Deep Learning - Foundations and Concepts

Chapter 15. Discrete Latent Variables

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Outline

1. K-means Clustering

2. Mixtures of Gaussians

3. Expectation-Maximization Algorithm

K-means clustering

Problem

Suppose we have a data set $\{x^1, \ldots, x^N\}$ consisting of N observations of a D-dimensional Euclidean variable x. Partition the data set into some number K of clusters, where we will suppose for the moment that the value of K is given.

K-means clustering

Problem'

Find:

- K cluster centers: $\mu_1, \ldots, \mu_K \in \mathbb{R}^D$.
- N data point assignment: $r^1, \ldots, r^N \in \{\mathrm{e}_1, \ldots, \mathrm{e}_K\}$.

such that the error function:

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_k^n ||x^n - \mu_k||^2$$

which represents the sum of the squares of the distances of each data point to its assigned cluster center, is minimized.

K-means clustering

We can do this through an iterative procedure:

1. Choose some initial values for the $\{\mu_k\}$.
2. E step: Minimize J with respect to the $\{r_k^n\}$, keeping the $\{\mu_k\}$ fixed.
3. M step: Minimize J with respect to the $\{\mu_k\}$, keeping the $\{r_k^n\}$ fixed.
4. Go to step 2 until convergence.

K-means clustering

Consider the E step. It's easy to see that we should assign the nth data point to the closest cluster center:

$$r_k^n = \begin{cases} 1, & \text{if } k = \text{argmin}_j ||x^n - \mu_j||^2 \\ 0, & \text{otherwise} \end{cases}$$

For the M step:

$$\frac{\partial J}{\partial \mu_k} = 2 \sum_{n=1}^{N} r_k^n (x^n - \mu_k)^T$$

$$\mu_k = \frac{\sum_{n=1}^{N} r_k^n x^n}{\sum_{n=1}^{N} r_k^n}$$

so μ_k is equal to the mean of all the data points x_n assigned to cluster k.

K-means clustering

Algorithm 1: K-means algorithm

```
$\{r_k^n\} \leftarrow 0$;
repeat
    $\{{}^{\text{old}}r_k^n\} \leftarrow \{r_k^n\}$;
    for $n \leftarrow 1$ to $N$ do
        $k \leftarrow \text{argmin}_j ||x^n - \mu_j||^2$;
        $r_k^n \leftarrow 1$;
        $r_{j \neq k}^n \leftarrow 0$;
    end
    for $k \leftarrow 1$ to $K$ do
        $\mu_k \leftarrow \frac{\sum_{n=1}^N r_k^n x^n}{\sum_{n=1}^N r_k^n}$;
    end
until $\{r_k^n\} = \{{}^{\text{old}}r_k^n\}$;
return $\{\mu_k\}, \{r_k^n\}$;
```

K-means clustering

When updating the prototype vectors, we can also derive a sequential update in which, for each data point x^n in turn, we update the nearest prototype μ_k using:

$$^{\text{new}}\mu_k = {}^{\text{old}}\mu_k + \frac{1}{N_k}(x^n - {}^{\text{old}}\mu_k)$$

where N_k is the number of data points that have so far been used to update μ_k.

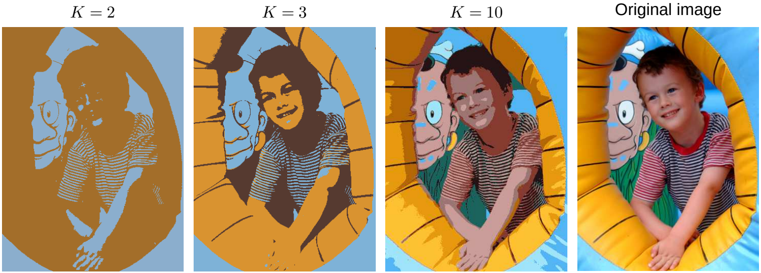
Image segmentation

Using the K-means algorithm to perform (toy) image segmentation:

- Each pixel in an image is a point in a three-dimensional space comprising the intensities of the red, blue and green channels.
- We treat each pixel in the image as a separate data point.
- We can apply the K-means algorithm to these pixels, and redraw the image in which we replace each pixel by the center μ_k to which that pixel has been assigned.

Image segmentation

Figure: Application of the K-means clustering algorithm to image segmentation



$K = 2$

$K = 3$

$K = 10$

Original image

Image segmentation

Using the K-means algorithm to perform lossy data compression:

- For each of the N data points, we store only the identity k of the cluster to which it is assigned.
- We also store the values of the K cluster centers $\{\mu_k\}$.

This framework is often called vector quantization, and the vectors $\{\mu_k\}$ are called codebook vectors.

Mixtures of Gaussians

Formulation of Gaussian mixtures in terms of discrete latent variables:

- Let z be a K-dimensional binary random variable having a 1-of-K representation:
  - $p(z) = \prod_{k=1}^{K} \pi_k^{z_k}$, where $0 \leq \pi_k \leq 1$ and $\sum_{k=1}^{K} \pi_k = 1$.
- Let x be a random variable whose distribution given a particular value for z is a Gaussian:
  - $p(x|z) = \prod_{k=1}^{K} \mathcal{N}(x; \mu_k, \Sigma_k)^{z_k}$.

Mixtures of Gaussians

We see that the marginal distribution for x is given by:

$$p(x) = \sum_{z} p(z)p(x|z) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x; \mu_k, \Sigma_k)$$

which is a Gaussian mixture. We are now able to work with the joint distribution $p(x, z)$ instead of the marginal distribution $p(x)$, and this will lead to significant simplifications.

Mixtures of Gaussians

Let's calculate $\gamma(z_k) = p(z_k = 1|x)$:

$$p(z_k = 1|x) = \frac{p(z_k = 1)p(x|z_k = 1)}{\sum_{k'=1}^{K} p(z_{k'} = 1)p(x|z_{k'} = 1)} = \frac{\pi_k \mathcal{N}(x; \mu_k, \Sigma_k)}{\sum_{k'=1}^{K} \pi_{k'} \mathcal{N}(x; \mu_{k'}, \Sigma_{k'})}$$

We will view π_k as the prior probability of $z_k = 1$, and the quantity $\gamma(z_k)$ as the corresponding posterior probability once we have observed x. $\gamma(z_k)$ can also be viewed as the responsibility that component k takes for explaining the observation x.

Likelihood function

Suppose we have a data set of observations $\{x^1, \ldots, x^N\}$, and we wish to model this data using a mixture of Gaussians. The log of the likelihood function is given by:

$$L = \sum_{n=1}^{N} \log(\sum_{k=1}^{K} \pi_k \mathcal{N}(x^n; \mu_k, \Sigma_k))$$

Likelihood function

We see that:

- Due to the presence of the summation over k that appears inside the logarithm, when maximizing this log likelihood function, we will no longer obtain a closed-form solution.
- The maximization of the log likelihood function is not a well-posed problem, because singularities will occur whenever one of the Gaussian components collapses onto a specific data point.
- Identifiability issue: For any given (non-degenerate) point in the space of parameter values, there will be a further $K! - 1$ additional points all of which give rise to exactly the same distribution.

Maximum likelihood

Let's find the conditions that must be satisfied at a maximum of the log likelihood function:

$$0 = \frac{\partial L}{\partial \mu_k} = \sum_{n=1}^{N} \gamma(z_k^n)(x^n - \mu_k)^T \Sigma_k^{-1} \implies \mu_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_k^n) x^n$$

$$0 = \frac{\partial L}{\partial \Lambda_k}(H) = \frac{1}{2} \sum_{n=1}^{N} \gamma(z_k^n) \mathrm{tr}((\Sigma_k - (x^n - \mu_k)(x^n - \mu_k)^T) H)$$

$$\implies \Sigma_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_k^n)(x^n - \mu_k)(x^n - \mu_k)^T$$

$$\lambda = \frac{\partial L}{\partial \pi_k} = \frac{N_k}{\pi_k} \implies \pi_k = \frac{N_k}{N}$$

where $N_k = \sum_{n=1}^{N} \gamma(z_k^n)$. We can interpret N_k as the effective number of points assigned to cluster k.

Maximum likelihood

We can maximize the log likelihood function through an iterative procedure:

1. Choose some initial values for the means, covariances and mixing coefficients.
2. E step: Use the current values for the parameters to evaluate the posterior probabilities.
3. M step: Use these probabilities to re-estimate the means, covariances and mixing coefficients.
4. Go to step 2 until convergence.

Maximum likelihood

Algorithm 2: EM algorithm for a Gaussian mixture model

```
repeat
    for $n \leftarrow 1$ to $N$ do
        for $k \leftarrow 1$ to $K$ do
            $\gamma(z_k^n) = \frac{\pi_k \mathcal{N}(x^n; \mu_k, \Sigma_k)}{\sum_{k'=1}^{K} \pi_{k'} \mathcal{N}(x^n; \mu_{k'}, \Sigma_{k'})}$;
        end
    end
    for $k \leftarrow 1$ to $K$ do
        $N_k \leftarrow \sum_{n=1}^{N} \gamma(z_k^n)$;
        $\mu_k \leftarrow \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_k^n) x^n$;
        $\Sigma_k \leftarrow \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_k^n)(x^n - \mu_k)(x^n - \mu_k)^T$;
        $\pi_k \leftarrow \frac{N_k}{N}$;
    end
    $L \leftarrow \sum_{n=1}^{N} \log(\sum_{k=1}^{K} \pi_k \mathcal{N}(x^n; \mu_k, \Sigma_k))$;
until convergence;
return $\{\mu_k\}, \{\Sigma_k\}, \{\pi_k\}$;
```

Expectation-maximization algorithm

Let's consider the EM algorithm under the more general situation:

- There are N observed data points: $x^1, \ldots, x^N \in \mathbb{R}^D$.
- The corresponding discrete latent variables $z^1, \ldots, z^N \in \mathbb{R}^K$ use a 1-of-K representation.
- The set of all model parameters is denoted by θ.

Expectation-maximization algorithm

The log likelihood function is given by:

$$L = \sum_{n=1}^{N} \log p(x^n; \theta) = \sum_{n=1}^{N} \log(\sum_{z^n} p(x^n, z^n; \theta))$$

The presence of the summation inside the logarithm results in complicated expressions for the maximum likelihood solution.

Expectation-maximization algorithm

The EM algorithm tries to maximize the log likelihood function through an iterative procedure:

1. Choose some starting value for the parameters θ_0.
2. E step: Calculate the posterior distribution of the latent variables $p(z^n|x^n;\theta^{\mathrm{old}})$, so that we can form the expected value of the complete-data log likelihood under this posterior distribution $\mathcal{Q}(\theta,\theta^{\mathrm{old}})=\sum_{n=1}^{N}\sum_{z^n} p(z^n|x^n;\theta^{\mathrm{old}})\log p(x^n,z^n;\theta)$.
3. M step: We maximize this expectation and determine the revised parameter estimate $\theta^{\mathrm{new}}=\mathrm{argmax}_{\theta}\mathcal{Q}(\theta,\theta^{\mathrm{old}})$.
4. Go to step 2 until convergence.

Expectation-maximization algorithm

Algorithm 3: General EM algorithm

```
repeat
    $\mathcal{Q}(\theta, \theta^{\text{old}}) \leftarrow \sum_{n=1}^{N} \sum_{z^n} p(z^n | x^n; \theta^{\text{old}}) \log p(x^n, z^n; \theta)$;
    $\theta^{\text{new}} \leftarrow \text{argmax}_{\theta} \mathcal{Q}(\theta, \theta^{\text{old}})$;
    $L \leftarrow \sum_{n=1}^{N} \log p(x^n; \theta^{\text{new}})$;
    $\theta^{\text{old}} \leftarrow \theta^{\text{new}}$;
until convergence;
return $\theta^{\text{new}}$;
```

Expectation-maximization algorithm

- The use of the expectation may seem somewhat arbitrary, we will see the motivation for this choice when we give a deeper treatment of EM in Section 15.4.
- In the definition of $\mathcal{Q}(\theta, \theta^{\mathrm{old}})$, the logarithm acts directly on the joint distribution $p(x^n, z^n; \theta)$, and so the corresponding M step maximization will be tractable.
- The EM algorithm has the property that each cycle of EM will increase the incomplete-data log likelihood, as we will see in Section 15.4.

Gaussian mixtures

Application of this latent-variable view of EM to the specific case of a Gaussian mixture model. For the E step:

$$p(z^n = \mathrm{e}_k | x^n; \theta^{\text{old}}) = p(z^n_k = 1 | x^n; \theta^{\text{old}})$$

$$= \frac{p(z^n_k = 1, x^n; \theta^{\text{old}})}{\sum_{k'=1}^{K} p(z^n_{k'} = 1, x^n; \theta^{\text{old}})} = \frac{\pi_k^{\text{old}} \mathcal{N}(x^n; \mu_k^{\text{old}}, \Sigma_k^{\text{old}})}{\sum_{k'=1}^{K} \pi_{k'}^{\text{old}} \mathcal{N}(x^n; \mu_{k'}^{\text{old}}, \Sigma_{k'}^{\text{old}})} = \gamma(z^n_k)$$

$$\mathcal{Q}(\theta, \theta^{\text{old}}) = \sum_{n=1}^{N} \sum_{z^n} p(z^n | x^n; \theta^{\text{old}}) \log p(x^n, z^n; \theta)$$

$$= \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z^n_k) (\log \pi_k + \log \mathcal{N}(x^n; \mu_k, \Sigma_k))$$

Gaussian mixtures

For the M step, we fix θ^{old} thus $\gamma(z_k^n)$, and maximize $\mathcal{Q}(\theta, \theta^{\text{old}})$ with respect to θ:

$$N_k = \sum_{n=1}^{N} \gamma(z_k^n)$$

$$0 = \frac{\partial \mathcal{Q}}{\partial \mu_k} = \sum_{n=1}^{N} \gamma(z_k^n)(x^n - \mu_k)^T \Sigma_k^{-1} \implies \mu_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_k^n) x^n$$

$$0 = \frac{\partial \mathcal{Q}}{\partial \Lambda_k}(H) = \frac{1}{2} \sum_{n=1}^{N} \gamma(z_k^n) \operatorname{tr}((\Sigma_k - (x^n - \mu_k)(x^n - \mu_k)^T) H)$$

$$\implies \Sigma_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_k^n)(x^n - \mu_k)(x^n - \mu_k)^T$$

$$\lambda = \frac{\partial \mathcal{Q}}{\partial \pi_k} = \frac{N_k}{\pi_k} \implies \pi_k = \frac{N_k}{N}$$

Relation to K-means

We can derive the K-means algorithm as a particular limit of EM for Gaussian mixtures. Consider a Gaussian mixture model in which:

- The mixing coefficients are fixed to $\frac{1}{K}$.
- The covariance matrices of the mixture components are given by ϵI, where ϵ is a fixed constant.

Relation to K-means

Consider the limit $\epsilon \to 0+$. For the E step:

$$\gamma(z_k^n) = \frac{\exp(-\frac{||x^n-\mu_k^{\text{old}}||^2}{2\epsilon})}{\sum_{k'=1}^{K} \exp(-\frac{||x^n-\mu_{k'}^{\text{old}}||^2}{2\epsilon})} \to \begin{cases} 1, & \text{if } k = \text{argmin}_j ||x^n - \mu_j^{\text{old}}||^2 \\ 0, & \text{otherwise} \end{cases}$$

Thus, in this limit, we obtain a hard assignment of data points to clusters, just as in the K-means algorithm, so that $\gamma(z_k^n) \to r_k^n$.

Relation to K-means

The expected complete-data log likelihood becomes:

$$
\begin{aligned}
\epsilon \mathcal{Q}(\theta, \theta^{\text{old}}) &= \epsilon \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_k^n)(-\log K + \log \mathcal{N}(x^n; \mu_k, \epsilon I)) \\
&\to -\frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} r_k^n ||x^n - \mu_k||^2
\end{aligned}
$$

We see that in this limit, maximizing the expected complete-data log likelihood is equivalent to minimizing the error measure J for the K-means algorithm.

Relation to K-means

For the M step:

$$\mu_k = \frac{\sum_{n=1}^{N} \gamma(z_k^n) x^n}{\sum_{n=1}^{N} \gamma(z_k^n)} \to \frac{\sum_{n=1}^{N} r_k^n x^n}{\sum_{n=1}^{N} r_k^n}$$

The EM re-estimation equation for the μ_k then reduces to the K-means result.

Mixtures of Bernoulli distributions

As a further example of mixture modelling and to illustrate the EM algorithm in a different context, we now discuss mixtures of descrete binary variables described by Bernoulli distributions:

- Let z be a K-dimensional binary random variable having a 1-of-K respresentation:
  - $p(z) = \prod_{k=1}^{K} \pi_k^{z_k}$, where $0 \leq \pi_k \leq 1$ and $\sum_{k=1}^{K} \pi_k = 1$.
- Let $x \in \mathbb{R}^D$ be a set of D binary variables, each of which is governed by a Bernoulli distribution given a particular value for z:
  - $\mathrm{Bern}(x; \mu) = \prod_{d=1}^{D} \mu_d^{x_d} (1 - \mu_d)^{1-x_d}$.
  - $p(x|z) = \prod_{k=1}^{K} \mathrm{Bern}(x; \mu^k)^{z_k}$.

Mixtures of Bernoulli distributions

Application of the EM algorithm to the specific case of a Bernoulli mixture model. For the E step:

$$\gamma(z_k^n) = p(z^n = \mathrm{e}_k | x^n; \theta^{\mathrm{old}}) = p(z_k^n = 1 | x^n; \theta^{\mathrm{old}})$$

$$= \frac{p(z_k^n = 1, x^n; \theta^{\mathrm{old}})}{\sum_{k'=1}^K p(z_{k'}^n = 1, x^n; \theta^{\mathrm{old}})} = \frac{\pi_k^{\mathrm{old}} \mathrm{Bern}(x^n; (\mu^k)^{\mathrm{old}})}{\sum_{k'=1}^K \pi_{k'}^{\mathrm{old}} \mathrm{Bern}(x^n; (\mu^{k'})^{\mathrm{old}})}$$

$$\mathcal{Q}(\theta, \theta^{\mathrm{old}}) = \sum_{n=1}^N \sum_{z^n} p(z^n | x^n; \theta^{\mathrm{old}}) \log p(x^n, z^n; \theta)$$

$$= \sum_{n=1}^N \sum_{k=1}^K \gamma(z_k^n)(\log \pi_k + \log \mathrm{Bern}(x^n; \mu^k))$$

Mixtures of Bernoulli distributions

For the M step, we fix θ^{old} thus $\gamma(z_k^n)$, and maximize $\mathcal{Q}(\theta, \theta^{\text{old}})$ with respect to θ:

$$
\begin{aligned}
N_k &= \sum_{n=1}^{N} \gamma(z_k^n) \\
0 &= \frac{\partial \mathcal{Q}}{\partial \mu_d^k} = \frac{1}{\mu_d^k(1-\mu_d^k)} \sum_{n=1}^{N} \gamma(z_k^n)(x_d^n - \mu_d^k) \\
&\implies \mu_d^k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_k^n) x_d^n \implies \mu^k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_k^n) x^n \\
\lambda &= \frac{\partial \mathcal{Q}}{\partial \pi_k} = \frac{N_k}{\pi_k} \implies \pi_k = \frac{N_k}{N}
\end{aligned}
$$