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Data Mining and Machine Learning
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  - There's a lot of "space" in higher dimensions!
  - Higher danger of overfitting

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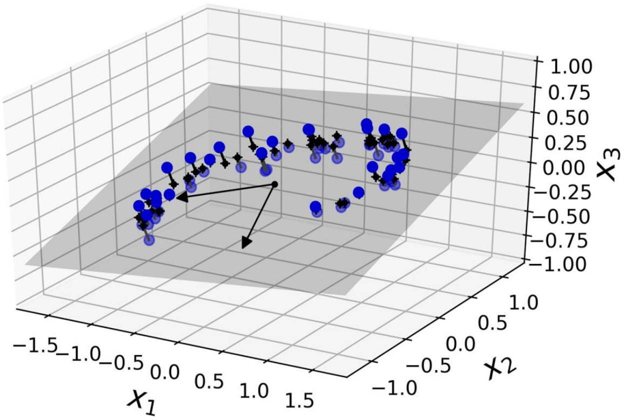

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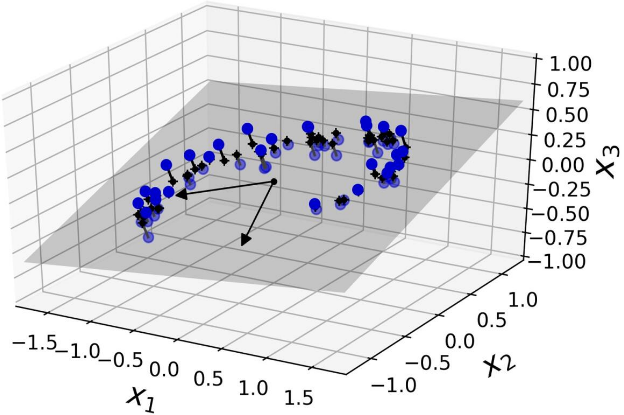
- Principal Component Analysis — transform d-dimensional input to k-dimensional input, preserving essential features



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  - $\boldsymbol{u}_i \cdot \boldsymbol{v}_i^\top$ describes components of rows of M along direction $\boldsymbol{v}_i$

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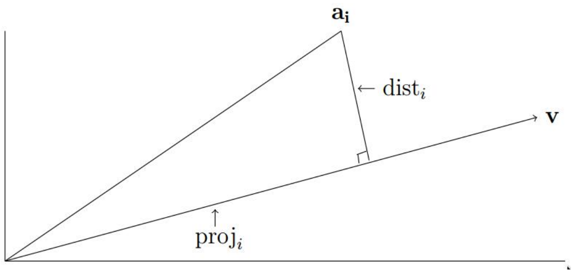

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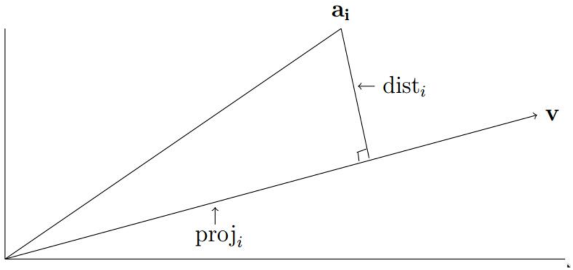
- Suppose we project $\mathbf{a}_i = (a_{i1}, a_{i2}, \ldots, a_{id})$ onto $\mathbf{v}$ through origin
- Minimizing distance of $\mathbf{a}_i$ from v is equivalent to maximizing the projection of $\mathbf{a}_i$ onto v
- Length of the projection is $\mathbf{a}_i \cdot \mathbf{v}$



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- Third singular vector — unit vector through origin, perpendicular to $\mathbf{v}_1$, $\mathbf{v}_2$, that maximizes the sum of projections of all rows in M

$$\mathbf{v}_3 = \arg\max_{\mathbf{v}\perp\mathbf{v}_1,\mathbf{v}_2;\ |\mathbf{v}|=1} |M\mathbf{v}|$$

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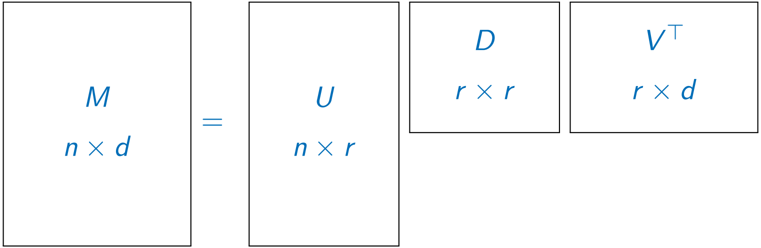
- Can show that $\{\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_r\}$ are also orthonormal

- M, dimension $n \times d$, of rank r uniquely decomposes as $M = UDV^\top$
  - $V = [\boldsymbol{v}_1 \ \boldsymbol{v}_2 \ \cdots \ \boldsymbol{v}_r]$ are the right singular vectors
  - D is a diagonal matrix with $D[i,i] = \sigma_i$, the singular values
  - $U = [\boldsymbol{u}_1 \ \boldsymbol{u}_2 \ \cdots \ \boldsymbol{u}_r]$ are the left singular vectors



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  - Matrix of first k right singular vectors $V_k = [\boldsymbol{v}_1 \;\; \boldsymbol{v}_2 \;\; \cdots \;\; \boldsymbol{v}_k]$,
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  - In other words, by truncating the SVD, we can focus on k most significant features implicit in M

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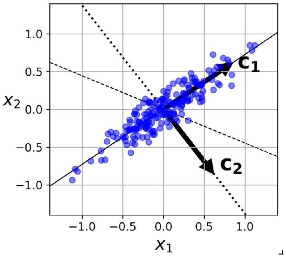

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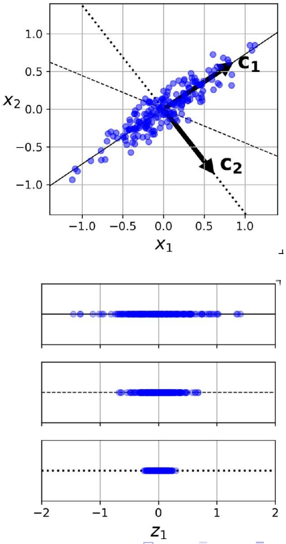
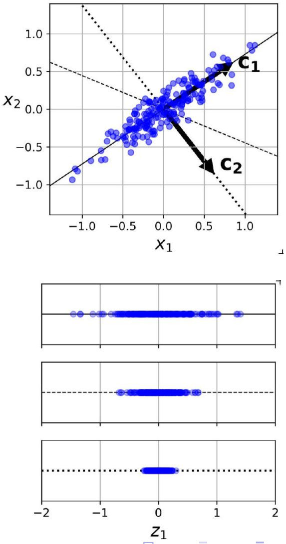


PCA and variance

- Interpret PCA in terms of preserving variance
- Different projections have different variance
- SVD orders projections in decreasing order of variance
- Criterion for choosing when to stop
  - Choose k so that a desired fraction of the variance is "explained"
  - $v_1, v_2, \dots, v_k$ are the first k Principal Components
  - Let V_k^T denote the matrix with $v_1, \dots, v_k$ as it's columns.
  - $M_k = MV_k^T$ is the projection of M to k dimensions



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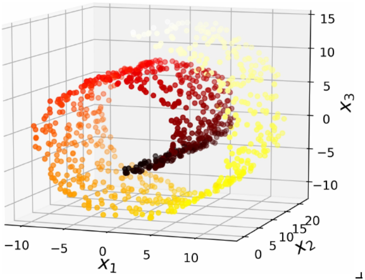

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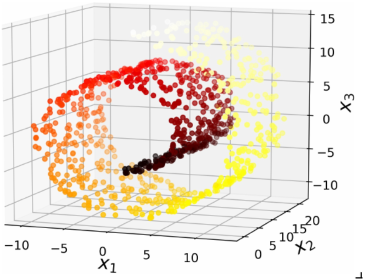

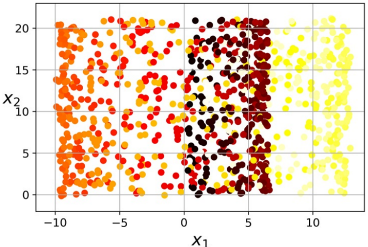

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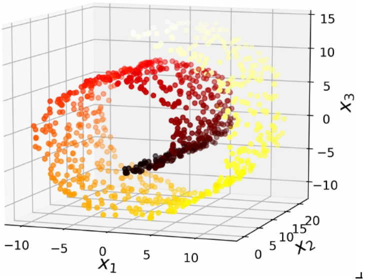

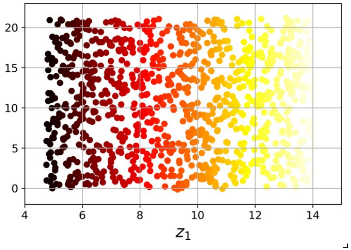

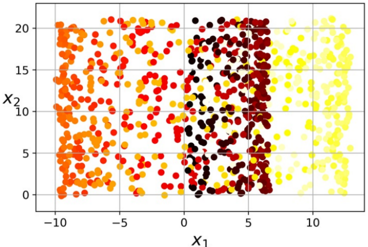

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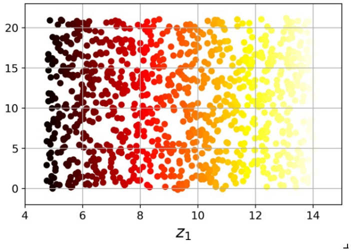

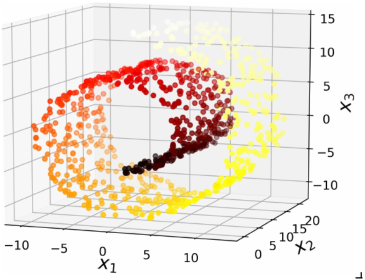

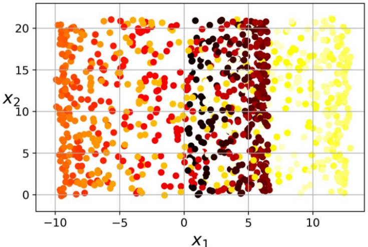

- Discover the manifold along which the data lies

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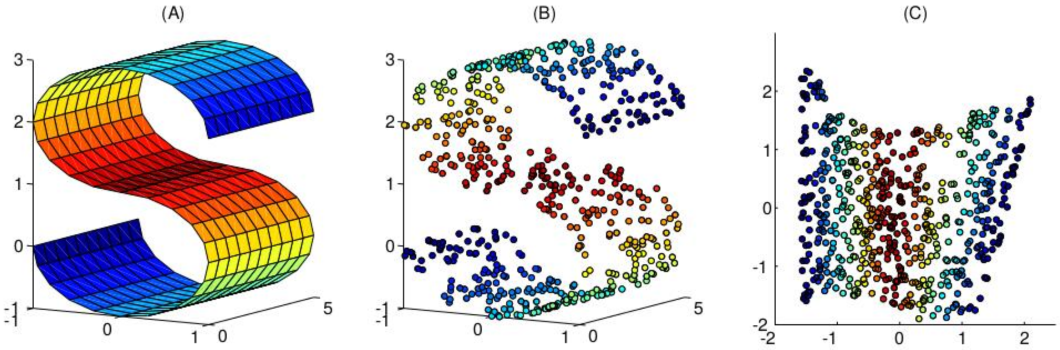
- Re-express each point in J dimensions

$$\hat{Z} = \arg\min_{Z} \sum_{i=1}^{m} \left(z_i - \sum_{j=1}^{m} w_{ij} z_j \right)^2$$



Original image | Sampled points | LLE reconstruction

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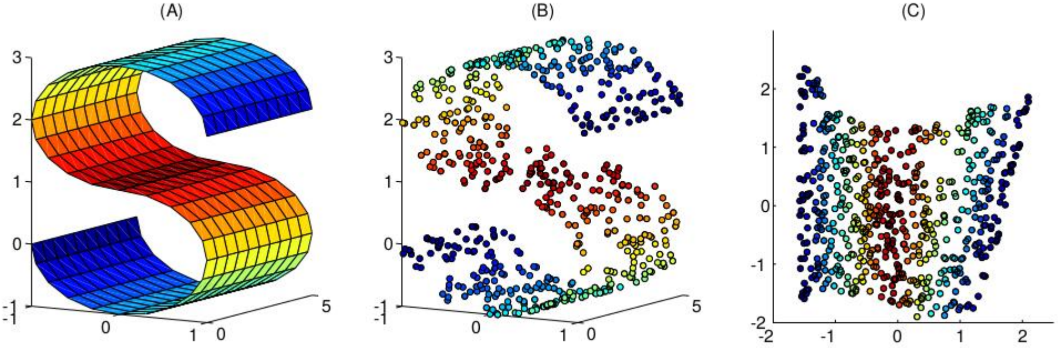


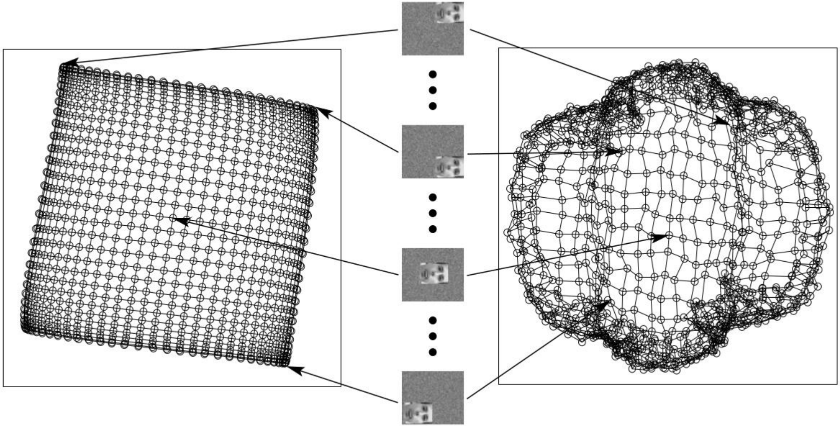
Original image

Sampled points

LLE reconstruction

- Need enough samples to discover the "curves"

Locally linear embeddings (LLE)



LLE reconstruction preserves neighbourhood structure

PCA distorts geometry

Summary

- Singular Value Decomposition (SVD) finds best fit k-dimensional subspace for any matrix M
- Principal Component Analysis uses SVD for dimensionality reduction
- Unsupervised technique — often helps simplify the problem, but may not
- SVD/PCA can only compress features that have a linear relationship
- More general techniques based on neural networks — autoencoders