Advances in Dimensionality Reduction

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DR Reduces the Feature Space

- p samples
- d dimensional ambient space
- Input dataset $\mathcal{D}$ (d features)
- Output: reduced dataset $\mathcal{R}$ (k features)

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

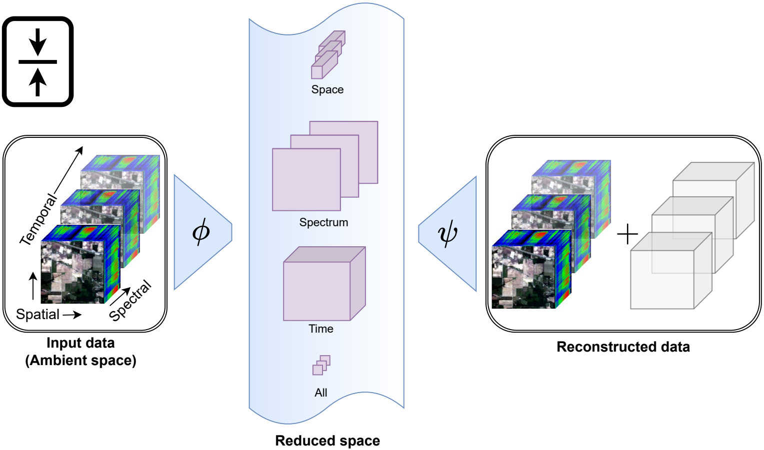
Question: Why do we want to use dimensionality reduction?

Dimensionality Reduction in Remote Sensing

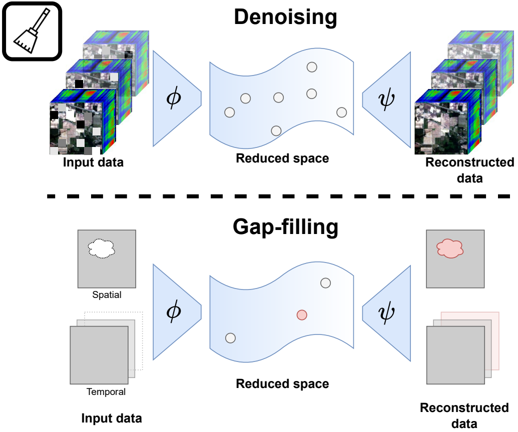
Input a data cube with spectral, spatial, and temporal dimensions.

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

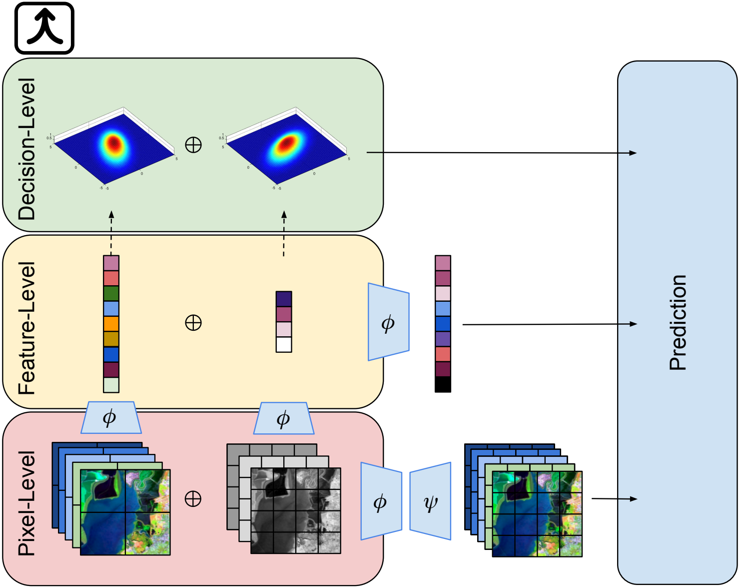
Compression



Denoising

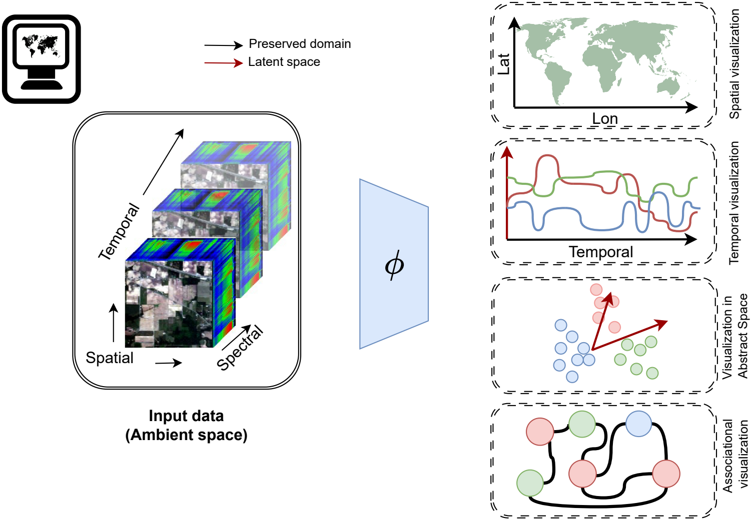

Denoising
ϕ
ψ
Input data
Reduced space
Reconstructed data
Gap-filling
Spatial
Temporal
ϕ
ψ
Reduced space
Input data
Reconstructed data

Fusion

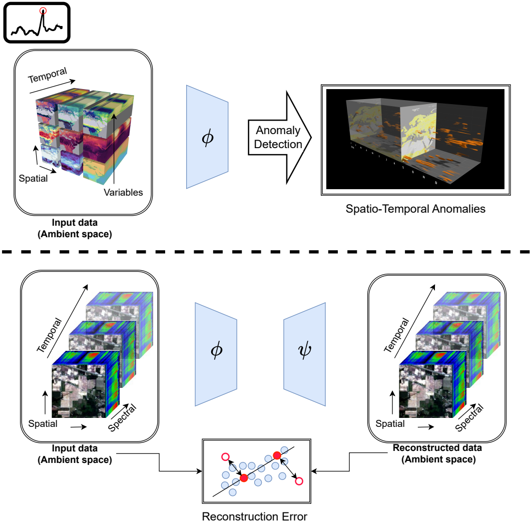


Decision-Level
⊕
Feature-Level
⊕
ϕ
Pixel-Level
⊕
ϕ
ϕ
ϕ
ψ
Prediction

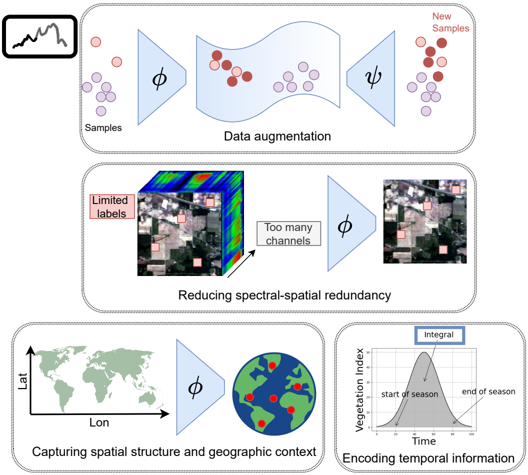
Visualization



Anomaly Detection

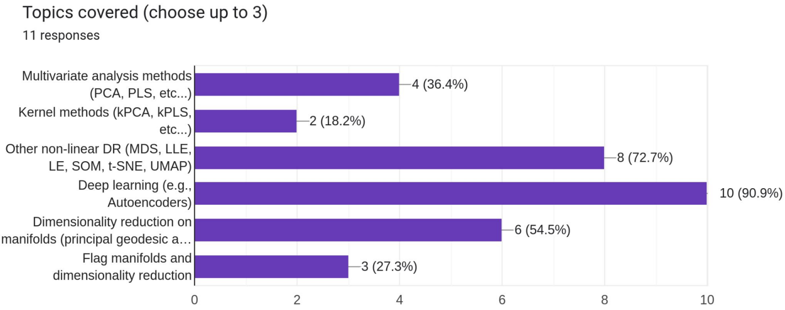


Improved Predictions



Course Survey Results

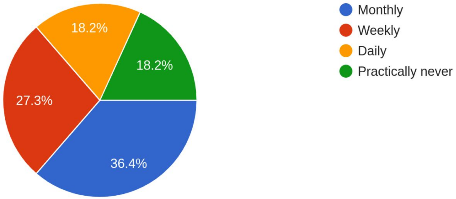
Survey Results



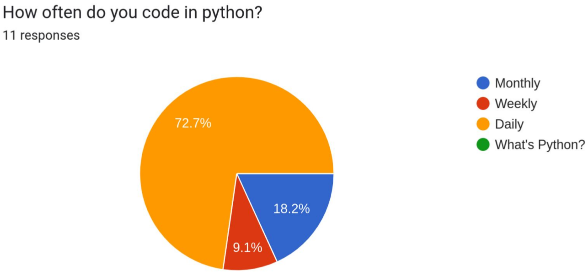
Survey Results

How often do you use linear algebra

11 responses



Survey Results



Course Outline

1. Linear Algebra Review
2. Intro to DR
3. Linear Dimensionality Reduction
4. Nonlinear Dimensionality Reduction
5. Autoencoders

Linear Algebra Review

Further reading [Strang, 2000]

Outline

1. Vectors & Inner Products
2. Subspaces, Orthogonality, Projections
3. Matrix Decompositions
4. Gradient Descent

Vectors & Inner Products

Field Axioms

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

- **Associativity:**
  - Addition: $a + (b + c) = (a + b) + c$
  - Multiplication: $a \cdot (b \cdot c) = (a \cdot b) \cdot c$
- **Commutativity:**
  - Addition: $a + b = b + a$
  - Multiplication: $a \cdot b = b \cdot a$
- **Identities:**
  - Additive identity: there exists $0 \in F$ such that $a + 0 = a$
  - Multiplicative identity: there exists $1 \in F$, $1 \neq 0$, such that $a \cdot 1 = a$
- **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 $a \cdot a^{-1} = 1$
- **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.

Vector Space Axioms

A vector space over a field F satisfies the following axioms for all $\mathbf{u}, \mathbf{v}, \mathbf{w} \in V$ and all scalars $a, b \in F$:

- **Associativity of addition:** $\mathbf{u} + (\mathbf{v} + \mathbf{w}) = (\mathbf{u} + \mathbf{v}) + \mathbf{w}$
- **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.

Dot Product & Friends

- **Transpose**

$$\mathbf{a}^\top = \begin{bmatrix} a_1 & a_2 \end{bmatrix}$$

- **Dot product**

$$\mathbf{a}^\top \mathbf{b} = a_1 b_1 + a_2 b_2$$

Two vectors are called "orthogonal" if their dot product is zero.

- 2-**Norm**

$$\|\mathbf{a}\|_2 = \sqrt{\mathbf{a}^\top \mathbf{a}}$$

- **Distance**

$$\|\mathbf{a} - \mathbf{b}\|_2$$

- **Angle between vectors**

$$\cos(\theta) = \frac{\mathbf{a}^\top \mathbf{b}}{\|\mathbf{a}\|_2 \|\mathbf{b}\|_2}$$

Span

The *span of two vectors* $\mathbf{a}, \mathbf{b}$ is the set of all vectors that can be written as a linear combination of $\mathbf{a}$ and $\mathbf{b}$

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

Linear Independence

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

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

In other words, the only solution to the linear combination equaling zero is the **trivial solution**.

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.

What is a Basis?

A **basis** of a vector space V is a set of vectors $\{v_1, v_2, \ldots, v_n\} \subset V$ such that:

1. The vectors are **linearly independent**.
2. The vectors **span** V, i.e., every vector in V can be written as a linear combination of $v_1, \ldots, v_n$.

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

$$\left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$$

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

Subspaces, Orthogonality, Projections

Matrices

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

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

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

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

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

Matrix multiplication

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

Projections

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

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

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

Lab 1: Vectors & Matrices

Go to Lab1_VectorsMatrices.ipynb

Matrix Decompositions

Singular Value Decomposition (SVD)

SVD of matrix $\mathbf{A} \in \mathbb{R}^{p \times d}$ of rank r:

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

- $\mathbf{U} \in \mathbb{R}^{p \times r}$: left singular vectors, $\mathbf{U}^\top\mathbf{U} = \mathbf{I}$
- $\boldsymbol{\Sigma} \in \mathbb{R}^{r \times r}$: diagonal matrix of singular values
- $\mathbf{V}^\top \in \mathbb{R}^{r \times d}$: right singular vectors, $\mathbf{V}^\top\mathbf{V} = \mathbf{I}$

Applications: dimensionality reduction, image compression, linear systems.

Eigenvalue Decomposition from SVD

Given the SVD

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

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

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

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

Exercises:

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

Eigenvalue Optimization Formulation

1. **Raleigh quotient:**

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

2. **Via trace**:

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

3. **Reconstruction error**:

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

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:

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

Big κ bad, Small κ good

Lab 2: Matrix Decompsitions

Go to Lab2_MatrixDecompositions.ipynb

Gradient Descent

Gradient Descent: Overview

- Gradient Descent is an optimization algorithm to minimize a function
- It iteratively moves in the direction of steepest descent (negative gradient)

Objective

Minimize a loss function $f(\theta)$, where:

- θ are the model parameters

Update Rule

At each iteration, the parameters are updated as:

$$\theta_{t+1} = \theta_t - \eta \nabla f(\theta_t)$$

- θ_t: Current parameters at iteration t
- η: Learning rate (step size)
- $\nabla f(\theta_t)$: Gradient of the loss function

The Landscape of Dimensionality Reduction

Inspired by Lee and Verleysen [2007]

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?

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:

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

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

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

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

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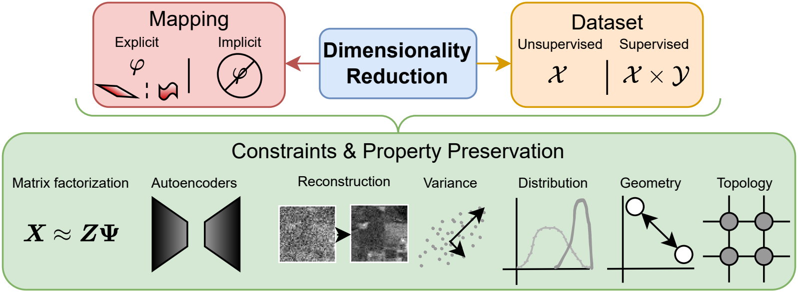
5. *"Autoencoders helped me compress my emotions. Now I only cry in low resolution."*
— **Dr. Dee Pression**, Deep Learning Enthusiast

DR Summary


Mapping
Explicit
φ
Implicit
Dimensionality Reduction
Dataset
Unsupervised
Supervised
$\mathcal{X}$
$\mathcal{X} \times \mathcal{Y}$
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

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

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

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

Reduced data matrix: $\mathbf{Z} = [\mathbf{z}_1 \cdots \mathbf{z}_p]^\top \in \mathbb{R}^{p \times k}$

The model:

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

Autoencoders

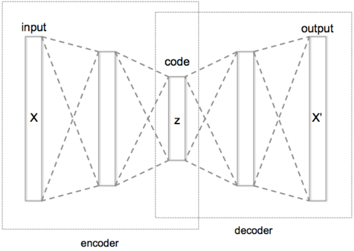


Figure: Image from
https://commons.wikimedia.org/wiki/File:Autoencoder_structure.png

- Neural networks trained to reconstruct input
- Bottleneck structure forces compression
- Encoder: $\phi(\mathbf{x}) = \mathbf{z}$, Decoder: $\psi(\mathbf{z}) = \hat{\mathbf{x}}$
- Loss: e.g., MSE $\sum_i \|\mathbf{x}_i - \psi \circ \phi(\mathbf{x}_i)\|^2$
- Variants: Denoising, Variational (VAE), Convolutional

DR as Optimization

$$\underset{\mathcal{Z}}{\arg\min} \quad L(\mathcal{X}, \mathcal{Z})$$

This general form preserves

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

Reconstruction-preserving

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

Useful when interpretability or invertibility is important.

Variance-preserving

Data $\mathbf{x}$ and DR mapping $\phi : \mathbb{R}^d \to \mathbb{R}^k$

$$\phi = \arg\max \mathbb{E}[\phi(\mathbf{x})^\top \phi(\mathbf{x})] \tag{2}$$

Distribution-preserving

- P "true" (target) distribution with distribution functon p
- Q "predicted" (modeled) distribution with distribution functon q

Entropy

$$H(p) = -\sum_{x \in \mathcal{X}} p(x) \log p(x)$$

Cross Entropy

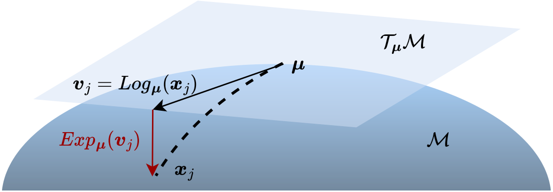
$$H(p, q) = -\sum_{x \in \mathcal{X}} p(x) \log q(x) = -\sum_{x \in \mathcal{X}} p(x) \log p(x) + \mathrm{KL}(p \,||\, q)$$

Kullback–Leibler (KL) Divergence

$$\mathrm{KL}(p \,||\, q) = H(p, q) - H(p) = \sum_{x \in \mathcal{X}} p(x) \log \frac{p(x)}{q(x)}$$

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

Geometry-preserving



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

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 $\mathbf{x}_i$.

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.

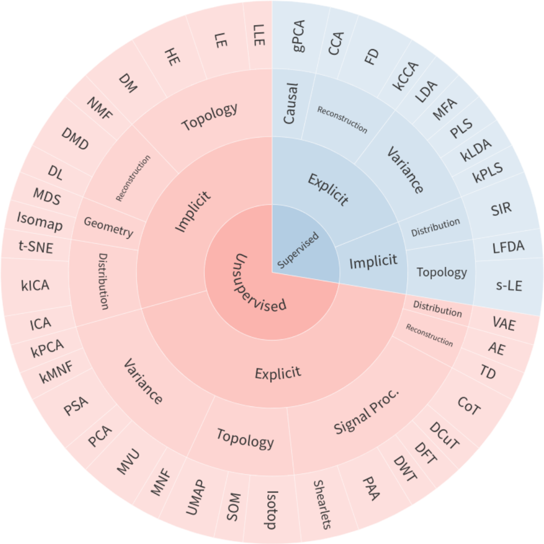
Data-driven topology (learned):

- 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

Predefined topology (fixed):

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

Too Many DR Methods..



Linear Dimensionality Reduction

Outline

1. Principal Component Analysis [Hotelling, 1933; Shlens, 2014]

2. Linear Discriminant Analysis [Tharwat et al., 2017]

3. Dynamic Mode Decomposition [Schmid, 2010]

Principal Component Analysis

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 describe the directions of maximum variance.

We find the jth direction of maximum variance as

$$\mathbf{v}_j = \underset{\substack{\mathbf{v}^\top \mathbf{v}=1 \\ \mathbf{v}^\top \mathbf{v}_\ell=0\ \forall \ell<i}}{\arg\max} \sum_i (\mathbf{v}\mathbf{x}_i)^\top (\mathbf{v}\mathbf{x}_i) \tag{3}$$

$$= \underset{\substack{\mathbf{v}^\top \mathbf{v}=1 \\ \mathbf{v}^\top \mathbf{v}_\ell=0\ \forall \ell<i}}{\arg\max} \sum_i \|\mathbf{x}_i\|_2^2 \cos\theta(\mathbf{v}, \mathbf{x}_i) \tag{4}$$

$$= \underset{\substack{\mathbf{v}^\top \mathbf{v}=1 \\ \mathbf{v}^\top \mathbf{v}_\ell=0\ \forall \ell<i}}{\arg\max} \ \mathbf{v}^\top \mathbf{X}^\top \mathbf{X} \mathbf{v} \tag{5}$$

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 we can find the EOFs (columns of $\mathbf{V}$) via eigendecomposition of $\mathbf{X}^\top \mathbf{X}$ or the SVD of $\mathbf{X}$.

PCA Objective Summary

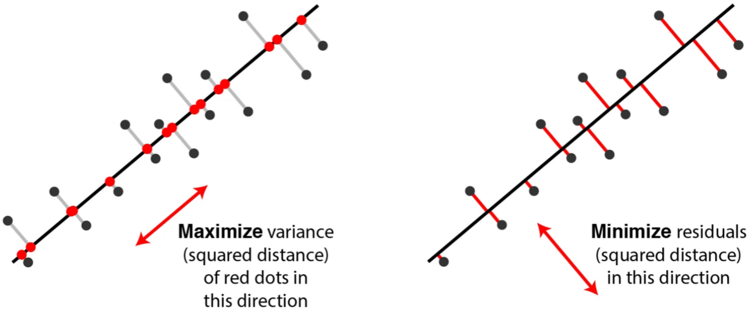


Figure: Image borrowed from `https://medium.com/@fraidoonomarzai99/principal-component-analysis-pca-in-depth-93c871f25dfa`.

Transformation

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

1st EOF is direction of maximum variance, 2nd EOF in direction of maximum variance that is orthogonal to 1st EOF, and so on ...

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

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

PCA map of an individual sample:

$$\mathbf{z} = \phi(\mathbf{x}) = \mathbf{V}^\top \mathbf{x} \in \mathbb{R}^k$$

PCA reconstruction of an individual sample:

$$\hat{\mathbf{x}} = \psi \circ \phi(\mathbf{x}) = \mathbf{V}\mathbf{V}^\top \mathbf{x} = \mathbf{\Pi}_{\mathbf{V}}(\mathbf{x}) \in \mathbb{R}^d$$

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:

$$\frac{\lambda_n}{\sum_{j=1}^{d} \lambda_j} = \frac{\lambda_n}{\mathrm{tr}(\mathbf{X}^\top \mathbf{X})}$$

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

Rule of thumb is select components that explain $> 90\%$ *of variance. (but there's other methods [Gavish and Donoho, 2014])*

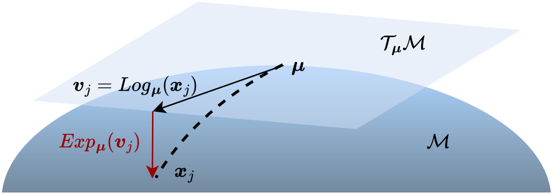
When to Use PCA

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

Beyond PCA... robust subspace recovery [Lerman and Maunu, 2018] & flag manifolds [Mankovich et al., 2024; Szwagier and Pennec, 2024, 2025]

Aside- PCA on Manifolds (Tangent-PCA)

Assume data samples from known, Riemannian manifold...



- Map data to tangent space
- Run PCA in tangent space
- Map back to manifold

Read more here: [Fletcher et al., 2004; Pennec, 2018]

Lab 3: PCA

Go to Lab3_PCA.ipynb

Linear Discriminant Analysis

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!"

LDA Intuition

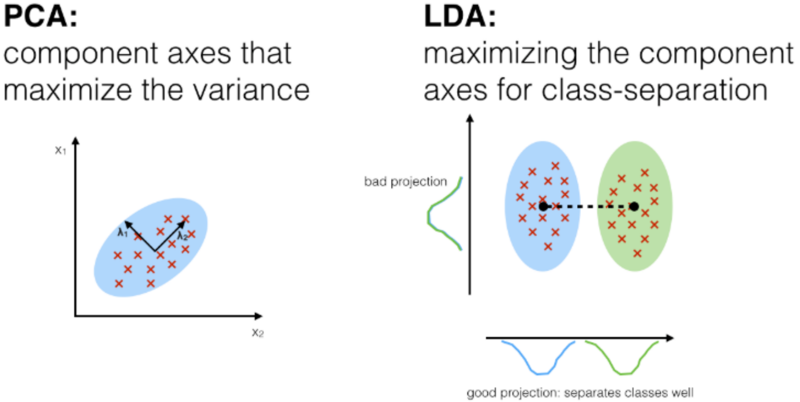


Figure: Image borrowed from
`https://sebastianraschka.com/Articles/2014_python_lda.html`

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:

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

Between-class scatter matrix:

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

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:

- $\mathbf{W} \in \mathbb{R}^{d \times k}$: DR mapping 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

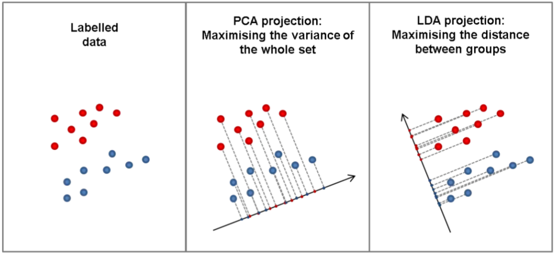


Figure: Image borrowed from `https://vivekmuraleedharan73.medium.com/what-is-linear-discriminant-analysis-lda-7e33ff59020a`.

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

Dynamic Mode Decomposition

Dynamical Systems

A **dynamical system** describes how a state evolves over time according to a fixed rule.

Discrete-time: $\mathbf{x}(t+\tau) = f(\mathbf{x}(t))$ Continuous-time: $\frac{d\mathbf{x}}{dt} = g(\mathbf{x}(t))$

- $\mathbf{x}(t) \in \mathbb{R}^n$: the state at time t
- f, g: a (possibly nonlinear) update rule
- Goal: Understand, predict, or control the evolution of $\mathbf{x}(t)$

Linear Systems
If $f(\mathbf{x}) = A\mathbf{x}$, the system is linear:

$$\mathbf{x}(t+\tau) = A\mathbf{x}(t)$$

$\Rightarrow$ Solutions evolve through powers of A: eigenvalues/eigenvectors govern behavior.

Dynamic Mode Decomposition

Assume that the data is sampled from the timeseries

$$\mathbf{x}(t+\tau) \; \approx \; \mathbf{A}\,\mathbf{x}(t).$$

Decompose the system into spatial and temporal patterns.

Analyzing **A** results in the DMD [Schmid, 2010]

$$\mathbf{x}(t) = \sum_{j=1}^{k} \phi_j e^{\omega_j t} b_j.$$

- $\phi_j \in \mathbb{C}^n$ **feature patterns** (dynamic modes)
- $\omega_j \in \mathbb{C}$ **temporal characteristics** (continuous time eigenvalues)
- $b_j \in \mathbb{R}$ scalar loadings (a.k.a. amplitudes)

Eigenvalue Interpretation

$$\lambda_j = e^{\omega_j \tau}$$

- Discrete time λ_j
- Continuous time ω_j

Write in polar form

$$\lambda_j = re^{i\theta}$$

- Trend: $r = |\lambda_j|$
- Oscillation frequency (per τ): $\theta = -i \log(\lambda_j / r)$

Exact Dynamic Mode Decomposition [Dawson et al., 2016]

1. Stack the data

$$\mathbf{X} = [\mathbf{x}(1) \,|\cdots|\mathbf{x}(T-\tau)] \in \mathbb{R}^{n\times p}, \quad \mathbf{X}' = [\mathbf{x}(1+\tau)\,|\cdots|\mathbf{x}(T)] \in \mathbb{R}^{n\times p},.$$

2. Want to solve

$$\min_{\mathbf{A}} \|\mathbf{X}' - \mathbf{A}\mathbf{X}\|_F$$

3. Rank-r truncated SVD $\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^\top$ leads to

$$\tilde{\mathbf{A}} = \mathbf{U}^\top \mathbf{X}'\mathbf{V}\boldsymbol{\Sigma}^{-1} \in \mathbb{R}^{k\times k}, \quad \tilde{\mathbf{A}}\mathbf{W} = \mathbf{W}\boldsymbol{\Lambda}, \text{ (eigendecomposition)}$$

4. Dynamic modes

$$\phi_j = \frac{1}{\lambda_j}\mathbf{X}'\mathbf{V}\boldsymbol{\Sigma}^{-1}\mathbf{w}_j$$

5. Eigenvalues (discrete time)

$$\lambda_j = e^{\omega_j \tau}$$

6. Loadings found by solving

$$\boldsymbol{\Phi}\mathbf{b} = \mathbf{x}(1).$$

My Interpretation

The system evolves in the low-dimensional reduced space mapped to by $\mathbf{U}^T \in \mathbb{R}^{k \times n}$

$$\mathbf{U}^\top \mathbf{x}(t+\tau) = \mathbf{z}(t+\tau) = \tilde{\mathbf{A}}\mathbf{z}(t) = \tilde{\mathbf{A}}\mathbf{U}^\top \mathbf{x}(t).$$

Projected dynamic modes:

$$\phi_j = \mathbf{U}\mathbf{w}_j$$

DMD analyzes the stability of this system and generates spatial patterns in $\mathbb{R}^n$ (ambient space)

Using Dynamic Mode Decomposition

- Spatial & temporal patterns of timeseries
- Ill-conditioning of $\mathbf{X}$ and $\mathbf{A}$
- Not robust to noise

Optimized Dynamic Mode Decomposition [Askham and Kutz, 2018]

Stack all the data together

$$\mathbf{X} = [\mathbf{x}(t_1)\,|\,\mathbf{x}(t_2)\ \cdots |\mathbf{x}(t_p)] \in \mathbb{R}^{n \times p}.$$

Optimize directly for DMD matrix decomposition

$$\min_{\mathbf{b}_j, \omega_j, b_j} \|\mathbf{X} - \sum_{j=1}^{r} \mathbf{b}_j e^{\omega_j t} b_j\|_F.$$

Translate to

$$\min_{\mathbf{A}} \|\mathbf{X}^\top - \boldsymbol{\Phi}(\boldsymbol{\alpha})\mathbf{B}\|_F.$$

- $\boldsymbol{\Phi}(\boldsymbol{\alpha})_{i,j} = \exp(\alpha_j t_i)$
- $b_j = \|\mathbf{B}^\top(:, j)\|_2$
- $\phi_j = \frac{\mathbf{B}^\top(:,j)}{b_j}$

Solve via variable projection method.

Further Reading

- Multiverse of DMD [Colbrook, 2023]
- Generalizing DMD: Modern Koopman theory [Brunton et al., 2021]

Bonus lab!

Tutorial 1 here: `https://github.com/PyDMD/PyDMD/blob/master/tutorials/tutorial1/tutorial-1-dmd.ipynb`

Nonlinear Dimensionality Reduction

Outline

1. Multidimensional Scaling (MDS) [Kruskal and Wish, 1978]
2. Isometric Mapping (Isomap) [Balasubramanian and Schwartz, 2002]
3. t-distributed Stochastic Neighborhood Embedding (t-SNE) [Van der Maaten and Hinton, 2008]
4. Uniform Manifold Approximation (UMAP) [McInnes et al., 2018]
5. Koopman Mode Decomposition [Brunton et al., 2021]

Multidimensional Scaling

What is MDS?

Multidimensional Scaling (MDS) recovers low-dimensional embeddings of abstract objects from a pairwise distance matrix.

Given:

- Abstract points $\{x_i\}_{i=1}^{p} \in \mathcal{M}$
- Distance function $d : \mathcal{M} \times \mathcal{M} \to \mathbb{R}$
- Distance matrix $\mathbf{D} \in \mathbb{R}^{p \times p}$, $d_{ij} = d(x_i, x_j)$

Goal: Find latent coordinates $\{\mathbf{z}_i\}_{i=1}^{p} \subset \mathbb{R}^k$ such that

$$\|\mathbf{z}_i - \mathbf{z}_j\|_2 \approx d(x_i, x_j)$$

Useful when there's a non-Euclidean distance between points in the ambient space.

Classical MDS Objective

We solve:

$$\{\mathbf{z}_i\}_{i=1}^{p} = \arg \min_{\{\mathbf{w}_i\} \subset \mathbb{R}^k} \sum_{i,j} \left(\|\mathbf{w}_i - \mathbf{w}_j\|_2 - d_{ij} \right)^2$$

Issue: The solution is not unique — distances are translation invariant.

Fix: Require mean centering:

$$\sum_{i=1}^{p} \mathbf{x}_i = \mathbf{0}, \quad \sum_{i=1}^{p} \mathbf{z}_i = \mathbf{0}$$

Eigenvalue Decomposition

Let $\mathbf{D}^{(2)}$ be the matrix of squared distances: d_{ij}^2.

Mean-centering matrix:

$$\mathbf{J} = \mathbf{I} - \frac{1}{p}\mathbf{1}\mathbf{1}^\top$$

Define the Gram matrix:

$$\mathbf{B} = -\frac{1}{2}\mathbf{J}\mathbf{D}^{(2)}\mathbf{J}$$

Compute eigenvalue decomposition:

$$\mathbf{B}\mathbf{V} = \mathbf{V}\boldsymbol{\Lambda}$$

Low-Dimensional Embedding

Truncate to top-k eigenvalues and eigenvectors:

$$\overline{\boldsymbol{\Lambda}},\ \overline{\mathbf{V}}$$

Construct the embedding:

$$\mathbf{Z} = \overline{\mathbf{V}}\,\overline{\boldsymbol{\Lambda}}^{1/2}$$

$\mathbf{Z}^\top = [\mathbf{z}_1, \ldots, \mathbf{z}_n]$ are the low-dimensional coordinates.

Note: When $\mathcal{M} = \mathbb{R}^d$ and $d(x_i, x_j) = \|\mathbf{x}_i - \mathbf{x}_j\|_2$, MDS recovers PCA.
(Details: `https://mlatcl.github.io/advds/notes/mds.pdf`)

Isometric Mapping

What is Isomap?

Isomap (Isometric Mapping) is a nonlinear dimensionality reduction method that:

- Preserves **geodesic distances** (not just Euclidean distances)
- Extends classical MDS to nonlinear manifolds

Key idea: Approximate manifold distances with shortest paths on a neighborhood graph, then apply MDS.

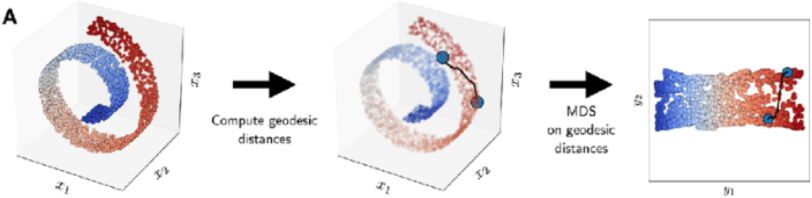


Figure: Figure borrowed from Tsai [2010].

Isomap vs MDS

The advantage of a nearest-neighbors approach...

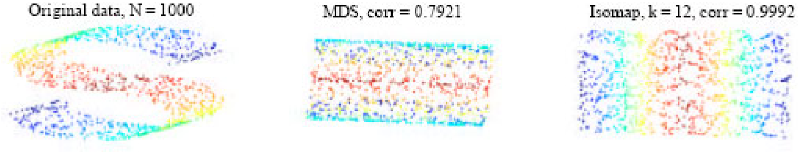


Figure: Figure borrowed from Tsai [2010].

Steps of Isomap

Inputs: Distance, & number of nearest neighbors

1. Construct a graph where:
   - Vertices correspond to samples
   - Edges E defined using k-nearest neighbors
2. Compute geodesic distance matrix $D^{\text{geo}} \in \mathbb{R}^{p \times p}$ using shortest path distances in G
3. Apply classical MDS to D^{geo}

When to Use Isomap

- Your data lies on a low-dimensional **nonlinear** manifold
- You want a global embedding that preserves intrinsic geometry
- You want a distance-preserving map like MDS, but for curved manifolds

Lab 5: MDS & Isomap

Go to Lab5_IsomapMDS.ipynb

t-SNE

Stochastic Neighbor Embedding (SNE): Overview

SNE constructs a probability distribution over neighbors for each point $\mathbf{x}_i$ based on distances in high-dimensional space.

$$g(\mathbf{x}_i, \mathbf{x}) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}\|_2^2}{2\sigma_i^2}\right).$$

The conditional probability that $\mathbf{x}_i$ picks $\mathbf{x}_j$ as neighbor:

$$p_{j|i} = \frac{g(\mathbf{x}_i, \mathbf{x}_j)}{\sum_{r \neq i} g(\mathbf{x}_i, \mathbf{x}_r)}.$$

Note: $p_{j|i} \neq p_{i|j}$ due to different σ_i values.

Perplexity and Bandwidth Selection

Perplexity controls local scale for each point:

$$\mathrm{Perp}(P_i) = 2^{H(P_i)}, \quad H(P_i) = -\sum_j p_{j|i} \log_2 p_{j|i}.$$

- Low perplexity $\implies$ tight local neighborhoods
- High perplexity $\implies$ broader neighborhoods

Binary search is used to find σ_i so that the perplexity matches a user-defined value.

- Small $\sigma_i \implies$ dense distribution
- Large $\sigma_i \implies$ sparse distribution

Low-dimensional Embedding

Embed points $\mathbf{z}_i \in \mathbb{R}^k$ with kernel

$$h(\mathbf{z}_i, \mathbf{z}_j) = \exp\left(-\|\mathbf{z}_i - \mathbf{z}_j\|_2^2\right),$$

and conditional probabilities

$$q_{j|i} = \frac{h(\mathbf{z}_i, \mathbf{z}_j)}{\sum_{r \neq i} h(\mathbf{z}_i, \mathbf{z}_r)}.$$

SNE minimizes the difference between two graphs

SNE minimizes the KL divergence between distributions of edge weights:

$$C = \sum_i \sum_j p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}.$$

- $p_{j|i}$ probability that $\mathbf{x}_i$ picks $\mathbf{x}_j$ as its neighbor in ambient space
- $q_{j|i}$ probability that $\mathbf{x}_i$ picks $\mathbf{x}_j$ as its neighbor in reduced space

SNE uses gradient descent on $\{\mathbf{z}_i\}$, where gradients resemble forces pulling embedded points closer or pushing them apart.

Challenges of SNE

1. **Asymmetry**: $p_{j|i} \neq p_{i|j}$ complicates interpretation.

2. **Crowding problem**: Moderate distances in high-D collapse into tight clusters in low-D.

3. **Optimization difficulty**: KL divergence is hard to optimize and sensitive.

t-SNE: *Symmetrized* Probabilities

t-SNE improves on SNE by:

- Using a **joint probability** distribution (with n samples)

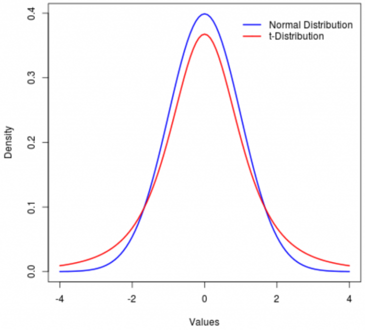
$$p_{ij} = \frac{p_{i|j} + p_{j|i}}{2n}$$

- Modeling q_{ij} in the low-dimensional space with a **Student's-t distribution**:

$$q_{ij} = \frac{(1 + \|\mathbf{z}_i - \mathbf{z}_j\|^2)^{-1}}{\sum_{r \neq s}(1 + \|\mathbf{z}_r - \mathbf{z}_s\|^2)^{-1}}$$

t-SNE: *Fixing the Crowding Problem*

Why use Student's-t?



The heavy tails of the t-distribution allow moderate distances to be represented more accurately — solving the **crowding problem**.

t-SNE: *Optimization*

t-SNE minimizes the KL divergence between p_{ij} and q_{ij}:

$$C = \sum_{i,j} p_{ij} \log\left(\frac{p_{ij}}{q_{ij}}\right)$$

Gradient with respect to $\mathbf{y}_i$:

$$\frac{\partial C}{\partial \mathbf{z}_i} = 4 \sum_j (p_{ij} - q_{ij})(\mathbf{y}_i - \mathbf{z}_j)(1 + \|\mathbf{z}_i - \mathbf{z}_j\|^2)^{-1}$$

Points repel or attract depending on similarity; repulsion is bounded (unlike in SNE) [Böhm et al., 2022]

Parameter Tuning

t-SNE parameters:

- **Perplexity** (typical range: 5–50)
- **Learning rate**
- **Number of iterations**

Effect of tuning: t-SNE is sensitive to parameter choices

See: a website for parameter tuning intuition

Summary

- SNE and t-SNE preserve local structure using probability distributions
- t-SNE improves SNE via:
  - Symmetric probabilities
  - Heavy-tailed Student's-t distribution
  - Better optimization
- Widely used for visualizing high-dimensional data
- t-SNE slow ($O(n^2)$), Barnes-Hut t-SNE is faster ($O(n(\log(n)))$)

Lab 6: t-SNE

Go to Lab6_tSNE.ipynb &
`https://distill.pub/2016/misread-tsne/`

UMAP

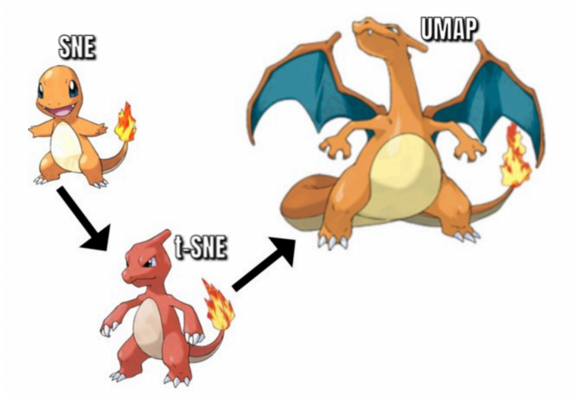


Figure: Image from https://arize.com/blog-course/reduction-of-dimensionality-top-techniques/.

Uniform Manifold Approximation (UMAP)

Goal: preserve the topological structure of the data manifold

Assumptions:

1. There exists an underlying manifold with uniform data distribution
2. The manifold is locally connected

Inputs

Given dataset $\{\mathbf{x}_1, \ldots, \mathbf{x}_p\}$

User-specified:

- Number of neighbors n
- Metric d
- Output dimension k
- Minimum distance *min_dist*

Choice of n:

- Small $n \Rightarrow$ fine detail structure (local)
- Large $n \Rightarrow$ coarser global structure

UMAP is based in category theory & mathematical topology.. we will sweep this foundation under the rug and consider the computational machinery instead

Algorithm Step 1: Ambient Graph Building

a. Define number of neighbors as n & minimum distance between $\mathbf{x}_i$ and neighbors ρ_i

b. Find σ_i via binary search:

$$\sum_{j=1}^{n} \exp\left(\frac{-\max(0, d(\mathbf{x}_i, \mathbf{x}_{i_j}) - \rho_i)}{\sigma_i}\right) = \log_2(n)$$

c. Edge weights from i to i_j:

$$\mathbf{w}_h(\mathbf{x}_i, \mathbf{x}_{i_j}) = \exp\left(\frac{-\max(0, d(\mathbf{x}_i, \mathbf{x}_{i_j}) - \rho_i)}{\sigma_i}\right)$$

d. Let $\mathbf{A}$ be adjacency matrix, then:

$$\mathbf{B} = \mathbf{A} + \mathbf{A}^\top - \mathbf{A} \circ \mathbf{A}^\top$$

Interpretation: edge weights are probabilities that a 1-simplex exists; combined weights: probability that at least one edge exists.

Algorithm Step 2: Reduced Graph Building

Edge weights between $\mathbf{z}_i$ and $\mathbf{z}_j$ in reduced space are

$$\mathbf{w}_l(\mathbf{z}_i, \mathbf{z}_j) = \frac{1}{a\|\mathbf{z}_i - \mathbf{z}_j\|_2^{2b}}.$$

Where a and b are hyperparameters chosen by a non-linear least squares fit to

$$\begin{cases} 1 & \|\mathbf{z}_i - \mathbf{z}_j\|_2 < min\_dist \\ \exp(-\|\mathbf{z}_i - \mathbf{z}_j\|_2 - min\_dist) & \text{otherwise} \end{cases}$$

But, when $a = b = 1$ edges are sampled from Student's-t distribution.

Default parameters: $a = 1.577$, $b = 0.8951$

Algorithm Step 3: Optimization

- Initialize with spectral embedding (e.g., Laplacian Eigenmaps from Belkin and Niyogi [2001])
- Use stochastic gradient descent to minimize cross-entropy:

$$C = \sum_e w_h(e) \log\left(\frac{w_h(e)}{w_l(e)}\right) + (1 - w_h(e)) \log\left(\frac{1 - w_h(e)}{1 - w_l(e)}\right)$$

Advantages of UMAP

- Preserves global and local structure
- Faster than vanilla t-SNE ($\mathcal{O}(n^{1.14})$ vs $\mathcal{O}(n^2)$)
- Based on topology + category theory
- Can be used for general dimensionality reduction (not just visualization)
- Approximately invertible
- Aligned UMAP for cross-dataset comparison

Parameter Tuning & Resources

Key Parameters:

- **Number of neighbors:** balance local vs. global structure
- **Minimum distance:** desired separation of points in latent space

Visualizing parameter tuning and comparison to t-SNE

Resources:

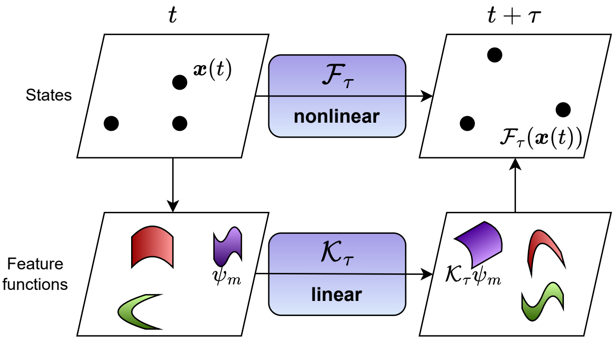
- UMAP: Uniform Manifold Approximation and Projection
- UMAP Documentation
- Understanding UMAP
- Inverse transform
- Aligned UMAP

Lab 7: UMAP

Go to Lab7_UMAP.ipynb &
`https://pair-code.github.io/understanding-umap/`

Koopman Mode Decomposition

Koopman Mode Decomposition



Koopman Mode Decomposition

ψ_m "observable" (a.k.a. feature) function
Koopman operator (denoted $\mathcal{K}_\tau$) [Koopman, 1931]

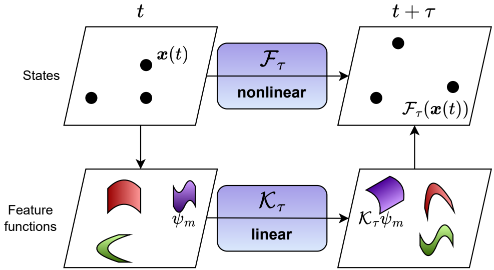
$$\mathcal{K}_\tau[\psi_m](\mathbf{x}(t)) \;=\; \psi_m\big(\mathcal{F}_\tau \mathbf{x}(t)\big) = \;\psi_m\big(\mathbf{x}(t+\tau)\big)$$

Koopman mode decomposition [Rowley et al., 2009; Mezić, 2013]

$$\mathbf{x}(t) = \sum_{j=1}^{r} \mathbf{b}_j e^{\omega_j t} \phi_j(\mathbf{x}(0)).$$

- $\mathbf{b}_j$ **spatial patterns** (dynamic modes)
- ω_j **temporal characteristics** (continuous time eigenvalues)
- ϕ_j Koopman eigenfunctions

Koopman Mode Decomposition



Koopman operator (denoted $\mathcal{K}_\tau$) [Koopman, 1931]

$$\mathcal{K}_\tau[\psi_m](\mathbf{x}(t)) \;=\; \psi_m(\mathcal{F}_\tau \mathbf{x}(t)) = \;\psi_m(\mathbf{x}(t+\tau))$$

Koopman mode decomposition [Rowley et al., 2009; Mezić, 2013]

$$\mathbf{x}(t) = \sum_{j=1}^{r} \mathbf{b}_j e^{\omega_j t} \phi_j(\mathbf{x}(0)).$$

- $\mathbf{b}_j$ **spatial patterns** (dynamic modes)
- ω_j **temporal characteristics** (continuous time eigenvalues)
- ϕ_j Koopman eigenfunctions

Kernel Koopman Mode Decomposition [Williams et al., 2015]

- Embed states into a Reproducing Kernel Hilbert Space (RKHS), denoted $\mathcal{H}$
- Let $\psi : \mathbb{R}^M \to \mathcal{H}$ be the feature map for some kernel $k(\cdot, \cdot)$
- Define the snapshot feature matrices

$$\boldsymbol{\Psi}_{\mathbf{X}} = \Big[\psi\big(\mathbf{x}(1)\big) \cdots \psi\big(\mathbf{x}(T-\tau)\big)\Big] \tag{6}$$

$$\boldsymbol{\Psi}_{\mathbf{X}'} = \Big[\psi\big(\mathbf{x}(\tau+1)\big) \cdots \psi\big(\mathbf{x}'(T)\big)\Big]. \tag{7}$$

- Seek finite-dimensional Koopman operator estimate is $\tilde{\mathbf{K}}$, which can be found via kernel Gram matrices

$$\mathbf{K}_{\mathbf{X}} = \boldsymbol{\Psi}_{\mathbf{X}}^{\top}\boldsymbol{\Psi}_{\mathbf{X}}, \quad \mathbf{K}_{\mathbf{X}',\mathbf{X}} = \boldsymbol{\Psi}_{\mathbf{X}'}^{\top}\boldsymbol{\Psi}_{\mathbf{X}}.$$

Kernel Koopman Mode Decomposition

- Using the eigendecomposition $\mathbf{K}_{\mathbf{X}} = \mathbf{Q}\boldsymbol{\Sigma}^2\mathbf{Q}^\top$
- The finite-dimensional Koopman operator estimate is $\tilde{\mathbf{K}} = \boldsymbol{\Sigma}^{-1}\mathbf{Q}^\top\mathbf{K}_{\mathbf{X}',\mathbf{X}}\mathbf{Q}\boldsymbol{\Sigma}^{-1}$
- Eigenvalue decomposition $\tilde{\mathbf{K}}\mathbf{W} = \mathbf{W}\boldsymbol{\Lambda}$

Name	Definition
Eigenfunctions of $\mathbf{X}$	$\boldsymbol{\Phi} = \mathbf{K}_{\mathbf{X}}\,\mathbf{Q}\,\boldsymbol{\Sigma}^\dagger\,\mathbf{W}$
Koopman modes	$\mathbf{B} = \mathbf{X}\mathbf{Q}^T\boldsymbol{\Sigma}^\dagger\mathbf{W}^{-1}$

Bonus lab!

Tutorials here:

- `https://github.com/PyDMD/PyDMD/blob/master/tutorials/tutorial17/tutorial-17-edmd.ipynb`
- `https://github.com/dynamicslab/pykoopman`

Autoencoders

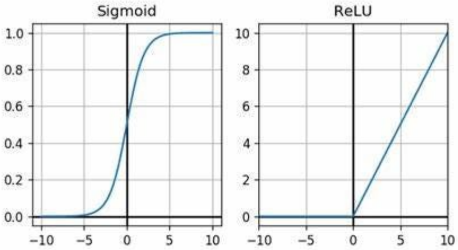
Outline

1. Vanilla Autoencoders
2. Denoising Autoencoders
3. Variational Autoencoders
4. Convolutional Autoencoders
5. Graph Autoencoders

Neural Networks

Composed of linear and nonlinear functions.

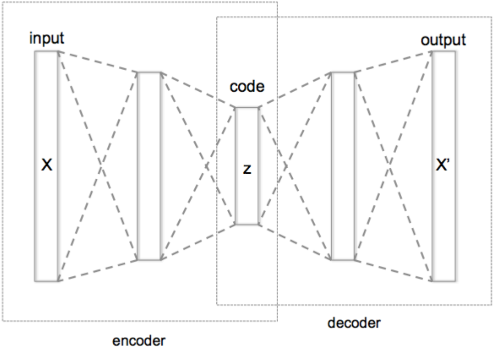
- **Linear functions: $\mathbf{W} \in \mathbb{R}^{\mathrm{out}\times\mathrm{in}}$**
- **Nonlinear (activation) functions: σ**



The "neural network function" maps

$$\mathbf{x} \mapsto \sigma(\mathbf{W}_\ell \sigma(\mathbf{W}_{\ell-1} \cdots \sigma(\mathbf{W}_1(\mathbf{x}))\cdots))$$

Vanilla Autoencoder



- Encoder compresses the input into a lower-D representation
- Decoder reconstructs the input from the lower-D representation
- Loss function: Typically Mean Squared Error (MSE) between the input and the reconstructed output

Autoencoders vs PCA

Autoencoders optimize

$$\arg\min_{\mathrm{Enc},\mathrm{Dec}} \sum_{i=1}^{n} L(\mathbf{x}_i, \mathrm{Dec} \circ \mathrm{Enc}(\mathbf{x}_i)).$$

- Define $\mathrm{Enc}(\mathbf{x}) = \mathbf{A}^\top \mathbf{x}$ and $\mathrm{Dec}(\mathbf{z}) = \mathbf{A}\mathbf{z}$.
- Take the mean squared error (MSE) loss $L(\mathbf{x}, \hat{\mathbf{x}}) = \|\mathbf{x} - \hat{\mathbf{x}}\|_2^2$.

$$\arg\min_{\mathbf{A}^\top \mathbf{A} = \mathbf{I}} \sum_{i=1}^{n} \|\mathbf{x}_i - \mathbf{A}\mathbf{A}^\top \mathbf{x}_i\|_2^2.$$

- This is *exactly* PCA

But, there's a deeper connection... see Rolinek et al. [2019]; Bao et al. [2020].

Denoising Autoencoder [Vincent et al., 2008]

- Similar to the vanilla autoencoder, but with ***noisy input data***
- The goal is to reconstruct the clean data from the noisy version
- Used for removing noise from data (e.g., images or signals)
- Loss function is also typically MSE, between clean data and reconstructions

Variational Autoencoder

Variational Autoencoder (VAE)

Goal: estimate true data distribution p_* given model parameters θ.

- **Estimated distribution:** p_θ
- Maximize $p_\theta(\mathbf{x})$ for each $\mathbf{x}$ in dataset.

Intuition p_* can be described by compressed features. E.g., reduced (a.k.a. latent) representation of a dataset of pictures of circles could be radius and center.

- Inference of latent space space: $p_\theta(\mathbf{z}|\mathbf{x})$ (likelihood)

- Generation from latent space: $p_\theta(\mathbf{x}|\mathbf{z})$ (posterior)

Problem: Marginal likelihood is intractable

$$p_\theta(\mathbf{x}) = \int_{\mathbf{z}} p_\theta(\mathbf{x}, \mathbf{z}) d\mathbf{z} = \int_{\mathbf{z}} p_\theta(\mathbf{z}) p_\theta(\mathbf{x}|\mathbf{z}) d\mathbf{z}$$

Enter Bayes

Bayes Rule:

$$p_\theta(\mathbf{z}|\mathbf{x}) = \frac{p_\theta(\mathbf{z})p_\theta(\mathbf{x}|\mathbf{z})}{p_\theta(\mathbf{x})}$$

- prior probability$p_\theta(\mathbf{x})$
- likelihood $p_\theta(\mathbf{z}|\mathbf{x})$
- marginal likelihood $p_\theta(\mathbf{z})$
- posterior probability $p_\theta(\mathbf{x}|\mathbf{z})$

Maximize prior equivalent to maximizing

$$p_\theta(\mathbf{x}) = \frac{p_\theta(\mathbf{z})p_\theta(\mathbf{x}|\mathbf{z})}{p_\theta(\mathbf{x})} = \frac{p_\theta(\mathbf{x},\mathbf{z})}{p_\theta(\mathbf{z}|\mathbf{x})}$$

But $p_\theta(\mathbf{z}|\mathbf{x})$ is also intractible...
But we can estimate $p_\theta(\mathbf{z}|\mathbf{x})$

Estimate $p_\theta(\mathbf{z}|\mathbf{x})$

Goal: approximate $p = p_\theta(\mathbf{z}|\mathbf{x})$ with $q = q_\phi(\mathbf{z}|\mathbf{x})$.
KL Divergence

$$
\begin{aligned}
\mathrm{D}_{\mathrm{KL}}(q||p) &= \int_{\mathbf{z}} q \log(q/p) d\mathbf{z} && (8)\\
&= \mathbb{E}_q\left[\log(q/p)\right] && (9)\\
&= \mathbb{E}_q[\log q] - \mathbb{E}_q[\log p] && (10)\\
&= \mathbb{E}_q[\log q] - \mathbb{E}_q[\log(p_\theta(\mathbf{z},\mathbf{x})/p_\theta(\mathbf{x}))] && (11)\\
&= \mathbb{E}_q[\log q] - \mathbb{E}_q[\log p_\theta(\mathbf{z},\mathbf{x})] + \mathbb{E}_q[\log p_\theta(\mathbf{x})] && (12)\\
&= \log p_\theta(\mathbf{x}) - \mathbb{E}_q[\log p_\theta(\mathbf{z},\mathbf{x}) - \log q_\phi(\mathbf{z}|\mathbf{x})] && (13)
\end{aligned}
$$

The expected information loss when we model p with q.
Problem: $\log p_\theta(\mathbf{x})$ intractible

More with KL Divergence

From before, we have

$$\log p_\theta(x) = \mathrm{D}_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})) + \mathbb{E}_q[\log p_\theta(\mathbf{z}, \mathbf{x}) - \log q_\phi(\mathbf{z}|\mathbf{x})]$$

Notice $\mathrm{D}_{\mathrm{KL}}(q||p) > 0$

Enter the Evidence Lower BOund! – **ELBO**

$$\log p_\theta(x) \geq \mathbb{E}_q[\log p_\theta(\mathbf{z}, \mathbf{x}) - \log q_\phi(\mathbf{z}|\mathbf{x})] = \mathrm{ELBO}$$

The Glory of ELBO

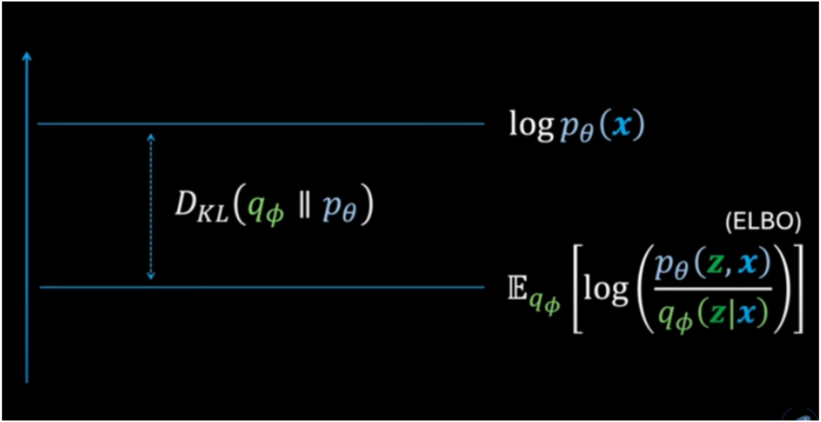


Figure: Image borrowed from
`https://www.youtube.com/watch?v=HBYQvKlaE0A`.

Maximizing ELBO maximizes $p_\theta(\mathbf{x})$ and $\mathrm{D}_{\mathrm{KL}}(q||p)$!

ELBO Optimization

Stochastic gradient descent on ELBO... but issues with estimation of gradient...

Reparameterization Trick:

- $q_\phi(\mathbf{z}|\mathbf{x}) = g(\phi, \mathbf{x}, \epsilon)$
- $\epsilon \sim p(\epsilon)$

Now expectation is taken over $p(\epsilon)$, rather than q

$$\mathcal{L}(\mathbf{x}) = \mathbb{E}_{p(\epsilon)}[\log p_\theta(\mathbf{z}, \mathbf{x}) - \log q_\phi(\mathbf{z}|\mathbf{x})]$$

Exercise: we approximate ELBO with L samples using

$$\mathrm{ELBO} \approx \frac{1}{L} \sum_{i=1}^{L} \log p_\theta(\mathbf{x}|\mathbf{z}) - \mathrm{D}_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x}) || p_\theta(\mathbf{z}))$$

Simplifying Assumptions

From before ...

$$\mathrm{ELBO} \approx \frac{1}{L}\sum_{i=1}^{L} \log p_\theta(\mathbf{x}|\mathbf{z}) - \mathrm{D}_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}))$$

Gaussian Assumptions

- **Prior:** $p(z) = \mathcal{N}(0, I)$
- **Posterior:** $q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\sigma})$
- $\boldsymbol{\mu}, \boldsymbol{\sigma} = f(\mathbf{x})$

Exercise: show that this loss becomes

$$\mathrm{D}_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z})) = \frac{-1}{2}[\log \boldsymbol{\sigma}^2 - \boldsymbol{\mu}^2 - \boldsymbol{\sigma}^2 + 1].$$

Modeling the log probability $\log p_\theta(\mathbf{x}|\mathbf{z})$

- Gaussian assumption: $(\mathbf{x} - \hat{\mathbf{x}})^2$ *(takes work to show)*
- Bernoulli assumption: $\mathrm{BCE}(\hat{\mathbf{x}}, \mathbf{x})$

VAE Architecture

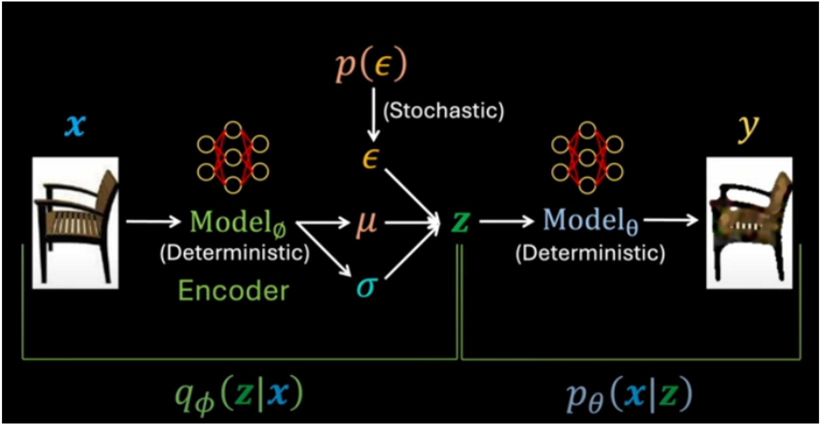


Figure: Image borrowed from
`https://www.youtube.com/watch?v=HBYQvKlaE0A`.

Convolutional Autoencoder

Continuous Convolution

Consider functions: $f, g : \mathbb{R} \to \mathbb{R}$.

$$f * g(x) = \int_u f(u)g(x-u)du$$

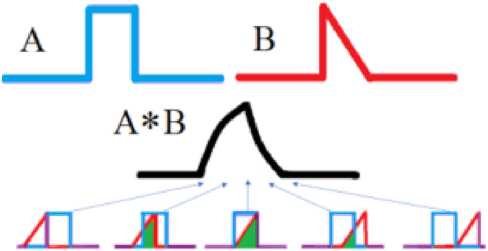


Figure:
`https://www.statisticshowto.com/convolution-integral-simple-definition/`

Discrete Convolution

Consider functions: $f, g : \mathbb{Z} \to \mathbb{Z}$.

$$f * g(n) = \sum_m f(m)g(n-m)$$

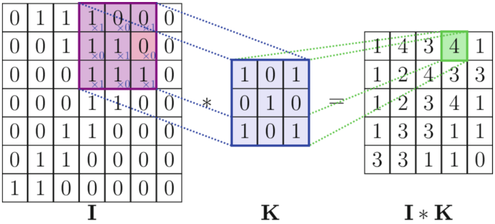


Figure: `https://www.researchgate.net/figure/A-visualization-of-the-discrete-convolution-operation-in-2D_fig5_372609466`

Convolutional Filter

Sliding convolutional filter.

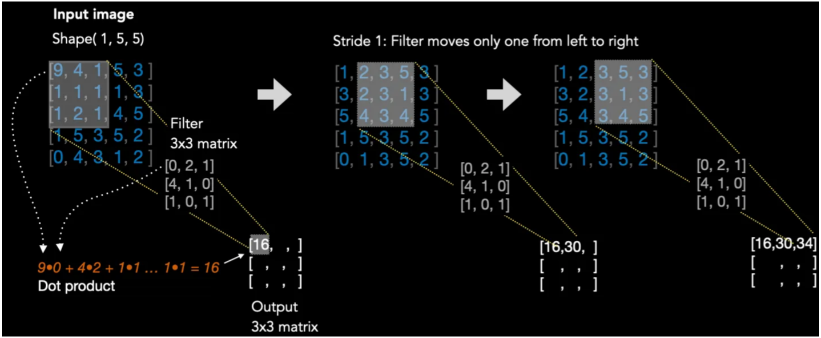


Figure:
https://medium.com/advanced-deep-learning/cnn-operation-with-2-kernels
-resulting-in-2-feature-mapsunderstanding-the-convolutional-filter-c4aad26cf32

Edge Detectors

Certain filters extract different patterns.

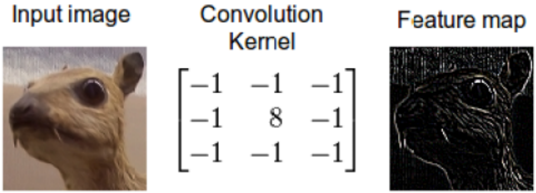


Figure: `https://timdettmers.com/2015/03/26/convolution-deep-learning/`

Convolutional Autoencoders

Encoder and decoder are convolutional filters

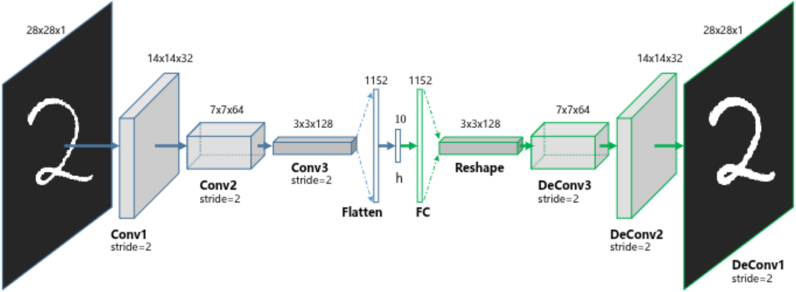


Figure: [Guo et al., 2017]

Graph Convolutional Autoencoder

Convolutions and Fourier Transform

Let $\mathcal{F}$ be the Fourier transform. Consider functions: $f, g : \mathbb{R} \to \mathbb{R}$. Then, under certain assumptions

$$\mathcal{F}(f * g) = \mathcal{F}(f)\mathcal{F}(g)$$

- Multiplication is easy!
- Decreases the computational cost of convolution

Discrete Fourier Transform (DFT)

Let $\omega := e^{-2\pi i/N} = \cos(-2\pi/N) + i\sin(-2\pi/N)$

$$\mathbf{V} = \frac{1}{\sqrt{N}} \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & \omega & \cdots & \omega^{d-1} \\ 1 & \omega^2 & \cdots & \omega^{2(d-1)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{p-1} & \cdots & \omega^{(d-1)(d-1)} \end{bmatrix}.$$

- The DFT of a timeseries $\mathbf{x} = [x(1)|x(2)|\cdots|x(d)]^\top$ is $\mathbf{Vx}$
- Transforms from time to frequency domain
- Can also be used on other signals (features other than time)

Graph Data

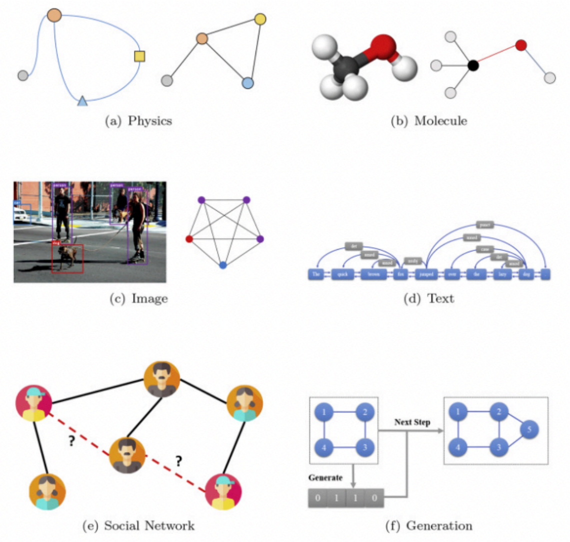
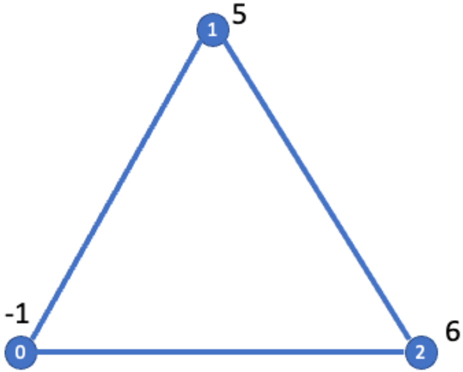


Figure: [Zhou et al., 2020]

Graph Signals

A graph signal is a vector with a value at every node on the graph.



Discrete Graph Fourier Transform (GFT)

1. $\mathbf{A}$ adjacency matrix for the graph
2. $\mathbf{x}$ signal on graph
3. $\mathbf{D}$ degree matrix
4. $\mathbf{L} = \mathbf{D} - \mathbf{A}$ graph Laplacian
5. $\mathbf{L}\mathbf{U} = \mathbf{U}\boldsymbol{\Lambda}$ eigenvalue decomposition
6. $\mathcal{F}(\mathbf{x}) = \mathbf{U}^\top \mathbf{x}$ discrete graph Fourier transform
7. $\mathcal{F}^{-1}(\mathbf{z}) = \mathbf{U}\mathbf{z}$ inverse discrete graph Fourier transform

On the cycle graph, the GFT reduces to the DFT.

Graph Convolution

Graph signals $\mathbf{x}, \mathbf{g}$

$$\mathcal{F}(\mathbf{x} * \mathbf{g}) = \mathcal{F}(\mathbf{x}) \cdot \mathcal{F}(\mathbf{g}) = \mathbf{\Lambda}_{\mathbf{U}^\top \mathbf{g}} \mathbf{U}^\top \mathbf{x}$$

Where $\cdot$ is point-wise multiplication and

$$\mathbf{\Lambda}_g = \begin{bmatrix} (\mathbf{U}^\top \mathbf{g})_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & (\mathbf{U}^\top \mathbf{g})_d \end{bmatrix}$$

Graph convolution

$$\mathbf{x} * \mathbf{g} = \mathcal{F}^{-1} \circ \mathcal{F}(\mathbf{x} * \mathbf{g}) = \mathbf{U} \mathbf{\Lambda}_{\mathbf{U}^\top \mathbf{g}} \mathbf{U}^\top \mathbf{x}$$

Graph Convolutional Layer [Kipf and Welling, 2016a]

Replace graph signal $\mathbf{g}$ with signal in frequency domain as a function of $\mathbf{\Lambda}$: $\mathbf{g}_\theta(\mathbf{\Lambda})$.
Convolution becomes

$$\mathbf{U}\mathbf{g}_\theta(\mathbf{\Lambda})\mathbf{U}^\top\mathbf{x}$$

Approximate using Chebyshev polynomials

$$\mathbf{U}\mathbf{g}_\theta(\mathbf{\Lambda})\mathbf{U}^\top\mathbf{x} \approx \theta_1\mathbf{x} - \theta_2\mathbf{L}\mathbf{x} \approx \theta(\mathbf{I} - \mathbf{L})\mathbf{x}$$

Renormalization trick & gives us the graph convolutional layer:

$$\mathrm{GC}(\mathbf{X}) = \sigma(\tilde{\mathbf{D}}^{-1/2}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-1/2}\mathbf{X}\mathbf{\Theta}) \tag{14}$$

- $\tilde{\mathbf{A}} = \mathbf{I} + \mathbf{A}$
- $\tilde{\mathbf{D}}$ degree matrix
- $\mathbf{X}$ input matrix of nodes $\times$ features
- Parameter matrix $\mathbf{\Theta}$

See Kipf and Welling [2016b] for details.

Graph (Variational) Autoencoders [Kipf and Welling, 2016b]

Reconstructed adjacency matrix: $\hat{\mathbf{A}} = \sigma(\mathbf{Z}\mathbf{Z}^\top)$

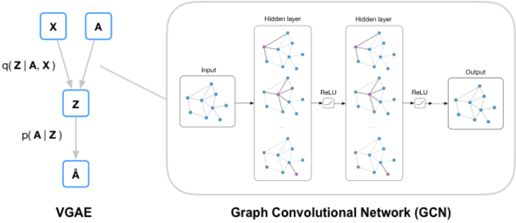


Figure: Code and image from `https://github.com/tkipf/gae`

Further reading: graph-based architectures [Wu et al., 2020] and generalizations of graph autoencoders [Hajij et al., 2021]

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