Unsupervised Learning

COMP 551 Applied Machine Learning

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Current participation rate: 49%.

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Thank you!

Outline

Acknowledgement

- The slides are adapted from Prof. Yue Li's slides.

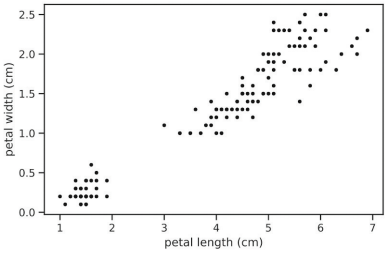
Unsupervised learning

- Instead of having a pair of input and output in the supervised learning tasks (Lectures 1-3), in **unsupervised learning**, we seek to find latent patterns from *only the inputs* data $\mathcal{D} = \{\mathbf{x}_n\}_{n=1}^N$ without any corresponding output y_n.
- Unsupervised learning forces the model to "explain" the high-dimensional inputs, rather than just the low-dimensional outputs (i.e., trying to "make sense of" the data)
- The reason we need unsupervised learning is that most of the data we have are *unlabelled*.
- Quoted from Geoffery Hinton 1996: "When we're learning to see, nobody's telling us what the right answers are – we just look. Every so often, your mother says "that's a dog", but that's very little information."

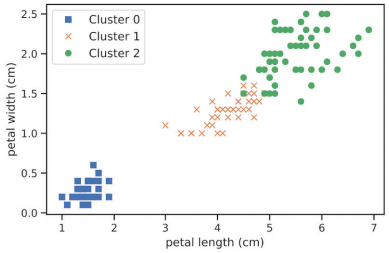
Clustering

The goal is to partition or cluster the input into regions that contain "similar" points.

2D data for the 149 iris flowers



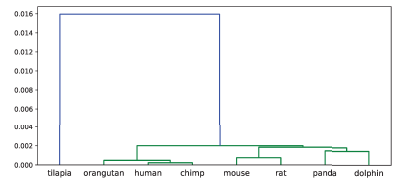
K-means



Sequence similarity among 8 species

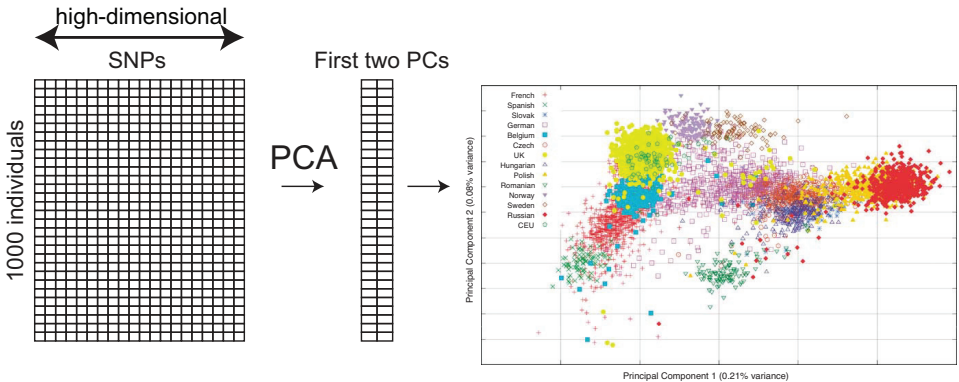
	human	chimp	orangutan	mouse	rat	panda	dolphin	tilapia
human	430	418	398	260	267	298	287	114
chimp	418	430	394	268	275	306	295	114
orangutan	398	394	430	252	259	286	283	118
mouse	260	268	252	426	381	296	269	104
rat	267	275	259	381	428	299	268	111
panda	298	306	286	296	299	430	319	110
dolphin	287	295	283	269	268	319	436	119
tilapia	114	114	118	104	111	110	119	446

Hierarchical clustering



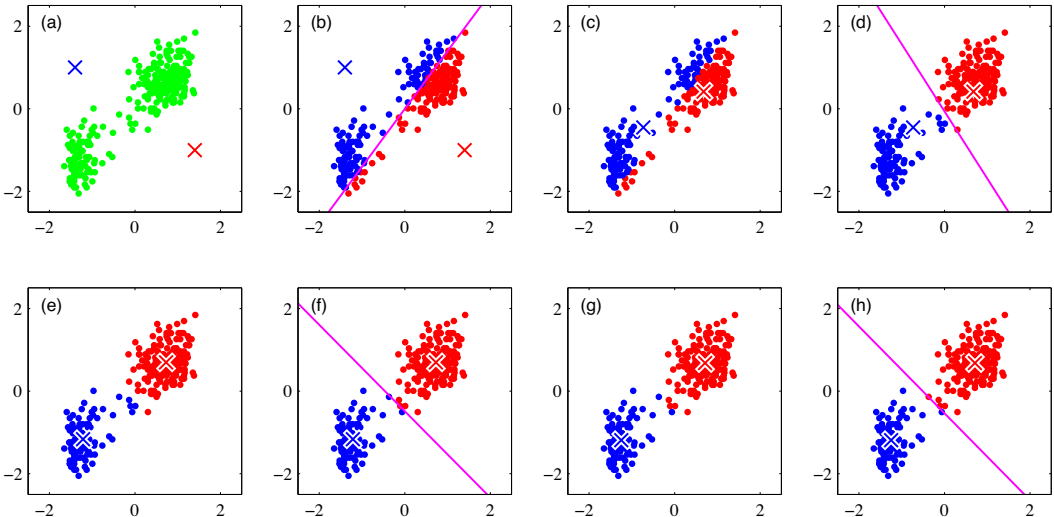
Discovering population structure from the genotype data

- It is often useful to reduce the high dimensional data by projecting it to a lower dimensional subspace to capture the "essence" of the data.
- Each observed high-dimensional data $\mathbf{x}_n \in R^D$ was generated by a set of hidden or unobserved low-dimensional latent factors $\mathbf{z}_n \in \mathbb{R}^K$.
- Below illustrates applying **Principal Component Analysis (PCA)** to 1000 human genomes, each having 1 million SNPs



Outline

K-means clustering algorithm for K=2, D=2



K-means clustering algorithm

Objective function:

$$J = \sum_{n=1}^{N} ||\mathbf{x}_n - \sum_{k=1}^{K} z_{n,k}\boldsymbol{\mu}_k||^2 = ||\mathbf{X} - \mathbf{ZM}||_F^2$$

where each row of $\mathbf{Z}$ is hot-encoding for the cluster assignment and $\mathbf{M} \in \mathbb{R}^{K \times D}$ are the K centroids for the D input features.

Algorithm 1 K-means clustering (ϵ)

1: Initialize K cluster centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$
2: **while** $J^{(t-1)} - J^{(t)} > \epsilon$ **do**
3: Assign each point $\mathbf{x}_n$ to the closest center k:

$$z_{n,k} = \begin{cases} 1 & \text{if } k = \arg\min_j ||\mathbf{x}_n - \boldsymbol{\mu}_j||^2 \\ 0 & \text{if otherwise} \end{cases}$$

4: Update the cluster centroids: $\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_n z_{n,k}\mathbf{x}_n$, where $N_k = \sum_n z_{n,k}$.
5: **end while**

Convergence on the cost function

- Cost function:

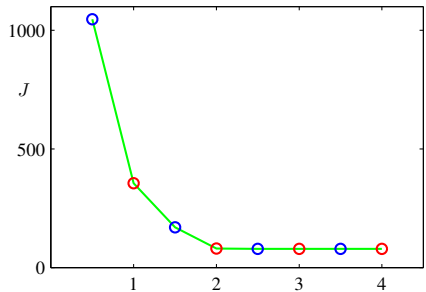
$$J = \sum_{n=1}^{N} ||\mathbf{x}_n - \sum_{k=1}^{K} z_{n,k}\boldsymbol{\mu}_k||^2$$

- K-means alternates between clustering and updating the K centers:
  1. Clustering:

$$z_{n,k} = \begin{cases} 1 & \text{if } k = \arg\min_j ||\mathbf{x}_n - \boldsymbol{\mu}_j||^2 \\ 0 & \text{if otherwise} \end{cases}$$

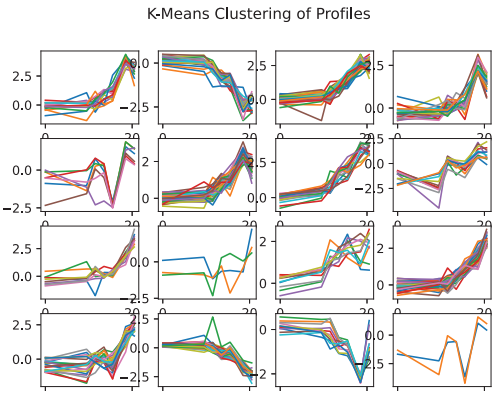
  2. Updating:

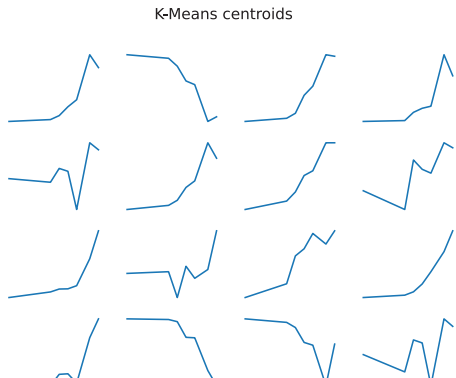
$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_n z_{nk}\mathbf{x}_k, \quad \text{where} \quad N_k = \sum_n z_{nk}$$



K-means minimize the reconstruction loss? (pop quiz: why?).

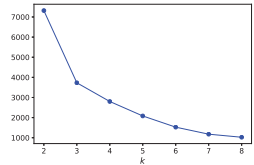
K-means clustering of the time-series yeast gene expression data



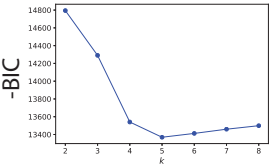


Evaluation metrics in choosing K

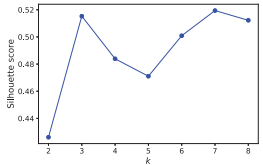
Validation error



Bayesian info criterion



ASW



$$J(K) = \sum_{n=1}^{N_{val}} ||\mathbf{x}_n^{(val)} - \sum_{k=1}^{K} z_{n,k}^{(val)} \hat{\boldsymbol{\mu}}_k||^2$$

$$BIC(K) = \log p(\mathcal{D}|\boldsymbol{\mu}) - \frac{D_K}{2} \log(N)$$

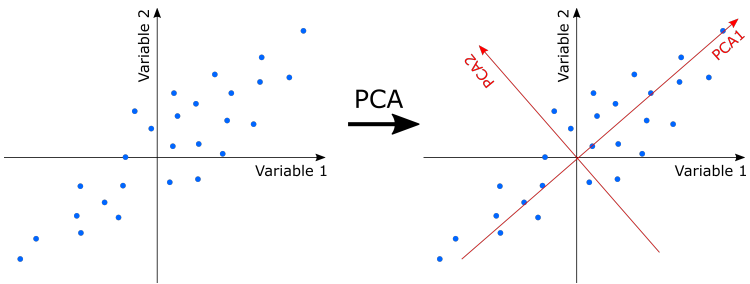
$$ASW(K) = \frac{1}{N} \sum_{i=1}^{N} \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$

- Reconstruction error on the validation set is not informative as it always decreases with increasing K. **But it's inflection point is a good heuristic to choosing K (called the Elbow or Hockey Stick Method)**.
- Bayesian information criteria (BIC) score penalizes more complex model besides the reconstruction loss and is informative of the best K (i.e., K=5)
- ASW suggests the best K at 3 or 7.

Outline

Principal Component Analysis

PCA main idea: find the directions which encode most of the difference (variance) between datapoints.



Principal Component Analysis

- Suppose we have an unlabelled dataset $\mathbf{X} \in \mathbb{R}^{D \times N}$ for D features and N examples.
- We would like to approximate each data point $\mathbf{x}_n \in \mathbb{R}^{D \times 1}$ by a low dimensional representation $\mathbf{z}_n \in \mathbb{R}^{K \times 1}$, where $K \leq D$.
- The variable $\mathbf{z}_n$ is known as the **latent factor**.
- The error produced by this approximation is called **reconstruction error**:

$$\begin{aligned}\mathcal{L}(\mathbf{W}) &= \frac{1}{N}\sum_{n=1}^{N} ||\mathbf{x}_n - \text{decode}(\text{encode}(\mathbf{x}_n; \mathbf{W}); \mathbf{W})||_2^2 \\ &\triangleq \frac{1}{N}\sum_{n=1}^{N} ||\mathbf{x}_n - \mathbf{W}\mathbf{z}_n||_2^2\end{aligned}$$

where in the context of PCA:

- we assume a *linear* encoder and decoder
- $\mathbf{Z} \in \mathbb{R}^{K \times N}$ is also known as the **loading matrix**.
- $\mathbf{W} \in \mathbb{R}^{D \times K}$ is called the **basis matrix**. It is *orthogonal* matrix: $\mathbf{W}^\top \mathbf{W} = \mathbf{I}$, which means that $\mathbf{w}_k^\top \mathbf{w}_{k'} = 1$ for $k = k'$ or 0 for $k \neq k'$.

PCA derivation

In what follows we assume $\mathbb{E}[\mathbf{x}] = \mathbf{0}$, if it is not true, we can simply redefine $\mathbf{x}_n = \hat{\mathbf{x}}_n - \mathbb{E}[\hat{\mathbf{x}}]$, where $\hat{\mathbf{x}}_n$ is the original data whose mean is not zero.

PCA derivation for the first PC

Let $\mathbf{z}_1 \in \mathbb{R}^{N\times 1}$ and $\mathbf{w}_1 \in \mathbb{R}^{D\times 1}$ be the loading and basis vector of the first PC. The reconstruction error is

$$\mathcal{L}(\mathbf{w}_1, \mathbf{z}_1) = \frac{1}{N}\sum_{n=1}^{N} ||\mathbf{x}_n - z_{1,n}\mathbf{w}_1||^2 = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - z_{1,n}\mathbf{w}_1)^\top(\mathbf{x}_n - z_{1,n}\mathbf{w}_1)$$

$$= \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n^\top\mathbf{x}_n - 2z_{1,n}\mathbf{w}_1^\top\mathbf{x}_n + z_{1,n}^2\underbrace{\mathbf{w}_1^\top\mathbf{w}_1}_{1}) = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n^\top\mathbf{x}_n - 2z_{1,n}\mathbf{w}_1^\top\mathbf{x}_n + z_{1,n}^2)$$

$$\frac{\partial\mathcal{L}(\mathbf{z}_1)}{\partial z_{1,n}} = \frac{1}{N}(-2\mathbf{w}_1^\top\mathbf{x}_n + 2z_{1,n}) \triangleq 0 \quad \Rightarrow \quad z_{1,n} = \mathbf{w}_1^\top\mathbf{x}_n$$

$$\mathcal{L}(\mathbf{w}_1) = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n^\top\mathbf{x}_n - 2z_{1,n}\mathbf{w}_1^\top\mathbf{x}_n + z_{1,n}^2) = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n^\top\mathbf{x}_n - 2z_{1,n}^2 + z_{1,n}^2) = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n^\top\mathbf{x}_n - z_{1,n}^2)$$

$$\propto -\frac{1}{N}\sum_{n=1}^{N} z_{1,n}^2 = -\frac{1}{N}\sum_{n=1}^{N}\mathbf{w}_1^\top\mathbf{x}_n\mathbf{x}_n^\top\mathbf{w}_1 = -\mathbf{w}_1^\top\hat{\Sigma}\mathbf{w}_1 \quad \text{where} \quad \hat{\Sigma} = \frac{1}{N}\mathbf{X}\mathbf{X}^\top$$

We see that minimizing the reconstruction error is equivalent to maximizing the variance of the latent representation w.r.t. $\mathbf{w}_1$ (since $\mathrm{Var}[z] = \mathbb{E}[z^2] - \mathbb{E}^2[z] = \mathbb{E}[z^2]$, where $\mathbb{E}[z] = \mathbf{w}_1^\top\mathbb{E}[\mathbf{x}]_n = 0$).

The first PC is the eigenvector of $\hat{\Sigma}$ with the largest eigenvalue

Because we want the projection to be orthonormal such that $\mathbf{w}_1^\top \mathbf{w} = 1$, we introduce the following constraint with the *Lagrange multiplier* λ_1 to the loss function:

$$\tilde{\mathcal{L}}(\mathbf{w}_1) = -\mathbf{w}_1^\top \hat{\Sigma} \mathbf{w}_1 + \lambda_1 (\mathbf{w}_1^\top \mathbf{w}_1 - 1) \tag{1}$$

$$\frac{\partial \tilde{\mathcal{L}}(\mathbf{w}_1)}{\partial \mathbf{w}_1} = -2\hat{\Sigma}\mathbf{w}_1 + 2\lambda_1 \mathbf{w}_1 \stackrel{\Delta}{=} 0 \quad \Rightarrow \quad \hat{\Sigma}\mathbf{w}_1 = \lambda_1 \mathbf{w}_1$$

Therefore, the optimal solution for $\mathbf{w}_1$ is an *eigenvector* of $\hat{\Sigma}$ and λ_1 corresponds to the *eigenvalue*. Multiplying $\mathbf{w}_1^\top$ on both side, we have

$$\hat{\Sigma}\mathbf{w}_1 = \lambda_1 \mathbf{w}_1 \quad \Rightarrow \quad \mathbf{w}_1^\top \hat{\Sigma} \mathbf{w}_1 = \lambda_1 \mathbf{w}_1^\top \mathbf{w}_1 \quad \Rightarrow \quad \mathbf{w}_1^\top \hat{\Sigma} \mathbf{w}_1 = \lambda_1$$

Since we want to maximize $\mathbf{w}_1^\top \hat{\Sigma} \mathbf{w}_1$ (i.e., minimizing the loss in Eq (1)), we pick the eigenvector that corresponds to the *largest* eigenvalue:

$$\mathbf{w}_1^* \leftarrow \arg\max_{\mathbf{w}_1} \mathbf{w}_1^\top \hat{\Sigma} \mathbf{w}_1 = \arg\max_{\mathbf{w}_1} \mathrm{Var}[\mathbf{z}_1] = \arg\min_{\mathbf{w}_1} \mathcal{L}(\mathbf{w}_1)$$

Computing the second PC

We can find the second PC to further minimize the reconstruction error:

$$\mathcal{L}(\mathbf{w}_2) = \frac{1}{N}\sum_{n=1}^{N} ||\mathbf{x}_n - z_{1,n}\hat{\mathbf{w}}_1 - z_{2,n}\mathbf{w}_2||^2 = \frac{1}{N}\sum_{n=1}^{N} ||\tilde{\mathbf{x}}_n - z_{2,n}\mathbf{w}_2||^2$$

$$= \frac{1}{N}\sum_{n=1}^{N} \tilde{\mathbf{x}}_n^\top \tilde{\mathbf{x}}_n - \mathbf{w}_2^\top \hat{\tilde{\Sigma}} \mathbf{w}_2 \quad \text{where}$$

$$\hat{\tilde{\Sigma}} = \frac{1}{N}\tilde{\mathbf{X}}\tilde{\mathbf{X}}^\top = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - z_{1,n}\hat{\mathbf{w}}_1)(\mathbf{x}_n - z_{1,n}\hat{\mathbf{w}}_1)^\top$$

$$= \underbrace{\frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n\mathbf{x}_n^\top}_{\hat{\Sigma}} - \hat{\mathbf{w}}_1\frac{1}{N}\sum_{n=1}^{N} z_{1,n}\mathbf{x}_n^\top - \left(\frac{1}{N}\sum_{n=1}^{N} z_{1,n}\mathbf{x}_n\right)\hat{\mathbf{w}}_1^\top + \left(\frac{1}{N}\sum_{n=1}^{N} z_{1,n}^2\right)\hat{\mathbf{w}}_1\hat{\mathbf{w}}_1^\top$$

Therefore

$$\mathbf{w}_2^\top \hat{\tilde{\Sigma}} \mathbf{w}_2 = \mathbf{w}_2^\top \hat{\Sigma} \mathbf{w}_2 - \underbrace{\mathbf{w}_2^\top \hat{\mathbf{w}}_1}_{0}\frac{1}{N}\sum_{n=1}^{N} z_{1,n}\mathbf{x}_n^\top \mathbf{w}_2 - \mathbf{w}_2^\top\left(\frac{1}{N}\sum_{n=1}^{N} z_{1,n}\mathbf{x}_n\right)\underbrace{\hat{\mathbf{w}}_1^\top \mathbf{w}_2}_{0} + \left(\frac{1}{N}\sum_{n=1}^{N} z_{1,n}^2\right)\underbrace{\mathbf{w}_2^\top \hat{\mathbf{w}}_1}_{0}\underbrace{\hat{\mathbf{w}}_1^\top \mathbf{w}_2}_{0}$$

$$= \mathbf{w}_2^\top \hat{\Sigma} \mathbf{w}_2$$

Computing the second PC

We can find the second PC to further minimize the reconstruction error:

$$\mathcal{L}(\mathbf{w}_2) = \frac{1}{N}\sum_{n=1}^{N} ||\mathbf{x}_n - z_{1,n}\hat{\mathbf{w}}_1 - z_{2,n}\mathbf{w}_2||^2 = \frac{1}{N}\sum_{n=1}^{N} ||\tilde{\mathbf{x}}_n - z_{2,n}\mathbf{w}_2||^2$$

$$= \frac{1}{N}\sum_{n=1}^{N} \tilde{\mathbf{x}}_n^\top \tilde{\mathbf{x}}_n - \mathbf{w}_2^\top \hat{\tilde{\Sigma}} \mathbf{w}_2 = \frac{1}{N}\sum_{n=1}^{N} \tilde{\mathbf{x}}_n^\top \tilde{\mathbf{x}}_n - \mathbf{w}_2^\top \hat{\Sigma} \mathbf{w}_2$$

Adding the orthogonal constraints $\mathbf{w}_1^\top \mathbf{w}_2 = 0$ and orthonormal constraint $\mathbf{w}_2^\top \mathbf{w}_2 = 1$:

$$\tilde{\mathcal{L}}(\mathbf{w}_2) = -\mathbf{w}_2^\top \hat{\Sigma} \mathbf{w}_2 + \lambda_2(\mathbf{w}_2^\top \mathbf{w}_2 - 1) + \lambda_{12}\mathbf{w}_2^\top \mathbf{w}_1$$

$$\frac{\partial \tilde{\mathcal{L}}(\mathbf{w}_2)}{\partial \mathbf{w}_2} = -2\hat{\Sigma}\mathbf{w}_2 + 2\lambda_2 \mathbf{w}_2 + \lambda_{12}\mathbf{w}_1 \stackrel{\Delta}{=} 0$$

Solving for $\mathbf{w}_2$:

$$2\hat{\Sigma}\mathbf{w}_2 = 2\lambda_2\mathbf{w}_2 + \lambda_{12}\mathbf{w}_1 \quad \overset{\mathbf{w}_1^\top \cdot}{\Rightarrow} \quad 2\overbrace{\mathbf{w}_1^\top \hat{\Sigma}\mathbf{w}_2}^{\lambda_1 \mathbf{w}_1^\top} = 2\lambda_2 \overbrace{\mathbf{w}_1^\top \mathbf{w}_2}^{0} + \lambda_{12}\overbrace{\mathbf{w}_1^\top \mathbf{w}_1}^{1} \Rightarrow 0 = \lambda_{12}$$

$$\Rightarrow \hat{\Sigma}\mathbf{w}_2 = \lambda_2 \mathbf{w}_2 \quad \Rightarrow \quad \mathbf{w}_2^\top \hat{\Sigma}\mathbf{w}_2 = \lambda_2$$

Therefore, the solution for $\mathbf{w}_2$ for the second PC is the second largest eigenvector.

Generalizing to computing all K PCs

Find the k^{th} PC can be done in the same way

$$\mathcal{L}(\mathbf{w}_k) = \frac{1}{N}\sum_{n=1}^{N} ||\mathbf{x}_n - \sum_{s=1}^{k-1} z_{s,n}\mathbf{w}_s - z_{k,n}\mathbf{w}_k||^2 = \frac{1}{N}\sum_{n=1}^{N} ||\tilde{\mathbf{x}}_n - z_{k,n}\mathbf{w}_k||^2$$

Iteratively computing the k^{th} eigenvector is slow.
For $N << D$ (e.g., $N = 100$ samples versus $D = 20,000$ genes), we can efficiently compute all eigenvectors by solving the *eigendecomposition* of the square and symmetric covariance matrix:

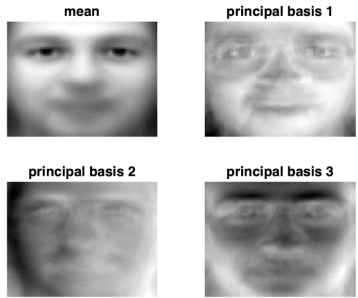
$$\underbrace{\mathbf{X}^\top\mathbf{X}}_{N\times N} = \mathbf{U}\Lambda\mathbf{U}^{-1}$$

where $\mathbf{U}$ contains all of the N eigenvectors and Λ is the diagonal matrix with the diagonal elements being the eigenvalues. Because $\mathbf{U}$ is a orthogonal matrix, $\mathbf{U}^\top\mathbf{U} = \mathbf{I}$ and $\mathbf{U}^\top = \mathbf{U}^{-1}$.
More efficiently, we can compute the truncated Singular Vector Decomposition (SVD) to get only the first $K < \min(N, D)$ PCs by $\mathbf{X} = \mathbf{USV}^\top$ (details omitted).

Eigen faces (Murphy22 Chapter 20.1)

PCA were performed on 64×64 pxiel images from the Olivetti face database (panel a). Mean and the first 3 PCA components $\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3$ are displayed in panel b.

(a)



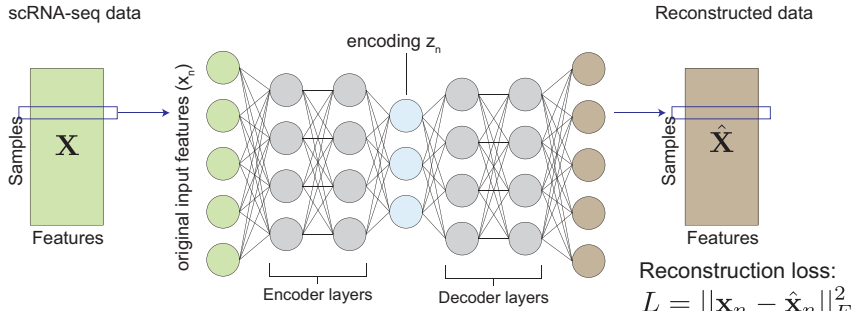
(b)

Outline

Autoencoders

AE main idea: same goal as PCA to describe data with as few parameters as possible, but allow for complex non-linear relationship between those parameters and the input data.

MLP autoencoder



Encoding by a 3-layer feedforward network (i.e., encoder):

$$z_n = f(f(\mathbf{x}_n \mathbf{W}_E^{(0)}) \mathbf{W}_E^{(1)}) \mathbf{W}_E^{(2)}$$

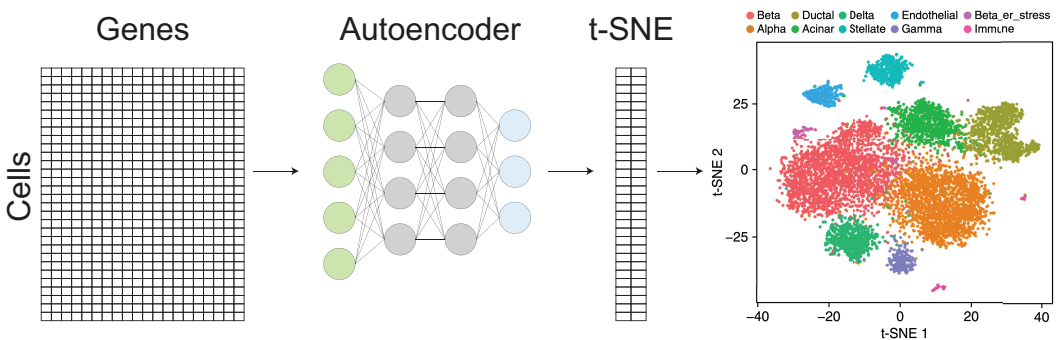
Decoding by another 3-layer feedforward network (i.e., decoder):

$$\hat{\mathbf{x}}_d = f(f(\mathbf{z}_n \mathbf{W}_D^{(0)}) \mathbf{W}_D^{(1)}) \mathbf{W}_D^{(2)}$$

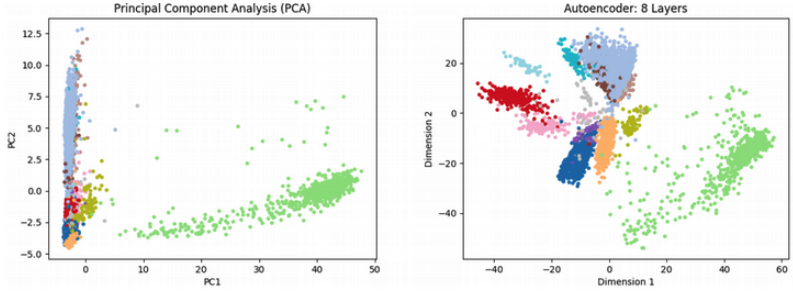
Loss: $L = \frac{1}{N} \sum_n ||\mathbf{x} - \hat{\mathbf{x}}_n||^2$; Backpropagation: $\mathbf{W}_{\cdot}^{(\ell)} \leftarrow \mathbf{W}_{\cdot}^{(\ell)} - \epsilon \nabla L(\mathbf{W}_{\cdot}^{(\ell)})$

Discovering cell types from single-cell gene expression data

- When dealing with high-dimensional data, it is useful to reduce the dimensionality to a lower dimensional subspace to capture the "essence" of the data.
- Below is an example of applying **Autoencoder** followed by **t-distributed stochastic neighbour embedding** (t-SNE) to thousands of cells, each having the expression of 20,000 genes



PCA vs Autoencoder



https://towardsdatascience.com/deep-learning-for-single-cell-biology-935d45064438

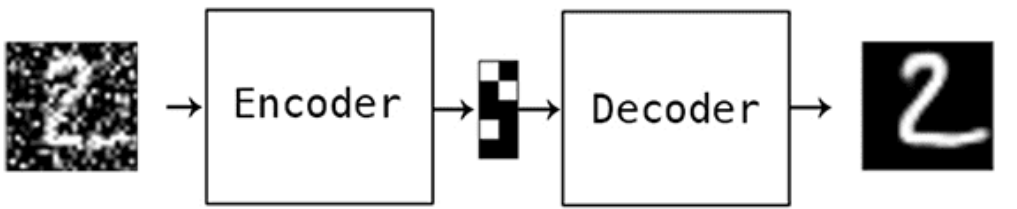
Denoising autoencoder (DAE) (?)

DAE takes the original input with added Gaussian or Bernoulli noise (for binary image):

$$\tilde{\mathbf{x}} \sim \mathcal{N}(\mathbf{x}, \sigma^2 \mathbf{I}), \quad \text{or} \quad \tilde{\mathbf{x}} \sim \mathbf{x}\mathcal{B}(p, 1-p)$$

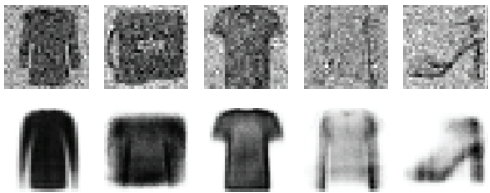
DAE are an extension of simple autoencoders to help:

- The hidden layers of the autoencoder learn more robust filters
- Reduce the risk of overfitting in the autoencoder
- Prevent the autoencoder from learning a simple identify function



Reconstructed Fashion MNIST images from validation set by DAE

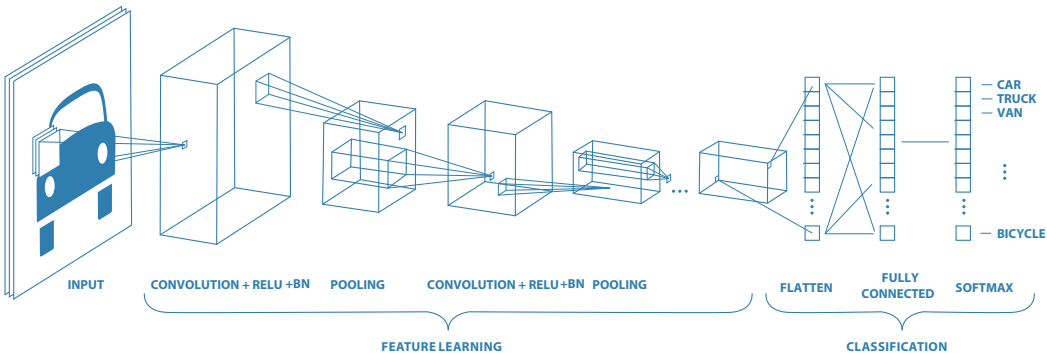
with Gaussian noise



with Bernoulli dropout noise

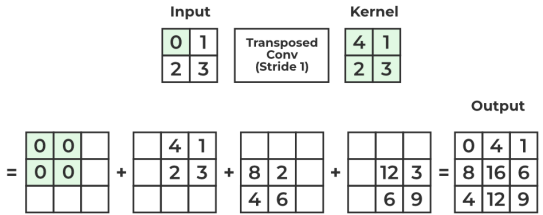
(Murphy22 Chapter 20.3 Figure 20.19)

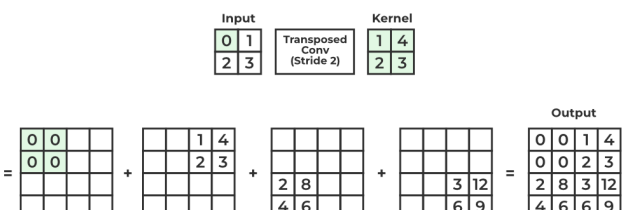
Convolutional neural network for classification on images (Lecture 3)



We can use CNN architectures in our autoencoders!

Transposed convolutional aka Deconvolution layer

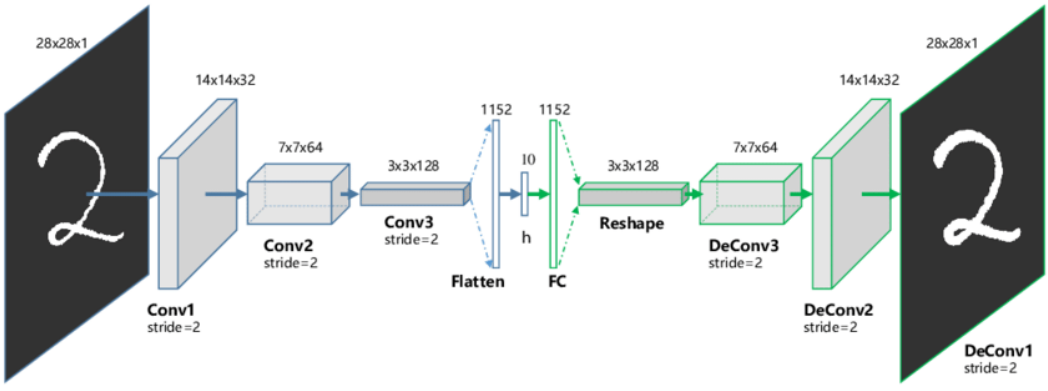




- Instead of sliding the kernel over the input pixels and performing element-wise multiplication and summation, a transposed convolutional layer **slides the input pixel over the kernel** and performs element-wise multiplication and summation.
- This results in an output that is larger than the input, and the size of the output can be controlled by the stride and padding parameters of the layer.

(source)

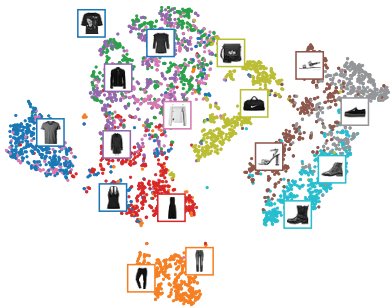
CNN autoencoder



source

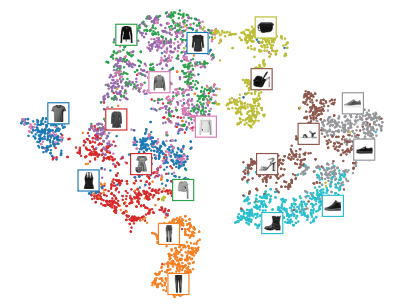
MLP AE vs CNN AE on Fashion MNIST (Murphy22 Fig 20.17 & 18)

MLP AE (784-100-30)



CNN AE

3x3 Conv (16), MaxPool (2x2), Conv (32, 3x3), MaxPool (2x2), Conv (64, 3x3), MaxPool (2x2)



Summary of Autoencoder

- Using network encoder and network decoder, we can train non-linear function that can project high-dimensional data onto low-dimensional latent space by minimizing the reconstruction loss via stochastic gradient decent.
- AE can have MLP or CNN architectures. When applied to images, CNN architecture works better because it benefits from the same induction bias as in the CNN classifiers.
- Denoising autoencoder learns more robust representation of the data than the vanilla autoencoder
- VAE can generate new samples by inferring the distribution of the latent embedding.

Summary of Unsupervised Learning

Goal: Find the regularities in the Data. That often means finding a compressed way to represent the data.

- Clustering: represent all data as a few different clusters.
- PCA & AE: represent the data as a low dimensional manifold of the main directions of variation.
  - PCA: linear submanifold, can find optimal sub-manifold analytically.
  - AE: non-linear, optimality not guaranteed.

Congratulations!