# CS4487 Lecture 7.1: The Expectation Maximization Algorithm

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Slides template by courtesy of Benjamin M. Marlin

#### Background

- Techniques for convincing manipulations of digital face images exist for decades via the use of visual effects
- Recent technologies in deep learning, especially "DeepFake," have led to a dramatic increase in the realism of fake content
- While there are entertaining applications of DeepFake, potential weaponization of such techniques has raised great concerns
- DeepFake detection has become a pressing issue and a hot spot of research



- **Task:** A binary classification problem
  - Input: RGB face images
  - Output: A binary label to indicate whether an image is fake or not
- **Training set**: 12,000 images, within which 8,000 images contain fake faces, and the rest images are real
  - Download link: https:
     //drive.google.com/drive/folders/1n18AqgUF\_
     KqKbcxuLXrTcLq-pyfhSJD9?usp=sharing
- **Test sets**: Will not be released to the students
  - Students have THREE chances to get access to the test sets
  - The best result among the three will be used for ranking
- **Tip**: It is a good practice to divide the available set further into training, validation, and test set

- **Group project:** A group of at most three students is allowed
- What to hand in: a single ipython notebook (.ipynb) as the project report with source code files included
  - Source files must contain the training code for reproduction
  - An extra PDF file as project report is not recommended
- When to hand in: Dec. 4, 2022, 11:59 pm
- Where to hand in:
  - Submit the clean and runable test code to the TAs and wait for the result update in a Kaggle in-class competition (link will be available soon)
  - Submit the .ipynb file via Canvas
- **GPUs**: Wait for the confirmation from the CS Lab

- **Grading** (Totally 30 points)
  - 30.0% Technical correctness (whether the methodologies/algorithms are correctly used)
  - 30.0% Experiment and analysis
    - More points for thoroughness and testing interesting cases (e.g., different parameter settings)
    - More points for insightful observations and analysis (e.g., failure analysis)
  - 20.0% Quality of the written report (organized, complete descriptions, etc.)
  - 10.0% Quality of project presentation (tentatively held in Week 13)
    - **Note**: you have the option **not** to present your project
  - 10.0% Reserved for Top-3 teams based on the test set performance

# Supervised vs Unsupervised Learning

- Supervised learning considers input-output pairs  $(\mathbf{x}, y)$ 
  - Learn a mapping f from input to output
  - Classification: output  $y \in \{-1, 1\}$
  - Regression: output  $y \in \mathbb{R}$
  - "Supervised" here means that the algorithm is learning the mapping that we want
- Unsupervised learning only considers the input data x
  - There is no output value
  - **Goal**: Try to discover inherent properties in the data
    - Clustering
    - Dimensionality reduction

# Expectation Maximization (EM)

■ EM solves a maximum likelihood problem of the form

$$L(\boldsymbol{\theta}) = \sum_{i=1}^{M} \log p(\mathbf{x}^{(i)}; \boldsymbol{\theta}) = \sum_{i=1}^{M} \log \sum_{z^{(i)}=1}^{K} p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta})$$

- $\bullet$ : Parameters of the probabilistic model we try to find
- $\{\mathbf{x}^{(i)}\}_{i=1}^{M}$ : Observed training examples
- $\{z^{(i)}\}_{i=1}^{M}$ : Unobserved latent variables (e.g., in GMM,  $z^{(i)}$  indicates which one of the K clusters  $\mathbf{x}^{(i)}$  belongs to, which is unobserved)

# Jensen's Inequality

■ Suppose  $f : \mathbb{R}^N \to \mathbb{R}$  is **concave**, then for all probability distributions p, we have

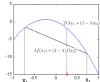
$$f(\mathbb{E}_{\mathbf{x} \sim p}[\mathbf{x}]) \ge \mathbb{E}_{\mathbf{x} \sim p}[f(\mathbf{x})]$$

- The subscript  $\mathbf{x} \sim p$  indicates that the expectation is taken w.r.t. random variable  $\mathbf{x}$  drawn from the probability distribution p
- The equality holds if and only if 1)  $\mathbf{x}$  is constant or 2) f is an affine function (i.e.,  $f(\mathbf{x}) = \mathbf{a}^T \mathbf{x} + b$ )
- The above inequality also holds if the expectation is computed for a deterministic function of  $\mathbf{x}$ , (e.g.,  $g(\mathbf{x})$ )

Illustration:

$$p(x_1) = \lambda,$$
  

$$p(x_2) = 1 - \lambda$$



$$\sum_{i=1}^{M} \log \sum_{z^{(i)}=1}^{K} p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta}) = \sum_{i=1}^{M} \log \sum_{z^{(i)}=1}^{K} q(z^{(i)}) \frac{p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta})}{q(z^{(i)})}$$

$$= \sum_{i=1}^{M} \log \mathbb{E}_{z^{(i)} \sim q} \left[ \frac{p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta})}{q(z^{(i)})} \right]$$

$$\geq \sum_{i=1}^{M} \mathbb{E}_{z^{(i)} \sim q} \log \left[ \frac{p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta})}{q(z^{(i)})} \right]$$

$$= \sum_{i=1}^{M} \sum_{z^{(i)}=1}^{K} q(z^{(i)}) \log p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta})$$

$$- \sum_{i=1}^{M} \sum_{z^{(i)}=1}^{K} q(z^{(i)}) \log q(z^{(i)})$$

$$L(\boldsymbol{\theta}) = \sum_{i=1}^{M} \log \sum_{z^{(i)}=1}^{K} p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta}) \ge \sum_{i=1}^{M} \sum_{z^{(i)}=1}^{K} q(z^{(i)}) \log p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta}) \\ - \sum_{i=1}^{M} \sum_{z^{(i)}=1}^{K} q(z^{(i)}) \log q(z^{(i)}) = \ell(\boldsymbol{\theta})$$

- $\ell(\theta)$  is a lower bound of the original objective  $L(\theta)$
- The equality holds when  $\frac{p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta})}{q(z^{(i)})}$  is constant
- This can be achieved for  $q(z^{(i)}) = p(z^{(i)}|\mathbf{x}^{(i)};\boldsymbol{\theta})$

■ The EM algorithm aims to optimize the lower bound  $\ell(\theta)$ 

$$\boldsymbol{\theta}^{\star} = \operatorname*{arg\,max}_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) = \operatorname*{arg\,max}_{\boldsymbol{\theta}} \sum_{i=1}^{M} \sum_{z^{(i)}=1}^{K} q(z^{(i)}) \log \frac{p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta})}{q(z^{(i)})}$$

- EM repeatedly performs the following two steps until convergence. At *t*-th iteration,
  - **1** E-step: For each index *i*, compute

$$q^{(t)}(z^{(i)}) = p(z^{(i)}|\mathbf{x}^{(i)};\boldsymbol{\theta}^{(t)})$$

2 M-step: Compute

$$\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{M} \sum_{\boldsymbol{z}^{(i)}} q^{(t)}(\boldsymbol{z}^{(i)}) \log p(\mathbf{x}^{(i)}, \boldsymbol{z}^{(i)}; \boldsymbol{\theta})$$

■ In E-step, we do not fill in the unobserved  $z^{(i)}$  with hard values, but find a posterior distribution  $q(z^{(i)})$ , given  $\mathbf{x}^{(i)}$  and  $\boldsymbol{\theta}^{(i)}$ , i.e.,

$$q^{(t)}(z^{(i)}) = p(z^{(i)}|\mathbf{x}^{(i)};\boldsymbol{\theta}^{(t)})$$

- In M-step, we maximize the lower bound  $\ell(\theta)$ , while holding  $q^{(t)}(z^{(i)})$  fixed, which is computed from the E-step
- M-step optimization can be done efficiently in most cases. For example, in GMM, we have closed-form solutions for all parameters

# EM Convergence

Assuming  $\theta^{(t)}$  and  $\theta^{(t+1)}$  are the parameters from two successive iterations of EM, we have

$$L\left(\boldsymbol{\theta}^{(t)}\right) \stackrel{(1)}{=} \sum_{i=1}^{M} \log p(\mathbf{x}^{(i)}; \boldsymbol{\theta}^{(t)}) \stackrel{(2)}{=} \sum_{i=1}^{M} \log \sum_{z^{(i)}=1}^{K} q(z^{(i)}) \frac{p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta}^{(t)})}{q(z^{(i)})}$$

$$\stackrel{(3)}{=} \sum_{i=1}^{M} \sum_{z^{(i)}=1}^{K} q^{(t)}(z^{(i)}) \log \frac{p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta}^{(t)})}{q^{(t)}(z^{(i)})}$$

$$\stackrel{(4)}{\leq} \sum_{i=1}^{M} \sum_{z^{(i)}=1}^{K} q^{(t)}(z^{(i)}) \log \frac{p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta}^{(t+1)})}{q^{(t)}(z^{(i)})}$$

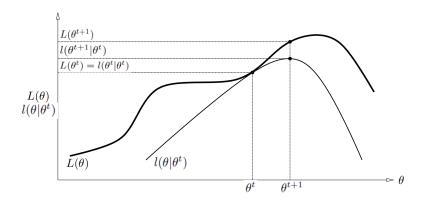
$$\stackrel{(5)}{\leq} \sum_{i=1}^{M} \log \sum_{z^{(i)}=1}^{K} q^{(t)}(z^{(i)}) \frac{p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta}^{(t+1)})}{q^{(t)}(z^{(i)})} \stackrel{(6)}{=} L\left(\boldsymbol{\theta}^{(t+1)}\right)$$

# EM Convergence

#### where

- (1): by definition likelihood of the data
- (2): by marginalization over  $z^{(i)}$  and multiplication an arbitrary distribution  $q(z^{(i)})$  to both numerator and denominator inside  $\log$
- (3): by Jensen's inequality where equality condition satisfied by setting  $q^{(i)}(z^{(i)}) = p(z^{(i)}|\mathbf{x}^{(i)};\boldsymbol{\theta}^{(t)})$
- (4): by M-step of EM, where we maximize (3), holding  $q^{(t)}(z^{(i)})$  fixed
- (5): by Jensen's inequality (in reverse order)
- (6): by definition
- Hence, EM causes the likelihood to increase monotonically

### EM Illustration for GMM



#### Remark

■ If we define

$$J(q, \theta) = \sum_{i=1}^{M} \sum_{z^{(i)}=1}^{K} q(z^{(i)}) \log \frac{p(\mathbf{x}^{(i)}, z^{(i)}; \theta)}{q(z^{(i)})},$$

■ EM can also be viewed as coordinate ascent on J, in which the E-step maximizes J w.r.t. q, and the M-step maximizes J with respect to  $\theta$ 

# Clustering Summary

#### Clustering task:

- Given a set of input vectors  $\mathcal{D} = \{\mathbf{x}^{(i)}\}_{i=1}^{M}$  with  $\mathbf{x}^{(i)} \in \mathbb{R}^{N}$ , group similar  $\mathbf{x}^{(i)}$  together into clusters
  - Estimate a cluster center, representing the data points in that cluster
  - Predict the cluster for a new data point

#### Exhaustive clustering

- Cluster shape: arbitrary shape
- Principle: minimize an assumed clustering criterion with brute-force search
- **Pros**: optimal under the given clustering criterion
- Cons: impractical to construct the clustering criterion; prohibitive to compute

# Clustering Summary

#### ■ K-means

- Cluster shape: circular
- **Principle**: minimize distance to cluster center
- **Pros**: simple and scalable (MiniBatchKMeans)
- **Cons**: sensitive to initialization; could get bad solutions due to local minima; need to choose *K*

#### **■** Gaussian mixture model (GMM)

- **Cluster shape**: elliptical
- **Principle**: maximum likelihood using expectation maximization
- **Pros**: elliptical cluster shapes
- **Cons**: sensitive to initialization; could get bad solutions due to local minima; need to choose *K*

# Other Things

#### **■** Feature normalization

- Feature normalization is typically required clustering
- E.g., algorithms based on Euclidean distance (*K*-means)