

# Unsupervised Learning

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Fall 2017

# Unsupervised Learning: What, Why, and When?

- 1 Only given inputs,  $\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^N$ ; not told what the desired output is for each input.
- 2 The goal is to find interesting patterns or structures in the data.
- 3 Knowledge discovery: density estimation, clustering, learning representations, dimensionality reduction, finding latent factors.
- 4 Humans are good at unsupervised learning. (E.g., Iron Chicken?)
- 5 “The next frontier in AI: unsupervised learning” — Yann LeCun.

# Example: Dimensionality Reduction for Data Visualization

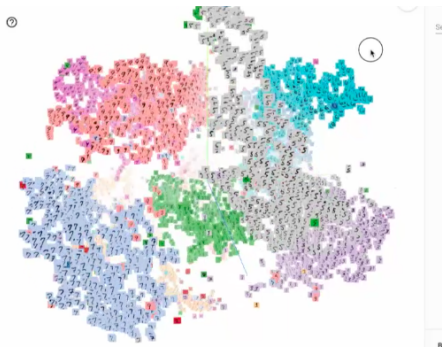


Figure 1: t-SNE visualization in TensorFlow.

# Topics of This Week

- 1 Model based clustering: mixture of Bernoullis, Gaussian mixture model (GMM)
- 2 Latent linear models: principal component analysis (PCA)
- 3 Sparse linear models: sparse coding
- 4 Nonlinear dimensionality reduction: locally linear embedding (LLE), t-distributed stochastic neighbor embedding (t-SNE)
- 5 Autoencoders: denoising autoencoder (DAE), variational autoencoder (VAE)

# Mixture of Gaussians/Gaussian Mixture Model (GMM)

Each distribution in the mixture is a multivariate Gaussian with mean  $\mu_k$  and covariance matrix  $\Sigma_k$ :

$$p(\mathbf{x}_i|\theta) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x}_i|\mu_k, \Sigma_k).$$

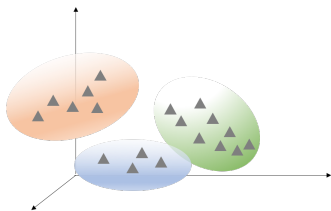


Figure 2: GMM.

$$\theta : \{\pi_k, \mu_k, \Sigma_k\}$$

# GMM for Clustering

## The responsibility and soft clustering

- 1 Fit the mixture model, and compute the posterior probability that a data point  $\mathbf{x}_i$  belongs to cluster  $k$ .
- 2 The *responsibility* of cluster  $k$  for data point  $\mathbf{x}_i$

$$r_{ik} = p(z_i = k | \mathbf{x}_i, \boldsymbol{\theta}) = \frac{p(z_i = k | \boldsymbol{\theta}) p(\mathbf{x}_i | z_i = k, \boldsymbol{\theta})}{\sum_{k'=1}^K p(z_i = k' | \boldsymbol{\theta}) p(\mathbf{x}_i | z_i = k', \boldsymbol{\theta})}.$$

$p(z_i = k | \boldsymbol{\theta})$ : the importance of component  $k$  in the mixture

$p(\mathbf{x}_i | z_i = k, \boldsymbol{\theta})$ : the likelihood of observing  $\mathbf{x}_i$  in component  $k$

# EM Algorithm for GMMs

Expectation maximization (EM), an iterative algorithm, with closed-form updates at each step.

E step:

$$r_{ik} = \frac{\pi_k p(\mathbf{x}_i | \boldsymbol{\theta}_k^{(t-1)})}{\sum_{k'} \pi_{k'} p(\mathbf{x}_i | \boldsymbol{\theta}_{k'}^{(t-1)})}.$$

M step:

$$\pi_k = \frac{1}{N} \sum_i r_{ik} = \frac{r_k}{N},$$

$$\boldsymbol{\mu}_k = \frac{\sum_i r_{ik} \mathbf{x}_i}{\sum_i r_{ik}} = \frac{\sum_i r_{ik} \mathbf{x}_i}{r_k},$$

$$\boldsymbol{\Sigma}_k = \frac{\sum_i r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T}{r_k}.$$

# Example of Using GMM: Video Object Cosegmentation

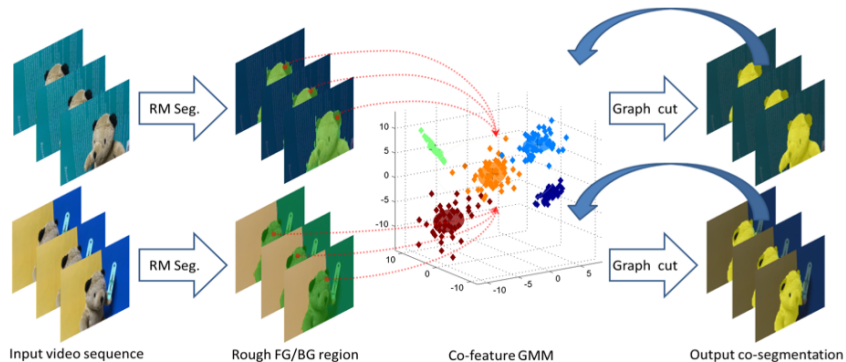


Figure 3: Video Object Cosegmentation.



# Mixture of Bernoullis for Binary Data

Consider binary variables  $\mathbf{x}_i \in \{0, 1\}$ .

## Multivariate Bernoulli

Like a binary image of  $D$  pixels or a bag of  $D$  coins:

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{j=1}^D \mu_j^{x_j} (1 - \mu_j)^{1-x_j}.$$

Mean and covariance:

$$\mathbb{E}[\mathbf{x}] = \boldsymbol{\mu}, \text{ cov}[\mathbf{x}] = \text{diag}\{\mu_j(1 - \mu_j)\}.$$

## Mixture of $K$ Bernoullis ( $K$ bags of $D$ coins)

$$p(\mathbf{x}|\{\boldsymbol{\mu}_k, \pi_k\}) = \sum_{k=1}^K \pi_k p(\mathbf{x}|\boldsymbol{\mu}_k).$$

# Mixture of Bernoullis for Binary Data

## Mixture of $K$ Bernoullis

Like  $K$  bags of  $D$  coins

$$p(\mathbf{x}|\{\boldsymbol{\mu}_k, \pi_k\}) = \sum_{k=1}^K \pi_k p(\mathbf{x}|\boldsymbol{\mu}_k).$$

Mean:

$$\mathbb{E}[\mathbf{x}] = \sum_k^K \pi_k \boldsymbol{\mu}_k,$$

Covariance (not diagonal anymore):

$$\text{cov}[\mathbf{x}] = \sum_k^K \pi_k [\text{diag}\{\mu_{kj}(1 - \mu_{kj})\} + \boldsymbol{\mu}_k \boldsymbol{\mu}_k^T] - \mathbb{E}[\mathbf{x}] \mathbb{E}[\mathbf{x}]^T.$$

# EM for Mixtures of Bernoullis

E step:

$$r_{ik} = \frac{\pi_k p(\mathbf{x}_i | \boldsymbol{\mu}_k^{(t-1)})}{\sum_{k'} \pi_{k'} p(\mathbf{x}_i | \boldsymbol{\mu}_{k'}^{(t-1)})} .$$

M step ( $k$ th component,  $j$ th dimension):

$$\mu_{kj} = \frac{\sum_i r_{ik} x_{ij}}{\sum_i r_{ik}} .$$

## Example: MNIST '3', '5', and '8'

Load MNIST data:

```
from tensorflow.examples.tutorials.mnist import input_data  
mnist = input_data.read_data_sets("MNIST_data/", one_hot=True)
```

# Principal Component Analysis (PCA)

## The synthesis view of PCA

Goal: to find an *orthogonal* set of  $L$  linear basis vectors  $\mathbf{w}_j \in \mathbb{R}^D$ , and the corresponding coefficients  $\mathbf{z}_i \in \mathbb{R}^L$  for each data point  $\mathbf{x}_i$ , such that the average reconstruction error is minimized:

$$J(\mathbf{W}, \mathbf{Z}) = \frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \mathbf{W}\mathbf{z}_i\|^2,$$

or equivalently

$$J(\mathbf{W}, \mathbf{Z}) = \|\mathbf{X}^T - \mathbf{W}\mathbf{Z}^T\|_F^2, \text{ with } \mathbf{X} \in \mathbb{R}^{N \times D}, \mathbf{Z} \in \mathbb{R}^{N \times L}, \mathbf{W}^T \mathbf{W} = \mathbf{I}_L.$$

The Frobenius norm of matrix  $\mathbf{A}$

$$\|\mathbf{A}\|_F = \sqrt{\sum_i \sum_j a_{ij}^2} = \sqrt{\text{tr}(\mathbf{A}^T \mathbf{A})} = \sqrt{\text{tr}(\mathbf{A} \mathbf{A}^T)} = \|\mathbf{A}(\cdot)\|_2.$$

# Principal Component Analysis (PCA)

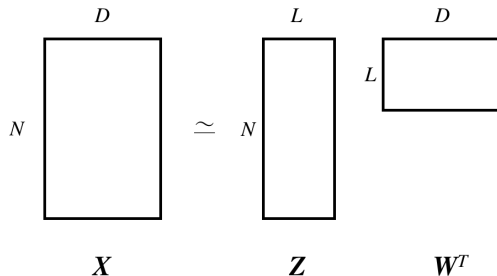


Figure 4: Matrix representation.

# Principal Component Analysis (PCA)

## The synthesis view of PCA

Solution: obtained by setting  $\mathbf{W} = \mathbf{V}_L$ , where  $\mathbf{V}_L$  consists of the  $L$  eigenvectors corresponding to the  $L$  largest eigenvalues of the empirical covariance matrix

$$\hat{\Sigma} = \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i \mathbf{x}_i^T.$$

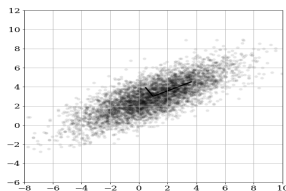


Figure 5: Gaussian PCA.

# Example of PCA: Eigenfaces

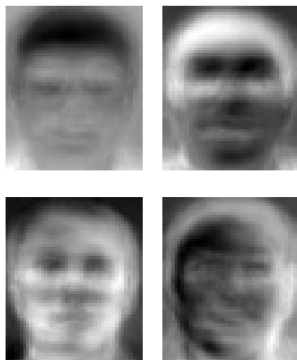


Figure 6: Eigenfaces.

Image credits: eigenface images from Wikipedia by MH & Ylebru, original dataset by AT&T Laboratories Cambridge



# Principal Component Analysis (PCA)

## The analysis view of PCA

Minimizing the reconstruction error is equivalent to maximizing the variance of the projected data.

The variance of the projected data can be written as

$$\frac{1}{N} \sum_{i=1}^N z_{1i}^2 = \frac{1}{N} \sum_{i=1}^N \mathbf{w}_1^T \mathbf{x}_i \mathbf{x}_i^T \mathbf{w}_1 = \mathbf{w}_1^T \hat{\Sigma} \mathbf{w}_1,$$

where

$$\hat{\Sigma} = \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i \mathbf{x}_i^T.$$

We need to impose the constraint  $\|\mathbf{w}_1\| = 1$ , and it can be shown that  $\mathbf{w}_1^T \hat{\Sigma} \mathbf{w}_1 = \lambda_1$  is an eigenvalue of  $\hat{\Sigma}$ .

# Singular Value Decomposition (SVD) and PCA

Decompose an  $N \times D$  data matrix  $\mathbf{X}$ :

$\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^T$ , where  $\mathbf{U}^T\mathbf{U} = \mathbf{I}_N$ ,  $\mathbf{V}^T\mathbf{V} = \mathbf{I}_D$ , and  $\mathbf{S}^2$  is a diagonal matrix.

To get  $\mathbf{U}$  and  $\mathbf{V}$ , compute the eigen-decomposition for

$$\mathbf{X}\mathbf{X}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T\mathbf{V}\mathbf{S}^T\mathbf{U}^T = \mathbf{U}(\mathbf{S}\mathbf{S}^T)\mathbf{U}^T,$$

$$\mathbf{X}^T\mathbf{X} = \mathbf{V}\mathbf{S}^T\mathbf{U}^T\mathbf{U}\mathbf{S}\mathbf{V}^T = \mathbf{V}(\mathbf{S}^T\mathbf{S})\mathbf{V}^T.$$

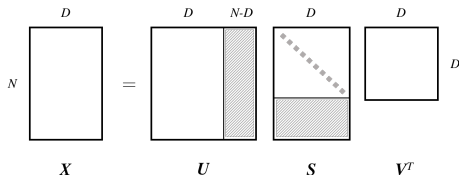


Figure 7: Singular Value Decomposition.

# Singular Value Decomposition (SVD) and PCA

Express the empirical covariance matrix in PCA by matrix multiplication

$$\hat{\Sigma} = \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i \mathbf{x}_i^T = \frac{1}{N} \mathbf{X}^T \mathbf{X}.$$

The eigenvectors of  $\hat{\Sigma}$  are equal to the right singular vectors of  $\mathbf{X}$ .

We can compute PCA using just a few lines of code based on (thin) SVD.

# Singular Value Decomposition (SVD) and PCA

The low-rank approximation view

$$\|\mathbf{X} - \mathbf{X}_L\|_F \approx \sigma_{L+1}$$

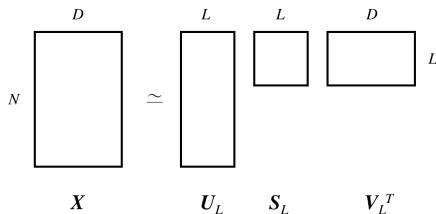


Figure 8: Truncated Singular Value Decomposition.

# Sparse Coding

Negative log-likelihood:

$$NLL(\mathbf{W}, \mathbf{Z}) = \sum_{i=1}^N \frac{1}{2} \|\mathbf{x}_i - \mathbf{W}\mathbf{z}_i\|_2^2 + \lambda \|\mathbf{z}_i\|_1.$$

$$\mathcal{C} = \{\mathbf{W} \in \mathbb{R}^{D \times L} \text{ s.t. } \mathbf{w}_j^T \mathbf{w}_j \leq 1\}.$$

$\mathbf{W}$  is called a dictionary.

The columns of  $\mathbf{W}$  are not required to be orthogonal.

Usually  $L > D$ : overcomplete representation.

$\mathbf{z}_i$  is sparse: only a few columns of  $\mathbf{W}$  are needed for reconstructing  $\mathbf{x}_i$ .

Learning a sparse coding dictionary

$$\min_{\mathbf{W} \in \mathcal{C}, \mathbf{Z} \in \mathbb{R}^{L \times N}} \sum_{i=1}^N \frac{1}{2} \|\mathbf{x}_i - \mathbf{W}\mathbf{z}_i\|_2^2 + \lambda \|\mathbf{z}_i\|_1.$$

# Why $\ell_1$ Regularization

$$\|\mathbf{z}\|_p = (|z_1|^p + |z_2|^p + \dots + |z_L|^p)^{1/p}$$

$$\|\mathbf{z}\|_\infty = \max\{|z_1|, |z_2|, \dots, |z_L|\}$$

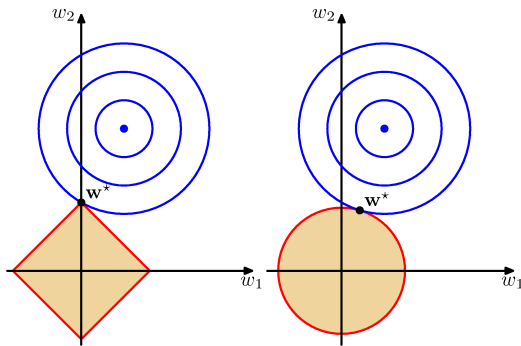


Figure 9:  $\ell_1$  vs.  $\ell_2$  regularization. (Lasso vs. ridge regression.) [Image from Bishop, PRML]

# Dictionary

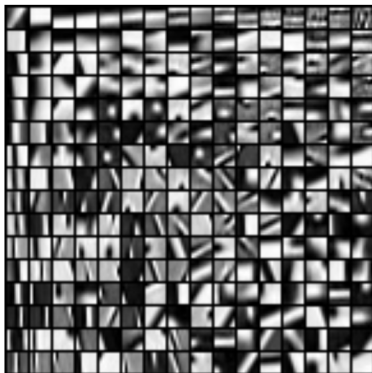


Figure 10: Dictionary. [Elad & Aharon]

# Dictionary Learning

Sparse coding: For a fixed dictionary  $\mathbf{W}$ , the optimization problem over  $\mathbf{Z}$  is identical to the lasso problem (least absolute shrinkage and selection operator [Tibshirani]), which can be solved by LARS algorithm (least angle regression)

SPAMS: J. Mairal, F. Bach and J. Ponce. Sparse Modeling for Image and Vision Processing. <http://spams-devel.gforge.inria.fr>  
Optimization with Sparsity-Inducing Penalties  
<https://hal.archives-ouvertes.fr/hal-00613125v1/document>

Dictionary update: With  $\mathbf{Z}$  fixed, solve for  $\mathbf{W}$  using projected gradient descent.



# Other Formulations

## $\ell_0$ regularization

Learn the dictionary using  $\ell_1$ -penalty. For the final reconstruction step,  $\ell_0$ -penalty is better:

$$\min_{\mathbf{z}_i \in \mathbb{R}^L} \|\mathbf{z}_i\|_0 \quad \text{s.t.} \quad \|\mathbf{x}_i - \mathbf{W}\mathbf{z}_i\|_2^2 \leq \epsilon,$$

which can be solved by orthogonal matching pursuit (OMP).

## Non-negative matrix factorization

$$\min_{\mathbf{W} \in \mathbb{C}, \mathbf{Z} \in \mathbb{R}^{L \times N}} \sum_{i=1}^N \frac{1}{2} \|\mathbf{x}_i - \mathbf{W}\mathbf{z}_i\|_2^2 \quad \text{s.t.} \quad \mathbf{W} \geq 0, \mathbf{z}_i \geq 0.$$

# Example: Learning Sparse Dictionaries for Saliency Detection

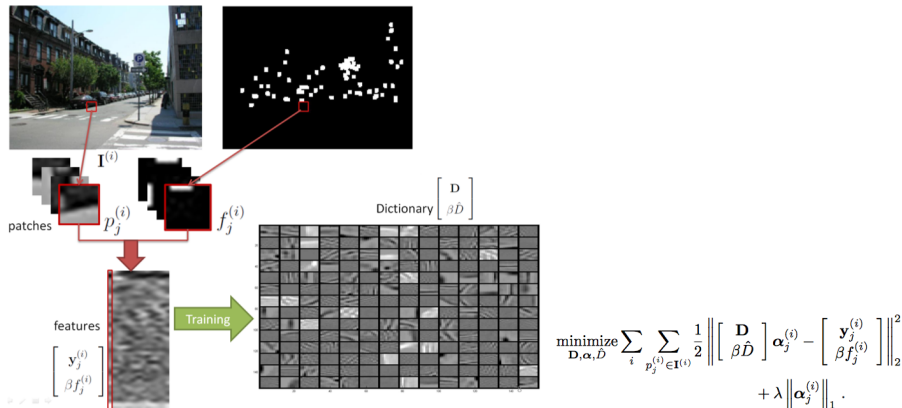


Figure 11: Overview of dictionary training for saliency detection.

# Locally Linear Embedding (LLE)

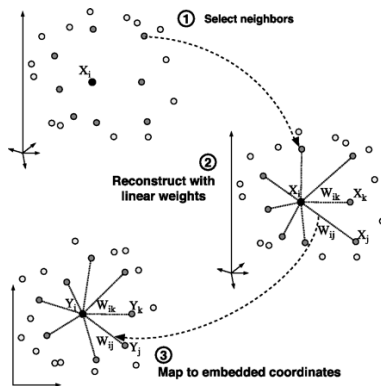


Figure 12: LLE.

## LLE

Each data point  $\mathbf{x}_i$  is reconstructed only from its neighbors. The rows of the weight matrix sum to one:  $\sum_j \mathbf{w}_{ij} = 1$ .

$$\mathcal{E}(\mathbf{W}) = \sum_i \left\| \mathbf{x}_i - \sum_j \mathbf{w}_{ij} \mathbf{x}_j \right\|^2.$$

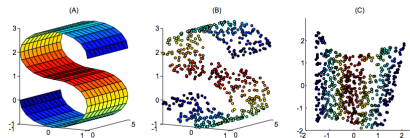


Figure 13: Discovering the 2D manifold in 3D space.

Solve for  $\mathbf{Y}$  by minimizing

$$\Phi(\mathbf{Y}) = \sum_i \left\| \mathbf{y}_i - \sum_j \mathbf{w}_{ij} \mathbf{y}_j \right\|^2.$$

# LLE

## LLE Algorithm

- 1 Compute the neighbors of each data point  $\mathbf{x}_i$ ;
- 2 Compute the weights  $\mathbf{w}_{ij}$  that best reconstruct each data point  $\mathbf{x}_i$  from its neighbors, minimizing the cost  $\mathcal{E}$  by constrained linear fits;
- 3 Compute the vectors  $\mathbf{y}_i$  best reconstructed by the weights  $\mathbf{w}_{ij}$ , minimizing the quadratic form  $\Phi$  by its bottom nonzero eigenvectors.

Solve  $\mathcal{E}(\mathbf{W})$  in LLE

For a data point  $\mathbf{x}$  and its  $K$  neighbors  $\boldsymbol{\eta}_j$ , the local reconstruction error

$$\epsilon = |\mathbf{x} - \sum_j w_j \boldsymbol{\eta}_j|^2 = |\sum_j w_j (\mathbf{x} - \boldsymbol{\eta}_j)|^2 = \sum_{j,k} w_j w_k C_{jk},$$

where  $C_{jk} = (\mathbf{x} - \boldsymbol{\eta}_j) \cdot (\mathbf{x} - \boldsymbol{\eta}_k)$  is the local covariance matrix.

The error can be minimized in closed form (with constraint  $\sum_j w_j = 1$ ):

$$w_j = \frac{\sum_k C_{jk}^{-1}}{\sum_{l,m} C_{lm}^{-1}}.$$

In practice, solve  $\sum_k C_{jk} w_k = 1$  and rescale the weights to make them sum to one.

Solve  $\Phi(\mathbf{Y})$  in LLE

Eigenvalue problem

$$\min_{\mathbf{Y}} \Phi(\mathbf{Y}) = \sum_i \left\| \mathbf{y}_i - \sum_j \mathbf{w}_{ij} \mathbf{y}_j \right\|^2.$$

$$\Phi(\mathbf{Y}) = \sum_{i,j} \mathbf{m}_{ij} (\mathbf{y}_i \mathbf{y}_j).$$

Constraints  $\sum_i \mathbf{y}_i = 0$  and  $\frac{1}{N} \sum_i \mathbf{y}_i \mathbf{y}_i^T = \mathbf{I}$ .

The optimal embedding is found by computing the bottom  $d + 1$  eigenvectors of the matrix  $\mathbf{M}$

$$\mathbf{M} = (\mathbf{I} - \mathbf{W})^T (\mathbf{I} - \mathbf{W}).$$

The bottom eigenvector is a unit vector enforcing the zero mean constraint.

# t-Distributed Stochastic Neighbor Embedding (t-SNE)

High-dimensional map  $p_{ij}$

$$p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2)}, \quad p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}.$$

Low-dimensional map  $q_{ij}$  (student t-distribution, heavy tailed, infinite mixture of Gaussians with different variances)

$$q_{ij} = \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_{k \neq l} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}}.$$

Symmetric SNE:

$$C = KL(P||Q) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}},$$

$p_{ij} = p_{ji}$ ,  $q_{ij} = q_{ji}$ ,  $p_{ii} = 0$ , and  $q_{ii} = 0$ .



## t-SNE

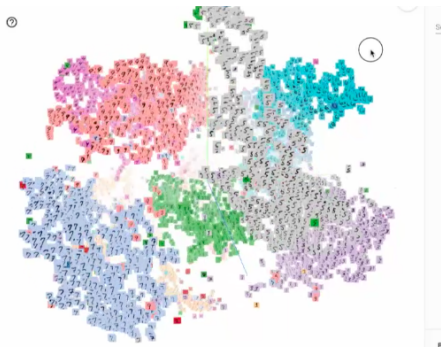


Figure 14: t-SNE visualization in TensorFlow.

# Derivation of the t-SNE gradient

Perplexity (a smooth measure of the effective number of neighbors) for  $\sigma_i$ :

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

Using binary search to find  $\sigma_i$  to make the entropy of the distribution over neighbors equal to  $\log \text{Perp}(P_i)$ .

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

## Algorithm

① Compute  $p_{j|i}$  with perplexity, and then compute  $p_{ij}$ .

② Loop:

Compute  $q_{ij}$  and  $\frac{\delta \mathcal{C}}{\delta \mathbf{Y}}$

Set  $\mathbf{Y}^{(t)} = \mathbf{Y}^{(t-1)} + \eta \frac{\delta \mathcal{C}}{\delta \mathbf{Y}} + \alpha(t)(\mathbf{Y}^{t-1} - \mathbf{Y}^{t-2})$

# Denosing Autoencoders (DAE)

An autoencoder is a neural network that is trained to attempt to copy its input to its output.

Autoencoders with linear neurons + squared loss = PCA

The *denoising autoencoder* (DAE) is an autoencoder that receives a corrupted data point as input and is trained to predict the original, uncorrupted data point as its output.

## DAE

- 1 From the original input  $\mathbf{x}$ , generate a corrupted input  $\tilde{\mathbf{x}} \sim q(\tilde{\mathbf{x}}|\mathbf{x})$ .  
(Simulating missing data, dropout)
- 2 Hidden representation  $\mathbf{z} = f_{\theta}(\tilde{\mathbf{x}})$ .
- 3 From  $\mathbf{z}$ , reconstruct  $\mathbf{y} = g_{\theta'}(\mathbf{z})$ .
- 4 Minimize the cross entropy  $\mathbb{E}_{\mathcal{B}(\mathbf{z})}[-\log \mathcal{B}(\mathbf{y})]$  or  $\|\mathbf{x} - \mathbf{y}\|^2$  as the reconstruction error between  $\mathbf{x}$  and  $\mathbf{y}$  to train the parameters  $\theta$  and  $\theta'$ .

# DAE Example

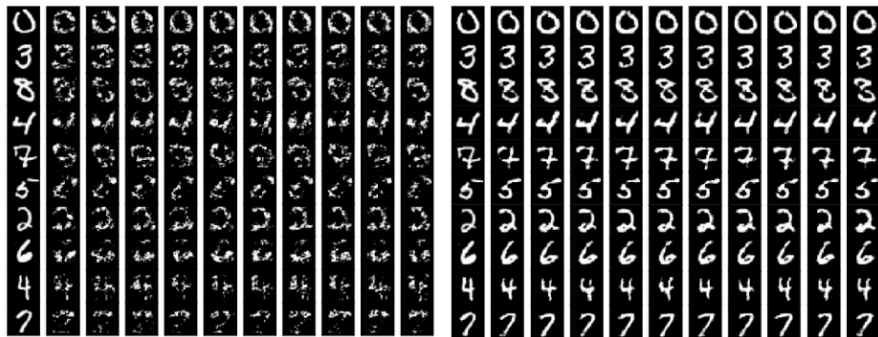


Figure 15: An example of denoising autoencoder.

# Variational Autoencoders (VAEs)

Maximize the probability of generating each data point  $\mathbf{x}$  in the dataset

$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z}; \theta) p(\mathbf{z}) d\mathbf{z},$$

where

$$p(\mathbf{x}|\mathbf{z}; \theta) = \mathcal{N}(\mathbf{x}|f(\mathbf{z}; \theta), \sigma^2 \mathbf{I}) \text{ and } p(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{I}).$$

How to define the latent variable  $\mathbf{z}$ ?

How to deal with the integral over  $\mathbf{z}$ ?

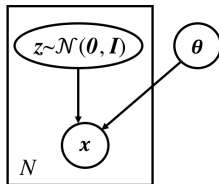


Figure 16: Probability model.

# Variational Autoencoders (VAEs)

Introduce a function  $q(\mathbf{z}|\mathbf{x})$  for sampling values of  $\mathbf{z}$  that are likely to have produced  $\mathbf{x}$ .

Kullback-Leibler divergence

$$KL[q(\mathbf{z}|\mathbf{x})||p(\mathbf{z}|\mathbf{x})] = \mathbb{E}_{\mathbf{z}\sim q}[\log q(\mathbf{z}|\mathbf{x}) - \log p(\mathbf{z}|\mathbf{x})] .$$

Bayes rule

$$KL[q(\mathbf{z}|\mathbf{x})||p(\mathbf{z}|\mathbf{x})] = \mathbb{E}_{\mathbf{z}\sim q}[\log q(\mathbf{z}|\mathbf{x}) - \log p(\mathbf{x}|\mathbf{z}) - \log p(\mathbf{z})] + \log p(\mathbf{x}) .$$

$$\log p(\mathbf{x}) - KL[q(\mathbf{z}|\mathbf{x})||p(\mathbf{z}|\mathbf{x})] = \mathbb{E}_{\mathbf{z}\sim q}[\log p(\mathbf{x}|\mathbf{z})] - KL[q(\mathbf{z}|\mathbf{x})||p(\mathbf{z})] .$$

Perform stochastic gradient descent on the right hand side of the above equation.

# Solving VAE

## Optimize

$$\mathbb{E}_{\mathbf{x} \sim D} [\log p(\mathbf{x}) - KL[q(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}|\mathbf{x})]] = \mathbb{E}_{\mathbf{x} \sim D} [\mathbb{E}_{\mathbf{z} \sim q} [\log p(\mathbf{x}|\mathbf{z})] - KL[q(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z})]]$$

- ① Let  $q(\mathbf{z}|\mathbf{x})$  be a multivariate Gaussian  $\mathcal{N}(\mu(\mathbf{x}; \theta), \Sigma(\mathbf{x}; \theta))$  depending on  $\mathbf{x}$ .
- ②  $\mu(\mathbf{x}; \theta)$  and  $\Sigma(\mathbf{x}; \theta)$  are implemented via neural networks.
- ③  $\Sigma(\mathbf{x}; \theta)$  is constrained to be a diagonal matrix.
- ④  $KL[q(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z})]$  is the KL divergence between two Gaussians, which can be computed in closed form.

Reparameterization trick: We can sample from  $\mathcal{N}(\mu(\mathbf{x}), \Sigma(\mathbf{x}))$  by sampling  $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ , and then computing  $\mathbf{z} = \mu(\mathbf{x}) + \Sigma^{1/2}(\mathbf{x})\epsilon$ .

# VAEs

VAEs are generative.  $q$  is the encoder and  $p$  ( $f$ ) is the decoder.

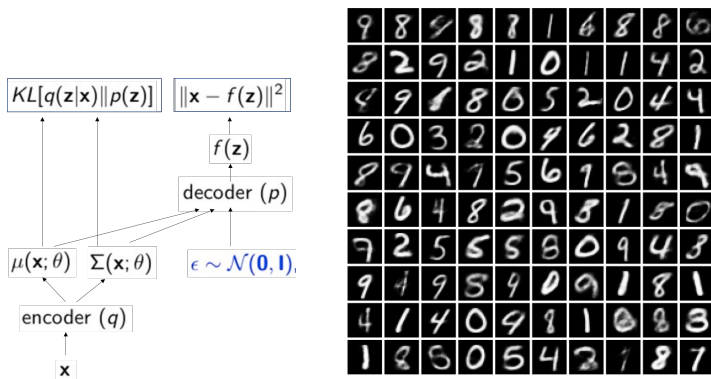


Figure 17: Left: Pipeline of VAE. Right: Samples generated by a trained VAE.



# Topics of This Week

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- 5 Autoencoders: denoising autoencoder (DAE), variational autoencoder (VAE)

# References

- ① Kevin P. Murphy, “Machine Learning: A Probabilistic Perspective”
- ② Christopher Bishop, “Pattern Recognition and Machine Learning”

# Thank You