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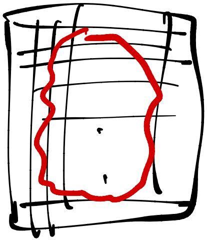
Data Mining and Machine Learning
January–April 2024

The curse of dimensionality

- ML data is often high dimensional — especially images
  - A 1000×1000 pixel image has 10^6 features



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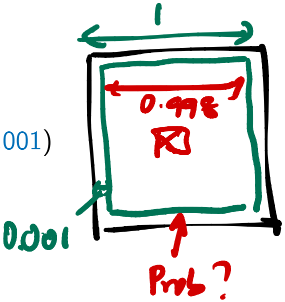
  - $2D$ unit square, 0.4% probability of being near the border (within 0.001)



$$(0.998)^2$$

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$$1 - (0.998)^n$$

$$n = 10^6 = 0.99 \sim 99$$

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

Dimensionality reduction

- Remove unimportant features by projecting to a smaller dimension

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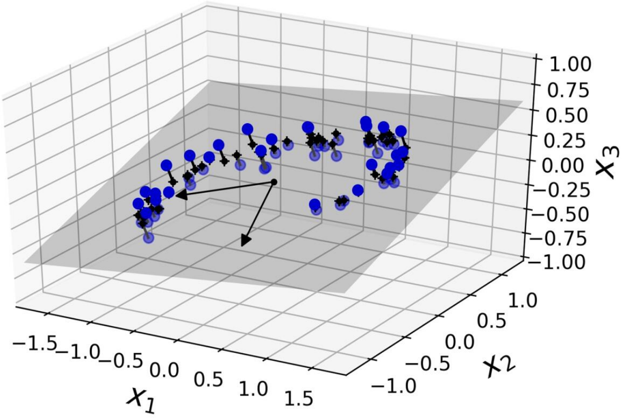
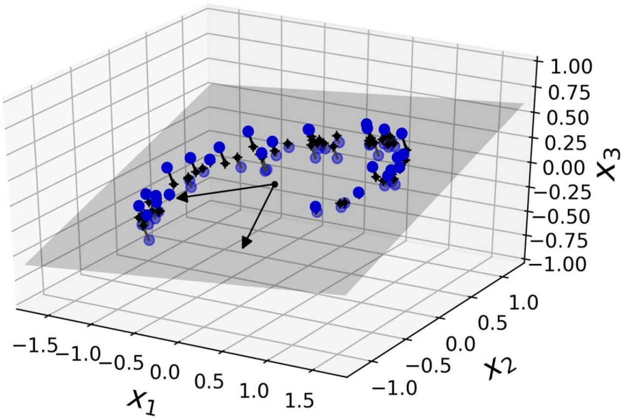
- Example: project blue points in 3D to black points in 2D plane



Dimensionality reduction

- Remove unimportant features by projecting to a smaller dimension
- Example: project blue points in 3D to black points in 2D plane
- Principal Component Analysis — transform d-dimensional input to k-dimensional input, preserving essential features



Singular Value Decomposition (SVD)

- Input matrix M, dimensions $n \times d$ — data
  - Rows are items, columns are features

row = 1 item
d features

$n \times k$

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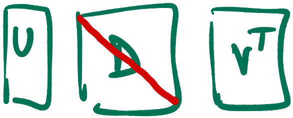

new dimension

d dimensional vector x in some basis

Represent in new basis $\langle v_1, .., v_d \rangle$

$$x \mapsto \langle x \cdot v_1, x \cdot v_2, \ldots, x \cdot v_d \rangle$$

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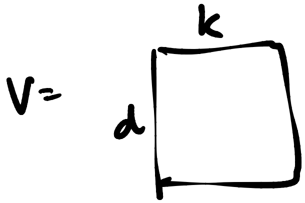

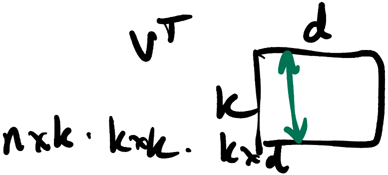

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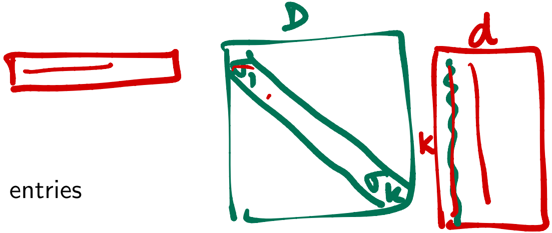
  - Rows of U describe decomposition of terms across features



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  - For columns $\mathbf{u}_i$ of U and $\mathbf{v}_i$ of V, $\mathbf{u}_i \cdot \mathbf{v}_i^\top$ is an $n \times d$ matrix, like M

$n \times 1$ $1 \times d$

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  - For columns $\mathbf{u}_i$ of U and $\mathbf{v}_i$ of V, $\mathbf{u}_i \cdot \mathbf{v}_i^\top$ is an $n \times d$ matrix, like M
  - $\mathbf{u}_i \cdot \mathbf{v}_i^\top$ describes components of rows of M along direction $\mathbf{v}_i$

Singular vectors

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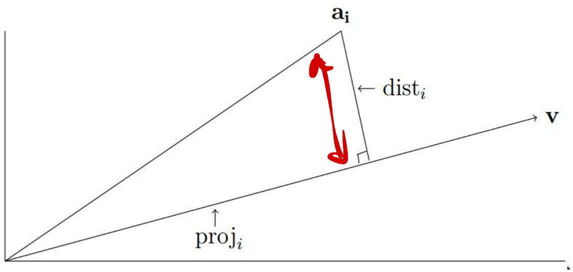
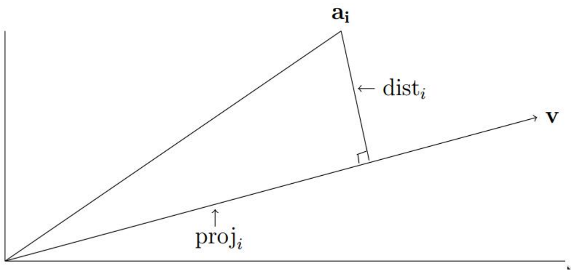


Singular vectors

- Unit vectors passing through the origin
- 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 $\boldsymbol{a_i} \cdot \boldsymbol{v}$



Singular vectors ...

- Sum of squares of lengths of projections of all rows in M onto $\boldsymbol{v}$ — $|M\boldsymbol{v}|^2$

Singular vectors . . .

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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

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

Extra constraint

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- Sum of squares of lengths of projections of all rows in M onto $\boldsymbol{v}$ — $|M\boldsymbol{v}|^2$

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$$\boldsymbol{v}_1 = \arg\max_{|\boldsymbol{v}|=1} |M\boldsymbol{v}|$$

$|Mv_1| \geq |Mv_2| \geq |Mv_3|$
$\geq \ldots$

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

$$\boldsymbol{v}_2 = \arg\max_{\boldsymbol{v}\perp\boldsymbol{v}_1;\ |\boldsymbol{v}|=1} |M\boldsymbol{v}|$$

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

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

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  - r turns out to be the rank of M
  - Vectors $\{\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_r\}$ are orthonormal right singular vectors

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

$$\underset{n \times d}{M} = \underset{n \times r}{U}\ \underset{r \times r}{D}\ \underset{r \times d}{V^\top}$$

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- We have
  - Matrix of first k right singular vectors $V_k = [\mathbf{v}_1 \ \mathbf{v}_2 \ \cdots \ \mathbf{v}_k]$,
  - Corresponding singular values $\sigma_1, \sigma_2, \ldots, \sigma_k$
  - Matrix of k left singular vectors $U_k = [\mathbf{u}_1 \ \mathbf{u}_2 \ \cdots \ \mathbf{u}_k]$
- Let D_k be the $k \times k$ diagonal matrix with entries $\sigma_1, \sigma_2, \ldots, \sigma_k$
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- In other words, by truncating the SVD, we can focus on k most significant features implicit in M

Principal Component Analysis

PCA and variance

- Interpret PCA in terms of preserving variance

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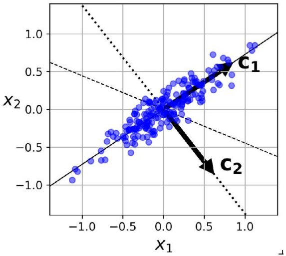

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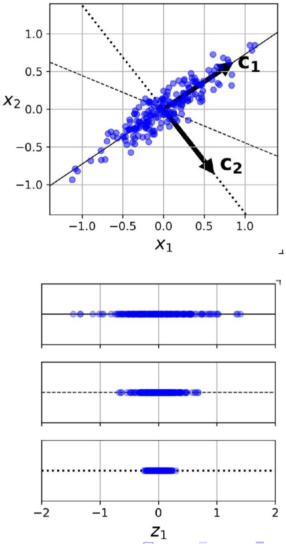
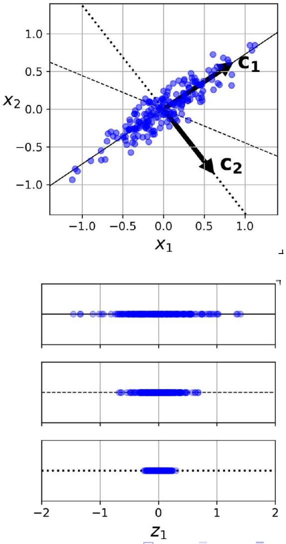


PCA and variance

- 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"



Manifold learning

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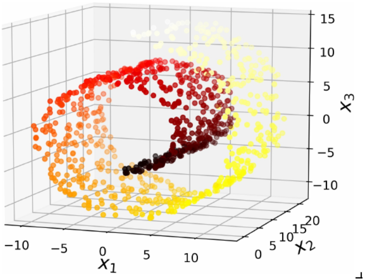

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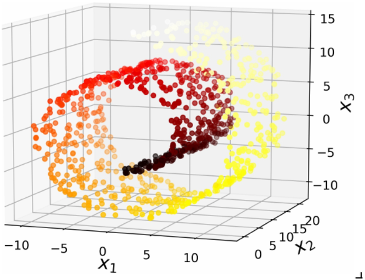

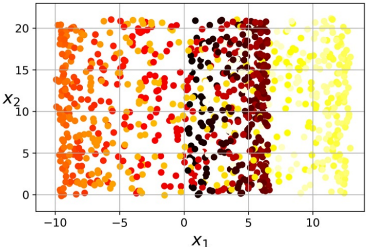

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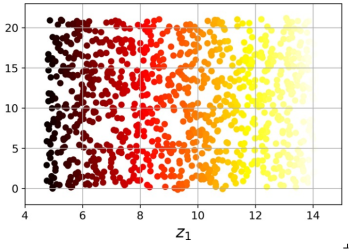

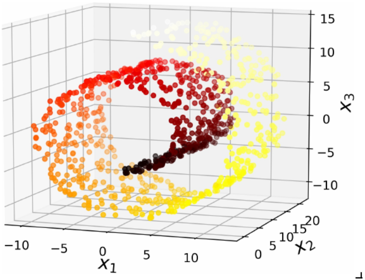

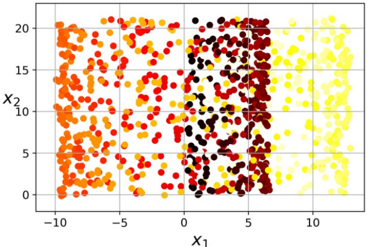

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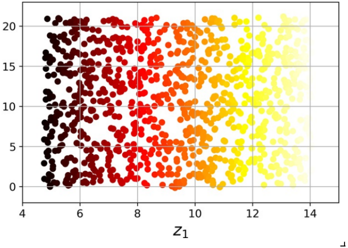

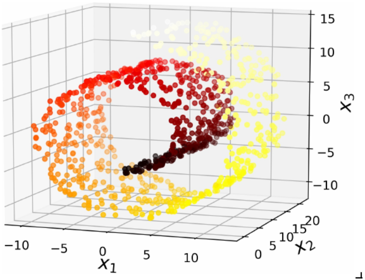

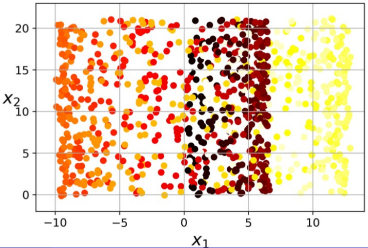

- Discover the manifold along which the data lies

Locally linear embeddings (LLE)

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

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

Locally linear embeddings (LLE)

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

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

k out of m
so all but k
W_{ij} are 0

- Choose weights to minimize the sum square distance

$$\hat{W} = \arg\min_{W} \sum_{i=1}^{m} \Big(\underbrace{x_i - \sum_{j=1}^{m} w_{ij} x_j}_{\text{discrepancy for } x_i} \Big)^2$$

$$W = \begin{array}{cc} & m \\ n & \left[\quad \right] \end{array}$$

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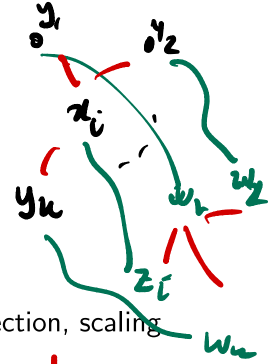

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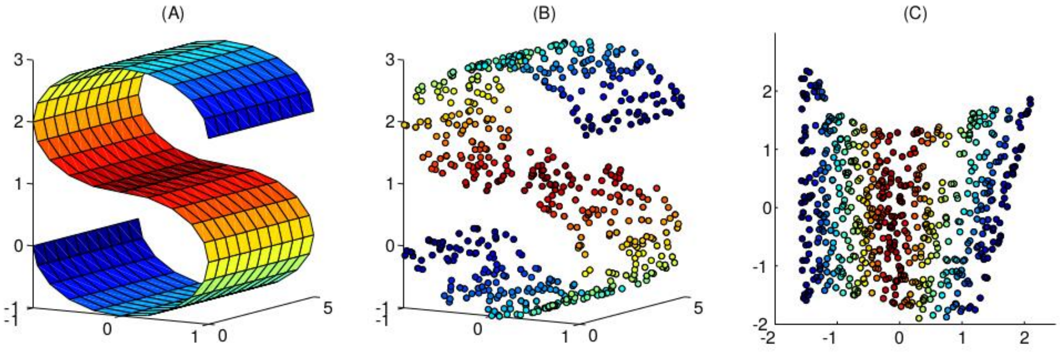
- Re-express each point in J dimensions

fixed above

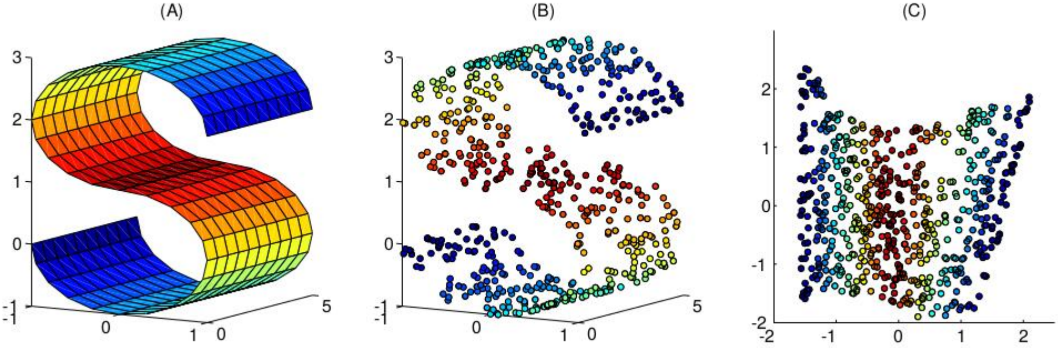
$$\hat{Z} = \arg\min_{Z} \sum_{i=1}^{m} \left(z_i - \sum_{j=1}^{m} w_{ij} z_j \right)^2$$

Locally linear embeddings (LLE)



Original image | Sampled points | LLE reconstruction

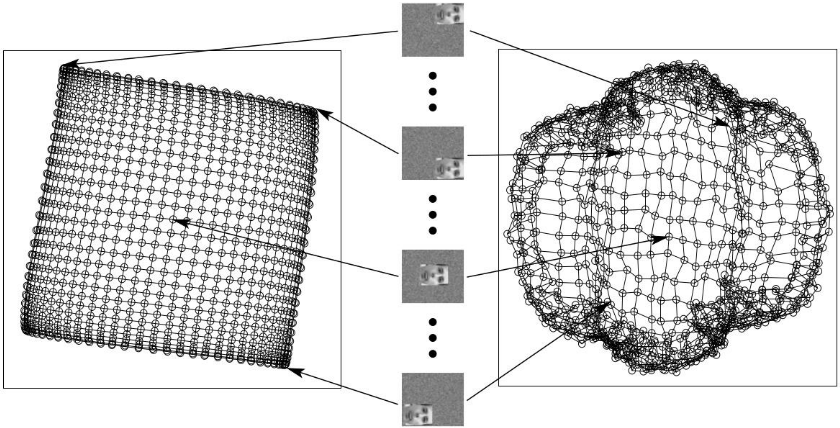
Locally linear embeddings (LLE)



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

Want $I' = I$

- More general techniques based on neural networks — autoencoders