Gaussian Mixture Models

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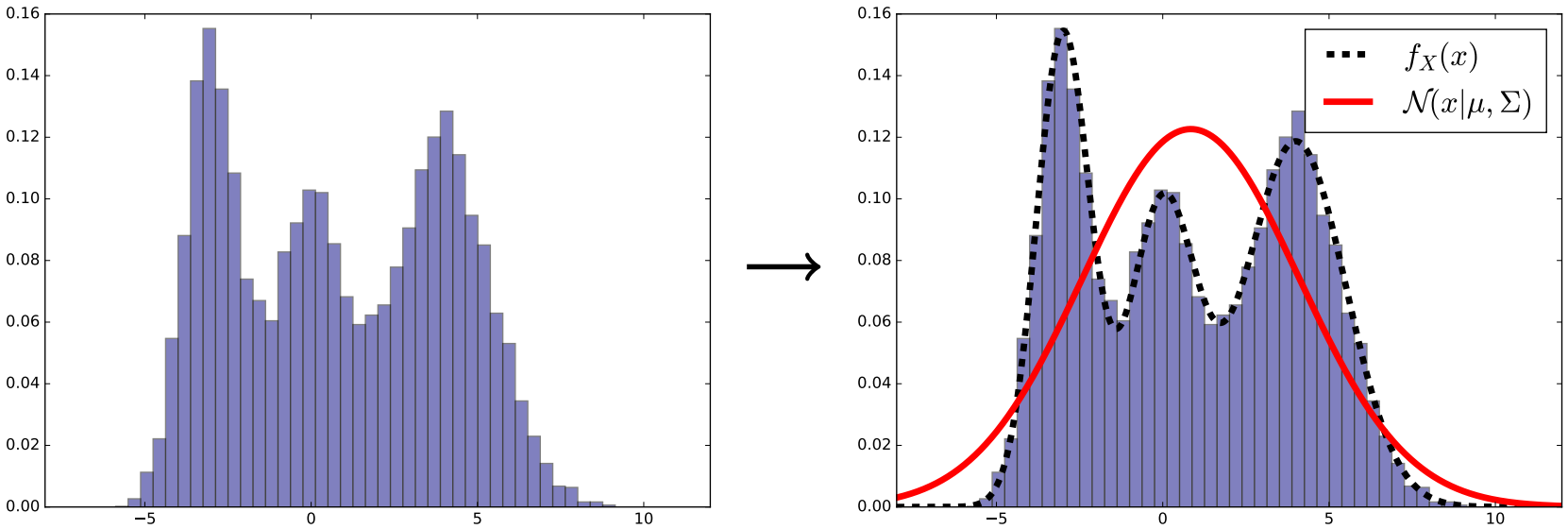
Gaussian Mixture models

We have seen that we can solve classification problems by building generative models that describe the distribution of samples

The Gaussian classifier is an example that assumes that class-conditional distributions are Gaussian

In many cases, however, the assumption can be quite inaccurate



Density estimation

Different distributions may be used in such cases

Depending on the task, we may be able to identify a reasonably good family of distributions

Gaussian Mixture Models are an alternative to model a generic distribution

They allow approximating any sufficiently regular distribution to a desired degree

Of course, since we are estimating the density from data, we require a sufficient amount of data to obtain good estimates

Density estimation

The use of GMMs is not restricted to classification

GMMs can be employed also in other tasks that require estimating a population density

As we will see, they also allow to solve different kind of problems

For example, GMMs provide an alternative to K-means for clustering

Gaussian Mixture Models

We have already encountered an example of GMM

Let's consider again the Gaussian classifier

The samples of each class are modeled by a Gaussian density

$$f_{X|C}(\boldsymbol{x}|c) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

To compute class posterior probabilities we had to compute the marginal density $f_X(\boldsymbol{x})$

If the class prior probabilities are $P(C = c) = \pi_c, c = 1 \dots K$, then $f_X(\boldsymbol{x})$ is given by

$$f_X(\boldsymbol{x}) = \sum_{c=1}^{K} f_{X|C}(\boldsymbol{x}|c)P(C = c) = \sum_{c=1}^{K} \pi_c \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) \qquad (1)$$

Gaussian Mixture Models

Expression (1) is an example of a K-components Gaussian Mixture Model:

$$\boldsymbol{X} \sim GMM(\boldsymbol{M}, \boldsymbol{\Sigma}, \boldsymbol{\Pi})$$

$$f_{\boldsymbol{X}}(\boldsymbol{x}) = \sum_{c=1}^{K} \pi_c \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

More in general, a Gaussian Mixture Model is a density model obtained as a weighted combination of Gaussians

$$f_{\boldsymbol{X}}(\boldsymbol{x}) = \sum_{c=1}^{K} w_c \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

The distribution parameters are the component means

$$\boldsymbol{M} = [\boldsymbol{\mu}_1 \dots \boldsymbol{\mu}_K]$$

the component covariances

$$\boldsymbol{\mathcal{S}} = [\boldsymbol{\Sigma}_1 \dots \boldsymbol{\Sigma}_K]$$

and the weights

$$\boldsymbol{w} = [w_1 \dots w_K]$$

Remember that, for f_X to be a density, we need that its integral is equal to 1. Integrating w.r.t. $\boldsymbol{x}$ we have:

$$\int f_X(\boldsymbol{x}) = \int \sum_{c=1}^{K} w_c \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) d\boldsymbol{x} = \sum_{c=1}^{K} w_c = 1$$

i.e., the weights must sum to 1

Gaussian Mixture Models

Given a dataset $\mathcal{D} = [\boldsymbol{x}_1 \dots \boldsymbol{x}_n]$ we can thus assume that the samples have been independently generated by a GMM

We assume that R.V.s describing the samples $\boldsymbol{X}_i$ are i.i.d., with $\boldsymbol{X}_i \sim \boldsymbol{X} \sim GMM(\boldsymbol{M}, \boldsymbol{\mathcal{S}}, \boldsymbol{w})$

Note: we are considering a density estimation problem

If we are using GMMs for classification $\mathcal{D}$ may correspond to the samples of a given class — however, in the following we do not assume any specific task, so that $\mathcal{D}$ is just a set of samples that we want to model by means of a GMM

In particular, we consider the dataset $\mathcal{D}$ as unlabeled

Gaussian Mixture Models

As we did with the Gaussian density, we can resort to Maximum Likelihood to estimate the model parameters of the GMM that best describes the dataset $\mathcal{D}$

In contrast with the Gaussian model, ML estimation for GMMs is an ill-posed problem

Indeed, as long as we have more than 1 component, we can devise degenerate solutions for which the likelihood is not bounded above

Care has to be taken to avoid these pathological solutions

In practice, the ML approach, combined with heuristics to avoid degeneracy, provides good density estimates

Gaussian Mixture Models

We can write the likelihood for the model parameters $\boldsymbol{\theta} = [\boldsymbol{M}, \boldsymbol{\mathcal{S}}, \boldsymbol{w}]$ as

$$\mathcal{L}(\boldsymbol{\theta}) = \prod_{i=1}^{n} f_{\boldsymbol{X}_i}(\boldsymbol{x}_i) = \prod_{i=1}^{n} GMM(\boldsymbol{x}_i | \boldsymbol{M}, \boldsymbol{\mathcal{S}}, \boldsymbol{w})$$
$$= \prod_{i=1}^{n} \left(\sum_{c=1}^{K} w_c \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) \right)$$

and the corresponding log-likelihood

$$\ell(\boldsymbol{\theta}) = \log \mathcal{L}(\boldsymbol{\theta}) = \sum_{i=1}^{n} \log \left(\sum_{c=1}^{K} w_c \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) \right)$$

Gaussian Mixture Models

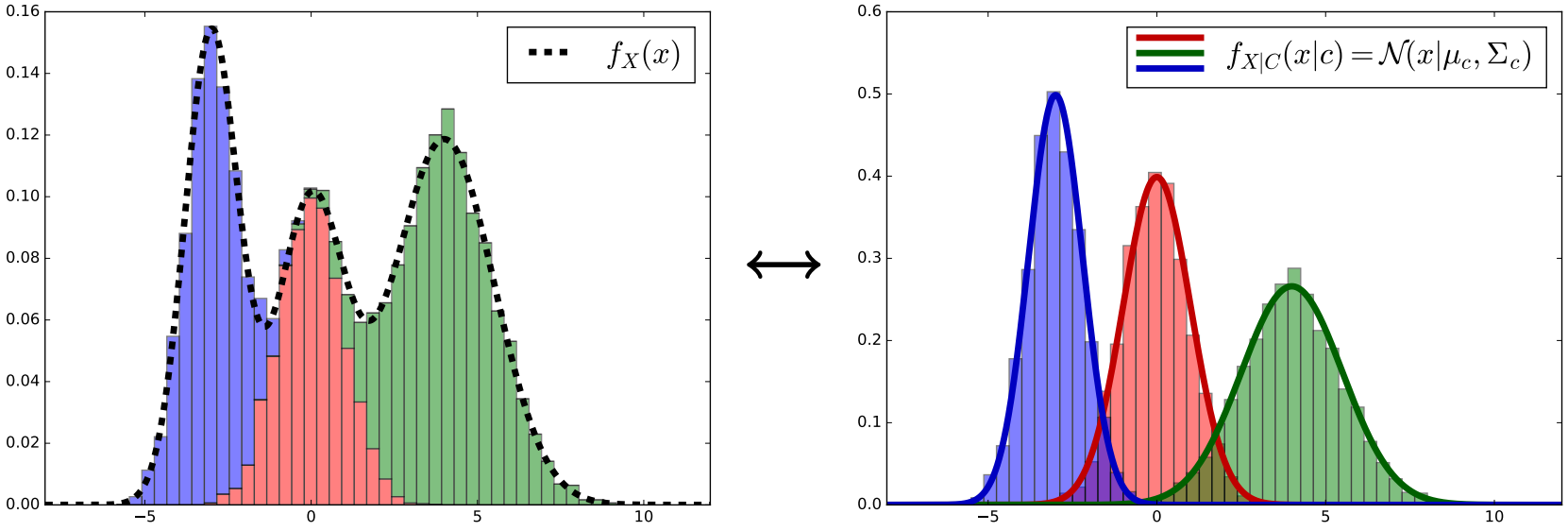
A GMM can be interpreted as the marginal of a joint distribution of data points and corresponding clusters

$$f_{\boldsymbol{X}_i}(\boldsymbol{x}_i) = \sum_{c=1}^{K} f_{\boldsymbol{X}_i|C_i}(\boldsymbol{x}_i|c)P(C_i = c) = \sum_{c=1}^{K} w_c \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

Although our training set cannot be well modeled by a Gaussian distribution, we can imagine that the set can be partitioned into subsets (components or clusters), in such a way that the distribution of the points of each component can be modeled by a Gaussian p.d.f.

If we knew the component responsible for each sample (i.e. its cluster label), we could estimate the parameters of each Gaussian by ML from the points of each cluster

Gaussian Mixture Models



Gaussian Mixture Models

Unfortunately, in general the clusters are unknown

We treat cluster membership as an unobserved (latent) random variables[1]

Intuitively, we want to estimate both cluster assignments and model parameters as to maximize the *marginal* distribution of the data

[1] Note that the model is not identifiable: for example, exchanging any two components results in the same marginal likelihood

Gaussian Mixture Models

Let's consider a set of GMM parameters $\boldsymbol{\theta} = (\boldsymbol{M}, \boldsymbol{\mathcal{S}}, \boldsymbol{w})$

The GMM defines a joint density of components (the clusters) and patterns. The density for sample $\boldsymbol{x}_i$ and component c is:

$$f_{\boldsymbol{X}_i, C_i}(\boldsymbol{x}_i, c) = w_c \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

We can compute cluster (component) posterior probabilities:

$$\gamma_{c,i} = P(C_i = c | \boldsymbol{X}_i = \boldsymbol{x}_i) = \frac{f_{\boldsymbol{X}_i, C_i}(\boldsymbol{x}_i, c)}{f_{\boldsymbol{X}_i}(\boldsymbol{x}_i)}$$

$$= \frac{w_c \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)}{\sum_{c'} w_{c'} \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_{c'}, \boldsymbol{\Sigma}_{c'})}$$

$\gamma_{c,i}$ are also called responsibilities

Gaussian Mixture Models

As a first approximation, we might decide to assign a point to the cluster c with highest posterior probability $P(C_i = c|\boldsymbol{X}_i = \boldsymbol{x}_i)$

We thus associate a cluster label

$$c_i^* = \arg\max_c P(C_i = c|\boldsymbol{X}_i = \boldsymbol{x}_i)$$

to each sample

Given the cluster assignments, we can then estimate by ML the new GMM parameters $\boldsymbol{\theta}^{new} = (\boldsymbol{M}^{new}, \boldsymbol{\mathcal{S}}^{new}, \boldsymbol{w}^{new})$

Gaussian Mixture Models

We treat the cluster assignments as if they were known class labels

The log-likelihood is similar to that of a (multivariate) Gaussian classifier:

$$\ell(\boldsymbol{\theta}) = \sum_{i=1}^{n} \left[\log f_{\boldsymbol{X}_i|C_i}(\boldsymbol{x}_i|c_i^*) + \log P(C_i = c_i^*)\right]$$
$$= \sum_{i=1}^{n} \left[\log \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_{c_i^*}, \boldsymbol{\Sigma}_{c_i^*})\right] + \sum_{i=1}^{n} \left[\log w_{c_i^*}\right]$$

and corresponds to a sum of two terms that depend on different subsets of the parameters

$$\ell(\boldsymbol{\theta}) = \ell_{\mathcal{N}}(\boldsymbol{M}, \boldsymbol{\mathcal{S}}) + \ell_{\mathcal{C}}(\boldsymbol{w})$$

We can observe that the first term

$$\ell_{\mathcal{N}}(\boldsymbol{M}, \boldsymbol{\mathcal{S}}) = \sum_{i=1}^{n} \left[\log \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_{c_i^*}, \boldsymbol{\Sigma}_{c_i^*}) \right]$$

corresponds to the log-likelihood of a (multivariate) Gaussian classification model, where the class labels are assumed to be the estimated c_i^*.

Let N_c be the number of samples for which $c_i^* = c$. The solution for $\boldsymbol{\mu}_c$ and $\boldsymbol{\Sigma}_c$ is thus

$$\boldsymbol{\mu}_c^* = \frac{1}{N_c} \sum_{i|c_i^*=c} \boldsymbol{x}_i \ , \quad \boldsymbol{\Sigma}_c^* = \frac{1}{N_c} \sum_{i|c_i^*=c} (\boldsymbol{x}_i - \boldsymbol{\mu}_c^*)(\boldsymbol{x}_i - \boldsymbol{\mu}_c^*)^T$$

The second term

$$\ell_{\mathcal{C}}(\boldsymbol{w}) = \sum_{i=1}^{n} \left[\log w_{c_i^*}\right] = \sum_{c=1}^{K} \sum_{i|c_i^*=c} \log w_c$$

corresponds to the log-likelihood of a categorical model with parameters w_c. The ML solution is thus

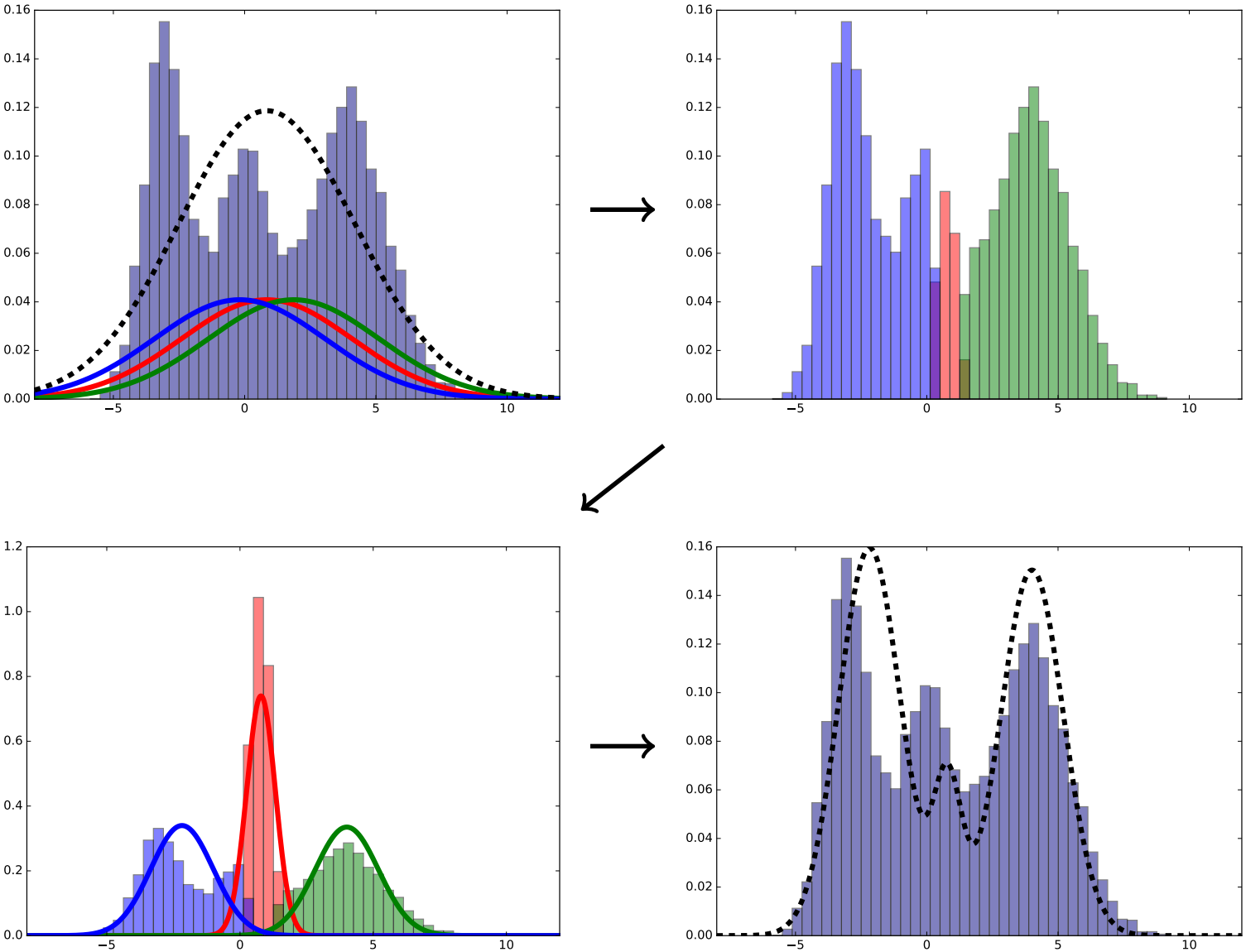
$$w_c^* = \frac{N_c}{\sum_{c=1}^{K} N_c}$$

Gaussian Mixture Models

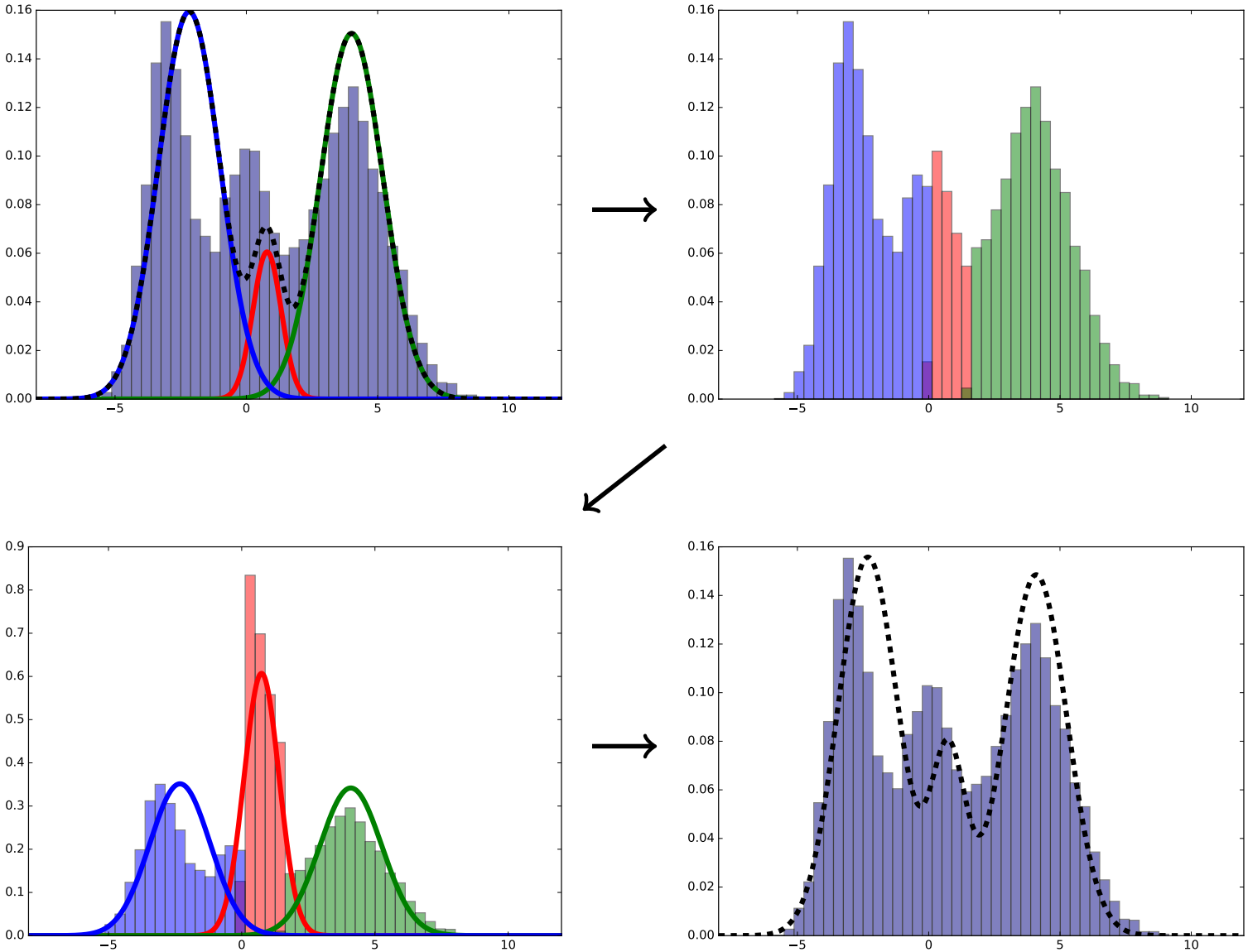
We could then obtain the updated set of model parameters $\boldsymbol{\theta}^{new} = (\boldsymbol{M}^*, \boldsymbol{\mathcal{S}}^*, \boldsymbol{w}^*)$

We could iterate the process by computing new cluster assignments using $\boldsymbol{\theta}^{new}$, and using the updated assignments to update once again the model parameters, stopping when some criterion is met

Gaussian Mixture Models



Gaussian Mixture Models



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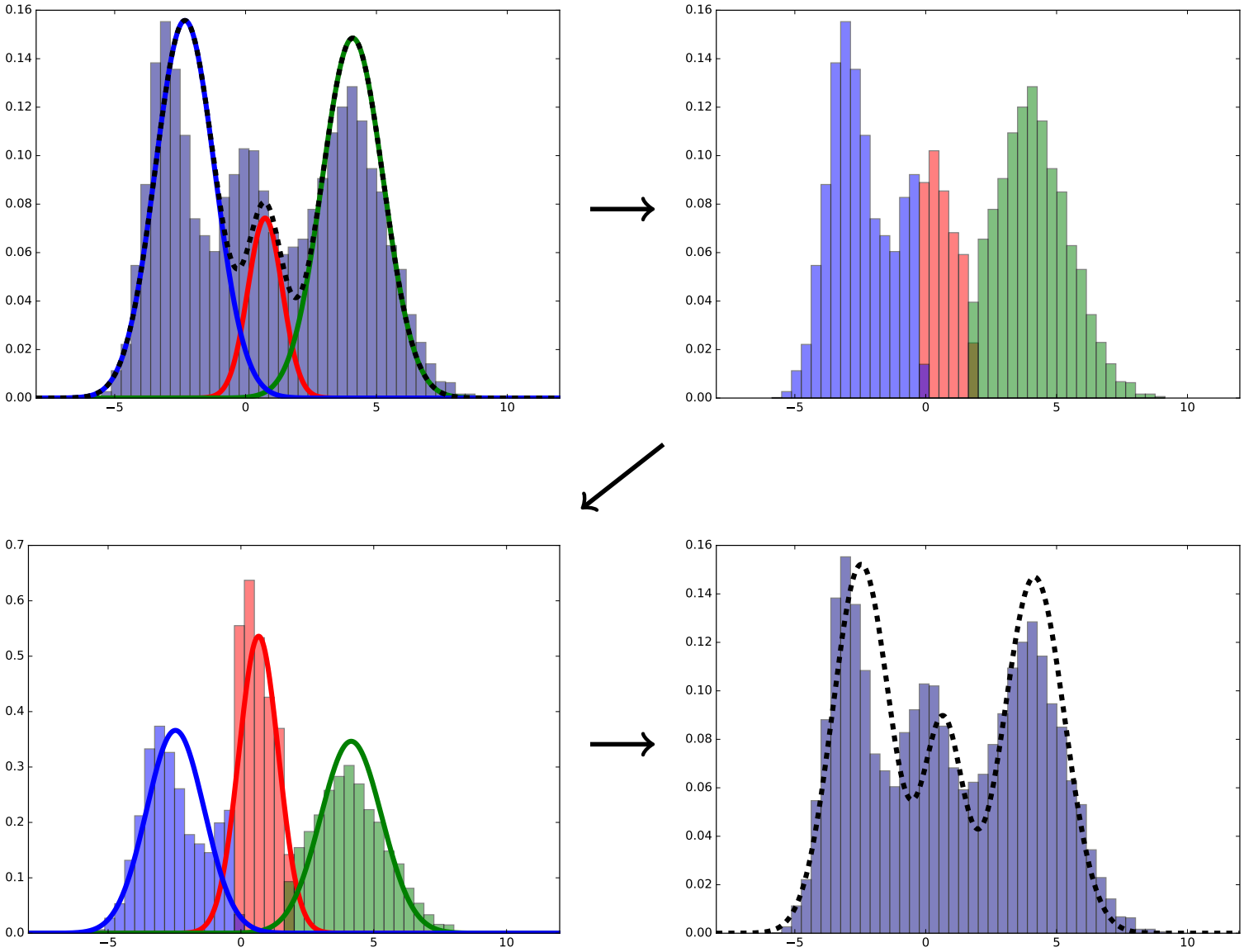

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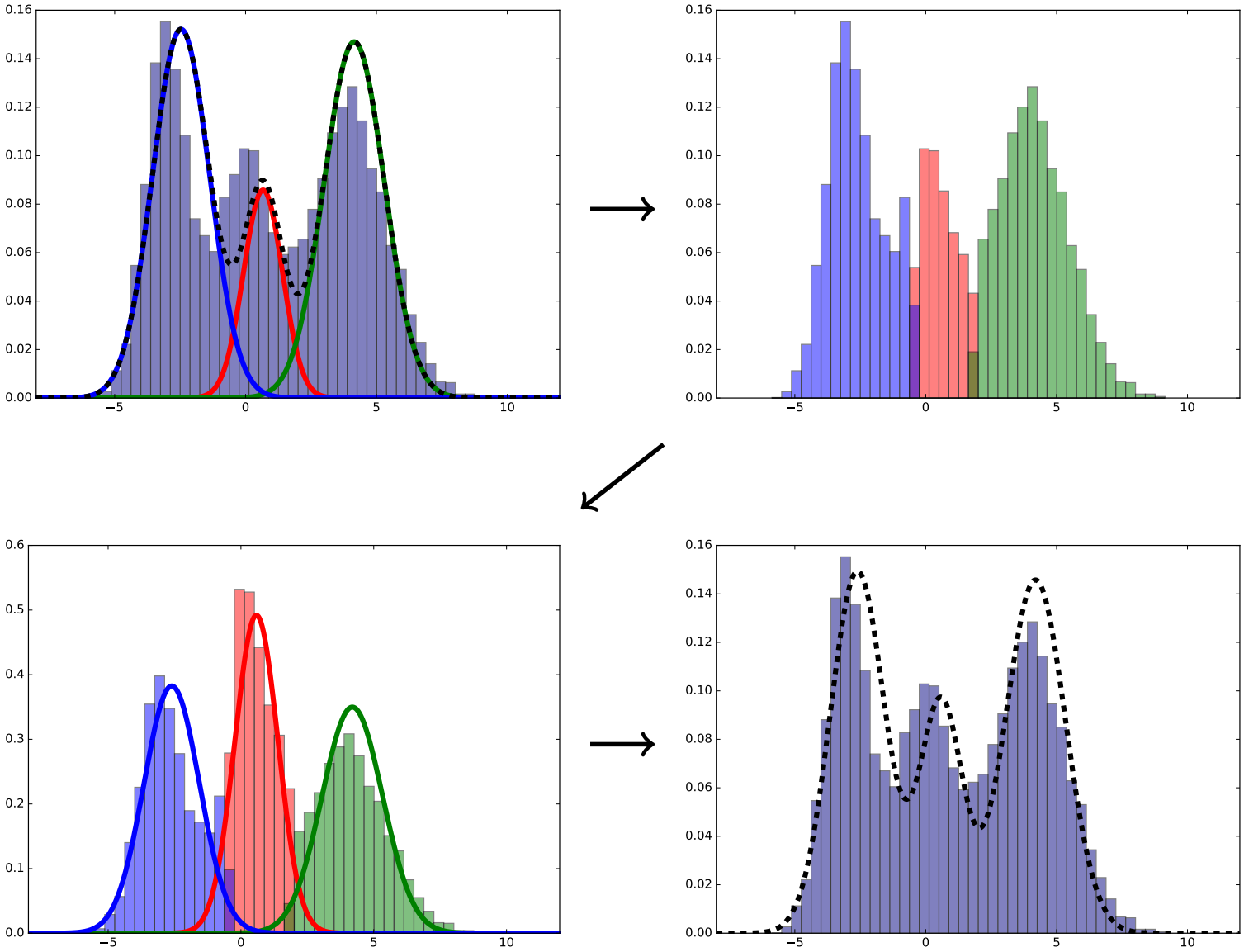
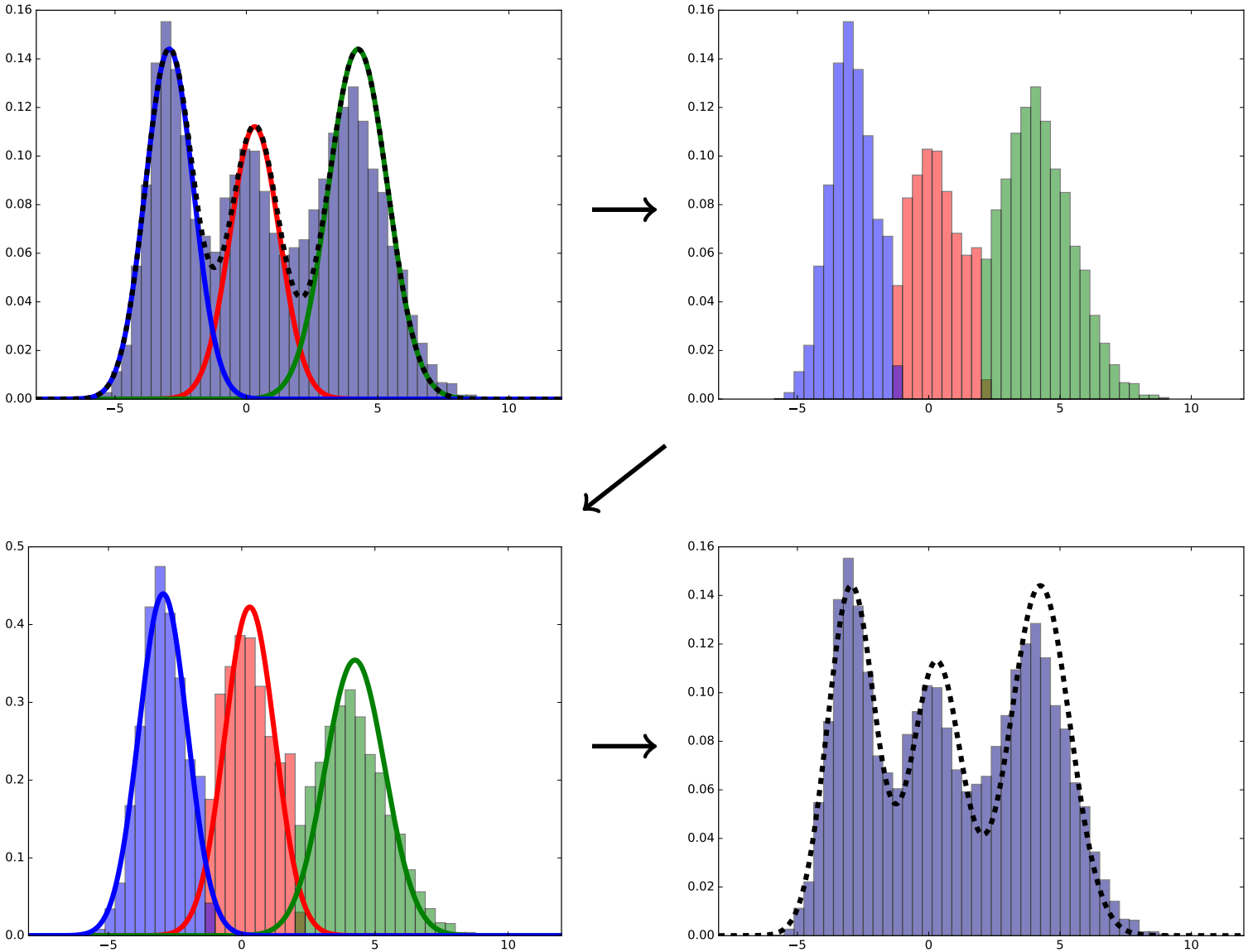


Gaussian Mixture Models



Gaussian Mixture Models

Problem: we form hard clusters — a point is assigned to one, and only one, component of the GMM

If $P(C_i = c_i^* | \boldsymbol{X}_i = \boldsymbol{x}_i) \approx 1$ then we can correctly assume that the point belongs to that component

However, when $P(C_i = c_1 | \boldsymbol{X}_i = \boldsymbol{x}_i) \approx P(C_i = c_2 | \boldsymbol{X}_i = \boldsymbol{x}_i)$ we are making a crude approximation: both c_1 and c_2 might have been responsible for the generation of $\boldsymbol{x}_i$

In general, the algorithm we discussed is not maximizing the likelihood of the observed samples $\boldsymbol{x}_i$

Gaussian Mixture Models

We will shortly see a method to estimate a local maximum of the likelihood

However, let's still consider hard-assignments

Let's also assume that we fix the covariance matrices of our GMM to $\boldsymbol{\Sigma}_c = \boldsymbol{I}$

We also fix the weights as $\boldsymbol{w}_c = \frac{1}{K}$

In this case cluster assignment corresponds to the rule

$$c_i^* = \arg\max_c P(C_i = c | \boldsymbol{X}_i = \boldsymbol{x}_i) = \arg\min_c \|\boldsymbol{x}_i - \boldsymbol{\mu}_c\|^2$$

Gaussian Mixture Models

Our algorithm becomes

- Compute the component or cluster c_i^* whose centroid $\boldsymbol{\mu}_{c_i^*}$ is closest to our point and assign $\boldsymbol{x}_i$ to that cluster
- Re-estimate the cluster centroids from the given points, and iterate until convergence

This is the K-Means clustering algorithm

GMMs can also be applied to clustering tasks as a generalization of K-Means

Gaussian Mixture Models

The algorithm we considered can be extended to handle soft assignments

We will see that a point is not completely associated to a single Gaussian component, but contributes to the estimation of different components according to its cluster (component) posterior probability

Consider the log-likelihood for our data (we now make explicitly the dependency on the model parameters in the conditional densities):

$$\sum_{i=1}^{n} \log f_{\boldsymbol{X}_i}(\boldsymbol{x}_i|\boldsymbol{\theta}) = \sum_{i=1}^{N} \log \left(\sum_{c=1}^{K} w_c \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) \right)$$

Let's take the gradient with respect to $\boldsymbol{\mu}_c$

$$\begin{aligned} \mathbf{0} &= -\sum_i \frac{w_c \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)}{\sum_{c'} w_{c'} \mathcal{N}(\boldsymbol{x}_i; \boldsymbol{\mu}_{c'}, \boldsymbol{\Sigma}_{c'})} \boldsymbol{\Sigma}_c (\boldsymbol{x}_i - \boldsymbol{\mu}_c) \\ &= -\sum_i \gamma_{c,i} \boldsymbol{\Sigma}_c (\boldsymbol{x}_i - \boldsymbol{\mu}_c) \end{aligned} \tag{2}$$

which gives

$$\boldsymbol{\mu}_c = \frac{\sum_i \gamma_{c,i} \boldsymbol{x}_i}{\sum_i \gamma_{c,i}} \tag{3}$$

Notice that the responsibilities $\gamma_{c,i}$ depend on $\boldsymbol{\mu}_c$. If we knew the responsibilities we could compute $\boldsymbol{\mu}_c$ as in (3)

We can interpret (3) as a weighted empirical mean. The weight of each sample is the corresponding responsibility.

The terms

$$N_c = \sum_{i=1}^{N} \gamma_{c,i}$$

and

$$\boldsymbol{F}_c = \sum_{i=1}^{N} \gamma_{c,i} \boldsymbol{x}_i$$

are also called zero and first order statistics

Note that we are summing over all samples in $\mathcal{D}$

Gaussian Mixture Models

We can adopt a similar strategy for the covariance matrix, obtaining

$$\boldsymbol{\Sigma}_c = \frac{1}{N_c} \sum_i \gamma_{c,i} \left(\boldsymbol{x}_i - \boldsymbol{\mu}_c\right) \left(\boldsymbol{x}_i - \boldsymbol{\mu}_c\right)^T = \frac{1}{N_c} \sum_i \gamma_{c,i} \boldsymbol{x}_i \boldsymbol{x}_i^T - \boldsymbol{\mu}_c \boldsymbol{\mu}_c^T$$

The terms

$$\boldsymbol{S}_c = \sum_i \gamma_{c,i} \boldsymbol{x}_i \boldsymbol{x}_i^T$$

are also called second order statistics

The weights can be re-estimated as

$$w_c = \frac{N_c}{N}$$

where N is the number of samples $N = \sum_{c=1}^{K} N_c$

Gaussian Mixture Models

Since we are not given $\gamma_{c,i}$, we can follow the same procedure we used for hard assignments:

- Given $\boldsymbol{\theta}$, we estimate the responsibilities, i.e. the cluster or component posterior probabilities

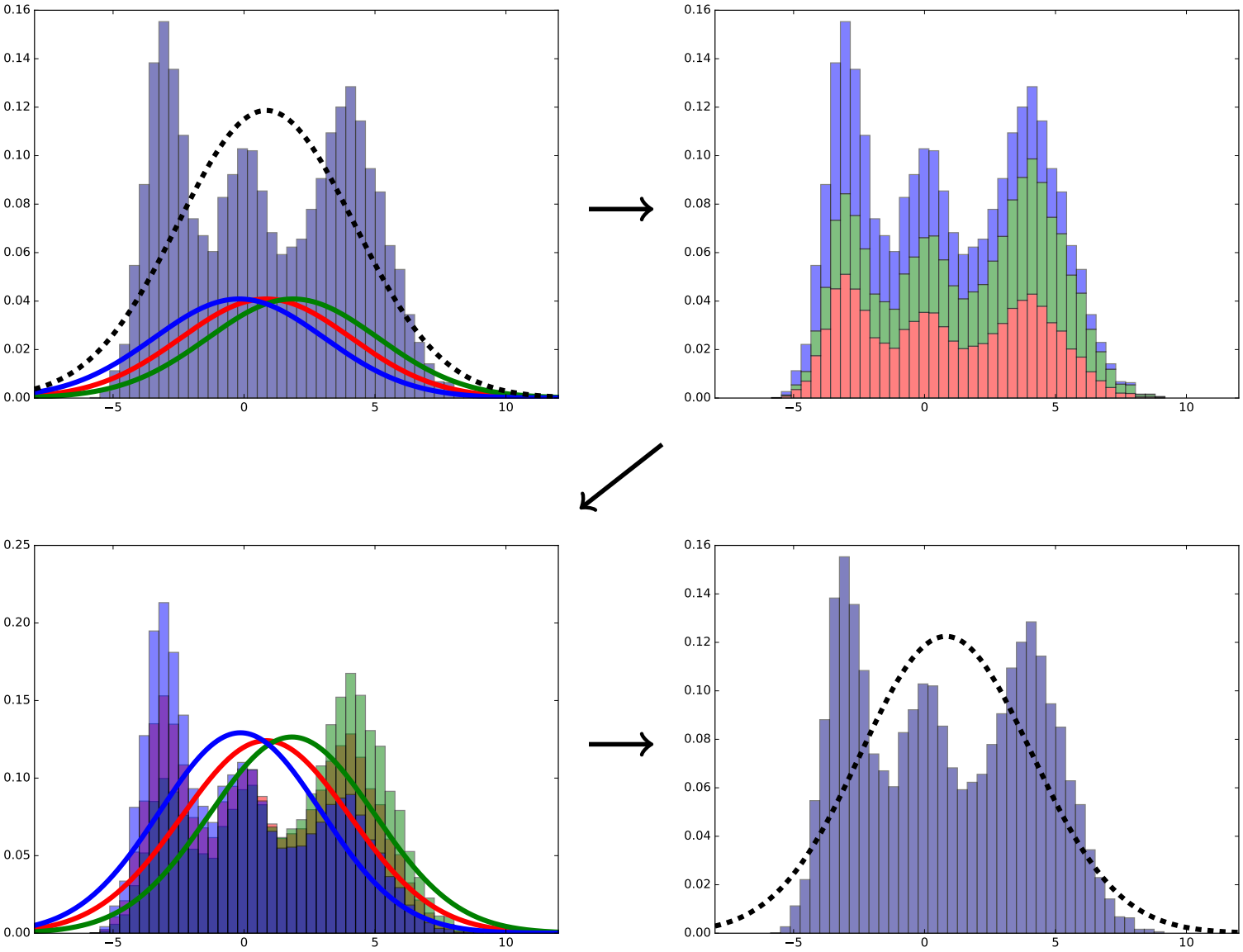
  $$\gamma_{c,i} = P(C_i = c | \boldsymbol{X}_i = \boldsymbol{x}_i)$$

  for each sample of our dataset $\mathcal{D}$

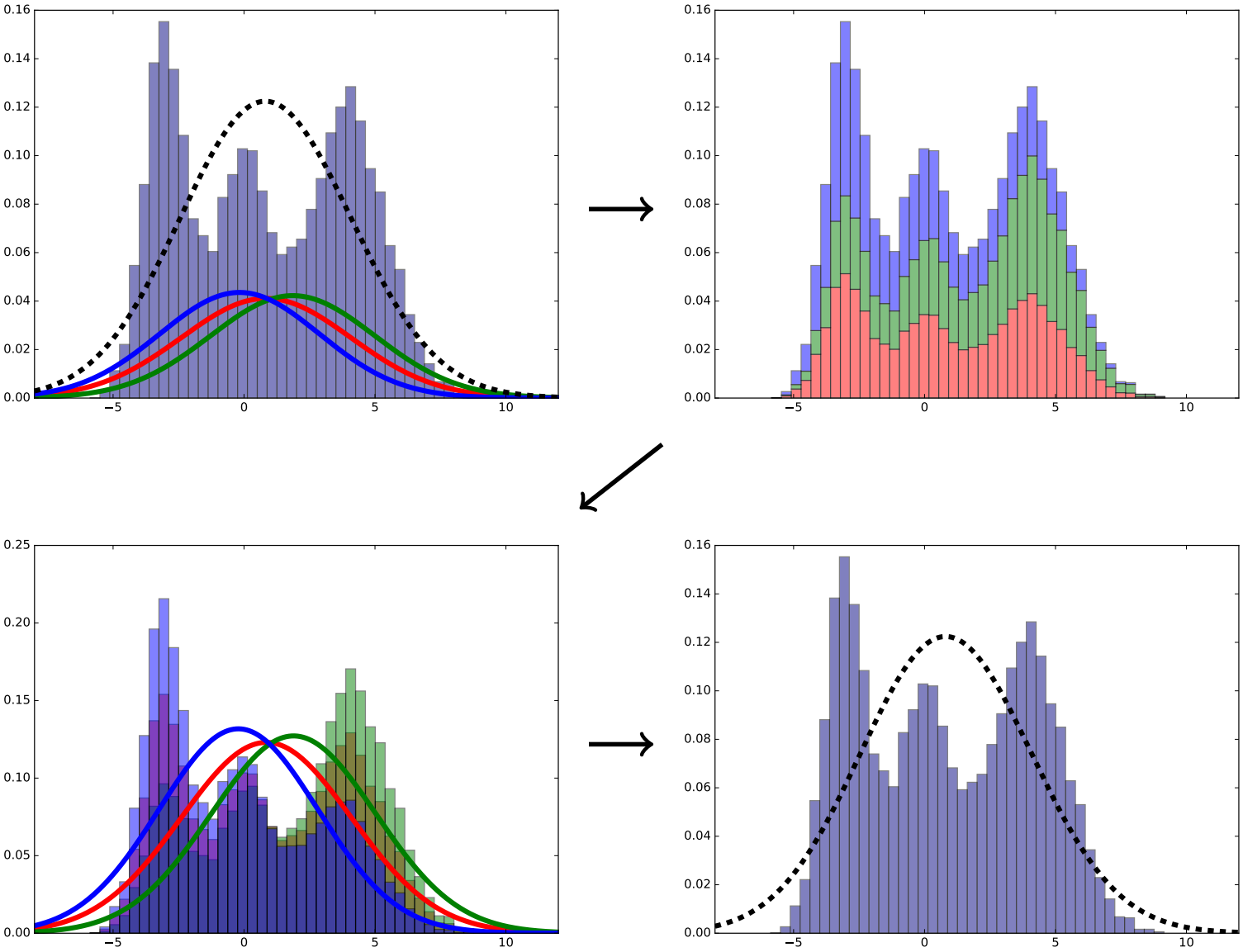
- Given the responsibilities, we re-estimate the GMM parameters $\boldsymbol{\theta}$ using the previous expressions

As we will shortly see, this procedure is a particular instance of an algorithm known as Expectation-Maximization

Gaussian Mixture Models



Gaussian Mixture Models



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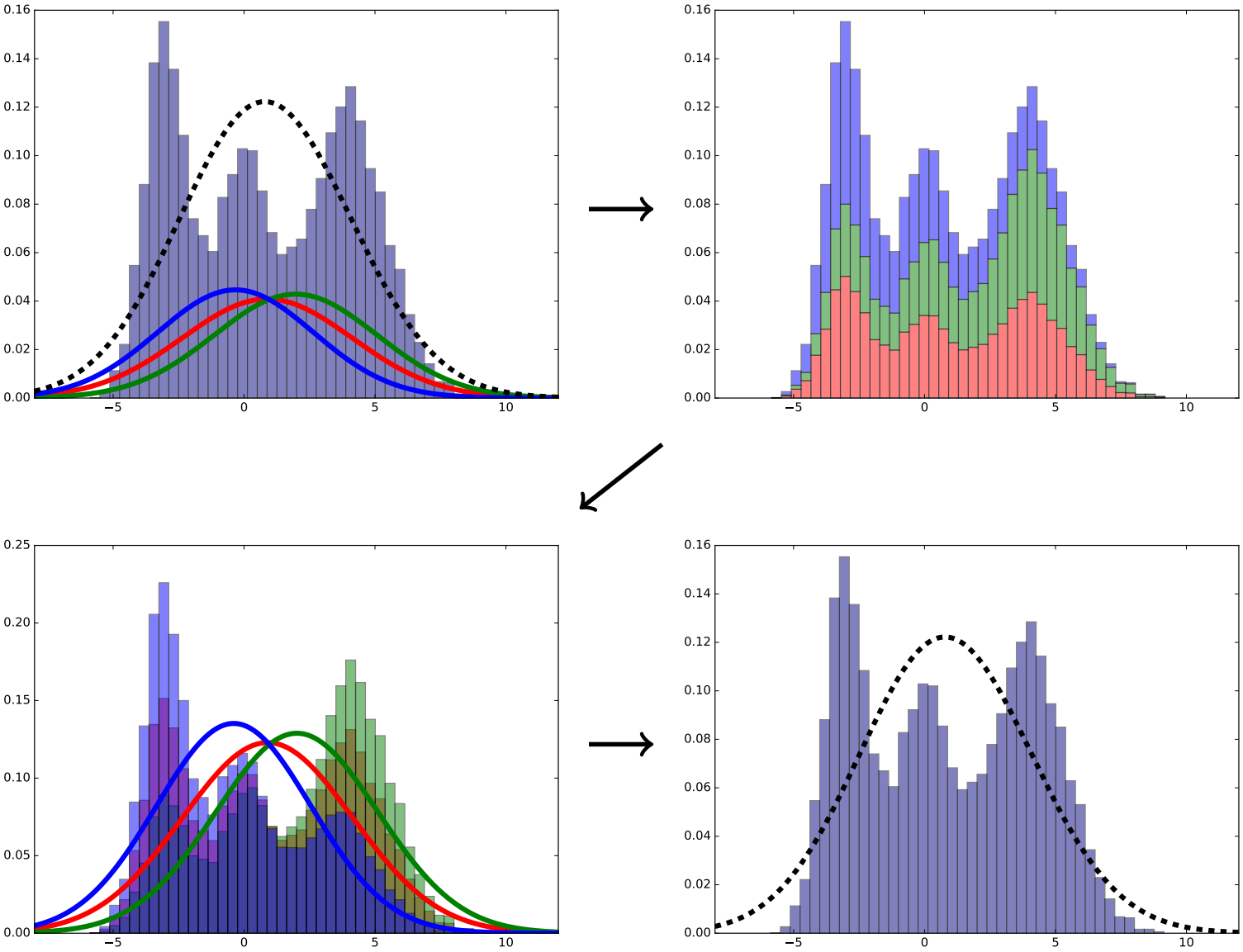

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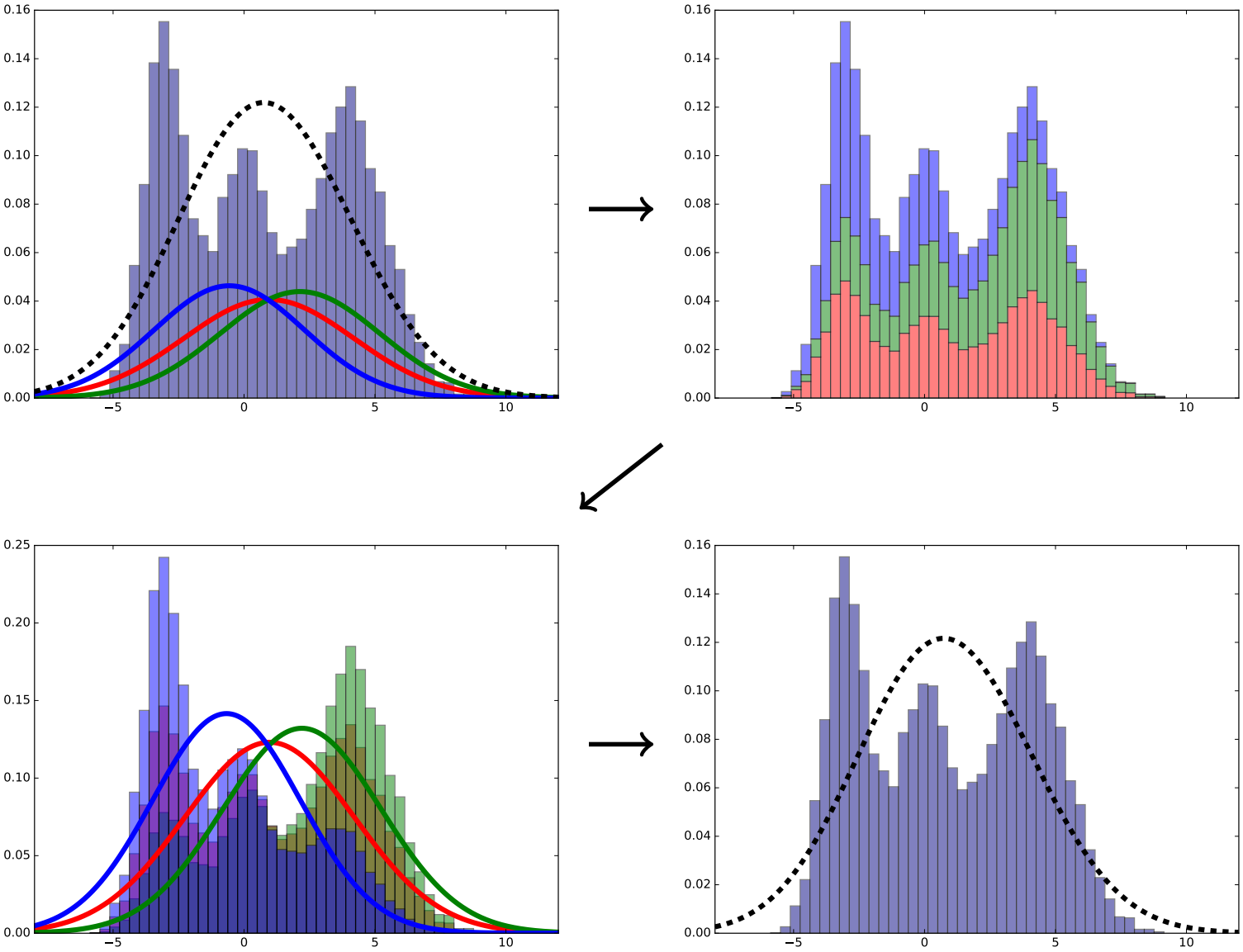

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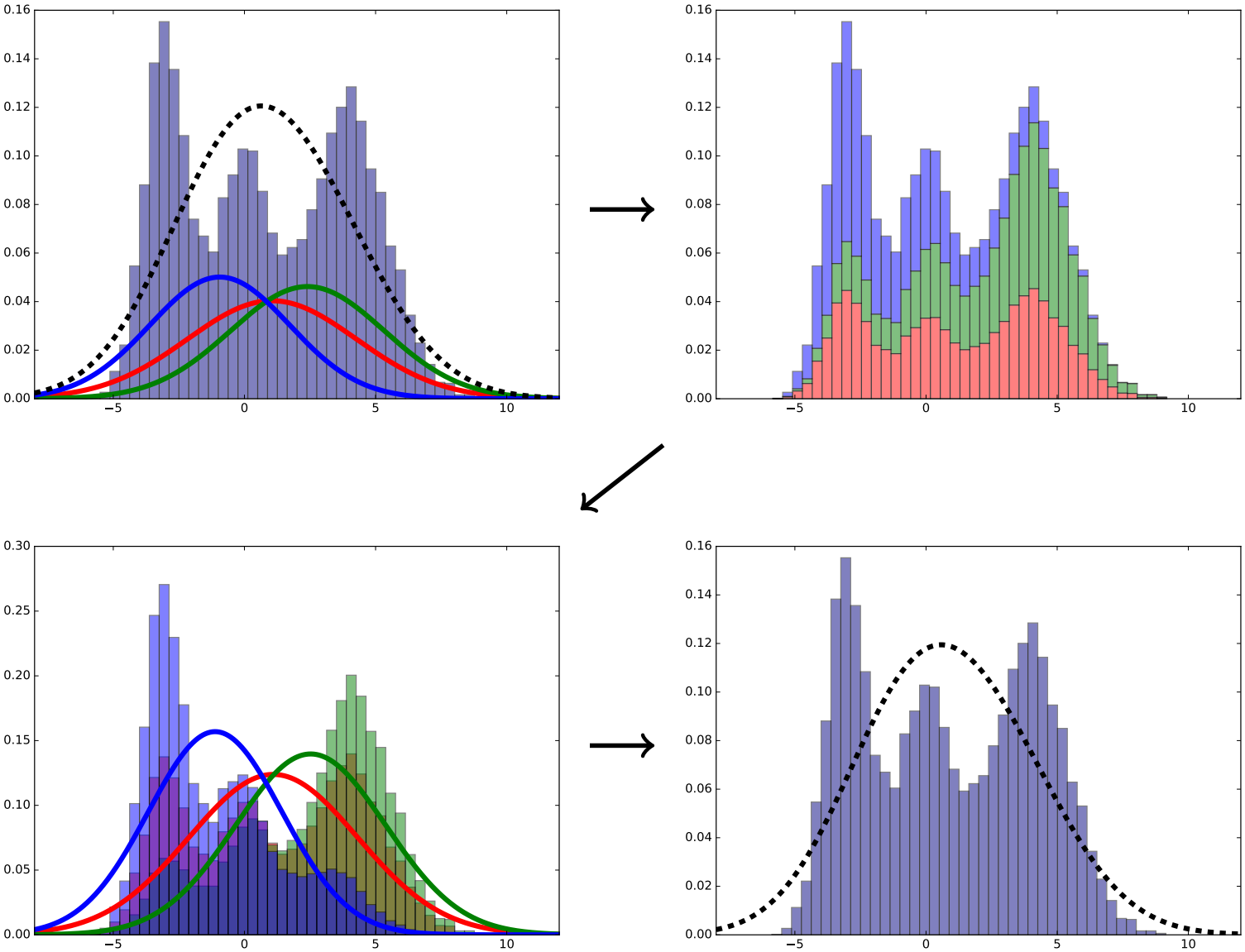

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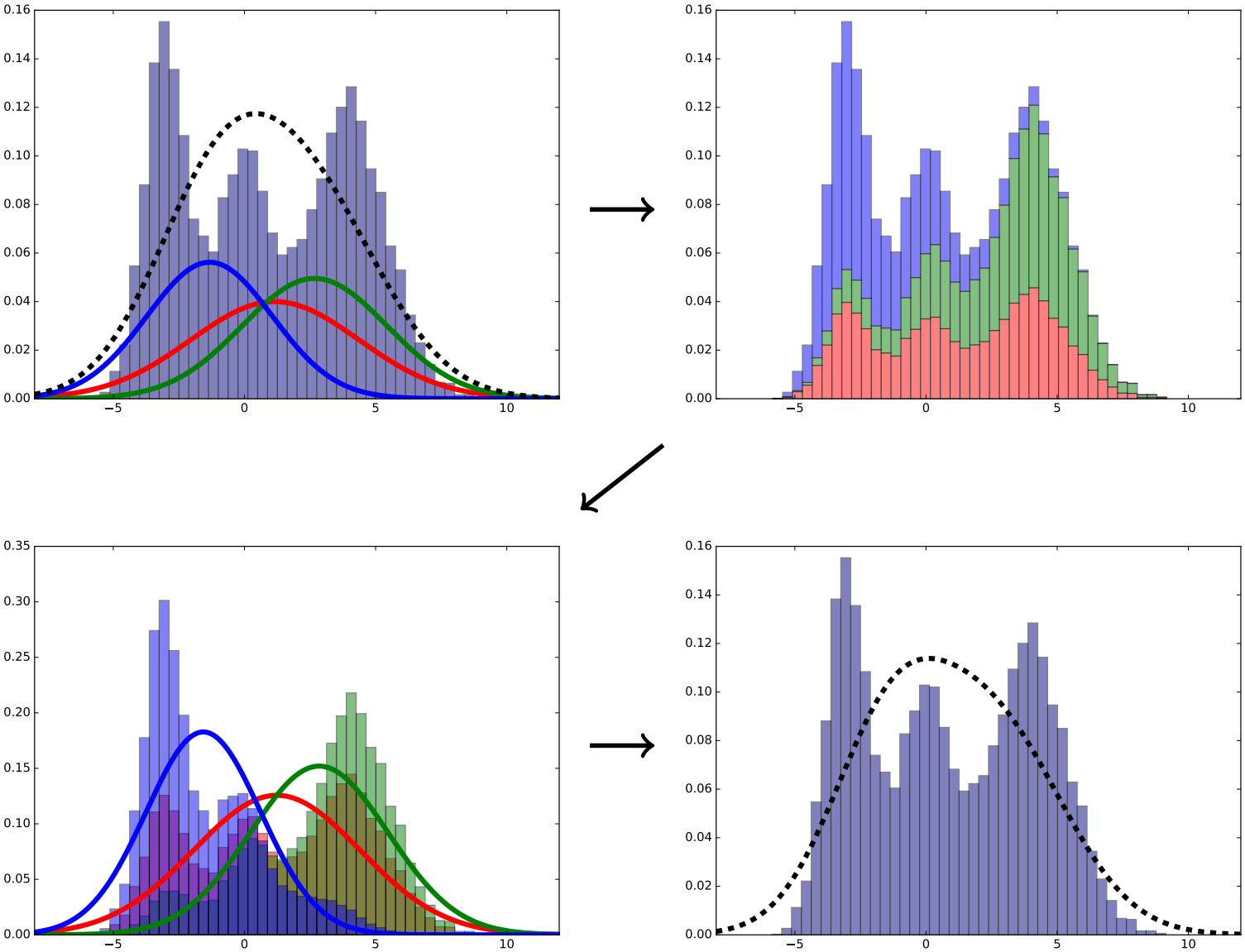

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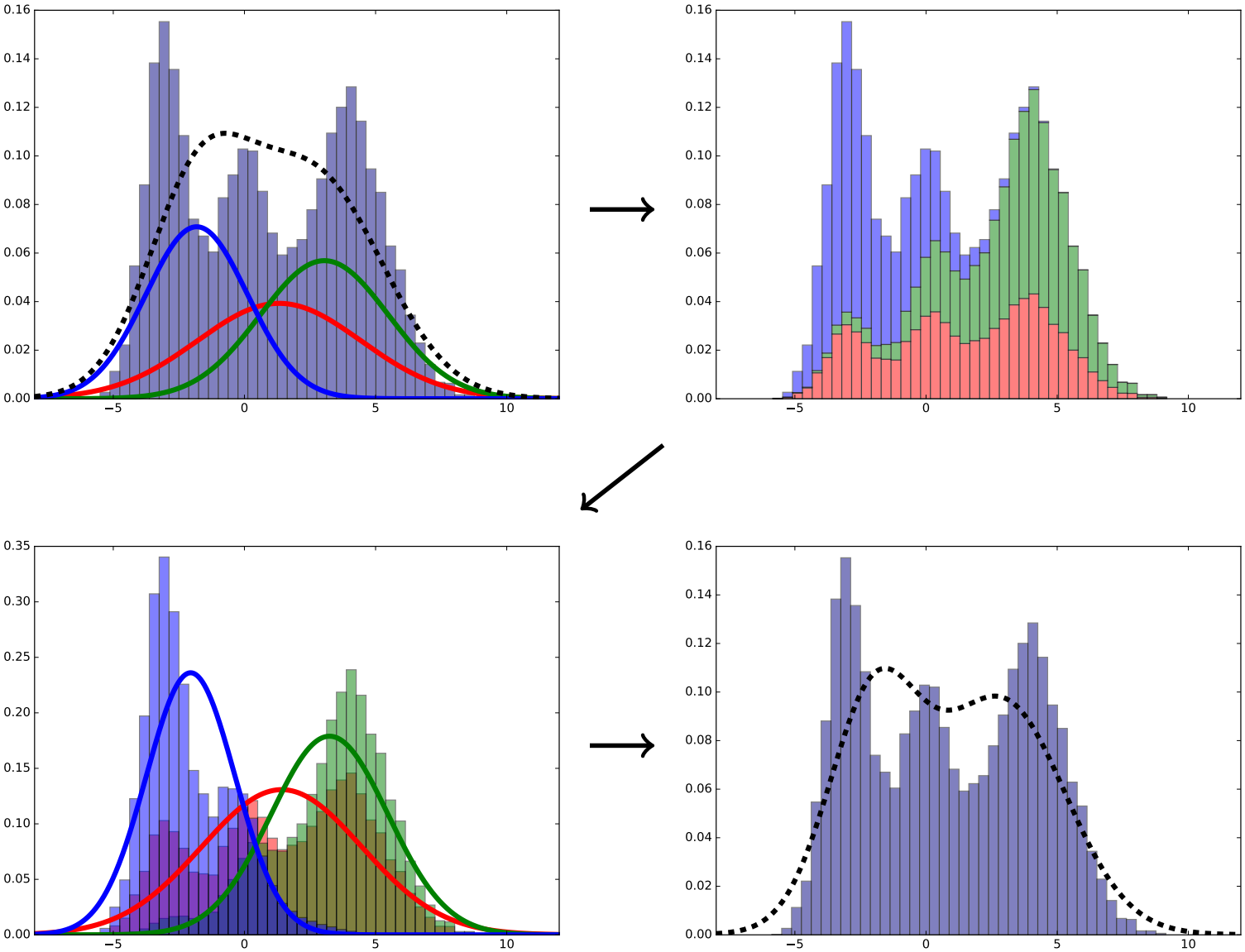

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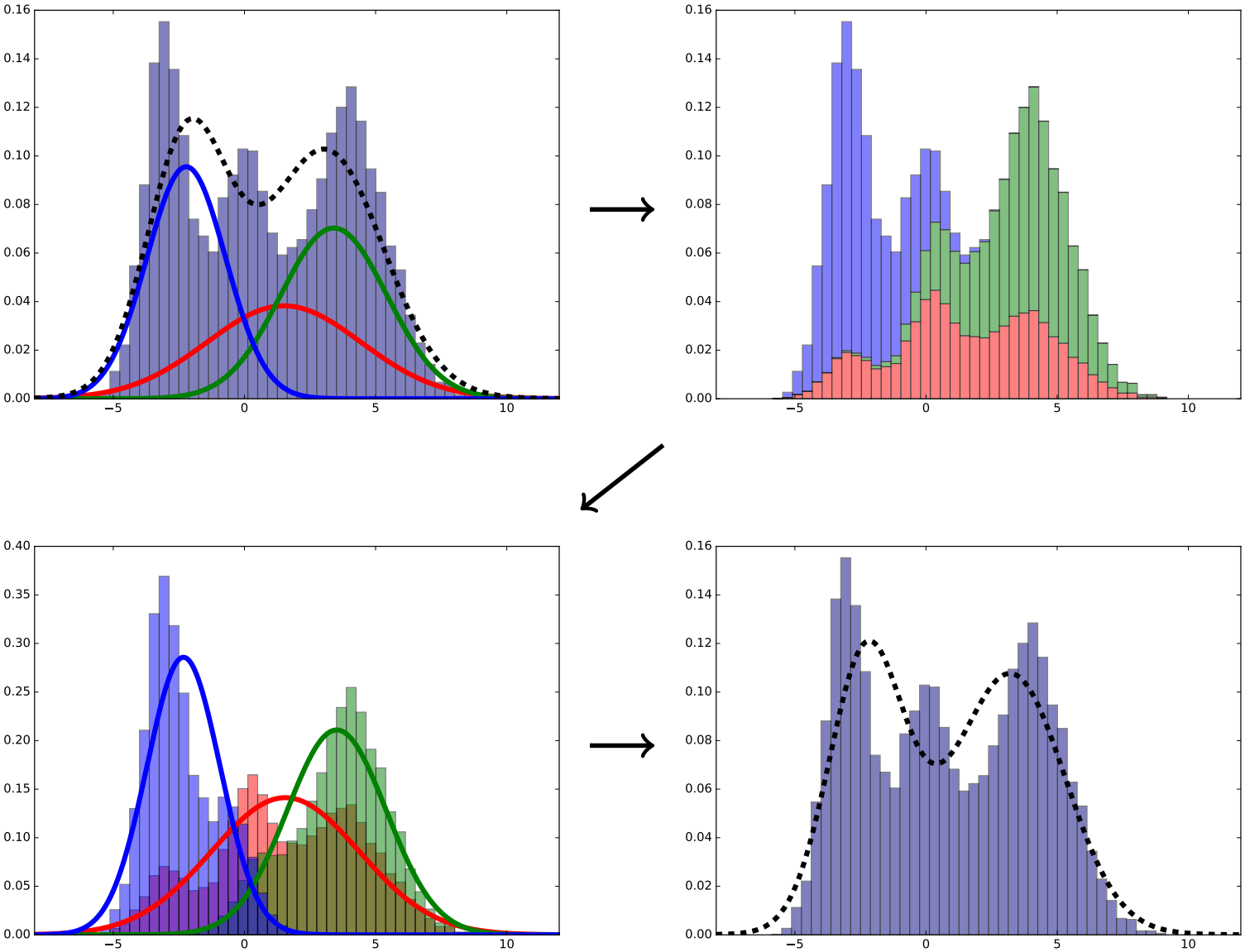

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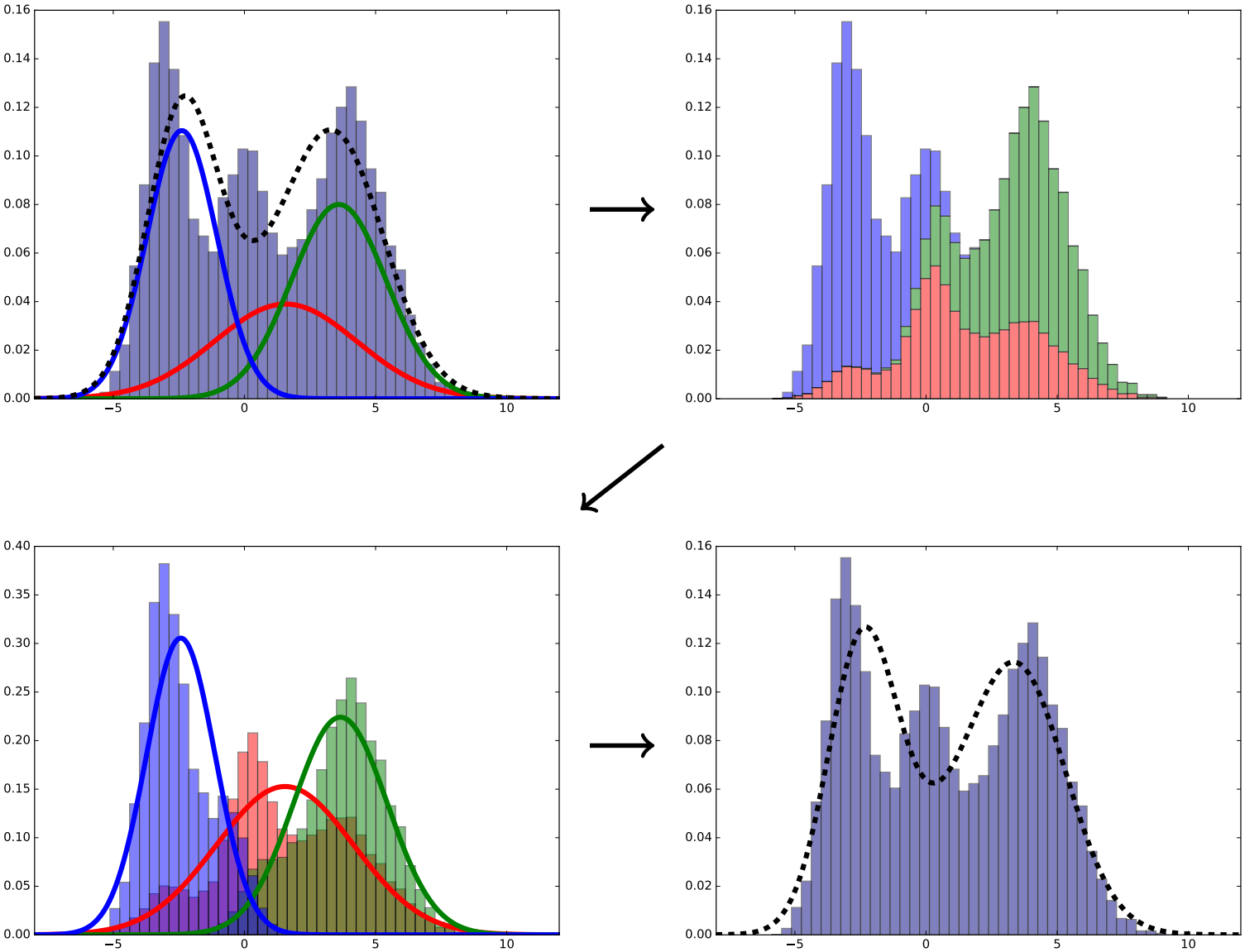

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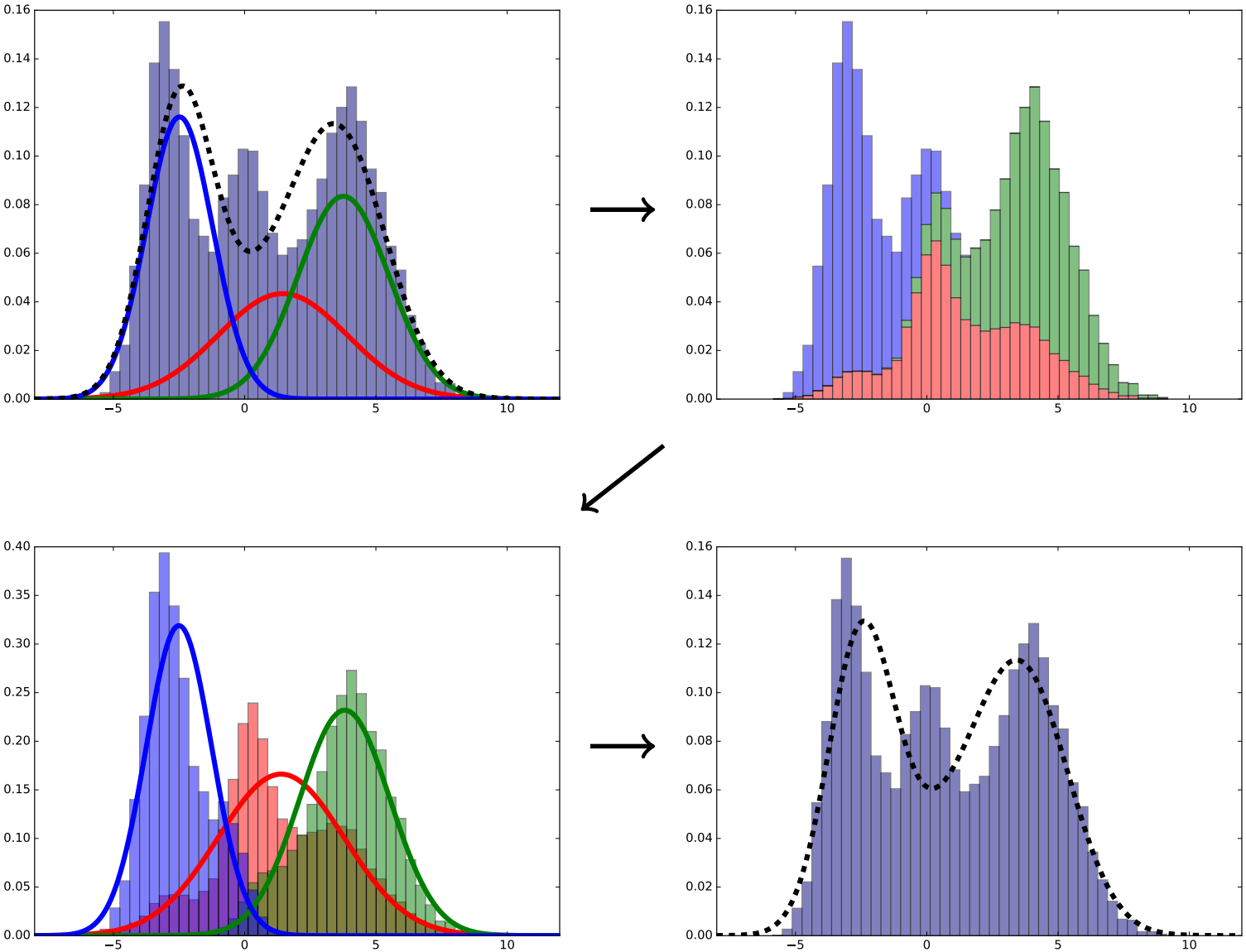

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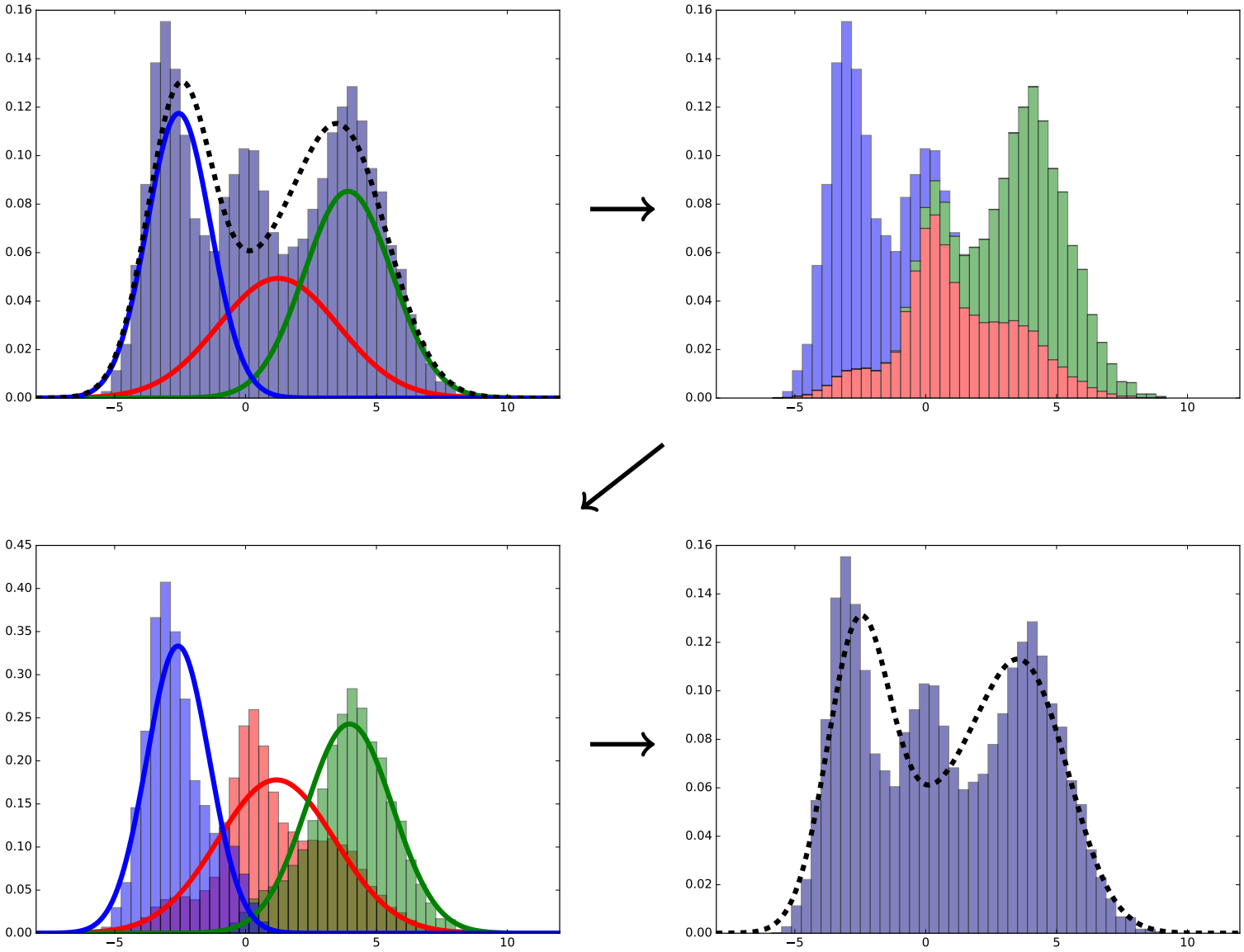

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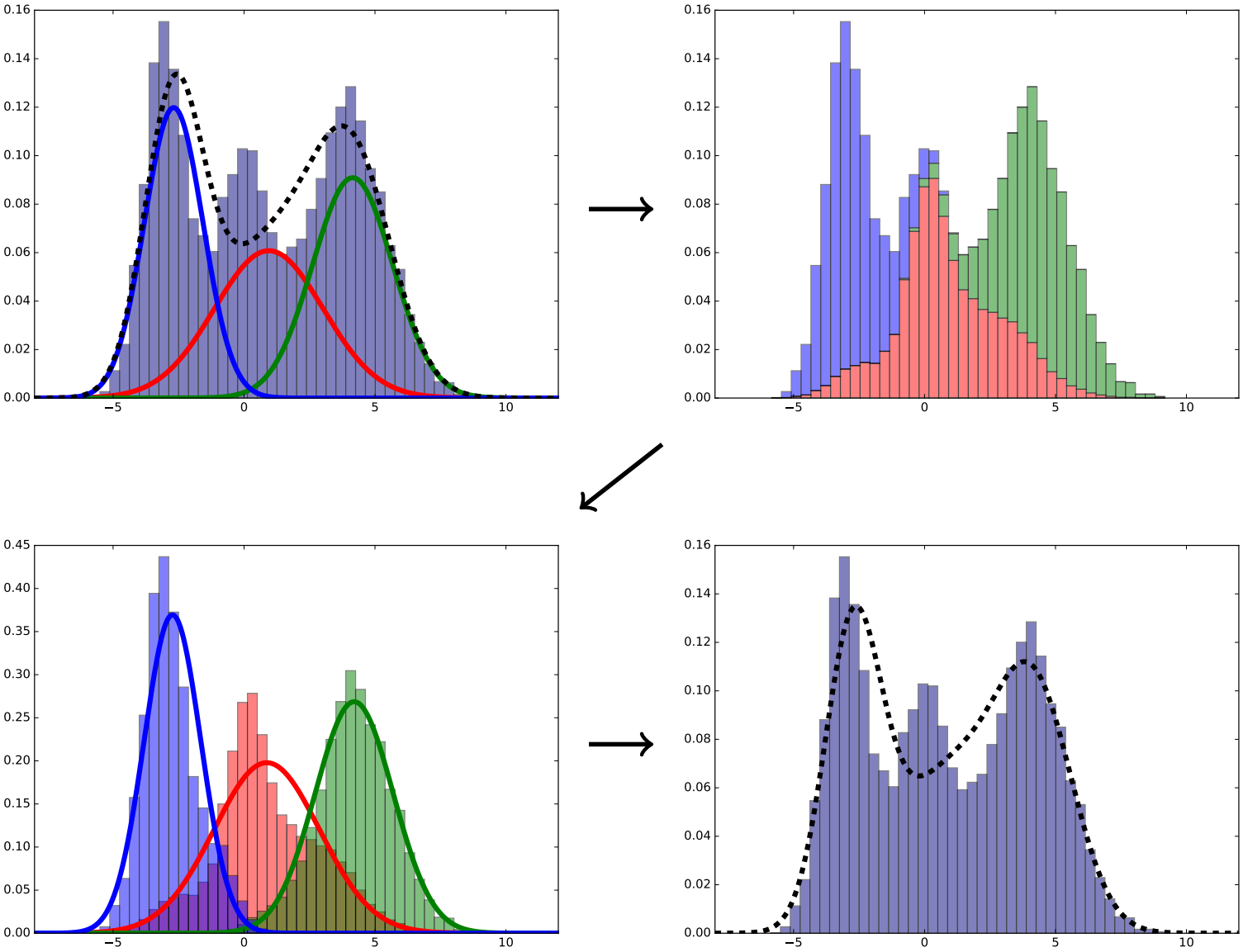

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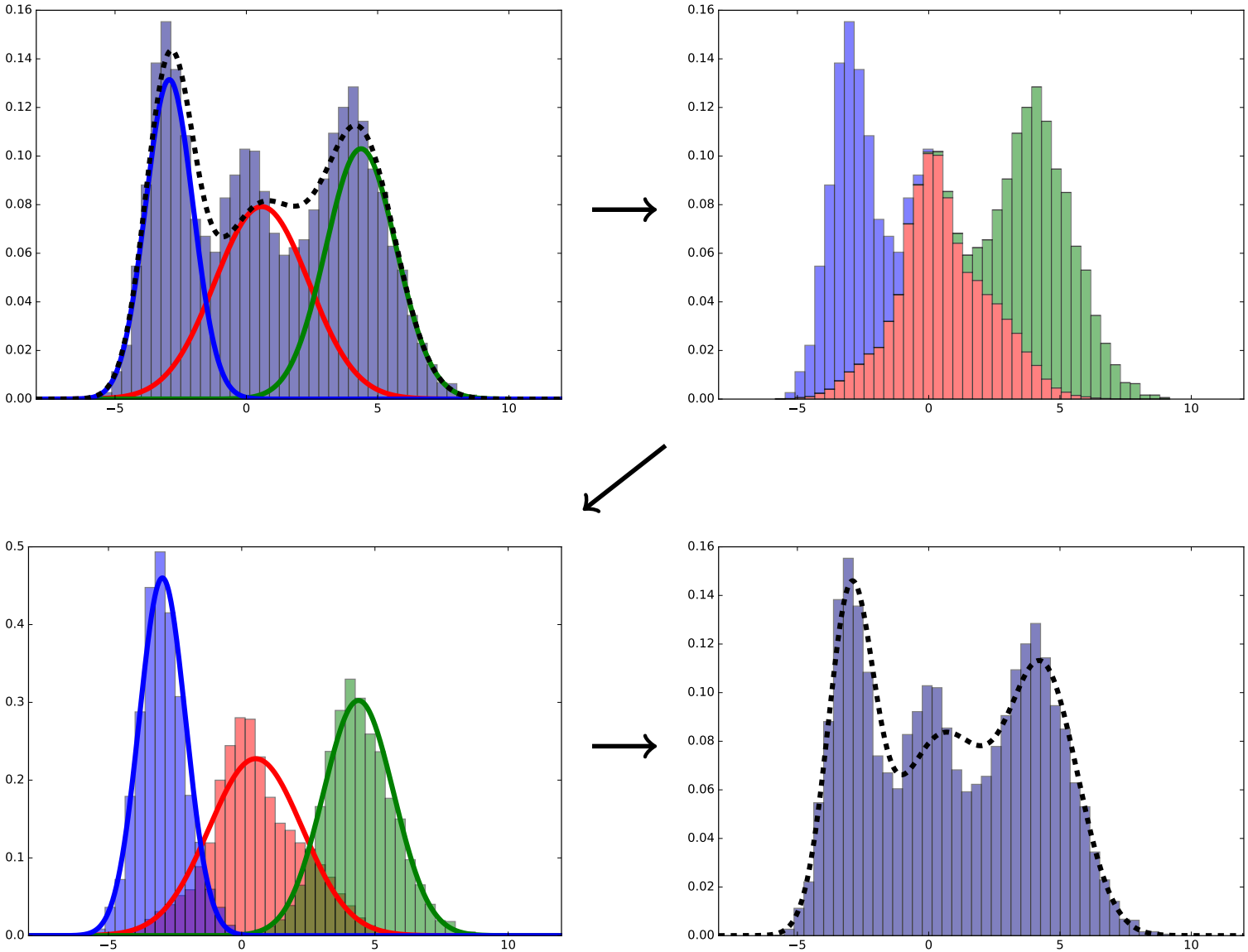

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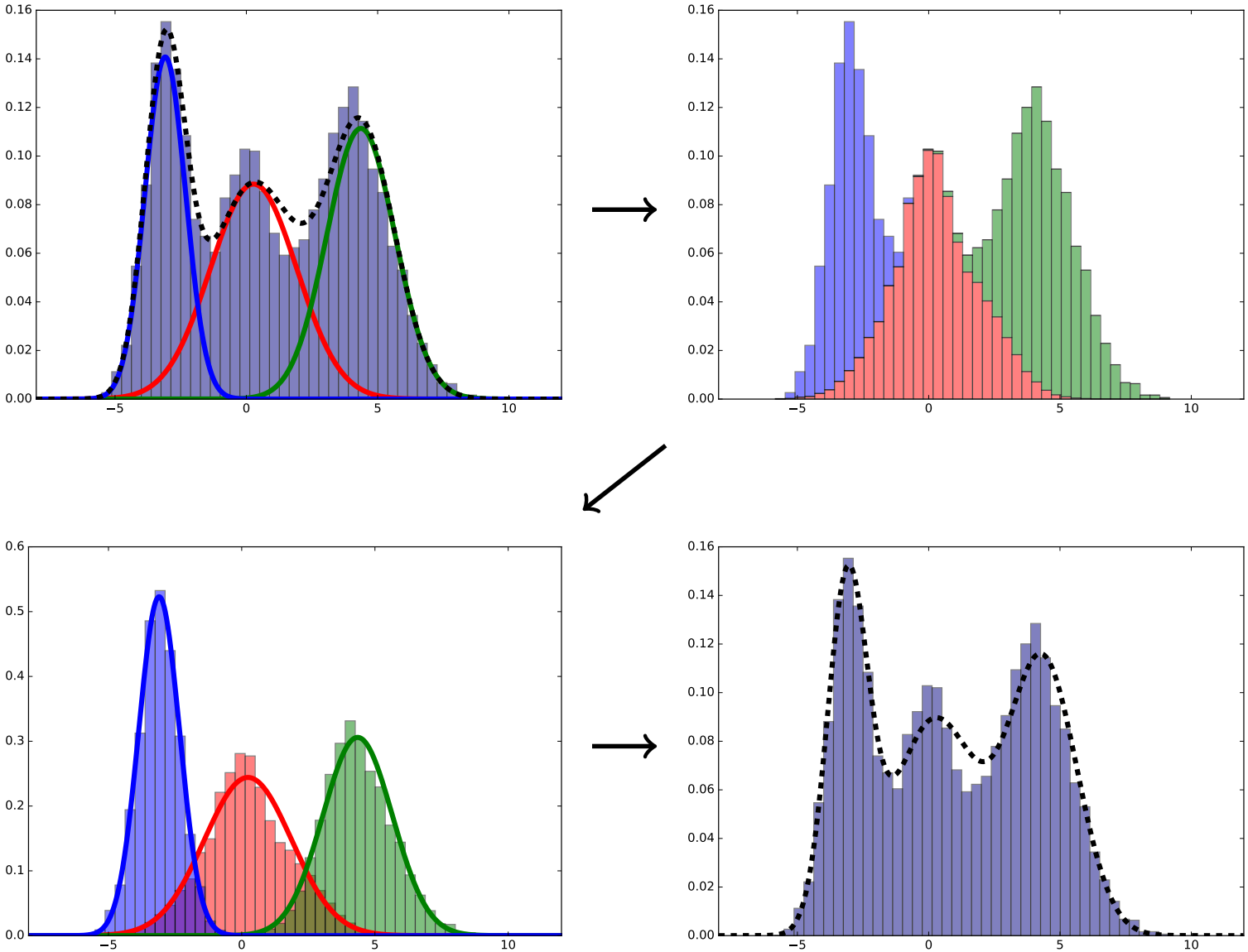

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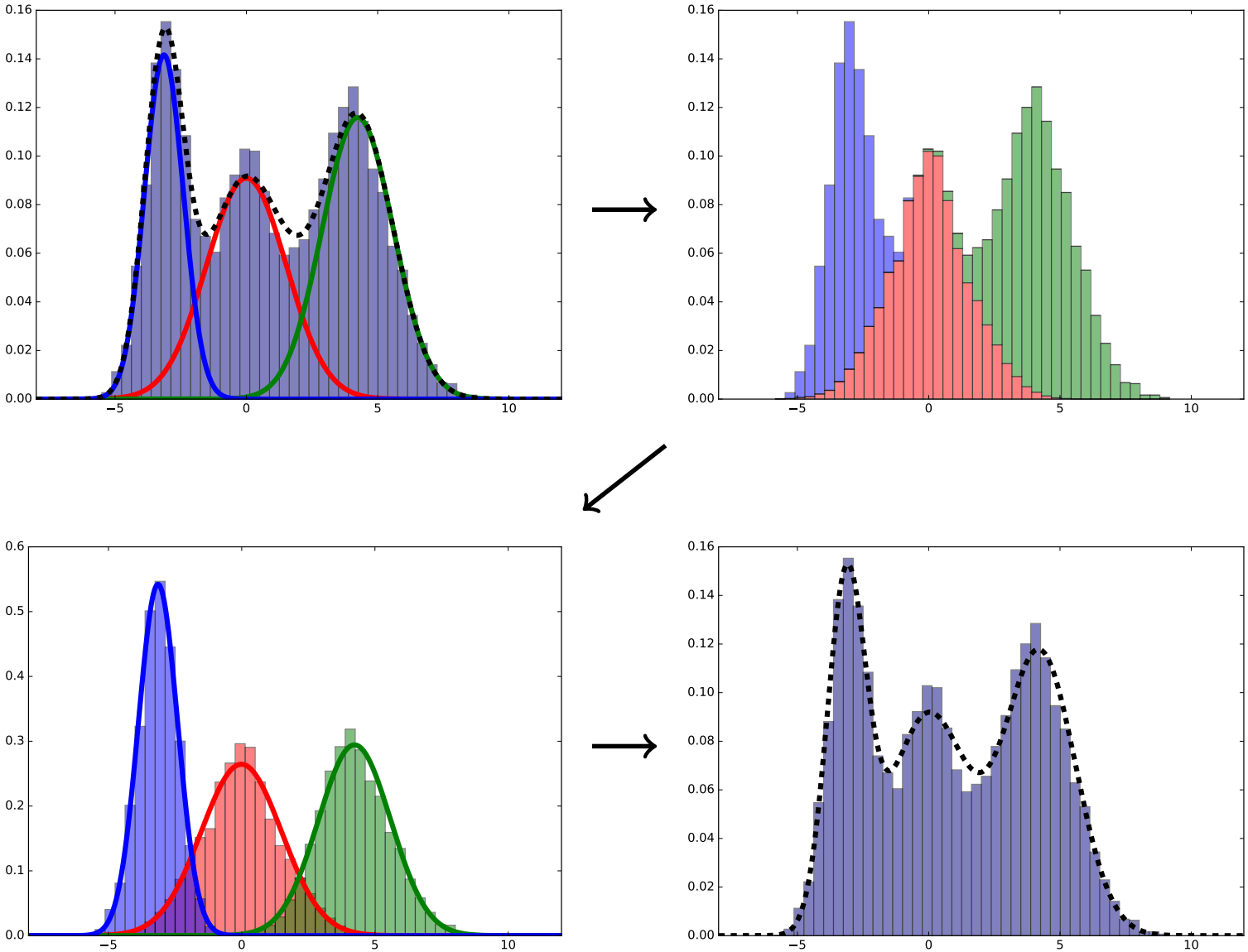

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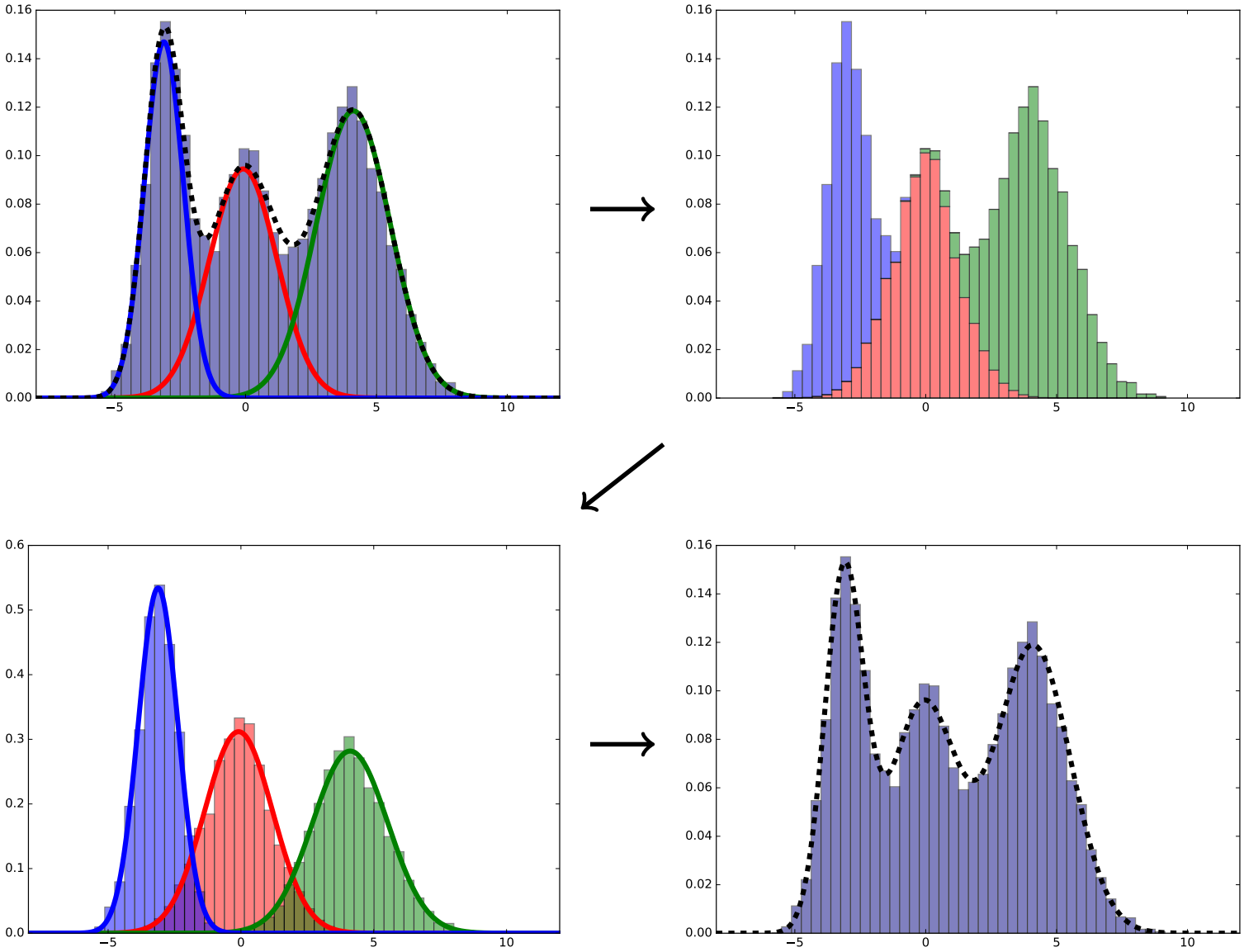
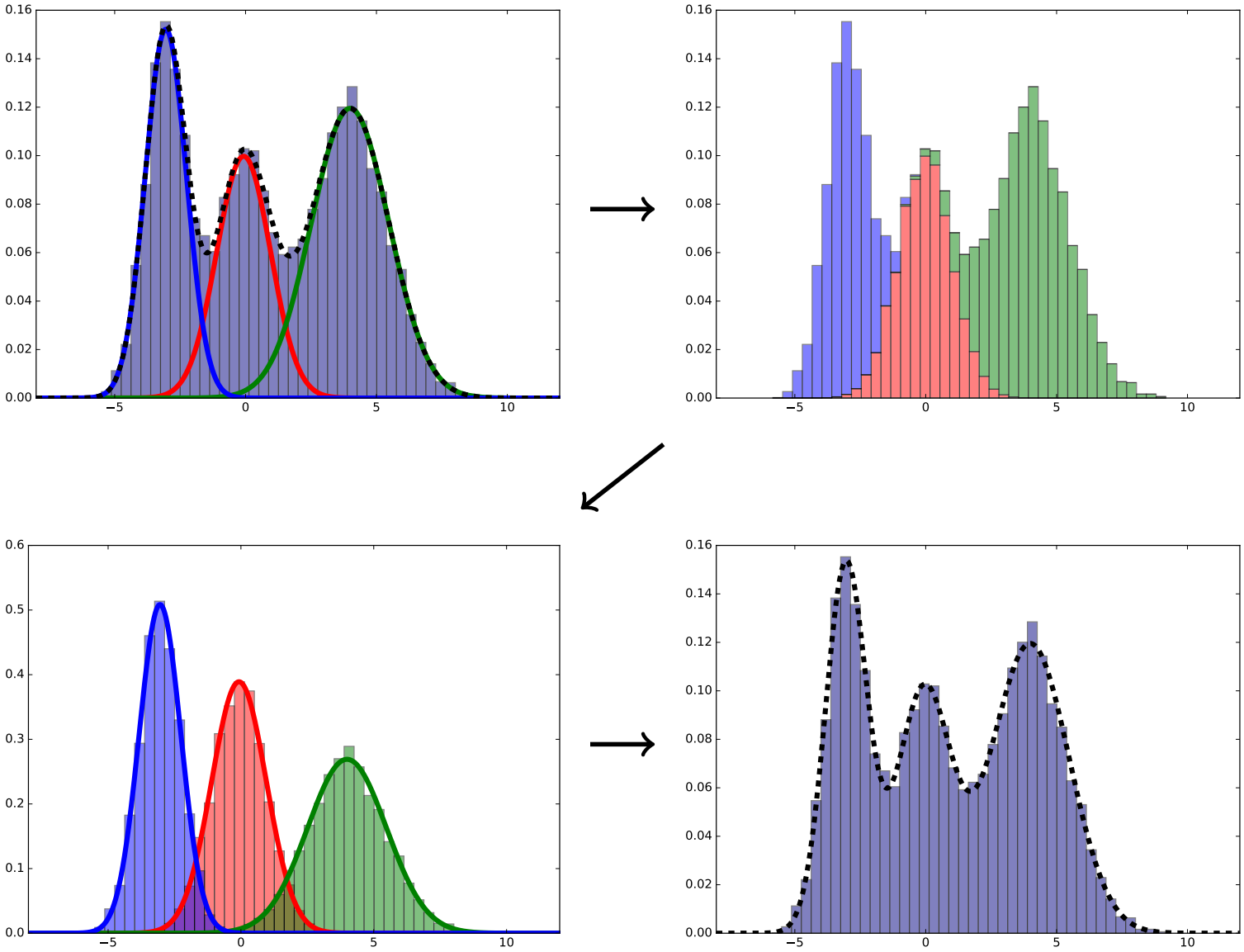
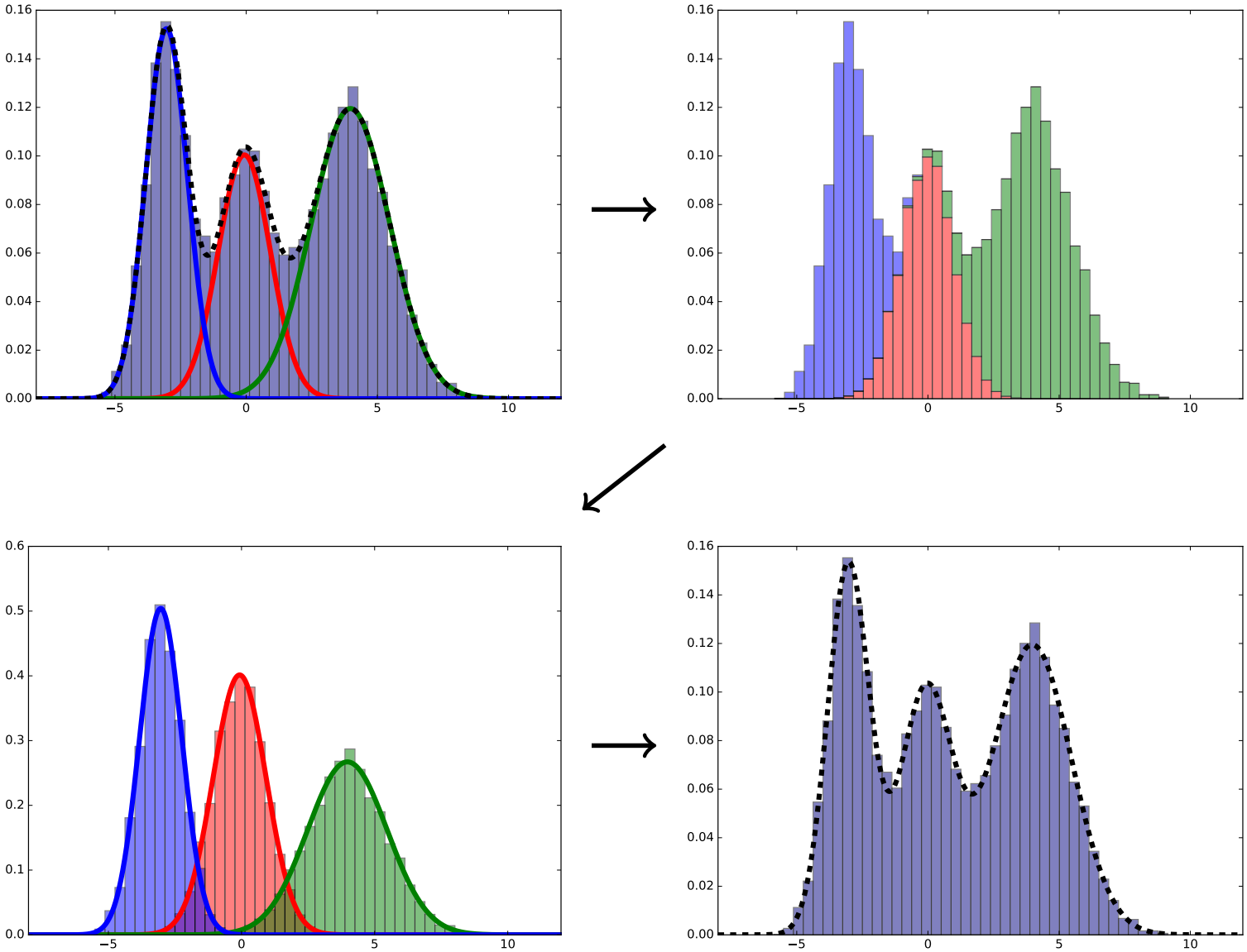


Gaussian Mixture Models

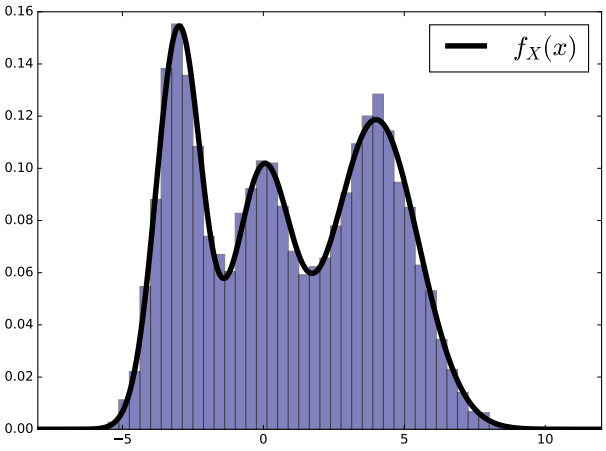


Gaussian Mixture Models

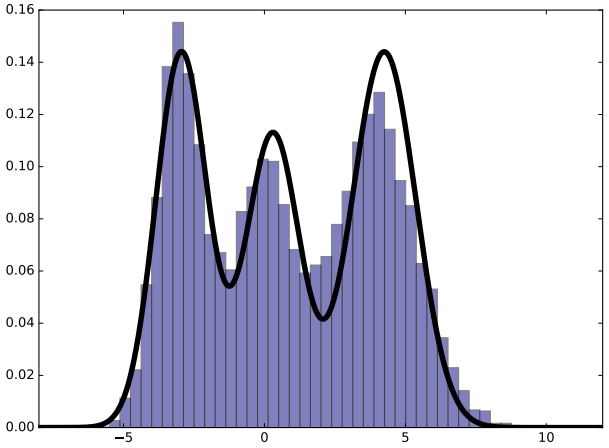


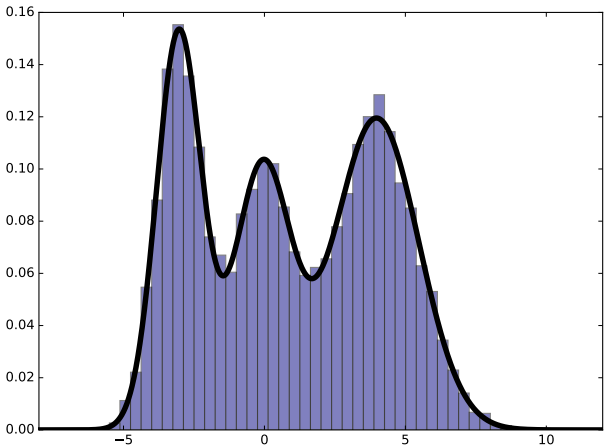
Gaussian Mixture Models

P.d.f.



Hard assignment





Soft assignment

Sampling parameters and estimated values

	π_1	π_2	π_3
P.d.f.	0.25	0.45	0.30
Hard	0.27	0.41	0.32
EM	0.25	0.45	0.30

	μ_1	μ_2	μ_3
P.d.f.	0.00	4.00	-3.00
Hard	0.30	4.25	-2.95
EM	-0.07	3.98	-3.03

	σ_1^2	σ_2^2	σ_3^2
P.d.f.	1.00	2.25	0.64
Hard	0.89	1.27	0.82
EM	0.99	2.23	0.63

Expectation Maximization

Direct maximization of the GMM log-likelihood proved difficult because of the form of the marginal log-density

$$\log f_{\boldsymbol{X}}(x|\boldsymbol{\theta}) = \log \left(\sum_{c=1}^{K} w_c \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) \right)$$

On the contrary, we have seen that the optimization of joint cluster-feature likelihoods is straightforward: the joint likelihood consists of the product of cluster-conditional normal log-densities and cluster prior probabilities

$$\log f_{X,C}(\boldsymbol{x}, c) = \log \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) + \log w_c$$

and has a simple expression

Expectation Maximization

The EM is an iterative procedure suited for the ML estimation of the parameters of complex likelihoods[2] $f_X(x|\theta)$ that can be expressed through marginalization of joint likelihoods $f_{X,H}(x,h|\theta)$:

$$f_X(x) = \int f_{X,H}(x,h)dh = \int f_{X|H}(x|h)f_H(h)dh$$

NOTE: Here and in the following we do not make any assumption on what X represents. We simply assume that it's a random variable or a random vector, for which we observe a value x. We shall see later that, for our GMM estimation task, X represents the set of random vectors that describe the feature vectors in our dataset $\mathcal{D}$

[2]The derivations hold for both continuous and discrete latent variables, replacing integrals with sums

Expectation Maximization

H represents a latent (or hidden) random variable (or vector) i.e. a R.V. whose value has not been observed, i.e., is unknown

As we shall see, the EM transforms the maximization of a log-likelihood $\log f_X(x|\theta)$ into a sequence of optimizations of expectations of the joint log-likelihood $\log f_{X,H}(x, h|\theta)$

Expectation Maximization

Let's consider again the marginal log-likelihood

$$\ell(\theta) = \log f_X(x|\theta) = \log \frac{f_{X,H}(x,h|\theta)}{f_{H|X}(h|x,\theta)}$$

Given a density $Q(h)$ with the same support of $f_H(h)$, we can rewrite the log-pdf as

$$\begin{aligned}
\log f_X(x|\theta) &= \int Q(h) \log f_X(x|\theta) dh \\
&= \int Q(h) \log \frac{f_{X,H}(x,h|\theta)}{f_{H|X}(h|x,\theta)} dh \\
&= \int Q(h) \log \frac{f_{X,H}(x,h|\theta)}{Q(h)} - \int Q(h) \log \frac{f_{H|X}(h|x,\theta)}{Q(h)} dh
\end{aligned} \tag{4}$$

The term

$$D_h(Q(h)\|f_{H|X}(h|x,\theta)) = -\int Q(h)\log\frac{f_{H|X}(h|x,\theta)}{Q(h)}dh$$
$$= -\mathbb{E}_Q\left[\log\frac{f_{H|X}(h|x,\theta)}{Q(h)}\right]$$

is called Kullback-Leibler (KL) divergence (usually denoted simply as $D(Q\|f_{H|X})$

As we will shortly see, the term

$$\mathcal{L}_h(Q(h),\theta) = \int Q(h)\log\frac{f_{X,H}(x,h|\theta)}{Q(h)}dh = \mathbb{E}_{Q(h)}\left[f_{X,H}(x,h|\theta)\right] + \mathcal{H}\left(Q(h)\right)$$

where $\mathcal{H}\left(Q(h)\right)$ is the entropy of distribution $Q(h)$, provides a lower bound of the log-likelihood (again, the suffix h is usually omitted, but we keep it to remember we are integrating w.r.t. h)

Expectation Maximization

Let's consider the KL divergence

$$D_h(Q(h)\|f_{H|X}(h|x,\theta)) = -\int Q(h)\log\frac{f_{H|X}(h|x,\theta)}{Q(h)}dh$$

Since for every $z > 0$, we have

$$\log z \leq z - 1$$

and $\log z = z - 1$ if and only if $z = 1$, then, for every value of h in the support of Q:

$$-\log\frac{f_{H|X}(h|x,\theta)}{Q(h)} \geq -\frac{f_{H|X}(h|x,\theta)}{Q(h)} + 1$$

with the equality holding if and only if

$$Q(h) = f_{H|X}(h|x,\theta)$$

Expectation Maximization

We thus have

$$-\int Q(h)\log\frac{f_{H|X}(h|x,\theta)}{Q(h)}dh \geq -\int Q(h)\frac{f_{H|X}(h|x,\theta)}{Q(h)}dh+\int Q(h)dh = 0$$

with the quality holding if and only if

$$Q(h) = f_{H|X}(h|x,\theta)$$

almost everywhere (a. e.)[3]

Therefore

$$D_h(Q(h)||f_{H|X}(h|x,\theta)) \geq 0$$

and

$$D_h(Q(h)||f_{H|X}(h|x,\theta)) = 0 \iff Q = f_{H|X} \text{ a. e.}$$

[3] i.e. over all the domain of H, except for at most a subset of zero measure

Expectation Maximization

We have decomposed the log-likelihood as

$$\log f_X(x|\theta) = \mathcal{L}_h(Q(h), \theta) + D_h\left(Q(h) \| f_{H|X}(h|x, \theta)\right)$$

Notice that the left hand side of the equation does not depend on the choice of Q

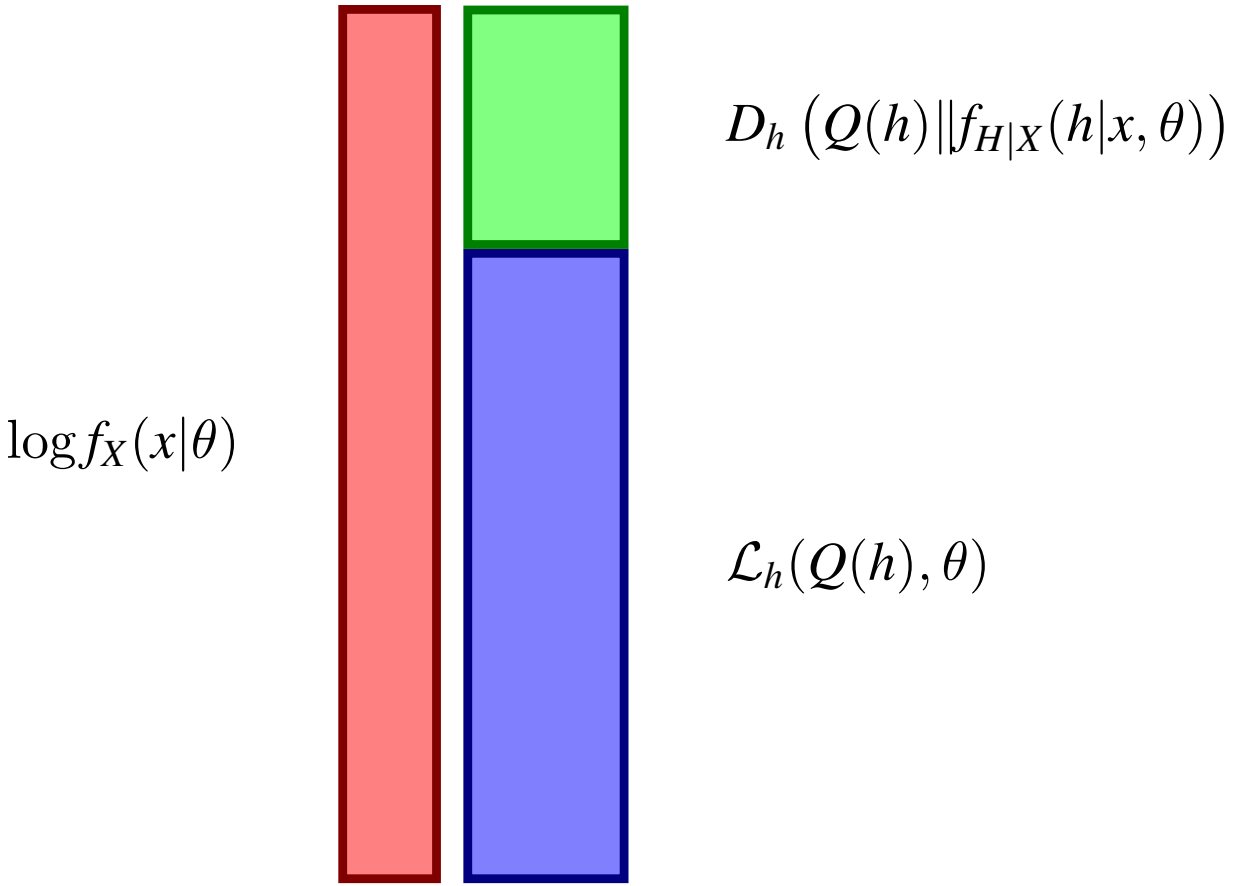
Furthermore,

$$D_h\left(Q(h) \| f_{H|X}(h|x, \theta)\right) \geq 0 \implies \mathcal{L}_h(Q(h), \theta) \leq \log f_X(x|\theta)$$

thus $\mathcal{L}_h(Q(h), \theta)$ is a lower bound on the log-likelihood

Expectation Maximization

Decomposition of $\log f_X(x|\theta) = \mathcal{L}_h(Q(h), \theta) + D_h\left(Q(h) \| f_{H|X}(h|x, \theta)\right)$



Expectation Maximization

The EM algorithm optimizes the log-likelihood by iteratively

- Maximizing the lower bound $\mathcal{L}_h(Q(h), \theta)$ with respect to Q
- Maximizing the lower bound $\mathcal{L}_h(Q(h), \theta)$ with respect to θ

From an initial sets of parameters θ_0:

- $Q_0 = \arg\max_Q \mathcal{L}_h(Q(h), \theta_0)$
- $\theta_1 = \arg\max_\theta \mathcal{L}_h(Q_0(h), \theta)$
- $Q_1 = \arg\max_Q \mathcal{L}_h(Q(h), \theta_1)$
- $\theta_2 = \arg\max_\theta \mathcal{L}_h(Q_1(h), \theta)$
- ...

Expectation Maximization

Let's consider the maximization of the lower bound w.r.t. $Q(h)$, with θ fixed: $\theta = \theta_t$

We have shown that

$$\mathcal{L}_h(Q, \theta_t) \leq \log f_X(x|\theta_t)$$

and

$$Q(h) = f_{H|X}(h|x, \theta_t) \implies \mathcal{L}_h(Q(h), \theta_t) = \log f_X(x|\theta_t)$$

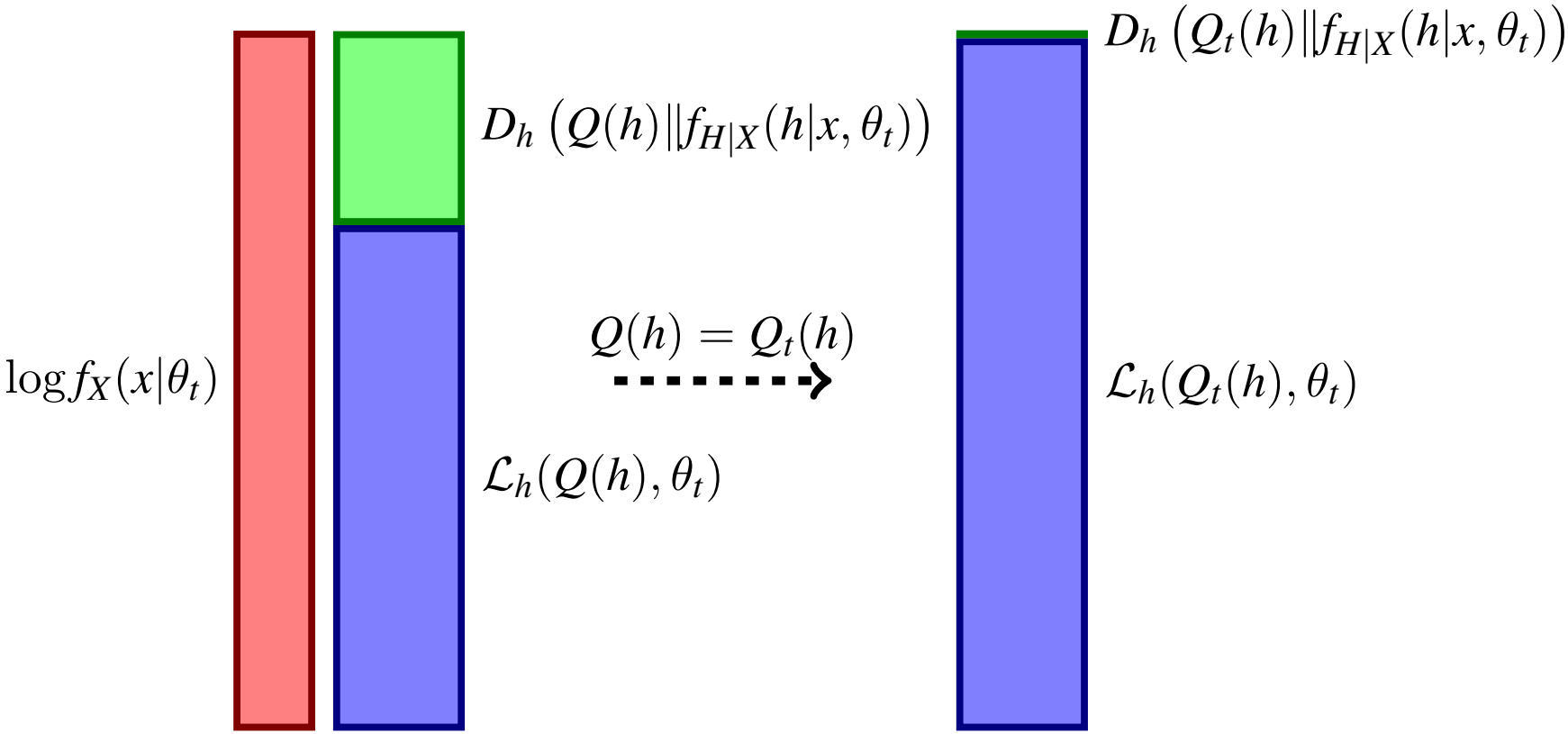
Therefore, we can maximize $\mathcal{L}_h(Q(h), \theta_t)$ w.r.t. Q by simply selecting

$$Q_t(h) = f_{H|X}(h|x, \theta_t)$$

i.e., the posterior for H given X and the fixed value θ_t for the parameters

Expectation Maximization

Setting $Q_t(h) = f_{H|X}(h|x, \theta_t)$ does not change the log-likelihood $\log f_X(x|\theta_t)$, but reduces to zero the KL divergence:



Expectation Maximization

We can now maximize $\mathcal{L}_h(Q_t, \theta)$ w.r.t. θ

This requires computing

$$\theta_{t+1} = \arg\max_{\theta} \mathbb{E}_{Q_t(h)} \log f_{X,h}(x, h|\theta)$$

Notice that the distribution we are taking the expectation with respect to does not involve θ anymore:

$$\begin{aligned}\mathbb{E}_{Q_t(h)} \log f_{X,h}(x, h|\theta) &= \int Q_t(h) \log f_{X,H}(x, h|\theta) dh \\ &= \int f_{H|X}(h|x, \theta_t) \log f_{X,H}(x, h|\theta) dh\end{aligned}$$

since the parameters used in the distribution

$$Q_t(h) = f_{H|X}(h|x, \theta_t)$$

are fixed to θ_t ($Q_t(h)$ does not depend on θ, but on θ_t)

Expectation Maximization

We can also rewrite the problem as maximization of

$$\mathbb{E}_{Q_t(h)} \log f_{X,H}(x,h|\theta) = \mathbb{E}_{Q_t(h)} \log f_{X|H}(x|h,\theta) + \mathbb{E}_{Q_t(h)} \log f_H(h|\theta)$$

which corresponds to the expression we used for the GMM

Since we are maximizing $\mathcal{L}_h(Q_t(h),\theta)$, we have

$$\mathcal{L}(Q_t,\theta_{t+1}) \geq \mathcal{L}(Q_t,\theta_t)$$

Expectation Maximization

$\mathcal{L}_h(Q_t, \theta_{t+1})$ is a lower bound of $\log f_X(x|\theta_{t+1})$, thus

$$\log f_X(x|\theta_{t+1}) \geq \mathcal{L}_h(Q_t, \theta_{t+1})$$

Indeed,

$$\log f_X(x|\theta_{t+1}) = \mathcal{L}(Q_t(h), \theta_{t+1}) + D\left(Q_t, f_{H|X}(h|x, \theta_{t+1})\right)$$

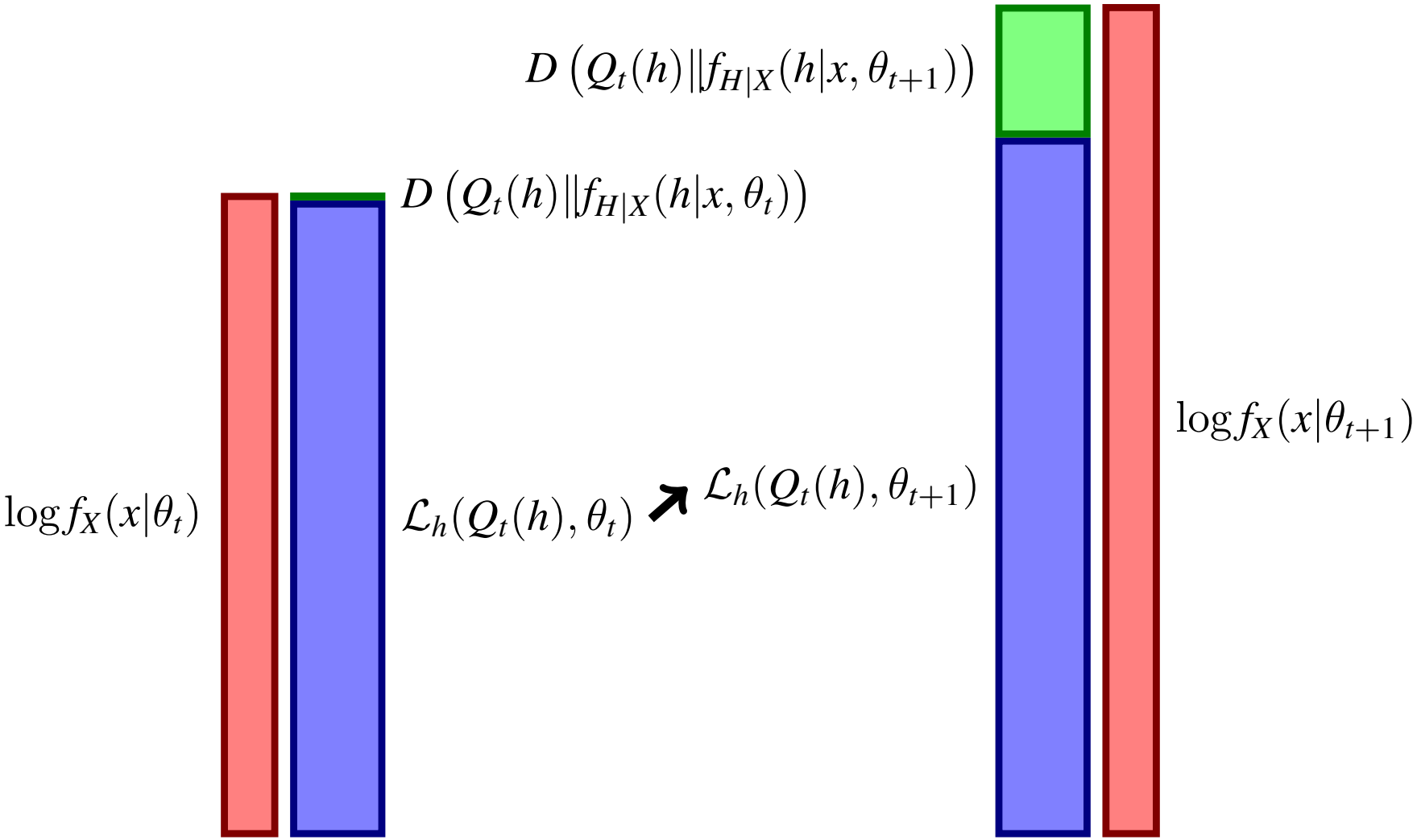
Maximization with respect to θ has increased both $\mathcal{L}_h$ and the KL-divergence, since, in general, $Q_t(h) \neq f_{H|X}(h|x, \theta_{t+1})$ unless we reached convergence

We thus have that

$$\log f_X(x|\theta_{t+1}) \geq \log f_X(x|\theta_t)$$

Expectation Maximization

Maximization w.r.t. θ of $\mathcal{L}_h(Q_t, \theta)$ increases the log-pdf $\log f_X(x|\theta)$



Expectation Maximization

The algorithm iterates between two steps

- **Expectation (E) step:** Compute the posterior distribution $f_{H|X}(h|x,\theta_t)$ and compute the auxiliary function:

$$\mathcal{Q}(\theta,\theta_t) = \mathbb{E}_{f_{H|X}(h|x,\theta_t)}\left[\log f_{X,H}(x,h|\theta)\right]$$

- **Maximization (M) step:** Maximize $\mathcal{Q}(\theta,\theta_t)$ w.r.t. θ to obtain

$$\theta_{t+1} = \arg\max_{\theta} \mathcal{Q}(\theta,\theta_t)$$

Expectation Maximization

Under very weak conditions it can be shown that the EM algorithm converges to a saddle point of the log-likelihood θ^*

Sufficient conditions for θ^* to be a local maximum exist, but are not easy to verify in practice

The saddle point will depend on the initial set of parameters

The choice of a good starting point is important for the estimation of good models

It is sometimes useful to apply several times the EM algorithm with different starting points

Gaussian Mixture Models

Let's apply the algorithm to the GMM

We have a set of n hidden variables $h = (C_1 \dots C_N)$ that represent the cluster assignments, i.e. the assignment of each sample to a component of the GMM

The GMM specifies the joint likelihood for samples and cluster assignments. For a single sample:

$$f_{X_i,C_i}(\boldsymbol{x}_i, c) = w_c \mathcal{N}(\boldsymbol{x}_i | \mu_c, \boldsymbol{\Sigma}_c)$$

The cluster R.V. C_i has a Categorical prior distribution

$$P(C_i = c) = w_c$$

whereas the sample conditional likelihood is

$$f_{X_i|C_i}(\boldsymbol{x}_i | c) = \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

Gaussian Mixture Models

We assume that samples are independent given the model parameters, so that we can express the log-likelihood for all the training set samples as

$$\log f_{\boldsymbol{X}_1 \ldots \boldsymbol{X}_N, C_1 \ldots C_N}(\boldsymbol{x}_1 \ldots \boldsymbol{x}_N, c_1 \ldots c_N | \boldsymbol{\theta}) = \sum_{i=1}^{N} \log f_{\boldsymbol{X}_i, C_i}(\boldsymbol{x}_i, c_i | \boldsymbol{\theta})$$

The EM algorithm requires computing the posterior for the hidden variables $C_1 \ldots C_N | \boldsymbol{X}_1 \ldots \boldsymbol{X}_N, \boldsymbol{\theta}$.

Due to the independence assumptions, also the posterior distribution factorizes as

$$f_{C_1 \ldots C_N | \boldsymbol{X}_1 \ldots \boldsymbol{X}_N}(c_1 \ldots c_N | \boldsymbol{x}_1 \ldots \boldsymbol{x}_N, \boldsymbol{\theta}) = \prod_{i=1}^{N} P(C_i = c_i | \boldsymbol{X}_i = \boldsymbol{x}_i, \boldsymbol{\theta})$$

The **E-step** requires computing the auxiliary function

$$\begin{aligned}\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}_t) &= \mathbb{E}_{C_1 \dots C_N | \boldsymbol{X}_1 = \boldsymbol{x}_1 \dots \boldsymbol{X}_N = \boldsymbol{x}_N, \boldsymbol{\theta}_t} \left[\log f_{\boldsymbol{X}_1 \dots \boldsymbol{X}_N, C_1 \dots C_N}(\boldsymbol{x}_1 \dots \boldsymbol{x}_N, c_1 \dots c_N | \boldsymbol{\theta}) \right] \\ &= \sum_{i=1}^{N} \mathbb{E}_{C_1 \dots C_N | \boldsymbol{X}_1 = \boldsymbol{x}_1 \dots \boldsymbol{X}_N = \boldsymbol{x}_N, \boldsymbol{\theta}_t} \left[\log f_{\boldsymbol{X}_i, C_i}(\boldsymbol{x}_i, c | \boldsymbol{\theta}) \right] \\ &= \sum_{i=1}^{N} \mathbb{E}_{C_i | \boldsymbol{X}_i = \boldsymbol{x}_i, \boldsymbol{\theta}_t} \left[\log f_{\boldsymbol{X}_i, C_i}(\boldsymbol{x}_i, c | \boldsymbol{\theta}) \right]\end{aligned}$$

The EM algorithm becomes:

E-step: Compute $\gamma_{c,i} = P(C_i = c|X_i = \boldsymbol{x}_i, \boldsymbol{\theta}^t)$. The auxiliary function is

$$\begin{aligned}
\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}_t) = & \sum_{i=1}^{N}\sum_{c=1}^{K} P(C_i = c|\boldsymbol{X}_i = \boldsymbol{x}_i, \boldsymbol{\theta}_t) \log f_{\boldsymbol{X}_i, C_i}(\boldsymbol{x}_i, c|\boldsymbol{\theta}) \\
= & \sum_{i=1}^{N}\sum_{c=1}^{K} \gamma_{c,i} \left[\log \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) + \gamma_{c,i} \log w_c\right] \\
= & \sum_{i=1}^{N}\sum_{c=1}^{K} \gamma_{c,i} \left(\frac{1}{2}\log|\boldsymbol{\Lambda}_c| - \frac{1}{2}(\boldsymbol{x}_i - \boldsymbol{\mu}_c)^T \boldsymbol{\Lambda}_c (\boldsymbol{x}_i - \boldsymbol{\mu}_c)\right) \\
& + \sum_{i=1}^{N}\sum_{c=1}^{K} \gamma_{c,i} \log w_c
\end{aligned}$$

The EM algorithm becomes:

M-step: Maximize $\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}_t)$ w.r.t. $\boldsymbol{\theta} = (\boldsymbol{M}, \boldsymbol{\mathcal{S}}, \boldsymbol{w})$, subject to $\sum_{k=1}^{K} w_k = 1$:

$$\boldsymbol{\mu}_c^* = \frac{\sum_i \gamma_{c,i} \boldsymbol{x}_i}{\sum_i \gamma_{c,i}}$$

$$\boldsymbol{\Sigma}_c^* = \frac{\sum_i \gamma_{c,i} (\boldsymbol{x}_i - \boldsymbol{\mu}_c)(\boldsymbol{x}_i - \boldsymbol{\mu}_c)^T}{\sum_i \gamma_{c,i}}$$

$$w_c^* = \frac{\sum_i \gamma_{c,i}}{\sum_i \sum_c \gamma_{c,i}}$$

The new estimate of the parameters is $\theta_{t+1} = (\boldsymbol{M}_{t+1}, \boldsymbol{\mathcal{S}}_{t+1}, w_{t+1})$:

$$\boldsymbol{M}_{t+1} = [\boldsymbol{\mu}_1^* \dots \boldsymbol{\mu}_K^*] \ , \quad \boldsymbol{\mathcal{S}}_{t+1} = [\boldsymbol{\Sigma}_1^* \dots \boldsymbol{\Sigma}_K^*] \ , \quad \boldsymbol{w}_{t+1} = [w_1^* \dots w_K^*]$$

Gaussian Mixture Models for classification

Just as we used Gaussian densities for modeling the samples of different classes in a classification task, we can use GMM to model the class conditional distribution

We can, for example, assume that the samples of class c are generated by a GMM with parameters $(\boldsymbol{M}_c, \boldsymbol{S}_c, \boldsymbol{w}_c)$

For each class we want to recognize, we can compute the ML estimate of a GMM for the samples of that class. We can then use the estimated densities to compute class conditional log-likelihoods and class posterior distributions or log-likelihood ratios

Gaussian Mixture Models for classification

MVG for classification:

- Fit a guassian density to samples of each class

$$X_i|C_i = c \sim \mathcal{N}(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$
$$f_{X_t|C_t}(\boldsymbol{x}_t|c) = \mathcal{N}(\boldsymbol{x}_t|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$
$$P(C_t = c|\boldsymbol{X}_t = \boldsymbol{x}_t) = \frac{\mathcal{N}(\boldsymbol{x}_t|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)P(C_t = c)}{\sum_c' \mathcal{N}(\boldsymbol{x}_t|\boldsymbol{\mu}_{c'}, \boldsymbol{\Sigma}_{c'})P(C_i = c')}$$

Gaussian Mixture Models for classification

GMM for classification:

- Choose the number of components for each class K_c
- Fit a GMM with K_c compoennts to samples of each class

$$X_i|C_i = c \sim GMM(\boldsymbol{M}_c, \boldsymbol{\mathcal{S}}_c, \boldsymbol{w}_c)$$

$$f_{\boldsymbol{X}_t|C_t}(\boldsymbol{x}_t|c) = \sum_{k=1}^{K_c} w_k \mathcal{N}(\boldsymbol{x}_t|\boldsymbol{\mu}_{c,k}, \boldsymbol{\Sigma}_{c,k})$$

$$P(C_t = c|\boldsymbol{X}_t = \boldsymbol{x}_t) = \frac{P(C_t = c)\sum_{k=1}^{K_c} w_{c,k}\mathcal{N}(\boldsymbol{x}_t|\boldsymbol{\mu}_{c,k}, \boldsymbol{\Sigma}_{c,k})}{\sum_{c'} P(C_t = c')\sum_{k=1}^{K'_c} w_{c',k}\mathcal{N}(\boldsymbol{x}_t|\boldsymbol{\mu}_{c',k}, \boldsymbol{\Sigma}_{c',k})}$$

Gaussian Mixture Models for classification

We can also exploit GMMs clustering capabilities for open-set multiclass classification

The difficulty in open-set classification consists in building a robust model for the none-of-the-others class

This class is usually very heterogeneous, and explicit modeling its sub-components requires labeled examples of its possible objects

We can partially alleviate the issue using a GMM.

Gaussian Mixture Models for classification

We can assume that samples of known classes can be modeled by MVG distributions

We can collect a large set of unlabeled samples for the none-of-the-others class

We can model the samples of the none-of-the-others class using a GMM

The GMM will find homogeneous clusters (sub-classes) of the none-of-the-others population, and can be used as an estimate for the conditional density of a test sample assuming that it belongs to the none-of-the-others class[4]

[4] Given the complexity of the task, and due to the fact that different amounts of parameters are used for modeling the none-of-the-others class these kind of models often provide class-conditional likelihoods that are not calibrated, and may require further score processing (e.g. score calibration) to obtain good decisions

Gaussian Mixture Models

As we did for MVG, we can train GMM with diagonal covariance matrices to reduce the number of parameters to estimate (reducing overfitting and computational costs).

The solution is again given by the diagonals of Σ_c^*'s we defined before

We may need more components to model more complex distributions

The diagonal covariance assumption DOES NOT correspond to the Naive Bayes assumption in this case

The Naive Bayes assumption would correspond to training a different GMM (possibly with different number of components) for each subset of features that is assumed independent from the other features

Gaussian Mixture Models for classification

We can also assume that all components of a GMM have the same covariance matrix (tied GMM)

Note that in this case we are tying the components of a single GMM, i.e. the Gaussian components of the GMM of a single class

This is different from the Tied Gaussian model, where parameters were shared across classes

Of course, we can extend GMM parameters tying across classes as well — we won't consider this model though, as it would require revisiting the EM estimation procedure, since sharing the parameters across classes would not allow us to independently estimate a GMM over the samples of each class

Gaussian Mixture Models for classification

MNIST — GMM (PCA 50)

Components:	1	2	4	8	16
FullCov	3.6%	3.4%	2.8%	2.3%	2.2%
Diagonal	12.3%	10.1%	8.9%	7.6%	6.2%

Components:	32	64	128	256
FullCov	2.3%			
Diagonal	5.1%	4.3%	4.3%	4.3%

Gaussian Mixture Models

Initialization plays an important role in GMM training

Hard-assignment with isotropic covariances $\longrightarrow$ K-means

K-means can be used as initializer

Alternative approach: LBG (can also be used for K-means)

LBG algorithm:

- Split the components of a G-components GMM

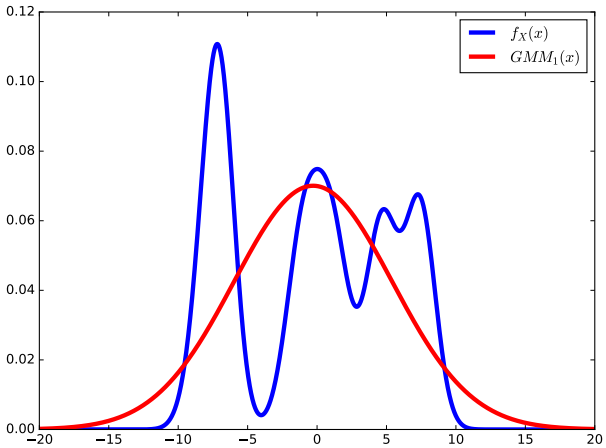
$$\boldsymbol{\mu}_c^+ = \boldsymbol{\mu}_c + \boldsymbol{\varepsilon}$$
$$\boldsymbol{\mu}_c^- = \boldsymbol{\mu}_c - \boldsymbol{\varepsilon}$$

  to obtain an initial $2G$-components GMM

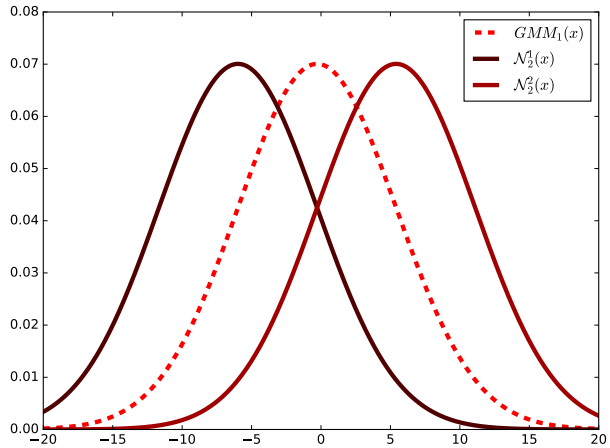
- Run the EM algorithm until convergence for the $2G$-components GMM
- Iterate until the desired number of Gaussians is reached

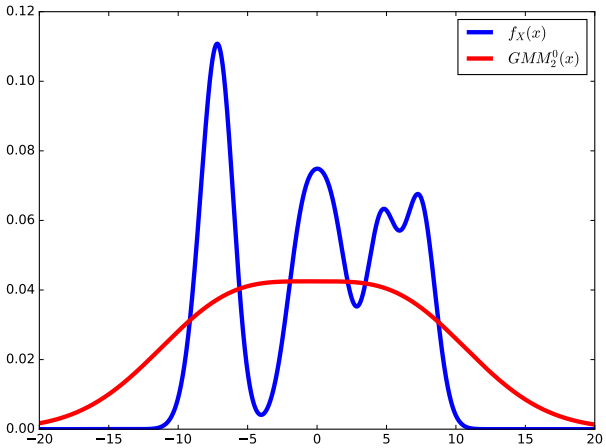
A good value for $\boldsymbol{\varepsilon}$ can be a displacement along the principal eigenvector of the covariance matrix $\boldsymbol{\Sigma}_c$

Gaussian Mixture Models



Split





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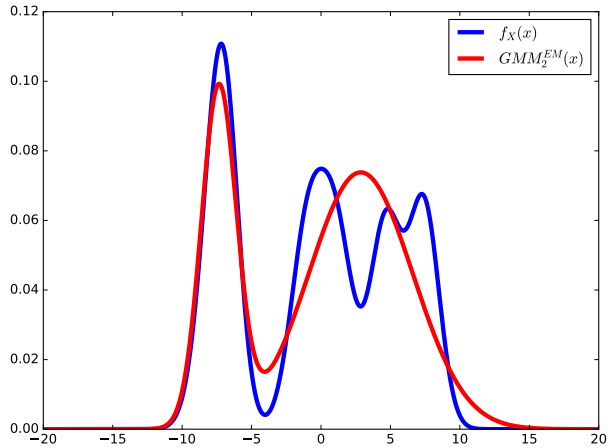
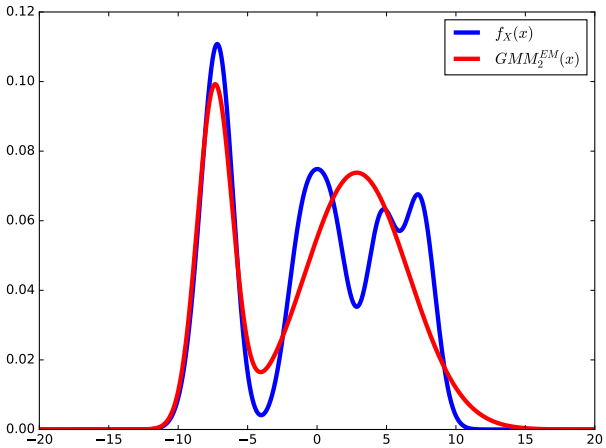


Gaussian Mixture Models



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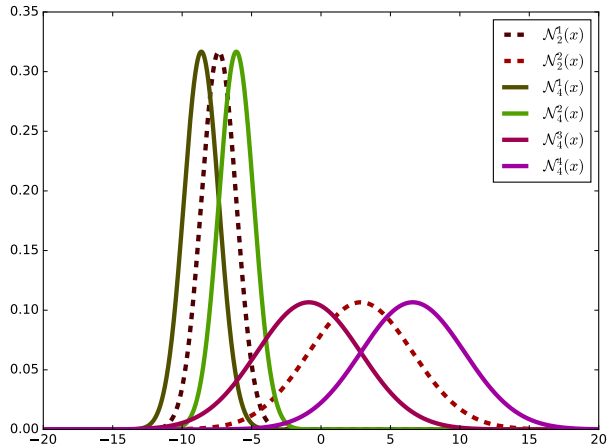

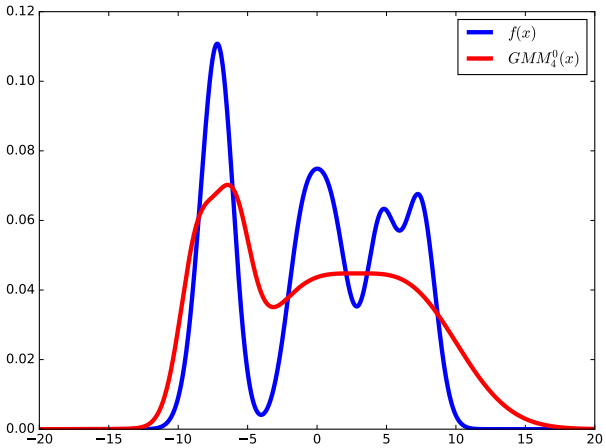

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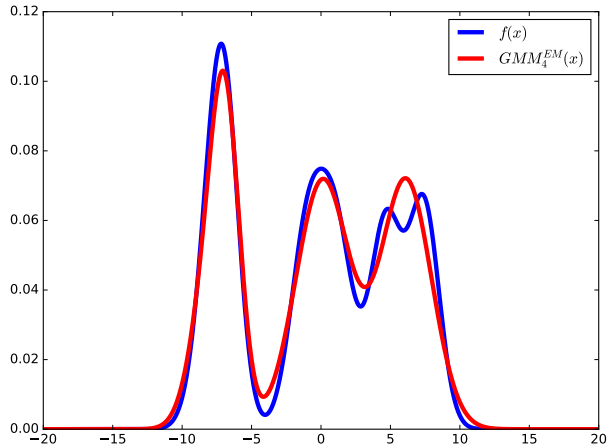

Gaussian Mixture Models

Problem: what is the “right” number of Gaussians?

If we increase the number of components, the likelihood will increase

We cannot choose based on likelihood alone

Several criteria, more or less successful, have been proposed (AIC, BIC)

We can also resort to cross-validation

Gaussian Mixture Models

We also need to pay attention to degenerate models

As we said at the beginning, the log-likelihood for a GMM, as long as we have at least two components, is unbounded

The EM algorithm will usually find local maxima that are well-behaved, however, especially if we have too many components, we may obtain degenerate models which cause numerical issues

Some heuristics can be used to force models to be well-behaved (e.g. impose minimum values for the eigenvalues of the covariance matrices, tie the covariance of different components)

We can also modify our initialization so that the algorithm may end up in a different local maximum