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Data Mining and Machine Learning
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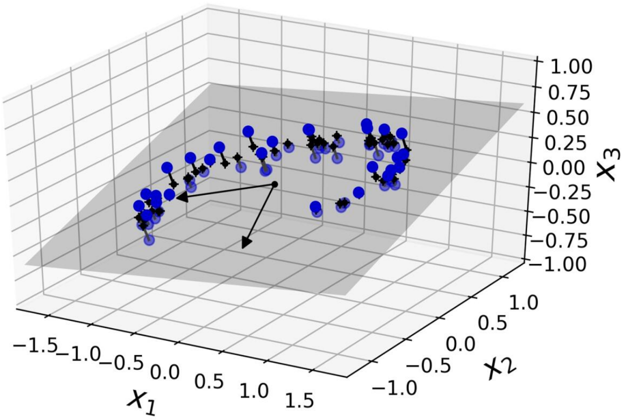
The curse of dimensionality

- ML data is often high dimensional — especially images
  - A 1000×1000 pixel image has 10^6 features
- Data behaves very differently in high dimensions
  - $2D$ unit square, 0.04% probability of being near the border (within 0.001)
  - $10^4 D$ hypercube, 99.999999% probability of being near the border
- Distances between items
  - $2D$ unit square, mean distance between 2 random points is 0.52
  - $3D$ unit cube, mean distance between 2 random points is 0.66
  - $10^6 D$ unit hypercube, mean distance between 2 random points is approximately 408.25
  - There's a lot of "space" in higher dimensions!
  - Higher danger of overfitting

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 Anaylsis — transform d-dimensional input to k-dimensional input, preserving essential features

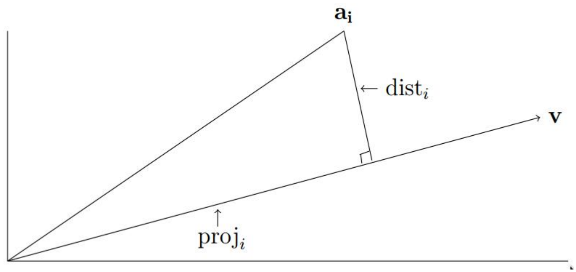


Singular Value Decomposition (SVD)

- Input matrix M, dimensions $n \times d$
  - Rows are items, columns are features
- Decompose M as $UDV^\top$
  - D is a $k \times k$ diagonal matrix, positive real entries
  - U is $n \times k$, V is $d \times k$
  - Columns of U, V are orthonormal — unit vectors, mutually orthogonal
- Interpretation
  - Columns of V correspond to new abstract features
  - Rows of U describe decomposition of terms across features
  - $M = \sum_i D_{ii}(\boldsymbol{u}_i \cdot \boldsymbol{v}_i^\top)$
  - For columns $\boldsymbol{u}_i$ of U and $\boldsymbol{v}_i$ of V, $\boldsymbol{u}_i \cdot \boldsymbol{v}_i^\top$ is an $n \times d$ matrix, like M
  - $\boldsymbol{u}_i \cdot \boldsymbol{v}_i^\top$ describes components of rows of M along direction $\boldsymbol{v}_i$

Singular vectors

- Unit vectors passing through the origin
- Want to find "best" k singular vectors to represent feature space
- 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 $\mathbf{a}_i \cdot \mathbf{v}$



Singular vectors . . .

- Sum of squares of lengths of projections of all rows in M onto $\boldsymbol{v}$ — $|M\boldsymbol{v}|^2$
- First singular vector — unit vector through origin that maximizes the sum of projections of all rows in M

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

- 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

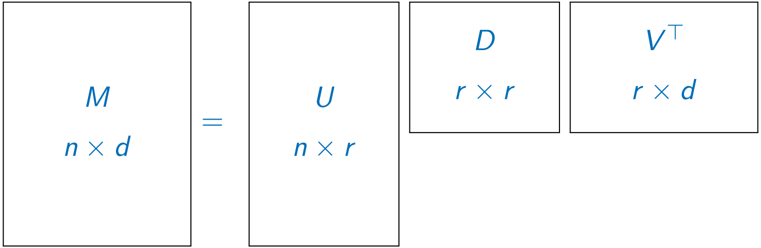
$$\boldsymbol{v}_3 = \arg \max_{\boldsymbol{v} \perp \boldsymbol{v}_1, \boldsymbol{v}_2;\ |\boldsymbol{v}|=1} |M\boldsymbol{v}|$$

Singular vectors ...

- With each singular vector $\boldsymbol{v}_j$, associated singular value is $\sigma_j = |M\boldsymbol{v}_j|$
- Repeat r times till $\displaystyle\max_{\boldsymbol{v}\perp\boldsymbol{v}_1,\boldsymbol{v}_2,\ldots,\boldsymbol{v}_r;\ |\boldsymbol{v}|=1} |M\boldsymbol{v}| = 0$
  - 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
- Our greedy strategy provably produces "best-fit" dimension r subspace for M
  - Dimension r subspace that maximizes content of M projected onto it
- Corresponding left singular vectors are given by $\boldsymbol{u}_i = \dfrac{1}{\sigma_i} M\boldsymbol{v}_i$
- Can show that $\{\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_r\}$ are also orthonormal

Singular Value Decomposition

- 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

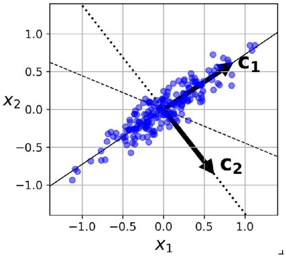


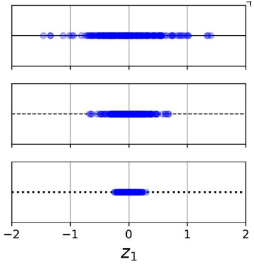
Rank-k approximation

- M has rank r, SVD gives rank r decomposition
- Singular values are non-increasing — $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r$
- Suppose we retain only k largest ones
- 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 $\sigma_1, \sigma_2, \ldots, \sigma_k$
- Then $U_k D_k V_k^\top$ is the best fit rank-k approximation of M
- In other words, by truncating the SVD, we can focus on k most significant features implicit in M

PCA and variance

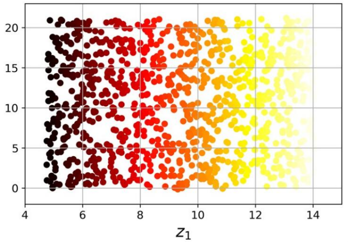
- Interpret PCA in terms of preserving variance
- Different projections have different variance
- SVD orders projections in decreasing order of variance
- Criterion for choosing when to stop
  - Choose k so that a desired fraction of the variance is "explained"

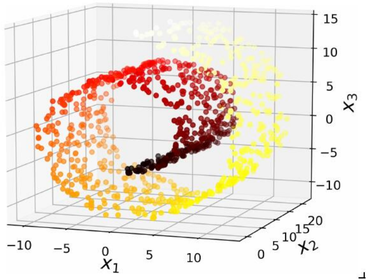


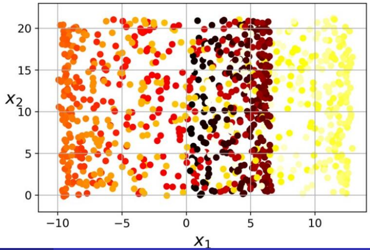


Manifold learning

- Projection may not always help
- Swiss roll dataset
- Projection onto 2 dimesions is not useful
- Better to unroll the image







- Discover the manifold along which the data lies