COMPSCI 514: Algorithms for Data Science

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Lecture 16

Summary

Last Class:

- No-distortion embeddings for data lying in a k-dimensional subspace via an orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$ for that subspace.
- View as low-rank matrix factorization. Introduce concept of low-rank approximation.
- Idea of approximating a data matrix $\mathbf{X}$ with $\mathbf{X}\mathbf{V}\mathbf{V}^T$ when the data points lie close to the subspace spanned by $\mathbf{V}$'s columns.
- 'Dual view' of low-rank approximation: data points that can be approximately reconstructed from a few basis vectors vs. linearly dependent features.

This Class:

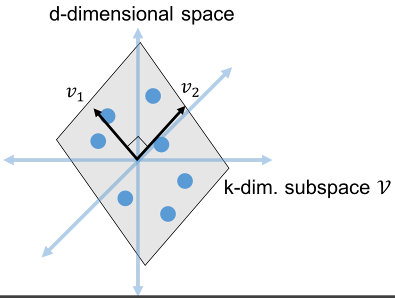
- How to find an optimal orthogonal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$ to minimize $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$.

Low-Rank Factorizatoin

Claim: If $\vec{x}_1, \ldots, \vec{x}_n$ lie in a k-dimensional subspace $\mathcal{V}$ with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be written as

$$\mathbf{X} = \mathbf{X}\mathbf{V}\mathbf{V}^T \text{ (Implies } \operatorname{rank}(\mathbf{X}) \leq k\text{)}$$

- $\mathbf{V}\mathbf{V}^T$ is a projection matrix, which projects the rows of $\mathbf{X}$ (the data points $\vec{x}_1, \ldots, \vec{x}_n$ onto the subspace $\mathcal{V}$.

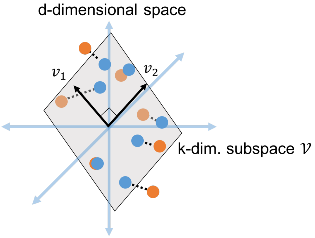


$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Low-Rank Approximation

Claim: If $\vec{x}_1, \ldots, \vec{x}_n$ lie close to a k-dimensional subspace $\mathcal{V}$ with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be approximated as:

$$\mathbf{X} \approx \mathbf{X}\mathbf{V}\mathbf{V}^T$$



$\mathbf{X}\mathbf{V}\mathbf{V}^T$ has rank k. It is a low-rank approximation of $\mathbf{X}$.

$$\mathbf{X}\mathbf{V}\mathbf{V}^\mathsf{T} = \underset{\mathbf{B} \text{ with rows in } \mathcal{V}}{\arg\min} \|\mathbf{X} - \mathbf{B}\|_F^2 = \sum_{i,j} (\mathbf{X}_{i,j} - \mathbf{B}_{i,j})^2.$$

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Properties of Projection Matrices

Quick Exercise 1 : Show that $\mathbf{V}\mathbf{V}^T$ is idempotent. I.e., $(\mathbf{V}\mathbf{V}^T)(\mathbf{V}\mathbf{V}^T)\vec{y} = (\mathbf{V}\mathbf{V}^T)\vec{y}$ for any $\vec{y} \in \mathbb{R}^d$.

Quick Exercise 2: Show that $\mathbf{V}\mathbf{V}^T(\mathbf{I} - \mathbf{V}\mathbf{V}^T) = \mathbf{0}$ (the projection is orthogonal to its complement).

Pythagorean Theorem

Pythagorean Theorem: For any orthonormal $\mathbf{V} \in \mathbb{R}^{d \times k}$ and any $\vec{y} \in \mathbb{R}^d$,

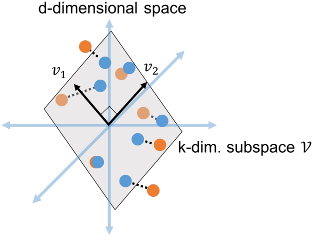
$$\|\vec{y}\|_2^2 = \|(\mathbf{V}\mathbf{V}^T)\vec{y}\|_2^2 + \|\vec{y} - (\mathbf{V}\mathbf{V}^T)\vec{y}\|_2^2.$$

Best Fit Subspace

If $\vec{x}_1, \ldots, \vec{x}_n$ are close to a k-dimensional subspace $\mathcal{V}$ with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be approximated as $\mathbf{X}\mathbf{V}\mathbf{V}^T$. $\mathbf{X}\mathbf{V}$ gives optimal embedding of $\mathbf{X}$ in $\mathcal{V}$.

How do we find $\mathcal{V}$ (equivilantly $\mathbf{V}$)?

$$\underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\min} \|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \sum_{i,j} (\mathbf{X}_{i,j} - (\mathbf{X}\mathbf{V}\mathbf{V}^T)_{i,j})^2 = \sum_{i=1}^{n} \|\vec{x}_i - \mathbf{V}\mathbf{V}^T\vec{x}_i\|_2^2 \quad \underset{\text{orthonor}}{\text{ar}}$$



$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Solution via Eigendecomposition

$\mathbf{V}$ minimizing $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$ is given by:

$$\underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\max} \|\mathbf{X}\mathbf{V}\|_F^2 = \sum_{i=1}^{n} \|\mathbf{V}^T \vec{x}_i\|_2^2 = \sum_{j=1}^{k} \|\mathbf{X}\vec{v}_j\|_2^2$$

Surprisingly, can find the columns of $\mathbf{V}$, $\vec{v}_1, \ldots, \vec{v}_k$ greedily.

$$\vec{v}_1 = \underset{\vec{v} \text{ with } \|v\|_2=1}{\arg\max} \|\mathbf{X}\vec{v}\|_2^2 \vec{v}^T \mathbf{X}^T \mathbf{X} \vec{v}.$$

$$\vec{v}_2 = \underset{\vec{v} \text{ with } \|v\|_2=1,\ \langle \vec{v}, \vec{v}_1 \rangle = 0}{\arg\max} \vec{v}^T \mathbf{X}^T \mathbf{X} \vec{v}.$$

$$\cdots$$

$$\vec{v}_k = \underset{\vec{v} \text{ with } \|v\|_2=1,\ \langle \vec{v}, \vec{v}_j \rangle = 0\ \forall j < k}{\arg\max} \vec{v}^T \mathbf{X}^T \mathbf{X} \vec{v}.$$

$\vec{v}_1, \ldots, \vec{v}_k$ are the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$ by the *Courant-Fischer Principle.*

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Review of Eigenvectors and Eigendecomposition

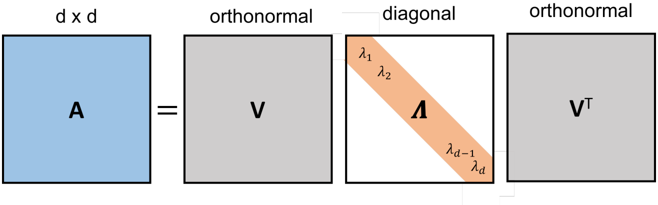
Eigenvector: $\vec{x} \in \mathbb{R}^d$ is an eigenvector of a matrix $\mathbf{A} \in \mathbb{R}^{d \times d}$ if $\mathbf{A}\vec{x} = \lambda \vec{x}$ for some scalar λ (the eigenvalue corresponding to $\vec{x}$).

- That is, $\mathbf{A}$ just 'stretches' x.
- If $\mathbf{A}$ is symmetric, can find d orthonormal eigenvectors $\vec{v}_1, \ldots, \vec{v}_d$. Let $\mathbf{V} \in \mathbb{R}^{d \times d}$ have these vectors as columns.

$$\mathbf{AV} = \begin{bmatrix} | & | & & | \\ \mathbf{A}\vec{v}_1 & \mathbf{A}\vec{v}_2 & \cdots & \mathbf{A}\vec{v}_d \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ \lambda_1\vec{v}_1 & \lambda_2\vec{v}_2 & \cdots & \lambda\vec{v}_d \\ | & | & & | \end{bmatrix} = \mathbf{V\Lambda}$$

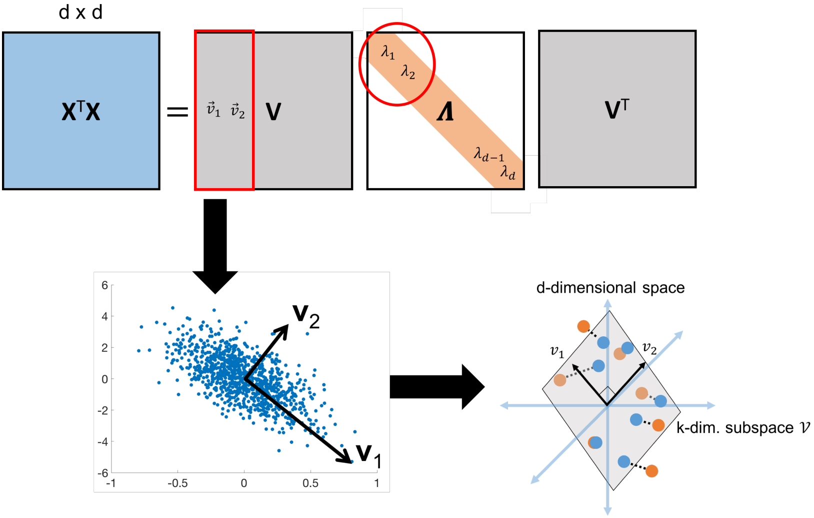
Yields eigendecomposition: $\mathbf{AVV}^T = \mathbf{A} = \mathbf{V\Lambda V}^T$.

Review of Eigenvectors and Eigendecomposition



Typically order the eigenvectors in decreasing order: $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$.

Low-Rank Approximation via Eigendecomposition



Low-Rank Approximation via Eigendecomposition

Upshot: Letting $\mathbf{V}_k$ have columns $\vec{v}_1, \ldots, \vec{v}_k$ corresponding to the top k eigenvectors of the covariance matrix $\mathbf{X}^T\mathbf{X}$, $\mathbf{V}_k$ is the orthogonal basis minimizing

$$\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2,$$

This is principal component analysis (PCA).

How accurate is this low-rank approximation? Can understand using eigenvalues of $\mathbf{X}^T\mathbf{X}$.

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $\mathbf{X}^T\mathbf{X}$, $\mathbf{V}_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Spectrum Analysis

Let $\vec{v}_1, \ldots, \vec{v}_k$ be the top k eigenvectors of X^TX (the top k principal components). Approximation error is:

$$\begin{aligned}
\|X - XV_kV_k^T\|_F^2 &= \|X\|_F^2 \operatorname{tr}(X^TX) - \|XV_kV_k^T\|_F^2 \operatorname{tr}(V_k^TX^TXV_k) \\
&= \sum_{i=1}^{d} \lambda_i(X^TX) - \sum_{i=1}^{k} \vec{v}_i^T X^T X \vec{v}_i \\
&= \sum_{i=1}^{d} \lambda_i(X^TX) - \sum_{i=1}^{k} \lambda_i(X^TX) = \sum_{i=k+1}^{d} \lambda_i(X^TX)
\end{aligned}$$

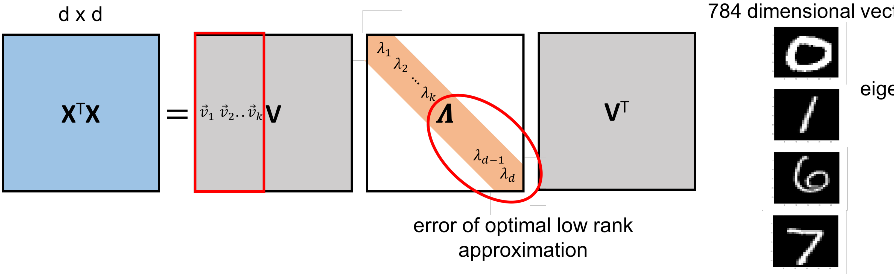
- **Exercise:** For any matrix A, $\|A\|_F^2 = \sum_{i=1}^{d} \|\vec{a}_i\|_2^2 = \operatorname{tr}(A^TA)$ (sum of diagonal entries = sum eigenvalues).

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $X \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of X^TX, $V_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Spectrum Analysis

Claim: The error in approximating $\mathbf{X}$ with the best rank k approximation (projecting onto the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$) is:

$$\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 = \sum_{i=k+1}^{d} \lambda_i(\mathbf{X}^T\mathbf{X})$$

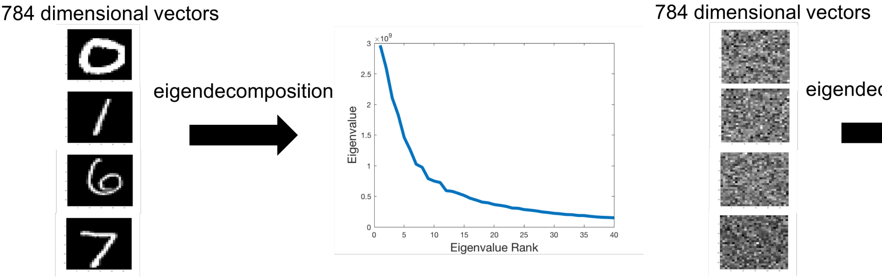


- Choose k to balance accuracy/compression – often at an ‘elbow’.

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $\mathbf{X}^T\mathbf{X}$, $\mathbf{V}_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

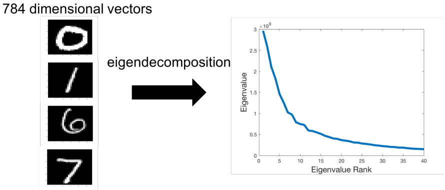
Spectrum Analysis

Plotting the spectrum of $X^T X$ (its eigenvalues) shows how compressible X is using low-rank approximation (i.e., how close $\vec{x}_1, \ldots, \vec{x}_n$ are to a low-dimensional subspace).



$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $X \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $X^T X$, $V_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Spectrum Analysis



Exercises:

1. Show that the eigenvalues of $\mathbf{X}^T\mathbf{X}$ are always positive. **Hint:** Use that $\lambda_j = \vec{v}_j^T\mathbf{X}^T\mathbf{X}\vec{v}_j$.
2. Show that for symmetric $\mathbf{A}$, the trace is the sum of eigenvalues: $\text{tr}(\mathbf{A}) = \sum_{i=1}^{n} \lambda_i(\mathbf{A})$. **Hint:** First prove the cyclic property of trace, that for any $\mathbf{M}\mathbf{N}$, $\text{tr}(\mathbf{M}\mathbf{N}) = \text{tr}(\mathbf{N}\mathbf{M})$ and then apply this to $\mathbf{A}$'s eigendecomposition.

Summary

- Many (most) datasets can be approximated via projection onto a low-dimensional subspace.
- Find this subspace via a maximization problem:

$$\max_{\text{orthonormal } \mathbf{V}} \|\mathbf{X}\mathbf{V}\|_F^2.$$

- Greedy solution via eigendecomposition of $\mathbf{X}^T\mathbf{X}$.
- Columns of $\mathbf{V}$ are the top eigenvectors of $\mathbf{X}^T\mathbf{X}$.
- Error of best low-rank approximation (compressibility of data) is determined by the tail of $\mathbf{X}^T\mathbf{X}$'s eigenvalue spectrum.

Interpretation in Terms of Correlation

Recall: Low-rank approximation is possible when our data features are correlated.

10000* bathrooms+ 10* (sq. ft.) ≈ list price

	bedrooms	bathrooms	sq.ft.	floors	list price	sale price
home 1	2	2	1800	2	200,000	195,000
home 2	4	2.5	2700	1	300,000	310,000
⋮	⋮	⋮	⋮	⋮	⋮	⋮
home n	5	3.5	3600	3	450,000	450,000

Our compressed dataset is $\mathbf{C} = \mathbf{X}\mathbf{V}_k$ where the columns of $\mathbf{V}_k$ are the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$.

Observe that $\mathbf{C}^T\mathbf{C} = \mathbf{\Lambda}_k$

C^TC is diagonal. I.e., all columns are orthogonal to each other, and correlations have been removed. Maximal compression.

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $\mathbf{X}^T\mathbf{X}$, $\mathbf{V}_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Algorithmic Considerations

Runtime to compute an optimal low-rank approximation:

- Computing $\mathbf{X}^T\mathbf{X}$ requires $O(nd^2)$ time.
- Computing its full eigendecomposition to obtain $\vec{v}_1, \ldots, \vec{v}_k$ requires $O(d^3)$ time (similar to the inverse $(\mathbf{X}^T\mathbf{X})^{-1}$).

Many faster iterative and randomized methods. Runtime is roughly $\tilde{O}(ndk)$ to output just to top k eigenvectors $\vec{v}_1, \ldots, \vec{v}_k$.

- Will see in a few classes (power method, Krylov methods).
- One of the most intensively studied problems in numerical computation.

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