Computational Intelligence Laboratory

Lecture 2
Principal Component Analysis

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Section 1

1D Linear Case

Line in $\mathbb{R}^m$

- Let us try to understand linear dimension reduction in a principled manner. For ease of presentation: start with 1 dimension
- Parametric form of a line in $\mathbb{R}^m$

$$\boldsymbol{\mu} + \mathbb{R}\mathbf{u} \equiv \{\mathbf{v} \in \mathbb{R}^m : \exists z \in \mathbb{R} \text{ s.t. } \mathbf{v} = \boldsymbol{\mu} + z\mathbf{u}\}$$

  - $\boldsymbol{\mu}$: offset or shift
  - $\mathbf{u}$: direction vector, $\|\mathbf{u}\| = 1$
  - $\|\cdot\|$ or $\|\cdot\|_2$: Euclidean vector norm, $\|\mathbf{v}\|^2 = \sum_j v_j^2 = \langle \mathbf{v}, \mathbf{v} \rangle$
  - $\langle \cdot, \cdot \rangle$: inner or dot product, $\langle \mathbf{u}, \mathbf{v} \rangle = \mathbf{u}^\top \mathbf{v} = \sum_j u_j v_j$

Orthogonal Projection (1 of 2)

- Approximate data point $\mathbf{x} \in \mathbb{R}^m$ by a point on the line
  - minimize (squared) Euclidean distance
  - formally:

$$\text{Dimension Reduction} \quad \leftarrow \operatorname*{arg\,min}_{z \in \mathbb{R}} \|\boldsymbol{\mu} + z\mathbf{u} - \mathbf{x}\|^2$$

or

$$\text{Reconstruction} \quad \leftarrow \operatorname*{arg\,min}_{\hat{\mathbf{x}} \in \boldsymbol{\mu} + \mathbb{R}\mathbf{u}} \|\hat{\mathbf{x}} - \mathbf{x}\|^2$$

  - We know the answer! ❣

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  - We know the answer! ❣ **Orthogonal projection**.

Orthogonal Projection (2 of 2)

- Warm-up exercise: first order optimality condition

$$\frac{d}{dz}\|\boldsymbol{\mu} + z\mathbf{u} - \mathbf{x}\|^2 = 2\langle \boldsymbol{\mu} + z\mathbf{u} - \mathbf{x}, \mathbf{u}\rangle \stackrel{!}{=} 0$$

$$\iff \underbrace{\langle \mathbf{u}, \mathbf{u}\rangle}_{\|\mathbf{u}\|^2=1} z \stackrel{!}{=} \langle \mathbf{x} - \boldsymbol{\mu}, \mathbf{u}\rangle$$

- Solution(s):

$$z = \langle \mathbf{x} - \boldsymbol{\mu}, \mathbf{u}\rangle$$

$$\hat{\mathbf{x}} = \boldsymbol{\mu} + \langle \mathbf{x} - \boldsymbol{\mu}, \mathbf{u}\rangle\,\mathbf{u}$$

- Procedure: (1) shift by $-\boldsymbol{\mu}$, (2) project onto $\mathbf{u}$, (3) shift back by $\boldsymbol{\mu}$

Optimal Line: Formulation

- Assume we are given data points $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \subset \mathbb{R}^m$.
- What is their optimal approximation by a line?
  - use orthogonal projection result

$$
\begin{aligned}
(\mathbf{u}, \boldsymbol{\mu}) \leftarrow \arg\min & \left[\frac{1}{n} \sum_{i=1}^{n} \| \underbrace{\boldsymbol{\mu} + \langle \mathbf{x}_i - \boldsymbol{\mu}, \mathbf{u} \rangle \mathbf{u}}_{=\hat{\mathbf{x}}_i} - \mathbf{x}_i \|^2 \right] \\
&= \left[\frac{1}{n} \sum_{i=1}^{n} \left\| \left(\mathbf{I} - \mathbf{u}\mathbf{u}^\top \right) (\mathbf{x}_i - \boldsymbol{\mu}) \right\|^2 \right]
\end{aligned}
$$

  - some simple algebra
  - exploit identity $\langle \mathbf{v}, \mathbf{u} \rangle \mathbf{u} = (\mathbf{u}\mathbf{u}^\top)\mathbf{v}$

I minus U2?

- What does this matrix represent? $\left(\mathbf{I} - \mathbf{u}\mathbf{u}^\top\right)$
  - in general: a matrix represents a linear map (in specific basis)
- Specifically: take argument $\mathbf{v}$, we get (by associativity)

$$\left(\mathbf{I} - \mathbf{u}\mathbf{u}^\top\right)\mathbf{v} = \mathbf{v} - \underbrace{\langle \mathbf{u}, \mathbf{v} \rangle \mathbf{u}}_{\text{projection}}$$

  - so this is the vector itself minus the projection to the line $\mathbb{R}\mathbf{u}$
  - which is the projection to the orthogonal complement $(\mathbb{R}\mathbf{u})^\perp$
  - it is idempotent, because

$$\left(\mathbf{u}\mathbf{u}^\top\right)\left[\mathbf{v} - \langle \mathbf{u}, \mathbf{v} \rangle \mathbf{u}\right] = \langle \mathbf{u}, \mathbf{v} \rangle \mathbf{u} - \langle \mathbf{u}, \mathbf{v} \rangle \mathbf{u} = \mathbf{0}$$

Optimal Line: Solving for μ

- First order optimality condition for $\boldsymbol{\mu}$

$$\nabla_{\boldsymbol{\mu}}[\cdot] \stackrel{!}{=} 0 \iff \frac{1}{n}\sum_{i=1}^{n}\left(\mathbf{I}-\mathbf{u}\mathbf{u}^\top\right)(\mathbf{x}_i-\boldsymbol{\mu}) \stackrel{!}{=} 0$$

$$\iff \left(\mathbf{I}-\mathbf{u}\mathbf{u}^\top\right)\frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i \stackrel{!}{=} \left(\mathbf{I}-\mathbf{u}\mathbf{u}^\top\right)\boldsymbol{\mu}$$

  - does not determine $\boldsymbol{\mu}$ uniquely ❣

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  - does not determine $\boldsymbol{\mu}$ uniquely ❣
  - however, there is a unique (simultaneous) solution for all $\mathbf{u}$:

$$\boldsymbol{\mu} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i \quad \equiv \quad \textbf{sample mean}$$

Optimal Line: Conclusion #1

- By **centering** the data:

$$\mathbf{x}_i \leftarrow \mathbf{x}_i - \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i$$

  - restrict to **linear** (instead of affine) subspaces
  - identify center of mass of data with origin
  - simplifies derivations and analyses w/o loss in modeling power
  - w.l.o.g.: assume data points are **centered**

Optimal Line: Solving for $\mathbf{u}$ (1 of 3)

- We are left with
$$\mathbf{u} \leftarrow \arg\min_{\|\mathbf{u}\|=1} \left[\frac{1}{n} \sum_{i=1}^{n} \|\langle \mathbf{u}, \mathbf{x}_i \rangle \mathbf{u} - \mathbf{x}_i\|^2 \right]$$
- Expanding the squared norm
  - general formula
$$\|\mathbf{v} - \mathbf{w}\|^2 = \langle \mathbf{v} - \mathbf{w}, \mathbf{v} - \mathbf{w} \rangle = \|\mathbf{v}\|^2 + \|\mathbf{w}\|^2 - 2\langle \mathbf{v}, \mathbf{w} \rangle$$
  - yields: const $- \langle \mathbf{u}, \mathbf{x} \rangle^{\mathbf{2}}$ as
$$\begin{aligned} \|\langle \mathbf{u}, \mathbf{x} \rangle \mathbf{u}\|^2 &= \langle \mathbf{u}, \mathbf{x} \rangle^2 \\ \|\mathbf{x}\|^2 &= \text{const.} \\ -2\langle \langle \mathbf{u}, \mathbf{x} \rangle \mathbf{u}, \mathbf{x} \rangle &= -2\langle \mathbf{u}, \mathbf{x} \rangle^2 \end{aligned}$$

Optimal Line: Solving for $\mathbf{u}$ (2 of 3)

- We can equivalently solve

$$\mathbf{u} \leftarrow \operatorname*{arg\,max}_{\|\mathbf{u}\|=1} \left[\frac{1}{n} \sum_{i=1}^{n} \langle \mathbf{u}, \mathbf{x}_i \rangle^2 \right] = \left[\mathbf{u}^\top \left(\frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^\top \right) \mathbf{u} \right]$$

- Key statistics: **variance-covariance matrix** of the data sample

$$\boldsymbol{\Sigma} \equiv \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^\top = \frac{1}{n} \mathbf{X}\mathbf{X}^\top \in \mathbb{R}^{m \times m}, \quad \mathbf{X} \equiv [\mathbf{x}_1 \ldots \mathbf{x}_n]$$

Optimal Line: Solving for $\mathbf{u}$ (3 of 3)

- Constrained optimization with Lagrange multiplier λ

$$\mathcal{L}(\mathbf{u}, \lambda) = \mathbf{u}^\top \mathbf{\Sigma} \mathbf{u} + \lambda \langle \mathbf{u}, \mathbf{u} \rangle$$

- Minimize over $\mathbf{u} \implies \mathbf{u}$ is an **eigenvector** of $\mathbf{\Sigma}$, because

$$\nabla_{\mathbf{u}} \mathcal{L}(\mathbf{u}, \lambda) = 2(\mathbf{\Sigma} \mathbf{u} - \lambda \mathbf{u})$$

$$\nabla_{\mathbf{u}} \mathcal{L}(\mathbf{u}, \lambda) \stackrel{!}{=} 0 \iff \mathbf{\Sigma} \mathbf{u} = \lambda \mathbf{u}$$

- Maximize over $\lambda \implies \mathbf{u}$ is a **principal** eigenvector of $\mathbf{\Sigma}$ (one with the largest eigenvalue λ - why?)

Linear Algebra: Eigen-{Values & Vectors}

- Let $\mathbf{A}$ be a squared matrix, $\mathbf{A} \in \mathbb{R}^{m \times m}$.
- $\mathbf{u}$ is an **eigenvector** of $\mathbf{A}$, if exists $\lambda \in \mathbb{R}$ such that $\mathbf{A}\mathbf{u} = \lambda\mathbf{u}$
- such a λ is called an **eigenvalue**
- if $\mathbf{u}$ is eigenvector with eigenvalue λ, so is any $\alpha\mathbf{u}$ with $\alpha \in \mathbb{R}$
- $\mathbf{A}$ is called **positive semi-definite**, if

$$\mathbf{v}^\top \mathbf{A}\mathbf{v} \geq 0 \quad (\forall \mathbf{v})$$

- If $\mathbf{A} = \mathbf{B}^\top\mathbf{B}$ for some $\mathbf{B} \in \mathbb{R}^{n \times m}$, then $\mathbf{A}$ is p.s.d.

$$\mathbf{v}^\top \left(\mathbf{B}^\top\mathbf{B}\right)\mathbf{v} = (\mathbf{B}\mathbf{v})^\top(\mathbf{B}\mathbf{v}) = \|\mathbf{B}\mathbf{v}\|^2 \geq 0$$

Optimal Line: Conclusion #2

- Optimal direction = **principal eigenvector** of the sample variance-covariance matrix

- Extremal characterization

$$\mathbf{u} \leftarrow \arg\max_{\mathbf{v}:\|\mathbf{v}\|=1} \left[\mathbf{v}^\top \mathbf{\Sigma} \mathbf{v} \right]$$

Variance Maximization

- Re-interpret in term of variance maximization in 1d representation

$$\mathsf{Var}[z] = \frac{1}{n}\sum_{i=1}^{n} z_i^2 = \frac{1}{n}\sum_{i=1}^{n}\langle \mathbf{x}_i, \mathbf{u}\rangle^2 = \mathbf{u}^\top \mathbf{\Sigma}\mathbf{u}$$

  - remember: we subtracted the mean
  - same objective as before

- Direction of **smallest reconstruction error** $\iff$

  Direction of **largest data variance**

Section 2

Principal Component Analysis

Residual Problem

- Residual: projection to $(\mathbb{R}\mathbf{u})^{\perp}$

$$\mathbf{r}_i := \mathbf{x}_i - \tilde{\mathbf{x}}_i = \left(\mathbf{I} - \mathbf{u}\mathbf{u}^{\top}\right)\mathbf{x}_i$$

- Variance-covariance matrix of residual vectors

$$\begin{aligned}
\frac{1}{n}\sum_{i=1}^{n}\mathbf{r}_i\mathbf{r}_i^{\top} &= \frac{1}{n}\sum_{i=1}^{n}\left(\mathbf{I} - \mathbf{u}\mathbf{u}^{\top}\right)\mathbf{x}_i\mathbf{x}_i^{\top}\left(\mathbf{I} - \mathbf{u}\mathbf{u}^{\top}\right)^{\top} \\
&= \left(\mathbf{I} - \mathbf{u}\mathbf{u}^{\top}\right)\boldsymbol{\Sigma}\left(\mathbf{I} - \mathbf{u}\mathbf{u}^{\top}\right)^{\top} \\
&= \boldsymbol{\Sigma} - 2\underbrace{\boldsymbol{\Sigma}\mathbf{u}}_{=\lambda\mathbf{u}}\mathbf{u}^{\top} + \mathbf{u}\underbrace{\mathbf{u}^{\top}\boldsymbol{\Sigma}\mathbf{u}}_{=\lambda}\mathbf{u}^{\top} = \boldsymbol{\Sigma} - \lambda\mathbf{u}\mathbf{u}^{\top}
\end{aligned}$$

Iterative View

- What does this mean? Note that

$$\left(\mathbf{\Sigma} - \lambda \mathbf{u}\mathbf{u}^\top\right)\mathbf{u} = \lambda\mathbf{u} - \lambda\mathbf{u} = 0$$

  - so $\mathbf{u}$ is now an eigenvector with eigenvalue 0
- Because $\mathbf{\Sigma}$ is p.s.d., all eigenvalues are non-negative
- Repeating the above procedure:
  - we find the principal eigenvector of $\left(\mathbf{\Sigma} - \lambda \mathbf{u}\mathbf{u}^\top\right)$
  - which is the 2nd principal eigenvector of $\mathbf{\Sigma}$
  - we keep iterating to identify the d principal eigenvectors of $\mathbf{\Sigma}$
  - eigenvectors are guaranteed to be pairwise orthogonal

Diagonalization

- Let us take a matrix view (to complement the iterative one ...)
- $\mathbf{\Sigma}$ can be **diagonalized** by **orthogonal matrices**

$$\mathbf{\Sigma} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top, \quad \mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \dots, \lambda_m), \quad \lambda_1 \geq \dots \geq \lambda_m$$

where $\mathbf{U}$ is an orthogonal matrix (unit length, orthogonal columns)

$$\mathbf{U} = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \dots & \mathbf{u}_m \end{pmatrix},$$
$$\mathbf{U}^\top \mathbf{u}_i = \mathbf{e}_i, \quad \mathbf{\Sigma}\mathbf{u}_i = \lambda_i \mathbf{u}_i$$

i.e. the columns are eigenvectors (form an eigenvector basis).

Results from Linear Algebra

- $\mathbf{\Sigma}$ is symmetric, $\mathbf{\Sigma} = \mathbf{\Sigma}^\top$
  - obvious as $\sigma_{jk} = \frac{1}{n} \sum_i x_{ij} x_{ik}$
- **Spectral Theorem**: Matrix $\mathbf{A}$ is diagonalizable by an orthogonal matrix if and only if it is symmetric
  - $\mathbf{U}$ orthogonal: $\mathbf{U}^\top \mathbf{U} = \mathbf{U}\mathbf{U}^\top = \mathbf{I}$ (i.e. transpose $=$ inverse)
    - columns are normalized and orthogonal: $\langle \mathbf{u}_j, \mathbf{u}_k \rangle = \delta_{jk}$
- **Theorem**: Distinct eigenvalues of symmetric matrices have orthogonal eigenvectors

$$\mathbf{u}_1^\top \mathbf{A} \mathbf{u}_2 = \langle \mathbf{u}_1, \lambda_2 \mathbf{u}_2 \rangle \overset{\text{symm}}{=} \mathbf{u}_2^\top \mathbf{A} \mathbf{u}_1 = \langle \mathbf{u}_2, \lambda_1 \mathbf{u}_1 \rangle$$

$$\Longrightarrow (\lambda_1 - \lambda_2) \langle \mathbf{u}_1, \mathbf{u}_2 \rangle = 0 \overset{\lambda_1 \neq \lambda_2}{\Longrightarrow} \langle \mathbf{u}_1, \mathbf{u}_2 \rangle = 0$$

PCA: Final Answer

- What is the optimal **reduction** to d dimensions?
  - diagonalize $\mathbf{\Sigma}$ and pick the d principal eigenvectors

$$\tilde{\mathbf{U}} = \begin{pmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_d \end{pmatrix}, \quad d \leq m$$

  - dimension reduction

$$\mathbf{Z} = \underbrace{\tilde{\mathbf{U}}^\top}_{\in \mathbb{R}^{d \times m}} \underbrace{\mathbf{X}}_{\in \mathbb{R}^{m \times n}} \in \mathbb{R}^{d \times n}$$

- What is the optimal **reconstruction** in d dimensions?
  - use eigenbasis

$$\tilde{\mathbf{X}} = \tilde{\mathbf{U}}\mathbf{Z} = \underbrace{\tilde{\mathbf{U}}\tilde{\mathbf{U}}^\top}_{\text{projection}} \mathbf{X}$$

Section 3

Algorithms & Interpretation

Power Method

- Simple algorithm for finding dominant eigenvector of $\mathbf{A}$
- **Power iteration**

$$\mathbf{v}_{t+1} = \frac{\mathbf{A}\mathbf{v}_t}{\|\mathbf{A}\mathbf{v}_t\|}$$

  - assumptions: $\langle \mathbf{u}_1, \mathbf{v}_0 \rangle \neq 0$ and $|\lambda_1| > |\lambda_j|$ $(\forall j \geq 2)$
- Then it follows:

$$\lim_{t\to\infty} \mathbf{v}_t = \mathbf{u}_1$$

  - recover λ_1 from Rayleigh quotient $\lambda_1 = \lim_{t\to\infty} \|\mathbf{A}\mathbf{v}_t\|/\|\mathbf{v}_t\|$

Power Method: Proof Sketch

- Focus on $\mathbf{\Sigma}$ (p.s.d. and symmetric): eigenbasis $\{\mathbf{u}_1, \ldots, \mathbf{u}_m\}$

$$\mathbf{v}_0 = \sum_{j=1}^{m} \alpha_j \mathbf{u}_j, \quad \alpha_1 \neq 0$$

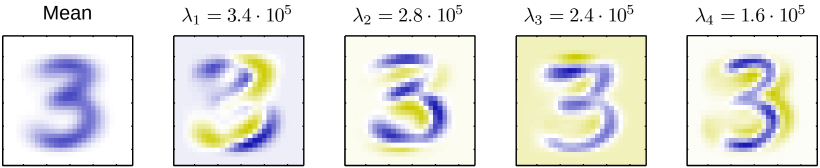
- Evolution equation:

$$\mathbf{v}_t = \frac{1}{c_t} \sum_{j=1}^{m} \alpha_j \lambda_j^t \mathbf{u}_j = \frac{\lambda_1^t \alpha_1}{c_t} \left[\mathbf{u}_1 + \sum_{j=2}^{m} \frac{\alpha_j}{\alpha_1} \underbrace{\left(\frac{\lambda_j}{\lambda_1} \right)^t}_{\to 0} \mathbf{u}_j \right] \stackrel{t \to \infty}{\longrightarrow} \mathbf{u}_1$$

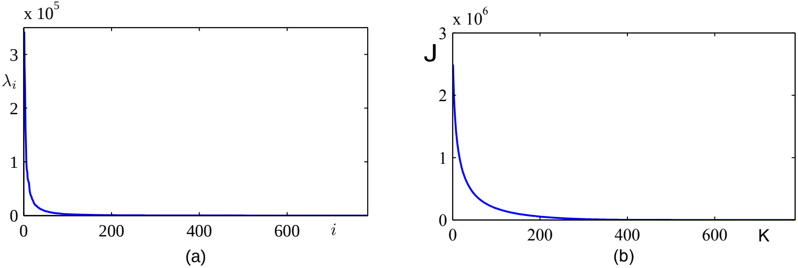
  - as $\lambda_j / \lambda_1 < 1$ and thus $c_t \to 1/(\lambda_1^t \alpha_1)$ (as $\|\mathbf{u}_1\| = 1$)

Digits Example

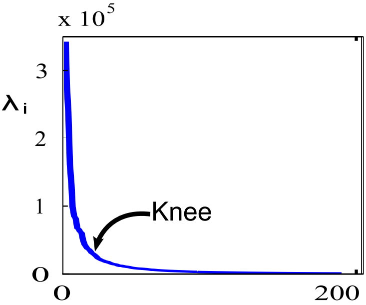
- Mean vector and first four principal directions:



- Eigenvalue spectrum (left), and approximation error (right):



Model Selection in PCA



- Eigenvalue spectrum: can help determine intrinsic dimensionality
- Heuristic: detect "knee" in eigenspectrum (= dimension)

Comparison w/ Linear Autoencoder Network

- PCA clarifies that one should (ideally) **center** the data
- PCA representation is unique (if no eigenvalue multiplicities) and as such (in principle) **interpretable**
- Linear autoencoder w/o weight sharing is highly non-interpretable (lack of identifiability)
- Linear autoencoder w/ weight sharing: $\mathbf{A} = \mathbf{B}^\top$ only identifies a subspace, but axis are non-identifiable
  - can an autoencoder be modified to identify the principle axes?
- General lesson: caution with naïvely interpreting learned (neural) representations

Algorithms: Comparison

- Compute PCA one component at a time via **power iterations**: good for small k, conceptually easy and robust
- Train a linear autoencoder via **backpropagation** (see subsequent lecture): easily extensible, stochastic optimization
- Compute PCA from **SVD**: good for mid-sized problems, can leverage wealth of numerical techniques for SVD (e.g. QR decomposition)

PCA via SVD (1 of 3)

- Can compute **eigen-decomposition** of $\mathbf{A}\mathbf{A}^\top$ via SVD
  - straightforward calculation

$$\begin{aligned}\mathbf{A}\mathbf{A}^\top &= \left(\mathbf{U}\mathbf{D}\mathbf{V}^\top\right)\left(\mathbf{V}\mathbf{D}^\top\mathbf{U}^\top\right) \\ &= \mathbf{U}\,\underbrace{\mathbf{D}\cdot\mathbf{I_n}\cdot\mathbf{D}^\top}_{\mathsf{diag}(\lambda_1,\ldots,\lambda_m)}\,\mathbf{U}^\top = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\top\end{aligned}$$

where **eigenvalues** relate to **singular values**

$$\lambda_i = \begin{cases}\sigma_i^2 & \text{for } 1 \le i \le \min\{m, n\} \\ 0 & \text{for } n < i \le m\end{cases}$$

PCA via SVD (2 of 3)

- Similarly $\mathbf{A}^\top \mathbf{A} = \mathbf{V}\mathbf{\Lambda}'\mathbf{V}^\top$, where

$$\mathbf{\Lambda}' = \text{diag}(\lambda'_1, \ldots, \lambda'_n), \quad \lambda'_i = \begin{cases} \lambda_i & \text{for } 1 \leq i \leq \min\{m, n\} \\ 0 & \text{for } m < i \leq n \end{cases}$$

- Interpretation
  - columns of $\mathbf{U}$: eigenvectors of $\mathbf{A}\mathbf{A}^\top$
  - columns of $\mathbf{V}$: eigenvectors of $\mathbf{A}^\top \mathbf{A}$
  - eigenvalues: $\mathbf{\Lambda}$ and $\mathbf{\Lambda}'$ (identical up to zero padding)
    - $\mathbf{\Lambda} = \mathbf{D}\mathbf{D}^\top \in \mathbb{R}^{m \times m}$
    - $\mathbf{\Lambda}' = \mathbf{D}^\top \mathbf{D} \in \mathbb{R}^{n \times n}$

PCA via SVD (3 of 3)

- Assume that $\mathbf{X}$ is a **centered data matrix**
- SVD of $\mathbf{X}$ can be used to compute eigendecomposition of $\mathbf{\Sigma}$
  - variance-covariance matrix: $\mathbf{\Sigma} = \frac{1}{n}\mathbf{X}\mathbf{X}^\top$
  - often $n \gg m$: reduced SVD sufficient