows the 2D embedding result of this analysis. We can see now a generation transition along the curved arrow in Figure 5. This result suggests that the kinship terms approximately lie on a 1D circle corresponding to Generation. The Sammon map weights seem to be able to preserve the local dissimilarities, and avoid collapsing the circular manifold as in Figure 3 when the weights $w_{ij} = 1 (\forall i, j)$ are used. Ideally, one would like to learn a 1D embedding for Generation, but unfolding a circle is no easy task for any manifold learning algorithm.

Figure 5. 2D embedding plot of condMDS, conditioning on Gender and Kinship Degree, with Sammon map weights $w_{ij} = 1/(\delta_{ij} \sum_{i<j} \delta_{ij}) (\forall i, j)$. The curved arrow indicates a generation transition of the kinship terms.
Let us now switch to condISOMAP, conditioning on Gender and Kinship Degree. Figures 6 and 7 show the 2D embedding results when using the weights $w_{ij} = 1$ ($\forall i,j$) and the Sammon map weights, respectively, and for different neighborhood size input $k$ in {3, 4, 5, 6}. For both types of weighting schemes, the embedding results vary with different value of $k$, which is a well known behavior of ISOMAP. When using $w_{ij} = 1$ ($\forall i,j$), condISOMAP puts most of the terms (except for Sibling) in the correct Generation (circular) order for $k = 5$ and 6, but not for $k = 3$ and 4 (see Figure 6). When using the Sammon map weights, condISOMAP orders all the terms correctly, except for the case of $k = 3$. In comparison with the result of condMDS in Figure 5, the kinship terms look more well spread in the results of condISOMAP.

![Figure 6. 2D embedding plots of condISOMAP, conditioning on Gender and Kinship Degree, with $w_{ij} = 1$ ($\forall i,j$) and different neighborhood size input $k$.](image-url)
Figure 7. 2D embedding plots of condISOMAP, conditioning on Gender and Kinship Degree, with Sammon map weights $w_{ij} = 1/(\delta_{ij} \sum_{i<j} \delta_{ij})$ (\forall i,j) and different neighborhood size input $k$.

4. Conclusions

Conditional manifold learning seeks for a low-dimensional manifold embedding of high-dimensional data, conditioning on auxiliary manifold information. This problem is ubiquitous in science and engineering, as the auxiliary manifold information can be often obtained from controllable or measurable conditions. This paper proposes a broad class of conditional MDS algorithms (including conditional ISOMAP) to solve this problem. A conditional SMACOF algorithm is presented to minimize the conditional stress function. These approaches are illustrated with the kinship terms example, which shows the benefit of conditional manifold learning for marginalizing out the known manifold parameters to uncover unknown manifold parameters.
References
Belkin, M., Niyogi, P., 2001. Laplacian eigenmaps and spectral techniques for embedding and clustering, in: Proceedings of the 14th International Conference on Neural Information Processing Systems: Natural and Synthetic. MIT Press, Cambridge.
Borg, I., Groenen, P.J.F., 2005. Modern Multidimensional Scaling: Theory and Applications, 2nd edition. Springer, New York.
Chao, G., Luo, Y., Ding, W., 2019. Recent Advances in Supervised Dimension Reduction: A Survey. Machine Learning and Knowledge Extraction 1, 341–358.
de Leeuw, J., 1977. Applications of convex analysis to multidimensional scaling. In: Barra, J.R., Brodeau, F., Romier, G., van Cutsen, B. (eds) Recent Developments in Statistics. North Holland, Amsterdam.
de Leeuw, J., Mair, P., 2009. Multidimensional Scaling Using Majorization: SMACOF in R. Journal of Statistical Software 31, 1–30.
Demartines, P., Herault, J., 1997. Curvilinear component analysis: a self-organizing neural network for nonlinear mapping of data sets. IEEE Transactions on Neural Networks 8, 148–154.
Donoho, D.L., Grimes, C., 2003. Hessian eigenmaps: Locally linear embedding techniques for high-dimensional data. PNAS 100, 5591–5596.
McInnes, L., Healy, J., Saul, N., and Großberger, L. 2018. UMAP: Uniform Manifold Approximation and Projection. Journal of Open Source Software 3, 861.
Rosenberg, S., and Kim, M. P. 1975. The method of sorting as a data gathering procedure in multivariate research. Multivariate Behavioral Research 10, 489–502.
Roweis, S.T., Saul, L.K., 2000. Nonlinear Dimensionality Reduction by Locally Linear Embedding. Science 290, 2323–2326.
Sammon, J.W., 1969. A Nonlinear Mapping for Data Structure Analysis. IEEE Transactions on Computers C–18, 401–409.
Tenenbaum, J.B., de Silva, V., Langford, J.C., 2000. A Global Geometric Framework for Nonlinear Dimensionality Reduction. Science 290, 2319–2323.
Torgerson, W.S., 1952. Multidimensional scaling: I. Theory and method. Psychometrika 17, 401–419.
vander Maaten, L., Hinton, G., 2008. Visualizing Data using t-SNE. Journal of Machine Learning Research 9, 2579–2605.