Laboratory 10

In this laboratory we will focus on Gaussian Mixture Models.

Gaussian Mixture Models

Gaussian Mixture Models allow approximating the density of a R.V. $\boldsymbol{X}$ when the density of $\boldsymbol{X}$ is not known. The GMM density consists of a weighted sum of M Gaussians:

$$\boldsymbol{X} \sim GMM(\boldsymbol{M}, \boldsymbol{\mathcal{S}}, \boldsymbol{w}) \implies f_{\boldsymbol{X}}(\boldsymbol{x}) = \sum_{g=1}^{M} w_g \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g)$$

where

$$\boldsymbol{M} = [\boldsymbol{\mu}_1 \dots \boldsymbol{\mu}_M] \ , \quad \boldsymbol{\mathcal{S}} = [\boldsymbol{\Sigma}_1 \dots \boldsymbol{\Sigma}_M] \ , \boldsymbol{w} = [w_1 \dots w_M]$$

are the components means, covariance matrices and weights, respectively.

We have seen that a GMM can be interpreted as the marginal distribution obtained by marginalizing the joint density

$$f_{\boldsymbol{X}_i, G_i}(\boldsymbol{x}_i, g) = w_g \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g) \ , \quad f_{\boldsymbol{X}_i}(\boldsymbol{x}_i) = \sum_{g=1}^{M} f_{\boldsymbol{X}_i, G_i}(\boldsymbol{x}_i, g) \ .$$

G_i is a discrete *hidden* random variable that represents the Gaussian component that was responsible for the generation of $\boldsymbol{x}_i$. The joint density can be expressed as a product of the component (cluster) conditional distribution for $\boldsymbol{X}_i$ and the prior distribution for G_i:

$$f_{\boldsymbol{X}_i|G_i}(\boldsymbol{x}_i|g) = \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g) \ , \quad P(G_i = g) = w_g \ , \quad f_{\boldsymbol{X}_i, G_i}(\boldsymbol{x}_i, g) = f_{\boldsymbol{X}_i|G_i}(\boldsymbol{x}_i|g) P(G_i = g)$$

Write a function `logpdf_GMM(X, gmm)` that computes the log-density of a GMM for a set of samples contained in matrix `X`. As we did in Laboratory 4, we will assume that `X` is a matrix of samples of shape `(D, N)`, where D is the size of a sample and N is the number of samples in `X`. As in Laboratory 4, you can either compute directly the 1-D vector of densities or use a `for` loop to compute the density for each sample. To encode a GMM you can use different ways. A possible, simple approach consists in representing a GMM as a list of component parameters:

```
gmm = [(w1, mu1, C1), (w2, mu2, C2), ...]
```

Suggestions:

- You can make use of the function `logpdf_GAU_ND` that you wrote for Laboratory 4 to compute the terms $\log \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g)$ for all samples $\boldsymbol{x}_i$, $i = 1 \dots N$ and for all components $g = 1 \dots M$.
- You can arrange the terms in a matrix `S` with shape `(M, N)`. Element `S[g, i]` of `S` contains the logarithm of the joint probability of sample $\boldsymbol{x}_i$ and component (cluster) g, and a row `S[g, :]` therefore contains all joint densities for all samples. These can be comptued as in LAboratory 5: `S[g, :] = logpdf_GAU_ND(X, mu, C) + numpy.log(w)` where `w, mu, C = gmm[g]`.
- Finally, you can compute the log-marginal $\log f_{\boldsymbol{X}_i}(\boldsymbol{x}_i)$ for all samples $\boldsymbol{x}_i$ by using the log-sum-exp function: `logdens = scipy.special.logsumexp(S, axis=0)`. The result will be an array of shape `(N,)`, whose component i will contain the log-density for sample $\boldsymbol{x}_i$.

NOTE: The process is the *same* we used to compute the log-densities $\log f_{\boldsymbol{X}_i}(\boldsymbol{x}_i) = \log \sum_c f_{\boldsymbol{X}_i, C_i}(\boldsymbol{x}_i, c)$ for the MVG classifier in Laboratory 5. Indeed, we can interpret each Gaussian component as representing a sub-class (i.e. clusters) of our data.

To check that the log-density is correct, you can compute the log-density over a reference dataset using a reference GMM. The file `GMM_data_4D.npy` contains a set $\boldsymbol{X}$ of 4-dimensional samples (as a numpy matrix of shape (4×1000)). It can be loaded using `numpy.load` . File `Data/GMM_4D_3G_init.json` contains a reference GMM. It can be loaded with function `load_gmm` contained in file `Data/GMM_load.py` .

The log-densities for all samples in $\boldsymbol{X}$ can be loaded using `numpy.load` from file `Data/GMM_4D_3G_init_ll.npy` . Check your log-density function provides the same results. You can also verify the log-density on 1-D data (stored as a 1×1000 matrix). You can find data, GMM and log-likelihoods in the `Data` folder. The names of the files are the same as for the 4-D dataset, replacing `4D` with `1D`.

GMM estimation: the EM algorithm

The EM algorithm can be used to estimate the parameters of a GMM that maximize the likelihood for a training set $\boldsymbol{X}$. The EM algorithm consists of two steps:

- E-step: compute the posterior probability for each component of the GMM for each sample, using an estimate $(\boldsymbol{M}_t, \boldsymbol{\mathcal{S}}_t, \boldsymbol{w}_t)$ of the model parameters. These quantities are also called *responsibilities*

$$\gamma_{g,i} = P(G_i = g | \boldsymbol{X}_i = \boldsymbol{x}_i, \boldsymbol{M}_t, \boldsymbol{\mathcal{S}}_t, \boldsymbol{w}_t)$$

- M-step: Update the model parameters. For each component, we can use the statistics

$$Z_g = \sum_{i=1}^{N} \gamma_{g,i} \ , \quad \boldsymbol{F}_g = \sum_{i=1}^{N} \gamma_{g,i} \boldsymbol{x}_i \ , \quad \boldsymbol{S}_g = \sum_{i=1}^{N} \gamma_{g,i} \boldsymbol{x}_i \boldsymbol{x}_i^T$$

  to obtain the new parameters

$$\boldsymbol{\mu}_{g_{t+1}} = \frac{\boldsymbol{F}_g}{Z_g} \ , \quad \boldsymbol{\Sigma}_{g_{t+1}} = \frac{\boldsymbol{S}_g}{Z_g} - \boldsymbol{\mu}_{g_{t+1}} \boldsymbol{\mu}_{g_{t+1}}^T \ , \quad w_{g_{t+1}} = \frac{Z_g}{\sum_{g'=1}^{M} Z_{g'}} = \frac{Z_g}{N} \ , \quad g = 1 \dots M$$

Implement the GMM EM estimation procedure. The estimation procedure should iterate from an initial estimate of the GMM, and keep computing E and M -steps until a convergence criterion is met.

Suggestions:

- The computation of the posterior distributions $\gamma_{g,i} = P(G_i = g | \boldsymbol{X}_i = \boldsymbol{x}_i, \boldsymbol{M}_t, \boldsymbol{\mathcal{S}}_t, \boldsymbol{w}_t)$ can be done in the same way as we computed class posterior probabilities for a MVG model. We can also re-use most of the code that was used to compute the log-densities in the previous section.
- Build matrix `S` containing component conditional densities, and add to each row the corresponding log-prior $\log P(G_i = g) = \log w_g$. The results is the matrix of joint densities $f_{\boldsymbol{X}_i, G_i}(\boldsymbol{x}_i, g)$ (the same matrix `S` that we built in the previous section).
- Compute the marginal densities using the log-sum-exp function (see previous section or the MVG laboratory)
- Compute the posterior distribution for each sample:

$$\gamma_{g,i} = P(G_i = g | \boldsymbol{X}_i = \boldsymbol{x}_i, \boldsymbol{M}_t, = \boldsymbol{\mathcal{S}}_t, \boldsymbol{w}_t) = \frac{f_{\boldsymbol{X}_i, G_i}(\boldsymbol{x}_i, g)}{f_{\boldsymbol{X}_i}(\boldsymbol{x}_i)} = e^{\log f_{\boldsymbol{X}_i, G_i}(\boldsymbol{x}_i, g) - \log f_{\boldsymbol{X}_i}(\boldsymbol{x}_i)}$$

  You can compute the logarithm of all $\gamma_{g,i}$'s by removing, from each row of the joint log-densities matrix `S`, the row vector containing the N marginal log-densities computed in the previous step. The $M \times N$ matrix of posterior probabilities can then be obtained by computing the exponential of each element of the result. This is the same procedure we used to compute class posterior probabilities for the MVG classifier.
- The statistics can be computed from the matrix of components posterior probabilities.
- As stopping criterion, we can use the log-likelihood of the training set

$$\ell(\boldsymbol{M}_t, \boldsymbol{\mathcal{S}}_t, \boldsymbol{w}_t) = \sum_{i=1}^{n} \log GMM(\boldsymbol{x}_i | \boldsymbol{M}_t, \boldsymbol{\mathcal{S}}_t, \boldsymbol{w}_t) = \sum_{i=1}^{n} f_{\boldsymbol{X}_i}(\boldsymbol{x}_i) \ .$$

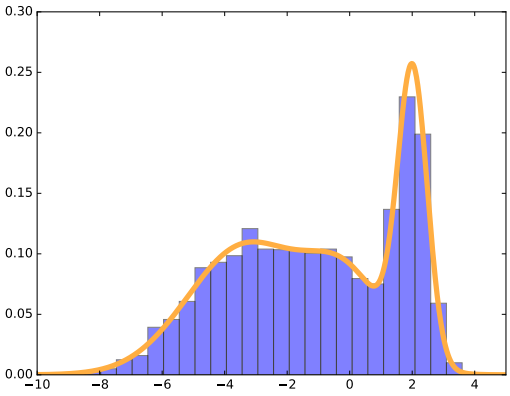
  The log-likelihood for the training set using the current parameter estimate can be computed from the outputs of function `logpdf_GMM`. Alternatively, you can compute the log-likelihood from the marginal densities at the end of the E-step

- NOTE: In this case you would obtain the log-likelihood for the previous M-step, not for the one of the current EM iteration
- NOTE: In the following we will use the *average* log-likelihood, i.e. we will divide the log-likelihood by N

We stop the iterations when the average log-likelihood increases by a value lower than a threshold: $\ell(\boldsymbol{M}_t, \boldsymbol{\mathcal{S}}_t, \boldsymbol{w}_t) - \ell(\boldsymbol{M}_{t-1}, \boldsymbol{\mathcal{S}}_{t-1}, \boldsymbol{w}_{t-1}) \leq \Delta_l$. In the examples below $\Delta_l = 10^{-6}$ was used.

- **To verify your implementation, check your log-likelihood is increasing. If the log-likelihood becomes smaller at some iteration, then your implementation is very likely to be incorrect**. We also suggest that, when your implementation seems stable, you let the EM run for more iterations than those required to reach the stopping criterion to check that the log-likelihood does not start decreasing. After this check, of course, these additional iterations can be removed.

Apply the EM algorithm to the data in `GMM_data_4D.npy` . You can use `Data/GMM_4D_3G_init.json` as initial GMM. You can find a solution in file `GMM_4D_3G_EM.json` . The *average* log-likelihood for the trained GMM is `-7.26325603` . The corresponding files are also available for the 1-D dataset. Below you can see the plot of the estimated density for the 1-D dataset.



LBG algorithm

The EM algorithm requires an initial guess for the GMM parameters. The LBG algorithm allows us to incrementally construct a GMM with $2G$ components from a GMM with G components. Starting with a single-component GMM (i.e. a Gaussian density), we can build a 2-component GMM and then use the EM algorithm to estimate a ML solution for the 2-components model. We can then split the 2 components to obtain a 4-components GMM, and re-apply the EM algorithm to estimate its parameters, and so on.

We can use the Maximum Likelihood solution for a Gaussian density as starting point:

```
GMM_1 = [(1.0, mu, C)]
```

where `mu` and `C` are the empirical mean and covariance matrix of the dataset.

A possible way to split the GMM consists in replacing component $(w_g, \boldsymbol{\mu}_g, \boldsymbol{\Sigma}_g)$ with two components

$$\left(\frac{w_g}{2}, \boldsymbol{\mu}_g - \boldsymbol{d}_g, \boldsymbol{\Sigma}_g\right) , \quad \left(\frac{w_g}{2}, \boldsymbol{\mu}_g + \boldsymbol{d}_g, \boldsymbol{\Sigma}_g\right) ,$$

The displacement vector $\boldsymbol{d}_g$ can be computed, for example, by taking the leading eigenvector of $\boldsymbol{\Sigma}_g$, scaled by the square root of the corresponding eigenvalue, multiplied by some factor α:

```
U, s, Vh = numpy.linalg.svd(Sigma_g)
d = U[:, 0:1] * s[0]**0.5 * alpha
```

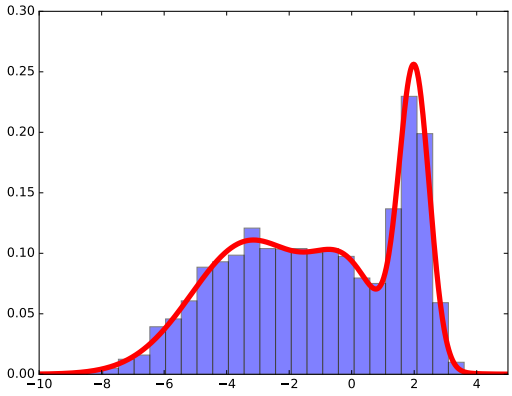
In practice, we are displacing the new components along the direction of maximum variance, using a step that is proportional to the standard deviation (i.e. the scale of the features along that direction) of the component we are splitting.

Implement the LBG algorithm. At each LBG iteration, we produce a 2G-components GMM from a G-components GMM. The 2G components GMM can be used as initial GMM for the EM algorithm. Retrain the 2G-GMM using the EM algorithm

NOTE: After the split, the initial iteration of the EM algorithm for the $2G$-components GMM may have a lower log-likelihood than you had at the end of the EM iterations for the G-components GMM.

NOTE: Depending on the order in which you insert the two components during the LBG updates your GMM may be equivalent, but with the components in a different order. If you want to obtain the same GMMs as in the files you should add the components in the same order as they appera in the above equation. File `GMM_4D_4G_EM_LBG.json` contains a 4-component GMM obtained using a factor $\alpha = 0.1$. The final average log-likelihood is `-7.25337844` .

You can also find the gmm for the 1-D dataset. Below you can see the plot of the estimated density.



Constraining the eigenvalues of the covariance matrices

The GMM log-likelihood is not bounded above for $M \geq 2$. Indeed, we can have arbitrarily high log-likelihood by centering one component at one of the N samples, and letting the corresponding covariance matrix shrink towards zero. To avoid these kind of degenerate solutions, we can constrain the minimum values of the eigenvalues of the covariance matrices.

A possible solution consists in constraining the eigenvalues of the covariance matrices to be larger or equal to a lower bound $\psi > 0$. It's possible to show that the solution can be obtained by modifying the output of the M-step in the previous section. In particular, after we have computed $\boldsymbol{\Sigma}_{g_{t+1}}$, we can compute its SVD:

$$\boldsymbol{U}_g, \boldsymbol{S}_g, \boldsymbol{U}_g^T = \boldsymbol{\Sigma}_{g_{t+1}}$$

where $\boldsymbol{S}_g$ is a diagonal matrix of singular values, and replace the estimated covariance with

$$\boldsymbol{\Sigma}_{g_{t+1}} = \boldsymbol{U}_g \boldsymbol{S}'_g \boldsymbol{U}_g^T \ , \quad \boldsymbol{S}'_{g_{ii}} = \max(\psi, \boldsymbol{S}_{g_{ii}})$$

where $\boldsymbol{S}'_{g_{ii}}$ is the i-th element of the diagonal of matrix $\boldsymbol{S}'_g$. Assuming that `covNew` is the variable that contains $\boldsymbol{\Sigma}_{g_{t+1}}$, the procedure can be implemented as

```
U, s, _ = numpy.linalg.svd(covNew)
s[s<psi] = psi
covNew = numpy.dot(U, mcol(s)*U.T)
```

NOTE: The log-likelihood should again increase at each iteration.

NOTE: When applying the eigenvalue threshold, you should make sure that the constraint is met also by the inital GMM estimate. In particular, when using the LBG algorithm, you should apply the transformation also to the initial, single-component (MVG) solution, otherwise the first EM iteration of the 2-components GMM may result in a decrease of the log-likelihood.

Diagonal and tied-covariance GMMs

The diagonal variant of the GMM we just implemented consists of a model whose components all have diagonal covariance matrices. The ML solution can be trivially obtained by modifying the M-step by keeping only the diagonal elements of $\mathbf{\Sigma}_{g_{t+1}}$. The approach is the same as for the diagonal covariance MVG model: after we have computed $\mathbf{\Sigma}_{g_{t+1}}$, we replace it with

$$\mathbf{\Sigma}_{g_{t+1}} \longleftarrow \text{Diag}(\mathbf{\Sigma}_{g_{t+1}})$$

i.e., `Sigma_g = Sigma_g * numpy.eye(Sigma_g.shape[0])` (a more efficient implementation would store and make use of only the diagonal terms of the covariance matrix, however simply zero-ing the out-of-diagonal elements is already enough to evaluate the goodness of the approach).

We can also compute ML solutions for tied models, where each component has a covariance matrix $\mathbf{\Sigma}_g = \mathbf{\Sigma}$. The tied solution can also be obtained by modifying the M-step of the non-tied approach. In particular, we can compute matrices $\mathbf{\Sigma}_{g_{t+1}}$ as in the standard M-step. Then, we can replace each matrix $\mathbf{\Sigma}_{g_{t+1}}$ with

$$\mathbf{\Sigma}_{g_{t+1}} \longleftarrow \frac{1}{N}\sum_{g=1}^{M} Z_g \mathbf{\Sigma}_{g_{t+1}} = \sum_{g=1}^{M} w_{g_{t+1}} \mathbf{\Sigma}_{g_{t+1}}$$

NOTE: the minimum eigenvalue constraints we have discussed in the previous section should be applied AFTER we have computed the diagonal or the tied updates.

GMM for classification

GMMs can be used for classification in a similar way as we did for the MVG classifier. In particular, we can train a GMM $GMM(\boldsymbol{M}_c, \boldsymbol{\mathcal{S}}_c, \boldsymbol{w}_c)$ for each class of the IRIS dataset, and then use the GMM log-density function to compute class-conditional distributions $f_{\boldsymbol{X}_t|C_t}(\boldsymbol{x}_t|c) = GMM(\boldsymbol{x}_t|\boldsymbol{M}_c, \boldsymbol{\mathcal{S}}_c, \boldsymbol{w}_c)$ for all classes. Results are in the table below (we consider only the accuracy / error rate metric in this laboratory; the LBG parameter α was set to 0.1; the minimum value for the eigenvalues of the covariance matrix ψ was set to 0.01; the EM stopping criterion was set to $\Delta_l = 10^{-6}$; the same number of components was chosen for all classes).

NOTE: The tied covariance GMM model assumes that the covariance of a single GMM $\mathbf{\Sigma}_{c,g} = \mathbf{\Sigma}_c$ are the same, but each GMM of each class has a different covariance matrix $\mathbf{\Sigma}_c$. **This is different from the tied MVG model.** In particular, for the 1-component model, the Tied GMM corresponds to the non-tied MVG model. We could implement also a globally tied GMM, which would correspond to the Tied MVG for 1-component GMMs, where the covariance matrices of each component of all the 3 GMMs would be the same. However, in this case we would not be able to train the 3 GMMs of each class independently, as the likelihood function would not factorize over the different parameters (as in the tied MVG case). We would then need to compute joint E and M steps to obtain the ML solution. You are free to try this on your own.

	Components				
GMM Type	1	2	4	8	16
Full Covariance (standard)	4.0%	4.0%	4.0%	4.0%	4.0%
Diagonal Covariance	4.0%	4.0%	6.0%	2.0%	4.0%
Tied Covariance	4.0%	4.0%	4.0%	4.0%	6.0%

For binary tasks we can also compute log-likelihood ratios

$$llr(\boldsymbol{x}_t) = \frac{GMM(\boldsymbol{x}_t|\boldsymbol{M}_1, \boldsymbol{\mathcal{S}}_1, \boldsymbol{w}_1)}{GMM(\boldsymbol{x}_t|\boldsymbol{M}_0, \boldsymbol{\mathcal{S}}_0, \boldsymbol{w}_0)}$$

and then proceed as we did for MVG and similar models.

In `Data/ext_data_binary.npy` and `Data/ext_labels_binary.npy` you can find an additional, artificial dataset with two classes, 1 and 0. Split the dataset in model training / validation sets with the usual split function, train a GMM for each class, and then compute the LLRs on the validation set. From the LLRs, compute minimum and actual DCF for an application $\pi_T = 0.5$. You can find below the results for different models (also in this case we use the same number of components for both classes). We used the same values for α and ψ we used for the multiclass Iris task.

	Components				
GMM Type	1	2	4	8	16
	minDCF / actDCF				
Full Covariance	0.4984 / 0.5398	0.4302 / 0.4416	0.5195 / 0.5706	0.5804 / 0.6177	0.6364 / 0.6640
Diagonal Covariance	0.5203 / 0.5625	0.4643 / 0.4643	0.4213 / 0.4513	0.4781 / 0.4781	0.4870 / 0.5446
Tied Covariance	0.4984 / 0.5398	0.4984 / 0.5398	0.4416 / 0.4643	0.4278 / 0.4846	0.4383 / 0.5252

Project

In this section we apply the GMM models to classification of the project data.

For each of the two classes, we need to decide the number of Gaussian components (hyperparameter of the model). Train full covariance models with different number of components for each class (suggestion: to avoid excessive training time you can restrict yourself to models with up to 32 components). Evaluate the performance on the validation set to perform model selection (again, you can use the minimum DCF of the different models for the target application). Repeat the analysis for diagonal models. What do you observe? Are there combinations which work better? Are the results in line with your expectation, given the characteristics that you observed in the dataset? Are there results that are surprising? (Optional) Can you find an explanation for these surprising results?

We have analyzed all the classifiers of the course. For each of the main methods (GMM, logistic regression, SVM — we ignore MVG since its results should be significantly worse than those of the other models, but feel free to test it as well) select the best performing candidate. Compare the models in terms of minimum and actual DCF. Which is the most promising method for the given application?

Now consider possible alternative applications. Perform a qualitative analysis of the performance of the three approaches for different applications (keep the models that you selected in the previous step). You can employ a Bayes error plot and visualize, for each model, actual and minimum DCF over a wide range of operating points (e.g. log-odds ranging from -4 to $+4$). What do you observe? In terms of minimum DCF, are the results consistent, preserving the relative ranking of the systems? What about actual DCF? Are there models that are well calibrated for most of the operating point range? Are there models that show significant miscalibration? Are there models that are harmful for some applications? We will see how to deal with these issue in the last laboratory.