Lecture 15: 21 March, 2022

Madhavan Mukund

https://www.cmi.ac.in/~madhavan

Data Mining and Machine Learning
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The curse of dimensionality

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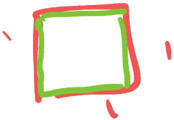

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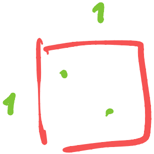

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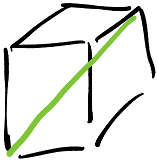

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  - There's a lot of "space" in higher dimensions!
  - Higher danger of overfitting

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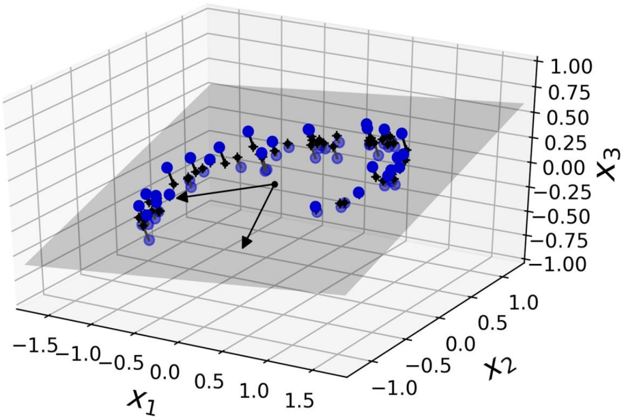
- Example: project blue points in 3D to black points in 2D plane



Dimensionality reduction

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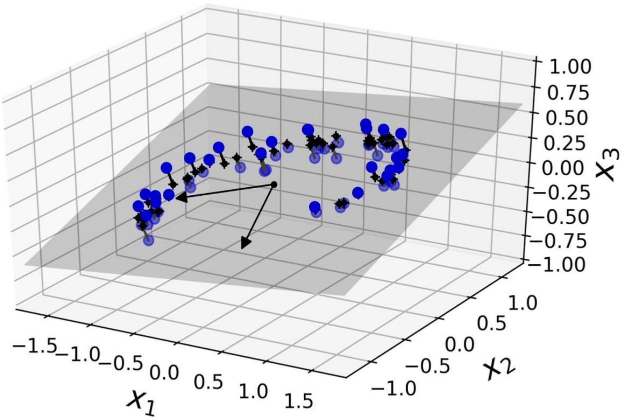
- Principal Component Analysis — transform d-dimensional input to k-dimensional input, preserving essential features



Singular Value Decomposition (SVD)

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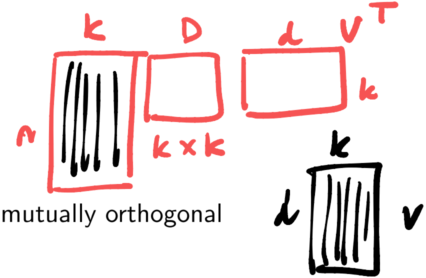

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nxk kxd

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

Singular vectors

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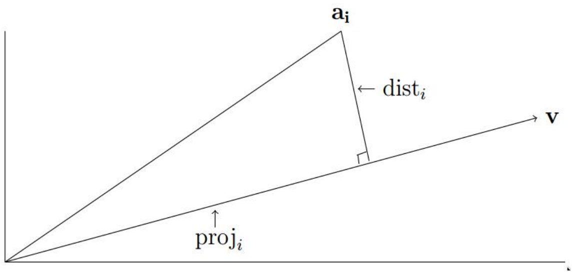

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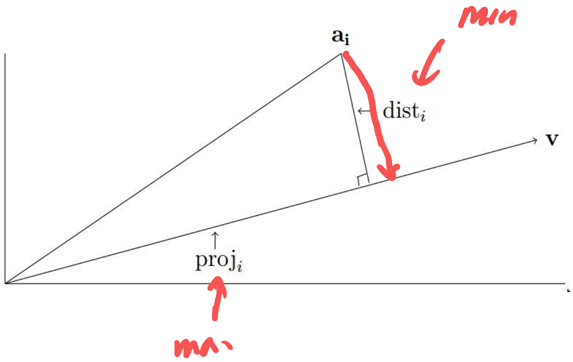
- Want to find "best" k singular vectors to represent feature space
- Suppose we project $\boldsymbol{a_i} = (a_{i1}, a_{i2}, \ldots, a_{id})$ onto $\boldsymbol{v}$ through origin
- Minimizing distance of $\boldsymbol{a_i}$ from v is equivalent to maximizing the projection of $\boldsymbol{a_i}$ onto v
- Length of the projection is $\boldsymbol{a_i} \cdot \boldsymbol{v}$



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

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If $|Mv_3| > |Mv_2|$ we would have picked v_3 before v_2

- 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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- Repeat r times till $\displaystyle\max_{\mathbf{v}\perp\mathbf{v}_1,\mathbf{v}_2,\ldots,\mathbf{v}_r;\ |\mathbf{v}|=1} |M\mathbf{v}| = 0$
  - r turns out to be the rank of M
  - Vectors $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_r\}$ are orthonormal right singular vectors

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  - Dimension r subspace that maximizes content of M projected onto it

Shrink M from d dimension to r dimension

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singular values

$M = U D V^T$ ← right sing. vectors

left sing vectors — $n \times k$ $V: d \times k$

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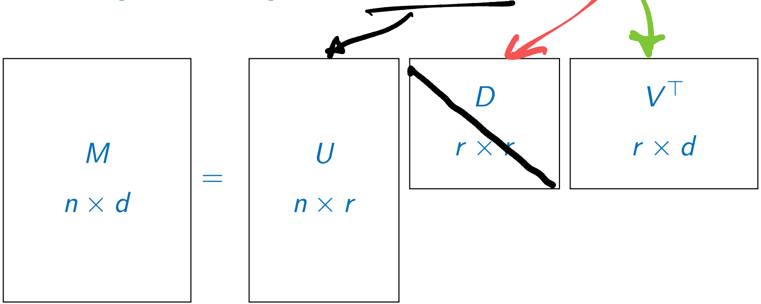
- Can show that $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_r\}$ are also orthonormal

Singular Value Decomposition

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



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- Suppose we retain only k largest ones

$k \leq r$

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- We have
  - Matrix of first k right singular vectors $V_k = [\boldsymbol{v}_1 \ \boldsymbol{v}_2 \ \cdots \ \boldsymbol{v}_k]$,
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- Let D_k be the $k \times k$ diagonal matrix with entries $\sigma_1, \sigma_2, \ldots, \sigma_k$
- Then $U_k D_k V_k^\top$ is the best fit rank-k approximation of M

$M = U_r D_r V_r^T$

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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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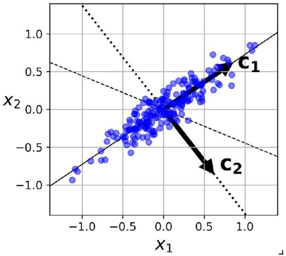

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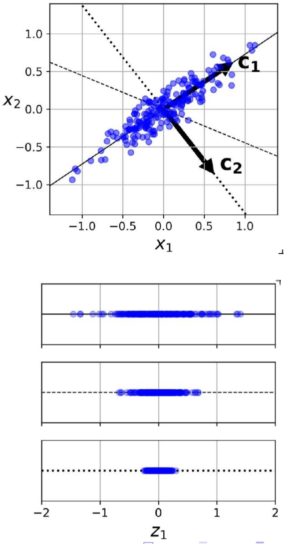
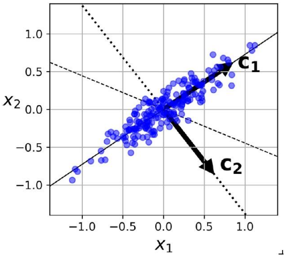
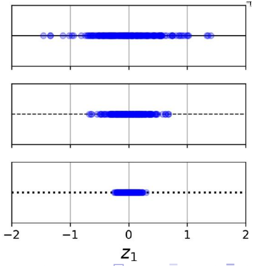
- SVD orders projections in decreasing order of variance



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"





Manifold learning

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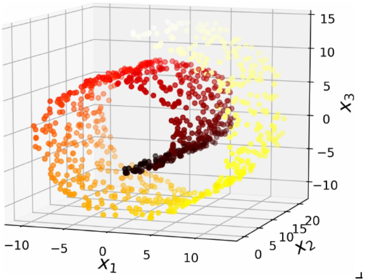

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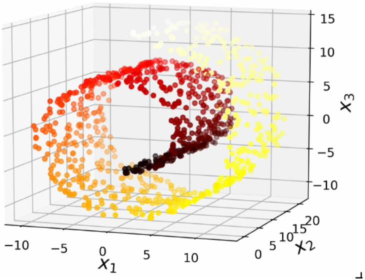

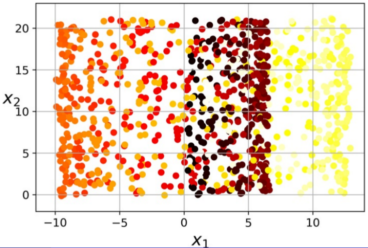

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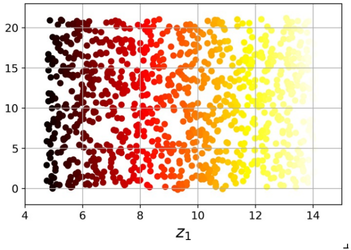

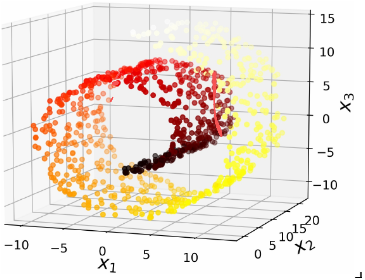

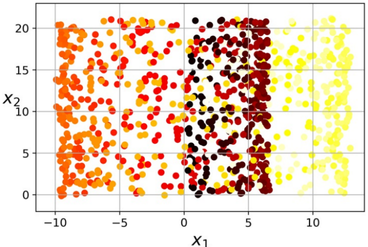

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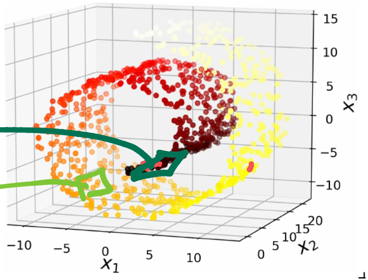
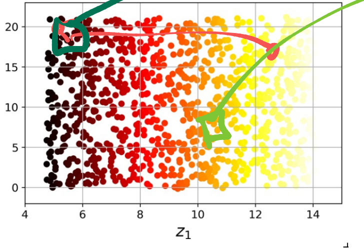
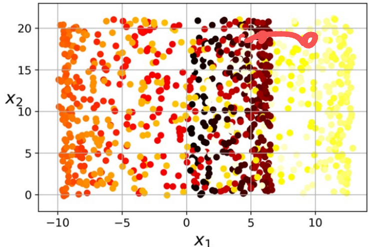






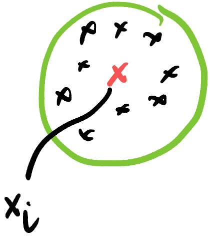
- Discover the manifold along which the data lies

Locally learning embeddings (LLE)

linear

- Describe each point x_i as a linear combination of k nearest neighbours, assume weight 0 for other neighbours

$$x_i = \sum_{j=1}^{m} w_{ij} x_j$$



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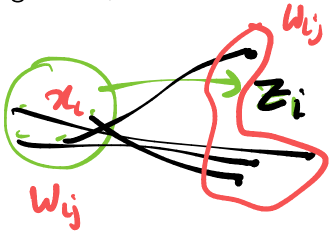

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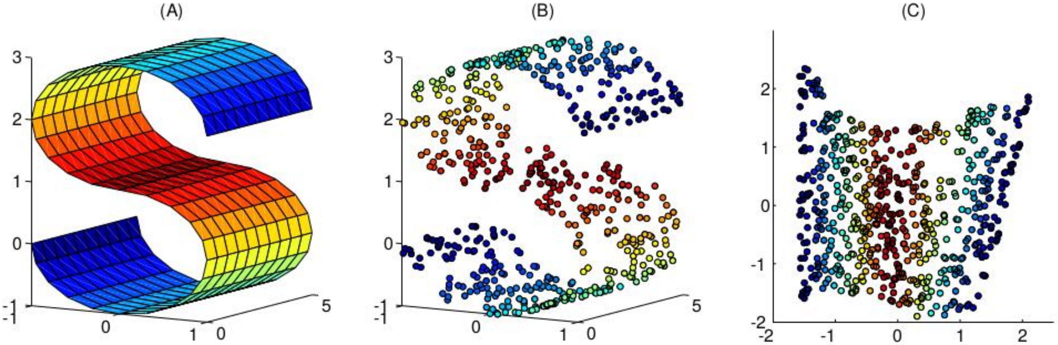
- Normalize weights — captures "local" geometry upto rotation, reflection, scaling
- Re-express each point in J dimensions

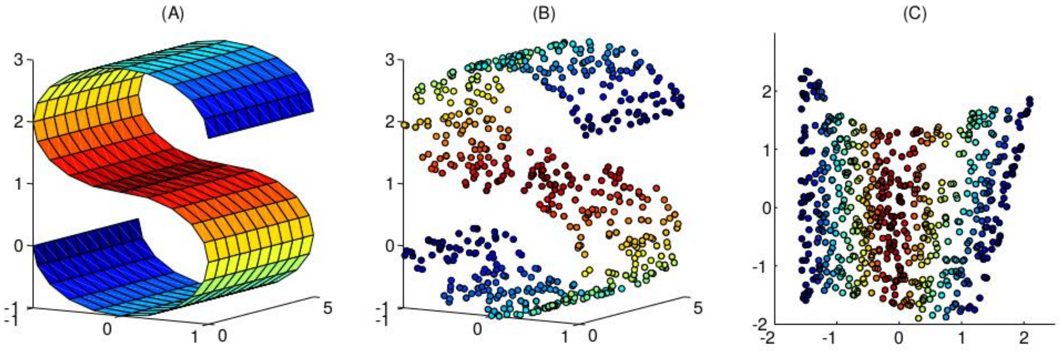
$$\hat{Z} = \arg\min_{Z} \sum_{i=1}^{m} \left(z_i - \sum_{j=1}^{m} w_{ij} z_j \right)^2$$

Locally learning embeddings (LLE)



Original image | Sampled points | LLE reconstruction

Locally learning embeddings (LLE)



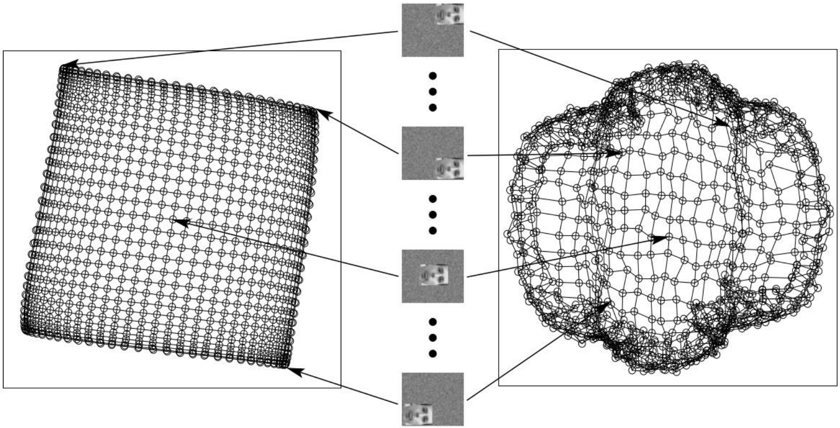
Original image

Sampled points

LLE reconstruction

- Need enough samples to discover the “curves”

Locally learning 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