COL866: Foundations of Data Science

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Best Fit Subspaces and Singular Value Decomposition (SVD)

Problem

Given an $n \times d$ matrix A, where we interpret the rows of the matrix as points in $\mathbb{R}^d$, find a best fit line through the origin for the given n points.

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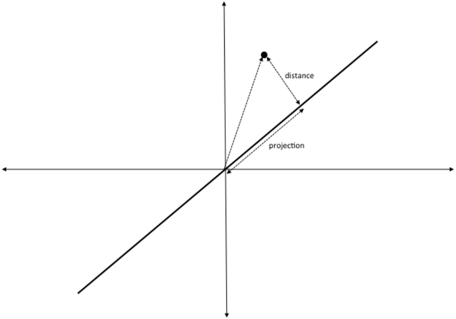
  - A line that minimises the sum of squared distance of the n points to the line.
  - Claim: The best fit line maximises the sum of projections squared of the n points to the line.



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- The best fit line through the origin is one that minimises the sum of squared distance of the n points to the line.
- Let $\mathbf{v}$ denote a unit vector ($d \times 1$ matrix) in the direction of the best fit line.
- Claim: The sum of squared lengths of projections of the points onto $\mathbf{v}$ is $||A\mathbf{v}||^2$.

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- Claim: The sum of squared lengths of projections of the points onto $\mathbf{v}$ is $||A\mathbf{v}||^2$.
- So, the best fit line is defined by unit vector $\mathbf{v}$ that maximises $||A\mathbf{v}||$.
- This is the first singular vector of the matrix A. So, the first singular vector is defined as:

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- So, σ_1^2 is equal to the sum of squared length of projections.
- Note that if all the data points are "close" to a line through the origin, then the first singular vector gives such a line.
- Question: if the data points are close to a plane (and in general close to a k-dimensional subspace), then how do we find such a plane?

Problem

Given an $n \times d$ matrix A, where we interpret the rows of the matrix as points in $\mathbb{R}^d$, find a best fit plane through the origin for the given n points.

- Let $\mathbf{v_1}$ denote the first singular vector of A.
- Idea: Find a unit vector $\mathbf{v}$ perpendicular to $\mathbf{v_1}$ that maximises $||A\mathbf{v}||$. Output the plane through the origin defined by vectors $\mathbf{v_1}$ and $\mathbf{v}$.
- Claim: The plane defined above indeed maximises sum of squared distances of all the points.
- The second singular vector is defined as:

$$\mathbf{v_2} = \arg\max_{||\mathbf{v}||=1, \mathbf{v} \perp \mathbf{v_1}} ||A\mathbf{v}||.$$

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Theorem

For any matrix A, the plane spanned by $\mathbf{v_1}$ and $\mathbf{v_2}$ is the best fit plane.

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Proof sketch

- Let W denote the best fit plane for A.
- Claim 1: There exists an orthonormal basis $(\mathbf{w_1}, \mathbf{w_2})$ of W such that $\mathbf{w_2}$ is perpendicular to $\mathbf{v_1}$.
- Claim 2: $||A\mathbf{w_1}||^2 \leq ||A\mathbf{v_1}||^2$.
- Claim 3: $||A\mathbf{w_2}||^2 \leq ||A\mathbf{v_2}||^2$.
- This gives $||A\mathbf{w_1}||^2 + ||A\mathbf{w_2}||^2 \leq ||A\mathbf{v_1}||^2 + ||A\mathbf{v_2}||^2$. □

- The first singular vector and first singular value is defined as:

$$\mathbf{v_1} = \arg\max_{||\mathbf{v}||=1} ||A\mathbf{v}|| \quad \text{and} \quad \sigma_1 = ||A\mathbf{v_1}||$$

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- The third singular vector and third singular value is defined as:

$$\mathbf{v_3} = \arg\max_{||\mathbf{v}||=1, \mathbf{v} \perp \mathbf{v_1}, \mathbf{v_2}} ||A\mathbf{v}|| \quad \text{and} \quad \sigma_3 = ||A\mathbf{v_3}||.$$

- ...and so on.
- Let r be the smallest positive integer such that: $\max_{||\mathbf{v}||=1, \mathbf{v} \perp \mathbf{v_1}, ..., \mathbf{v_r}} ||A\mathbf{v}|| = 0$. Then A has r singular vectors $\mathbf{v_1}, ..., \mathbf{v_r}$.

Theorem

Let A be any $n \times d$ matrix with r singular vectors $\mathbf{v_1}, ..., \mathbf{v_r}$. For $1 \leq k \leq r$, let V_k be the subspace spanned by $\mathbf{v_1}, ..., \mathbf{v_k}$. For each k, V_k is the best-fit k-dimensional subspace for A.

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- The vectors $\mathbf{v_1}, ..., \mathbf{v_r}$ are more specifically called the right singular vectors.
- For any singular vector $\mathbf{v_i}$, $\sigma_i = ||A\mathbf{v_i}||$ may be interpreted as the component of the matrix A along $\mathbf{v_i}$.
- Given this interpretation, the "*the components should add up to give the whole content of A*".

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- For any row a_j in the matrix A, we can write $||a_j||^2 = \sum_{i=1}^{r} (a_j \cdot \mathbf{v_i})^2$. This further gives:

$$\sum_{j=1}^{n} ||a_j||^2 = \sum_{j=1}^{n} \sum_{i=1}^{r} (a_j \cdot \mathbf{v_i})^2 = \sum_{i=1}^{r} ||A\mathbf{v_i}||^2 = \sum_{i=1}^{r} \sigma_i^2.$$

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- The LHS of the above equation may be interpreted as "*content of the matrix*" defines the Frobenius Norm of the matrix A.

Definition (Frobenius Norm)

The Frobenius norm of a given $n \times d$ matrix A, denoted by $||A||_F$, is defined as: $||A||_F = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{d} A_{i,j}^2}$.

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Theorem

For any matrix A, the sum of squares of the right singular values equals the square of the Frobenius norm of the matrix.

- Let $\mathbf{v}_1, ..., \mathbf{v}_r$ be the right singular vectors and $\sigma_1, ..., \sigma_r$ be the corresponding singular values of matrix A.
- The left singular vectors are defined as $\mathbf{u}_i = \frac{1}{\sigma_i} A\mathbf{v}_i$.
- $\sigma_i \mathbf{u}_i$ may be interpreted as a vector whose components are the projections of the rows of A onto $\mathbf{v}_i$.

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- The left singular vectors are defined as $\mathbf{u}_i = \frac{1}{\sigma_i} A\mathbf{v}_i$.
- $\sigma_i \mathbf{u}_i$ may be interpreted as a vector whose components are the projections of the rows of A onto $\mathbf{v}_i$.
- $\sigma_i \mathbf{u}_i \mathbf{v}_i^T$ is a rank one matrix whose rows can be interpreted as component of rows of A along $\mathbf{v}_i$.
- Given this, the following decomposition of A into rank one matrices should make sense (we will prove this): $A = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$.

Theorem

Let A be any $n \times d$ matrix with right singular vectors $\mathbf{v}_1, ..., \mathbf{v}_r$, left-singular vectors $\mathbf{u}_1, ..., \mathbf{u}_r$, and corresponding singular values $\sigma_1, ..., \sigma_r$. Then $A = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$.

Singular Value Decomposition (SVD)

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Proof sketch

- Lemma: Matrices A and B are identical iff for all vectors $\mathbf{v}$, $A\mathbf{v} = B\mathbf{v}$.
- Let $B = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$.
- For any j, $A\mathbf{v}_j = \sigma_j \mathbf{u}_j$ from the definition of u_j.
- $B\mathbf{v}_j = \left(\sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^T\right) \mathbf{v}_j = \sigma_j \mathbf{u}_j$ from orthonormality.
- Fact: Any vector $\mathbf{v}$ can be written as a linear combination of right eigenvectors $\mathbf{v}_1, ..., \mathbf{v}_r$ and a vector perpendicular to $\mathbf{v}_1, ..., \mathbf{v}_r$. □

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- The decomposition $A = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$ is called the Singular Value Decomposition (or SVD in short).
- In matrix notation, we can write $A = UDV^T$ where:
  - U is a $n \times r$ matrix where the i^{th} column is $\mathbf{u}_i$.
  - D is a $r \times r$ diagonal matrix with the i^{th} diagonal element σ_i.
  - V is a $d \times r$ matrix where the i^{th} column is $\mathbf{v}_i$.
- Question: How do we compute the SVD?
- Question: What are the applications of SVD?

- Let $A = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$ be the SVD of an $n \times d$ matrix A.
- For $k \in \{1, ..., r\}$ let

$$A_k = \sum_{i=1}^{k} \sigma_i \mathbf{u}_i \mathbf{v}_i^T \quad \text{(i.e., sum truncated to first } k \text{ elements)}$$

- Claim 1: A_k has rank k.
- Claim 2: The rows of A_k are the projections of the rows of A onto the subspace V_k spanned by the first k singular vectors of A.
- We will prove that A_k is the best rank k approximation to A where the error is measured in terms of the Frobenius norm.

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- The above theorem tells us that A_k is a good approximation for A (w.r.t. Frobenius norm).
- The approximation A_k also is good for computation of product with any vector $\mathbf{x}$ with $||\mathbf{x}|| \leq 1$.
  - Computing $A\mathbf{x}$ would cost $O(nd)$ multiplications.
  - However, computing $A_k = \sum_{i=1}^{k} \sigma_i \mathbf{u}_i \mathbf{v}^T$ only costs $O(kd + nk)$ multiplications.
- Question: Is A_k best rank-k approximation to A w.r.t. the computation $A\mathbf{x}$ for an arbitrary $\mathbf{x}$ with $||\mathbf{x}|| \leq 1$?
  - We want a rank-k matrix B such that $\max_{||\mathbf{x}|| \leq 1} ||(A - B)\mathbf{x}||$ is minimized.

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Theorem

Let A be any $n \times d$ matrix. For any matrix B of rank at most k:

$$||A - A_k||_2 \leq ||A - B||_2.$$

- First, we show that the left singular vectors $\mathbf{u}_1, ..., \mathbf{u}_r$ are pairwise orthogonal.

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The left singular vectors $\mathbf{u}_1, ..., \mathbf{u}_r$ *are pairwise orthogonal.*

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- We will also need the following theorem.

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$||A - A_k||_2^2 = \sigma_{k+1}^2$.

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$||A - A_k||_2^2 = \sigma_{k+1}^2$.

- Finally, we show the following:

Theorem

Let A be an $n \times d$ matrix. For any matrix B of rank at most k:

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- Exercise: Show that u_i's are the right singular vectors for the matrix A^T.

End