Solving Large Scale Non-metric Multidimensional Scaling Problems Using ADMM Optimization

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INTRODUCTION + OBJECTIVE

The goal of this research project is to use an algorithm based on the alternating direction method of multipliers (ADMM), to solve large-scale non-metric multidimensional scaling (NMDS) problems with randomly generated datasets and more interesting and real-world datasets such as the Swiss roll, S curve, and related images. Our hypothesis is that the calculated Gram matrix will preserve the ordering of the original distances between points in our initial dataset.

PRINCIPLES

NMDS: attempts to preserve the original distances between inputs in a dataset.
ADMM: a method for large-scale optimization which performs alternating optimizations over two vector variables x and y.
Convex optimization: A convex objective function is subject to inequality constraints that are summarized by a slack variable that we seek to minimize.

Figures: S curve and Swiss roll.

Source: https://www.semanticscholar.org/paper/Nonlinear-Manifold-Learning-6-.-454-Summary-Ihler/62bc7f7507f8f3e7c9c4ac62215d31b06e45da98/figure/0

MATERIALS

Python: Optimization package cvxpy
Matlab: Optimization package CVX
Datasets: Random datasets of size 50, Swiss roll dataset, S curve dataset, images

METHODS

1. Generate datasets with random data points, Swiss roll, S curve, images.
2. Code optimization problem along with ADMM solution into Python and then into Matlab.
3. Analyze results in Python and Matlab.
4. Make necessary adjustments to code and repeat.

$$
\begin{array}{ll}
\min\limits_{K,\xi_{ijkl}} & \sum\limits_{(i,j,k,l)\in\mathcal{S}} \xi_{ijkl} + \lambda\,\mathrm{Trace}(K) \\
\text{subject to} & k_{kk} - 2k_{kl} + k_{ll} - k_{ii} + 2k_{ij} - k_{jj} \geq 1 - \xi_{ijkl} \\
& \sum\limits_{ab} k_{ab} = 0, \quad K \succeq 0. \qquad\qquad (\text{GNMDS})
\end{array}
$$

This is the optimization problem with inequality constraints represented as linear equations of Gram matrix K which define a unique K which can solve the problem and have specifications that disallow translations, rotations, and scalings of K.
Source: Agarwal et al.

$$
\begin{array}{ll}
\text{minimize} & \sum\limits_{k=1}^{m} \max\{0, u_k\} + \lambda \mathbf{1}^T x + g(x) + h(y) \\
\text{subject to} & \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} x \\ u \end{bmatrix} + \begin{bmatrix} -I \\ -A \end{bmatrix} y = \begin{bmatrix} 0 \\ \mathbf{1} \end{bmatrix}.
\end{array}
$$

This is the optimization problem in an ADMM-ready form, which consists of first optimization over x and u, then optimization over y, and lastly the dual update. Source: Boyd et al.

RESULTS

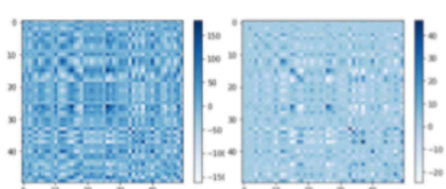
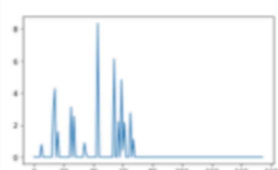


Figure: Shows the original Gram matrix calculated from the original distances matrix (left) and the calculated Gram matrix obtained by solving the non-metric multidimensional scaling problem (right).

Figure: Shows the values of the slack variable (error); ordering of distances is overall preserved.



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