Density Estimation with Autoregressive Bayesian Predictives

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Abstract

Bayesian methods are a popular choice for statistical inference in small-data regimes due to the regularization effect induced by the prior, which serves to counteract overfitting. In the context of density estimation, the standard Bayesian approach is to target the posterior predictive. In general, direct estimation of the posterior predictive is intractable and so methods typically resort to approximating the posterior distribution as an intermediate step. The recent development of recursive predictive copula updates, however, has made it possible to perform tractable predictive density estimation without the need for posterior approximation. Although these estimators are computationally appealing, they tend to struggle on non-smooth data distributions. This is largely due to the comparatively restrictive form of the likelihood models from which the proposed copula updates were derived. To address this shortcoming, we consider a Bayesian nonparametric model with an autoregressive likelihood decomposition and Gaussian process prior, which yields a data-dependent bandwidth parameter in the copula update. Further, we formulate a novel parameterization of the bandwidth using an autoregressive neural network that maps the data into a latent space, and is thus able to capture more complex dependencies in the data. Our extensions increase the modelling capacity of existing recursive Bayesian density estimators, achieving state-of-the-art results on tabular data sets.

1 Introduction

Modelling the joint distribution of multivariate random variables with density estimators is a central topic in modern unsupervised machine learning research [13, 35, 43]. As well as providing insight into the statistical properties of the data, density estimates are used in a number of downstream applications, including image restoration [56], density-based clustering [40], and simulation-based inference [38]. In small-data regimes, Bayesian methods are a popular choice for a wide range of machine learning tasks, including density estimation, thanks to their attractive generalization capacities. Nonparametric methods, such as the

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Dirichlet Process Mixture Model (DPMM) \cite{15}, are particularly appealing due to their flexibility. For density estimation, the typical Bayesian approach is to target the Bayesian predictive density, $p_n(x) = \int f(x|\theta)\pi_n(\theta)d\theta$, where $\pi_n$ denotes the posterior density of the model parameters $\theta$ after observing $x_1, \ldots, x_n$, and $f$ denotes the sampling distribution.

De Finetti's representation theorem \cite{10, 27} states that an exchangeable joint density fully characterises a Bayesian model, which then implies a sequence of predictive densities. Furthermore, Fong et al. \cite{17} recently showed that a sequence of predictive densities, under some assumptions, is sufficient for carrying out full Bayesian posterior inference. The above provides theoretical motivation for an iterative approach to Bayesian predictive density estimation by updating the predictive $p_{i-1}(x)$ to $p_i(x)$ given an observation $x_i$ for $i = 1, \ldots, n$.

The idea of recursive Bayesian updates goes back to at least Hill \cite{28}, but was only recently made more widely applicable through the relaxation of the assumption of exchangeability in favour of conditionally identically distributed \cite{5} sequences. Here, we focus on a particular class of one-step-ahead predictive updates $p_{i-1}(x) \rightarrow p_i(x)$ based on bivariate copulas. These copula updates do not correspond exactly, nor approximately, to a traditional Bayesian likelihood-prior model, and can instead be viewed as a separate class of predictive models. Importantly, this class retains many desirable Bayesian properties, such as coherence and regularization, and moreover are fully tractable. The copula characterization of the update step was introduced by Hahn et al. \cite{25} for univariate data, and extended by Fong et al. \cite{17} to the multivariate setting and to regression analyses.

The resulting density estimator, henceforth referred to as the Recursive Bayesian Predictive (RBP), lacks flexibility to model highly complex data distributions (see Figure 1). This is because the existing copula updates rely on a Gaussian copula with a single scalar bandwidth parameter, corresponding to a Bayesian model with a likelihood that factorizes over dimensions. We also note that popular neural network based approaches, such as MAF \cite{43}, and RQ-NSF \cite{13} can struggle in small-data regimes (Figure 1).

**Contributions.** This motivates our main contribution, namely the formulation of a more flexible autoregressive (AR) copula update. In particular:

- By considering an AR likelihood with a Gaussian process (GP) prior, we formulate a copula update with a data-dependent bandwidth that is equivalent to a Euclidean metric on the data space. Our method, Autoregressive Recursive Bayesian Predictives (AR-BP), significantly outperforms traditional density estimators on tabular data sets of moderate size.
- We observe in practice that the Euclidean metric used in AR-BP can be inadequate for highly non-smooth data distributions. For such cases, we propose using an AR neural network \cite{2, 20, 21, 36} that maps the observations into a latent space before bandwidth estimation. This introduces additional non-linearity through the dependence of the bandwidth on the data, leading to a density estimator, ARnet-BP, that is more accurate on non-smooth densities.

2 Background

We briefly recap predictive density estimation via bivariate copula updates for univariate and multivariate data, before describing a particular such update inspired by DPMMs.

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Figure 1: Scatter plot and density estimates of 600 observations sampled from a chessboard data distribution, reported with mean and standard deviation of test log likelihoods over a test data set. For a comparison with larger training sizes, please see Supplement C.2.
2.1 Univariate Predictive Density Updates

To compute predictive densities quickly, Hahn et al. [25] propose an iterative approach. For \( x \in \mathbb{R} \), any sequence of Bayesian posterior predictive densities \( p_i(x) \) with likelihood \( f \) and posterior \( \pi_i \), conditional on \( x_{1:i} \), can be expressed as

\[
p_i(x) = \int f(x|\theta)\pi_i(\theta)d\theta = p_{i-1}(x)h_i(x,x_i),
\]

for some bivariate function \( h_i(x,x_i) \) [25]. Rearranging for \( h_i \), we have

\[
h_i(x,x_i) = \frac{p_i(x)}{p_{i-1}(x)} = \frac{p_{i-1}(x,x_i)}{p_{i-1}(x)p_{i-1}(x_i)}.
\]

The key observation made by Hahn et al. [25] is that \( h_i(x,x_i) \) is in fact the transformation of a bivariate copula density. A \textit{bivariate copula} is a bivariate cumulative distribution function (CDF) \( C : [0,1]^2 \to [0,1] \) with uniform marginal distributions. Sklar’s theorem [18] states that for any bivariate density \( p(y_1,y_2) \) with continuous marginal CDFs \( P_1(y_1) \) and \( P_2(y_2) \), there exists a unique bivariate copula \( C \) with density \( c \) such that

\[
p(y_1,y_2) = c \{ P_1(y_1), P_2(y_2) \} p_1(y_1)p_2(y_2).
\]

Applying this copula factorization to (2) yields \( h_i(x,x_i) = c_i\{ P_{i-1}(x), P_{i-1}(x_i) \} \), where \( P_{i-1} \) is the CDF corresponding to the predictive density \( p_{i-1} \), and \( c_i \) is defined as the copula that exists according to Sklar’s theorem for \( p_{i-1}(x) \) and \( p_{i-1}(x_i) \). Given prior \( \pi \) and likelihood \( f \), Equation 2 suggests that the update function can be written as

\[
h_i(x,x_i) = \frac{\int f(x|\theta)f(x_i|\theta)\pi_{i-1}(\theta)d\theta}{\int f(x|\theta)\pi_{i-1}(\theta)d\theta} \frac{\int f(x_n|\theta)\pi_{i-1}(\theta)d\theta}{\int f(x|\theta)\pi_{i-1}(\theta)d\theta}.
\]

For each Bayesian model, there is thus a unique sequence of symmetric copula densities \( c_i(u,v) = c_i(v,u) \). This sequence has the property that \( c_n \to 1 \) as \( n \to \infty \), ensuring that the predictive density converges asymptotically with sample size \( n \).

Note that in general, (3) is intractable due to the posterior so it is not possible to compute the iterative update in (1) for fully Bayesian models. However, we may still consider alternative, tractable formulations for \( h_i \). In particular we will consider sequences that match the Bayesian model for \( i = 1 \), but not for \( i > 1 \). As mentioned above, this copula update no longer corresponds to a Bayesian model, nor are the resulting predictive density estimates approximations to a Bayesian model. Nevertheless, if the copula updates are \textit{conditionally identically distributed} (c.i.d), they still exhibit desirable Bayesian characteristics such as coherence and regularization. The sequence \( X_1, X_2, \ldots \) is c.i.d if we have \( P(X_{i+k} \leq x|x_{1:i}) = P_1(x), \forall k > 0 \) almost surely for each \( x \in \mathbb{R} \); refer to [5, 17, 25] for more details. A particular example of tractable and c.i.d copula updates, proposed by Hahn et al. [25], is motivated by DPMMs for univariate density estimation. We introduce this update for the multivariate setting in the next subsection.

2.2 Multivariate Predictive Density Updates

The above arguments cannot directly be extended to multivariate \( x \in \mathbb{R}^d \) since \( h_i \) cannot necessarily be written as \( c_i\{ P_{i-1}(x), P_{i-1}(x_n) \} \) for \( d > 1 \). However, (2) still holds, and recursive predictive updates with bivariate copulas as building blocks can be derived explicitly given a likelihood model and a prior, which we now exhibit.

Hahn et al. [25] and Fong et al. [17] propose DPMMs as a general-use nonparametric model, where the DPMM [14, 15] can be written as

\[
f(x|G) = \int_{\Theta} K(x|\theta)dG(\theta), \text{ with } G \sim \text{DP}(c,G_0),
\]

where \( \theta \in \Theta = \mathbb{R}^d \) are parameter vectors, \( K(x|\theta) \) is a user-specified kernel, and the prior assigned to \( G \) is a Dirichlet process (DP) prior with base measure \( G_0 \) and concentration parameter \( c > 0 \) [19]. In particular, Fong et al. [17] consider the base measure \( G_0 = \ldots \)
\( \mathcal{N}(0, \tau^{-1}I_d) \) for some precision parameter \( \tau \in \mathbb{R}_{>0} \), and the factorized kernel \( K(x|\theta) = \mathcal{N}(x|\theta, I_d) \) where \( I_d \) is the \( d \)-dimensional identity matrix. The likelihood is then

\[
f(x|G) = \int \prod_{j=1}^{d} \mathcal{N}(x^j | \theta^j, 1) \, dG(\theta), \tag{5}
\]

where the dimensions of \( x \) are conditionally independent given \( \theta \), and we denote the dimension \( j \) of a vector \( y \) with \( y^j \). We note that the strong assumption of a factorised kernel form drastically impacts the performance of the regular \textbf{DPMM} and also influences the form and modelling capacity of the corresponding copula update.

This model inspires the following recursive predictive density update \( p_1(x) = h_i(x, x_i)p_{i-1}(x) \) for which the first \( d' \in \{1, \ldots, d\} \) marginals take on the form

\[
p_1 \left( x^{1:d'} \right) = \left\{ 1 - \alpha_i + \alpha_i \prod_{j=1}^{d'} c \left( u_{i-1}^j(x^j), v_{i-1}^j; \rho_0 \right) \right\} p_{i-1} \left( x^{1:d'} \right), \tag{6}
\]

\[
u_{i-1}^j(x^j) := P_{i-1} \left( x^j | x^{1:j-1} \right), \quad \alpha_i := \left( 2 - \frac{1}{\alpha_1} \right)^{\frac{1}{2}} \tag{7}
\]

where \( c(u, v; \rho_0) \) is the bivariate Gaussian copula density with correlation \( \rho_0 = 1/(1 + \tau) \), \( \rho_0 \) can be any chosen prior density, and \( \alpha_i = \left( 2 - \frac{1}{\alpha_1} \right)^{\frac{1}{2}} \) (see Supplement A and [17]). Note that the above update requires a specific ordering of the feature dimensions, and the Gaussian copula follows from the Gaussian distribution in the kernel and \( G_0 \) for the \textbf{DPMM}.

While \( \rho_0 \) is a scalar here, Fong et al. [17] also consider the setting with a distinct bandwidth parameter for each dimension. We refer to the resulting predictive density estimator as \textbf{R}_{d-BP}, or simply \textbf{R-BP} if the dimensions share a single bandwidth.

### 3 AR-BP: Autoregressive Bayesian Predictives

For smooth data distributions, the recursive update defined in [6] generates density estimates that are highly competitive against other popular density estimation procedures such as \textbf{kernel density estimation (KDE)} and \textbf{DPMM} [17]. Moreover, the iterative updates provide a fast estimation alternative to fitting the full \textbf{DPMM} through \textbf{Markov chain Monte Carlo (MCMC)}. When considering more structured data, however, performance suffers due to the choices of the factorized kernel \( K(\cdot|\theta) = \mathcal{N}(\cdot|\theta, I_d) \) and base measure \( G_0 = \mathcal{N}(0, \tau^{-1}I_d) \) in the \textbf{DPMM}. These choices induce a priori independence between the dimensions of the data, and are thus insufficiently flexible to capture more complex dependencies.

We therefore propose employing more general kernels and base measures in the \textbf{DPMM} and show that these inspire a more general tractable recursive predictive update. In particular, we allow the kernel to take on an autoregressive structure

\[
K(x|\theta) = \prod_{j=1}^{d} \mathcal{N} \left( x^j | \theta^j \left( x^{1:j-1} \right), 1 \right),
\]

where \( \theta^j : \mathbb{R}^{j-1} \rightarrow \mathbb{R} \) is now an unknown mean function for dimension \( x^j \), which we allow to depend on the previous \( j - 1 \) dimensions of \( x \). Correspondingly, specifying our \textbf{DPMM} requires the specification of a base measure supported on the function space in which \( (\theta^1, \ldots, \theta^d) \) is valued. We specify this base measure as a product of independent \textbf{GP} priors on the functional parameters

\[
\theta^j \sim \text{GP}(0, \tau^{-1}k^j) \quad \text{for } j = 1, \ldots, d \text{ where } k^j : \mathbb{R}^{j-1} \times \mathbb{R}^{j-1} \rightarrow \mathbb{R}
\]

and \( k^j \) can be any given covariance function that takes as input a pair of \( x^{1:j-1} \) values. In practice, we use the same functional form of \( k \) for each \( j \), so we will drop the superscript \( j \) for later convenience. We have also written the scaling term \( \tau^{-1} \) explicitly. We highlight that for \( j = 1, \theta^1 \sim \mathcal{N}(0, \tau^{-1}) \). Under this choice, the mean of the normal kernels in the \textbf{DPMM} for each dimension \( j \) is thus a flexible function of the first \( j - 1 \) dimensions \( x^{1:j-1} \), on which we elicit independent \textbf{GP} priors. The conjugacy of the \textbf{GP} with the Gaussian kernel in [7] is crucial for deriving a tractable density update.
Remark. The proposed kernel in (7) is in fact more flexible than a general multivariate kernel, \( K(x \mid \theta) = \mathcal{N}(x \mid \theta, \Sigma) \). This is because the multivariate kernel also implies an AR form like (7) but where the \( \theta^j \) are restricted to be linear in \( x^{1:j-1} \); see [53] for details.

3.1 Iterative Predictive Density Updates

Computing the Bayesian posterior predictive density induced by the [DPMM] with kernel given by (7) and base measure given by (8) through posterior estimation is intractable and requires [MCMC]. However, as before, we can utilize the model to derive tractable iterative copula updates. In Supplement [A.1] we show that the corresponding recursive predictive density update \( p_i(x) = h_i(x, x_i)p_{i-1}(x) \) for the first \( d' \) marginals takes on the form

\[
p_i \left( x^{1:d'} \right) = \begin{cases} 1 - \alpha_i + \alpha_i \prod_{j=1}^{d'} e \left( u_{i-1}^{j-1}(x^j), v_{i-1}^{j-1}; \rho^j \left( x^{1:j-1}, x_i^{1:j-1} \right) \right) \\ p_{i-1} \left( x^{1:d'} \right) \end{cases},
\]

with \( u_{i-1}^{j-1}(x^j), v_{i-1}^{j-1} \) defined as in (9), \( \alpha_i = \left( 2 - \frac{1}{\tau} \right) \frac{1}{1+i} \), and the bandwidth given by

\[
\rho^j \left( x^{1:j-1}, x_i^{1:j-1} \right) = \rho_0 k \left( x^{1:j-1}, x_i^{1:j-1} \right),
\]

for \( \rho_0 = 1/(1+\tau) \), and \( \rho_1 = \rho_0 \). Where appropriate, we henceforth drop the argument \( x \) for brevity. The conditional CDFs \( u_{i-1}^{j-1} \) can also be computed through an iterative closed form expression similarly to (9) (Supplement [B.3]). Note that this is almost identical to the update given in (6) induced by the factorised kernel, except for the key difference that the bandwidth \( \rho \) is no longer a constant, but is now data-dependent. More precisely, the bandwidth for dimension \( j \) is a function of the GP covariance function on the first \( j-1 \) dimensions. As we shall see, the additional flexibility afforded by the inclusion of covariance function \( k \) enables us to capture more complex dependency structures in the data, as we do not enforce a-priori independence between the dimensions of the parameter \( \theta \). Similarly to the extension of R-BP to \( \text{R}_{d'}\text{-BP} \), we can also define \( \text{AR}_{d'}\text{-BP} \) by introducing dimension dependence in \( \rho_0 \).

Remark. The data-dependent bandwidth also appears when starting from other Bayesian nonparametric models, such as dependent [DPs] and [GPs] (see Supplement [A.2.2]).

Our approach can be viewed as a Bayesian version of an online [KDE] procedure. To see this, note that a [KDE] trained on \( i-1 \) observations – yielding the density estimate \( q_{i-1}(x) \) – can be updated after observing the \( i \)th observation \( x_i \) via \( q_i(x) = (1-\alpha_i)q_{i-1}(x) + \alpha_i d(x, x_i) \), where \( \alpha_i = 1/i \) and \( d(\cdot, \cdot) \) denotes the kernel of the [KDE]. Rather than adding a weighted kernel term directly, AR-BP instead adds an adaptive kernel that depends on a notion of distance between \( x \) and \( x_i \) based on the predictive CDF conditional on \( x_{1:i-1} \).

To better understand the impact of the data-dependent bandwidth, we can compare the conditional predictive mean of R-BP and AR-BP in the bivariate setting \( X \times Y \). Under the
simplifying assumption of Gaussian predictive densities (Supplement A.3), the conditional mean, \( \mu_i(x) \), of \( Y \mid X \) is given by

\[
\mu_i(x) = \mu_{i-1}(x) + \alpha_i(x, x_i)p(x, x_i)(y_i - \mu_{i-1}(x_i)),
\]

where \( \alpha_i(x, x_i) = \alpha_c(P_{x-1}(x), P_{x-1}(x_i); \rho_0) / \left[1 - \alpha_c(P_{x-1}(x), P_{x-1}(x_i); \rho_0)\right] \). Note that \( \rho(x, x_i) = \rho_0 \) for R-BP. Intuitively, the updated mean is the previous mean plus a residual term at \( y_i \), scaled by some notion of distance between \( x \) and \( x_i \). For R-BP, this distance between \( x \) and \( x_i \) depends only on their predictive CDF values through \( \alpha_i(x, x_i) \). This can result in undesirable behaviour as shown in the upper plot in Figure 2(a), where the peak of \( \alpha_i(x, x_i) \), as a function of \( x \), is not centred at \( x_i \). Counterintuitively, there is thus an \( x > x_i \) where \( \mu_i(x) \) is updated more than at the actual observed \( x = x_i \). This follows from the lack of focus on conditional density estimates for R-BP, which is alleviated by AR-BP. In the AR case, \( \rho(x, x_i) \) takes into account the Euclidean distance between \( x \) and \( x_i \) in the data space. We see in the lower plot in Figure 2(a) that the peak is closer to \( x_i \). Figure 2(b) further demonstrates this difference on a toy example - we see that R-BP struggles to fit a linear conditional mean function for \( n = 4 \), while AR-BP succeeds.

**Training the update parameters** In order to compute the predictive density \( p_n(x^*) \), we require the vector of conditional CDFs \( \vec{v}_n = [v'_1, \ldots, v'_{n-1}] \) where \( v'_i = P_i(x'_{i+1} | x_{i+1}^*) \). Given a bandwidth parameterisation, obtaining this vector thus amounts to model-fitting, and each \( v'_i \) requires \( i-1 \) iterations (Supplement B.3), for \( i \in \{1, \ldots, n\} \). We note that the order of samples and dimensions influences the prediction performance in AR density estimators. In practice, averaging over different permutations of these improves performance (Supplement B.3). Full implementation details, including all the algorithms used, can be found in Supplement B.

**Computational complexity** The above procedure results in a computational complexity of \( \mathcal{O}(dn^2) \) at the training stage. At test time, we have already obtained the necessary conditional prequential CDFs \( v'_i \) in computing the prequential log-likelihood above. As a result, we have a computational complexity \( \mathcal{O}(dn) \) for each test observation. Note that the introduction of a data-dependent bandwidth does not increase the computational complexity at train or test time relative to R-BP.

### 3.2 Parameterisation of the Bandwidth

The choice of covariance function in [8] provides substantial modelling flexibility in our AR-BP framework. Moreover, the additional parameters associated with a given covariance function allow us to tune the implied covariance structure according to the observed data. This formulation enables us to draw upon the rich literature on the choice of covariance functions for Gaussian processes [55]. For simplicity we only consider the most popular such choice. The radial basis function (RBF) covariance function is defined as \( k_d(x_{i:j-1}, x_{i:j-1}') = \exp\left[-\sum_{k=1}^{j-1} \|x^k - x^k'\|^2 / \ell^2 \right] \), where \( \ell = [\ell^1, \ldots, \ell^{d-1}] \in \mathbb{R}_{>0}^{d-1} \) is the length scale vector.

**Neural parameterisation** As we saw in the motivating example of the density estimation of a checkerboard distribution in Figure 1, the RBF kernel can restrict the capacity of the predictive density update to capture intricate nonlinearities if the training data size is not sufficient. While the parameterization of the bandwidth in [10] was initially derived via the first predictive update for a DPMM, all we require is that the bandwidth function \( \rho^d : \mathbb{R}^{d-1} \times \mathbb{R}^{d-1} \to \mathbb{R} \) lies in \((0, 1)\). We would also like \( \rho^d(x, y) \) to take larger values when \( x \) and \( y \) are ‘close’ in some sense. Motivated by this observation, we now consider more expressive bandwidth functions that can lead to increased predictive performance. In particular, we formulate an AR neural network \( f_w : \mathbb{R}^d \to \mathbb{R}^{d \times d} \) for \( d \in \mathbb{N} \) with the property that the \( j^{th} \) row of the output depends only on the first \( j - 1 \) dimensions of the input. Let \( Z = f_w(x) \) and denoting \( z^j \) to be the \( j^{th} \) row of the matrix \( Z \), the covariance function is then computed as \( \rho^d = \rho_0 \exp\left(\sum_{k=1}^{j-1} \|z^k - z'^k\|^2 \right) \).

Numerous AR neural network models have been extensively used for density estimation [11] [30] [34]. In our experiments, we use a relatively simple model with parameter sharing.
inspired by NADE, an AR neural network designed for density estimation [36]. More advanced properties like the permutation invariance of MADE [43] create an additional overhead that cannot be used in the copula formulation as the predictive update is not permutation-invariant. We refer to Bayesian predictive densities estimated using AR neural networks as ARnet Bayesian predictives (ARnet-BP).

Tuning the bandwidth function Recall that the bandwidths $\rho_i(\cdot, \cdot)$ are parameterised by $\rho_0$ and the parameters of the chosen covariance functions or neural embedders. For AR-BP, these are the length scales $\ell$ of the RBF covariance function, while for ARnet-BP, these are the parameters $w$ of the AR neural network. We fit these tunable parameters in a data-driven approach by maximising the prequential [9] log-likelihood $\sum_{i=1}^{n} \log p_i(x_i)$ which is analogous to the Bayesian marginal likelihood – the tractable predictive density allows us to compute this exactly, and this approach is analogous to empirical Bayes. Specifically, we use gradient descent optimisation with Adam [33], sampling a different random permutation of the training data at each optimisation step (Supplement B.3).

4 Related Work

Our work falls into the broad area of multivariate density estimation [47]. While AR networks have been previously used directly for the task of density estimation [2, 20, 21, 36], we use them to elicit a data-dependent bandwidth in the predictive update to mitigate the smoothing effect observed in AR-BP. Neural network based approaches, however, often underperform in small-data regimes. Deep learning approaches that do target few-shot density estimation require complex meta-learning and pre-training pipelines [23, 44].

Our work directly extends the contributions of Hahn et al. [25] and Fong et al. [17] through an alternative specification of the nonparametric Bayesian model in the recursive predictive update scheme. R-BP has recently been used for nonparametric solvency risk prediction [29], and survival analysis [18]. Berti et al. [3, 4, 5] also focus on univariate predictive updates in the Bayesian nonparametric paradigm, specifically exploring the use of the conditionally identically distributed condition as a relaxation of the standard exchangeability assumption. Other studies have investigated recursive Bayesian updates in the special case of the mixing distribution in nonparametric mixture models [12, 15, 39, 50], though these typically focus on univariate or low-dimensional spaces. See also [40] for a survey.

Finally, copulas are a well-studied tool for modelling the correlations in multivariate data (see e.g. [22, 37, 42]). Copula density estimation aims to construct density estimates whose univariate marginals are uniform [22], and often focus on modelling strong tail dependencies [54]. In contrast to this literature stream, in this work we employ bivariate copulas as a tool to model the correlations between subsequent subjective predictive densities, rather than across the data dimensions directly.

5 Experiments

We demonstrate the benefits of AR-BP, ARd-BP and ARnet-BP for density estimation and prediction tasks in an experimental study with five baseline approaches and 13 different data sets. All copula examples were implemented in JAX [6] and run on a single Tesla V100 GPU. The code and data used is provided in the Supplementary Material, and will be made available online. See Supplement C for additional experimental details and results, including a sensitivity study, an ablation study, further illustrative examples, a preliminary investigation into image examples, and an empirical study of the computational complexity of the proposed methods. We stress that introducing the data-dependent bandwidth comes with little computational overhead compared to R-BP.

5.1 Density Estimation

Baseline models We compared our models against KDEs, DPMMs, masked autoregressive flows (MAFs) [43] and rational-quadratic neural spline flows (RQ-NSFs) [13]. The bandwidth of the KDEs was found by five-fold cross validation over a grid of 80 log-scale-equidistant
values from $\rho = 0.1$ to 100. For the DPMM, we considered versions with a diagonal (Diag) and full (Full) covariance matrix for each mixture component. We optimized over the weight concentration prior of the DPMM by five-fold cross validation with values ranging from $10^{-40}$ to 1. The model was trained with variational inference using \texttt{sklearn}. The hyperparameters of MAFs and RQ-NSFs were found with a Bayesian optimisation search. See Supplement C.2 for further information.

Small UCI data sets  See Table 1 for the negative log-likelihood (NLL) estimated on five UCI data sets \cite{fong2019} of moderate size, as investigated by Fong et al. \cite{fong2019}. We used a train/test split of 50\%. Our proposed methods display highly competitive performance: ARd-BP achieved the best test log-likelihood on four of the data sets, while ARnet-BP prevailed on the remaining data set.

Table 1: Average NLL with standard error over five runs on five UCI data sets of small-to-moderate size

| n/d     | WINE   | BREAST | PARKIN | IONO   | BOSTON |
|---------|--------|--------|--------|--------|--------|
| KDE     | $13.69_{0.00}$ | $10.49_{0.24}$ | $12.83_{0.27}$ | $32.08_{0.00}$ | $8.34_{0.00}$ |
| DPMM (Diag) | $17.46_{0.6}$  | $16.26_{0.71}$ | $22.28_{0.66}$ | $35.30_{1.28}$ | $7.64_{0.09}$ |
| DPMM (Full) | $32.88_{0.82}$ | $26.67_{1.32}$ | $39.95_{1.56}$ | $86.18_{10.22}$ | $9.45_{0.43}$ |
| MAF     | $39.60_{1.41}$ | $10.13_{0.40}$ | $11.76_{0.45}$ | $140.09_{4.03}$ | $56.01_{27.74}$ |
| RQ-NSF  | $38.34_{0.63}$ | $26.41_{0.57}$ | $31.26_{0.31}$ | $54.49_{0.65}$ | $-2.20_{0.11}$ |
| R-BP    | $13.57_{0.04}$ | $7.45_{0.02}$ | $9.15_{0.04}$ | $21.15_{0.04}$ | $4.56_{0.04}$ |
| Rd-BP   | $13.32_{0.01}$ | $6.12_{0.05}$ | $7.52_{0.05}$ | $19.82_{0.08}$ | $-13.50_{0.59}$ |
| AR-BP   | $13.40_{0.05}$ | $6.18_{0.05}$ | $8.29_{0.11}$ | $17.16_{0.25}$ | $-6.40_{0.77}$ |
| ARd-BP  | $13.22_{0.04}$ | $6.11_{0.04}$ | $7.21_{0.12}$ | $16.48_{0.26}$ | $-14.75_{0.89}$ |
| ARnet-BP| $14.41_{0.11}$ | $6.87_{0.23}$ | $8.29_{0.17}$ | $15.32_{0.35}$ | $-5.71_{0.62}$ |

Benchmark UCI data sets  A number of UCI data sets have become the standard evaluation benchmark for deep AR models \cite{quinonero2006,quinonero2005,quinonero2004}. These include low-dimensional data sets with up to 63 features, but at least 29,000 observations. To investigate performance as a function of sample size, we trained the models on subsets of the full data set. To compare density estimation across different data set sizes, we first normalized the data sets thus changing the log density estimates by a constant. We do not report results for the KDEs and the DPMM estimators as these were significantly worse than the other approaches. Similarly, we do not report the deep learning results for sample sizes smaller than $10^2$. See Supplement C.3 for complete results.

In the small-data regime, we observe that the R-BP methods significantly outperform the neural density estimators (Figure 3). As the sample size increases, the gap in performance decreases until eventually the neural density estimators outcompete the R-BP methods. The performance between the R-BP methods and our proposed AR extensions is largely similar, though we note that the AR-BP methods were generally more effective on the GAS dataset.

5.2 Supervised Learning

R-BP methods, including AR-BP and ARnet-BP, can be used for prediction tasks such as regression and classification \cite{fong2019}. In short, this is achieved by estimating the conditional predictive density $p_n(y|x)$ of the labels $y$ directly by assuming a dependent Dirichlet process.
An appealing feature of AR-BP is that it requires no manual hyperparameter tuning. Further, via a data-dependent bandwidth. Additionally, ARnet-BP provides a useful illustration of density via a sequential Monte Carlo algorithm, but note that its effectiveness is restricted by observations in less than an hour.

Results As with the density estimation tasks, our proposed methods were highly competitive (Table 2). ARt-BP achieved the best average test log-likelihood on two of the regression tasks and one of the classification tasks. ARnet-BP was substantially better than the remaining methods on the CONCR data set and also performed best on the PARKIN data set. On the other hand, the MLP model was best on the MNIST digits data set.

Table 2: Average NLL over five runs reported with standard error for supervised tasks

| n/d | Regression | Classification |
|-----|------------|----------------|
|     |           | BOSTON | CONCR | DIAB | IONO | PARKIN | MNIST01 |
| Linear | 506/13 | 1.030/8 | 442/10 |
| GP | 0.03,0.03 | 0.99,0.01 | 1.07,0.01 | 0.34,0.01 | 0.35,0.01 | 0.003,0.000 |
| MLP | 0.42,0.08 | 0.36,0.02 | 1.06,0.02 | 0.30,0.02 | 0.42,0.02 | 0.035,0.000 |
| R-BP | 1.42,0.01 | 2.01,0.08 | 3.32,0.05 | 0.26,0.05 | 0.31,0.02 | 0.003,0.000 |
| R-BP | 0.76,0.09 | 0.87,0.03 | 1.05,0.03 | 0.26,0.01 | 0.37,0.01 | 0.015,0.001 |
| ARt-BP | 0.40,0.03 | 0.42,0.00 | 1.00,0.02 | 0.34,0.02 | 0.27,0.03 | 0.018,0.001 |
| ARt-BP | 0.52,0.13 | 0.42,0.01 | 1.06,0.02 | 0.21,0.02 | 0.29,0.02 | 0.015,0.001 |
| ARnet-BP | 0.37,0.10 | 0.39,0.01 | 0.99,0.02 | 0.20,0.02 | 0.28,0.03 | 0.017,0.001 |
| ARnet-BP | 0.45,0.11 | -0.03,0.00 | 1.41,0.07 | 0.24,0.04 | 0.26,0.04 | 0.014,0.001 |

6 Discussion

Density estimation for high-dimensional data is a challenging task. Although Bayesian methods generally perform well in the small sample setting, the conventional Bayesian approach to density estimation via the posterior predictive is computationally intensive. Here, we build upon newly developed methodology that enables fast density estimation via recursive updates of the predictive distribution whilst maintaining the attractive features typical of Bayesian methods [17, 25].

An appealing feature of AR-BP is that it requires no manual hyperparameter tuning. Further, on small data sets, AR-BP shows state-of-the-art generalization and is faster than competing deep learning models. It significantly increases the modelling capacity of the baseline R-BP via a data-dependent bandwidth. Additionally, ARnet-BP provides a useful illustration of how powerful neural network models can be incorporated into R-BP methods to improve density estimation. Future work can investigate alternative architectures for structured data. Our work adds to the rich body of density estimators and thus we do not anticipate any additional negative societal impact arising from our proposal.

A limitation of R-BP methods, including AR-BP, is the quadratic time dependence on the number of training observations. Subsampling techniques thus offer a particularly promising avenue to reduce the overall computational cost and warrant further investigation. Another limitation is the dependence on the sample and covariate ordering, though we note that it is possible to estimate the R-BP over multiple permutations in parallel. Nevertheless, the algorithm is relatively fast: with a single GPU, we were able to train models with 100,000 observations in less than an hour.

In Supplement [3.1] we describe a procedure to sample new data points from the estimate density via a sequential Monte Carlo algorithm, but note that its effectiveness is restricted by
the failure of importance sampling methods in high dimensional settings. As such, AR-BP is more suited to evaluating densities, rather than generating synthetic data. Promising applications of AR-BP include anomaly detection [11], Monte Carlo sampling (i.e. in the form of importance weights) [49], or streaming risk prediction tasks [29].

The use of a GP prior greatly increases the flexibility of our framework. Moreover, it opens the door to future research to incorporate ideas from the vast GP literature to further boost performance in high-dimensional settings. For example, we anticipate that the use of recent advances in convolutional kernels [51] would be particularly suited for computer vision tasks.

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A Derivations

A.1 Derivation of AR-BP

For illustration purposes, we first start by summarising the derivation of the update without autoregression, closely following Appendix E.1.2 in Fong et al. [17].

A.1.1 No Autoregression (R-BP)

The multivariate DPMM with factorized kernel has the form

$$f_G(x) = \prod_{j=1}^d N(x_j \mid \theta_j^*, 1) dG(\theta), \quad G \sim \text{DP}(a, G_0), \quad G_0 = \prod_{j=1}^d N(\theta_j \mid 0, \tau^{-1}).$$

Given

$$p_i(x) = p_{i-1}(x)h_i(x, x_i),$$

Hahn et al. [25] and Fong et al. [17] derive the predictive density updates for R-BP by initially only considering the first step update $h_1$

$$p_1(x) = p_0(x)h_1(x, x_1).$$

From

$$h_1(x, x_1) = \frac{\int f(x|\theta) f(x_i|\theta) \pi_{i-1}(\theta) d\theta}{\int f(x|\theta) \pi_{i-1}(\theta) d\theta \int f(x_i|\theta) \pi_{i-1}(\theta) d\theta},$$

it follows that

$$h_1(x, x_1) = \frac{E[f_G(x) f_G(x_1)]}{p_0(x) p_0(x_1)}$$

(11)

where the expectation is over $G$ coming from the prior. Following the stick-breaking representation of the DP, Fong et al. [17] write $G$ as

$$G = \sum_{k=1}^{\infty} w_k \delta_{\theta_k^*}$$

where $w_k = v_k \prod_{j<k} (1 - v_j)$, $v_k \overset{iid}{\sim} \text{Beta}(1, a)$ and $\theta_k^* \overset{iid}{\sim} G_0$. Fong et al. [17] then derive the numerator as

$$E \left[ \sum_{j=1}^\infty \sum_{k=1}^\infty w_j w_k K(x \mid \theta_j^*) K(x_1 \mid \theta_k^*) \right]$$

$$= \left(1 - E \left[ \sum_{k=1}^\infty w_k^2 \right] \right) E[K(x \mid \theta^*)] E[K(x_1 \mid \theta^*)] + E \left[ \sum_{k=1}^\infty w_k^2 \right] E[K(x \mid \theta^*)] E[K(x_1 \mid \theta^*)]$$

where they have used the fact that $\sum_{k=1}^\infty w_k = 1$ almost surely. As $p_0(x) = E[K(x \mid \theta^*)]$, it follows that (11) can be expressed as

$$1 - \alpha_1 + \alpha_1 \frac{E[K(x \mid \theta^*)] K(x_1 \mid \theta^*)}{p_0(x) p_0(x_1)}.$$

for some fixed $\alpha_1$. For R-BP, the kernel $K$ factorises with independent priors on each dimension, and $p_0(x) = \prod_{j=1}^d p_0(x_j) = \prod_{j=1}^d N(x_j \mid 0, 1 + \tau^{-1})$, so

$$\frac{E[K(x \mid \theta^*)] K(x_1 \mid \theta^*)}{p_0(x) p_0(x_1)} = \prod_{j=1}^d \frac{E[K(x_j \mid \theta_j^*)] K(x_1 \mid \theta_j^*)}{p_0(x_j) p_0(x_1)}$$

(12)

Fong et al. [17] then show that each univariate term corresponds to the bivariate Gaussian copula density,

$$c(u, v ; \rho) = \frac{\mathcal{N}_2 \left( \Phi^{-1}(u), \Phi^{-1}(v) \mid 0, 1, \rho \right)}{\mathcal{N}(\Phi^{-1}(u) \mid 0, 1) \mathcal{N}(\Phi^{-1}(v) \mid 0, 1)},$$

where $\Phi$ is the normal CDF and $\mathcal{N}_2$ is the standard bivariate density with correlation parameter $\rho = 1/(1 + \tau)$. They then suggest an alternative sequence $h_1$ which iteratively repeats $h_1$, with the key feature that $\alpha_1 = (2 - 1/\tau) 1/\tau$. See Appendix E.1.1. in [17] for a derivation of this sequence $\alpha_1$. 

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A.1.2 With Autoregression (AR-BP)

For the derivation of the AR-BP update, we can follow the arguments in the previous section until (12) where the factorised kernel assumption applies for the first time. For AR-BP, we instead have

\[
\frac{E[K(x \mid \theta^*) K(x_1 \mid \theta^*)]}{p_0(x) p_0(x_1)} = \prod_{j=1}^{d} \frac{E[K(x^j \mid \theta^{*j}(x^{1:j-1})) K(x_1^j \mid \theta^{*j}(x^{1:j-1}))]}{p_0(x^j) p_0(x_1^j)},
\]

(13)

The factorisation of the denominator follows from

\[
p_0(x) = E\left[\prod_{j=1}^{d} K(x^j \mid \theta^{*j}(x^{1:j-1}))\right] = \prod_{j=1}^{d} E[K(x^j \mid \theta^{*j}(x^{1:j-1}))]
\]

as we have independent GP priors on each function \(\theta^{*j}\). For notational convenience we write \(\{y, x\}\) in place of \(\{x^j, x^{1:j-1}\}\) in the following. With the autoregressive kernel assumption, there is the additional complexity

\[
E[\mathcal{N}(y \mid \theta(x), 1) \mathcal{N}(y_1 \mid \theta(x_1), 1)]
\]

where \(\theta(\cdot) \sim \text{GP}(0, \tau^{-1}k)\). The marginal distribution of the GP is normal, so we have

\[
[\theta(x), \theta(x_1)]^T \sim \mathcal{N}_2(x, x_1 \mid 0, \Sigma_{x,x_1})
\]

where

\[
\Sigma_{x,x_1} = \begin{bmatrix}
\tau^{-1} & \tau^{-1} k(x, x_1) \\
\tau^{-1} k(x, x_1) & \tau^{-1}
\end{bmatrix}.
\]

Again from the conjugacy of the normal, we can show that

\[
E[\mathcal{N}(y \mid \theta(x), 1) \mathcal{N}(y_1 \mid \theta(x_1), 1)] = \mathcal{N}(y, y_1 \mid 0, K_{x,x_1})
\]

where

\[
K_{x,x_1} = \begin{bmatrix}
1 + \tau^{-1} & \tau^{-1} k(x, x_1) \\
\tau^{-1} k(x, x_1) & 1 + \tau^{-1}
\end{bmatrix}.
\]

Here \(p_0(y) = E[\mathcal{N}(y \mid \theta(x))]\) is the same as above, since marginally \(\theta(x) \sim \mathcal{N}(0, \tau^{-1})\). Plugging in \(y = P_0^{-1}(\Phi(z))\) again gives us the Gaussian copula density with correlation parameter

\[
\rho_1(x) = \rho_0 k(x, x_1)
\]

for \(\rho_0 = 1/(1 + \tau)\).

A.2 Derivation of Gaussian Process Posterior

In this section, we derive the copula sequence for the Gaussian Process, which is fully tractable. This section is mostly for insight, but it would however be interesting to investigate any potential avenues for methodological development.

A.2.1 First Update Step

We consider a univariate regression setting with \(\{y, x\}\). For the GP, we have the model

\[
f_\theta(y \mid x) = \mathcal{N}(y \mid \theta(x), \sigma^2), \quad \theta(\cdot) \sim \text{GP}(0, \tau^{-1}k).
\]

Like in the above, we can derive the function \(h_1(x, x_1)\). Following a similar argument to the AR-BP derivation, the first step GP copula density is

\[
\frac{\mathcal{N}_2(y, y_1 \mid 0, K_2 + \sigma^2 I)}{p_0(y \mid x) p_0(y_1 \mid x_1)}
\]

where \(K_i\) is the \(i \times i\) Gram matrix, with kernel

\[
k(x, x') = \tau^{-1} \exp \left\{-0.5(x - x')^2/\ell^2\right\}.
\]
Writing in terms of $P_0$, we have
\[ c\{P_0(y \mid x), P_0(y_1 \mid x_1); \rho_1(x)\} \]
where $c$ is again the Gaussian copula density, but we have the correlation parameter as
\[ \rho_1(x) = \exp \left\{ -0.5(x - x_1)^2/\ell \right\} / (1 + \tau \sigma^2) . \]

From this, we can derive the first step of the update scheme:
\[ p_1(y \mid x) = c\{P_0(y \mid x), P_0(y_1 \mid x_1); \rho_1(x)\} p_0(y \mid x) \]
where $c(u; v; \rho)$ is again the Gaussian copula density, and $p_0(y \mid x) = N(y; 0, \sigma^2 + \tau^{-1})$.

A.2.2 All Update Steps

We can even derive the copula update scheme for $i > 1$, as the Gaussian process posterior is tractable. After observing $i - 1$ observations, we have
\[ \pi(\theta_x, \theta_{x_1} \mid y_{1:i-1}, x_{1:i-1}) = N(\mu_{i-1}, \Sigma_{i-1}) \]
where each element of $\Sigma_{i-1}$ has the entry
\[ k_{i-1}(x, x') = k(x, x') - k(x, x_{1:i-1}) \left[ K_{i-1} + \sigma^2 I \right]^{-1} k(x_{1:i-1}, x') \]
where the subscript $i - 1$ indicates it is the posterior kernel and $\mu_{i-1}$ is the posterior mean vector of the GP at $x$ and $x_1$. Marginally, the GP copula after $i - 1$ data points is
\[ N_2 \{y, y; \mu_{i-1}, \Sigma_{i-1} + \sigma^2 I\} = N \{y; \mu_{i-1}^y, k_{i-1}(x, x) + \sigma^2\} N \{y_{i+1}; \mu_{i-1}^{y_{i+1}}, k_{i-1}(x_i, x_i) + \sigma^2\} \]
where $\mu_{i-1}^y$ is the posterior mean of the GP at $x$ and likewise for $\mu_{i-1}^{y_{i+1}}$. This is equivalent to the bivariate Gaussian copula density $c(u, v; \rho_i(x))$, where as before $u = P_{i-1}(y \mid x)$ and $v = P_{i-1}(y_1 \mid x_{1:i})$. The correlation parameter is now
\[ \rho_i(x) = \sqrt{\frac{k_{i-1}(x, x_i)}{\{k_{i-1}(x, x) + \sigma^2\}\{k_{i-1}(x_i, x_i) + \sigma^2\}}} \]
In summary, we have the update
\[ p_i(y \mid x) = c\{P_{i-1}(y \mid x), P_{i-1}(y_1 \mid x_1); \rho_i(x)\} p_{i-1}(y \mid x) . \]
This gives the same predictives as fitting a full GP. While this update form does not offer any computational gains, it gives us insight into the GP update. The copula update corresponds to the regular normal update [25] with a data-dependent bandwidth $\rho_i(x)$ which measures the distance between $x$ and $x_i$ based on the posterior kernel. A potential interesting direction of research is to seek approximations of the expensive $\rho_i(x)$ to aid with the computation of the GP.

A.3 Intuition for AR Copula

As in the main paper, we consider bivariate data, $(x, y)$. As shown in [17], the update for the conditional density for R-BP takes the form
\[ p_i(y \mid x) = [1 - \alpha_i(x, x_i) + \alpha_i(x, x_i) c\{P_{i-1}(y \mid x), P_{i-1}(y_1 \mid x_1); \rho\}] p_{i-1}(y \mid x) , \]
where
\[ \alpha_i(x, x_i) = \frac{\alpha_i c\{P_{i-1}(x), P_{i-1}(x_1); \rho\}}{1 - \alpha_i + \alpha_i c\{P_{i-1}(x), P_{i-1}(x_1); \rho\}} . \]
To show the effect of the AR update, we make simplifying assumptions to derive the update for the conditional mean function, $\mu_i(x) = \int y p_i(y \mid x) dy$. Let us assume that our predictive densities are normally distributed, that is $P_{i-1}(y \mid x) = N(y \mid \mu_{i-1}(x), \sigma_y^2)$. This is an accurate approximation if the truth is normal and we have observed sufficient observations. Without loss of generalizability, we assume that $\sigma_y^2 = 1$. This then gives the
form \( P_{i-1}(y \mid x) = \Phi(y - \mu_{i-1}(x)) \), which will help us in the calculation of the bivariate Gaussian copula. If we multiply by \( y \) and integrate on both sides of (14), we get

\[
\mu_i(x) = (1 - \alpha_i(x, x_i))\mu_{i-1}(x) + \alpha_i(x, x_i) \int c(P_{i-1}(y \mid x), P_{i-1}(y_i \mid x_i); \rho) \ y \ p_{i-1}(y \mid x) \ dy.
\]

Plugging in \( P_{i-1}(y \mid x) = \Phi(y - \mu_{i-1}(x)) \) (and similarly for the density) to the above gives

\[
\int c(P_{i-1}(y \mid x), P_{i-1}(y_i \mid x_i); \rho) \ y \ dy = \frac{N(y, y_i \mid [\mu_{i-1}(x), \mu_{i-1}(x_i)], 1, \rho)}{N(y_i \mid \mu_{i-1}(x_i), 1)} \ y \ dy.
\]

The above is simply the expectation of a conditional normal distribution, giving us

\[
\int c(P_{i-1}(y \mid x), P_{i-1}(y_i \mid x_i); \rho) \ y \ dy = \mu_{i-1}(x) + \rho(y_i - \mu_{i-1}(x_i)).
\]

Putting it all together, we thus have

\[
\mu_i(x) = \mu_{i-1}(x) + \alpha_i(x, x_i)\rho(y_i - \mu_{i-1}(x_i)).
\]

In the autoregressive case, we have

\[
\mu_i(x) = \mu_{i-1}(x) + \alpha_i(x, x_i)\rho(x, x_i)(y_i - \mu_{i-1}(x_i)),
\]

where we use the notations \( \rho_i(x) = \rho(x, x_i) \) interchangeably to highlight the dependence of \( \rho \) on the distance between \( x \) and \( x_i \). Further assuming \( P_{i-1}(x) = \mathcal{N}(x \mid 0, 1) \) returns a tractable form for \( \alpha_i(x, x_i) \), giving us Figure 2 in the main paper.

### A.4 Derivation of Copula Update for Supervised Learning

We now derive the predictive density update for supervised learning tasks, closely following the derivations of Pang et al. [17] for the conditional methods in Supplements E.2 and E.3. We assume fixed design points \( x_{1:n} \in \mathbb{R}^{n \times d} \) and random response \( y_{1:n} \in \mathbb{R}^n \).

#### A.4.1 Conditional Regression with Dependent Stick-Breaking

We follow Appendix E.2.2 in [17], and derive the regression copula update inspired by the dependent DP. Consider the general covariate-dependent stick-breaking mixture model

\[
f_{G_x}(y) = \int \mathcal{N}(y \mid \theta, 1) \ dG_x(\theta), \quad G_x = \sum_{l=1}^{\infty} w_l(x) \delta_{\theta_l(x)}.
\]

For the weights, we elicit the stick-breaking prior \( w_l(x) = v_l(x) \prod_{j<l} \{1 - v_j(x)\} \) where \( v_l(x) \) is a stochastic process on \( \mathcal{X} \) taking values in \([0,1]\), and is independent across \( l \). For the atoms, which are now dependent on \( x \), we assume they are independently drawn from a Gaussian process,

\[
\theta_l^x(\cdot) \overset{iid}{\sim} \text{GP}(0, \tau^{-1} k),
\]

where \( k \) is the covariance function. Once again, we want to compute

\[
\frac{E \left[ f_{G_x}(y) f_{G_{x_1}}(y_1) \right]}{p_0(y \mid x) p_0(y_1 \mid x_1)}
\]

Following the stick-breaking argument as in Section A.1.1 we can write the numerator as

\[
\{1 - \beta_1(x, x_1)\} E \left[ K \{y \mid \theta^*(x)\} \right] E \left[ K \{y_1 \mid \theta^*(x_1)\} \right] + \beta_1(x, x_1) E \left[ K \{y \mid \theta^*(x)\} \right] K \{y_1 \mid \theta^*(x_1)\}
\]

where

\[
K \{y \mid \theta^*(x)\} = \mathcal{N}(y \mid \theta^*(x), 1), \quad \theta^*(\cdot) \sim \text{GP}(0, \tau^{-1} k),
\]

and

\[
\beta_1(x, x_1) = \sum_{k=1}^{\infty} E \left[ w_k(x) w_k(x_1) \right].
\]
As before, we have

\[
E \left[ f_{G_x}(y) f_{G_{x_1}}(y_1) \right] \frac{p_0(y \mid x) p_0(y_1 \mid x_1)}{p_0(y \mid x) p_0(y_1 \mid x_1)} = c \{ P_0(y \mid x), P_0(y_1 \mid x_1); \rho_1(x) \}
\]

where \( \rho_1(x) = \rho_0 k(x, x_1) \) and \( p_0 = 1/(1 + \tau) \). We thus have the copula density as a mixture of the independent and Gaussian copula density. This then implies the copula update step of the form

\[
p_i(y \mid x) = [1 - \beta_i(x, x_i) + \beta_i(x, x_1) c \{ P_{i-1}(y \mid x), P_{i-1}(y_1 \mid x_1); \rho_i(x) \}] p_{i-1}(y \mid x),
\]

where we write \( \rho_i(x) = \rho_i^{d+1}(x) \). As in [17], we turn to the multivariate update for inspiration where we do not update \( P_n(x) \) and instead keep it fixed at \( P_0(x) = \Phi(x) \) (for each dimension). This gives us

\[
\beta_i(x, x_i) = \frac{\alpha_i \prod_{j=1}^d \Phi(x^j), \Phi(x^j_1) ; \rho_i^{q_i(x^{1:j-1})}}{1 - \alpha_i + \alpha_i \prod_{j=1}^d \Phi(x^j), \Phi(x^j_1) ; \rho_i^{q_i(x^{1:j-1})}}.
\]

(16)

A.4.2 Classification with Beta-Bernoulli Copula Update

In the classification setting (Appendix E.3.1 in [17]), Fong et al. [17] assume a beta-Bernoulli mixture for \( y_i \in \{0, 1\} \). As the derivation is written w.r.t \( \rho \), we simply replace \( \rho \) with our definition of \( \rho_i^{q_i(x^{1:j-1})} \), giving the update

\[
p_i(y \mid x) = (1 - \beta_i(x, x_i) + \beta_i(x, x_1) b \{ q_{i-1}, r_{i-1} ; \rho_i(x) \}) p_{i-1}(y \mid x)
\]

where \( q_{i-1} = p_{i-1}(y \mid x), r_i = p_{i-1}(y_i \mid x_i), \rho_i(x) \) as in Equation (16), \( \beta_i(x, x_i) \) similarly as in (16), and finally the copula-like function \( b \) given by

\[
b(q_{i-1}, r_{i-1} ; \rho_i(x)) = \begin{cases} 
1 - \rho_i(x) + \rho_i(x) \frac{q_{i-1} \land r_{i-1}}{q_{i-1} r_{i-1}} & \text{if } y = y_i \\
1 - \rho_i(x) + \rho_i(x) \frac{q_{i-1} - (q_{i-1} \land (1 - r_{i-1}))}{q_{i-1} r_{i-1}} & \text{if } y \neq y_i.
\end{cases}
\]

B Methodology

In this section, we provide more details on the methodology referred to in the main part of the paper.

B.1 Generative Modelling

First, we consider three approaches to generative modelling

1. Inverse sampling
2. Importance sampling
3. Sequential Monte Carlo (SMC)

B.1.1 Inverse Sampling

Univariate setting As noted by Fong et al. [17], we can sample from \( x^* \sim P_n(x) \) by inverse sampling, that is

\[
u \sim U[0, 1], \quad x^* \sim P_n^{-1}(u).
\]

As we cannot evaluate \( P_n^{-1}(u) \) directly, we instead solve an optimisation problem

\[
x^* = \arg\min_x |P_n(x) - u|
\]
**Multivariate setting**  The univariate procedure can be repeated iteratively in the multivariate setting given the conditional distribution

\[ u^1 \sim U[0, 1], \quad x^1 = P_{n^{-1}}^{-1}(u^1) \]

\[ u^2 \sim U[0, 1], \quad x^2 = P_{n^{-1}}^{-1}(u^2 | x^1) \]

\[ \ldots \]

\[ u^d \sim U[0, 1], \quad x^d = P_{n^{-1}}^{-1}(u^d | x^{1:d-1}) \]

**B.1.2 Importance Sampling**

In practice, inverse sampling is unstable and is highly dependent on the performance of the optimization. An alternative approach to data generation is importance sampling. This includes two steps

1. Sampling a set of particles \( z_1, \ldots, z_B \) from the initial predictive \( p_0 \).
2. Re-sampling \( z_1, \ldots, z_B \) with replacement based on the weights \( w_1 = p_n(z_1)/p_0(z_1), \ldots, w_B = p_n(z_B)/p_0(z_B) \).

**B.1.3 Sequential Monte Carlo**

Importance sampling will perform poorly if \( p_n \) and \( p_0 \) are far apart. Instead, we propose a SMC procedure. A similar SMC sampling scheme has been proposed for univariate imputation of censored survival data by Fong and Lehmann [18]. Here, the goal is parameter inference, and thus only requires implicit sample observations by drawing the marginal CDF \( w^i_j \) from a uniform distribution. In our case, we generate new explicit data directly by sampling from the data space. Please see Algorithm 6 for a complete overview. As this sampling approach is similar to evaluating the density at test data points (Algorithm 5), we highlighted the differences in blue. In short,

1. We sample a set of particles \( z_1, \ldots, z_B \) from the initial predictive \( p_0 \), and set the particle weights to \( w_k^{[0]} = 1 \) for all \( k = 1, \ldots, B \).
2. We update the predictive \( p_{i-1} \rightarrow p_i \), and the particle weights \( w_k^{[i]} = w_k^{[i-1]} \cdot p_i(z_k^{[i-1]})/p_{i-1}(z_k^{[i-1]}) \) for each training observation.
3. If the effective sample size (ESS) is smaller than half of the number of particles, we resample \( z_1, \ldots, z_B \) and \( w_1^{[i]}, \ldots, w_B^{[i]} \) based on their weights.

Note that particle diversity can be improved by introducing move steps, for example using Markov kernels [8, 24].

In Figure 4, we see that inverse sampling struggles on a simple GMM example. On the other hand, importance sampling and SMC provide reasonable samples. Similar sampling schemes have been proposed for Restricted Boltzmann Machines [36, 45] where samples can only be drawn from the model approximately by Gibbs sampling.

**B.2 Supervised Learning**

We briefly recap how joint density estimation can be extended to conditional supervised learning (regression and classification), as outlined by Fong et al. [17]. Please see Supplement A.4 for the derivation. Given fixed design points \( x_1:n \) and random response \( y_1:n \), the problem at hand is to infer a family of conditional densities \( \{ f_x(y) : x \in \mathbb{R}^d \} \).

**B.2.1 Regression**

For the regression case, Fong et al. [17] posit a Bayesian model with the nonparametric likelihood being a covariate-dependent stick-breaking DPMM

\[ f_{G_x}(y) = \int \mathcal{N}(y | \theta, 1) dG_x(\theta), \quad G_x = \sum_{k=1}^{\infty} w_k(x) \delta_{\theta_k}, \quad (17) \]
Figure 4: 100 samples generated from AR\textsubscript{d}-BP trained on 50 samples from a GMM with 4 components.

where \( w_k(x) \) follows an \( x \)-dependent stick-breaking process. Our contribution is to assume an autoregressive factorisation of the kernel and independent GP priors on \( \theta^*_i \). See Supplement A.4.1 for the derivation of the predictive density update that is now given by

\[
p_i(y \mid x) = [1 - \beta_i(x, x_i) + \beta_i(x, x_i) c \{ P_{i-1}(y \mid x), P_{i-1}(y_i \mid x_i) ; \rho_i(x) \}] p_{i-1}(y \mid x),
\]

where \( \rho_i(x) = \rho_i^{d+1}(x) \) and \( \beta \) as in (16).

**B.2.2 Classification**

For \( y_i \in \{0, 1\} \), Fong et al. [17] assume a beta-Bernoulli mixture. As explained in Supplement A.4.2 and [17], this gives the same update as in the regression setting with the difference that the copula \( c \) in (18) is replaced with

\[
b(q_{i-1}, r_{i-1}; \rho_i(x)) = \begin{cases} 1 - \rho_i(x) + \rho_i(x) \frac{q_{i-1} \wedge r_{i-1}}{q_{i-1} r_{i-1}} & \text{if } y = y_i \\ 1 - \rho_i(x) + \rho_i(x) \frac{q_{i-1} - (q_{i-1} \wedge (1 - r_{i-1}))}{q_{i-1} r_{i-1}} & \text{if } y \neq y_i \end{cases}
\]

where \( \rho_i(x) = \rho_i^{d+1}(x), q_{i-1} = p_{i-1}(y \mid x), r_{i-1} = p_{i-1}(y_i \mid x_i) \) and \( \rho_y \in (0, 1) \).

**B.3 Implementation Details**

Please see Algorithm 1 for the full estimation procedure, Algorithm 2 for the optimisation of the bandwidth parameters, Algorithm 4 for the fitting procedure of the predictive density updates, and eventually Algorithm 5 for the steps during test-time inference. All algorithms are written for one specific permutation of the dimensions, and are repeated for different permutations.
Note that at both training time and test time, we need to consider the updates on the scale of the CDF, that is for the terms such as $u_i^j(x^i)$, which appear in the update step \[9\]. Given

$$u_i^j(x^i) = P_i(x^i | x^{1:j-1}) = \int_{-\infty}^{x_i^j} p_i(x^{1:j-1}, x^i) / p_i(x^{1:j-1}) dx^i,$$

and \[9\], the CDF $u_i^j(x^i)$ take on the tractable update

$$u_i^j = \left\{ (1 - \alpha_i)u_i^{j-1} + \alpha_i H \left( u_i^{j-1}, v_i^{j-1}; \rho_i \right) \prod_{r=1}^{k-1} c \left( u_i^{r-1}, v_i^{r-1}; \rho_i \right) \right\} p_{i-1} \left( x^{1:k-1} \right) / p_i \left( x^{1:k-1} \right),$$

and set $v_i^{j-1} = u_i^{j-1}(x_i)$ which holds by definition, where we dropped the argument $x$ for simplicity from $\rho_i$ and $u_i^j$, and $H(u, v; \rho)$ denotes the conditional Gaussian copula distribution with correlation $\rho$, that is

$$H(u, v; \rho) = \int_0^u c(u', v; \rho) \, du' = \Phi \left\{ \frac{\Phi^{-1}(u) - \rho \Phi^{-1}(v)}{\sqrt{1 - \rho^2}} \right\}.$$ 

The Gaussian copula density $c(u, v; \rho)$ is given by

$$c(u, v; \rho) = \frac{\mathcal{N}_2 \left\{ \Phi^{-1}(u), \Phi^{-1}(v) \mid 0, 1, \rho \right\}}{\mathcal{N} \left\{ \Phi^{-1}(u) \mid 0, 1 \right\} \mathcal{N} \left\{ \Phi^{-1}(v) \mid 0, 1 \right\}},$$

where $\Phi$ is the normal CDF and $\mathcal{N}_2$ is the standard bivariate density with correlation $\rho \in (0, 1)$.

**Ordering** Note that the predictive density update depends on the ordering of both the training data and the dimensions. This permutation dependence is not an additional assumption on the data generative process, and the only implication is that the subset of ordered marginal distributions continue to satisfy \[6\] (main paper). In the absence of a natural ordering of the training samples or the dimensions, we take multiple random permutations, observing in practice that the resulting averaged density estimate performs better. More precisely, for a given permutation of the dimensions, we first tune the bandwidth parameters, and then calculate density estimates based on multiple random permutations of the training data. We then average over each of the resulting estimates to obtain a single density estimate for each dimension permutation, and subsequently take the average across these estimates to obtain the final density estimate. Importantly, our method is parallelizable over permutations and thus able to exploit modern multi-core computing architectures.

**Algorithm 1** Full density estimation pipeline

**Input:**
- $x_{1:n}$: training observations;
- $x_{n+1:n+n'}$: test observations;
- $M$: number of permutations over observations to average over;
- $n_p$: number of train observations used for the optimisation of bandwidth parameters;

**Output:**
- $p_n(x_{n+1}), \ldots, p_n(x_{n+n'})$: density of test points

1: procedure FULL_DENSITY_ESTIMATION
2: Compute optimal bandwidth parameters $\triangleright \mathcal{O}(Mn_0^2d \cdot \#gradient\ steps)$
3: Compute $v_i^{j,(m)}$ for $i \in \{1, \ldots, n\}, j \in \{1, \ldots, d\}, m \in \{1, \ldots, M\}$ $\triangleright \mathcal{O}(Mn^2d)$
4: Evaluate density at test observations $x_{n+1:n+n'}$ $\triangleright \mathcal{O}(Mnn'd)$
5: end procedure

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Algorithm 2 Estimate optimal bandwidth parameters

Input:
- $x_{1:n}$: training observations;
- $M$: number of permutations over samples to average over;
- $n_\rho$: number of train observations used for the optimisation of bandwidth parameters;
- maxiter: number of iterations;

$\mathcal{R}^{(0)}$: initialisation of bandwidth parameters:
- $\mathcal{R}^{(0)} = \{\rho_0^{(0)}, t_1^{(0)}, \ldots, t_{d-1}^{(0)}\}$ (by default, $\rho_0^{(0)} \leftarrow 0.9, t_i^{(0)} \leftarrow 1, \ldots, t_{d-1}^{(0)} \leftarrow 1$) for AR-BP,
- $\mathcal{R}^{(0)} = \{\rho_0^{(0)}, w\}$ (by default, $\rho_0^{(0)} \leftarrow 0.9$, and $w$ initialised as implemented in Haiku by default) for ARnet-BP

Output:
- $\mathcal{R}^{(\text{maxiter})}$: optimal bandwidth parameters

1: procedure OPTIMAL_BANDWIDTH_AND_LENGTHScales
2: Subsample $\{x'_1, \ldots, x'_{n_\rho}\}$ from $x_{1:n}$
3: for $s \leftarrow 1$ to maxiter do
4:    _, $\{p_{i-1}^{(m)}(x'_i)\}_{1,m} \leftarrow \text{FITCONDITIONAL_PREDICTIVE_CDF}($
5:        $\mathcal{R}^{(s-1)}, \{x'_1, \ldots, x'_{n_\rho}\}, M, \text{fit}_\text{density}=\text{True})$
6:    Compute $L(x'_1, \ldots, x'_{n_\rho}) = -\sum_{m=1}^M \sum_{i=1}^{n_\rho} \log p_{i-1}^{(m)}(x'_i)$
7:    $\mathcal{R}^{(s)} \leftarrow \text{ADAMSTEP}(\mathcal{R}^{(s-1)}, L)$
8: end for
9: return $\mathcal{R}^{(s)}$
10: end procedure
Algorithm 3 Single copula update

**Input:**
\[ \mathcal{R} \]: bandwidth parameters;
\( z \): observation to update the log density;
\( x_i \): observation to update with;
\( j \): feature index;
\( u_{i-1}^j(z) \): predictive CDF for \( z \);
\( v_{i-1}^{j(m)} \): prequential CDF

**Output:**
\( u_i(z) \)

1: `procedure UPDATE_U`
2: \[ \rho_{i}^{j}(z_{1:j-1}) \leftarrow \rho_{0k_{\mathcal{R}}}(z_{1:j-1}, x_{1:j-1}) \]
   \[ \text{where } k_{\mathcal{R}} \text{ denotes the user-defined kernel} \]
3: Compute the bivariate Gaussian copula density
   \[ c_{\{u_{i-1}^{j}(z), v_{i-1}^{j(m)}; \rho_{i}^{j}\}} \leftarrow \frac{\mathcal{N}_{2} \{ \Phi^{-1}(u_{i-1}^{j}(z)), \Phi^{-1}(v_{i-1}^{j(m)}) | 0, 1, \rho_{i}^{j}(z) \}}{\mathcal{N}\{\Phi^{-1}(u_{i-1}^{j}(z)) | 0, 1\} \mathcal{N}\{\Phi^{-1}(v_{i-1}^{j(m)}) | 0, 1\}} \]
4: Compute the conditional Gaussian copula CDF
   \[ H_{\{u_{i-1}^{j}(z), v_{i-1}^{j(m)}; \rho_{i}^{j}(z)\}} \leftarrow \Phi \left\{ \frac{\Phi^{-1}(u_{i-1}^{j}(z)) - \rho_{i}^{j}(z)\Phi^{-1}(v_{i-1}^{j(m)})}{\sqrt{1 - \rho_{i}^{j}(z)^2}} \right\} \]
5: Compute \( \alpha_i = (2 - \frac{1}{\tau + 1}) \]
6: Compute \( u_i^{j}(z) = P_{i}^{j}(z | z_{1:j-1}) \) by
   \[ u_i^{j}(z) \leftarrow \{1 - \alpha_i\} u_{i-1}^{j}(z) + \alpha_i \prod_{l=1}^{j-1} c_{\{u_{i-1}^{j}(z), v_{i-1}^{j(l)}; \rho_{i}^{j}(z)\}} \]
   \[ \cdot \prod_{j=1}^{d} c_{\{u_{i-1}^{j}(z), v_{i-1}^{j(m)}; \rho_{i}^{j}(z)\}} \]
7: `{return } u_i(z)
8: `end procedure`
Algorithm 4 Estimate prequential CDFs at train observations

Input:
\( \mathcal{R} \): bandwidth parameters
\( x_{1:n} \): training observations;
\( M \): number of observations over features to average over;
compute_density (by default, False);

Output:
\( \{v_{i-1}^{j(m)}\}_{i,j,m}, \{p_{i-1}^{(m)}(x_i)\}_{i,m} \) if compute_density, else \( \{v_{i-1}^{j(m)}\}_{i,j,m} \)

1: procedure fit_conditional_predictive_cdf
2: \hspace{1em} for \( m \leftarrow 1 \) to \( M \) do
3: \hspace{2em} Sample permutation \( \pi \in \Pi(n) \)
4: \hspace{2em} Change the ordering of the training observations \( \{x_{1}^{(m)}, \ldots, x_{n}^{(m)}\} \leftarrow \{\pi(x_1), \ldots, \pi(x_n)\} \) \hspace{1em} For simplicity we will drop the superscript in the following
5: \hspace{2em} for \( j \leftarrow 1 \) to \( d \) do
6: \hspace{3em} for \( k \leftarrow 1 \) to \( n \) do
7: \hspace{4em} Initialise \( u_{0}^{j}(x_k) \leftarrow \Phi(x_{k}^{j}) \) \hspace{1em} \( u \) also depends on the permutation \( m \), but since we do not reuse \( u \) after \( m \) is updated, we drop the index for simplicity
8: \hspace{3em} end for
9: \hspace{2em} end for
10: \hspace{2em} for \( i \leftarrow 1 \) to \( n \) do
11: \hspace{3em} Set \( v_{i-1}^{j(m)} \leftarrow u_{i-1}^{j}(x_i) \) for \( j \leftarrow 1 \) to \( d \)
12: \hspace{3em} for \( k \leftarrow 1 \) to \( d \) do
13: \hspace{4em} UPDATE_U(x_k, x_i, j, u_{i-1}^{j}(x_k), v_{i-1}^{j(m)})
14: \hspace{3em} end for
15: \hspace{2em} if compute_density then
16: \hspace{3em} end if
17: \hspace{2em} end for
18: \hspace{2em} end for
19: \hspace{2em} return \( \{v_{i-1}^{j(m)}\}_{i,j,m}, \{p_{i-1}^{(m)}(x_i)\}_{i,m} \) if compute_density else \( \{v_{i-1}^{j(m)}\}_{i,j,m} \)
20: end procedure
Algorithm 5 Evaluate density at test observations

Input:
\( \mathcal{R} \): bandwidth parameters
\( x_{n+1:n+n'} \): test observations;
\( \{x_1^{(1)}, \ldots, x_n^{(1)}\}, \ldots, \{x_1^{(M)}, \ldots, x_n^{(M)}\} \): sets of permuted train observations;
\( \{v_{i,j,m}^{(m)}\}_{i,j,m} \): prequential conditional CDFs at train observations;
\( M \): number of observations over features to average over;

Output:
\( \{p_n(x_{n+1}), \ldots, p_n(x_{n+n'})\} \)

procedure EVAL_DENSITY
for \( m \leftarrow 1 \) to \( M \) do
  for \( j \leftarrow 1 \) to \( d \) do
    for \( k \leftarrow 1 \) to \( n' \) do
      Initialise \( u_0^j(x_{n+k}) \leftarrow \Phi(x_{n+k}^j) \)
    end for
  end for
for \( i \leftarrow 1 \) to \( n \) do
  for \( k \leftarrow 1 \) to \( n' \) do
    for \( j \leftarrow 1 \) to \( d \) do
      UPDATE_U(x_{n+k}, x_i, j, u_{i-1}^j(x_{n+k}), v_{i-1}^{j,(m)})
    end for
  end for
  Compute density
  \[ p_{i-1}^{(m)}(x_{n+k}) \leftarrow \left\{ 1 - \alpha_i + \alpha_i \prod_{j=1}^{d} c \left( u_{i-1}^j(x_{n+k}), v_{i-1}^{j,(m)}, p_{i-1}^j(x_{n+k}) \right) \right\} p_{i-1}^{(m)}(x_{n+k}) \]
end for
\( \triangleright \) Average density over permutations
for \( i \leftarrow n + 1 \) to \( n + n' \) do
  \[ p_n(x_i) \leftarrow \frac{1}{M} \sum_{m=1}^{M} p_{n}^{(m)}(x_i) \]
end for
return \( \{p_n(x_{n+1}), \ldots, p_n(x_{n+n'})\} \)
end procedure
Algorithm 6 Sample new observations

Input:
\( \mathcal{R} \): bandwidth parameters
\( \{z_1^0, \ldots, z_B^0\} \): initial samples from proposal distribution;
\( \{q(z_1^0), \ldots, q(z_B^0)\} \): proposal density evaluated at initial samples;
\( \{x_1^1, \ldots, x_n^1\}, \ldots, \{x_1^M, \ldots, x_n^M\} \): sets of permuted train observations;
\( \{z_i^{(m)}\}_{i,j,m} \): prequential conditional CDFs at train observations;

Output: 
\( \{z_1^n, \ldots, z_B^n\} \) and \( \{p_n(z_1^n), \ldots, p_n(z_B^n)\} \)

1: \textbf{procedure} SAMPLE
2: \hspace{1em} \textbf{for} \( m \leftarrow 1 \) \textbf{to} \( M \) \textbf{do}
3: \hspace{2em} \textbf{for} \( k \leftarrow 1 \) \textbf{to} \( B \) \textbf{do}
4: \hspace{3em} \textbf{for} \( j \leftarrow 1 \) \textbf{to} \( d \) \textbf{do}
5: \hspace{4em} Initialise \( u_0^j(z_k^0) \leftarrow \Phi(z_k^0) \)
6: \hspace{3em} \textbf{end for}
7: \hspace{2em} Initialise \( w_0^0 \leftarrow p_0(z_k^0)/q(z_k^0) \)
8: \hspace{1em} \textbf{end for}
9: \textbf{end for}
10: \textbf{for} \( i \leftarrow 1 \) \textbf{to} \( n \) \textbf{do}
11: \hspace{1em} \textbf{for} \( k \leftarrow 1 \) \textbf{to} \( B \) \textbf{do}
12: \hspace{2em} \textbf{for} \( m \leftarrow 1 \) \textbf{to} \( M \) \textbf{do}
13: \hspace{3em} \textbf{for} \( j \leftarrow 1 \) \textbf{to} \( d \) \textbf{do}
14: \hspace{4em} UPDATE\_U(z_k^{[i-1]}, x_i, j, u_{i-1}^j(z_k^{[i-1]}), v_{i-1}^{(m)})
15: \hspace{3em} \textbf{end for}
16: \hspace{2em} Compute density
17: \hspace{3em} \hspace{1em} \( p_i^{(m)}(z_k^{[i-1]}) \leftarrow 1 - \alpha_i + \alpha_i \sum_{j=1}^d c \left( u_{i-1}^j(x_{n+k}), v_{i-1}^{(m)}; p_i^{(m)}(z_k^{[i-1]}) \right) p_{i-1}(z_k^{[i-1]}) \)
18: \hspace{3em} \hspace{1em} \( p_i(z_k^{[i-1]}) \leftarrow \frac{1}{M} \sum_{m=1}^M p_i^{(m)}(z_k^{[i-1]}) \)
19: \hspace{3em} \hspace{1em} \( w_i^k \leftarrow w_i^{[i-1]} \cdot p_i(z_k^{[i-1]})/p_{i-1}(z_k^{[i-1]}) \)
20: \hspace{2em} \textbf{end for}
21: \hspace{1em} \textbf{end for}
22: \hspace{1em} \textbf{if} ESS < 0.5 \cdot B \textbf{then}
23: \hspace{2em} \textbf{RESAMPLE\_WITH\_REPLACEMENT}(\{z_k^{[i-1]}\}_k, \{w_k^i\}_k)
24: \hspace{2em} \textbf{else}
25: \hspace{3em} \( z_k^i \leftarrow z_k^{[i-1]} \) for \( k = 1, \ldots, B \)
26: \hspace{2em} \textbf{end if}
27: \hspace{1em} \textbf{end if}
28: \hspace{1em} \textbf{return} \( \{z_k^i\}_k \)
29: \hspace{1em} \textbf{end procedure}
Table 3: Hyperparameters for MAF and RQ-NSF

| data        | batch size | learning rate | flow steps | hidden nodes | bins | transform blocks | dropout |
|-------------|------------|---------------|------------|--------------|------|------------------|---------|
| MAF         |            |               |            |              |      |                  |         |
| WINE        | 10000      | 0.0003        | 20         | 512          | -    | 1                | 0.2     |
| BREAST      | 10000      | 0.0004        | 20         | 512          | -    | 1                | 0.2     |
| PARKINSONS  | 10000      | 0.0004        | 20         | 512          | -    | 1                | 0.2     |
| IONOSPHERE  | 10000      | 0.0003        | 20         | 512          | -    | 1                | 0.2     |
| BOSTON      | 10000      | 0.0003        | 10         | 512          | -    | 1                | 0.2     |
| CONCRETE    | 1024       | 0.0003        | 20         | 512          | -    | 1                | 0.2     |
| DIABETES    | 10000      | 0.0004        | 20         | 512          | -    | 1                | 0.2     |
| CHECKERBOARD| 10000      | 0.0003        | 20         | 512          | -    | 1                | 0.2     |
| RQ-NSF      |            |               |            |              |      |                  |         |
| WINE        | 10000      | 0.0004        | 20         | 512          | 8    | 1                | 0.2     |
| BREAST      | 10000      | 0.0005        | 10         | 512          | 8    | 1                | 0.2     |
| PARKINSONS  | 10000      | 0.0005        | 20         | 512          | 8    | 1                | 0.2     |
| IONOSPHERE  | 10000      | 0.0003        | 10         | 512          | 8    | 1                | 0.2     |
| BOSTON      | 10000      | 0.0003        | 10         | 512          | 8    | 1                | 0.2     |
| CONCRETE    | 1024       | 0.0004        | 20         | 256          | 8    | 2                | 0.1     |
| DIABETES    | 256        | 0.0004        | 10         | 512          | 8    | 2                | 0.2     |
| CHECKERBOARD| 1024       | 0.0004        | 10         | 512          | 8    | 2                | 0.1     |

C Experiments

C.1 Experimental Details

The UCI data sets [1] we used are: wine, breast, parkinson (PARKIN), ionosphere (IONO), boston housing (BOSTON), concrete (CONCR), diabetes (DIAB), and digits.

**Code** We downloaded the code for MAF and NSF from [https://github.com/bayesiains/nsf](https://github.com/bayesiains/nsf) and the code for R-BP from [https://github.com/edfong/MP/tree/main/pr_copula](https://github.com/edfong/MP/tree/main/pr_copula) and implemented EarlyStopping with patience 50, and 200 minimal, and 2000 maximal iterations. Note that we chose the autoregressive version of RQ-NSF over the coupling variant as the former seemed to generally outperform the latter in [13]. The neural network in ARnet-BP was implemented with [Haiku](https://github.com/haiku). The remaining methods are implemented in [sklearn](https://github.com/scikit-learn). For the DPMM with VI (mean-field approximation), we use both the diagonal and full covariance function, with default hyperparameters for the priors. The code used to generate these results is available as an additional supplementary directory.

**Initialisation** We initialise the predictive densities with a standard normal, the bandwidth parameter with $\rho_0 = 0.9$, the length scales with $l_2 = 1, \ldots, l_{d-1} = 1$, and the neural network weights inside ARnet-BP by sampling from a truncated normal with variance proportional to the number of input nodes of the layer [31].

**Data pre-processing** For each dataset, we standardized each of the attributes by mean-centering and rescaling to have a sample standard deviation of one. Following [33], we eliminated discrete-valued attributes. To avoid issues arising from collinearity, we also eliminated one attribute from each pair of attributes with a Pearson correlation coefficient greater than 0.98.

**Hyperparameter tuning** Please see Section 5 in the main paper for details on the hyperparameter search of the [sklearn](https://github.com/scikit-learn) benchmark models. For MAF and RQ-NSF, we applied a Bayesian optimisation search over the learning rate $\{3 \cdot 10^{-4}, 4 \cdot 10^{-4}, 5 \cdot 10^{-4}\}$, the batch size $\{512, 1024\}$, the flow steps $\{10, 20\}$, the hidden features $\{256, 512\}$, the number of bins $\{4, 8\}$, the number of transform blocks $\{1, 2\}$ and the dropout probability $\{0, 0.1, 0.2\}$. On each data set, the hyperparameter search ran for more than 5 days. Please see Table 3 for the optimal parameters found. For the benchmark UCI data sets, we did not tune the hyperparameters for neither MAF nor RQ-NSF but instead used the standard parameters given by [13].
We observe that none of these ablations consistently outperforms ARnet-BP. In Table 4, we also show results on the small UCI datasets for:

- a different choice of covariance function, namely a rational quadratic covariance function, defined by $k(x, x_i) = \left(1 + \frac{|x - x_i|^2}{2\gamma^2}\right)^{-\gamma}$, where $\ell, \gamma > 0$ and
- a different choice of initial distribution, namely a uniform distribution (unif).

Table 4: Average NLL with standard error over five runs on five UCI data sets of small-to-moderate size

| n/d | WINE | BREAST | PARKIN | IONO | BOSTON |
|-----|------|--------|--------|------|--------|
| AR-BP | 13.22±0.04 | 6.11±0.04 | 7.21±0.12 | 16.48±0.26 | -14.75±0.89 |
| AR-BP (RQ) | 13.53±0.02 | 7.39±0.06 | 8.79±0.08 | 21.26±0.08 | 4.49±0.00 |
| AR-BP (unif) | 13.39±0.04 | 6.18±0.03 | 7.85±0.08 | 20.25±0.09 | -20.41±1.28 |
| AR-BP (unif) | -5.18±0.04 | -15.51±0.11 | -16.58±0.06 | -47.77±1.77 | -10.73±1.63 |

We observe that none of these ablations consistently outperforms AR-BP.

**Benchmark UCI data sets** As we only presented a subset of the results on the benchmark data sets introduced by [43] in Section 5, we present more results for density estimation on the complete data set in Table 3. These results underscore that 1) MAF and RQ-NSF outperform any other baseline, the more data is available; 2) KDE underperforms in high-dimensional settings; 3) DPMM is not suitable for every data distribution. Note that evaluation of the R-BP variants take at least 4 days to run on any of the data sets with more than 800,000 observations which is why we omitted those results here.

**Image examples** We provide preliminary results on two image datasets, digits and MNIST, in Table 3. Note that the AR-BP copula updates investigated here were not designed with computer vision tasks in mind. The rich parameterization allows the model to overfit to the data leading to a prequential negative log-likelihood of at least -684 at train time while the test NLL is considerably higher. ARnet-BP, on the other hand, helps to model the complex data structure more efficiently. We expect that further extensions based on, for instance, convolutional covariance functions [51] may prove fruitful.
Figure 5: Computational study: computational time measured in elapsed seconds for a simple GMM example.
Figure 6: Sensitivity analysis: Average test NLL over 5 runs reported with standard error for a simple GMM example over a range of simulation and parameter settings.

Table 5: Average NLL with standard error over five runs on benchmark UCI data from [43].

| Model         | POWER | GAS   | HEPMASS | MINIBOONE | BSDS300 |
|---------------|-------|-------|---------|-----------|---------|
| Gaussian      | 1.659/917/6 | 852/174/8 | 315/123/21 | 29/556/43 | 1,000/0,000/63 |
| KDE           | 29.39 ±0.00  | -9.61±0.00 | 26.44±0.00 | 43.88±7.32 | 63.70±10.00 |
| DPMM (Diag)   | 0.51±0.01   | 1.20±0.02  | 25.80±0.00 | 39.16±0.01 | 37.55±0.02 |
| DPMM (Full)   | 0.33±0.00   | -5.57±0.04 | 23.40±0.02 | 18.82±0.01 | 4.47±0.00 |
| MAF           | 0.52±0.00   | -2.21±0.54 | 21.10±0.04 | 12.81±0.08 | 2.76±0.17 |
| RQ-NSF        | 0.00±0.01   | -6.41±0.14 | 19.46±0.08 | 12.51±0.19 | 2.44±0.56 |

**Toy examples**  Figure 7 shows density estimates for the introductory example of the checkerboard distribution in a large data regime. We observe that neural-network-based methods outperform the AR-BP alternatives. Nevertheless, AR-BP performs better than the baseline R-BP. An illustration of this behaviour on another toy example is also given in Figure 8. Figure 9 shows density estimates from AR-BP on a number of complex distributions.
Table 6: Image datasets: average test NLL over five runs displayed with standard error

| Dataset   | DIGITS      | MNIST      |
|-----------|-------------|------------|
| MAF       | $-8.76 \pm 0.10$ | $-7.14 \pm 0.48$ |
| RQ-NSF    | $-6.17 \pm 0.13$ | $-8.49 \pm 0.03$ |
| R-BP      | $-8.80 \pm 0.00$ | $-9.04 \pm 0.07$ |
| $R_d$-BP  | $-7.46 \pm 0.12$ | $-7.73 \pm 0.07$ |
| AR-BP     | $-8.66 \pm 0.03$ | $-7.31 \pm 0.42$ |
| $AR_d$-BP | $-7.46 \pm 0.18$ | $-8.32 \pm 0.61$ |
| ARnet-BP  | $-7.72 \pm 0.28$ | $-9.20 \pm 0.10$ |

Figure 8: Illustration of the importance of an autoregressive kernel. We trained the models on 500 data points sampled according to a sine wave distribution (given in Figure 9). We visualise the predictive density after observing a different number, $n$, of observations, highlighting the last five points with $\times$. We observe that for highly non-linear relationships between $x^1$ and $x^2$, the optimal bandwidth of R-BP is quite high ($\rho = 0.93$) which results in strong overfitting. Even when we choose $\rho_0 = 0.93$ for AR-BP and ARnet-BP, we observe that these models learn the true data distribution with fewer samples than R-BP does.

Figure 9: Scatter plots of 60,000 samples from different data distributions in the first row, and corresponding autoregressive predictive density estimates in the second row.