Advances in Dimensionality Reduction

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DR Reduces the Feature Space

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Data

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Data

- p samples

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- p samples
- d dimensional ambient space

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- p samples
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- Dataset $\mathcal{D}$ (d features)

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- Dataset $\mathcal{D}$ (d features)
- Reduced dataset $\mathcal{R}$ (k features)

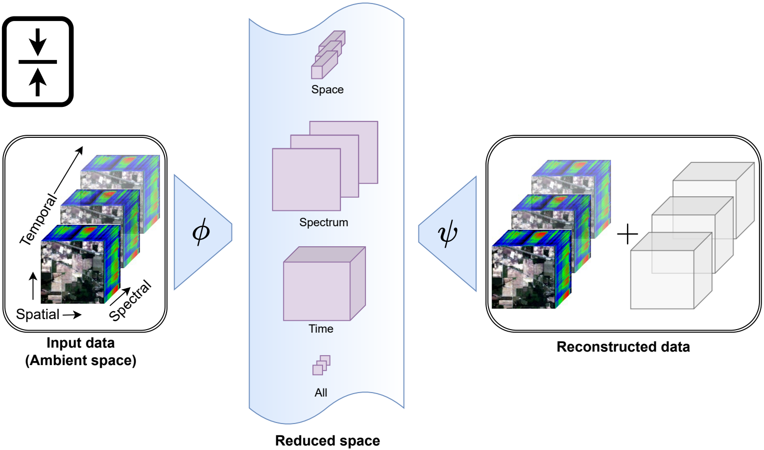
Dimensionality Reduction (DR) maps d-dimensional features to k-dimensional features ($k < d$).

Why DR?

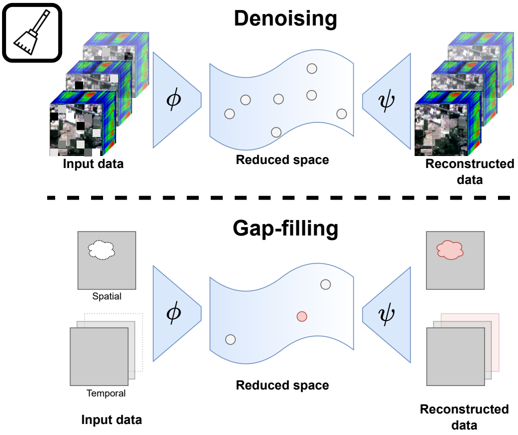
Why DR?

- Compression
- Denoising
- Fusion
- Visualization y D
- Anomaly detection
- Improving predictions

Compression

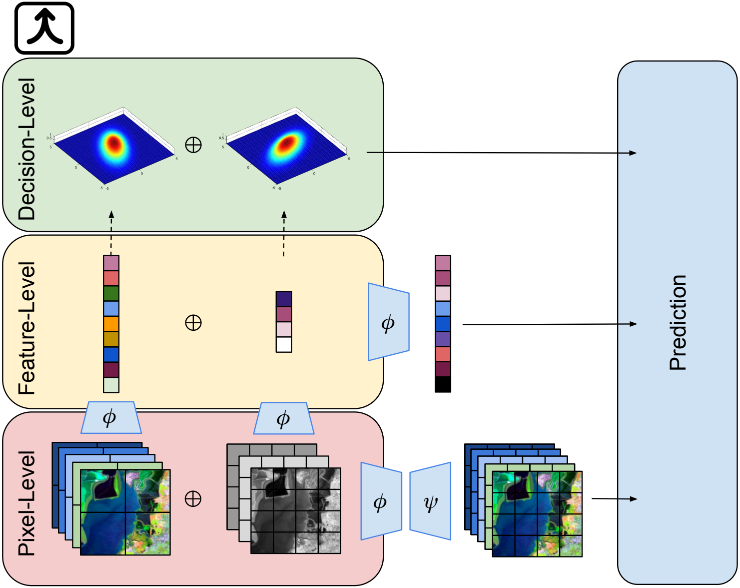


Denoising

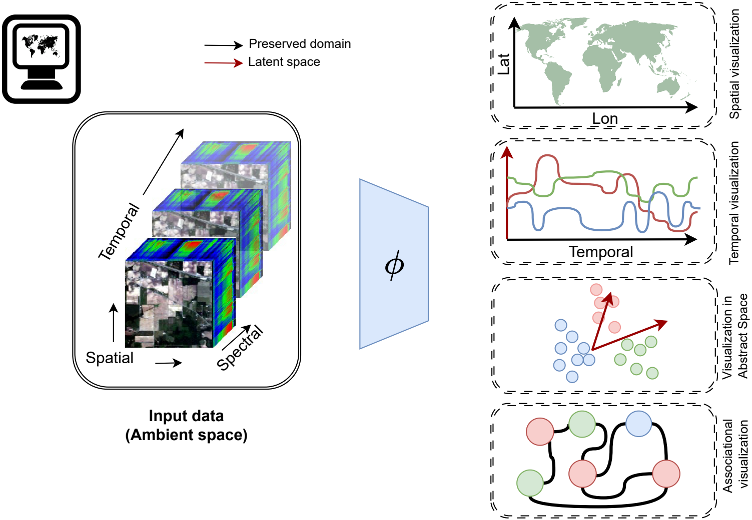


Denoising
Input data
ϕ
Reduced space
ψ
Reconstructed data
Gap-filling
Spatial
Temporal
Input data
ϕ
Reduced space
ψ
Reconstructed data

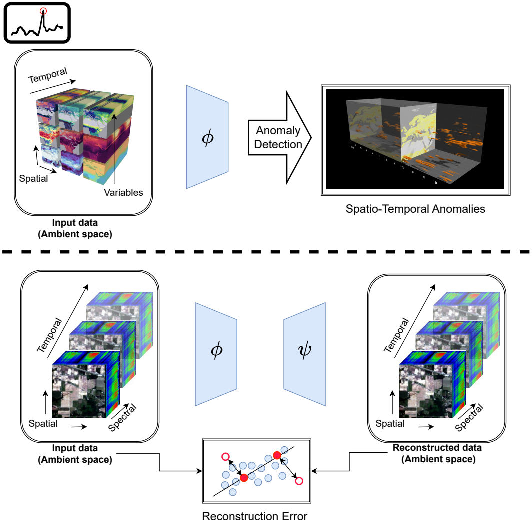
Fusion


Decision-Level
Feature-Level
Pixel-Level
Prediction
$\oplus$
ϕ
ψ

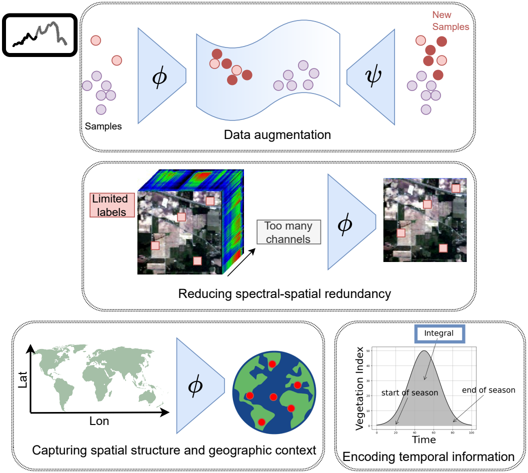
Visualization



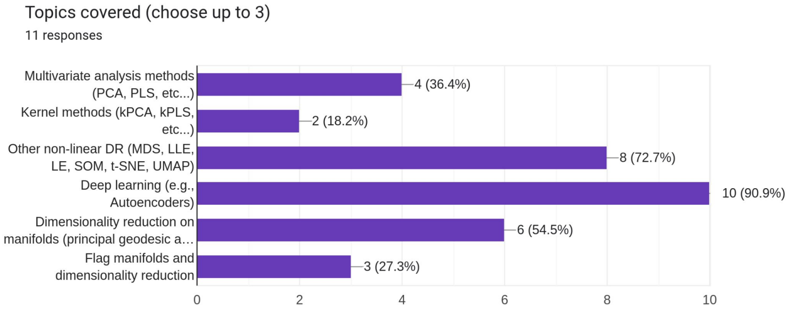
Anomaly Detection



Improved Predictions



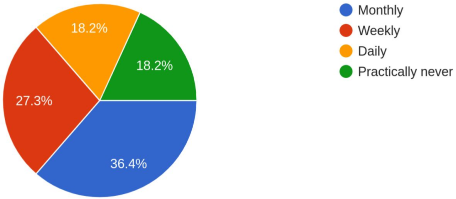
Survey Results



Survey Results

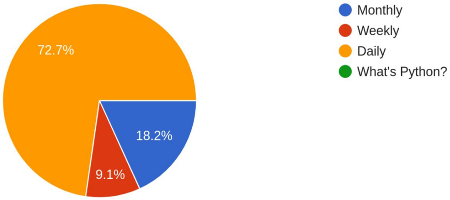
How often do you use linear algebra

11 responses



Survey Results

How often do you code in python?
11 responses



Course Outline

1. Linear Algebra Review
2. Intro to DR
3. Linear Dimensionality Reduction
4. Nonlinear Dimensionality Reduction
5. Neural Network-Based Methods

Linear Algebra Review

Further reading [Strang, 2000]

Outline

1. Vectors & Inner Products
2. Subspaces, Orthogonality, Projections
3. Singular Value Decomposition (SVD)
4. Eigenvalue Decomposition

Field Axioms

A field F is a set equipped with two operations (addition and multiplication) satisfying the following axioms for all $a, b, c \in F$:

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- **Inverses:**
  - Additive inverse: for every $a \in F$, there exists $-a \in F$ such that $a + (-a) = 0$
  - Multiplicative inverse: for every $a \neq 0$ in F, there exists $a^{-1} \in F$ such that $a \cdot a^{-1} = 1$

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- **Distributivity:** $a \cdot (b + c) = (a \cdot b) + (a \cdot c)$

The set of all real numbers (denoted $\mathbb{R}$) is a Field

- Addition and multiplication operations
- Additive identity is 0
- Multiplicative identity is 1

Exercise: Show that $\mathbb{R}$ satisfies the axioms of a field, whereas $\mathbb{Z}$ (the set of all integers) does not.

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- **Commutativity of addition:** $\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u}$
- **Additive identity:** There exists $\mathbf{0} \in V$ such that $\mathbf{v} + \mathbf{0} = \mathbf{v}$
- **Additive inverse:** For each $\mathbf{v} \in V$, there exists $-\mathbf{v} \in V$ such that $\mathbf{v} + (-\mathbf{v}) = \mathbf{0}$
- **Compatibility with scalar multiplication:** $a(b\mathbf{v}) = (ab)\mathbf{v}$
- **Identity element of scalar multiplication:** $1\mathbf{v} = \mathbf{v}$, where 1 is the multiplicative identity in F
- **Distributivity over vector addition:** $a(\mathbf{u} + \mathbf{v}) = a\mathbf{u} + a\mathbf{v}$
- **Distributivity over field addition:** $(a + b)\mathbf{v} = a\mathbf{v} + b\mathbf{v}$

$\mathbb{R}^2$ is a Vector Space

$\mathbb{R}^2$ is a Vector Space over $\mathbb{R}$.

$$\mathbb{R}^2 = \left\{\mathbf{a} = \begin{bmatrix} a_1 & a_2 \end{bmatrix} \,:\, a_1, a_2 \in \mathbb{R}\right\}$$

Exercise: Show that $\mathbb{R}^2$ satisfies the axioms of a vector space.

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- **Angle between vectors**

$$\cos(\theta) = \frac{\mathbf{a}^\top \mathbf{b}}{\mathbf{a}^\top \mathbf{a} \mathbf{b}^\top \mathbf{b}}$$

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$$\operatorname{span}(\mathbf{a}, \mathbf{b}) = \alpha\mathbf{a} + \beta\mathbf{b} \;:\; \alpha, \beta \in \mathbb{R} \tag{1}$$

Linear Independence

A set of vectors $\{v_1, v_2, \ldots, v_k\}$ in a vector space V is **linearly independent** if:

$$c_1 v_1 + c_2 v_2 + \cdots + c_k v_k = 0 \quad \Rightarrow \quad c_1 = c_2 = \cdots = c_k = 0$$

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Example:

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

are linearly independent in $\mathbb{R}^2$, since neither can be written as a multiple of the other.

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Example: The standard basis for $\mathbb{R}^3$ is:

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The **dimension** of a vector space V is the number of elements in a basis for V.

Matrices

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix}$$

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- The **row space** of $\mathbf{A}$ (denoted $\mathrm{row}(\mathbf{A})$) is the set of linear combinations of rows.
- The **column space** of $\mathbf{A}$ (denoted $\mathrm{col}(\mathbf{A})$) is the set of linear combinations of columns.

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- The **rank** of **A** is the dimension of its column space.

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- The **rank** of $\mathbf{A}$ is the dimension of its column space.
- The **trace** of $\mathbf{A}$ is the sum of the diagonal entries

$$\mathrm{tr}(\mathbf{A}) = a_{11} + a_{22}$$

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- The Frobenius norm of $\mathbf{A}$ is

$$\|\mathbf{A}|_F = \sqrt{\mathrm{tr}(\mathbf{A}^\top \mathbf{A})}$$

Matrix multiplication

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}$$

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Lab 1: Vectors & Matrices

Go to Lab1_VectorsMatrices.ipynb

Projections

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Projection of **b** onto col(**A**):

$$\mathbf{\Pi}_{\mathbf{A}}(\mathbf{b}) = \mathbf{A}(\mathbf{A}^\top\mathbf{A})^{-1}\mathbf{A}^\top\mathbf{b}$$

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Projection of $\mathbf{b}$ onto $\mathrm{col}(\mathbf{A})$:

$$\mathbf{\Pi}_{\mathbf{A}}(\mathbf{b}) = \mathbf{A}(\mathbf{A}^\top \mathbf{A})^{-1}\mathbf{A}^\top \mathbf{b}$$

Exercise: If the columns of $\mathbf{A}$ are orthogonal, show that the projection onto the column space of $\mathbf{A}$ is $\mathbf{A}\mathbf{A}^\top$.

Singular Value Decomposition (SVD)

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- $\mathbf{U} \in \mathbb{R}^{p \times r}$: left singular vectors, $\mathbf{U}^\top\mathbf{U} = \mathbf{I}$
- $\boldsymbol{\Sigma} \in \mathbb{R}^{r \times r}$: diagonal matrix of singular values
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Applications: dimensionality reduction, image compression, linear systems.

Eigenvalue Decomposition from SVD

Given the SVD

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The Eigenvalue Decomposition of $\mathbf{A}^\top\mathbf{A}$ is

$$\mathbf{C} = \mathbf{A}^\top\mathbf{A} = \mathbf{V}\boldsymbol{\Sigma}^\top\boldsymbol{\Sigma}\mathbf{V}^\top = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^\top$$

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- **Eigenvectors**: columns of $\mathbf{V}$, $\mathbf{V}^\top\mathbf{V} = \mathbf{I}$
- **Eigenvalues**: diagonal of $\boldsymbol{\Sigma}$

Eigenvalue Decomposition from SVD

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Exercises:

- Show the eigenvalue decomposition of $\mathbf{A}^\top\mathbf{A}$ is $\mathbf{U}\mathbf{\Sigma}\mathbf{\Sigma}^\top\mathbf{U}^\top$
- Show the trace of $\mathbf{C}$ is the sum of its eigenvalues

Eigenvalue Optimization Formulation

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1. **Raleigh quotient:**

$$\lambda_i = \max_{\mathbf{v}^\top \mathbf{v}_j = 0 \ \forall j < i} \frac{\mathbf{v}^\top \mathbf{C} \mathbf{v}}{\mathbf{v}^\top \mathbf{v}}$$

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3. **Reconstruction error**:

$$\mathbf{V} = \arg\min_{\mathbf{W}^\top \mathbf{W} = \mathbf{I}} \|\mathbf{A} - \mathbf{A}\mathbf{W}\mathbf{W}^\top\|_F^2$$

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Exercise: Show that these optimizations are equivalent.

Generalized Eigenvalue Decomposition

Solve:

$$\mathbf{C}_A \mathbf{w} = \lambda \mathbf{C}_B \mathbf{w}$$

Optimization form:

$$\lambda_i = \max_{\mathbf{w}^\top \mathbf{w}_j = 0 \; \forall j < i} \frac{\mathbf{w}^\top \mathbf{C}_A \mathbf{w}}{\mathbf{w}^\top \mathbf{C}_B \mathbf{w}}$$

Approximate with:

$$\mathbf{C}_B^{-1} \mathbf{C}_A$$

Use SVD for pseudo-inverse:

- $\mathbf{C}_B = \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^\top$
- $\mathbf{C}_B^\dagger = \mathbf{V} \boldsymbol{\Sigma}^{-1} \mathbf{U}^\top$

Condition number:

$$\kappa(\mathbf{C}_B) = \frac{\sigma_{\max}}{\sigma_{\min}}$$

Big κ bad, Small κ good

Lab 2: Matrix Decompsitions

Go to Lab2_MatrixDecompositions.ipynb

The Landscape of Dimensionality Reduction

Inspired by Lee and Verleysen [2007]

DR Reduces the Feature Space

DR Reduces the Feature Space

Data

DR Reduces the Feature Space

Data

- p samples

DR Reduces the Feature Space

Data

- p samples
- d dimensional ambient space

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- p samples
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- Dataset $\mathcal{D}$ (d features)

DR Reduces the Feature Space

Data

- p samples
- d dimensional ambient space
- Dataset $\mathcal{D}$ (d features)
- Reduced dataset $\mathcal{R}$ (k features)

Dimensionality Reduction (DR) maps d-dimensional features to k-dimensional features ($k < d$).

Why DR?

Why DR?

give me 5 fake and funny quotes from researchers about how DR changed their life

Sure! Here are 5 fake and funny quotes from fictional researchers on how dimensionality reduction (DR) changed their lives:

---

1. *"Before PCA, my life was just noise. Now it's all principal components — including my dating life!"*
— **Dr. Ada Scatter**, Romantic Data Scientist

---

2. *"I applied t-SNE to my thoughts and finally found out why I kept forgetting my keys."*
— **Prof. Moe Mentz**, Cognitive Chaos Lab

---

3. *"After discovering manifold learning, I realized my career path wasn't linear either — just locally Euclidean."*
— **Dr. Lin E. Ar**, Nonlinear Trajectory Researcher

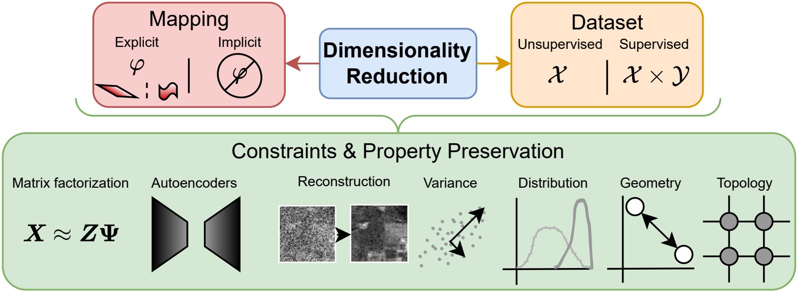
---

4. *"With UMAP, I reduced my midlife crisis to just two dimensions: wine and existential dread."*
— **Dr. Max E. Stress**, Professor of Reduced Expectations

---

5. *"Autoencoders helped me compress my emotions. Now I only cry in low resolution."*
— **Dr. Dee Pression**, Deep Learning Enthusiast

DR Summary



Mapping
Explicit
φ
Implicit
Dimensionality Reduction
Dataset
Unsupervised
$\mathcal{X}$
Supervised
$\mathcal{X} \times \mathcal{Y}$
Constraints & Property Preservation
Matrix factorization
$\boldsymbol{X} \approx \boldsymbol{Z\Psi}$
Autoencoders
Reconstruction
Variance
Distribution
Geometry
Topology

Dataset

Unsupervised
$\mathcal{D} = \mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_p\} \subset \mathbb{R}^d$

e.g., Visualize data in 2D to see if there are any patterns

Dataset

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$\mathcal{D} = \mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_p\} \subset \mathbb{R}^d$

e.g., Visualize data in 2D to see if there are any patterns

Supervised
$\mathcal{D} = \{\mathcal{X}, \mathcal{Y}\}, = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_p\}, \{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_p\}$

e.g., Find a low-dimensional, discriminatory feature space w.r.t. $\mathcal{Y}$

DR Mapping

DR Mapping

Explicit DR mapping outputs ϕ where

$$\phi(\mathbf{x}_i) = \mathbf{z}_i$$

- Approximate inverse $\psi \approx \phi^{-1}$
- Reconstructions: $\mathbf{x}_i \approx \hat{\mathbf{x}}_i = \psi(\phi(\mathbf{x}_i))$

e.g., Want to fit a model on some data, then apply it to "unseen" data.

Implicit: ϕ, ψ are not explicitly defined but inferred

e.g., Model fit on all the data to be reduced

Matrix Factorization

Matrix Factorization

Data matrix: $\mathbf{X} = [\mathbf{x}_1 \cdots \mathbf{x}_p]^\top \in \mathbb{R}^{p \times d}$

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The model:

$$\mathbf{X} \approx \mathbf{Z}\boldsymbol{\Psi}$$

Autoencoders

Autoencoders

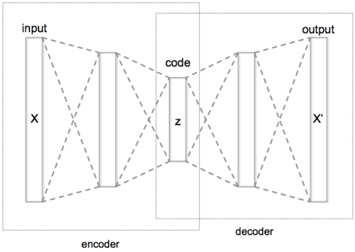
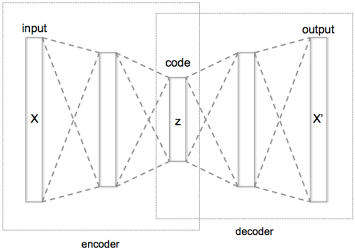


Figure: Image from
https://commons.wikimedia.org/wiki/File:Autoencoder_structure.png

Autoencoders



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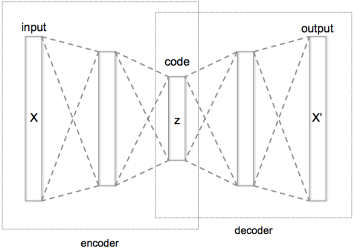
- Neural networks trained to reconstruct input

Autoencoders



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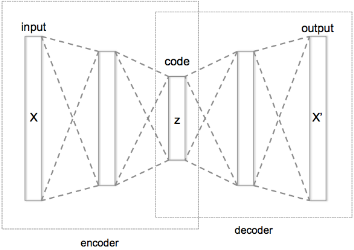
- Neural networks trained to reconstruct input
- Bottleneck structure forces compression

Autoencoders



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- Encoder: $\phi(\mathbf{x}) = \mathbf{z}$, Decoder: $\psi(\mathbf{z}) = \hat{\mathbf{x}}$

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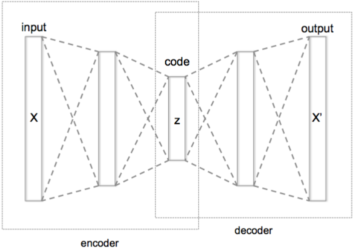

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- Encoder: $\phi(\mathbf{x}) = \mathbf{z}$, Decoder: $\psi(\mathbf{z}) = \hat{\mathbf{x}}$
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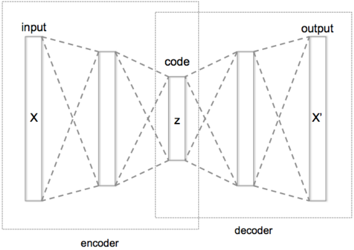
Autoencoders



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- Loss: e.g., MSE $\sum_i \|\mathbf{x}_i - \psi \circ \phi(\mathbf{x}_i)\|^2$
- Variants: Denoising, Variational (VAE), Convolutional

DR as Optimization

$$\arg\min_{\mathcal{Z}} \quad L(\mathcal{X}, \mathcal{Z}) \tag{3}$$

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$$\arg\min_{\mathcal{Z}} \quad L(\mathcal{X}, \mathcal{Z}) \tag{3}$$

This general form preserves

- Reconstructions
- Variance
- Probability distributions
- Geometry
- Graph structures

Reconstruction-preserving

Reconstruction-preserving

$$
\begin{aligned}
&\min_{\psi,\phi} \sum_{i=1}^{p} \|\mathbf{x}_i - \psi \circ \phi(\mathbf{x}_i)\|^2 \\
&\text{s.t. } \phi : \mathbb{R}^d \to \mathbb{R}^k, \quad \psi : \mathbb{R}^k \to \mathbb{R}^d
\end{aligned} \tag{4}
$$

Reconstruction-preserving

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$$\text{s.t. } \phi : \mathbb{R}^d \to \mathbb{R}^k, \quad \psi : \mathbb{R}^k \to \mathbb{R}^d \tag{4}$$

Useful when interpretability or invertibility is important.

Variance-preserving

Data matrix: $\mathbf{X} = [\mathbf{x}_1 \cdots \mathbf{x}_p]^\top$

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$$\begin{aligned} \Phi = \arg\max \ & \mathrm{Tr}(\mathbf{W}^\top \mathbf{X}^\top \mathbf{X} \mathbf{W}) \\ \text{s.t. } & \mathbf{W}^\top \mathbf{W} = I \end{aligned} \tag{5}$$

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Here, we assume the DR mapping is linear: $\phi(\mathbf{x}_i) = \mathbf{W}^\top \mathbf{x}_i$

Distribution-preserving

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- P "true" (target) data distribution
- Q "predicted" (modeled) data distribution

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$$H(P, Q) = -\sum_{x \in \mathcal{X}} P(x) \log Q(x) = -\sum_{x \in \mathcal{X}} P(x) \log P(x) + \mathrm{KL}(P \,||\, Q)$$

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Kullback–Leibler (KL) Divergence

$$\mathrm{KL}(P \,||\, Q) = H(P, Q) - H(P) = \sum_{x \in \mathcal{X}} P(x) \log \frac{P(x)}{Q(x)} \tag{6}$$

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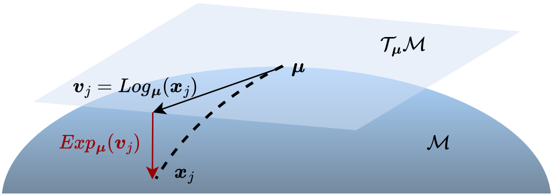
1. Determine two distributions to compare
2. Minimize KL divergence directly
3. With conditional distributions, max Evidence Lower BOund (ELBO)

Geometry-preserving



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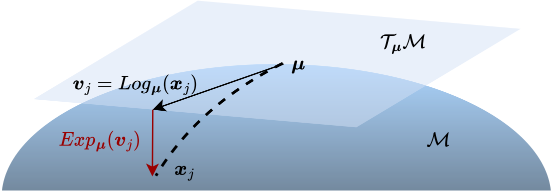

Manifold Hypothesis: High-dimensional data lies (approximately) on a low-dimensional manifold $\mathcal{M} \subset \mathbb{R}^d$.

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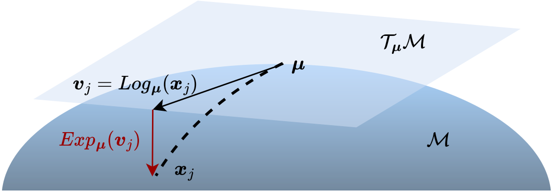

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Local Linearity: Around each $\mathbf{x}_i \in \mathcal{M}$, there exists a neighborhood U such that:

$$\mathcal{M} \cap U \approx T_{\mathbf{x}_i}\mathcal{M}$$

where $T_{\mathbf{x}_i}\mathcal{M}$ is the tangent space at $\mathbf{x}_i$.

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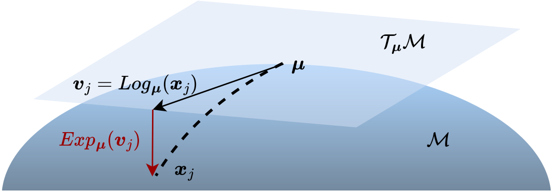

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where $T_{\mathbf{x}_i}\mathcal{M}$ is the tangent space at $\mathbf{x}_i$.

Geodesic Distances: For $\mathbf{x}_i, \mathbf{x}_j \in \mathcal{M}$, define

$$d_{\mathcal{M}}(\mathbf{x}_i, \mathbf{x}_j) = \text{length of shortest path on } \mathcal{M}$$

Improves global geometry preservation.

Topology-preserving

Goal: Dimensionality reduction often assumes a topology that determines local neighborhoods and connectivity.

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Data-driven topology (learned):

- Construct graph $G = (\mathcal{X}, E)$ from data.
- Edge weights: $w_{ij} = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{\sigma^2}\right)$ or k-nearest neighbors.
- Preserve graph in low-dimensional representation

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- Preserve graph in low-dimensional representation

Predefined topology (fixed):

- Impose grid or lattice structure: $\mathcal{G} = 1\text{D}$ or 2D lattice.
- Each reduce-space representation $\mathbf{z}_i$ corresponds to a fixed node in $\mathcal{G}$.

Linear Dimensionality Reduction

Outline

1. Principal Component Analysis Hotelling [1933]; Shlens [2014]
   - Dataset
   - Optimization Problem
   - Transformation
   - Explained Variance
2. Linear Discriminant Analysis Tharwat et al. [2017]
   - What is LDA?
   - Mathematical Formalization
   - Optimization Problem

Dataset

We consider a dataset of p samples with d features:

$$\{\mathbf{x}_i\}_{i=1}^{p} \subset \mathbb{R}^d$$

We collect the dataset into a matrix:

$$\mathbf{X} \in \mathbb{R}^{p \times d}$$

Important: The data must be **mean-centered**:

$$\frac{1}{p}\sum_{i=1}^{p} \mathbf{x}_i = \mathbf{0}$$

Optimization Goal

We aim to extract $k < p$ features that provide an accurate low-dimensional reconstruction of the samples.

We want to find directions of **maximum variance**:

$$\mathbf{V} = \arg\max_{\mathbf{W}^\top\mathbf{W}=\mathbf{I}} \sum_i (\mathbf{W}\mathbf{x}_i)^\top (\mathbf{W}\mathbf{x}_i)$$

$$= \arg\max_{\mathbf{W}^\top\mathbf{W}=\mathbf{I}} \mathrm{tr}(\mathbf{W}^\top \mathbf{X}^\top \mathbf{X}\mathbf{W})$$

Alternative Formulation: Reconstruction Error

This is equivalent to finding the rank-k projection:

$$\mathbf{\Pi}_{\mathbf{W}}(\mathbf{x}) := \mathbf{W}\mathbf{W}^\top\mathbf{x}$$

We solve:

$$\mathbf{V} = \arg\min_{\mathbf{W}^\top\mathbf{W}=\mathbf{I}} \mathbb{E}\left[\|\mathbf{x}_i - \mathbf{W}\mathbf{W}^\top\mathbf{x}_i\|_2^2\right]$$

Exercise Show that this is an eigenvalue problem.

Transformation

We call $\mathbf{V}$ the matrix of **PCA weights** or **Empirical Orthogonal Functions (EOFs)**.

The first k principal components of $\mathbf{X}$:

$$\hat{\mathbf{X}} = \mathbf{X}\mathbf{V} \in \mathbb{R}^{p \times k}$$

PCA map of an individual sample:

$$\hat{\mathbf{x}} = \mathbf{V}^\top \mathbf{x} \in \mathbb{R}^{k}$$

Explained Variance

The **explained variance** is how much variance each principal component captures:

Variance of component *i*:

$$\lambda_i = \mathbf{v}_i^\top \mathbf{X}^\top \mathbf{X} \mathbf{v}_i$$

Explained variance ratio of component *n*:

$$\frac{\lambda_n}{\sum_{j=1}^{n} \lambda_j}$$

This helps select the number of components to keep...

Rule of thumb is select components that explain $> 90\%$ *of variance.*

When to Use PCA

- Have unlabeled data
- Want to reduce dimensionality while preserving variance
- Want a fast, interpretable linear projection
- Want to decorrelate features
- Few outliers

Lab 3: PCA

Go to Lab3_PCA.ipynb

What is LDA?

Linear Discriminant Analysis (LDA) is a supervised dimensionality reduction technique.

Goal: Project high-dimensional data onto a lower-dimensional space that best separates multiple classes.

- Maximizes **between-class variance**
- Minimizes **within-class variance**

"PCA with class information!"

Mathematical Formulation

Given labeled dataset:

$$\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{p}, \quad \mathbf{x}_i \in \mathbb{R}^d$$

Number of classes: C.

Within-class scatter matrix:

$$S_W = \sum_{c=1}^{C} \sum_{\mathbf{x}_i \in c} (\mathbf{x}_i - \mu_c)(\mathbf{x}_i - \mu_c)^\top$$

Between-class scatter matrix:

$$S_B = \sum_{c=1}^{C} (\mu_c - \mu)(\mu_c - \mu)^\top$$

Optimization Problem

We solve the following generalized eigenvalue problem:

$$\mathbf{W} = \arg\max_{\mathbf{W}} \frac{\mathrm{tr}(\mathbf{W}^\top S_B \mathbf{W})}{\mathrm{tr}(\mathbf{W}^\top S_W \mathbf{W})}$$

Output:

- $\mathbf{W} \in \mathbb{R}^{d \times k}$: projection matrix
- $k \leq C - 1$: max number of discriminative components

Reduced data:

$$\mathbf{z}_i = \mathbf{W}^\top \mathbf{x}_i$$

When to Use LDA

- Labeled data
- Want low-dimensional features that separate classes well
- Want a fast, interpretable linear projection
- Linearly separable classes
- Each class follows a multivariate normal distribution with equal covariances

LDA vs PCA

Aspect	**PCA** Shlens [2014]	**LDA** Tharwat et al. [2017]
Supervised?	No	Yes
Objective	Maximize variance	Maximize class separation
Axes chosen	max variance	best separation
Max dimensions	$\leq$ input dimension	$\leq$ number of classes -1

Lab 3: LDA

Go to Lab4_LDA.ipynb

Harold Hotelling. Analysis of a complex of statistical variables into principal components. *Journal of educational psychology*, 24(6):417, 1933.

John A Lee and Michel Verleysen. *Nonlinear dimensionality reduction*. Springer Science & Business Media, 2007.

Jonathon Shlens. A tutorial on principal component analysis. *arXiv preprint arXiv:1404.1100*, 2014.

Gilbert Strang. *Linear algebra and its applications*. 2000.

Alaa Tharwat, Tarek Gaber, Abdelhameed Ibrahim, and Aboul Ella Hassanien. Linear discriminant analysis: A detailed tutorial. *AI communications*, 30(2):169–190, 2017.