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Science 290, 2323 (2000);
DOI: 10.1126/science.290.5500.2323

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Nonlinear Dimensionality Reduction by Locally Linear Embedding
Sam T. Roweis¹ and Lawrence K. Saul²

Many areas of science depend on exploratory data analysis and visualization. The need to analyze large amounts of multivariate data raises the fundamental problem of dimensionality reduction: how to discover compact representations of high-dimensional data. Here, we introduce locally linear embedding (LLE), an unsupervised learning algorithm that computes low-dimensional, neighborhood-preserving embeddings of high-dimensional inputs. Unlike clustering methods for local dimensionality reduction, LLE maps its inputs into a single global coordinate system of lower dimensionality, and its optimizations do not involve local minima. By exploiting the local symmetries of linear reconstructions, LLE is able to learn the global structure of nonlinear manifolds, such as those generated by images of faces or documents of text.

How do we judge similarity? Our mental representations of the world are formed by processing large numbers of sensory inputs—including, for example, the pixel intensities of images, the power spectra of sounds, and the joint angles of articulated bodies. While complex stimuli of this form can be represented by points in a high-dimensional vector space, they typically have a much more compact description. Coherent structure in the world leads to strong correlations between inputs (such as between neighboring pixels in images), generating observations that lie on or close to a smooth low-dimensional manifold. To compare and classify such observations—in effect, to reason about the world—depends crucially on modeling the nonlinear geometry of these low-dimensional manifolds.

Scientists interested in exploratory analysis or visualization of multivariate data (1) face a similar problem in dimensionality reduction. The problem, as illustrated in Fig. 1, involves mapping high-dimensional inputs into a low-dimensional "description" space with as many coordinates as observed modes of variability. Previous approaches to this problem, based on multidimensional scaling (MDS) (2), have computed embeddings that attempt to preserve pairwise distances [or generalized disparities (3)] between data points; these distances are measured along straight lines or, in more sophisticated usages of MDS such as Isomap (4), along shortest paths confined to the manifold of observed inputs. Here, we take a different approach, called locally linear embedding (LLE), that eliminates the need to estimate pairwise distances between widely separated data points. Unlike previous methods, LLE recovers global nonlinear structure from locally linear fits.

The LLE algorithm, summarized in Fig. 2, is based on simple geometric intuitions. Suppose the data consist of N real-valued vectors \( \mathbf{x}_i \), each of dimensionality \( D \), sampled from some underlying manifold. Provided there is sufficient data (such that the manifold is well-sampled), we expect each data point and its neighbors to lie on or close to a locally linear patch of the manifold. We characterize the local geometry of these patches by linear coefficients that reconstruct each data point from its neighbors. Reconstruction errors are measured by the cost function

\[
\epsilon(W) = \sum_i \left( \mathbf{x}_i - \sum_j W_{ij} \mathbf{x}_j \right)^2
\]

which adds up the squared distances between all the data points and their reconstructions. The weights \( W_{ij} \) summarize the contribution of the \( i \)th data point to the \( j \)th reconstruction. To compute the weights \( W_{ij} \), we minimize the cost

![Fig. 1. The problem of nonlinear dimensionality reduction, as illustrated (10) for three-dimensional data (B) sampled from a two-dimensional manifold (A). An unsupervised learning algorithm must discover the global internal coordinates of the manifold without signals that explicitly indicate how the data should be embedded in two dimensions. The color coding illustrates the neighborhood-preserving mapping discovered by LLE; black outlines in (B) and (C) show the neighborhood of a single point. Unlike LLE, projections of the data by principal component analysis (PCA) (28) or classical MDS (2) map faraway data points to nearby points in the plane, failing to identify the underlying structure of the manifold. Note that mixture models for local dimensionality reduction (29), which cluster the data and perform PCA within each cluster, do not address the problem considered here: namely, how to map high-dimensional data into a single global coordinate system of lower dimensionality.](https://www.sciencemag.org/content/suppl/2000/12/22/vo290n5500/DC1/2323.F1.jpg)

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function subject to two constraints: first, that each data point \( X_i \) is reconstructed only from its neighbors (5), enforcing \( W_{ij} = 0 \) if \( X_i \) does not belong to the set of neighbors of \( X_j \); second, that the rows of the weight matrix sum to one: \( \sum W_{ij} = 1 \). The optimal weights \( W_{ij} \) subject to these constraints (6) are found by solving a least-squares problem (7).

The constrained weights that minimize these reconstruction errors obey an important symmetry: for any particular data point, they are invariant to rotations, rescalings, and translations of that data point and its neighbors. By symmetry, it follows that the reconstruction weights characterize intrinsic geometric properties of each neighborhood, as opposed to properties that depend on a particular frame of reference (8). Note that the invariance to translations is specifically enforced by the sum-to-one constraint on the rows of the weight matrix.

Suppose the data lie on or near a smooth nonlinear manifold of lower dimensionality \( d \ll D \). To a good approximation then, there exists a linear mapping—consisting of a translation, rotation, and rescaling—that maps the high-dimensional coordinates of each neighborhood to global internal coordinates on the manifold. By design, the reconstruction weights \( W_{ij} \) reflect intrinsic geometric properties of the data that are invariant to exactly such transformations. We therefore expect their characterization of local geometry in the original data space to be equally valid for local patches on the manifold. In particular, the same weights \( W_{ij} \) that reconstruct the \( i \)th data point in \( D \) dimensions should also reconstruct its embedded manifold coordinates in \( d \) dimensions.

LLE constructs a neighborhood-preserving mapping based on the above idea. In the final step of the algorithm, each high-dimensional observation \( X_i \) is mapped to a low-dimensional vector \( Y_i \) representing global internal coordinates on the manifold. This is done by choosing \( d \)-dimensional coordinates \( Y_i \) to minimize the embedding cost function

\[
\Phi(Y) = \sum_i \left| Y_i - \sum_w W_{ij} Y_j \right|^2 \tag{2}
\]

This cost function, like the previous one, is based on locally linear reconstruction errors, but here we fix the weights \( W_{ij} \) while optimizing the coordinates \( Y_i \). The embedding cost in Eq. 2 defines a quadratic form in the vectors \( Y_i \). Subject to constraints that make the problem well-posed, it can be minimized by solving a sparse \( N \times N \) eigenvalue problem (9), whose bottom \( d \) nonzero eigenvectors provide an ordered set of orthogonal coordinates centered on the origin.

Implementation of the algorithm is straightforward. In our experiments, data points were reconstructed from their \( K \) nearest neighbors, as measured by Euclidean distance or normalized dot products. For such implementations of LLE, the algorithm has only one free parameter: the number of neighbors, \( K \). Once neighbors are chosen, the optimal weights \( W_{ij} \) and coordinates \( Y_i \) are

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**Fig. 2.** Steps of locally linear embedding: (1) Assign neighbors to each data point \( X_i \) (for example by using the \( K \) nearest neighbors). (2) Compute the weights \( W_{ij} \) that best linearly reconstruct \( X_i \) from its neighbors, solving the constrained least-squares problem in Eq. 1. (3) Compute the low-dimensional embedding vectors \( Y_i \) best reconstructed by \( W_{ij} \), minimizing Eq. 2 by finding the smallest eigenmodes of the sparse symmetric matrix in Eq. 3. Although the weights \( W_{ij} \) and vectors \( Y_i \) are computed by methods in linear algebra, the constraint that points are only reconstructed from neighbors can result in highly nonlinear embeddings.

**Fig. 3.** Images of faces (11) mapped into the embedding space described by the first two coordinates of LLE. Representative faces are shown next to circled points in different parts of the space. The bottom images correspond to points along the top-right path (linked by solid line), illustrating one particular mode of variability in pose and expression.
LLE scales well with the intrinsic manifold dimensionality, $d$, and does not require a discretized gridding of the embedding space. As more dimensions are added to the embedding space, the existing ones do not change, so that LLE does not have to be rerun to compute higher dimensional embeddings. Unlike methods such as principal curves and surfaces (18) or additive component models (19), LLE is not limited in practice to manifolds of extremely low dimensionality or codimensionality. Also, the intrinsic value of $d$ can itself be estimated by analyzing a reciprocal cost function, in which reconstruction weights derived from the embedding vectors $Y_i$ are applied to the data points $X_i$.

LLE illustrates a general principle of manifold learning, elucidated by Martinetz and Schulten (20) and Tenenbaum (4), that overlapping local neighborhoods—collectively analyzed—can provide information about global geometry. Many virtues of LLE are shared by Tenenbaum’s algorithm, Isomap, which has been successfully applied to similar problems in nonlinear dimensionality reduction. Isomap’s embeddings, however, are optimized to preserve geodesic distances between general pairs of data points, which can only be estimated by computing shortest paths through large sublattices of data. LLE takes a different approach, analyzing local symmetries, linear coefficients, and reconstruction errors instead of global constraints, pairwise distances, and stress functions. It thus avoids the need to solve large dynamic programming problems, and it also tends to accumulate very sparse matrices, whose structure can be exploited for savings in time and space.

LLE is likely to be even more useful in combination with other methods in data analysis and statistical learning. For example, a parametric mapping between the observation and embedding spaces could be learned by supervised neural networks (21) whose target values are generated by LLE. LLE can also be generalized to harder settings, such as the case of disjoint data manifolds (22), and specialized to simpler ones, such as the case of time-ordered observations (23).

Perhaps the greatest potential lies in applying LLE to diverse problems beyond those considered here. Given the broad appeal of traditional methods, such as PCA and MDS, the algorithm should find widespread use in many areas of science.

**References and Notes**


5. The set of neighbors for each data point can be assigned in a variety of ways: by choosing the $K$ nearest neighbors in Euclidean distance, by considering all data points within a ball of fixed radius, or by using prior knowledge. Note that for fixed number of neighbors, the maximum number of embedding dimensions LLE can be expected to recover is strictly less than the number of neighbors.

6. For certain applications, one might also constrain the weights to be positive, thus requiring the reconstruction of each data point to lie within the convex hull of its neighbors.

7. Fits the constrained weights that best reconstruct each data point from its neighbors can be computed in closed form. Consider a particular data point $x$ with neighbors $y_i$ and sum-to-one reconstruction weights $w_i$. The reconstruction error $J = \sum_i w_i^2$ is minimized in three steps. First, evaluate inner products between neighbors to compute the neighborhood correlation matrix $C_{ij} = y_i \cdot y_j$, and its matrix inverse, $C^{-1}$. Second, compute the Lagrange multiplier, $\lambda = \mu_i$, that enforces the sum-to-one constraint, where $\mu = 1 - \sum_i C_{ij} \mu_j$ and $\beta = C_{ii} \mu_i$. Third, compute the reconstruction weights:

$$w_i = C_{ii}^2 \{ y_i \cdot \mu_i - \lambda \}.$$ Noting that the correlation matrix $C$ is unitary, one has $C^2 = I$. In this case, $C_{ii} \mu_i = y_i \cdot \mu_i$, and $C_{ii}^2 = 1$. The reconstruction weights $w_i$ are then

$$w_i = \frac{C_{ii} \mu_i - \lambda}{\mu_i}.$$
nearly singular, it can be conditioned (before inver-
sion) by adding a small multiple of the identity
matrix. This amounts to penalizing large weights
that exploit correlations beyond some level of precision in
the data sampling process.

8. Indeed, LLE does not require the original data
to be described in a single coordinate system, only
that each data point be located in relation to its
neighbors.

9. The embedding vectors $\tilde{Y}$ are found by minimizing
the cost function $\Phi(\tilde{Y}) = \sum_{i=1}^{N} \sum_{j=1}^{K} \| \tilde{W}_{ij} \|_2^2$ over $\tilde{Y}$, with fixed
weights $W_{ij}$. This optimization is performed subject to
constraints that make the problem well posed. It is clear
that the coordinates $\tilde{Y}$ can be translated by a constant
displacement without affecting the cost, $\Phi(\tilde{Y})$. We re-
move this degree of freedom by requiring the coordi-
nates to be centered on the origin: $\sum_{i=1}^{N} \tilde{Y}_i = 0$. Also, to
avoid degenerate solutions, we constrain the embed-
ding vectors to have unit covariance, with outer prod-
ucts that satisfy $\sum_{i=1}^{N} \tilde{Y}_i \otimes \tilde{Y}_i = I$, where $I$ is the $d \times d$
identity matrix. Now the cost defines a quadratic form,
$\Phi(\tilde{Y}) = \sum_{i=1}^{N} M_i (\tilde{Y}_i - \tilde{Y})$, involving inner products of
the embedding vectors and the symmetric $N \times N$
matrix

$$M_i = \delta_{ij} - \tilde{W}_{ij} - \tilde{W}_{ii} + \sum_{k \neq i} \tilde{W}_{ik} \tilde{W}_{kj}$$

where $\delta_{ij}$ is 1 if $i = j$ and 0 otherwise. The optimal
embedding, up to a global rotation of the embedding
space, is found by computing the bottom $d + 1$
eigenvectors of this matrix (24). The bottom eigen-
vector of this matrix, which we discard, is the unit
vector with all equal components; it represents a free
translation mode of eigenvalue zero. (Discarding it
enforces the constraint that the embeddings have zero
mean.) The remaining $d$ eigenvectors form the $d$
embedding coordinates found by LLE. Note that the
matrix $M$ can be stored and manipulated as the
sparse banded matrix. (Discarding it makes the problem
well posed.) It is clear that the coordinates $\tilde{Y}$ can be
translated by a constant displacement without affecting the cost, $\Phi(\tilde{Y})$. We remove this degree of freedom by requiring the coordinates to be centered on the origin: $\sum_{i=1}^{N} \tilde{Y}_i = 0$. Also, to avoid degenerate solutions, we constrain the embedding vectors to have unit covariance, with outer products that satisfy $\sum_{i=1}^{N} \tilde{Y}_i \otimes \tilde{Y}_i = I$, where $I$ is the $d \times d$ identity matrix. Now the cost defines a quadratic form, $\Phi(\tilde{Y}) = \sum_{i=1}^{N} M_i (\tilde{Y}_i - \tilde{Y})$, involving inner products of the embedding vectors and the symmetric $N \times N$ matrix

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well posed.)

10. Manifold: Data points in Fig. 1B (N = 2000) were
sampled from the manifold (d = 3) shown in Fig. 1A.
Nearest neighbors (K = 20) were determined by Euclidean
distance. This particular manifold was in-
troduced by Tenenbaum (4), who showed that its
global structure could be learned by the Isomap
algorithm.

11. Faces: Multiple photographs (N = 2000) of the same
face were digitized as 20 \times 20 grayscale images. Each
image was treated by LLE as a data vector with D =
560 elements corresponding to raw pixel intensities.
Nearest neighbors (K = 12) were determined by Euclidean
distance in pixel space.

12. Words: Word-document counts were tabulated for
N = 5000 words from D = 31,000 articles in Grolier’s
Encyclopedia (26). Nearest neighbors (K = 20) were
determined by dot products between count vectors
normalized to unit length.

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21. Although in all the examples considered here, the
data had a single connected component, it is possible
to formulate LLE for data that lies on several disjoint
manifolds, possibly of different underlying dimen-
sionality. Suppose we form a graph by connecting
each data point to its neighbors. The number of
connected components (27) can be detected by ex-
amining powers of its adjacency matrix. Different
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folds, and are best analyzed separately by LLE.

23. If neighbors correspond to nearby observations in
time, then the reconstruction weights can be com-
puted online (as the data itself is being collected) and
the embedding can be found by diagonalizing a
sparse banded matrix.

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30. We thank G. Hinton and M. Revow for sharing their
unpublished work (at the University of Toronto) on
segmentation and pose estimation that motivated us to
“think globally, fit locally”; J. Tenenbaum (Stanford
University) for many stimulating discussions about
his work (4) and for sharing his code for the Isomap
algorithm; D. D. Lee (Bell Labs) and B. Frey (University
of Waterloo) for making available word and face data
from previous work (26); and C. Brody, A. Buja, P.
Dayan, Z. Ghahramani, G. Hinton, T. Jaakkola, D. Lee,
F. Pereira, and M. Sahani for helpful comments. S.T.R.
acknowledges the support of the Gatsby Charitable
Foundation, the U.S. National Science Foundation,
and the National Sciences and Engineering Research
Council of Canada.

7 August 2000; accepted 17 November 2000