CS5489 Lecture 7.1: The Expectation Maximization Algorithm

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Background

- Techniques for creating convincing naturalistic images have existed for decades
- Recent advances in deep learning, particularly in generative adversarial networks (GANs) and diffusion models, have significantly increased the photorealism of generated content
- While these techniques have entertaining applications, their potential weaponization has raised serious concerns
- Detecting AI-generated content (AIGC) has become a pressing issue and a prominent research topic













Photographic Images

AI-generated Images

Dataset Description

- The dataset contains photographic and AI-generated images
- Photographic images, with arbitrary sizes, are gathered from the ImageNet dataset
- AI-generated images, with a fixed size of 512 × 512 × 3, are created using the text-to-image diffusion model *Stable Diffusion v1.4*, which is trained on the LAION dataset containing billions of image-text pairs
- Photographic and AI-generated images have similar semantic content to avoid any content bias
- Only binary labels are provided for training and testing

- Main task: A binary classification problem
 - Input: RGB images
 - Output: A binary label to indicate whether an image is AI-generated or not
- **Training and validation sets**: 45,000 images for training and 5,000 images for validation
 - Download link:

```
https://portland-my.sharepoint.com/:f:
/g/personal/haoychen3-c_my_cityu_edu_hk/
EvfnkWdVX4lOmFLWOn-dZCOBJCq-ngYWwj8wuBoiwKMolg
```

- **Test set:** Will not be released to the students
 - Students have THREE chances to get access to the test set
 - The best result among the three will be used for ranking
- **Tip**: It is a good practice to have a test set divided from the available training (or validation) set

- **Group project:** A group of at most four 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. 15, 2024, 11:59:59 pm
- Where to hand in:
 - Submit the clean and runable test code to the TAs and wait for the result update in a Kaggle-style 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, concise 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

Outline

- 1 Review
- 2 Expectation Maximization
- 3 Clustering Summary

Supervised vs Unsupervised Learning

- Supervised learning considers input-output pairs (\mathbf{x}, y)
 - \blacksquare 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
 - Density estimation
 - Clustering
 - Dimensionality reduction
 - Manifold embedding

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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

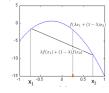
$$f(\mathbb{E}_{\mathbf{x} \sim p}[\mathbf{x}]) \ge \mathbb{E}_{\mathbf{x} \sim p}[f(\mathbf{x})]$$

- 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) **x** is constant or 2) f is an affine function (i.e., $f(\mathbf{x}) = \mathbf{a}^T \mathbf{x} + b$)

Illustration:

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

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



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

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

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

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

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

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

- \bullet $\ell(\theta)$ 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,
 - **I** E-step: For each index *i*, compute

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

2 M-step: Compute

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

■ 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 $\boldsymbol{\theta}^{(t)}$, 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

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

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

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

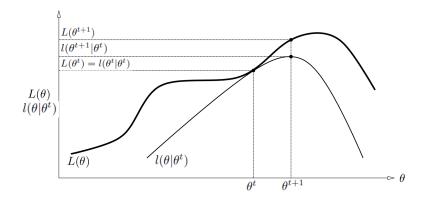
$$\stackrel{(5)}{\leq} \sum_{i=1}^{M} \log \sum_{z^{(i)}=1}^{K} q^{(t)}(z^{(i)}) \frac{p(\mathbf{x}^{(i)}, z^{(i)}; \boldsymbol{\theta}^{(t+1)})}{q^{(t)}(z^{(i)})} \stackrel{(6)}{=} L\left(\boldsymbol{\theta}^{(t+1)}\right)$$

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 $q^{(t)}(z^{(i)}) = p(z^{(i)}|\mathbf{x}^{(i)};\boldsymbol{\theta}^{(t)})$
- (4): by M-step of EM, where we maximize (3), holding $q^{(t)}(z^{(i)})$ fixed
- (5): by Jensen's inequality (in reverse order). Note that we have already updated θ from $\theta^{(t)}$ to $\theta^{(t+1)}$, $q^{(t)}(z^{(i)}) = p(z^{(i)}|\mathbf{x}^{(i)};\theta^{(t)})$ now may not satisfy the equality condition
- (6): by definition
- Hence, EM causes the likelihood to increase monotonically

EM Illustration for GMM



Remark

If we define

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

EM 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 θ

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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)