Sampling from mixtures with negative weights: application to density approximation by Gaussian processes

Luca Martino*
* Università di Catania, Italy.
email: luca.martino@unict.it

Abstract

Mixtures of probability densities are widely used in statistics and machine learning. While classical mixtures restrict weights to be non-negative, allowing negative weights enables more flexible density approximation. However, negative weights introduce challenges in handling and sampling such distributions. For this purpose, we propose efficient Monte Carlo (MC) methods (including MC quadratures, rejection sampling and importance sampling schemes) for computing integrals and generating samples from these mixtures. A tailored proposal density ensures accurate and efficient generation of (unweighted) samples. Applications in Gaussian process-based density estimation demonstrate the practical relevance and efficiency of proposed schemes.

Keywords: Non-convex mixtures, mixtures with negative weights, Gaussian processes, rejection sampling, importance sampling

1. Introduction

Mixtures of probability densities are fundamental tools in statistics, signal processing, and machine learning [2]. A mixture model represents a probability distribution as a convex combination of simpler component distributions, such as Gaussians, exponentials, or Gamma distributions, to name a few. Mixture models provide a powerful and flexible framework for modeling complex data [4, 15, 16].
While classical mixture models restrict weights to be non-negative, allowing negative weights opens new theoretical and practical possibilities. When

weights can be negative, the resulting function may no longer be a proper probability density. In this work, we focus on the case where the mixture remains positive and proper. Mixtures with negative components are also referred to as non-convex or pseudo-convex mixtures [1, 6, 5]. In statistics and machine learning, mixtures with negative weights can be particularly useful for density approximation [10, 12, 25]. For example, Gaussian process (GP) regressors, often used for density estimation, can lead to expansions with both positive and negative coefficients [12, 17, 18, 19]. In this context, negative weights can enable better approximation of sharp features, heavy tails, and periodic behaviorspatterns that may be difficult to capture with strictly non-negative mixtures. However, negative weights also introduce significant challenges. The resulting function may not always be a proper density, and classical sampling methods cannot be directly applied [7, 14, 21].
In this work, we describe several Monte Carlo quadrature and sampling methods for mixtures with (possibly) negative coefficients (Mix-NCs). First, we focus on the efficient computation of integrals involving non-convex mixtures. Second, we propose an efficient proposal density to be used within rejection sampling (RS) and/or importance sampling with resampling (IS+R) schemes. In both cases, we obtain (unweighted) samples (exactly in RS, or asymptotically in IS+R) that are distributed according to the target mixture with negative weights. The proposal density introduced here ensures good performance in both RS and IS schemes, as it is itself a "piece" of the target density. We also describe in detail the application of these methods to GP-based density approximation. Theoretical discussions are also provided. Numerical simulations demonstrate the efficiency and accuracy of the proposed techniques.

2. Framework and main notation

Let consider a finite mixture of densities, $\phi_n(\mathbf{x})$, with potentially negative associated weights, i.e.,

$$\bar{p}(\mathbf{x}) \propto p(\mathbf{x}) = \sum_{n=1}^{N} \alpha_n \phi_n(\mathbf{x}), \tag{1}$$

$$= p_+(\mathbf{x}) + p_-(\mathbf{x}), \tag{2}$$

$$= \sum_{i=1}^{M} \alpha_i^+ \phi_i(\mathbf{x}) + \sum_{k=1}^{N-M} \alpha_k^- \phi_k(\mathbf{x}) \geq 0, \qquad \forall \mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^{d_X}, \tag{3}$$

where $\alpha_i^+ > 0$ and $\alpha_i^- < 0$. We have also set $p_+(\mathbf{x}) = \sum_{i=1}^{M} \alpha_i^+ \phi_i(\mathbf{x}) \geq 0$ and $p_-(\mathbf{x}) = \sum_{k=1}^{N-M} \alpha_k^- \phi_k(\mathbf{x}) \leq 0$. Clearly, we have

$$\alpha_1 = \alpha_1^+ > 0, ..., \alpha_M = \alpha_M^+ > 0, \quad \alpha_{M+1} = \alpha_1^- < 0, ..., \alpha_N = \alpha_{N-M}^- < 0.$$

Without loss of generality, we are assuming that the components are ordered: the first M components are associated to positive weights, α_i^+, and the rest of $N-M$ components have assigned to the negative weights, α_i^-. Additional assumptions are:

- $\phi_n(\mathbf{x}) \geq 0$ and $\int_{\mathcal{X}} \phi_n(\mathbf{x}) d\mathbf{x} = 1$, for all n.
- We can evaluate and we can draw samples from each component $\phi_n(\mathbf{x})$.

Given the assumptions above, and since we consider a proper/normalized mixture density, i.e.,$\bar{p}(\mathbf{x}) \geq 0$ and $\int_{\mathcal{X}} \bar{p}(\mathbf{x}) d\mathbf{x} = 1$, we can write

$$\bar{p}(\mathbf{x}) = \frac{p(\mathbf{x})}{\sum_{j=1}^{N} \alpha_j} = \frac{\sum_{n=1}^{N} \alpha_n \phi_n(\mathbf{x})}{\sum_{j=1}^{N} \alpha_j} = \sum_{n=1}^{N} \bar{\alpha}_n \phi_n(\mathbf{x}), \tag{4}$$

where we have defined

$$\bar{\alpha}_n = \frac{\alpha_n}{\sum_{j=1}^{N} \alpha_j}, \qquad n = 1, ..., N. \tag{5}$$

Note that:

- $\sum_{n=1}^{N} \bar{\alpha}_n = 1$ (since $\int_{\mathcal{X}} \bar{p}(\mathbf{x}) d\mathbf{x} = 1$ and $\int_{\mathcal{X}} \phi_n(\mathbf{x}) d\mathbf{x} = 1$ for all n),
- even if we have $\bar{\alpha}_n > 0$ for $n = 1, ..., M$,
- and $\bar{\alpha}_n < 0$ for $n = M+1, ..., N$.

Hence, Eq. (4) is *not* a convex combination of $\phi_n(\mathbf{x})$. Thus, we also have the condition $\sum_{i=1}^{M} \alpha_i^+ > \sum_{k=1}^{N-M} \alpha_k^-$, since we need $\sum_{n=1}^{N} \alpha_n > 0$ to have $p(\mathbf{x}) \geq 0$. We can also define the two *partial-mixtures*,

$$\bar{p}_+(\mathbf{x}) = \frac{p_+(\mathbf{x})}{\sum_{i=1}^{M} \alpha_i^+} = \sum_{m=1}^{M} \bar{\alpha}_m^+ \phi_m(\mathbf{x}), \quad \bar{p}_-(\mathbf{x}) = \frac{p_-(\mathbf{x})}{\sum_{i=1}^{N-M} \alpha_i^-} = \sum_{m=1}^{M} \bar{\alpha}_k^- \phi_k(\mathbf{x}), \tag{6}$$

where

$$\bar{\alpha}_m^+ = \frac{\alpha_m^+}{\sum_{i=1}^{M} \alpha_i^+}, \qquad \bar{\alpha}_k^- = \frac{\alpha_k^-}{\sum_{j=1}^{N-M} \alpha_j^-}, \tag{7}$$

Note that:

- $\bar{p}_+(\mathbf{x}) \geq 0$ and $\bar{p}_-(\mathbf{x}) \geq 0$ (despite $\alpha_j^- < 0$ and $p_-(\mathbf{x}) \leq 0$),
- and they are both proper classical mixtures with non-negative weights, i.e., $\bar{\alpha}_m^+ \geq 0$, $\bar{\alpha}_k^- \geq 0$ and $\sum_{m=1}^{M} \bar{\alpha}_m^+ = 1$, $\sum_{k=1}^{N-M} \bar{\alpha}_k^- = 1$ (despite $\alpha_j^- < 0$).

Finally, we can also write the complete mixture $\bar{p}(\mathbf{x})$, in Eq. (4), as function of the partial mixtures $\bar{p}_+(\mathbf{x})$ and $\bar{p}_-(\mathbf{x})$ in Eq. (6), i.e.,

$$\begin{aligned}
\bar{p}(\mathbf{x}) &= \frac{p(\mathbf{x})}{\sum_{j=1}^{N} \alpha_j}, \\
&= \frac{p_+(\mathbf{x})}{\sum_{j=1}^{N} \alpha_j} + \frac{p_-(\mathbf{x})}{\sum_{j=1}^{N} \alpha_j}, \\
&= \frac{\sum_{i=1}^{M} \alpha_i^+}{\sum_{i=1}^{M} \alpha_i^+} \frac{p_+(\mathbf{x})}{\sum_{j=1}^{N} \alpha_j} + \frac{\sum_{i=1}^{N-M} \alpha_i^-}{\sum_{i=1}^{N-M} \alpha_i^-} \frac{p_-(\mathbf{x})}{\sum_{j=1}^{N} \alpha_j}, \\
&= \frac{\sum_{i=1}^{M} \alpha_i^+}{\sum_{j=1}^{N} \alpha_j} \bar{p}_+(\mathbf{x}) + \frac{\sum_{i=1}^{N-M} \alpha_i^-}{\sum_{j=1}^{N} \alpha_j} \bar{p}_-(\mathbf{x}) \\
&= \underbrace{\beta^+}_{>1} \bar{p}_+(\mathbf{x}) + \underbrace{(1-\beta^+)}_{<0} \bar{p}_-(\mathbf{x}),
\end{aligned} \tag{8}$$

where

$$\beta^+ = \frac{\sum_{i=1}^{M} \alpha_i^+}{\sum_{j=1}^{N} \alpha_j} > 1. \tag{9}$$

Therefore, even if the sum of two weights β^+ and $1 - \beta^+$ is one, the linear combination $\beta^+ \bar{p}_+(\mathbf{x}) + (1 - \beta^+)\bar{p}_-(\mathbf{x})$ is not a convex combination.

3. Quadratures for integral approximations involving Mix-NCs

The best procedure for approximating integral involving to a mixture $\bar{p}(\mathbf{x})$ of densities with possibly negative weights (Mix-NCs) is related to a quadrature trick [11, 18]. Indeed, if we are interested to approximate a

generic moment or any integral involving to the distribution $\bar{p}(\mathbf{x})$, i.e.,

$$I_{\bar{p}} = \mathbb{E}_{\bar{p}}[f(\mathbf{x})] = \int_{\mathcal{X}} f(\mathbf{x})\bar{p}(\mathbf{x})d\mathbf{x}, \tag{10}$$

$$= \frac{1}{\sum_{j=1}^{N}\alpha_j}\sum_{n=1}^{N}\alpha_n \int_{\mathcal{X}} f(\mathbf{x})\phi_n(\mathbf{x})d\mathbf{x}, \tag{11}$$

$$= \sum_{n=1}^{N}\bar{\alpha}_n J_n. \tag{12}$$

where $f(\mathbf{x})$ is a generic integrable function. Note that above we have set $J_n = \int_{\mathcal{X}} f(\mathbf{x})\phi_n(\mathbf{x})d\mathbf{x}$ and $\bar{\alpha}_n = \frac{\alpha_n}{\sum_{j=1}^{N}\alpha_j}$. Since we are able to draw from $\phi_n(\mathbf{x})$, we can approximate each J_n by a simple Monte Carlo procedure (i.e., a stochastic quadrature rule) [14],

$$\widehat{J}_n = \frac{1}{S}\sum_{s=1}^{S} f(\mathbf{x}_n^{(s)}), \qquad \mathbf{x}_n^{(s)} \sim \phi_n(\mathbf{x}). \tag{13}$$

Therefore, replacing in the expressions above into $I = \sum_{n=1}^{N}\bar{\alpha}_n J_n$, we obtain the final estimator:

$$\widehat{I}_{\bar{p}} = \sum_{n=1}^{N}\bar{\alpha}_n\widehat{J}_n = \frac{1}{S}\sum_{n=1}^{N}\sum_{s=1}^{S}\bar{\alpha}_n f(\mathbf{x}_n^{(s)}). \tag{14}$$

As $S \to \infty$, we have $\widehat{I}_{\bar{p}} \to I_{\bar{p}}$ [7, 14, 21]. Recall that $\bar{\alpha}_n > 0$ for $n = 1, ..., M$ and $\bar{\alpha}_n < 0$ for $n = M+1, ..., N$.

4. Sample generation from Mix-NCs

In this section, we discuss two sampling schemes: a rejection sampling method and an importance sampling technique. Note that we are able to generate samples from

$$\bar{p}_+(\mathbf{x}) = \frac{p_+(\mathbf{x})}{\sum_{i=1}^{M}\alpha_i^+} = \sum_{m=1}^{M}\bar{\alpha}_m^+\phi_m(\mathbf{x}), \qquad \bar{\alpha}_m^+ = \frac{\alpha_m^+}{\sum_{i=1}^{M}\alpha_i^+}, \tag{15}$$

in a classical way, since $0 \leq \bar{\alpha}_m^+ \leq 1$ and $\sum_{m=1}^{M}\bar{\alpha}_m^+ = 1$. Moreover, by construction,

$$p_+(\mathbf{x}) \geq p(\mathbf{x}), \tag{16}$$

that is the inequality required for applying the RS technique [14, Chapter 3]. Furthermore, $\bar{p}_+(\mathbf{x})$ represents a part (a "piece") of the target density $p(\mathbf{x})$. Namely, a generic proposal density $q(\mathbf{x})$ must satisfy the inequality $q(\mathbf{x}) \geq p(\mathbf{x})$ in order to apply rejection sampling correctly. If this condition is violated, the samples generated by the algorithm are no longer distributed according to the target density $p(\mathbf{x})$, but instead follow $\tilde{p}(\mathbf{x}) \propto \min\{p(\mathbf{x}), q(\mathbf{x})\}$ [14, Chapter 3]. This observation highlights the relevance and ability of constructing proposals that satisfy the bound (16). In particular, the proposed choice $q(\mathbf{x}) = p_+(\mathbf{x})$ automatically fulfills this requirement. Moreover, $p_+(\mathbf{x})$ is typically an efficient proposal within an RS scheme, since it is assembled directly from components of the target density $p(\mathbf{x})$, thereby preserving its main structural features and generally remaining close to it in shape.... L1 distance...

Hence, $\bar{p}_+(\mathbf{x})$ constitutes an appropriate choice of proposal density in Monte Carlo methods, specially in a RS technique. Below we outline the proposed RS scheme.

Rejection sampling (RS) for Mix-NCs:

1. Set $s = 1$.
2. Draw a candidate $\mathbf{z}' \sim \bar{p}_+(\mathbf{x})$,
3. With probability

$$p_A(\mathbf{z}') = \frac{p(\mathbf{z}')}{p_+(\mathbf{z}')}, \tag{17}$$

   set $\mathbf{x}^{(s)} = \mathbf{z}'$ and increase $s \leftarrow s+1$. Otherwise, with prob. $1 - p_A(\mathbf{z}')$ discard $\mathbf{z}'$.
4. if $s \leq S$, repeat from step 2.

Note that $p_A \in [0, 1]$. The algorithm provides exact samples from $\bar{p}(\mathbf{x})$ and its validity is ensured by the inequality (16) [14, Chapter 3]. The acceptance

rate A_r is:

$$A_r = \int_{\mathcal{X}} \frac{p(\mathbf{x})}{p_+(\mathbf{x})} \bar{p}_+(\mathbf{x}) d\mathbf{x} = \frac{1}{\sum_{i=1}^{M} \alpha_i^+} \int_{\mathcal{X}} p(\mathbf{x}) d\mathbf{x}, \tag{18}$$

$$= \frac{\sum_{n=1}^{N} \alpha_n}{\sum_{i=1}^{M} \alpha_i^+}, \tag{19}$$

$$= 1 - \frac{\sum_{k=1}^{N-M} \alpha_k^-}{\sum_{i=1}^{M} \alpha_i^+} = 1 - \rho, \tag{20}$$

where we set $\rho = \frac{\sum_{k=1}^{N-M} \alpha_k^-}{\sum_{i=1}^{M} \alpha_i^+}$. If $\rho \to 0$ then $A_r \to 1$ and we have a perfect sampler [14, 21]. Hence, the acceptance rate A_r is close to 1 is the sum of negative weights is close to zero, or the sum of positive weights is much larger than the sum of negative weights. This is particularly interesting for the Gaussian process application: in a GP approximation of a density, the number of negative weights should tend to disappear as the number of points in the regression grows, and the hyper-parameters are updated and optimized. The corresponding importance sampling (IS) 'plus' resampling scheme is described below.

Importance sampling plus resampling (IS+R) for Mix-NCs:

1. Draw $\mathbf{z}_1, ..., \mathbf{z}_S \sim \bar{p}_+(\mathbf{x})$,
2. Assign the weight

$$w_s = \frac{p(\mathbf{z}_s)}{\bar{p}_+(\mathbf{z}_s)} = \left[\sum_{i=1}^{M} \alpha_i^+ \right] p_A(\mathbf{z}_s), \quad s = 1, ..., S, \tag{21}$$

   where we have used $p_A(\mathbf{z})$ given in Eq. (17).
3. Define the normalized weights

$$\bar{w}_s = \frac{w_s}{\sum_{i=1}^{S} w_i}, \qquad s = 1, ..., S. \tag{22}$$

4. Resample S times within the set $\{\mathbf{z}_1, ..., \mathbf{z}_S\}$ according to the probability mass function defined by the normalized weights $\bar{w}_s$, with $s = 1, ..., S$, obtaining a new set of unweighted samples $\{\mathbf{x}^{(1)}, ..., \mathbf{x}^{(S)}\}$.

Unlike RS, the IS+R does not return exact samples, but provides samples

$\{\mathbf{x}^{(1)}, ..., \mathbf{x}^{(S)}\}$ that are approximately and asymptotically distributed as $\bar{p}(\mathbf{x})$. However, the quality of this approximation improves as S grows [7, 8, 21]. Furthermore, no samples are rejected/discarded as in the RS scheme. It is also important to remark that the weights w_s present good theoretically properties due to the choice of the proposal density. For instance, since $w_s \propto p_A(\mathbf{z}_s)$, the IS weights are bounded

$$w_s \in \left[0, \sum_{i=1}^{M} \alpha_i^+\right], \tag{23}$$

hence their distribution has not heavy tails, and the variance of the weights is always bounded [3, 10, 22, 24]. Standard IS can produce highly variable estimates, especially when weights have heavy right tails [23]. Namely, extreme values of the weights lead to unstable estimates [22, 23] or yield estimators with infinite variance (see numerical experiments in [9]). However, these undesirable scenarios cannot occur in the proposed IS scheme, due to the property in Eq. (23). Recall that the proposal density, described in this work, provides good performance within RS and IS schemes since it is itself a piece of the target density [8].

Histograms. Histograms can be constructed in the usual way using the unweighted samples, that are generated by the RS or by IS+R schemes as well. Alternatively, one can directly use the weighted samples $\{\mathbf{z}_s, w_s\}_{s=1}^{S}$ obtained by the IS procedure. Indeed, in each bin of the histogram, instead of considering the number of samples inside the bin, we can sum the corresponding weights. Namely, let consider the bin $\mathcal{B} \subset \mathcal{X}$. The value of the histogram in the bin must be $\sum_{\mathbf{z}_j \in \mathcal{B}} w_j$, where we sum each w_j with j such that $\mathbf{z}_j \in \mathcal{B}$ (for the underlying theory see [13]). The histogram can be normalized dividing all the values by the complete sum of the weights, i.e., $\sum_{s=1}^{S} w_s$.

5. Mix-NCs as proposal densities within IS methods

In many applications, a good approximation of a distribution is needed. For instance, let us consider a target-posterior distribution $\bar{\pi}(\mathbf{x}) = \frac{1}{Z}\pi(\mathbf{x})$ where $Z = \int_{\mathcal{X}} \pi(\mathbf{x}) d\mathbf{x}$. In order to extract information about the posterior $\bar{\pi}(\mathbf{x})$, often we are interested in computing integrals which generally involve

the product of a generic function f and the posterior $\bar{\pi}$,

$$I_{\bar{\pi}} = \mathbb{E}_{\bar{\pi}}[f(\mathbf{x})] = \int_{\mathcal{X}} f(\mathbf{x})\bar{\pi}(\mathbf{x})d\mathbf{x} = \frac{1}{Z}\int_{\mathcal{X}} f(\mathbf{x})\pi(\mathbf{x})d\mathbf{x}. \tag{24}$$

Note that the expectation above $\mathbb{E}_{\bar{\pi}}[f(\mathbf{x})]$ is different from the expectation $\mathbb{E}_{\bar{p}}[f(\mathbf{x})]$ given in Eq. (10), since in Eq. (24) the density involved is the posterior $\bar{\pi}$ instead of the mixture $\bar{p}$, i.e., $I_{\bar{\pi}} = \int_{\mathcal{X}} f(\mathbf{x})\bar{\pi}(\mathbf{x})d\mathbf{x}$. Note that we can write:

$$\begin{aligned}
I_{\bar{\pi}} = \mathbb{E}_{\bar{\pi}}[f(\mathbf{x})] &= \int_{\mathcal{X}} f(\mathbf{x})\bar{\pi}(\mathbf{x})d\mathbf{x}, && (25)\\
&= \int_{\mathcal{X}} \frac{f(\mathbf{x})\bar{\pi}(\mathbf{x})}{\bar{p}(\mathbf{x})}\bar{p}(\mathbf{x})d\mathbf{x},\\
&= \int_{\mathcal{X}} \frac{f(\mathbf{x})\bar{\pi}(\mathbf{x})}{\bar{p}(\mathbf{x})}\left(\beta^+\bar{p}_+(\mathbf{x}) + (1-\beta^+)\bar{p}_-(\mathbf{x})\right)d\mathbf{x},\\
&= \beta^+\int_{\mathcal{X}} \frac{f(\mathbf{x})\bar{\pi}(\mathbf{x})}{\bar{p}(\mathbf{x})}\bar{p}_+(\mathbf{x})d\mathbf{x} + (1-\beta^+)\int_{\mathcal{X}} \frac{f(\mathbf{x})\bar{\pi}(\mathbf{x})}{\bar{p}(\mathbf{x})}\bar{p}_-(\mathbf{x})d\mathbf{x},\\
&= \beta^+\mathbb{E}_{\bar{p}_+}[f(\mathbf{x})\bar{\pi}(\mathbf{x})] + (1-\beta^+)\mathbb{E}_{\bar{p}_-}[f(\mathbf{x})\bar{\pi}(\mathbf{x})], && (26)\\
&= \frac{\beta^+}{Z}\mathbb{E}_{\bar{p}_+}[f(\mathbf{x})\pi(\mathbf{x})] + \frac{1-\beta^+}{Z}\mathbb{E}_{\bar{p}_-}[f(\mathbf{x})\pi(\mathbf{x})], && (27)
\end{aligned}$$

The expression (26) induces the design of an importance sampling scheme with positive and negative IS weights. The idea is to apply the MC approach to approximate the expectations $\mathbb{E}_{\bar{p}_+}[f(\mathbf{x})\pi(\mathbf{x})]$ and $\mathbb{E}_{\bar{p}_-}[f(\mathbf{x})\pi(\mathbf{x})]$, as shown below.

Importance sampling with an Mix-NCs as proposal density:

1. Draw S samples from $\bar{p}_+(\mathbf{x})$ and S samples from $\bar{p}_-(\mathbf{x})$, i.e.,

$$\mathbf{x}_s^+ \sim \bar{p}_+(\mathbf{x}), \qquad \mathbf{x}_s^- \sim \bar{p}_-(\mathbf{x}), \qquad s = 1, ..., S. \tag{28}$$

2. To each sample, assign the weights

$$w_s^+ = \beta^+ \frac{\pi(\mathbf{x}_s^+)}{\bar{p}(\mathbf{x}_s^+)} \geq 0, \qquad w_s^- = (1-\beta^+) \frac{\pi(\mathbf{x}_s^-)}{\bar{p}(\mathbf{x}_s^-)} \leq 0, \tag{29}$$

   with $s = 1, ..., S$. Note that, both denominators of weights in Eq. (29) contain the complete mixture $\bar{p}(\mathbf{x})$.

3. **If Z is known**, the resulting estimator is given by the formula:

$$\widehat{I}_{\bar{\pi}} = \frac{1}{SZ} \left(\sum_{j=1}^{S} w_j^+ f(\mathbf{x}_j^+) + \sum_{j=1}^{S} w_j^- f(\mathbf{x}_j^-) \right). \tag{30}$$

4. **If Z is unknown**, estimate and replace Z above with:

$$\widehat{Z} = \frac{1}{S} \left(\sum_{j=1}^{S} w_j^+ + \sum_{j=1}^{S} w_j^- \right). \tag{31}$$

The estimator in Eq. (31) is based on the following equality:

$$\begin{aligned} Z &= \beta^+ \int_{\mathcal{X}} \frac{\pi(\mathbf{x})}{\bar{p}(\mathbf{x})} \bar{p}_+(\mathbf{x}) d\mathbf{x} + (1-\beta^+) \int_{\mathcal{X}} \frac{\pi(\mathbf{x})}{\bar{p}(\mathbf{x})} \bar{p}_-(\mathbf{x}) d\mathbf{x}, \\ &= \beta^+ \mathbb{E}_{\bar{p}_+}[\pi(\mathbf{x})] + (1-\beta^+) \mathbb{E}_{\bar{p}_-}[\pi(\mathbf{x})]. \end{aligned} \tag{32}$$

Note that the samples $\mathbf{x}_s^-$ generated from $\bar{p}_-(\mathbf{x})$ have associated negative weights w_s^-.

6. Applications to GP approximation of a density - emulators

In some adaptive Monte Carlo scheme, the key idea is the construction (via regression) of a non-parametric density (a.k.a., emulator/surrogate model), which mimics a posterior distribution [10, 12]. More precisely, let us consider again a target-posterior distribution $\bar{\pi}(\mathbf{x}) \propto \pi(\mathbf{x})$. Related to this target density, we have a (possibly noisy) set of points $\{\mathbf{x}_n, t_n\}$ with

$n = 1, ..., N$, where $t_n = \pi(\mathbf{x}_n)$ or $t_n = \pi(\mathbf{x}_n) + \epsilon_n$ (where ϵ_n is a noise perturbation) but always we have $t_n \geq 0$ [10, 12].
Let us assume to apply a GP regression method [20]. We consider a (proper) kernel function $k(\mathbf{x}, \mathbf{z}) : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, then we can define a $N \times N$ kernel matrix $\mathbf{K}$ where each entry is $[\mathbf{K}]_{ij} := k(\mathbf{x}_i, \mathbf{x}_j)$, and a $N \times 1$ kernel vector $\mathbf{k}(\mathbf{x}) = [k(\mathbf{x}, \mathbf{x}_1), ..., k(\mathbf{x}, \mathbf{x}_N)]^\top$. For simplicity, we assume Gaussian kernels,

$$k(\mathbf{x}, \mathbf{z}) = \left(\frac{1}{2\pi\lambda^2}\right)^{\frac{d_X}{2}} \exp\left(-\frac{||\mathbf{x} - \mathbf{z}||^2}{2\lambda^2}\right), \quad \lambda > 0. \tag{33}$$

Defining also the vector $\mathbf{t} = [t_1, ..., t_J]^\top$, the density approximation is given by the formulas:

$$\bar{p}(\mathbf{x}) \propto p(\mathbf{x}) = \mathbf{k}(\mathbf{x})^\top (\mathbf{K} + \eta \mathbf{I}_J)^{-1} \mathbf{t}, \tag{34}$$

$$= \mathbf{k}(\mathbf{x})^\top \boldsymbol{\alpha}, \tag{35}$$

$$= \sum_{n=1}^{N} \alpha_n k(\mathbf{x}, \mathbf{x}_n), \qquad \eta \geq 0, \tag{36}$$

where $\boldsymbol{\alpha} = [\alpha_1, ..., \alpha_N]^\top$ is defined as

$$\boldsymbol{\alpha} = (\mathbf{K} + \eta \mathbf{I}_J)^{-1} \mathbf{t}. \tag{37}$$

Note that $p(\mathbf{x})$ is a mixture of Gaussian kernels ($k(\mathbf{x}, \mathbf{x}_n)$ plays the role of $\phi_n(\mathbf{x})$) and, generally, the coefficients α_n's can be positive or negative.
We can assume of choosing a vector of hyper-parameters $[\lambda, \eta]$ such that $p(\mathbf{x}) \geq 0$, for all $\mathbf{x} \in \mathcal{X}$. It is always possible to find such hyper-parameters. For instance, decreasing the value of λ helps to obtain $p(\mathbf{x}) \geq 0$ for all $\mathbf{x}$. This assumption can be avoided just defining $\widetilde{p}(\mathbf{x}) = \max[p(\mathbf{x}), 0]$. However, this issue tends to disappear as N grows and the hyper-parameters are optimized. if a suitable optimization criterion is employed for updating the hyper - parameters $[\lambda, \eta]$ (as the classical marginal likelihood optimization [9, 20]), the number of negative values of α_n's should decrease as the number N of acquired data, $\{\mathbf{x}_n, t_n\}_{n=1}^N$, grows. However, for a finite N, we can have negative values of α_n. Since the emulator $\bar{p}(\mathbf{x}) \propto p(\mathbf{x})$ is often used as proposal density in a sophisticated sampling schemes, we need to be able to draw from it. The RS and IS+R schemes proposed here can be employed for this purpose.

7. Numerical Simulations

Let us consider the multi-modal target density

$$\bar{\pi}(x) \propto \pi(x) = \sin(x)^2 \exp\left(-\frac{x^2}{30}\right),$$

that is shown in solid line in Figure 1(a). We consider two scenarios.[1]

Scenario 1: We consider $N = 9$ points in the regression, more precisely,

$$x_i \in \{-5, -4, -1, 0, 0.5, 1, 2, 5, 10\}, \tag{38}$$

and $t_i = \pi(x_i)$. We apply the GP regressor with Gaussian kernel and hyper-parameters $\lambda = 1$, $\eta = 0$. In this case, we obtain 6 positive coefficients and 3 negative coefficients in the vector $\boldsymbol{\alpha}$. The 3 negative coefficients are associated to the kernels localized at $x_i = 0, 0.5$ and 2. Applying the proposed RS scheme, the histogram of the accepted samples is given in Figure 1(d). The acceptance rate $A_r = 1 - \rho = 0.417$. The unnormalized densities $p(x)$, $p_+(x)$ and the corresponding versions are also shown in Figure 1.

Scenario 2: Now, we consider $N = 11$ points in the regression,

$$x_i \in \{-8, -5, -4, -1.2, -0.8, 0.5, 1, 2, 5, 8, 10\}, \tag{39}$$

and again $t_i = \pi(x_i)$. We apply the GP regressor with Gaussian kernel and hyper-parameters $\lambda = 0, 5$, $\eta = 0$. In this case, we have a unique negative coefficient, α_6, corresponding to $x_6 = 0.5$. The acceptance rate $A_r = 1 - \rho = 0.974$, that is sensibly greater than in scenario 1. However, in both scenarios, we obtain more than reasonable acceptance rates, due to the suitable choice of the proposal density.

8. Conclusions

In this work, we focused on mixtures with negative coefficients. These generalized mixture models enable more flexible and accurate density approximations, though they introduce challenges for handling and sampling such

[1]Related Matlab code is given at `http://www.lucamartino.altervista.org/public_code_NegMix2025.zip`.

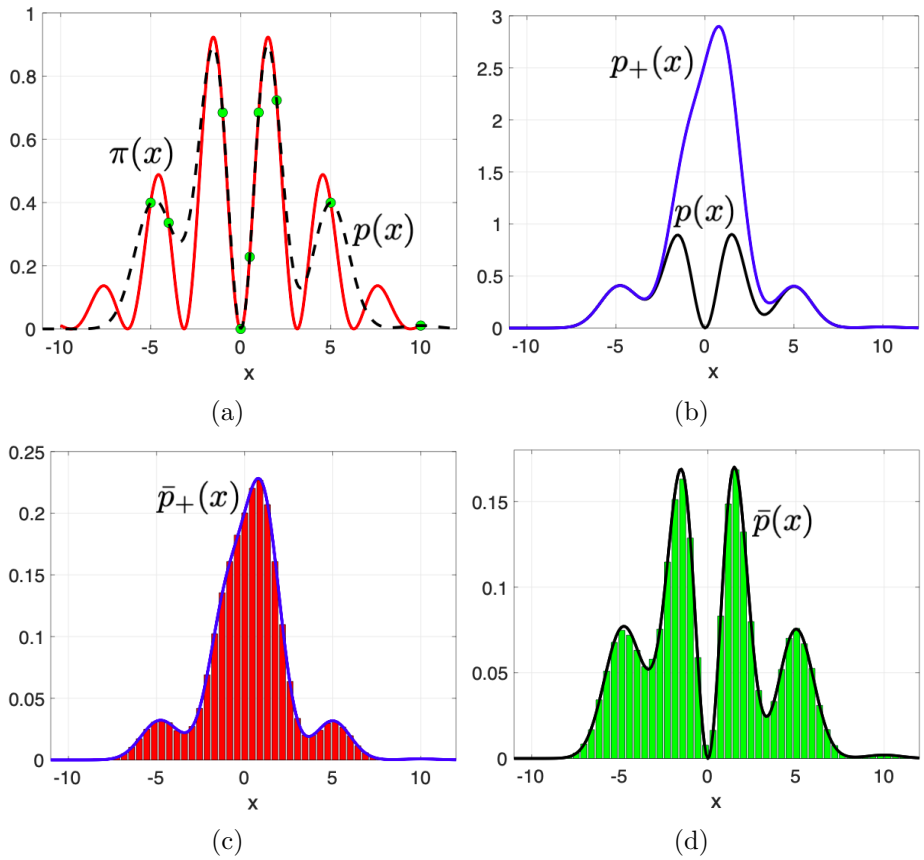
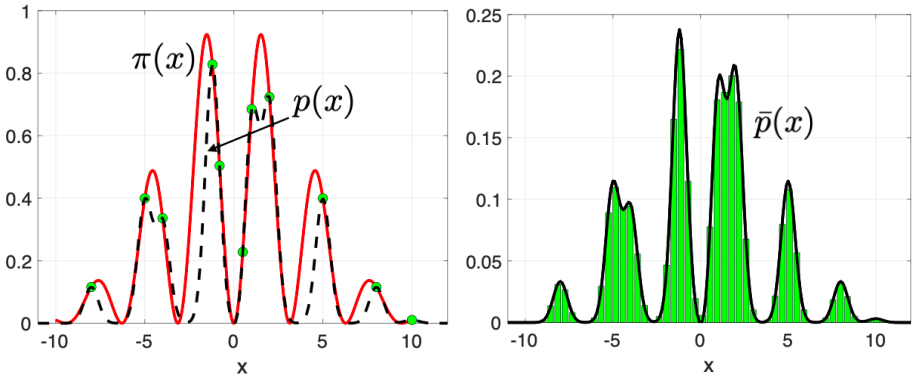


Figure 1: **Scenario 1:** $N = 9$ input points $x_i \in \{-5, -4, -1, 0, 0.5, 1, 2, 5, 10\}$ in regression; in this scenario, with $\lambda = 1$, $\eta = 0$, we have 6 positive coefficients and 3 negative coefficients in $\boldsymbol{\alpha}$. The 3 negative coefficients are associated to the kernels localized at $x_i = 0,\ 0.5$ and 2. the theoretical acceptance rate is $A_r = 1 - \rho = 0.417$, and the empirical acceptance rate is ≈ 0.416, in line with the theoretical expression. This means that drawing 20000 samples from $\bar{p}_+(x)$, in one run we obtain $S = 8326$ samples from $\bar{p}(x)$. The corresponding histogram is depicted in figure (d).

distributions. To address these challenges, we proposed efficient Monte Carlo methods (including quadrature techniques, rejection sampling, and importance sampling schemes) capable of accurately approximating integrals and generating (unweighted) samples from these non-convex mixtures. The use of a tailored proposal density ensures both accuracy and efficiency. Applications to Gaussian processbased density estimation illustrate the practical relevance and effectiveness of the proposed methods, highlighting their po-



(a) (b)

Figure 2: **Scenario 2:** we have $N = 11$ input points, $x_i \in \{-8, -5, -4, -1.2, -0.8, 0.5, 1, 2, 5, 8, 10\}$ in regression; in this scenario, with $\lambda = 0.6$, $\eta = 0$, we have only one negative coefficient in $\boldsymbol{\alpha}$. the theoretical acceptance rate $A_r = 1 - \rho = 0.974$ which is virtually identical with the empirical acceptance rate obtained, i.e., ≈ 0.974. This means that drawing 20000 samples from $\bar{p}_+(x)$, in one run we obtain $S = 19481$ samples from $\bar{p}(x)$. The corresponding histogram is depicted in figure (b).

tential for broader use in complex density modeling tasks.

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Author Contribution declaration

Luca Martino is the single author of this work.

Data availability and related code

The datasets generated and analyzed during the current study are available (jointly with the related Matlab code) at `http://www.lucamartino.altervista.org/public_code_NegMix2025.zip`.

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