COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Fall 2021.
Lecture 16

LOGISTICS

A/A- 85%

C - 50-55%

B 65-75%

- Problem Set 3 is posted. Due Monday 11/8, 11:59pm.
- I strongly encourage you to work together on the problems, rather than split them up.
- Midterms can be collected after class today. Solutions were posted in Moodle. The class average was a 34/40.
- Quiz this week due Monday at 8pm.

Last Class: Optimal Low-Rank Approximation

- When data lies close to $\mathcal{V}$, the optimal embedding in that space is given by projecting onto that space.

$$\mathbf{X}\mathbf{V}\mathbf{V}^T = \underset{\mathbf{B} \text{ with rows in } \mathcal{V}}{\arg\min} \|\mathbf{X} - \mathbf{B}\|_F^2.$$

- Optimal $\mathbf{V}$ maximizes $\|\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F$ and can be found greedily. Equivilantly by computing the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$.

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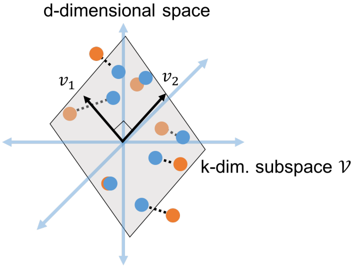
This Class:

- How do we assess the error of this optimal $\mathbf{V}$.
- Connection to the singular value decomposition.

BASIC SET UP

Reminder of Set Up: Assume that $\vec{x}_1, \ldots, \vec{x}_n$ lie close to any k-dimensional subspace $\mathcal{V}$ of $\mathbb{R}^d$. Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be the data matrix.



$$\begin{bmatrix} - x_1^T - \\ X \\ - x_n^T - \end{bmatrix}$$

Let $\vec{v}_1, \ldots, \vec{v}_k$ be an orthonormal basis for $\mathcal{V}$ and $\mathbf{V} \in \mathbb{R}^{d \times k}$ be the matrix with these vectors as its columns.

- $\mathbf{V}\mathbf{V}^T \in \mathbb{R}^{d \times d}$ is the projection matrix onto $\mathcal{V}$.
- $\mathbf{X} \approx \mathbf{X}(\mathbf{V}\mathbf{V}^T)$. Gives the closest approximation to $\mathbf{X}$ with rows in $\mathcal{V}$.

> $\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: 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 $\vec{v}_1, \ldots, \vec{v}_k$.

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

Pythagorean thm

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

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Solution via eigendecomposition: Letting $\mathbf{V}_k$ have columns $\vec{v}_1, \ldots, \vec{v}_k$ corresponding to the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$,

$$\mathbf{V}_k = \underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\max} \|\mathbf{X}\mathbf{V}\|_F^2$$

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: 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 $\vec{v}_1, \ldots, \vec{v}_k$.

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

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- Proof via Courant-Fischer and greedy maximization.

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: 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 $\vec{v}_1, \ldots, \vec{v}_k$.

V minimizing $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$ is given by: $\left[x_1 \; x_2 \; X^T \right]$

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

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- Proof via Courant-Fischer and greedy maximization.
- 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, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

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

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

$$V_k = \begin{array}{cc} & k \\ d & \begin{bmatrix} v_1 \; v_2 \cdots v_k \end{bmatrix} \end{array}$$

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: 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 $\vec{v}_1, \ldots, \vec{v}_k$.

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

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

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

$$\|XV_kV_k^T\|_F^2 = \|XV_k\|_F^2$$

$$n \left[XV_kV_k^T \right]$$

$$x_i^T V_k V_k^T$$

$$\|x_i^T V_k V_k^T\|_2^2 = \|x_i^T V_k\|_2^2$$

$$V_k^T V_k = I$$

A

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: 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 $\vec{v}_1, \ldots, \vec{v}_k$.

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$(A^TA)_{ii} = \|a_i\|_2^2$

A^TA

$n \times d$

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

$= tr(AA^T)$

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

$$\|X\|_F^2 - \|XV_k\|_F^2$$

$$\|X - XV_kV_k^T\|_F^2 = \text{tr}(X^TX) - \text{tr}(V_k^TX^TXV_k)$$

- **Exercise:** For any matrix A, $\|A\|_F^2 = \sum_{i=1}^d \|\vec{a}_i\|_2^2 = \text{tr}(A^TA)$ (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

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

$$\|X - XV_kV_k^T\|_F^2 = \mathrm{tr}(X^TX) - \mathrm{tr}(V_k^T X^T X V_k)$$

$$= \sum_{i=1}^{d} \lambda_i(X^TX) - \sum_{i=1}^{k} \underbrace{\vec{v}_i^T X^T X \vec{v}_i}_{?}$$

$1\times d \quad d\times d \quad d\times 1$

$$v_i^T (X^T X) v_i = v_i^T(\lambda_i \cdot v_i)$$
$$= \lambda_i \cdot v_i^T v_i = \lambda_i$$

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SPECTRUM ANALYSIS

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

$\|\mathbf{X}\|_F^2$ $\qquad$ $\|\mathbf{X}\mathbf{V}_k\|_F^2$

$$\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 = \text{tr}(\mathbf{X}^T\mathbf{X}) - \text{tr}(\mathbf{V}_k^T\mathbf{X}^T\mathbf{X}\mathbf{V}_k)$$
$$= \sum_{i=1}^{d} \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^{k} \vec{v}_i^T\mathbf{X}^T\mathbf{X}\vec{v}_i$$
$$= \sum_{i=1}^{d} \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^{k} \lambda_i(\mathbf{X}^T\mathbf{X})$$

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

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

$$\begin{aligned}\boxed{\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2} &= \operatorname{tr}(\mathbf{X}^T\mathbf{X}) - \operatorname{tr}(\mathbf{V}_k^T\mathbf{X}^T\mathbf{X}\mathbf{V}_k) \\ &= \sum_{i=1}^{d} \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^{k} \vec{v}_i^T\mathbf{X}^T\mathbf{X}\vec{v}_i \\ &= \sum_{i=1}^{d} \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^{k} \lambda_i(\mathbf{X}^T\mathbf{X}) = \boxed{\sum_{i=k+1}^{d} \lambda_i(\mathbf{X}^T\mathbf{X})}\end{aligned}$$

$\lambda_1(X^TX) \geq \lambda_2(X^TX) \geq \ldots \geq \lambda_d(X^TX)$

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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:

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

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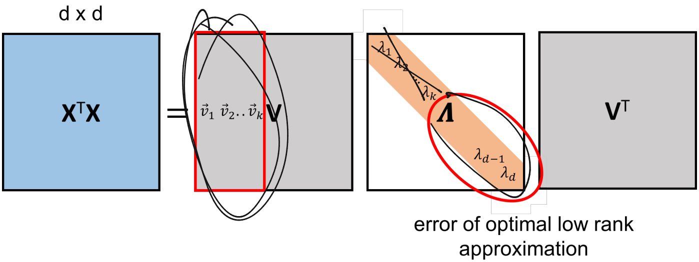

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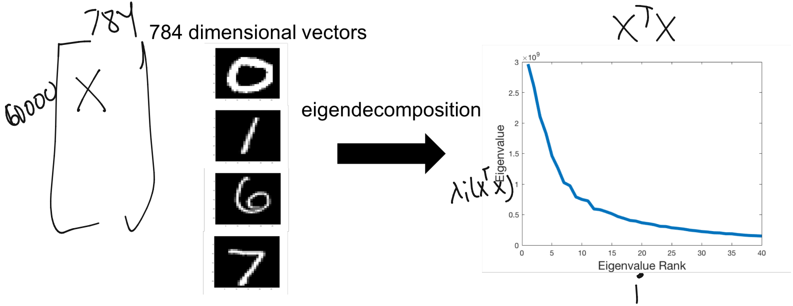

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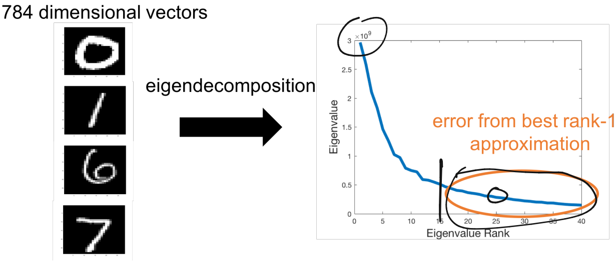

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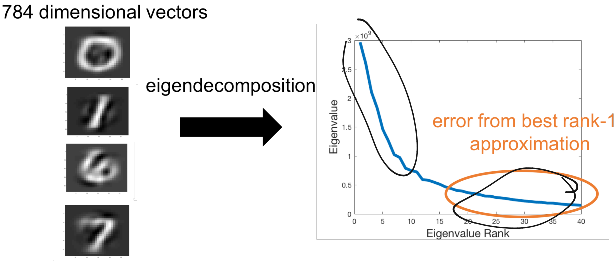

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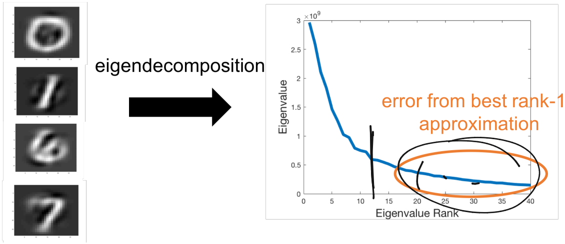
SPECTRUM ANALYSIS

Claim: The error in approximating X with the best rank k approximation (projecting onto the top k eigenvectors of X^TX is:

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

784 dimensional vectors



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

> $\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: 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 $\vec{v}_1, \ldots, \vec{v}_k$.

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

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SPECTRUM ANALYSIS

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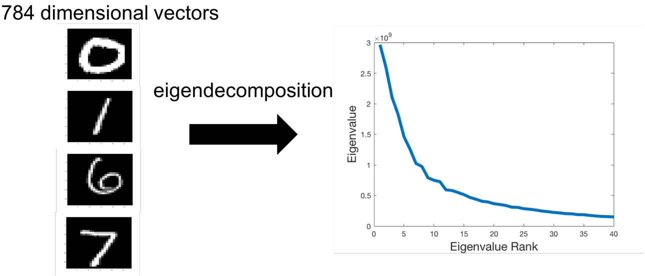

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Plotting the spectrum of $X^T X$ (its eigenvalues) shows how compressible X is using low-rank approximation (i.e., how close $\vec{x}_1, \ldots, \vec{x}_n$ are to a low-dimensional subspace).

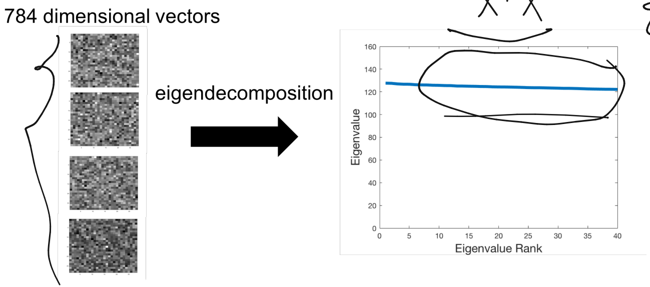
$\|X - XVV^T\|$ large

$\|X - XVV^T\|_F$

$\sum \|x_i - VV^T x_i\|_2$

$\frac{\log n}{\varepsilon^2}$

$X^T X$



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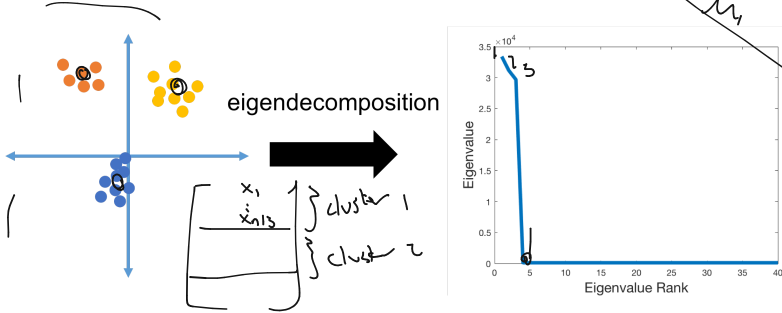
Plotting the spectrum of $\mathbf{X}^T\mathbf{X}$ (its eigenvalues) shows how compressible $\mathbf{X}$ is using low-rank approximation (i.e., how close $\vec{x}_1, \ldots, \vec{x}_n$ are to a low-dimensional subspace).



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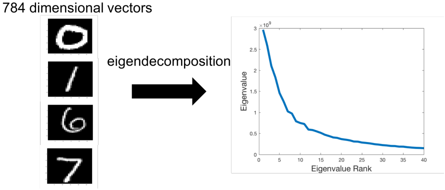
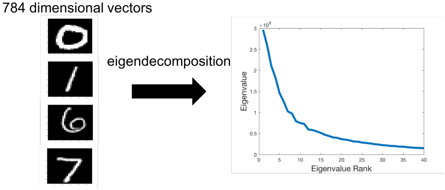
SPECTRUM ANALYSIS



Exercises:

, positive semidefinite

1. Show that the eigenvalues of $\mathbf{X}^T\mathbf{X}$ are always positive. **Hint:** Use that $\underline{\lambda_j = \vec{v}_j^T\mathbf{X}^T\mathbf{X}\vec{v}_j}$.



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 $\mathbf{MN}$, $\text{tr}(\mathbf{MN}) = \text{tr}(\mathbf{NM})$ and then apply this to $\mathbf{A}$'s eigendecomposition.

- 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.

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

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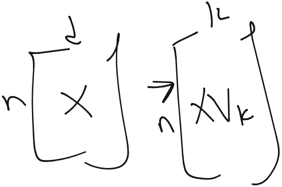
INTERPRETATION IN TERMS OF CORRELATION

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



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

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$d \times d$

$$\begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_d \end{bmatrix}$$

$$\begin{bmatrix} - & v_1^T & - \\ & \vdots & \\ - & v_k^T & - \end{bmatrix} V_k \begin{bmatrix} | & & | \\ v_1 & \cdots & v_d \\ | & & | \end{bmatrix}$$

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Observe that $\mathbf{C}^T\mathbf{C} = V_k^T X^T X V_k = \underbrace{V_k^T V}_{} \Lambda V^T V_k$

$k \times d \quad d \times d$

$$X^T X = V \Lambda V^T$$

$$\begin{array}{c} k \\ \begin{bmatrix} I & \vdots & 0 \end{bmatrix} k \end{array} \begin{bmatrix} \Lambda \end{bmatrix} \begin{bmatrix} I \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} \Lambda_k \end{bmatrix} k$$

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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.

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Runtime to compute an optimal low-rank approximation:

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$$d\left[\; \overset{n}{X^T} \;\right] \overset{d}{\left[\, X \,\right]} n = \overset{d}{\left[\; X^T X \;\right]} d$$

Runtime to compute an optimal low-rank approximation:

- Computing $X^T X$ requires $O(nd^2)$ time.

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Runtime to compute an optimal low-rank approximation:

- Computing $X^T X$ 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 $(X^T X)^{-1}$).

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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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