STA 414/2104

Statistical Methods for Machine Learning and Data Mining

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Week 7

Clustering and Mixture Models

Unsupervised Learning, Clustering, and Mixture Distributions

Recall that *unsupervised learning* does not focus on predicting anything in particular, but rather tries to find "interesting" aspects of the data.

One possible informal objective is to find *clusters* of similar items. One possible formal objective is modeling the *probability distribution* of all observed variables.

It can be useful to model a probability distribution in which variables are dependent using *latent* (also called *hidden*) variables to express some or all of the dependencies.

When there is one discrete latent variable, the model will express the distribution as a *mixture* of distributions. The latent variable can also be seen as identifing the cluster an item belongs to.

Example: We have data on symptoms of patients (body temperature, blood pressure, etc.). We could cluster the patients, hoping the clusters will correspond to "diseases". We could model the distribution of symptoms using a discrete latent variable, hoping it will represent the disease a patient has. The distribution of symptoms will be a mixture of distributions for each disease.

K-Means Clustering

Suppose we have data $x_1, \ldots, x_n$, with each x_i being a vector of p variables.

We aim to divide the data into K clusters of similar items, measuring similarity by Euclidean distance (perhaps rescaling variables to all have standard deviation one).

The *K-means algorithm* iteratively finds K centres for the clusters, and assigns each item to the cluster whose centre it is nearest to:

1) Initialize $\mu_1, \ldots, \mu_K$ somehow (eg, set them to randomly selected data items).

2) Repeat the following:

    a) For $i = 1, \ldots, n$, assign data item i to the cluster, k, for which $||x_i - \mu_k||$ is smallest. (Prefer the current assignment if it is tied for the best.)

    b) For $k = 1, \ldots, K$, set μ_k to the mean of data items assigned to cluster k.

    until there is no change in the cluster assignments from the previous iteration.

It's easy to see that this process converges, since each step reduces the value of

$$J \;=\; \sum_{i=1}^{n} ||x_i - \mu_{c_i}||^2$$

where c_i is the cluster assigned to data item i. The algorithm may not find the global minimum of J, however.

From Clustering to Mixture Models

K-means clustering assigns a definite cluster to each data item. But often this is unrealistic — eg, some patients have combinations of the symptoms we have measured that are consistent with more than one disease.

The clusters found by the K-means algorithm are described only by the mean of the data items in the cluster. We might like a more complete description of what items in a cluster are like.

Both of these issues can be addressed by modeling the data as coming from a *mixture* distribution, with mixture components corresponding to clusters.

Mixture Distributions

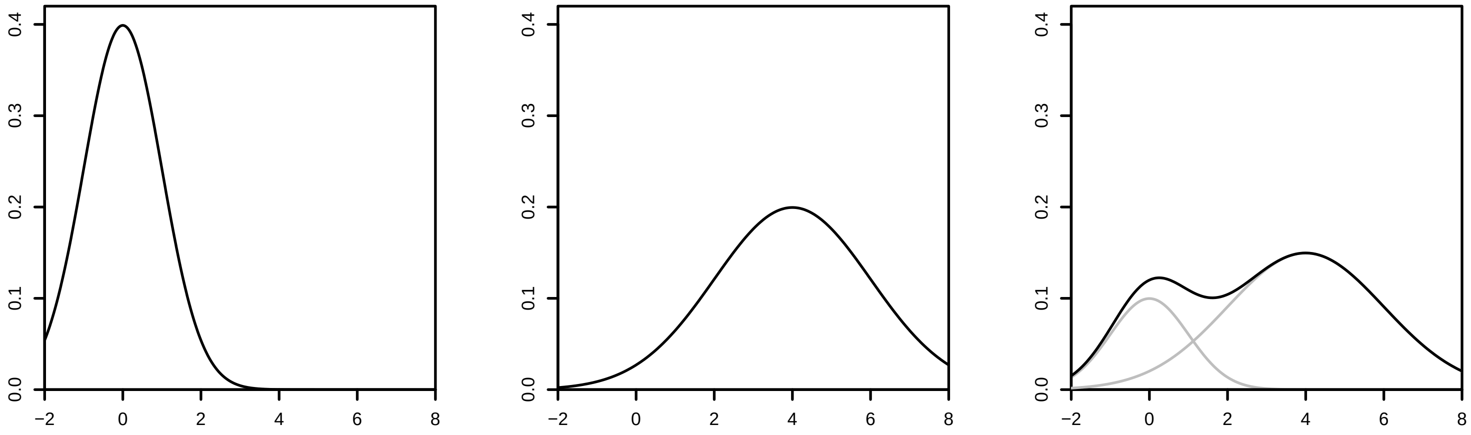
K distributions with probability/density functions $P_1(x), \ldots, P_K(x)$ can be mixed in proportions $\pi_1, \ldots, \pi_K$ to give a mixture distribution with probability/density function

$$P(x) \;\;=\;\; \sum_{k=1}^{K} \pi_k \, P_k(x)$$

For example, when x is one dimensional, we can mix $N(0, 1^2)$ and $N(4, 2^2)$ with proportions 1/4 and 3/4, giving the density function

$$P(x) \;\;=\;\; \frac{1}{4}\frac{1}{\sqrt{2\pi}}\exp(-(1/2)x^2) \;+\; \frac{3}{4}\frac{1}{2\sqrt{2\pi}}\exp(-(1/2)(x-4)^2/2^2)$$

as pictured below:



$N(0, 1)$ $\quad$ $N(4, 2^2)$ $\quad$ $(1/4)N(0, 1) \;+\; (3/4)N(4, 2^2)$

Gaussian Mixture Models

When data items are real vectors, it may be reasonable to model the data as a mixture of Gaussian distributions, using the data to estimate the mixing proportion, the mean vector, and covariance matrix for each component.

The density function for this model, with K components, can be written as

$$P(x|\pi, \mu, \Sigma) \;\; = \;\; \sum_{k=1}^{K} \pi_k \, N(x|\mu_k, \Sigma_k)$$

We might allow Σ_k to be any valid covariance matrix, or we might constrain Σ_k to be a diagonal matrix. If the Σ_k are diagonal, *all* the dependence between the variables in x is a consequence of the distribution being a mixture.

A natural idea is to estimate π_k, μ_k, and Σ_k for $k = 1, \ldots, K$ by maximizing the likelihood. Assuming that data items are independent, the log likelihood is

$$L(\pi, \mu, \Sigma) \;\; = \;\; \sum_{i=1}^{n} \log P(x_i|\pi, \mu, \Sigma)$$

where x_i is the data vector for item i.

Issues with Maximum Likelihood for Gaussian Mixture Models

Non-identifiability: The global maximum of the likelihood for a mixture model is not unique, since permuting the labels of the mixture components will produce a different set of parameter values that fits the data just as well.

Other local maxima: Even aside from re-labellings, there is often more than one local maximum of the likelihood. Finding one of the global maxima (or at least a good local maximum) may require searching for the maximum from many different starting points.

We don't want the global maximum anyway: When $K > 1$, the actual global maximum will be at a point with infinite likelihood, in which for some component, k, and some data item, i, we have $0 < \pi_k < 1$, $\mu_k = x_i$, and $\Sigma_k = 0$. This gives an infinite spike of probability density at one point, while other points have non-zero probability density from other components.

Because of this problem, we need to try as many starting points as needed to find a good local maximum that *isn't* one where some $\Sigma_k \to 0$.

The EM algorithm

The EM Algorithm for Gaussian Mixture Models

We could use some general purpose optimization method (eg, R's nlm function) to find the parmeters of a mixture model that maximize the likelihood (avoiding the singular solutions with $\Sigma_k \to 0$). But a method known as the *EM algorithm* is commonly used, because it is simple to implement, and very stable. (Though it can unfortunately also be rather slow.)

The idea: If we knew which mixture component each data item came from, estimating the mixing proportions and the parameters of each component distribution would be easy. We don't know this, but given an initial guess at the parameters, we can probabilistically assign a component to each data item, and then get a better estimate of the parameters based on these assignments.

This is sort of like the K-means algorithm, but in a probabilistic setting, with a proof that the algorithm will reach a (local) maximum of the likelihood.

Details of the EM Algorthim for Gaussian Mixture Models

Here are the details of the EM algorithm for a Gaussian mixture model with Σ_k being diagonal, with diagonal elements of σ_{kj}^2.

We alternate between "E" (Expectation) steps and "M" (Maximization) steps:

E Step: Using the current values of the parameters, compute the "responsibilities" of components for data items, by applying Bayes' Rule:

$$r_{ik} \;=\; P(\text{data item } i \text{ came from component } k \,|\, x_i) \;=\; \frac{\pi_k\, N(x_i|\mu_k, \Sigma_k)}{\displaystyle\sum_{k'} \pi_{k'}\, N(x_i|\mu_{k'}, \Sigma_{k'})}$$

M Step: Using the current responsibilities, re-estimate the parameters, using weighted averages, with weights given by the responsibilities:

$$\pi_k \;=\; \frac{1}{n}\sum_i r_{ik}, \quad \mu_k \;=\; \sum_i r_{ik} x_i \Big/ \sum_i r_{ik}, \quad \sigma_k^2 \;=\; \sum_i r_{ik}(x_i - \mu_k)^2 \Big/ \sum_i r_{ik}$$

We start with some initial guess at the parameter values (perhaps random), or perhaps with some initial guess at the responsibilities (in which case we start with an M step). We continue alternating E and M steps until there is little change.

The EM Algorithm in General

Consider model for observed data x (which might be a vector of n independent items) that is accompanied by a latent (unobserved) z (also possibly a vector of n independent values). A model with parameters θ describes the joint distribution of x and z, as $P(x, z|\theta)$.

We want to estimate θ by maximum likelihood, which means finding the θ that maximizes

$$P(x|\theta) \quad = \quad \sum_z P(x, z|\theta)$$

(This assumes z is discrete; if it's continuous the sum is replaced by an integral.)

We assume that this isn't easy. But suppose that we *can* easily find the θ that maximizes $P(x, z|\theta)$, for any known x and z. We try to use (something related to) this capability in an iterative algorithm for maximizing $P(x|\theta)$.

The EM Algorithm in General — Details

The general EM algorithm alternates these steps:

E Step: Using the current value of the parameter, θ, find the distribution, Q, for the latent z, given the observed x:

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

M Step: Maximize the expected value of $\log P(x,z|\theta)$ with respect to θ, where the expectation is with respect to the distribution Q found in the E step:

$$\theta \quad = \quad \arg\max_{\theta}\, E_Q[\log P(x,z|\theta)]$$

For many models (specifically, those in the "exponential family"), maximizing $E_Q[\log P(x,z|\theta)]$ will be feasible if maximizing $\log P(x,z|\theta)$ for known z is feasible.

Justification of the EM algorithm

To see that the EM algorithm maximizes (at least locally) the log likelihood, consider the following function of the distribution Q over z and the parameters θ:

$$\begin{aligned} F(Q,\theta) &= E_Q[\log P(x,z|\theta)] \;-\; E_Q[\log Q(z)] \\ &= \log P(x|\theta) \;+\; E_Q[\log P(z|x,\theta)] \;-\; E_Q[\log Q(z)] \\ &= \log P(x|\theta) \;-\; E_Q[\log(Q(z)/P(z|x,\theta))] \end{aligned}$$

The final term above is the "Kullback-Leibler (KL) divergence" between the distribution $Q(z)$ and the distribution $P(z|x,\theta)$. One can show that this divergence is always non-negative, and is zero only when $Q(z) = P(z|x,\theta)$.

We can now justify the EM algorithm by showing that

a) The E step maximizes $F(Q,\theta)$ with respect to Q — a consequence of KL divergence being minimized when $Q(z) = P(z|x,\theta)$.

b) The M step maximizes $F(Q,\theta)$ with respect to θ — clear since $E_Q[\log Q(z)]$ doesn't depend on θ.

c) The maximum of $F(Q,\theta)$ occurs at a θ that maximizes $P(x|\theta)$ — if instead $P(x|\theta^*) > P(x|\theta)$ for some θ^*, then $F(Q^*,\theta^*) > F(Q,\theta)$ with $Q^*(z) = P(z|x,\theta^*)$.

How this Translates to the Mixture Version

For the mixture example, the model parameters are $\theta = (\pi,\ \mu,\ \sigma)$.

We'll let the latent variables be $z_{ik} = 1$ if data item i comes from component k, and 0 otherwise.

In the E step, we find the distribution of the z_{ik} given x_i and the model parameters. It turns out that all we actually need from this distribution is the expected value of each z_{ik} (same as the probability that $z_{ik} = 1$), which we define to be r_{ik}, and find by Bayes' Rule as shown before.

In the M step, we need to maximize $E_Q\Big(\sum_{i=1}^{n} \log P(x_i, z_i|\theta)\Big)$.

Suppose we knew the value of both x_i and $z_i = (z_{i1}, \ldots, z_{iK})$ for data item i. The log probability (dropping constant factors) for that item can be written as

$$\log \left[\prod_{k=1}^{K} \left(\pi_k \prod_{j=1}^{p} \left(\frac{1}{\sigma_{kj}} \exp(-(1/2)(x_{ij} - \mu_{kj})^2 / \sigma_{kj}^2) \right) \right)^{z_{ik}} \right]$$

Note that all but one factor in the outer product will have the value one.

We maximize the expected value of the sum of the above for all i, with respect to the distribution of z_i found in the E step. We'll see how this works out next...

Details of the Mixture Version of EM

Taking the expectation of the log probability of data item i with respect to the distribution of z_i (denoted by Q), we get

$$
\begin{aligned}
& E_Q\left\{\log\left[\prod_{k=1}^{K}\left(\pi_k\prod_{j=1}^{p}\left(\frac{1}{\sigma_{kj}}\exp(-(1/2)(x_{ij}-\mu_{kj})^2/\sigma_{kj}^2)\right)\right)^{z_{ik}}\right]\right\} \\
&\quad = \quad E_Q\left\{\sum_{k=1}^{K} z_{ik}\left(\log(\pi_k)-\frac{1}{2}\sum_{j=1}^{p}\left(\log(\sigma_{kj}^2)+(x_{ij}-\mu_{kj})^2/\sigma_{kj}^2\right)\right)\right\} \\
&\quad = \quad \sum_{k=1}^{K} r_{ik}\left(\log(\pi_k)-\frac{1}{2}\sum_{j=1}^{p}\left(\log(\sigma_{kj}^2)+(x_{ij}-\mu_{kj})^2/\sigma_{kj}^2\right)\right)
\end{aligned}
$$

where $r_{ik} = E_Q(z_{ik})$. To maximize the sum of the above for all i, we separately maximize $\sum_{i=1}^{n}\sum_{k=1}^{K} r_{ik}\log(\pi_k)$ with respect to π, and $-\frac{1}{2}\sum_{i=1}^{n} r_{ik}(x_{ij}-\mu_{kj})^2$ with respect to each μ_{kj}, and finally $-\frac{1}{2}\sum_{i=1}^{n} r_{ik}\left(\log(\sigma_{kj}^2)+(x_{ij}-\mu_{kj})^2/\sigma_{kj}^2\right)$ with respect to each σ_{kj}^2. This gives the algorithm presented earlier.

How Many Mixture Components Should We Use?

Non-Bayesian Ways of Setting K

If we estimate the parameters of a mixture of K distributions by maximum likelihood, we will "overfit" if we choose K to be too big. Letting $K = n$ is the extreme — then every data point can have its own mixture component, which can give it infinite probability density.

Many, many schemes have been devised for picking an appropriate value for K, most without a convincing justification.

One plausible way is to look at performance on a validation set, with parameters estimated from a separate estimation set (or use S-fold cross validation).

To do this, we need a measure of performance.

We could use the average log probabability of the validation observations.

Or we could use something else that reflects our actual intended use of the results. For instance, we might intend to use a mixture model to fill in missing covariates in a regression model, in which case we might use squared error in prediction of left-out values from other values.

Bayesian Mixture Models

A different approach is to use a Bayesian model, in which we don't predict using a single estimate of the parameters. This will avoid overfitted solutions in which each component models just one data point, infinitely well.

We need to specify a prior distributions for the parameters (eg, mean vector and covariance matrix) of each mixture component.

We might let this prior be independent for each component.

We *cannot* let this prior be improper. If we do, only one component will be used, since the prior probability of a second component having reasonable parameter values will be zero!

We also need a prior for the mixing proportions...

A Prior for Mixing Proportions

A Bayesian mixture model needs to have a prior distribution for the mixing proportions, $\pi_1, \ldots, \pi_K$. One possibility is the *Dirichlet distribution*, which has the following density on the simplex where $\pi_k > 0$ and $\sum \pi_k = 1$:

$$P(\pi_1, \ldots, \pi_K) \;\;=\;\; \frac{\Gamma(\Sigma_k \alpha_k)}{\Pi_k \, \Gamma(\alpha_k)} \prod_{k=1}^{K} \pi_k^{\alpha_k - 1}$$

The parameters $\alpha_1, \ldots, \alpha_K$ can be any positive reals.

If $Z_1, Z_2, \ldots$ are i.i.d. given π, with $P(Z_i = k) = \pi_k$, the posterior distribution after observing $z_1, \ldots, z_n$, with n_1 of the z_i having value 1, n_2 having value 2, etc. is a Dirichlet distribution with parameters $\alpha_1 + n_1, \ldots, \alpha_K + n_K$.

The predictive distribution for Z_{n+1} given $Z_1, \ldots, Z_n$ is

$$P(Z_{n+1} = k \,|\, Z_1 = z_1, \ldots, Z_K = z_k) \;\;=\;\; \frac{n_k + \alpha_k}{n + \Sigma_{k'} \alpha_{k'}}$$

Implementing Bayesian Mixture Models

Bayesian mixture models are usually implemented using Markov chain Monte Carlo methods, which we aren't covering in this course.

Just like the EM algorithm for maximum likelihood fitting of mixtures can converge to a bad local maximum, a Markov chain Monte Carlo method for a mixture model can get stuck for a long time in a local mode of the posterior distribution — though it should get out eventually.

Choosing K Using Marginal Likelihood

We can choose among Bayesian mixture models with different numbers of components, K, using the marginal likelihood for each value of K.

The marginal likelihood for these models is rather hard to compute, but it's possible.

But does this procedure make sense? Do we really believe that there is some true (even if unknown) value of K?

Consider a mixture model for symptoms of patients, where we hope the mixture components will represent "diseases". Do we expect only K diseases, for some reasonably small value of K?

As the number of patients, n, increases, we actually expect to see more and more diseases (some of which will be quite rare).

Letting K be Infinite

We can let K go to infinity in a Bayesian mixture model with a Dirichlet prior for $\pi_1, \ldots, \pi_K$ — giving what's called a *Dirichlet process mixture model*.

If we use a Dirichlet prior for $\pi_1, \ldots, \pi_K$ with all parameters being α/K, the limiting form of the "law of succession" for the predictive distribution of Z_i, representing which mixture component to use for item i, is

$$P(Z_i = k \mid z_1, \ldots, z_{i-1}) \;\; = \;\; \frac{n_{i,k} + \alpha/K}{i-1+\alpha} \;\; \to \;\; \frac{n_{i,k}}{i-1+\alpha}$$

$$P(Z_i \neq Z_j \text{ for all } j < i \mid z_1, \ldots, z_{i-1}) \;\; \to \;\; \frac{\alpha}{i-1+\alpha}$$

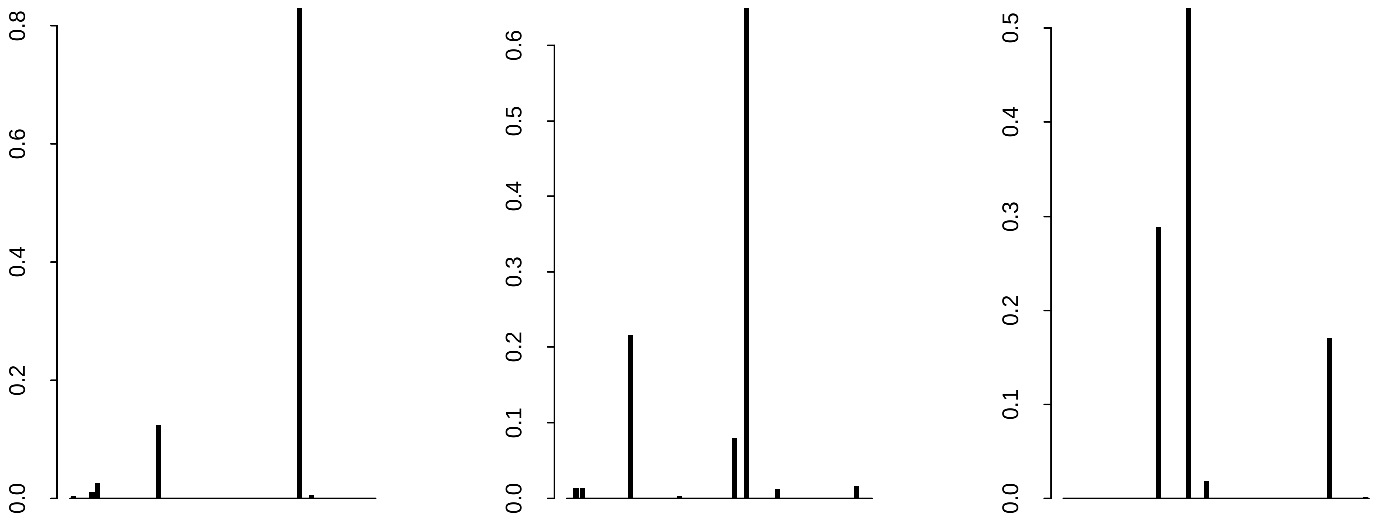
where $n_{i,k}$ is the number of $z_1, \ldots, z_{i-1}$ that are equal to k.

So even with infinite K, behaviour is reasonable: The probability of the next data item being associated with a new mixture component is neither 0 nor 1.

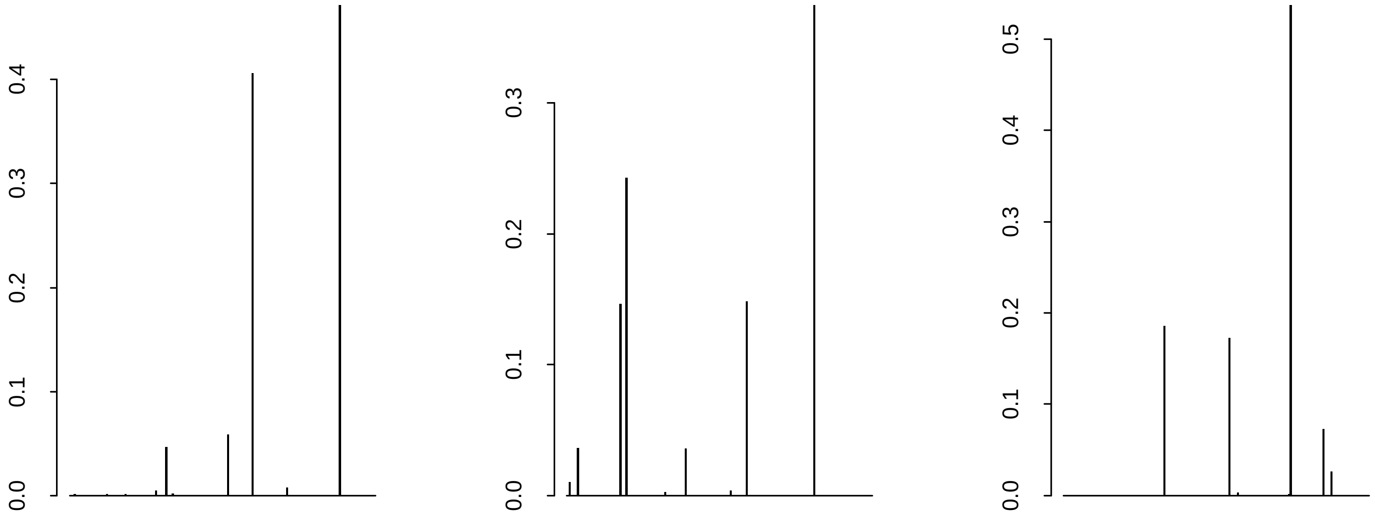
The Prior for Mixing Proportions as K Increases

Three random values from priors for $\pi_1, \ldots, \pi_K$:

$\alpha = 1, \quad K = 50:$



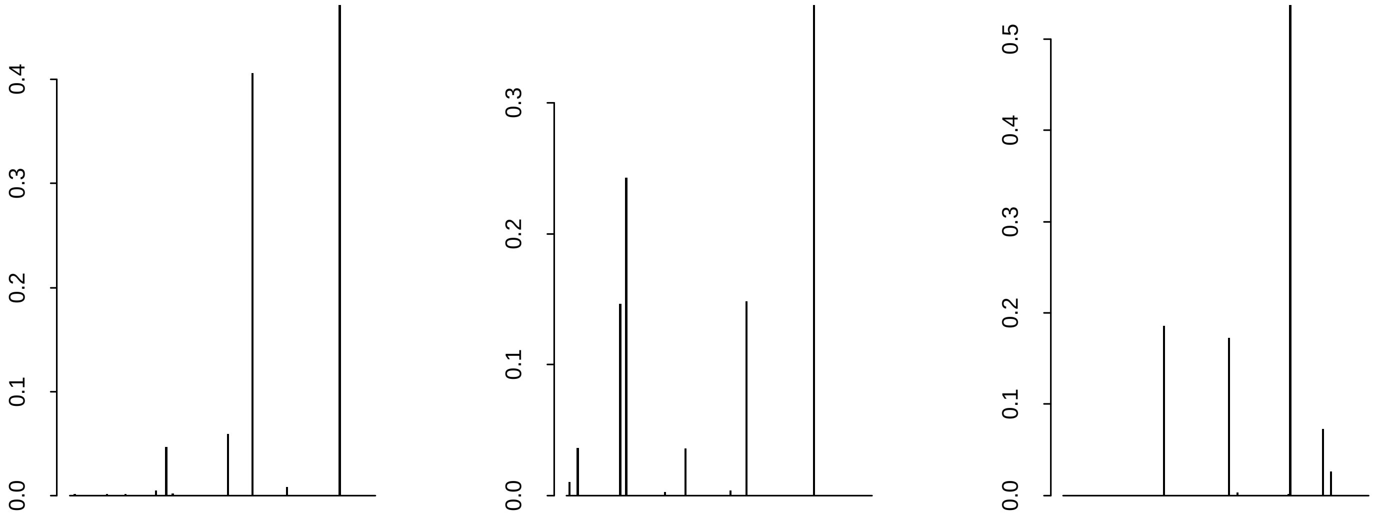
$\alpha = 1, \quad K = 150:$



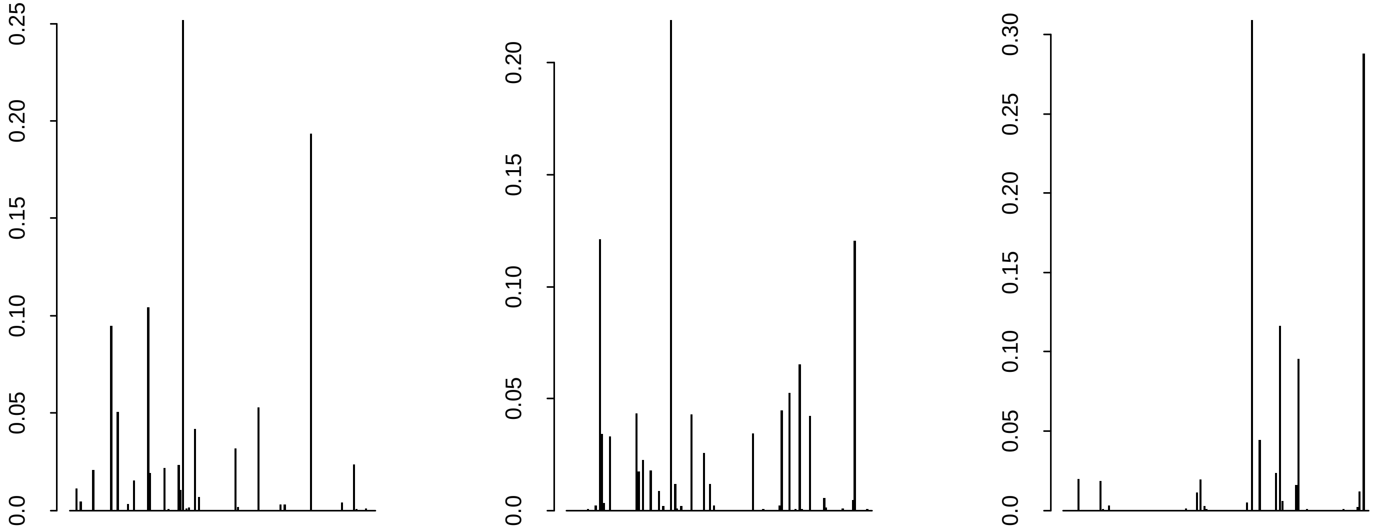
The Prior for Mixing Proportions as α Varies

Three random values from priors for $\pi_1, \ldots, \pi_K$:

$\alpha = 1, \quad K = 150:$



$\alpha = 5, \quad K = 150:$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