Combining Disparate Information by Nonmetric Multidimensional Scaling

Brent Castle
Indiana University

This is joint work with Michael Trosset (IU) and in collaboration with Carey E. Priebe, Youngser Park, and others (JHU).

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Disparate Information Fusion (DIF) is the combination of data of heterogeneous type and/or structure, e.g., text and images.

In text mining, image analysis, and many other disciplines, the ambient feature spaces are complicated and high-dimensional. Domain experts have developed specialized measures of (dis)similarity, e.g., for retrieval.

We assume that we have $n$ objects and pairwise dissimilarities for each data type. Our goal is to construct a common representation of the $n$ objects to be used for subsequent analysis. Our present concern is with classification.
Product Embedding Approach

Given: \( n \) objects and \( k \) \( n \times n \) pairwise dissimilarity matrices \( \Delta_1, \Delta_2, \ldots, \Delta_k \)

Goal: construct a Euclidean representation of the objects

\[
\begin{align*}
\Delta_1 & \rightarrow X_1 \\
\vdots & \vdots \quad X_* \\
\Delta_k & \rightarrow X_k
\end{align*}
\]

1. Construct a representation, \( X_i \), for each of the \( k \) disparate measures.
2. Form the product, \( X_* = [X_1|\ldots|X_k] \).
3. Apply standard multivariate methods for dimension reduction, classification, etc.
Multidimensional Scaling

Metric multidimensional scaling are techniques for embedding points in Euclidean space such that $d_{ij} \approx \delta_{ij}$.

- Uses actual values of the observed dissimilarities
- Scale equivariant

Nonmetric multidimensional scaling are techniques for embedding points in Euclidean space such that the interpoint distances are monotonically related to the dissimilarities.

- Uses only the rank order of the observed dissimilarities
- Scale invariant
Kruskal (1964) formulated nonmetric multidimensional scaling to minimize the normalized stress criterion:

$$\sigma_n(X) = \sqrt{\frac{\sum_{i<j}(\hat{d}_{ij} - d_{ij}(X))^2}{\sum_{i<j}d_{ij}^2(X)}}$$

where $d_{ij}$ is the distance between objects $i$ and $j$ and $\hat{d}_{ij}$ is the monotone regression of $d_{ij}(X)$ on the ranks of the observed dissimilarities.

Normalizing ensures scale invariance and precludes degenerate solutions.

Kruskal proposed minimizing $\sigma_n$ by a gradient method.
Our Formulation

Our approach to nonmetric MDS is unconventional, motivated by a desire to embed large data sets.

We are less concerned with precise global minimizers than with plausible embeddings of large data sets. For each $\Delta_r$, we seek small values of

$$\sigma(\Delta, X) = \sum_{i<j}[\delta_{ij} - d_{ij}(X)]^2$$

subject to

$(1)$ $\Delta \in M(\Delta_r)$ [monotonicity constraint]

$(2)$ $\sum_{i<j} \delta_{ij}^2 \geq \sum_{\ell=1}^{n(n-1)/2} \ell^2$ [nondegeneracy constraint]

Trosset (1998) proposed (2) as an alternative to normalization.
Our Algorithm

1. Construct an inexpensive initial embedding using the method of standards. We embed $d + 1$ anchor points by Classical MDS, then position each remaining point by solving a $d \times d$ linear system.

2. Decrease $\sigma$ by several cycles of the following variable alternation scheme:
   
   a. Fix $\Delta$ and modify $X$ by several iterations of a fixed point method, e.g., Guttman majorization or diagonal majorization (Trosset and Groenen 2005).
   
   b. Fix $X$ and modify $\Delta$ by projecting $D(X)$ into the closed and convex set of feasible $\Delta$. This is accomplished by projecting $D(X)$ into $M(\Delta_r)$ by isotonic regression (Grotzinger & Witzgall 1984), followed by rescaling the projected $D(X)$ to satisfy the nondegeneracy constraint (Lemma 2, Trosset 1998).
Two Classification Examples

Example 1: Classify images as one of four classes using two measures

Example 2: Classify yeast genes with functional labels given five measures

For each example we:

1. Construct a Euclidean representation as the product of the separate embeddings constructed by nonmetric MDS.

2. Perform linear discriminant analysis in product representation (or a subspace). Subspaces identified by various methods, e.g., variable selection (McHenry 1978), discriminant coordinates, etc.
Example 1 - Tiger Images

Given \( n = 1520 \) images that contain the word “tiger” in their caption.

The images range in size from \( 186 \times 245 \) pixels to \( 406 \times 450 \) pixels. Each pixel is represented as a vector of RGB values.

Each object is labeled by the following:

- animal 148
- golf 897
- baseball 145
- rebel 330
Example 1 - Color

1. Transform each image from RGB space to CIE L*a*b* space.  

2. For each image, compute pixel representatives $m_1, \ldots, m_8$ by a fast algorithm for $k$-means clustering. An image’s color signature is the discrete measure that weights each $m_i$ by the proportion of pixels associated with $m_i$.

3. Use $\|m_i - m_j\|_2$ to compute the earth mover’s distance between pairs of color signatures.  

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Example 1 - Texture


1. Convolve each image with 24 Gabor filters (6 orientations \(\times\) 4 scales), each with a fixed size of 13 \(\times\) 13 pixels. This procedure associates a vector of 24 features with each pixel.

2. For each image, compute pixel representatives \(m_1, \ldots, m_8\) by \(k\)-means clustering the pixel feature vectors. An image’s texture signature is the discrete probability measure that weights each \(m_i\) by the proportion of pixels associated with \(m_i\).

3. Use \(\|m_i - m_j\|_1\) to compute the earth mover’s distance between pairs of texture signatures.
Example 1 - Product Embedding

\[ \Delta_{color} \rightarrow X_{color} \]

\[ \Delta_{texture} \rightarrow X_{texture} \]
Example 1 - Results

5-fold cross validated error rate

# of variables selected for discrimination

Chance
Texture
Color
Color & Texture

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Example 2 - Yeast gene function

Given \( n = 3588 \) yeast genes, each with 13 binary labels:

<table>
<thead>
<tr>
<th>Function</th>
<th>Count</th>
<th>Function</th>
<th>Count</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metabolism</td>
<td>1048</td>
<td>Cell Rescue, Defense &amp; Virulence</td>
<td>264</td>
</tr>
<tr>
<td>Energy</td>
<td>242</td>
<td>Interaction w/ cell. env.</td>
<td>193</td>
</tr>
<tr>
<td>Cell Cycle &amp; DNA proc.</td>
<td>600</td>
<td>Cell Fate</td>
<td>411</td>
</tr>
<tr>
<td>Transcription</td>
<td>753</td>
<td>Control of cellular organization</td>
<td>192</td>
</tr>
<tr>
<td>Protein Synthesis</td>
<td>335</td>
<td>Transport Facilitation</td>
<td>306</td>
</tr>
<tr>
<td>Protein Fate</td>
<td>578</td>
<td>Others</td>
<td>81</td>
</tr>
<tr>
<td>Cellular Transportation</td>
<td>479</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Five measures were taken between each pair of genes:

1. Inner product of binary vectors (presence of Pfam domains) (Pfam)
2. Distance in a graph of genetic interaction information (GI)
3. Distance in a graph of protein-protein interaction information (PPI)
4. Distance in a graph of co-participation in a protein complex (TAP)
5. Dissimilarity measure between expression profiles (Exp)

Deng (2003) used a Markov Random Field to fuse the five measures and predict gene function. Lanckriet et al. (2004) formed an optimal linear combination of the five measures in a kernel representation.
Example 2 - Product Embedding

\[ \Delta_{Pfam} \rightarrow X_{Pfam} \]

\[ \vdots \]

\[ \Delta_{Exp} \rightarrow X_{Exp} \]
Example 2 - Results

Following the methods in Deng (2003) and Lanckriet (2004) we present the results as the area under the receiver operating characteristic (ROC) curve (AUC).

The ROC curve is a plot of the true positive rate (sensitivity) vs. the false positive rate (1-specificity) for various discrimination thresholds. The AUC statistic is a means of summarizing the curve in a single number.
Example 2 - Results

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Summary

- Motivated the use of nonmetric MDS in the product embedding
- Formulated a scalable implementation of nonmetric MDS
- Results from image classification and gene function classification show the technique works on complex data
Thank you!