Dimensionality Reduction

COMP 527 Data Mining

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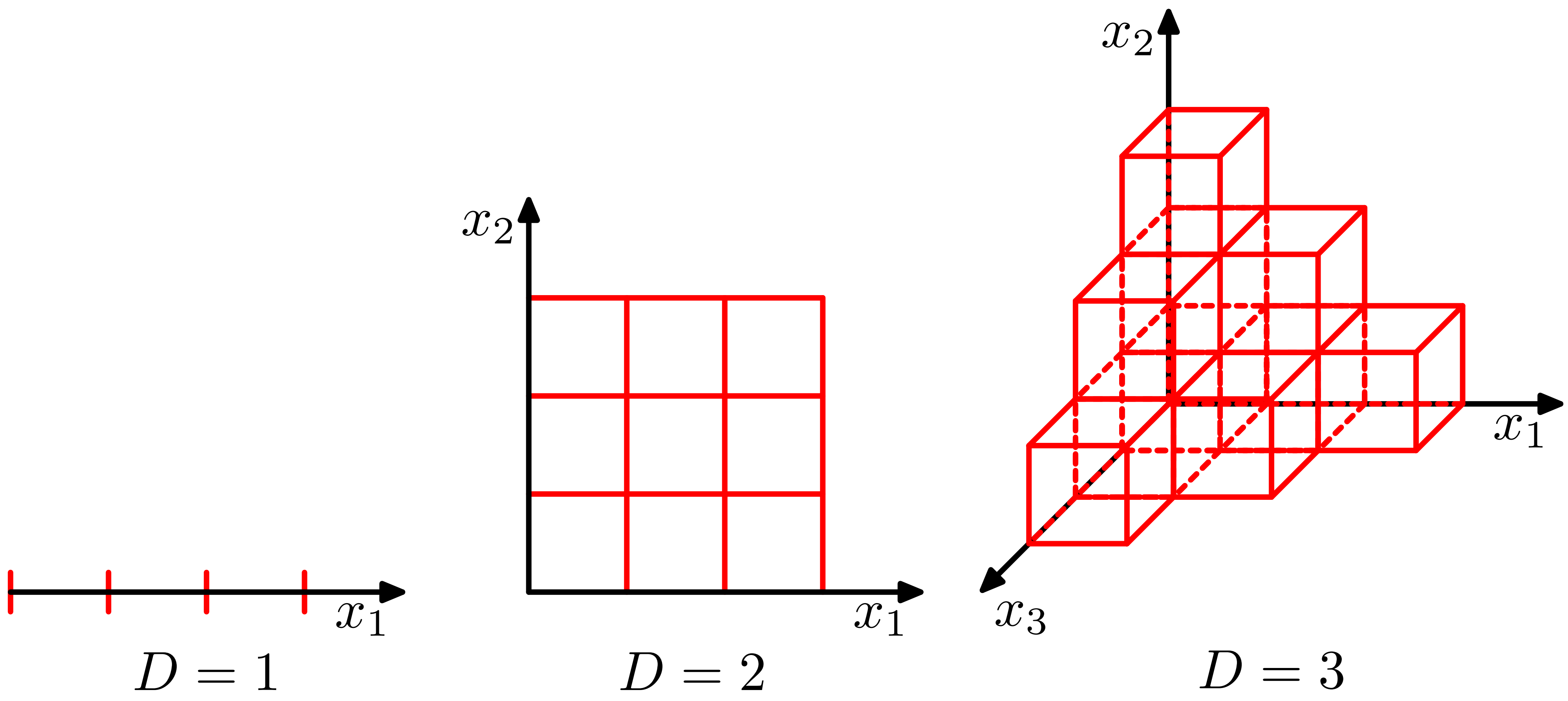
Outline

- Problems with high dimensional data
- Dimensionality Reduction Methods
  - Singular Value Decomposition (SVD)
  - Principal Component Analysis (PCA)

Problems in High Dimensions

- Curse of dimensionality
  - We need exponentially large number of data points to cover a high dimensional space

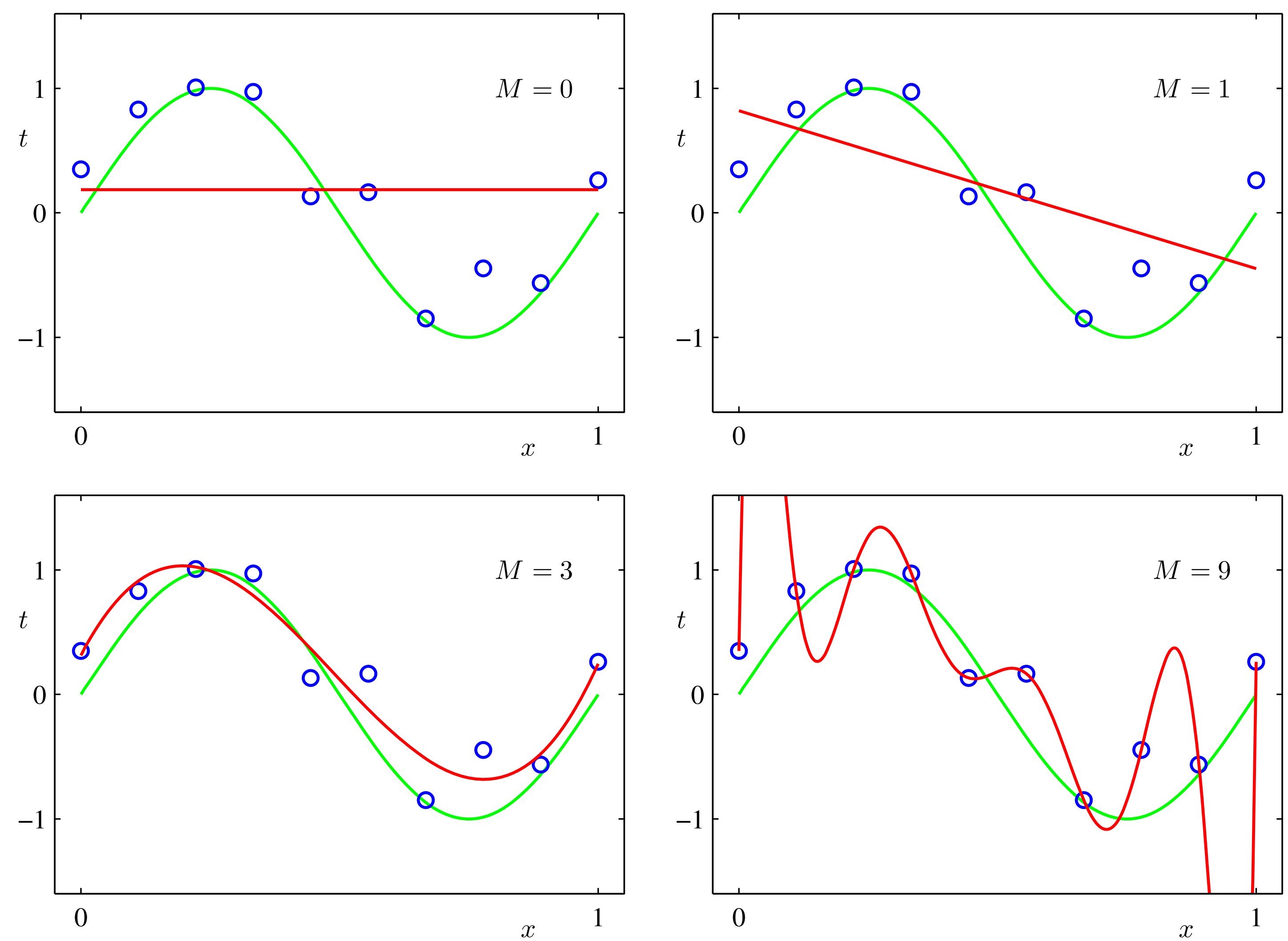


Problems in High Dimensions

- Data Sparseness
  - Although we have a large feature space (lots of dimensions to the data), we only observe a small number of non-zero features in any instance
  - This was the case for texts (in particular with the bag-of-words model)

Problems in High Dimensions

- Overfitting
  - Given n train data points, we can come up with an n-dimensional (n-th order) polynomial that passes through all those data points.
  - But it is very unlikely that it will fit well for the test data points



Problems in High Dimensions

- Time consuming (time complexity is large)
  - Consider computing cosine similarity between two n dimensional vectors, when n increases.
- Memory issues (space complexity is large)
  - Storing high dimensional dense vectors can be problematic when
    - the dimensionality of the vectors is large
    - there are lots of vectors (instances) to store

Solution

- Dimensionality Reduction
  - Try to *project* the original vectors to a *lower dimensional* space L
- What constraints do we have
  - Try to minimise the error due to the projection
    - If X and Y are neighbours in the original space, then they must also be neighbours in the projected space
  - Try to retain salient/important/principal dimensions as much as possible and remove the non-salient/ unimportant/auxiliary dimensions as much as possible

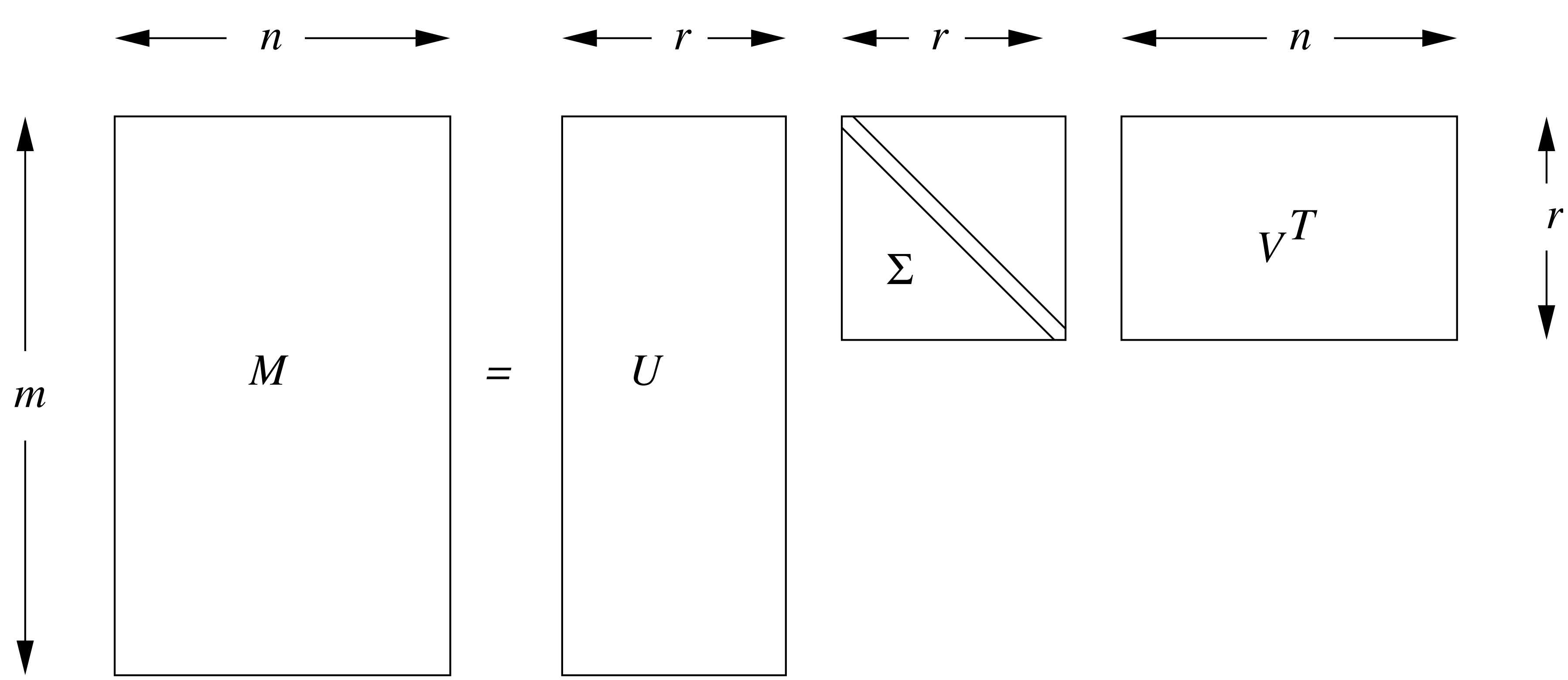
Eigenvalue Decomposition

- Linear Algebra Revision
  - Eigenvalues and Eigenvectors of a Square Matrix
  - $A\mathbf{x} = \lambda\mathbf{x}$
    - $\mathbf{x}$ is the eigenvector of A corresponding to the eigenvalue λ
- Compute the eigenvalues and eigenvectors of the following matrix

$$\begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix}$$

Singular Value Decomposition

- Eigenvalue decomposition can be performed only for square matrices.
- Singular Value Decomposition (SVD) is a operation that can be applied to any matrix
  - $M = U\Sigma V^T$
  - U and V are unitary (perpendicular) matrices, Σ is a diagonal matrix (singular values of M are diagonal elements of Σ).
  - Columns of U and V are perpendicular. $U^TU = I$ and $V^TV = I$.



SVD?

Snayperskaya Vintovka sistem'y Dragunova obraz’tsa
(Dragunov Sniper Rifle or SVD)

Example

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 3 & 3 & 3 & 0 & 0 \\ 4 & 4 & 4 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 4 & 4 \\ 0 & 0 & 0 & 5 & 5 \\ 0 & 0 & 0 & 2 & 2 \end{bmatrix} = \begin{bmatrix} .14 & 0 \\ .42 & 0 \\ .56 & 0 \\ .70 & 0 \\ 0 & .60 \\ 0 & .75 \\ 0 & .30 \end{bmatrix} \begin{bmatrix} 12.4 & 0 \\ 0 & 9.5 \end{bmatrix} \begin{bmatrix} .58 & .58 & .58 & 0 & 0 \\ 0 & 0 & 0 & .71 & .71 \end{bmatrix}$$

M $\quad U \quad \Sigma \quad V^T$

To perform SVD in python (scipy) use scipy.linalg.svd

http://docs.scipy.org/doc/scipy/reference/generated/scipy.linalg.svd.html

Dimensionality Reduction with SVD

- Procedure
  - Perform SVD on M. Retain the top-*k* (largest) singular values in Σ and set the remainder to zero.
  - Let us denote the diagonal matrix produced by the previous step by Σ_k
  - The *k*-dimensional approximation (projection) M_k of M is then given by
    - $M_k = U \Sigma_k V^T$

Reason

- The *k*-dimensional matrix M_k that minimises the Frobenius norm $||M-M_k||$ is given by the matrix M_k computed as described in the previous slide
- Frobenius norm
  - Extension of the vector L2 norm to matrices
  - Frobenius norm of a matrix M is given by $\sqrt{\sum_{ij} \mathbf{M}_{ij}{}^2}$

Proof

- By performing SVD on M, let
  - $M = PQR^T$

$$m_{ij} = \sum_k \sum_\ell p_{ik} q_{k\ell} r_{\ell j} \qquad \|M\|^2 = \sum_i \sum_j (m_{ij})^2 = \sum_i \sum_j \Big(\sum_k \sum_\ell p_{ik} q_{k\ell} r_{\ell j} \Big)^2$$

$$\Big(\sum_k \sum_\ell p_{ik} q_{k\ell} r_{\ell j} \Big)^2 = \sum_k \sum_\ell \sum_m \sum_n p_{ik} q_{k\ell} r_{\ell j} p_{in} q_{nm} r_{mj}$$

$$\|M\|^2 = \sum_i \sum_j \sum_k \sum_\ell \sum_n \sum_m p_{ik} q_{k\ell} r_{\ell j} p_{in} q_{nm} r_{mj}$$

$$\|M\|^2 = \sum_i \sum_j \sum_k \sum_n p_{ik} q_{kk} r_{kj} p_{in} q_{nn} r_{nj}$$

Much easier proof exists if you use
the trace of a matrix and its properties

$$\|M\|^2 = \sum_j \sum_k q_{kk} r_{kj} q_{kk} r_{kj}$$

$$\|M\|^2 = \sum_k (q_{kk})^2$$

Proof using Trace

$$\mathbf{M} = \mathbf{P}\mathbf{Q}\mathbf{R}^\top$$

$$||\mathbf{M}||_2^2 = \mathrm{tr}(\mathbf{M}^\top\mathbf{M})$$

$$||\mathbf{M}||_2^2 = \mathrm{tr}(\mathbf{R}\mathbf{Q}\mathbf{P}^\top\mathbf{P}\mathbf{Q}\mathbf{R}^\top)$$

$$||\mathbf{M}||_2^2 = \mathrm{tr}(\mathbf{R}\mathbf{Q}\mathbf{Q}\mathbf{R}^\top)$$

$$||\mathbf{M}||_2^2 = \mathrm{tr}(\mathbf{R}\mathbf{Q}^2\mathbf{R}^\top)$$

$$||\mathbf{M}||_2^2 = \mathrm{tr}(\mathbf{R}^\top\mathbf{R}\mathbf{Q}^2)$$

$$||\mathbf{M}||_2^2 = \mathrm{tr}(\mathbf{Q}^2)$$

SVD and Approximation Error

$$\mathbf{M} = \mathbf{P} \begin{bmatrix} \sigma_1 & & & & & \\ & \ddots & & & & \\ & & \sigma_k & & & \\ & & & \sigma_{k+1} & & \\ & & & & \ddots & \\ & & & & & \sigma_n \end{bmatrix} \mathbf{R}^\top$$

If M_k is the matrix with (k+1) and above singular values set to zero (k-th rank approximation)

$$\mathbf{M}_k = \mathbf{P} \begin{bmatrix} \sigma_1 & & & & & \\ & \ddots & & & & \\ & & \sigma_k & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{bmatrix} \mathbf{R}^\top$$

SVD and Approximation error

- Then, the approximation error, $||M - M_k||^2$ becomes

$$||\mathbf{M} - \mathbf{M}_k||^2 = \mathrm{tr}\left(\mathbf{P}\begin{bmatrix} 0 & & & & & \\ & \ddots & & & & \\ & & 0 & & & \\ & & & \sigma_{k+1} & & \\ & & & & \ddots & \\ & & & & & \sigma_n \end{bmatrix}\mathbf{R}^\top\right)$$

$$||\mathbf{M} - \mathbf{M}_k||^2 = \sigma_{k+1}^2 + \ldots + \sigma_n^2$$

If we want to minimize this error, then we must select the largest singular values for the first 1…k positions!

Applications of SVD

- Latent Semantic Analysis
  - words vs. document matrix
  - Find similar words (query expansion)
  - Find similar documents (similarity search)
- Recommendation Systems
  - users vs. items/products
  - Recommend similar products to users

Two uses of SVD

- SVD for dimensionality reduction
  - Compute $M = U\Sigma V^T$
  - Get the largest *k* singular values from Σ to construct a diagonal matrix Σ_k
  - Get the corresponding left singular vectors from U to construct a matrix U_k
  - Reduce the number of columns of M to *k* to construct the matrix M_k
    - $M_k = U_k\Sigma_k$

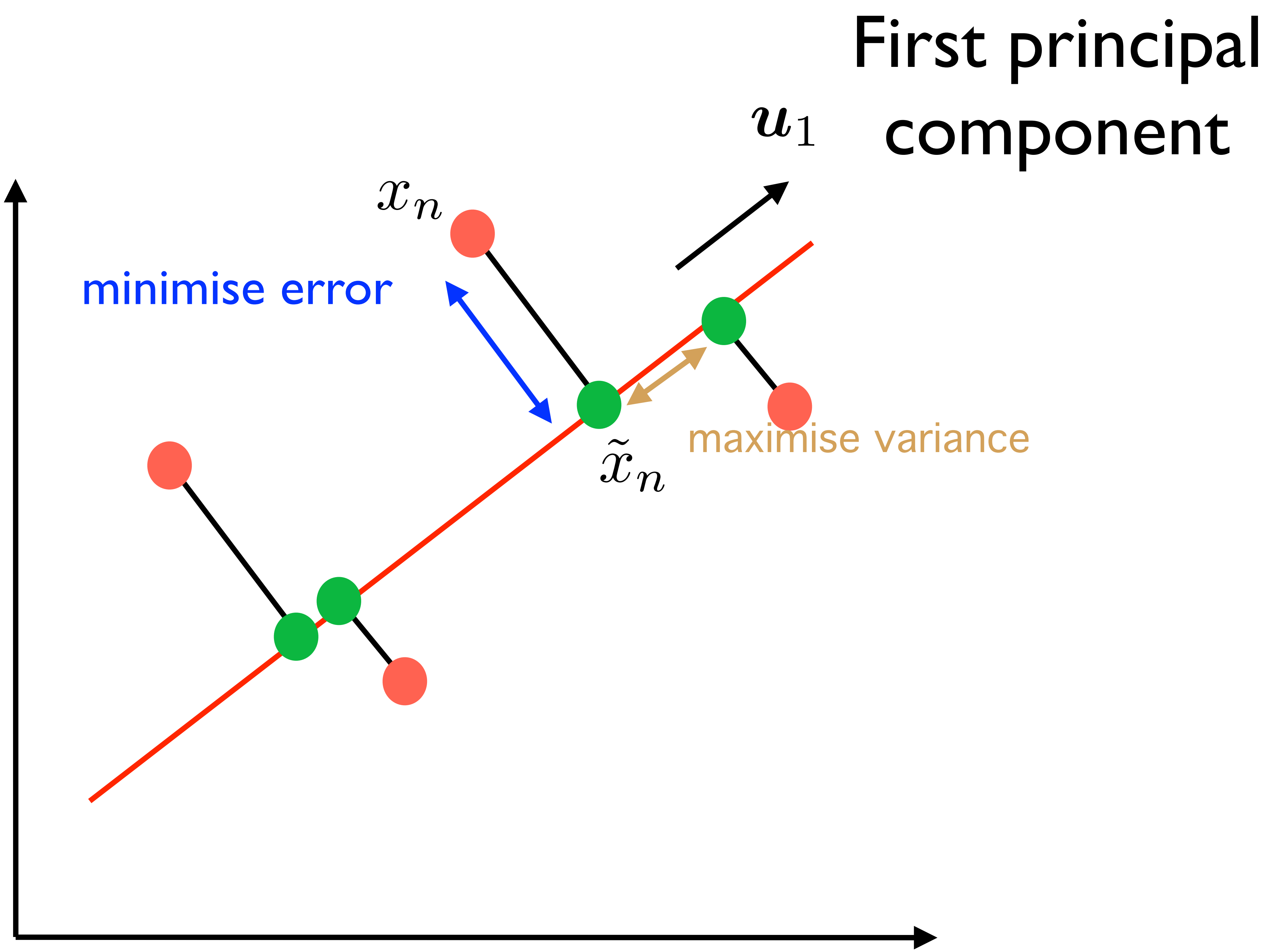
Two uses of SVD

- SVD to increase the density of a matrix
  - Compute $M = U\Sigma V^T$
  - Get the largest *k* singular values from Σ to construct a diagonal matrix Σ_k
  - Get the corresponding left singular vectors from U to construct a matrix U_k
  - Get the corresponding right singular vectors from U to construct a matrix V_k
  - Reproduce a dense version of M, M_k
    - $M_k = U_k \Sigma_k V_k^T$
    - Lesser number of non-zero values in M_k
    - However, we end up with negative values in M_k even though M is a matrix with all non-negative values!

Principal Component Analysis

- We would like to *project* our *high dimensional* data points to a *low dimensional* space by *preserving the geometric properties* in the original space as much as possible
- Two ways to do this:
  - Maximise the variance of the projected data
  - Linear projection that minimises the average projection cost
- PCA is also known as the *Karhunen-Loève Transform*

Idea



First principal component
$\boldsymbol{u}_1$
x_n
minimise error
maximise variance
$\tilde{x}_n$

Maximum Variance Formulation

- Problem
  - Given D dimensional N data points $\{\mathbf{x}_n\}$, where $n=1,\ldots,N$, we must project those into a $M<D$ dimensional space
  - M is given
- Let us consider the case $M=1$ (one-dimensional projection)
- The projection direction is given by the unit vector $\mathbf{u}_1$
  - $\mathbf{u}_1^\top \mathbf{u}_1 = 1$

$$\tilde{x}_n = \boldsymbol{u}_1{}^\top \boldsymbol{x}_n$$

Maximum Variance Formulation

- Mean of the data points

$$\bar{\boldsymbol{x}} = \frac{1}{N}\sum_{n=1}^{N}\boldsymbol{x}_n$$

- Variance of the projected data

$$\frac{1}{N}\sum_{n=1}^{N}(\boldsymbol{u}_1{}^\top\boldsymbol{x}_n - \boldsymbol{u}_1{}^\top\bar{\boldsymbol{x}})^2 = \boldsymbol{u}_1{}^\top\mathbf{S}\boldsymbol{u}_1$$

- S is the covariance matrix given by

$$\mathbf{S} = \frac{1}{N}\sum_{n=1}^{N}(\boldsymbol{x}_n - \bar{\boldsymbol{x}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^\top$$

Maximum Variance Formulation

- We must maximize the variance subjected to the normalization constraint on $\mathbf{u}_1$

Lagrange multiplier method
(see SVM slides)

$$L(\boldsymbol{u}_1, \lambda_1) = \boldsymbol{u}_1{}^\top \mathbf{S} \boldsymbol{u}_1 + \lambda_1 (1 - \boldsymbol{u}_1{}^\top \boldsymbol{u}_1)$$

$$\frac{\partial L(\boldsymbol{u}_1, \lambda_1)}{\partial \boldsymbol{u}_1} = 0 \quad \Rightarrow \quad \mathbf{S} \boldsymbol{u}_1 = \lambda_1 \boldsymbol{u}_1$$

$$\boldsymbol{u}_1{}^\top \mathbf{S} \boldsymbol{u}_1 = \lambda_1$$

This is variance!

$\mathbf{u}_1$ is the eigenvector of S that corresponds to the largest eigenvalue of S

PCA Algorithm

- INPUT
  - D dimensional N data points $\{x_n\}$, where $n=1,\ldots,N$
  - Dimensionality M
- Procedure
  - Compute the covariance matrix S for the dataset
  - Compute the first M eigenvectors of S
- return the computed eigenvectors

A Word on Complexity

- Eigenvalue decomposition of a DxD matrix is $O(D^3)$
- However, we only need the largest M eigenvectors of S
- This can be computed efficiently using truncated methods such as the power-iteration method in $O(MD^2)$
- Reference
    - Golub & Van Loan, *Matrix Computations*, John Hopkins University Press, 1996.

References

- Mining of Massive Datasets
  - http://infolab.stanford.edu/~ullman/mmds.html#original
  - Chapter 11 on Dimensionality Reduction (SVD)
- Pattern Recognition and Machine Learning
  - Section 1.1 (overfitting)
  - Section 1.4 (curse of dimensionality)
  - Page 561 onwards: PCA