# Error Metrics for Learning Reliable Manifolds from Streaming Data

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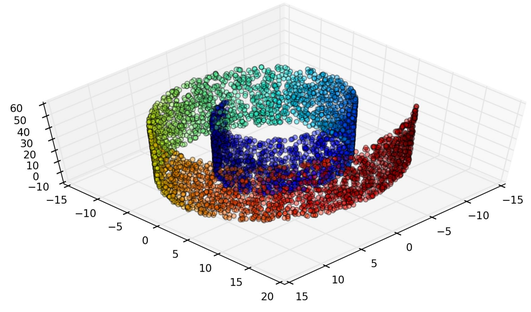
## Motivation

- Progress in science and engineering depends more than ever on our ability to analyze huge amounts of data.
- Huge amounts of data is coming from high-performance high-fidelity numerical simulations, high-resolution scientific instruments or Internet of Things feeds.
- Real-world data is typically a result of complex non-linear processes, but can often times be described by a low-dimensional manifold.
- Manifold learning has numerous applications in scientific computing and bio-medical research, including fMRI analysis, clustering of oncology data, gene profiling, and many others.
- Isomap is a common method for manifold learning that has been widely-adopted in many application areas.

## Challenges

- Widely used manifold learning methods have been designed for off-line or batch processing.
- Standard methods are computationally expensive or impractical to apply to high-throughput data streams.
- Error in manifold learning is not yet completely understood, making error measurement on streaming data all the more complex.
- Until now, applying Isomap to data streams and understanding the collective error has not been well studied.



## Proposed Approach

- We formalize a notion of *collective error* in Isomap and describe strategies to quantify it using Procrustes Analysis.
- We assume that there exists a function $f\colon \mathbb{R}^d \rightarrow \mathbb{R}^D$ which maps $\boldsymbol{y_i} \in \mathbb{R}^d$ to $\boldsymbol{x_i} \in \mathbb{R}^D$. The goal of Isomap is to learn the inverse mapping, $f^{-1}(\cdot)$ that can be used to map high-dimensional $\boldsymbol{x_i}$ to low-dimensional $\boldsymbol{y_i}$ i.e. $\boldsymbol{y_i} = f^{-1}(\boldsymbol{x_i})$.
- Let $Y$ denote the data matrix containing the true low-dimensional mapping for the samples in $X$, i.e. $Y = [\boldsymbol{y_1}, \boldsymbol{y_2}, \cdots, \boldsymbol{y_n}]^T$ and $\hat{Y}$ denote the matrix with the approximate mapping, i.e. $\hat{Y} = \left[\hat{f}^{-1}(\boldsymbol{x_1}), \hat{f}^{-1}(\boldsymbol{x_2}), \cdots, \hat{f}^{-1}(\boldsymbol{x_n})\right]^T$.
- We then use Procrustes error to measure the difference between the true low-dimensional samples and the approximate samples.

$$\epsilon = d_{Proc}(Y, \hat{Y}) = \min_{R,t,s} \left\| sR\hat{Y} + t - Y \right\|_F$$

- We propose a new efficient algorithm call *Streaming Isomap (S-Isomap)* to incorporate streamed data into a stable Isomap manifold.

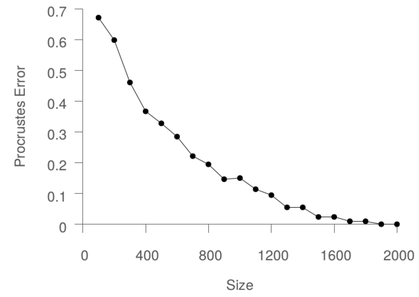
**Algorithm 1** STREAMING ISOMAP (S-ISOMAP)

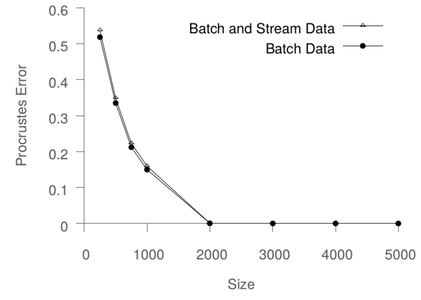
**Input:** $G_b$, $X_b$, $\mathbf{x}_s$, $k$
**Output:** $\mathbf{y_s}$

1: $\mathbf{kNN}, \mathbf{kDist} \leftarrow \mathrm{KNN}(\mathbf{x_s}, X_b, k)$ //Determine kNN
2:
3: **for** $1 \leq i \leq n$ **do**
4: $\quad g_i \leftarrow \min_{1 \leq j \leq k} \{\mathbf{kDist}_j + (G_b)_{kNN_j, i}\}$
5:
6: $\mathbf{g}_i^2 \leftarrow \mathbf{g_i}^2$
7: $\mathbf{G}_{ij}^2 \leftarrow \mathbf{G_{ij}}^2$
8:
9: $\mathbf{c} \leftarrow \frac{1}{2}(\bar{\mathbf{g}}^{\mathbf{2}} \cdot \mathbf{1}_n - \mathbf{g}^2 - \bar{\bar{G}} \cdot \mathbf{1}_n + \bar{\mathbf{G}})$
10: $\mathbf{p} \leftarrow (Y_b^\top Y_b)^{-1} Y_b^\top \mathbf{c}$ //least squares estimate
11: $\hat{Y} \leftarrow [Y_b; \mathbf{p}]$
12: $\mathbf{y}_s \leftarrow \mathbf{p} - \hat{Y}$
13: **return** $\mathbf{y}_s$

## Experiments

- We investigate the behavior of error in Isomap when applied to the Swiss Roll dataset, where we have low-dimensional ground truth available for comparison.
- A Reference-Sample method, for use where ground truth is not available, is shown to have similar behavior, making it a reliable method for error measurement on real-world data.
- Using these strategies to quantify error, we identify a **transition point** where a reliable manifold has been learned, and we can switch to our lightweight algorithm, S-Isomap.




## Reference

- F. Schoeneman, S. Mahapatra, V. Chandola, N. Napp, and J. Zola. Error Metrics for Learning Reliable Manifolds from Streaming Data. Under review for *SIAM International Conference on Data Mining*, 2017.