6.7900 Machine Learning (Fall 2024)

Lecture 21: more detailed derivations for mixtures, ELBO

Log-likelihood gradient for a mixture model

- Consider a k-component spherical Gaussian mixture model in $\mathbb{R}^d$ with parameters
$$\theta = \{\pi_1, \ldots, \pi_k, \mu_1, \ldots, \mu_k, \sigma_1^2, \ldots, \sigma_k^2\}$$
where, e.g., $\mu_j \in \mathbb{R}^d, \sigma_j^2 \in \mathbb{R}^+$ (one overall variance per cluster)
- We will write the mixture model in a generic form to keep the formulas simpler
$$\log P(x\,|\,\theta) = \log[\,\sum_{z=1}^{k} P(z\,|\,\theta)P(x\,|\,z,\theta)\,]$$
where now, $P(z\,|\,\theta) = p_z$ (mixing proportion for zth cluster), and
$$P(x\,|\,z,\theta) = \frac{1}{(2\pi\sigma_z^2)^{d/2}}\exp(-\frac{1}{2\sigma_z^2}\|x-\mu_z\|^2)$$
- We wish to calculate $\nabla_\theta \log P(x\,|\,\theta)$

Log-likelihood gradient for a mixture model

$$\nabla_\theta \log P(x\,|\,\theta) = \nabla_\theta \log[\, \sum_z P(z\,|\,\theta) P(x\,|\,z,\theta)\,]$$

$$= \frac{1}{\sum_z P(z\,|\,\theta) P(x\,|\,z,\theta)} \nabla_\theta \sum_z P(z\,|\,\theta) P(x\,|\,z,\theta)$$

$$= \sum_z \frac{1}{P(x\,|\,\theta)} \nabla_\theta [P(z\,|\,\theta) P(x\,|\,z,\theta)]$$

$$\nabla_\theta P = P\, \nabla_\theta \log P$$

$$= \sum_z \frac{1}{P(x\,|\,\theta)} [P(z\,|\,\theta) P(x\,|\,z,\theta)]\, \nabla_\theta \log[P(z\,|\,\theta) P(x\,|\,z,\theta)]$$

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

$$= \sum_z P(z\,|\,x,\theta)\, \nabla_\theta \log[P(z\,|\,\theta) P(x\,|\,z,\theta)]$$

i.e., posterior weighted average of gradients
of log-complete log-likelihoods

ELBO lower bound

- We will show that the ELBO lower bound

$$\log P(x \mid \theta) \geq \sum_z Q(z \mid x) \log [\, P(z \mid \theta) P(x \mid z, \theta) \,] + H(Q_{z|x})$$

holds for all choices of Q (conditional distribution) and parameters θ

- Here $H(Q_{z|x}) = -\sum_z Q(z \mid x) \log Q(z \mid x)$ (entropy)

ELBO lower bound cont'd

$$\sum_z Q(z|x)\log[\,P(z|\theta)P(x|z,\theta)\,] - \sum_z Q(z|x)\log Q(z|x)$$

$$= \sum_z Q(z|x)\log[\,P(z|\theta)P(x|z,\theta)\,] + \sum_z Q(z|x)\log\frac{1}{Q(z|x)}$$

$$= \sum_z Q(z|x)\log[\,\frac{P(z|\theta)P(x|z,\theta)}{Q(z|x)}\,]$$

$$\leq \log[\,\sum_z Q(z|x)\frac{P(z|\theta)P(x|z,\theta)}{Q(z|x)}\,]$$

Jensen's inequality: log() is concave (convex down) so taking the expectation inside the log increases (does not decrease) the value

$$= \log[\,\sum_z P(z|\theta)P(x|z,\theta)\,]$$

$$= \log P(x|\theta)$$

ELBO lower bound: alternative derivation

$$\sum_z Q(z|x)\log[\,P(z|\theta)P(x|z,\theta)\,] + \sum_z Q(z|x)\log\frac{1}{Q(z|x)}$$

$$= \sum_z Q(z|x)\log[\frac{P(z|\theta)P(x|z,\theta)}{Q(z|x)}] = \sum_z Q(z|x)\log[\,P(x|\theta)\frac{P(z|\theta)P(x|z,\theta)}{P(x|\theta)Q(z|x)}\,]$$

$$= \log P(x|\theta) + \sum_z Q(z|x)\log[\frac{P(z|\theta)P(x|z,\theta)}{P(x|\theta)Q(z|x)}]$$

$$= \log P(x|\theta) + \sum_z Q(z|x)\log[\frac{P(z|x,\theta)}{Q(z|x)}]$$

$$= \log P(x|\theta) - \sum_z Q(z|x)\log[\frac{Q(z|x)}{P(z|x,\theta)}]$$

$$= \log P(x|\theta) - KL(Q_{z|x}\|P_{z|x,\theta})$$

where $KL(Q_{z|x}\|P_{z|x,\theta}) \geq 0$

$KL(Q_{z|x}\|P_{z|x,\theta}) = 0$

iff $Q(z|x) = P(z|x,\theta)$