RafterNet: Probabilistic Predictions in Multi-Response Regression

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ABSTRACT
A fully nonparametric approach for making probabilistic predictions in multi-response regression problems is introduced. Random forests are used as marginal models for each response variable and, as novel contribution of the present work, the dependence between the multiple response variables is modeled by a generative neural network. This combined modeling approach of random forests, corresponding empirical marginal residual distributions and a generative neural network is referred to as RafterNet. Multiple datasets serve as examples to demonstrate the flexibility of the approach and its impact for making probabilistic forecasts.

1. Introduction
We consider a fairly general class of problems, where the joint distribution of a d-dimensional random vector \( X_k \) = \( (X_{k,1}, \ldots, X_{k,d}) \) allows for the Sklar decomposition (Sklar 1959),
\[
F_{X_k}(x_k) = C(F_{X_{k,1}}(x_{k,1}), \ldots, F_{X_{k,d}}(x_{k,d})),
\]
in which the copula \( C \) (Embrechts, McNeil, and Straumann 2002; Nelsen 2006) remains the same across all \( k \) and satisfies the “simplifying assumption” in the sense of Côté, Genest, and Omelka (2019), but the marginal distributions \( F_{X_{k,1}}, \ldots, F_{X_{k,d}} \) can depend on a (vector) covariate, say, \( z_k \), and hence vary with \( k \).

1.1. Background
Since Song (2000) and Oakes and Ritz (2000) first presented multi-response regression modeling using copulas, it has been explored in a few different contexts, including insurance applications (Frees and Wang 2005, 2006; Frees and Valdez 2008; Côté, Genest, and Omelka 2019) and survival analysis (He and Lawless 2005; Barriga et al. 2010). Typically, each marginal distribution is assumed to follow a parametric model,
\[
F_{X_{k,j}}(x_{k,j}) = F_j(x_{k,j}; \theta_j(z_k)), \quad j = 1, \ldots, d,
\]
with parameter \( \theta_j(z_k) \) depending on the covariate \( z_k \), for example specified by a generalized linear model (GLM) with \( \theta_j(z_k) = \eta_j(\beta^T z_k) \), where \( \eta_j \) is a pre-specified link function specific to the parametric family of \( F_j \). Then, a parametric copula model (for example normal, t, Frank, Gumbel, and so on) is chosen as \( C \); see Gijbels, Omelka, and Veraverbeke (2015) and Côté, Genest, and Omelka (2019) for investigations into the estimation and selection of \( C \) in copula-based regression setups.

In any dimension \( j \), the function \( \theta_j(\cdot) \) can be estimated from training data \( \{(X_{k,j}, z_k)\}_{k=1}^{n_{trn}} \). Afterwards, one can apply the probability integral transform to each training observation
\[
\tilde{U}_{k,j} = F_j(X_{k,j}; \hat{\theta}_j(z_k)), \quad k = 1, \ldots, n_{trn}, \quad (3)
\]
and estimate the copula \( C \) from the transformed sample,
\[
\{\tilde{U}_k = (\tilde{U}_{k,1}, \ldots, \tilde{U}_{k,d})\}_{k=1}^{n_{trn}}.
\]
The goal is to make probabilistic predictions for any \( k \), either a training observation \( k \leq n_{trn} \) or a future observation \( k > n_{trn} \). This can be done by first generating a sample of size \( n_{gen} \),
\[
\{U_k^{(i)} = \{U_{k,1}^{(i)}, \ldots, U_{k,d}^{(i)}\}_{i=1}^{n_{gen}}
\]
from the estimated copula \( \hat{C} \), and then letting
\[
\hat{X}_{k,j}^{(i)} = F_j^{-1}(U_{k,j}^{(i)}; \hat{\theta}_j(z_k)), \quad i = 1, \ldots, n_{gen},
\]
The resulting collection
\[
\{\hat{X}_k = (\hat{X}_k^{(1)}, \ldots, \hat{X}_k^{(n_{gen})})\}_{i=1}^{n_{gen}}
\]
is an empirical predictive distribution for \( X_k \). We can then make probabilistic forecasts such as predicting \( \mathbb{P}(X_{k,j} > c_j, X_{k,\ell} > c_\ell) \) by \( 1/n_{gen} \sum_{i=1}^{n_{gen}} \mathbb{1}(\hat{X}_{k,j}^{(i)} > c_j, \hat{X}_{k,\ell}^{(i)} > c_\ell) \), something that point predictions/forecasts are incapable of; see Appendix C for such an example based on our fully nonparametric approach.
to be detailed below. For these types of predictions, correctly capturing the dependence structure $C$ is critical.

1.2. Our Contribution

The aforementioned classic, and fully parametric, approach will be illustrated using one dataset later in Appendix A as a comparison. For the main part of this article, however, we will propose a fully nonparametric approach. For the marginal models $F_{X_{k,1}}, \ldots, F_{X_{k,d}}$, this objective is easy to achieve. Instead of the parametric approach (2), we model the mean in each dimension $j$ as a function of the covariate,

$$
E(X_{k,j}) = \theta_j(z_k),
$$

fitted with a random forest (Breiman 2001), and the distribution of the ensuing residual,

$$
X_{k,j} - E(X_{k,j}) \sim F_j,
$$

with its empirical (rather than a specific parametric) distribution function.

Our key contribution, and the main focus of this article, is to model the joint distribution of the transformed variables

$$(F_1(X_{k,1} - E(X_{k,1})), \ldots, F_d(X_{k,d} - E(X_{k,d}))) \sim C$$

by a generative neural network. Instead of fitting and then sampling from a parametric copula for $C$, we train a neural network to directly provide us with samples from an estimate of $C$.

We have found this approach to be quite powerful in practice, to a large extent due to its considerable flexibility at all three levels: $\theta_j(z_k)$ for $E(X_{k,j})$, $F_j$ for $X_{k,j} - E(X_{k,j})$, $j = 1, \ldots, d$, and a neural network for $(F_1(X_{k,1} - E(X_{k,1})), \ldots, F_d(X_{k,d} - E(X_{k,d})))$. Therefore, we refer to our model as RafterNet, for “random forests + empirical residuals + generative neural network”. The English word “rafter” means “one of several internal beams extending from the eaves to the peak of a roof and constituting its framework.” The analogy is especially apt here: The $j$th beam represents the $j$th marginal model, and these marginal models are then connected by the neural network which learns the dependence across all dimensions $j = 1, \ldots, d$; see Figure 1 for a schematic illustration.

Any nonparametric regression technique can be used to model $\theta_j(\cdot)$; the random forest is merely being used as a generic choice which has the reputation of being both relatively robust and easy to apply. In Appendix A, we illustrate with an example that, even when using classic GLMs as marginal models, it can still be beneficial to model the dependence across all dimensions with a neural network, as opposed to a parametric copula.

2. The RafterNet

2.1. Modeling and Probabilistic Prediction

Fitting a random forest to estimate the marginal regression function $\theta_j(\cdot)$ is straightforward. For any observation $k$, let $\tilde{R}_{k,j} = X_{k,j} - \hat{\theta}_j(z_k)$ denote the realized residual in the $j$th coordinate after having removed the estimated effect of the covariate. As typical in copula modeling, we use

$$
\hat{F}_j(t) = \frac{1}{n_{trn}} + \sum_{\ell=1}^{n_{trn}} 1 \left(\tilde{R}_{\ell,j} \leq t\right)
$$

as the empirical distribution of $\tilde{R}_{1,j}, \ldots, \tilde{R}_{n_{trn},j}$. Thus, for us, Equation (3) corresponds to

$$
\tilde{U}_{k,j} = \hat{F}_j(X_{k,j} - \hat{\theta}_j(z_k)).
$$

By letting $\tilde{U}_k = (\tilde{U}_{k,1}, \ldots, \tilde{U}_{k,d})$ for all $k = 1, \ldots, n_{trn}$, we then train a neural network $G$ in such a way that, given any sample $(V_{\ell,i})_{i=1}^{n_{gen}}$ from a “simple” distribution (e.g., the uniform or the independent standard normal), the two samples

$$
\{\tilde{U}_{k,i} = (\hat{V}_{k,1}, \ldots, \hat{V}_{k,d})\}_{i=1}^{n_{gen}} \quad \text{and} \quad \{U_\ell = G(V_\ell)\}_{\ell=1}^{n_{gen}}
$$

follow approximately the same distribution; more details about this step are given in Section 2.2. For any given $k$, this allows us to generate samples

$$
(U_k^{(i)} = G(V_{k}^{(i)}))_{i=1}^{n_{gen}}
$$

![Figure 1](image-url). Illustration of the idea behind RafterNet. Random forests provide marginal models, the empirical residuals of which are then used as input to a neural network that models the dependence structure.
from an *implicit* estimate of $C$, say, $\hat{C}$, without making any parametric assumptions about $C$. Finally, by using the quantile function $F_j^{-1}$ of $\hat{F}_j$, Equation (4) becomes

$$\hat{X}_{kj}^{(i)} = F_j^{-1}(U_{kj}^{(i)}) + \hat{g}(z_k). \quad (4')$$

Algorithm 2.1 summarizes the main steps used by our suggested RafterNet model to make probabilistic predictions given a covariate $z$.

**Algorithm 2.1 (Using the RafterNet to make probabilistic predictions given a covariate).**

1. From the trained neural network $G$, generate $U^{(i)} = (U_1^{(i)}, \ldots, U_d^{(i)}) \sim \hat{C}, i = 1, \ldots, n_{\text{gen}}$.
2. For all $i = 1, \ldots, n_{\text{gen}}$ and $j = 1, \ldots, d$, let $\hat{X}_j^{(i)} = F_j^{-1}(U_j^{(i)}) + \hat{g}(z)$.
3. Return $\{(\hat{X}_1^{(i)}, \ldots, \hat{X}_d^{(i)})\}_{i=1}^{n_{\text{gen}}}$ as a sample from the empirical predictive distribution.

### 2.2. The Optimization Problem

We now briefly describe how to train a neural network $G$ capable of generating samples of approximately the same distribution as a given training sample; for us, the latter is $\{(U_k)_{k=1}^{n_{\text{trn}}}\}$. We use a technique introduced independently by Li, Swersky, and Zemel (2015) and Dziugaite, Roy, and Ghahramani (2015).

Let $G$ denote a family of feedforward neural networks $G$ with a pre-determined architecture, and let $K$ be a kernel function. Given $\{V_\ell \in \mathbb{R}^{d_{\text{gen}}}, \ell = 1, \ldots, n_{\text{gen}}\}$ from a “simple” distribution (e.g., the uniform or the independent standard normal), we solve the optimization problem

$$\min_{G \in \mathcal{G}} \left\{ \frac{1}{n_{\text{trn}}^2} \sum_{k=1}^{n_{\text{trn}}} \sum_{k'=1}^{n_{\text{trn}}} K(\hat{U}_k, \hat{U}_{k'}) - \frac{2}{n_{\text{trn}} n_{\text{gen}}} \sum_{k=1}^{n_{\text{trn}}} \sum_{\ell=1}^{n_{\text{gen}}} K(\hat{U}_k, G(V_\ell)) + \frac{1}{n_{\text{gen}}^2} \sum_{\ell_1=1}^{n_{\text{gen}}} \sum_{\ell_2=1}^{n_{\text{gen}}} K(G(V_{\ell_1}), G(V_{\ell_2})) \right\} \quad (5)$$

by stochastic gradient descent. The first term in (5) does not depend on $G$, so it does not have any direct impact on the optimization problem itself, but retaining it in the equation will make the optimization problem easier to understand.

In particular, the kernel function computes inner products in an implicit feature space (Mercer 1909) in the sense that $K(u, v) = \varphi(u)^\top \varphi(v)$ for a feature map $\varphi$. Therefore, (5) is equivalent to

$$\min_{G \in \mathcal{G}} \left\| \frac{1}{n_{\text{trn}}} \sum_{k=1}^{n_{\text{trn}}} \varphi(\hat{U}_k) - \frac{1}{n_{\text{gen}}} \sum_{\ell=1}^{n_{\text{gen}}} \varphi(G(V_\ell)) \right\|^2. \quad (6)$$

The feature map implicitly specified by the Gaussian kernel (here, with bandwidth parameter $h$),

$$K(u, v) = \exp\left(-\frac{\|u - v\|^2}{h}\right), \quad (7)$$

is an infinite-dimensional vector function $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}^N$. With such a choice, the two terms in (6) will contain all empirical moments of $\{\hat{U}_k\}_{k=1}^{n_{\text{trn}}}$ and $\{G(V_\ell)\}_{\ell=1}^{n_{\text{gen}}}$, respectively. It is in this sense that the solution $G$ can generate samples that “match” the training sample in distribution.

In practice, we always set $d' = d$. We also follow the suggestion of Li, Swersky, and Zemel (2015) and use a mixture of Gaussian kernels with different bandwidths (instead of a single Gaussian kernel) in order to avoid having to select an “optimal” bandwidth parameter; this is particularly convenient as the output of our neural network always lies in the unit hypercube. For an investigation into these neural networks, an application to generating quasi-random numbers from complex dependence structures, and details about training these neural networks, see Hofert, Prasad, and Zhu (2021).

### 2.3. Remarks

One may ask why we have chosen the technique of Li, Swersky, and Zemel (2015) and Dziugaite, Roy, and Ghahramani (2015), instead of some other techniques such as variational auto-encoders (VAEs), for training generative neural networks. The short, and not-so-surprising, answer is that this technique works while others do not. It is true that learning a VAE (Kingma and Welling 2013) will also allow us to generate from $\{V_\ell \in \mathbb{R}^{d_{\text{gen}}}, \ell = 1, \ldots, n_{\text{gen}}\}$ a sample $\{G(V_\ell) \in \mathbb{R}^{d_{\text{gen}}} : \ell = 1, \ldots, n_{\text{gen}}\}$ that follows a certain target distribution, but VAEs make the explicit assumption that this target distribution is concentrated around a smooth manifold in $\mathbb{R}^d$, usually having a much lower intrinsic dimensionality than $d$. The main effort of the VAE is to learn this unknown manifold from training data. For our learning problem, however, this crucial assumption does not apply. Our target distributions are copulas in $\mathbb{R}^d$, and they usually do not concentrate around some lower-dimensional manifold. As a result, VAEs—and other techniques which also rely heavily on this “manifold assumption”—simply cannot be used to learn what we really want to learn here. We shall present some empirical evidence to this effect in Appendix B.

### 3. Examples

In this section we apply RafterNet to a variety of multi-response regression examples. We focus on our key innovation, the non-parametric modeling of $C$, and compare our approach based on a neural network with the conventional approach of using a parametric copula. For a fair comparison, we also combine the latter with random forests as models for each $E(X_j)$. For ease of comparison with RafterNets, we refer to the latter model based on a parametric copula as "RafterCop." Both RafterCops and RafterNets therefore share the same marginal models and that the residuals $X_j - E(X_j), j = 1, \ldots, d,$ are modeled empirically, but we replace the neural network (the “Net” part) with a conventional copula (the “Cop” part) when modeling the joint distribution of $(F_1(X_1 - E(X_1)), \ldots, F_d(X_d - E(X_d)))$. A summary of our findings across all datasets is provided in Section 3.2.

#### 3.1. Datasets

First, we consider a demographic dataset containing observations of height and weight of the !Kung San people in Botswana.
collected by Howell (1985). The exact dataset we use can be found on the webpage by McElreath (2020) under the name Howell1.csv; see also Appendix C. We are interested in modeling the distribution of the height and weight of individuals conditional on their age and sex. All models we consider are trained on $n_{\text{trn}} = 1959$ randomly chosen athletes to train all models we consider and the remaining $n_{\text{tst}} = 1000$ samples serve as test data to evaluate the models.

Second, we consider a dataset with results from the 2019 Ironman World Championship held in Hawaii. It can be downloaded from Esipov (2019). Using these data, we aim to model the joint distribution of swimming, biking and running times of all competitors conditional on their "region of representation" (or continent) and "race category" (indicating the professional status, age group and sex of each competitor). We use results from $n_{\text{trn}} = 444$ randomly selected individuals and the remaining $n_{\text{tst}} = 100$ samples serve as test data to evaluate them.

Third, we consider a dataset obtained from the National Education Longitudinal Study (NELS) of 1988 (Curtin et al. 2002). It can be downloaded from National Center for Education Statistics (2021); on this website, follow the link "1988-00," then "Download," under "Statistical Software Formats" use "R" and finally download the dataset and its explanations from the two appearing links. The NELS was a major study in the U.S. that measured the educational achievement and growth of a nationally representative sample of middle school students (from 1052 public and private schools) along with numerous factors that could potentially impact a student’s academic performance. In this example, we are particularly interested in modeling the joint distribution of the standardized scores (in the base year 1988) for mathematics, science, reading comprehension and social studies, conditional on 10 covariates, which are sex, race, socioeconomic status, minority, family size, family composition, school size, urbanicity, school type and student–teacher ratio. We use $n_{\text{trn}} = 9888$ randomly chosen observations to train RafterNet and RafterCop models and the remaining $n_{\text{tst}} = 1000$ observations to assess the quality of probabilistic predictions produced by these models.

Fourth, we consider a dataset extracted from the air quality system database of the Environmental Protection Agency (EPA), see (EPA 2021), with the help of the R package RQAQAPI that provides an API to the EPA database. The dataset contains air sample data collected by state, local, tribal and federal air pollution control agencies from various monitoring stations across the US. Because of missing data, we aggregate the data across all monitoring sites (and over potentially multiple measurement devices per site). We have $d = 8$ variables of interest, which are the levels of Carbon Monoxide (CO; measured in parts per millions (ppm)), Nitrogen Dioxide (NO2; measured in parts per billion (ppb)), Oxides of Nitrogen (NOx; ppb), Ozone (O3; ppm), Sulfur Dioxide (SO2; ppb), Carbon Dioxide (CO2; ppm), particulate matter in the air with diameter of 10 microns or less (PM10; measured in micrograms per cubic meter ($\mu g/m^3$)) and particulate matter in the air with diameter of 2.5 or less (PM2.5; $\mu g/m^3$). We are then interested in modeling the distribution of these eight air pollutants conditional on six covariates, which are barometric pressure (measured in millibar), temperature (measured in degrees Fahrenheit), relative humidity (in percent), wind speed (measured in knots), rain (measured as a total in inches over a 24 hr period) and the day of the week. We use $n_{\text{trn}} = 1322$ randomly chosen observations for training our models and the remaining $n_{\text{tst}} = 300$ observations for assessing probabilistic predictions generated from the models.

3.2. Results

We created a variety of RafterCops, each using a different copula (such as normal, t, vine, Frank, Gumbel, empirical and empirical beta) to model $C$. We compared these RafterCops with a variety of RafterNets, each using a different neural network architecture, referred to by the notation "RnFx," where $f$ is the number of hidden layers and $h$ the number of neurons per hidden layer.

We assess two aspects of the out-of-sample performance of RafterCops and RafterNets. First, we evaluate how close generated samples from the neural networks and copulas are to the underlying dependence of response observations $X_k$ in the test dataset. To do so, we use a two-sample Cramér-von-Mises type test statistic (Rémillard and Scaillet 2009) that is averaged over $n_{\text{rep}}$-many replications and is defined by

$$ACvM = \frac{1}{n_{\text{rep}}} \sum_{i=1}^{n_{\text{rep}}} \left( \frac{1}{n_{\text{tst}}} \int_{[0,1]^d} \left( C_{n_{\text{tst}}}^i(u) - C_{n_{\text{gen}}}^i(u) \right)^2 \, du \right),$$

where $C_{n_{\text{tst}}}^i$ is the empirical copula of the $n_{\text{tst}}$ observations in the test dataset and $C_{n_{\text{gen}}}^i$ is the empirical copula of the $n_{\text{gen}}$ samples generated from either a neural network or a copula in replication $i$. Let $T$ denote the set of indices $k$ for which $(X_k, z_k)$ is in the test dataset. We can extract the $C_{n_{\text{tst}}}^i$ of the test dataset observations by computing $\hat{F}_k = (\hat{F}_{1}(X_k, z_k), \ldots, \hat{F}_{d}(X_k, z_k))$ for $k \in T$, where, for $j = 1, \ldots, d$, $\theta_j$ and $\hat{F}_j$ are the marginal fitted random forests and empirical distributions based on the training data $((X_k, z_k))_{k=1}^{n_{\text{tst}}}$. In our experiments, we use $n_{\text{rep}} = 25$ replications to compute the ACvM metric (8).

Second, we evaluate the quality of probabilistic predictions produced by RafterCops and RafterNets using the average mean squared error over all test observations

$$\text{AMSE} = \frac{1}{|T|} \sum_{k \in T} \left( \frac{1}{n_{\text{gen}}} \sum_{i=1}^{n_{\text{gen}}} \| \hat{X}_k^i - X_k \|_2^2 \right).$$

We use $n_{\text{gen}} = 1000$ samples when computing the AMSE metric.

Figure 2 shows scatterplots of AMSE versus ACvM for the four examples considered. From these plots, we observe that, in most cases, the samples generated from the five neural network models more closely match the underlying dependence $C_{n_{\text{tst}}}$ of the test data than those generated from competing copula models. Moreover, this better dependence modeling (as assessed by ACvM) does, in most cases, translate into better probabilistic
predictions (as assessed by the AMSE metric). The five RafterNets therefore typically produce better empirical predictive distributions when compared with various RafterCops.

4. Conclusion and Outlook

We suggested a fully nonparametric approach, the RafterNet, for making probabilistic predictions in multi-response regression problems. First, random forests are used to model the mean of each response variable $\mathbb{E}(X_j)$ as flexible functions of the covariates. Then, empirical distributions are used to model the marginal distributions of the residuals $X_j - \mathbb{E}(X_j)$. Finally, as a novel contribution, we introduced generative neural networks to model the joint distribution of $(F_1(X_1 - \mathbb{E}(X_1)), \ldots, F_d(X_d - \mathbb{E}(X_d)))$ in place of conventional copulas. The flexibility of RafterNets were showcased in four different data examples, where we demonstrated how using neural networks yielded superior probabilistic predictions compared to various copula models.

It would be desirable to relax the restriction in Equation (1) that $C$ is generic for all $k$ and does not depend on the covariate. However, $C$ is much harder to model nonparametrically than $\theta_j(\cdot)$ and $F_j$. If, for a random variable $U \in \mathbb{R}^d$ (here, with uniform margins), its distribution $C_z(u_1, \ldots, u_d)$ behaves differently over the space of covariates $z$, then, in order to understand the difference between $C_z$ and $C_{z'}$ without any parametric assumption, it will be necessary to have observed $U$ near both $z$ and $z'$ a relatively large number of times. If not, then surely some sort of smoothness assumptions will be required to describe the behavior of $C_z$ in the space of $z$. This is a challenging problem in the realm of generative neural networks that is open for future research.
Appendix A. The Air Pollution Data with Different Marginal Models

In Section 3, we have naturally focused on empirical results produced by performing (3)–(4). In this appendix, we use the air pollution dataset to illustrate the effect of performing (3)–(4) instead. Specifically, for every \( j = 1, \ldots, d \), we model the marginal distribution \( f_j(x_k; \theta_j) \) as a gamma distribution having density function

\[
f_j(x_k; \theta_j) = \frac{\theta_j (x_k)^{\alpha_j - 1}}{\Gamma(\alpha_j)} e^{-\theta_j (x_k) x_k}
\]

or, in short, as \( \Gamma(\alpha_j, \exp(\beta_j^\top z_k)) \). But as in Section 3, we still focus mainly on comparing our approach of using neural networks to model the copula \( C \) (referred to as “GLM Nets” in accordance with “RafterNets”) with the conventional approach of using parametric copulas (referred to as “GLM Cops” in accordance with “RafterCops”).

The left panel of Figure A.1 shows that GLM Nets (using different neural network architectures) generally outperform GLM Cops (using different parametric copulas) in both metrics, so there is clearly benefit in using neural nets rather than parametric copulas to model dependence regardless of how the marginal distributions are modeled. This is the main point of our article.

The right panel of Figure A.1 merely reproduces the bottom-right panel of Figure 2, for ease of direct comparison. After comparing the \( y \)-axis with the left panel, we can see that RafterNets and RafterCops outperform GLM Nets and GLM Cops in the AMSE metric. This is not surprising since random forests are more flexible than GLMs, but there are exceptions, for example, if the true marginal distributions are very close to (9), then one would expect GLM Nets and GLM Cops to be superior, but that is both obvious and not the main point of our article.

Appendix B. Evidence that VAEs do not Properly Learn Dependence

We now provide some empirical evidence to support what we have said in Section 2.3, namely that VAEs are not effective for our specific learning task. We consider the simple task of learning to generate from a few well-known copula models. Specifically, we learn to generate from 2-dimensional and 10-dimensional Clayton and \( t_4 \) copulas with pairwise Kendall’s tau set to \( \tau = 0.5 \), using training samples of size \( n_{\text{trn}} = 50,000 \) from the true copula.

First, we use the same five neural networks from Section 3, that is \( G^{\text{ks}}_{\ell, h} \) with \([\ell, h] = [1, 100], [1, 300], [1, 600], [2, 600], \) and \([3, 300] \). Then, we perform the same task with VAEs. We use the same five architectures, for both the encoder network (mapping from the training sample to \( V \)) and the decoder network (mapping from \( V \) to the output) within each VAE. For VAEs, we also experiment with different dimensions of \( V \). We denote each VAE architecture by \( V_{\ell, d} \), where \( d \) is the dimension of \( V \).

After each \( G^{\text{ks}}_{\ell, h} \) and \( V_{\ell, d} \) is trained, each for \( n_{\text{epo}} = 300 \) epochs which we are empirically sure is more than necessary for a fair comparison, we use it to generate \( B = 25 \) samples, each of size \( n_{\text{gen}} = 1000 \). We then assess the quality of each generated sample against the ground truth using the one-sample Cramér–von Mises statistic, defined as

\[
\text{CvM} = \int_{[0,1]^d} n_{\text{gen}}(C_{\text{gen}}(u) - C(u))^2 dC_{\text{gen}}(u),
\]

where \( C_{\text{gen}} \) is the empirical copula of the \( n_{\text{gen}} \) generated samples and \( C \), the true copula we are trying to learn. These 25 measurements of CvM are summarized by boxplots in Figure C.1 for learning Clayton copulas and in Figure C.2 for learning \( t_4 \) copulas.

When \( d' = d \), the samples generated by VAEs are significantly worse than those generated by the neural networks we have adopted (which also use \( d' = d \)). Even when \( d' \gg d \), VAEs still cannot learn the distributions properly, although their performance improves. However, it should be immediately clear to anyone that, even if the VAEs could be made to perform equally well as our neural networks, perhaps by using a very large \( d' \) indeed, it would still be highly inefficient if, in order to learn a two-dimensional distribution, one must first “embed” it onto a manifold that lies in \( \mathbb{R}^{200} \) or even \( \mathbb{R}^{500} \).

Appendix C. Demonstration in R with Height and Weight Data

In this section, we illustrate how to implement our RafterNet approach in R based on the height and weight dataset. To begin with, we load the
required R packages; note that your system needs Python’s Keras and TensorFlow installed for neural network training and evaluation.

As mentioned in Section 3.1, the dataset can be found on the webpage McElreath (2020) under the name Howell1.csv. The following chunk downloads and reads this dataset.

```
## Loading height and weight data
url <- "https://raw.githubusercontent.com/rmcelreath/rethinking/master/data/"
file <- "Howell1.csv"
if(!file.exists(file)) # if not yet exists, download
download.file(paste0(url,file), destfile = file)
raw <- read.csv("Howell1.csv", sep = ";") # read
dat <- as.matrix(raw) # convert raw to a matrix
```

To model the distribution of the height and weight of individuals conditional on their age and sex we use observations from \( n_{\text{trn}} = 444 \) individuals to train the RafterNet and the remaining \( n_{\text{tst}} = 100 \) observations as a test sample.

```
## Split the dataset into training and test data
n.tst <- 100 # number of test samples
set.seed(271) # for reproducibility
## Indices of observations in test data
tst.obs <- sample(1:nrow(dat), size = n.tst)
## Training and test data
dat.trn <- dat[-tst.obs,] # training data
dat.tst <- dat[tst.obs,] # test data
## Responses and covariates in training data
X.trn <- dat.trn[, c("height", "weight")]
z.trn <- dat.trn[, c("age", "male")]
## Responses and covariates in test data
X.tst <- dat.tst[, c("height", "weight")]
z.tst <- dat.tst[, c("age", "male")]
```

First, we separately model the mean height and mean weight \( \mathbb{E}(X_{k,j}), j = 1, 2, \) of individuals as flexible functions of the covariates \( z_k, k = 1, \ldots, n_{\text{trn}} \) (age and sex of individuals) using random forests \( \hat{\theta}_j(z_k) \).

Next, we use the fitted random forests \( \hat{\theta}_j(z_k), j = 1, 2, \) to compute the realized residuals \( \hat{R}_{k,j} = X_{k,j} - \hat{\theta}_j(z_k), k = 1, \ldots, n_{\text{trn}}, j = 1, 2 \). Thereafter we nonparametrically model the marginal distributions of
Figure C.2. Boxplot of CvM values evaluating samples generated by our five neural network models and the ten considered VAE models, which were trained on $d = 2$-dimensional (top) and $d = 10$-dimensional (bottom) $t_4$ copulas with $r = 0.5$.

the realized residuals $\hat{R}_{k,j}, k = 1, \ldots, n_{\text{trn}}, j = 1, 2$, by computing the pseudo-observations $\hat{U}_k, k = 1, \ldots, n_{\text{trn}}$, as described in (3).

Now we can model the pseudo-observations $\hat{U}_k, k = 1, \ldots, n_{\text{trn}}$, using a neural network $G$. For this illustration, we work with a neural network with a single hidden layer consisting of 100 neurons. Due to its non-expensive and non-vanishing gradients, we use a ReLU activation function $\phi(x) = \max\{0, x\}$ in the hidden layer. Since our target output (the pseudo-observations) lie in $(0,1)^2$, we use a sigmoid activation function $\phi(x) = 1/(1+e^{-x})$ in the output layer. This neural network architecture can be specified as follows.

We take as input to the neural network, a sample $\{V_i\}_{i=1}^{n_{\text{trn}}}$ from $N(0, I_2)$. As explained in Section 2.2, we then train the neural network based on the optimization problem described in (5), where the kernel function $K$ is a mixture of Gaussian kernels with different bandwidth parameters $h = (0.001, 0.01, 0.15, 0.25, 0.50, 0.75)$. Additionally, we use batch normalization and dropout regularization (with dropout rate 0.1) in the hidden layer to help control possible overfitting while training. The neural network is trained for 1000 epochs and the network with the best weights over the entire training process is selected.

```
## NN setup
n.trn <- nrow(U.hat) # number of training obs.
dim.in.out <- d # dimension input and output layers
dim.hid <- 100 # dimension (single) hidden layer
NN.dim <- c(dim.in.out, dim.hid, dim.in.out) # NN
## Define the NN model
NN.model <- FNN(dim = NN.dim,
activation = c("relu", "sigmoid"),
batch.norm = TRUE,
dropout.rate = 0.1,
loss.fun = "MMD")

## Compute residuals and their pseudo-observations
R.hat <- sapply(1:d, function(j) X.trn[,j] - raft.fits[[j]]$predicted)
U.hat <- pobs(R.hat) # corresponding pseudo-obs.

Now we can model the pseudo-observations $\hat{U}_k, k = 1, \ldots, n_{\text{trn}}$, using a neural network $G$. For this illustration, we work with a neural network with a single hidden layer consisting of 100 neurons. Due to its non-expensive and non-vanishing gradients, we use a ReLU activation function $\phi(x) = \max\{0, x\}$ in the hidden layer. Since our target output (the pseudo-observations) lie in $(0,1)^2$, we use a sigmoid activation function $\phi(x) = 1/(1+e^{-x})$ in the output layer. This neural network architecture can be specified as follows.

We take as input to the neural network, a sample $\{V_i\}_{i=1}^{n_{\text{trn}}}$ from $N(0, I_2)$. As explained in Section 2.2, we then train the neural network based on the optimization problem described in (5), where the kernel function $K$ is a mixture of Gaussian kernels with different bandwidth parameters $h = (0.001, 0.01, 0.15, 0.25, 0.50, 0.75)$. Additionally, we use batch normalization and dropout regularization (with dropout rate 0.1) in the hidden layer to help control possible overfitting while training. The neural network is trained for 1000 epochs and the network with the best weights over the entire training process is selected.

```
```
Figure C.3. Scatterplots of empirical predictive distributions produced by RafterNet, one for each of four given covariate realizations along with the corresponding true response realizations (red points) for the height and weight dataset.

### Take the best weights
```r
callbacks = callback_early_stopping
  (monitor = "loss",
   min_delta = 0,
   patience = n.epo,
   restore_best_weights = TRUE))
```

We can now use our trained RafterNet, to make probabilistic predictions for a given covariate $z_k$ by following the procedure summarized in Algorithm 2.1. For our illustration here, we select the observations corresponding to six year old males from our test sample (there was one such observation) and make a probabilistic prediction using $n_{gen} = 1000$ samples of the height and weight for such individual(s).

We repeat the prediction step described in the code above for three additional sets of observations from the test sample, corresponding to 10-year-old females, 43-year-old males, and 67-year-old females, respectively.

### Generate samples from the trained NN
```
n.gen <- 1000 # number of samples to generate
## Generate new observations from hat(C)
U.gen <- rGNN(NN, size = n.gen, pobs = TRUE)
## Convert to empirical margins (residuals)
R.pred <- toEmpMargins(U.gen, x = R.hat)
## Probabilistic prediction using RafterNet
## for the covariate (six year old male)

z1 <- c(age = 6.0, male = 1)
stopifnot(sum( # check for one such combination
  apply(z.tst, 1, function(x) all(x == z1))) == 1)
X.pred1 <- sapply(1:d, # transform to margins
  function(j)
  predict(raft.fits[[j]],
    newdata = z1) + R.pred[,j])
```

### Probabilistic predictions for other covariate combinations (checks also passed)
```
R.pred2 <- toEmpMargins(rGNN(NN, size = n.gen, pobs = TRUE),
  x = R.hat)
## for the covariate (six year old male)

t2 <- c(age = 10, male = 0)
X.pred2 <- sapply(1:d, function(j)
  predict(raft.fits[[j]], newdata = t2) + R.pred2[,j])
```
Figure C.3 displays the probabilistic predictions of the heights and weights for each of these four sets of covariates along with the corresponding true heights and weights of such individuals (represented by red points). From these plots we observe that the empirical predictive distributions indeed roughly concentrate around each of the corresponding height and weight observations.

For each of these four individuals defined by the covariate $z_k = (\text{age}_k, \text{sex}_k)$, we can also predict joint tail probabilities such as $P(X_{k,1} > c_1, X_{k,2} < c_2)$ for any fixed constants $(c_1, c_2)$. Here are some examples.

```r
define the range

mean(X.pred1[,1] >116 & X.pred1[,2] <21) #~ = 0.1
mean(X.pred2[,1] >116 & X.pred2[,2] <21) #~ = 0.247
mean(X.pred3[,1] <158 & X.pred3[,2] >46) #~ = 0.122
mean(X.pred4[,1] <158 & X.pred4[,2] >46) #~ = 0.082
```

Thus, we are able to predict (based on $n_{\text{gen}} = 1000$) that, for a six-year-old male, the probability of him having a height of > 116 and a weight of < 21 is about 10%; for a 10-year-old female, the probability of her having a height of > 116 and a weight of < 21 is about 25%; for a 43-year-old male, the probability of him having a height of < 158 and a weight of > 46 is about 12%; and finally, for a 67-year-old female, the probability of her having a height of < 158 and a weight of > 46 is about 8%.

Finally, we use our RafterNet to make probabilistic predictions of height and weight for all given covariates in the test sample,
$z_k, k = 1, ..., n_{\text{test}}$. As before, we follow the procedure in Algorithm 2.1, but now generate five samples for each given $z_k$ as we iterate over all the $n_{\text{test}} = 100$ observations.

Besides five samples for each $z_k$, we repeat the algorithm outlined in the code above to also construct probabilistic predictions based on one and two samples for each given $z_k$. Figure C.4 displays a scatterplot of the test data of the height and weight dataset in the top panel, along with scatterplots of the three probabilistic predictions considered in the bottom panel. From these plots, we see that the probabilistic predictions essentially match the height and weight test data.

**Disclosure Statement**

The authors report there are no competing interests to declare.

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