Marginally-calibrated deep distributional regression

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August 27, 2019

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Abstract

Deep neural network (DNN) regression models are widely used in applications requiring state-of-the-art predictive accuracy. However, until recently there has been little work on accurate uncertainty quantification for predictions from such models. We add to this literature by outlining an approach to constructing predictive distributions that are ‘marginally calibrated’. This is where the long run average of the predictive distributions of the response variable matches the observed empirical margin. Our approach considers a DNN regression with a conditionally Gaussian prior for the final layer weights, from which an implicit copula process on the feature space is extracted. This copula process is combined with a non-parametrically estimated marginal distribution for the response. The end result is a scalable distributional DNN regression method with marginally calibrated predictions, and our work complements existing methods for probability calibration. The approach is first illustrated using two applications of dense layer feed-forward neural networks. However, our main motivating applications are in likelihood-free inference, where distributional deep regression is used to estimate marginal posterior distributions. In two complex ecological time series examples we employ the implicit copulas of convolutional networks, and show that marginal calibration results in improved uncertainty quantification. Our approach also avoids the need for manual specification of summary statistics, a requirement that is burdensome for users and typical of competing likelihood-free inference methods.

Keywords: Calibration, Copula, Deep neural network, Distributional regression, Likelihood-free Inference.
1 Introduction

Deep models involving multiple layers of latent variables have become extremely popular in applications requiring high predictive accuracy (Goodfellow et al., 2016). In addition to being flexible, these models are scalable to large datasets with high-dimensional features. However, in some applications it is crucial to represent uncertainty in predictions accurately, which is something that naïve applications of deep learning models often fail to do. This has motivated recent research on extensions that are able to capture aspects of the predictive distributions beyond the mean, and on methods to calibrate the full predictive distributions accurately. Our aim in the present work is to review and add to this existing literature in the area of distributional calibration methods for deep neural network (DNN) models.

To do so we develop a new scalable method for ‘distributional deep regression’, by which we mean a DNN regression method that provides predictions for the full distribution. The proposed method uses the implicit copula (Nelsen, 2006, p.51) of a vector of values on a response variable that arises from a DNN regression. We call this variable a ‘pseudo-response’ because it is not observed directly. The resulting copula is a highly flexible deep function of the feature vector, which we combine with a non-parametrically estimated marginal distribution for the observed response variable. The predictive distributions from the model are marginally-calibrated (where the long-run average of the predictive distributions matches the empirically observed margin) and the approach extends the marginally-calibrated regression copula models of Klein and Smith (2019) and Smith and Klein (2019) to deep models. Even though the proposed implicit copula is of very high dimension, the likelihood is easy to compute using Bayesian methods and efficient existing neural net libraries optimized for scalability.

Importantly, all aspects of the predictive distribution—such as the mean, variance, higher order moments and tail behaviour—are learned jointly in this deep regression. To illustrate this, and other advantages of our approach, we first consider the implicit copula of a dense layer feed-forward network, and apply the resulting distributional deep regression to two popular benchmark datasets. In both cases, our approach provides substantially more accurate predictive densities, compared to those obtained from applying the feed-forward network directly to the data with, or without, probability calibration.

However, our main application of this new distributional deep regression model is in
likelihood-free inference. Here, we estimate Bayesian posterior distributions for models with intractable likelihood functions. A posterior distribution is a conditional distribution for the parameters, given data, derived from a data generating process and a Bayesian prior. In cases where the likelihood is intractable, distributional regression methods can be employed to estimate the posterior density using training samples simulated under the joint model, with the parameter as response and the data as features. After fitting the regression, the approximate posterior is obtained as the predictive distribution from the regression with features given by the observed data. The approach we propose is quite general, but in likelihood-free inference applications we show that the marginal calibration property acts to improve uncertainty quantification significantly.

To illustrate the advantages of our approach in likelihood-free inference, we construct the implicit copula of a convolutional network, and apply the resulting distributional deep regression to compute inference for two complex applications in ecological time series considered in Wood (2010) and Fasiolo et al. (2016). Wood (2010) considered the use of likelihood-free inference methods based on summary statistics for inference in state space models where the likelihood may be highly irregular. Wood (2010) developed an approximate likelihood, called the synthetic likelihood, which is based on a Gaussian model for a vector-valued non-sufficient summary statistic, where the summary statistic mean and covariance are estimated for each parameter value by Monte Carlo simulation. Discarding some information by using a non-sufficient summary of the data can lead to a better behaved likelihood function. A recent comparison of full likelihood and synthetic likelihood inference is given in Fasiolo et al. (2016), where some typical applications in ecology and epidemiology are described. Bayesian implementations of synthetic likelihood are discussed in detail in Price et al. (2018). There are alternative likelihood-free inference methods that can be applied for time series data, most notably the approximate Bayesian computation (ABC) framework (Sisson et al., 2018). A recent discussion of ABC methods for time series is given in Frazier et al. (2019). Frazier et al. (2019) consider ABC approaches to forecasting, and suggest that accurate estimation of the posterior on parameters may not be needed for this purpose. However, like synthetic likelihood and its extensions, ABC methods require suitable summary statistics for the data. Even without the requirement that these statistics be multivariate normal for every parameter value, choosing statistics that are informative and low-dimensional is difficult. A major advantage of our proposed approach is that manually specified summary
statistics are not required, and instead the whole dataset is used as the feature vector in
a regression model. A further comparison of our approach and alternative likelihood-free
inference methods is given in Section 5.

The rest of the paper is organized as follows. Section 2 introduces deep learning regression
models, including uncertainty quantification of predictions from such models. Section 3
shows how the copula smoother of Klein and Smith (2019) can be extended to the DNN case,
including efficient implementation and calculation of the predictive distributions. Section 4
illustrates our approach using dense layer feed-forward networks for two benchmark datasets.
Section 5 reviews likelihood-free inference, and uses an implicit copula constructed from a
convolutional network to compute likelihood-free inference in two complex ecological time
series models. A comparison to some leading alternative approaches is also provided, while
Section 6 concludes.

2 Deep Learning for Regression

In this section we briefly introduce deep learning regression models, and review the existing
literature on uncertainty quantification for deep learning.

2.1 Deep learning regression models

Suppose we observe \( n \) response and features pairs \((Z_i, x_i), i = 1, \ldots, n\), where \( Z_i \) is the
\( i \)th scalar response and \( x_i = (x_{i1}, \ldots, x_{ip})^\top \) is the corresponding vector of \( p \) feature values.

A feed-forward neural network specifies a function of the input features as a convolution,
written as a sequence of transformations called ‘layers’. The feature vector, \( x \), enters the
model at an initial input layer, while the final transformation gives the predicted response at
an output layer; the intermediate component transformations are the hidden layers. For an
introduction to neural network terminology from a statistical perspective see recent overviews
by Polson and Sokolov (2017) and Fan et al. (2019).

In this paper we consider DNNs for regression with a single output, so that the response
is scalar-valued. The function defined by a DNN can be written as \( f_\eta(x) \), where \( \eta \) is the set
of all parameters (weights) in the network. We assume that the activation function for the
output layer is linear, so that \( f_\eta(x) \) can be written as

\[
f_\eta(x) = \psi_\zeta(x)^\top \beta + \beta_0,
\]

where \( \beta \) are the output layer coefficients, \( \zeta \) are the coefficients of all other layers (so that
\( \eta = (\beta_0, \beta^\top, \zeta^\top)^\top \), and \( \psi_\zeta(x) \) is the vector of \( q \) basis functions defined by the last hidden layer of the network. In general an intercept \( \beta_0 \) is also included, although later in Section 3 we set \( \beta_0 = 0 \) in the output layer because implicit copulas are location free.\(^1\)

Training of a neural network such as (1) is usually done by minimizing a penalized empirical loss function with respect to \( \eta \). A popular loss in regression problems is the squared error over the observed values \( z = (z_1, \ldots, z_n)^\top \) of the response, given by

\[
L(z, f_\eta) = \sum_{i=1}^{n} (z_i - f_\eta(x_i))^2.
\] (2)

A regularization penalty—such as the \( L2 \) or \( L1 \) norm of the weights—is usually added to prevent over-fitting and simplify the optimization. Regularization can also be undertaken in an implicit manner in the optimization algorithm, using a variety of methods such as early stopping, drop-out or batch normalization; see Goodfellow et al. (2016) for an introduction to these ideas. For posterior mode estimation in a Bayesian framework, the loss is equivalent to the negative log-likelihood and an explicit penalty is equivalent to the negative log prior density. When (2) is used in a regression setting, it is equivalent to assuming a homoscedastic Gaussian model, and the simplest way to construct predictive distributions for future responses is to use a Gaussian predictive density, after estimating the response variance. However, in many applications more sophisticated uncertainty quantification is necessary, which is the focus of the current paper.

In our approach we consider an initial DNN regression fit, from which data-dependent basis functions \( \psi_\zeta(x) \) are obtained. We make use of highly optimized standard neural network libraries for the adaptive construction of the basis functions, which will be employed in our Bayesian copula regression model outlined in Section 3. Our methodology is related to that in Nalenz and Villani (2018), where data-dependent basis functions from tree ensemble methods were further used within a Bayesian statistical model with shrinkage priors to obtain uncertainty quantification. The work of Nalenz and Villani (2018), however, is not concerned with marginal calibration, DNN basis functions or any applications to likelihood-free inference.

### 2.2 Uncertainty quantification for deep learning

Gneiting et al. (2007) discuss different ways to gauge the accuracy of uncertainty quan-

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\(^1\)Note that in Section 3 the random variable \( Z_i \) is a pseudo-response, and we construct the implicit copula of its data distribution.
titification in prediction. In this paper we focus on two of these: ‘probability calibration’
and ‘marginal calibration’. Gneiting et al. (2007) define notions of calibration formally by
considering a sequence of forecasting problems indexed by time. “Nature” chooses a distri-
bution \( H_t \) at time \( t \), from which an outcome is drawn, and the forecaster gives a predictive
distribution \( F_t \). Intuitively, probability calibration means that an event predicted to have
probability \( p \) occurs with relative frequency \( p \). This is formalized in Gneiting et al. (2007)
by the requirement that
\[
\lim_{T \to \infty} \frac{1}{T} H_t \circ F_t^{-1}(p) = p,
\]
for all \( p \in (0, 1) \). Roughly speaking, marginal calibration is where the average of nature’s
true distribution should match the average forecast distribution. Marginal calibration occurs
if
\[
\lim_{T \to \infty} \frac{1}{T} \sum_{t=1}^{T} H_t = \lim_{T \to \infty} \frac{1}{T} \sum_{t=1}^{T} F_t,
\]
and if the limits on the left- and right-hand sides above exist. In practice, \( H_t \) is not observed,
but only observations drawn from \( H_t \), and we can consider replacing \( H_t \) with a point mass
at the observed value, which makes the average of \( H_t \) an empirical distribution. In the
current work, the forecaster is a regression model, and \( F_t \) will be a predictive distribution
from such a model. We do not follow the above theoretical framework strictly in our later
development. For example, the definition of a particular ordering of the observations into a
time sequence is artificial in our applications. However, as noted in Gneiting et al. (2007), the
above theoretical framework can be inspirational for related empirical notions of calibration
that are useful in their own right.

In the deep learning literature previous approaches to achieve accurate uncertainty quan-
tification are of two main types, which we discuss separately below.

### 2.2.1 Post-processing calibration adjustments

The first type of approach to deep learning uncertainty quantification uses post-processing
adjustments to achieve probability calibration. The early machine learning literature on this
topic is concerned with classification problems (see Platt (2000) for an early example), while
calibration in regression has received far less attention. One approach for regression is due
to Keren et al. (2018), who consider discretizing a continuous response so that calibration
methods developed for classifiers can be applied. A related method is described in Li et al.
(2019), who consider classification methods which account for the ordering of the discretized response, and where the estimation remains stable even for a fine discretization with possibly very few observations in each class.

Another approach, which we compare to our own later, is due to Kuleshov et al. (2018) and can be briefly explained as follows. Suppose we have a training set of features and responses, and a regression model has been fitted to them. The fitted model provides predictive distributions for the response for any value of the feature vector. Now consider a calibration set of features and responses, which may be disjoint from the training set. For every probability $p \in [0, 1]$ we can ask what is the value $p' = p'(p)$ such that the $p'$-quantiles of the predictive distributions upper bound a relative frequency of $p$ of the responses in the calibration set? We then adjust all predictive distributions such that the $p$-quantile is changed to the corresponding $p'$-quantile. This adjustment can be achieved using isotonic regression for a set of $p$ and $p'$ pairs, and is a form of probability calibration.

The method we describe in Section 3 ensures that the marginal distribution of the model response matches an empirically estimated marginal distribution. However, whether the ergodic averaging of predictive distributions leads to equality with the model marginal distribution is something that depends on the properties of the implicit regression copula. We show that the average predictive distribution from our method reproduces the empirically estimated marginal well in the examples.

Kuleshov et al. (2018), in their discussion of the notion of marginal calibration in Gneiting et al. (2007), state that “We found that their notion of marginal calibration was too weak for our purposes, since it only preserves guarantees relative to the average distribution.” We show that, in certain cases, the notion of marginal calibration can be highly constraining, so that marginal calibration methods are an interesting complement to probability calibration post-processing methods. In our experience, these methods are particularly useful when the response distribution is skewed, heavy-tailed, or involves a range constraint.

2.2.2 Distributional regression approaches

Post-processing calibration methods are not the only way to improve uncertainty quantification for deep learning models in regression. An alternative is to use more flexible models which are able to capture complex features of the response distribution beyond the mean. In the context of deep learning, loss functions equivalent to Gaussian log-likelihoods with
heteroscedasticity have been considered (Kendall and Gal (2017); Lakshminarayanan et al. (2017), among others) where both the mean and log-variance are modelled as functions of the features in a flexible way. However, with such an approach the response distribution is still conditionally Gaussian, which will result in a lack of calibration in some problems. These authors also consider various other innovations designed to improve uncertainty quantification, including uncertainties relating to feature vectors which are unusual compared to the training set. A deep version of quantile regression has been recently considered by Tagasovska and Lopez-Paz (2018) as a method for modelling the whole distribution, but a difficulty here is enforcing monotonicity in the estimated quantiles – although regularization can reduce the extent of any violation of monotonicity it does not prevent it from occurring. Rodrigues and Pereira (2018) consider a deep multi-task quantile learning approach which can help to avoid the crossing quantiles problem. Mixture density networks and their extensions are another neural approach to distributional regression giving enormous flexibility (Bishop, 1994; Uria et al., 2013) but estimation of such models is extremely challenging. Tran et al. (2019) consider using deep learning predictors within conventional generalized linear and generalized linear mixed models. Hubin et al. (2018) also consider generalized linear models with deep learning predictors, focusing on the difficult problem of accounting for model uncertainty in the architecture and suggesting several MCMC algorithms for computation.

Moving beyond neural network methods, there are a wide variety of interesting methods for distributional regression in the wider statistical and machine learning literature. Approaches include Bayesian nonparametric methods of many kinds (Foti and Williamson 2015) and the generalized additive models for location, scale and shape framework of Rigby and Stasinopoulos (2005). The latter authors suggest using complex parametric response distributions which might not lie in the exponential family, and model the mean, scale and shape parameters such as skewness and kurtosis as functions of the covariates. See also Mayr et al. (2012); Klein et al. (2015); Wood et al. (2010) and Umlauf et al. (2018) for related developments. A problem with many existing distributional regression methods is that they do not scale well to large datasets, and so there is certainly a role for computationally cheap distributional regression methods based on calibrating or modifying a simpler model that is easier to fit.

Research on Bayesian methods for training neural networks has also been motivated partly by problems of improved uncertainty quantification. The Bayesian machinery for
constructing predictive distributions where parameter uncertainty is integrated out according to the posterior distribution is a very convenient way of accounting for such uncertainties in predictive inference. Recent work in this direction includes Blundell et al. (2015); Hernandez-Lobato and Adams (2015); Gal and Ghahramani (2016); Khan et al. (2018); Kingma et al. (2015) and Teye et al. (2018) among many others. Pioneering work on Bayesian neural networks was done by MacKay (1992) and Neal (1996). A recent review of deep learning methods emphasizing the connections between existing algorithms and models and Bayesian thinking is given by Polson and Sokolov (2017).

3 Marginally-Calibrated Deep Learning Regression

Klein and Smith (2019) and Smith and Klein (2019) introduce a new approach to distributional regression that uses a copula decomposition to ensure marginal calibration. We outline how to extend this approach to deep learning regression.

3.1 Copula model

Consider $n$ realizations $Y = (Y_1, \ldots, Y_N)^\top$ of a continuous-valued response, with corresponding feature values $x = \{x_1, \ldots, x_n\}$. Following Sklar (1959), the joint density of the distribution $Y|x$ can always be written as

$$p(y|x) = c^\dagger(F(y_1|x_1), \ldots, F(y_n|x_n)|x) \prod_{i=1}^n p(y_i|x_i),$$

(3)

with $y = (y_1, \ldots, y_n)^\top$. Here, $c^\dagger(u|x)$ is a $n$-dimensional copula density with $u = (u_1, \ldots, u_n)^\top$, and $F(y_i|x_i)$ is the distribution function of $Y_i|x_i$; both of which are typically unknown. We call such a copula a ‘regression copula’ because it is a function of the features $x$. In copula modelling it is common to replace $c^\dagger$ in (3) with the density of a parametric copula with parameters $\theta$, and we do so here with $c_{\text{DNN}}(u|x, \theta)$, which is the implicit copula of a DNN regression specified below in Section 3.2. Klein and Smith (2019) suggest calibrating the distribution of $Y_i|x_i$ to its invariant margin, so that density $p(y_i|x_i) = p_{Y}(y_i)$ with distribution function $F_Y$ estimated non-parametrically. Thus, we can write

$$p(y|x, \theta) = c_{\text{DNN}}(F_Y(y_1), \ldots, F_Y(y_n)|x, \theta) \prod_{i=1}^n p_{Y}(y_i).$$

(4)
We stress that even though \( Y_i \big| x_i \) is assumed invariant with respect to \( x_i \), the response is still affected by the features \( x \) though the joint distribution. For example, we show in Section 3.4 that the entire predictive distribution of a future response \( Y_0 \) is a function of the feature vector \( x_0 \).

### 3.2 Regression copula

The key to the success of our approach is the specification of the regression copula with density \( c_{\text{DNN}} \). For this we employ the implicit copula of a pseudo-response vector from a DNN regression model derived as follows. Consider a pseudo-response given by the output layer observed with Gaussian noise, so that if \( \varepsilon_i \) is distributed independently \( N(0, \sigma^2) \),

\[
\tilde{Z}_i = f_{\eta}(x_i) + \varepsilon_i. \tag{5}
\]

Then from (1), the vector of \( n \) realizations \( \tilde{Z} = (\tilde{Z}_1, \ldots, \tilde{Z}_n)^\top \) is given by the linear model

\[
\tilde{Z} = B_\zeta(x)\beta + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2 I), \tag{6}
\]

with \( B_\zeta(x) = [\psi_\zeta(x_1)| \cdots | \psi_\zeta(x_n)]^\top \) an \((n \times q)\) matrix. We assume that \( \zeta \) is known so that the basis functions are fixed, and the procedure for obtaining \( \zeta \) is described later. To produce smooth and efficient estimates we regularize the basis coefficient vectors \( \beta \). In a Bayesian context this corresponds to adopting a shrinkage prior, with a common choice being the conditionally Gaussian prior

\[
\beta | \theta, \sigma^2 \sim N(0, \sigma^2 P(\theta)^{-1}),
\]

where \( P(\theta) \) is a sparse precision matrix that is a function of the regularization parameters \( \theta \).

We extract the copula of the distribution of the pseudo-response vector \( \tilde{Z} \) with \( \beta \) integrated out. Such a copula is either called an ‘implicit’ (McNeil et al., 2005, p.190) or ‘inversion’ (Nelsen, 2006, p.51) copula because it is constructed by inverting Sklar’s theorem. The copula is \( n \)-dimensional with a dependence structure that is a function of the feature values \( x \). To derive this copula, first notice that integrating \( \beta \) out of the linear model at (6) gives the Gaussian distribution

\[
\tilde{Z} | x, \sigma^2, \theta \sim N \left( 0, \sigma^2 \left( I + B_\zeta(x)P(\theta)^{-1}B_\zeta(x)^\top \right) \right),
\]

which is derived in Sec.2.1 of Klein and Smith (2019). The implicit copula of this distribution is called the Gaussian copula (Song, 2000), and it is constructed by standardizing
the distribution above to have zero mean and unit variances. To do so here, we set $Z = (Z_1, \ldots, Z_n)\top = \sigma^{-1}S(x, \theta)\tilde{Z}$, where $S(x, \theta) = \text{diag}(s_1, \ldots, s_n)$ is a diagonal scaling matrix with elements $s_i = (1 + \psi_\zeta(x_i)^\top P(\theta)^{-1}\psi_\zeta(x_i))^{-1/2}$, which ensures that $Z_i|x, \sigma^2, \theta \sim N(0, 1)$.

Following Song (2000) and many others, the resulting Gaussian copula has density

$$c_{\text{DNN}}(u|x, \theta) = \frac{p(z|x, \sigma^2, \theta)}{\prod_{i=1}^n p(z_i|x, \sigma^2, \theta)} = \frac{\phi_n(z; \mathbf{0}, R(x, \theta))}{\prod_{i=1}^n \phi_1(z_i)},$$

where

$$R(x, \theta) = S(x, \theta) \left(I + B_\zeta(x)P(\theta)^{-1}B_\zeta(x)^\top\right) S(x, \theta),$$

$z_i = \Phi_1^{-1}(u_i)$, $z = (z_1, \ldots, z_n)\top$, and $\phi_n(\cdot; \mathbf{0}, R)$ and $\phi_1$ are the densities of $N_n(\mathbf{0}, R)$ and $N(0, 1)$ distributions, respectively.

Because $\sigma^2$ does not feature in the expression for $c_{\text{DNN}}$, it is therefore unidentified, so that we simply set it equal to 1 throughout the rest of the paper. This is because implicit copulas are always invariant to the scale of the pseudo-response. Also, while the copula is $n$-dimensional—and therefore potentially of very high dimension—the matrix $R$ at (8) is a parsimonious function of $\theta$. Klein and Smith (2019) give expressions for $R$ for three different shrinkage priors, and we consider two different choices here:

**Horseshoe:** The horseshoe prior is attractive due to its robustness, local adaptivity and analytical properties (Carvalho and Polson, 2010). It is a scale mixture, where $\beta_j|\lambda_j \sim N(0, \lambda_j^2)$, with prior $\pi_0(\lambda_j|\tau) = \text{Half-Cauchy}(0, \tau)$ and $\pi_0(\tau) = \text{Half-Cauchy}(0, 1)$. With this prior $\theta = \{\lambda, \tau\}$, with $\lambda = (\lambda_1, \ldots, \lambda_q)'$, while

$$R(x, \theta) = S(x, \theta) \left(I + B_\zeta(x)\text{diag}(\lambda_1, \ldots, \lambda_q)^2B_\zeta(x)^\top\right) S(x, \theta).$$

**Ridge:** The ridge prior is one of the simplest forms of shrinkage priors, where $\beta_j|\tau^2 \sim N(0, \tau^2)$ and we use the scale-dependent prior of Klein and Kneib (2016) for $\tau^2$. With this prior $\theta = \{\tau^2\}$, while

$$R(x, \theta) = S(x, \theta) \left(I + \tau^2B_\zeta(x)B_\zeta(x)^\top\right) S(x, \theta).$$

Last, to see the link between the two regression copulas in (3) and (4), it is straightforward to see that $c^\dagger(u|x) = \int c_{\text{DNN}}(u|x, \theta)p(\theta)d\theta$ for some prior density $p(\theta)$. Klein and Smith (2019) highlight that even though $c_{\text{DNN}}$ is a Gaussian copula, $c^\dagger$ can be far from a Gaussian.

\footnote{We stress that this does not mean the observed response $Y_i$ has unit variance, but instead has a marginal variance given by $F_Y$.}
copula, although its computation through integration with respect to \( \theta \) has to be undertaken numerically.

### 3.3 Estimation

We employ a multi-stage estimator with the following three steps:

**Algorithm 1 (Estimation of Distributional Deep Regression)**

1. Estimate the marginal \( F_Y \) using a non-parametric estimator, for which we use the kernel density estimator of Shimazaki and Shinomoto (2010).
2. Given \( F_Y \), compute pseudo-response values \( z_i = \Phi_1^{-1}(F_Y(y_i)) \), for \( i = 1, \ldots, n \). Using existing neural net libraries applied to \( z = (z_1, \ldots, z_n) \top \), construct output layer basis functions, and evaluate them at the feature values to obtain \( B_{\zeta}(x) \).
3. Given \( F_Y \) and \( B_{\zeta}(x) \), compute the posterior distribution \( \theta|y \) of the copula parameters using Markov chain Monte Carlo.

Step 2 is dependent upon the choice of architecture, which we discuss later in the context of each application. Step 3 is the main challenge, where computing the posterior requires evaluation of the likelihood, which is given by the copula decomposition at (4). To do so directly requires evaluation of the copula density at (7), which is computationally infeasible in general because of the need to invert the \( n \times n \) matrix \( R \). Klein and Smith (2019) solve this problem by instead using the likelihood conditional on \( \beta \), which is

\[
p(y|x, \beta, \theta) = p(z|x, \beta, \theta) \prod_{i=1}^{n} \frac{p_Y(y_i)}{\phi_1(z_i)}
\]

\[
= \phi_n(z; S(x, \theta)\beta, S(x, \theta)^2) \prod_{i=1}^{n} \frac{p_Y(y_i)}{\phi_1(z_i)},
\]

and can be evaluated in \( O(n) \) operations because \( S(x, \theta) \) is diagonal. These authors propose standard MCMC schemes that generate \( \beta \) and \( \theta \), so that \( \beta \) is integrated out in a Monte Carlo manner and direct computation of \( R \) is avoided. We refer readers to Klein and Smith (2019) for further details on these samplers, which produce draws \{\((\beta^1, \theta^1), \ldots, (\beta^J, \theta^J)\)\} from the augmented posterior distribution \( \beta, \theta|y \).
3.4 Predictive densities

The predictive density \(p(y_0| x_0)\) of a new observation of the response \(Y_0\), given new feature values \(x_0 = (x_{01}, \ldots, x_{0p})^\top\), is estimated using its Bayesian posterior predictive density

\[
p(y_0| x_0, x, y) = \int p(y_0| x_0, x, \beta, \theta)p(\beta, \theta| y) d(\beta, \theta).
\]

If \(z_0 = \Phi^{-1}(F_Y(y_0))\), then \(\frac{dz_0}{dy_0} = \phi_1\), and the first term in the integrand above can be computed by changing variables from \(y_0\) to \(z_0\), giving

\[
p(y_0| x_0, x, \beta, \theta) = \frac{p_Y(y_0)}{\phi_1(\Phi^{-1}(F_Y(y_0)))} \frac{1}{s_0} \phi_1 \left( \frac{\Phi^{-1}(F_Y(y_0)) - f_n(x_0)}{s_0} \right),
\]

which follows from (5) with \(\sigma^2 = 1\), so that \(Z_i = s_i \tilde{Z}_i \sim N(s_i f_n(x_i), s_i^2)\).

Last, the predictive regression density is evaluated using the Monte Carlo draws to compute the integral, giving the density estimate

\[
\hat{p}_0(y_0| x_0) = \frac{p_Y(y_0)}{\phi_1(\Phi^{-1}(F_Y(y_0)))} \left\{ \frac{1}{J} \sum_{j=1}^J \phi_1 \left( \frac{\Phi^{-1}(F_Y(y_0)) - \hat{f}_n^j(x_0)}{s^{[j]}_0} \right) \right\},
\]

where \(\hat{f}_n^j(x_0) = B_\zeta(x_0)^\top \hat{\beta}^{[j]}\) and \(s^{[j]}_0 = (1 + \psi_\zeta(x_i)^\top P(\theta^{[j]})^{-1} \psi_\zeta(x_i))^{-1/2}\).

The density forecast (10) is readily computed using the output of Algorithm 1 for any point in the feature space. This is the approach we employ throughout our empirical work. However, to speed up calculation [Klein and Smith (2019)] suggest a second estimator obtained by replacing the summation in (10) with a single term evaluated at the plug-in values \(\hat{\beta} = \frac{1}{J} \sum_{j=1}^J \beta^{[j]}\) and \(\hat{s}_0 = \frac{1}{J} \sum_{j=1}^J s^{[j]}_0\). Empirical work by these authors suggests that using the plug-in values provides a density forecast that is very close to (10).

Last, we stress that in (10) the entire density \(\hat{p}_0(y_0| x_0)\) varies with the feature vector \(x_0\), something that we now highlight in the examples below.

4 Dense Feed-Forward Network Examples

To illustrate our approach we construct a regression copula from a dense layer deep feed-forward network, and apply it to two widely used benchmark regression datasets.

**Description of datasets** The first dataset is the Boston housing data ([Harrison and Rubinfeld](1978)) with \(n = 506\) observations and 14 features, while the second is the Framingham
cholesterol data (Zhang and Davidian, 2001) with $n = 1,044$ observations and 202 features. Both feature sets include binary, categorical and continuous variables, the latter of which we standardize to the unit interval.

**Architecture and benchmarks** We considered our DNN copula (labelled ‘DNCC’) with both ridge and horseshoe regularization priors. For the feed-forward network we used ReLU activation functions for one to three hidden layers, along with a linear activation function for the output layer. At Step 2 of Algorithm 1, we obtained the basis functions of the linear activation layer using the package **keras** in R (Chollet and Allaire, 2018). We found that two hidden layers of size 64 are sufficient and use them combined with L2 regularization and a dropout rate of 0.5. In training the network early stopping was used based on ten-fold cross-validation in both cases, with the optimization run for 200 epochs.

The predictions from the DNCC are compared to two benchmarks. The first is a feed-forward network with the same architecture above, but applied directly to the response data $y$ with $N(0, \sigma^2)$ disturbances and non-zero intercept $\beta_0$ for the output layer (labelled ‘DNN’). The second benchmark is a recalibration of the predictive densities from the DNN obtained using the approach of Kuleshov et al. (2018) (labelled ‘DNN-recalibrated’).

**Measuring accuracy** To judge accuracy of the predictive distributions, they are evaluated at the observed feature values to give predictive densities $\{\hat{p}_1(\cdot|x_1), \ldots, \hat{p}_n(\cdot|x_n)\}$ using (10), from which distribution functions $\{\hat{F}_1(\cdot|x_1), \ldots, \hat{F}_n(\cdot|x_n)\}$ are also computed. From these we constructed the following three measures of accuracy.

(i) The first is a plot of the average predictive density

$$\hat{p}_{\text{marg},n}(y) \equiv \frac{1}{n} \sum_{i=1}^{n} \hat{p}_i(y|x_i),$$

overlaid on a histogram of the response values. We use this plot to assess marginal calibration of the different methods.

(ii) The second is a plot to assess probability calibration. Consider an increasing set of values $0 \leq p_1 < p_2 < \ldots < p_k \leq 1$, and define

$$\tilde{p}_j \equiv \frac{1}{n} \# \left\{ y_i \left| \hat{F}_{i}(y_i|x_i) \leq p_j, \ i = 1, \ldots, n \right. \right\}, \text{ for } j = 1, \ldots, k,$$

The first dataset is available on many webpages, while the second was taken from the **qrLMM** package in R. The latter is longitudinal data, where extra dummy variables were included to account for different individuals.
to be the relative frequency of observations falling below the \(p_j\)-quantile of the predictive distribution, where \# denotes the cardinality of a set. A plot of \(\hat{p}_j\) against \(p_j\) should be close to a 45 degree line if a method produces probability calibrated predictive distributions.

(iii) The third is the mean in- and out-of-sample logarithmic score. To compute the latter we use ten-fold cross-validation as follows. Partition the data into ten approximately equally-sized sub-samples of sizes \(n_k\), denoted here as \(\{(y_{i,k}, x_{i,k}); i = 1, \ldots, n_k\}\) for \(k = 1, \ldots, 10\). For each observation in sub-sample \(k\) we compute the predictive density using the remaining nine sub-samples as the training data, and denote these densities here as \(\hat{p}_{i,k}(y_{i,k}|x_{i,k})\). The ten-fold mean out-of-sample logarithmic score is then

\[
\text{MLS} = \frac{1}{10} \sum_{k=1}^{10} \frac{1}{n_k} \sum_{i=1}^{n_k} \log \hat{p}_{i,k}(y_{i,k}|x_{i,k}).
\]

**Empirical results** To first illustrate the difference in methods, Figures 1 and 2 plot the predictive densities \(\hat{p}_i(\cdot|x_i)\), evaluated at observations in the Boston housing and cholesterol datasets, respectively. For visual clarity, we only plot densities for observations that correspond to every fifth (Boston) and tenth (cholesterol) ordered response values, resulting in roughly 100 predictive densities. Each panel corresponds to a different method, and also includes a histogram of the response values and an adaptive kernel density estimate (KDE). In panel (a) the DNN produces homoscedastic Gaussian densities, whereas in panel (b) the DNN-recalibrated method produces densities that are non-Gaussian, but nevertheless still homoscedastic. In contrast, the DNNC provides non-parametric predictions in panels (c) and (d) which are highly heteroscedastic. As discussed in depth in Smith and Klein (2019), a key strength of the regression copula modelling approach is that the entire predictive distribution—including higher order moments—can vary with feature values.

Figures 3 and 4 show both calibration plots for the different methods and two datasets, and we make three observations. First, the DNN is neither marginally nor probability calibrated. Second, the DNN-recalibrated is probability calibrated well by construction, but this does not lead to marginal calibration, which can be very poor, such as in Figure 3(b). Third, in contrast, the DNNC—whether using either the horseshoe or ridge prior for regularization—exhibits accurate marginal calibration, along with near probability calibration.

Finally, Table 1 reports the in- and out-of-sample mean logarithmic scores for the two
datasets, and we make three observations. First, the DNN performs poorly, which is because
the response distributions are non-Gaussian in both examples. Second, the shrinkage prior
considered for $\beta$ matters, with the predictions from the horseshoe prior superior to those
from the ridge prior in both examples. Last, the predictive performance of the DNNC is
clearly higher than the benchmarks DNN and DNN-recalibrated.

5 Application to Likelihood-Free Inference

In this section we discuss likelihood-free inference. We will discuss here only regression
approaches to likelihood-free inference. For a recent comprehensive overview of alternative
methods see [Sisson et al. (2018)]. We show how to use the distributional deep regression
copula model in Section 3 to compute likelihood-free inference, and highlight the advantage
of marginal calibration—which is an intrinsic aspect of the copula model—in this context. To
illustrate, a regression copula is constructed from a convolutional network, and the resulting
copula model is used to construct likelihood-free inference in two empirical applications.
Convolutional networks are used in situations where the features take the form of a time series
or an image, and the layers of the network can be thought of as extracting local characteristics
of the input and then combining these into increasingly abstract representations. See [Polson
and Sokolov (2017) and Fan et al. (2019)] for further background.

5.1 Likelihood-free inference

5.1.1 Introduction

Let $\rho$ denote the parameters in a parametric statistical model for data observed from a
sampling distribution with density $p(d|\rho)$. Consider Bayesian inference with prior density
$p(\rho)$, and observed data denoted as $d_{\text{obs}}$, so that the posterior density is $p(\rho|d_{\text{obs}})$. Suppose
we can simulate data $(\rho_i, d_i)$, $i = 1, \ldots, n$ as $\rho_i \sim p(\rho)$, $d_i \sim p(d|\rho)$. We refer to the
density $p(\rho, d) = p(\rho)p(d|\rho)$ as the ‘joint model’ for the data and parameters. By definition,
the posterior density is the conditional density of $\rho$ given $d = d_{\text{obs}}$ obtained from this
joint density. In cases where the likelihood function $p(d|\rho)$ is intractable (but can still be simulated from), we can use a regression fitted to the simulated data to approximate the conditional density of $\rho$ given $d$ in the joint model. Fitting a regression model to data $(\rho_i, d_i)$,
$i = 1, \ldots, n$, where $\rho_i$ is the response and $d_i$ is the feature vector, will give a predictive density

5We denote the data vector as $d$, rather than $y$, to avoid confusion with the response values from the distributional deep regression copula model outlined in Section 3.
\( \tilde{p}(\rho|\mathbf{d}) \) for any \( \mathbf{d} \). The predictive density \( \tilde{p}(\rho|\mathbf{d}_{\text{obs}}) \) is then an approximation to the posterior density based on the regression model. Thus, selecting a regression method that produces an accurate density estimate \( \tilde{p}(\rho|\mathbf{d}) \) is key to conducting accurate likelihood-free inference in this approach.

Later we consider only modelling scalar functions of \( \rho \) in the regression, rather than a multivariate regression model. Posterior distributions for one-dimensional functions of the parameter are enough for scientific inferences in most cases, although the joint posterior is needed for some purposes such as full posterior predictive inference. Multivariate extensions of our methods are left to future work.

### 5.1.2 Advantage of marginal calibration

For simplicity, we denote scalar functions of \( \rho \) as \( \rho \). Then the marginal distribution for the regression training data \( \rho_i \sim p(\rho), \ i = 1, \ldots, n \) is the prior \( p(\rho) \). In this case, marginal calibration as defined in Section 2.2 occurs when the marginal distribution for \( \rho \) (i.e. \( p(\rho) \) here) matches the average posterior predictive density \( \frac{1}{n} \sum_{i=1}^{n} \tilde{p}(\rho|\mathbf{d}_i) \) from the regression model. Moreover, this average is a sample-based estimate of \( \int \tilde{p}(\rho|\mathbf{d}) p(\mathbf{d}) d\mathbf{d} \), because the values \( \mathbf{d}_i \) are simulated from density \( p(\mathbf{d}) = \int p(\rho)p(\mathbf{d}|\rho) d\rho \). Therefore, if the marginal calibration property holds for the regression method then we have

\[
\frac{1}{n} \sum_{i=1}^{n} \tilde{p}(\rho|\mathbf{d}_i) \approx \int \tilde{p}(\rho|\mathbf{d}) p(\mathbf{d}) d\mathbf{d} = p(\rho). \tag{11}
\]

To highlight why it is advantageous for such a property to hold, write the joint Bayesian model as \( p(\rho, \mathbf{d}) = p(\mathbf{d})p(\rho|\mathbf{d}) \) and then notice that

\[
p(\rho) = \int p(\rho|\mathbf{d})p(\mathbf{d}) d\mathbf{d}, \tag{12}
\]

which shows that marginal calibration always holds for the true posterior density. Thus it is desirable for the regression-based approximations to the posterior to respect this kind of calibration also.

### 5.1.3 Previous flexible regression models for likelihood-free inference

The use of flexible regression models for conditional density estimation in likelihood-free inference is not new. For example, \cite{Fan2013} consider flexible regression models for approximating the summary statistic distribution, and hence the likelihood, based on a copula of a mixture and flexible mixture of experts regression estimates of summary statistic marginal distributions. \cite{Raynal2018} consider applying the quantile regression forests
method of Meinshausen (2006) to likelihood-free inference. Izbicki and Lee (2017) describe methods for converting high-dimensional regression methods into flexible conditional density estimators using orthogonal series estimators, and Izbicki et al. (2019) consider initial estimates obtained from an ABC sampler, and then applying nonparametric conditional density estimators which make use of a surrogate loss function to estimate the conditional density locally. Papamakarios and Murray (2016) consider a neural network approach using a sequential decomposition of the posterior into conditional distributions and mixture density network models for the conditionals. They also consider the use of a sequential design strategy to concentrate more on the high posterior probability region of the parameter space. Further improvements on this methodology are given in Lueckmann et al. (2017). Papamakarios et al. (2019) consider autoregressive flows to learn approximations to the likelihood, avoiding the difficulties of removing the bias arising from the use of proposal in the sequential design step in Papamakarios and Murray (2016) and Lueckmann et al. (2017). However, methods such as those of Papamakarios et al. (2019) and Fan et al. (2013) require use of a conventional Bayesian computational algorithm for summarizing the posterior once the approximate likelihood has been obtained. Heteroscedastic neural network methods have also been used in post-processing adjustments of conventional ABC samplers (Blum and François, 2010), where empirical residuals are used within the fitted regression model to give particle approximations to the posterior. The method of Blum and François (2010) builds on an earlier seminal paper of Beaumont et al. (2002).

Many of the regression methods discussed above require the use of summary statistics for their application. The method we develop here does not require summary statistics, and makes use of convolutional neural networks for the mean specification, where the time series is used directly for the features in the regression. Jiang et al. (2017) is the first work that we know of considering the use of deep learning methods to automate the choice of summary statistics in likelihood-free inference, although they do not consider convolutional networks. Convolutional networks have been used in likelihood-free inference for time series by Dinev and Gutmann (2018), where similar to Jiang et al. (2017) the regression is being used as an automated way of obtaining summary statistics, rather than for density estimation in itself. Greenberg et al. (2019) suggest a way to use a proposal which focuses on a relevant part of the parameter space without the difficulties of the proposal corrections in Papamakarios and Murray (2016) and Lueckmann et al. (2017), and also avoiding additional computations after
the conditional density estimation step. In their method, a parametrized family of approximations is considered, such as Gaussian or a mixture of Gaussians, and a mapping from the data to the parameters in the approximation is learned using a certain loss function. In the case of time series data, it may be possible to avoid the use of summary statistics using this approach for a suitable neural network parametrization of the function mapping the data to the parameters of the approximation. The difficulties of training increase with increasingly flexible parametric approximating families, as one would expect. In contrast, the semiparametric approach proposed here has only very modest computational demands. The general principle of marginal calibration could be applied in conjunction with some of the other flexible regression methods described above, and in that sense it represents a complementary direction in the existing literature on flexible regression methods in likelihood-free inference.

5.2 Convolutional network examples

In the context of likelihood-free inference for time series models, Dinev and Gutmann (2018) considered using a convolutional neural network (CNN) regression model to predict the components of the parameter vector $\rho \in \mathbb{R}^p$ based on data $d = (d_1^T, \ldots, d_T^T)^T$, using a training set of simulations of pairs $(\rho_k, d_k)$ which are generated from the joint model. Dinev and Gutmann (2018) consider multivariate outputs to predict all parameters jointly and use the predictions of the network as an automated summary statistic choice. Here we will use the DNN regression copula model in Section 3 as a distributional regression method to directly estimate marginal posterior distributions of the elements of $\rho$.

In the following we show the potential of our proposed approach (labelled as DNNC as in the previous subsection) in two complex ecological time series examples. In both examples we consider 10,000 data sets simulated under the prior, and use 8,000 data sets for training and 2,000 for testing, denoted as $\{d_i\}$ and $\{d_i^*\}$, respectively. The simulated series have the same length $T$ as the observed data. Since for simulated data the true parameter values are known, we can assess different likelihood-free inference methods according to how well the true parameter values are predicted from the corresponding data. We also report results for the real data and use data splitting and predictive assessment of the quality of point estimates using a composite scoring role to to judge the accuracy of different methods.

Nicholson’s blowfly model As the first example we consider the Nicholson’s Blowflies data of experiment E2 of a series of laboratory experiments to elucidate the population
dynamics of sheep blowfly (*Lucilia cuprina*) under resource limitation reported by Nicolson (1954). To model the observed dynamics and to make the model feasible, Wood (2010) propose the model \( d_t = r_t + s_t \) for the population at time \( t \), where

\[
r_t \sim \text{Poi}(Pn_{t-\tau} \exp(-n_{t-\tau}/n_0)e_t).
\]

represents the delayed recruitment process with model parameters \( P, n_0, \tau, \delta \), while

\[
s_t \sim \text{Binom}(\exp(-\delta e_t), n_{t-1}),
\]

is the adult survival process and \( e_t, \epsilon_t \) are independent gamma disturbances with unit mean and variances \( \sigma^2_p \) and \( \sigma^2_d \) respectively. Consequently, \( p = 6, \rho = (\delta, P, n_0, \sigma^2_p, \tau, \sigma^2_d) \) and the length of the series is \( T = 275 \). We use the prior for \( p(\rho) \) specified in Table 13 of Fasiolo et al. (2016), see Table 2 for details.

**A chaotic prey-predator model for modelling voles abundance** The second model we consider has been used by Fasilio and Wood (2018) to describe the dynamics of Fennoscandian voles (*Microtus and Clethrionomys*). There has been an observed shift in voles abundance dynamics from low-amplitude oscillations in central Europe and southern Fennoscandia to high-amplitude fluctuations in the north. One possible reason is the absence of generalist predators in the north, where voles are hunted primarily by weasels (*Mustela nivalis*). In the notation of Fasilio and Wood (2018), the predator-prey dynamics are given by the following system of differential equations (Turchin and Ellner, 2000)

\[
\frac{dN}{dt} = r(1 - e \sin(2\pi t))N - \frac{r}{K}N^2 - \frac{GN^2}{N^2 + H^2} - \frac{CNP}{N + D} + N \frac{dw}{K dt}
\]

\[
\frac{dP}{dt} = s(1 - e \sin(2\pi t))P - sQ\frac{P^2}{N},
\]

where \( dw(t_2) - dw(t_1) \sim N(0, \sigma^2(t_2 - t_1)), t_2 > t_1, \) is a Brownian motion process with constant volatility \( \sigma \); and \( N \) and \( P \) represent voles and weasels abundances, respectively. Turchin and Ellner (2000) considered a mechanistic version of this model without the driving Brownian motion, and investigate the effects of environmental noise through perturbing the model parameters. The model is formulated in continuous time, with the parameters \( r \) and \( s \) representing intrinsic population growth rates of voles and weasels respectively, while \( K \) is the carrying capacity of \( r \). Averaging of these parameters is done over the seasonal component with amplitude \( e \) and period equal to one year. Peak growth is achieved in summer. Further, \( G \) and \( H \) as well as \( C \) and \( D \) are the parameters of type II and III functional response models of generalist predation and predation by weasels, respectively;
see Fasilio and Wood (2018) for further details. These authors assume the number of trapped voles to be Poisson distributed, \( d_t \sim \text{Poi}(\Phi N_t) \), at times \( t \in \{1, \ldots, T\} \) when trapping took place. Finally, the model is not fitted directly to data but rescaled to a dimensionless form, where

\[
\frac{dn}{dt} = r(1 - e \sin(2\pi t))n - rn^2 - \frac{gn^2}{n^2 + h^2} - \frac{anp}{n + \delta} + n \frac{dw}{dt}
\]

\[
\frac{dp}{dt} = s(1 - e \sin(2\pi t))p - s \frac{p^2}{n}
\]

\( d_t \sim \text{Poi}(\phi n_t) \).

We used the same strategy as Fasilio and Wood (2018) to arrive at \( T = 90 \) data points collected during the spring (mid-June) and autumn (September) of each year between 1952 and 1997. The prior on the parameter \( \rho = (r, e, g, h, a, \delta, s, \sigma, \phi) \) is specified in Table 3.

**CNN specification** To set up the basis functions for our DNNC in Step 2 of Algorithm 1, we fitted separate CNNs for each model parameter in turn (six parameters in the case of the blowfly model, nine in the case of the voles abundance model) with pseudo-responses \( z \) as outputs and the simulated series as features. Beginning with the generic architecture suggested in Dinev and Gutmann (2018) and experimenting also with other specifications, we ended up using two convolutional layers with \( 31/7 \) filters, and kernel sizes of \( 31/10 \) for the blowfly and voles data respectively. In the later cross-validation comparisons where training based on the first 80% of the series is considered, the kernel sizes were \( 31/8 \) for the blowfly and voles data, respectively. We used ReLU activation functions for the convolutional layers followed by two dense layers of sizes \( 100/1 \) and ReLU/linear activation functions for the first and second dense layers respectively. It is important to not normalize the inputs as this may destroy the time series structure. Instead we use batch normalization after each layer. As proposed by Dinev and Gutmann (2018) we apply a max-pooling layer after the first convolutional layer and a flattening layer after the second one. Extracting the resulting basis functions was done as in the previous subsection using the keras package.

**Benchmark models** To compare or DNNC method with, we consider the following leading benchmark methods:

(i) **DNN**: the same DNN as used to construct the copula, but applied directly to the
original response values as outputs, and with Gaussian errors in the output layer.

(ii) **ABC**: the method of [Blum and François, 2010] with a DNN regression adjustment, as implemented in the R package `abc` by [Csilléry et al., 2012]. We found that using the maximal possible size of 30 for the number of nodes in the hidden layer of the DNN worked best. The $L2$ regularization parameter for the weights in the neural network was chosen by cross-validation, and with a tolerance of one that corresponds to no rejection step in the ABC procedure, which is recommended for high-dimensional settings. Bounded parameters were transformed to the real line used logistic transformations.

(iii) **ABCrF**: ABC with random forests, as implemented in the R package `abcrf` by [Marin et al., 2017]. For tuning the ABCrF method, we used 500 trees and tuned several other algorithmic parameters (mtry, the number of randomly chosen features to consider for splits in the trees, sample.fraction the sample fraction of points used in constructing the trees and min.node.size, the node size at which splitting stops) using the `tuneRanger` package [Probst et al., 2018], see Tables 4 and 5 for the optimal hyperparameter settings obtained. Raynal et al. (2018) emphasize increasing training sample size to control variability and monitoring out-of-bag error. However, in a simulation study it is not possible to adaptively increase the training sample size based on one of the methods. The default random forests implementation gives poor results with the sample size used here, with overfitting evident in both examples, but after tuning with the `tuneRanger` package performance was greatly improved.

(iv) **BSL**: the Bayesian synthetic likelihood approach implemented in the R package `BSL` by [An et al., 2019]). This is the most computationally expensive method considered, and which is why this method is not included in the assessments based on the simulated data. The BSL is run with $10^4$ steps and a diagonal covariance for the proposal until convergence. We then take the covariance of these samples as a proposal for the final run.

(v) **semiBSL**: a semi-parametric version of BSL which estimates the marginal distributions non-parametrically and combines them with a Gaussian copula, as implemented in the R package `BSL`. The settings are the same as for BSL estimator. Both the BSL and semiBSL can experience numerical difficulties if the MCMC starting value is in the posterior tail, so we initialized these using the posterior mean parameters of ABC. The methods BSL, semiBSL, ABC and ABCrF require summary statistics, and we used
the same choices as Fasiolo et al. (2016) and Fasiolo and Wood (2018) (23 statistics for the blowfly data and 16 for the voles data) and implemented in the R packages synlik (Fasiolo and Wood, 2018) and volesModel (available on Github).

**Measures of performance** Tables 6 and 7 report mean squared errors and coverage rates of 95% credible intervals for the logarithm of the parameters in the simulated test data sets for both applications. Figures 5 and 6 depict the average marginal posteriors of the six/nine log-parameters averaging over the 2,000 test replicates, to examine marginal calibration of different methods.

Comparison of the performance of different methods when applied to the observed data, is undertaken using data splitting. Here, the first 80% of the time series is used as training data, while the last 20% is test data used to assess out-of-sample predictive performance. Full posterior predictive inference is not considered, because our own method as well as the ABCrf approach estimates only marginal posterior distributions, but not the full posterior distribution. Figures 7 and 8 show the estimated marginal posterior densities of the parameters $\rho$ for all competing methods. The figures show that inferences can differ substantially between different methods for some of the parameters, particularly for the blowfly data. To examine whether the different fits are reasonable, our predictive comparison of the different methods using data splitting uses a composite scoring rule (Dawid and Musio, 2014) based on plug-in predictive densities using posterior mean point estimates for different methods.

Consider a sequence of pairwise marginal predictive distributions \( \{\hat{p}(d_t, d_{t+1}|\hat{\rho})\} \), with $\hat{\rho}$ being the posterior mean parameters and \((t, t+1)\) consecutive time points in the test part of the series. With point estimates $\hat{\rho}$ obtained from training data $d_1, \ldots, d_K$, and test data consisting of $d_{K+1}, \ldots, d_T$, out of sample predictive performance is measured by the composite logarithmic score (CLS) and composite energy score (CES) defined as

$$\text{CLS} = 1/(T-K-1) \sum_{t=K+1}^{T-1} \log \hat{p}(d_t, d_{t+1}|\hat{\rho}) \quad \text{and} \quad \text{CES} = 1/(T-K-1) \sum_{t=K+1}^{T-1} S_t(d_t, d_{t+1}),$$

where $S_t(\cdot, \cdot)$ is the multivariate energy score for the pair $(d_t, d_{t+1})$ (Gneiting et al., 2008). The multivariate energy score is the natural generalization of the continuous ranked probability score to a multivariate setting. The composite scores CLS and CES are easier to compute than alternative scoring rules that involve looking at a full joint distribution for $(d_{K+1}, \ldots, d_T)^\top$. The bivariate predictive densities are estimated using kernel estimates.
based on Monte Carlo simulation from the model. We report the scores in Table 8, where we compute the negative values so that higher values are better.

**Results** We make four observations on the simulations. First, our DNNC outperforms all benchmark models, with smallest simulation MSE values, and with coverage rates closest to the nominal levels. ABCrf was also a strong performer for the Voles data, although with slightly conservative uncertainty assessments. Second, ABC, DNNC and ABCrf calibrate well marginally, while DNN is poorly calibrated in general. Third, simulation MSE values and coverage rates for the ABC and ABCrf are very similar for the Blowfly example. Finally, in the comparison of different methods based on the composite scoring rules, DNNC is second best for the Blowfly data and the best for the Voles data for the composite energy score. For the composite logarithmic score, DNNC is fourth best for the Blowfly data and second best for the Voles data.

6 Discussion

In this work we have contributed to the growing literature on uncertainty quantification for deep neural network regression models, exploring a marginal calibration approach derived from a deep neural network implicit copula. Our approach is complementary to existing post-processing adjustments of neural network regression approaches which attempt to achieve probability calibration. We have focused particularly on applications to likelihood-free inference for times series models using convolutional networks to avoid the need for hand-crafted summary statistics. In these likelihood-free applications the marginal calibration property has a strong motivation as imposing a consistency requirement on regression approximations to the posterior density that holds for the true posterior density.

We have only been concerned in this work with regressions for a scalar response. In the case of our motivating likelihood-free applications, mostly posterior densities for scalar functions of the parameter are all that are required for scientific inferences, but the joint posterior may be required for purposes such as full posterior predictive inference. It would be possible to extend the approach considered here to a multivariate response. It would also be interesting in future work to apply the marginal calibration principle to other regression-based likelihood-free approximations that have been suggested in the literature.
References

An, Z., South, L. F. and Drovandi, C. C. (2019). *BSL: Bayesian Synthetic Likelihood*. R package version 2.0.0.

Beaumont, M. A., Zhang, W. and Balding, D. J. (2002). Approximate Bayesian computation in population genetics, *Genetics* **162**: 2025–2035.

Bishop, C. (1994). Mixture density networks, Technical Report NCRG/4288, Aston University, Birmingham, UK.

Blum, M. G. B. and François, O. (2010). Non-linear regression models for approximate Bayesian computation, *Statistics and Computing* **20**: 63–75.

Blundell, C., Cornebise, J., Kavukcuoglu, K. and Wierstra, D. (2015). Weight uncertainty in neural network, in F. Bach and D. Blei (eds), *Proceedings of the 32nd International Conference on Machine Learning*, Vol. 37 of *Proceedings of Machine Learning Research*, PMLR, Lille, France, pp. 1613–1622.

Carvalho, C. M. and Polson, Nicholas, G. (2010). The horseshoe estimator for sparse signals, *Biometrika* **97**: 465–480.

Chollet, F. and Allaire, J. J. (2018). *Deep Learning with R*, 1st edn, Manning Publications Co., Greenwich, CT, USA.

Csilléry, K., François, O. and Blum, M. G. B. (2012). ABC: an R package for approximate Bayesian computation (ABC), *Methods in Ecology and Evolution* **3**: 475–479.

Dawid, A. P. and Musio, M. (2014). Theory and applications of proper scoring rules, *METRON* **72**(2): 169–183.

Dinev, T. and Gutmann, M. (2018). Dynamic likelihood-free inference via ratio estimation (DIRE), *arXiv:1810.09899*.

Fan, J., Ma, C. and Zhong, Y. (2019). A selective overview of deep learning, *arXiv preprint arXiv:1904.05526*.

Fan, Y., Nott, D. J. and Sisson, S. A. (2013). Approximate Bayesian computation via regression density estimation, *Stat* **2**(1): 34–48.

Fasiolo, M. and Wood, S. (2018). ABC in ecological modelling, in S. A. Sisson, Y. Fan and M. Beaumont (eds), *Handbook of Approximate Bayesian Computation*, Chapman & Hall, CRC, Boca Raton, pp. 597–623.

Fasiolo, M., Pya, N. and Wood, S. N. (2016). A comparison of inferential methods for highly nonlinear state space models in ecology and epidemiology, *Statistical Science* **31**(1): 96–118.

Fasiolo, M. and Wood, S. (2018). *An introduction to synlik (2014)*. R package version 0.1.2.

Foti, N. J. and Williamson, S. A. (2015). A survey of non-exchangeable priors for Bayesian nonparametric models, *IEEE Transactions on Pattern Analysis and Machine Intelligence* **37**(2): 359–371.
Frazier, D. T., Maneesoonthorn, W., Martin, G. M. and McCabe, B. P. (2019). Approximate Bayesian forecasting, *International Journal of Forecasting* **35**(2): 521–539.

Gal, Y. and Ghahramani, Z. (2016). Dropout as a Bayesian approximation: Representing model uncertainty in deep learning, in M. F. Balcan and K. Q. Weinberger (eds), *Proceedings of The 33rd International Conference on Machine Learning*, Vol. 48 of *Proceedings of Machine Learning Research*, PMLR, New York, New York, USA, pp. 1050–1059.

Gneiting, T., Balabdaoui, F. and Raftery, A. E. (2007). Probabilistic forecasts, calibration and sharpness, *Journal of the Royal Statistical Society Series B* **69**(2): 243–268.

Gneiting, T., Stanberry, L. I., Grimit, E. P., Held, L. and Johnson, N. A. (2008). Assessing probabilistic forecasts of multivariate quantities, with an application to ensemble predictions of surface winds, *TEST* **17**(2): 211–235.

Goodfellow, I., Bengio, Y. and Courville, A. (2016). *Deep Learning*, MIT Press. [http://www.deeplearningbook.org](http://www.deeplearningbook.org).

Greenberg, D. S., Nonnenmacher, M. and Macke, J. H. (2019). Automatic posterior transformation for likelihood-free inference, [https://arxiv.org/abs/1905.07488](https://arxiv.org/abs/1905.07488).

Harrison, D. and Rubinfeld, D. L. (1978). Hedonic prices and the demand for clean air, *Journal of Environmental Economics and Management* **5**: 81–102.

Hernandez-Lobato, J. M. and Adams, R. (2015). Probabilistic backpropagation for scalable learning of Bayesian neural networks, in F. Bach and D. Blei (eds), *Proceedings of the 32nd International Conference on Machine Learning*, Vol. 37 of *Proceedings of Machine Learning Research*, PMLR, Lille, France, pp. 1861–1869.

Hubin, A., Storvik, G. and Frommlet, F. (2018). Deep Bayesian regression models, *arXiv preprint arXiv:1806.02160*.

Izbicki, R. and Lee, A. B. (2017). Converting high-dimensional regression to high-dimensional conditional density estimation, *Electronic Journal of Statistics* **11**: 2800–2831.

Izbicki, R., Lee, A. B. and Pospisil, T. (2019). ABCCCDE: Toward approximate Bayesian computation with complex high-dimensional data and limited simulations, *Journal of Computational and Graphical Statistics* (To appear).

Jiang, B., Wu, T.-y., Zheng, C. and Wong, W. H. (2017). Learning summary statistic for approximate bayesian computation via deep neural network, *Statistica Sinica* pp. 1595–1618.

Kendall, A. and Gal, Y. (2017). What uncertainties do we need in Bayesian deep learning for computer vision?, *Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, 4-9 December 2017, Long Beach, CA, USA*, pp. 5580–5590.

Keren, G., Cummins, N. and Schuller, B. (2018). Calibrated prediction intervals for neural network regressors, *arXiv preprint arXiv:1803.09546*.
Khan, M., Nielsen, D., Tangkaratt, V., Lin, W., Gal, Y. and Srivastava, A. (2018). Fast and scalable Bayesian deep learning by weight-perturbation in Adam, in J. Dy and A. Krause (eds), *Proceedings of the 35th International Conference on Machine Learning, ICML 2018, Stockholmsmässan, Stockholm, Sweden, July 10-15, 2018*, Vol. 80 of *Proceedings of Machine Learning Research*, PMLR, pp. 2611–2620.

Kingma, D. P., Salimans, T. and Welling, M. (2015). Variational dropout and the local reparameterization trick, in C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama and R. Garnett (eds), *Advances in Neural Information Processing Systems 28*, Curran Associates, Inc., pp. 2575–2583.

Klein, N. and Kneib, T. (2016). Scale-dependent priors for variance parameters in structured additive distributional regression, *Bayesian Analysis* 11(4): 1071–1106.

Klein, N., Kneib, T. and Lang, S. (2015). Bayesian generalized additive models for location, scale, and shape for zero-inflated and overdispersed count data, *Journal of the American Statistical Association* 110(509): 405–419.

Klein, N. and Smith, M. S. (2019). Implicit copulas from Bayesian regularized regression smoothers, *To appear in Bayesian Analysis*.

Kuleshov, V., Fenner, N. and Ermon, S. (2018). Accurate uncertainties for deep learning using calibrated regression, *Proceedings of the 35th International Conference on Machine Learning, ICML 2018, Stockholmsmässan, Stockholm, Sweden, July 10-15, 2018*, pp. 2801–2809.

Lakshminarayanan, B., Pritzel, A. and Blundell, C. (2017). Simple and scalable predictive uncertainty estimation using deep ensembles, in I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan and R. Garnett (eds), *Advances in Neural Information Processing Systems 30*, Curran Associates, Inc., pp. 6402–6413.

Li, R., Bondell, H. D. and Reich, B. J. (2019). Deep distribution regression, *https://arxiv.org/abs/1903.06023*.

Lueckmann, J.-M., Goncalves, P. J., Bassetto, G., Öcal, K., Nonnenmacher, M. and Macke, J. H. (2017). Flexible statistical inference for mechanistic models of neural dynamics, in I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan and R. Garnett (eds), *Advances in Neural Information Processing Systems 30*, Curran Associates, Inc., pp. 1289–1299.

MacKay, D. J. C. (1992). A practical Bayesian framework for backpropagation networks, *Neural Computation* 4(3): 448–472.

Marin, J.-M., Raynal, L., Pudlo, P., Robert, C. and Estoup, A. (2017). *abcrf: approximate Bayesian computation via random forests*. R package version 1.7.

Mayr, A., Fenske, N., Hofner, B., Kneib, T. and Schmid, M. (2012). Generalized additive models for location, scale and shape for high dimensional dataa flexible approach based on boosting, *Journal of the Royal Statistical Society: Series C (Applied Statistics)* 61(3): 403–427.
McNeil, A. J., Frey, R. and Embrechts, R. (2005). Quantitative Risk Management: Concepts, Techniques and Tools, Princeton University Press, Princton: NJ.

Meinshausen, N. (2006). Quantile regression forests, J. Mach. Learn. Res. 7: 983–999.

Nalenz, M. and Villani, M. (2018). Tree ensembles with rule structured horseshoe regularization, The Annals of Applied Statistics 12(4): 2379–2408.

Neal, R. (1996). Bayesian Learning for Neural Networks, Lecture Notes in Statistics, Springer New York.

Nelsen, R. B. (2006). An Introduction to Copulas., Springer-Verlag, New York, Secaucus, NJ, USA.

Nicolson, A. J. (1954). An outline of the dynamics of animal populations, Australian Journal of Zoology 2: 9–65.

Papamakarios, G. and Murray, I. (2016). Fast $\epsilon$-free inference of simulation models with bayesian conditional density estimation, in D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon and R. Garnett (eds), Advances in Neural Information Processing Systems 29, Curran Associates, Inc., pp. 1028–1036.

Papamakarios, G., Sterratt, D. and Murray, I. (2019). Sequential neural likelihood: Fast likelihood-free inference with autoregressive flows, in K. Chaudhuri and M. Sugiyama (eds), Proceedings of Machine Learning Research, Vol. 89, pp. 837–848.

Pitt, M., Chan, D. and Kohn, R. (2006). Efficient Bayesian inference for Gaussian copula regression models, Biometrika 93: 537–554.

Platt, J. (2000). Probabilistic outputs for support vector machines and comparison to regularize likelihood methods, in A. Smola, P. Bartlett, B. Schoelkopf and D. Schuurmans (eds), Advances in Large Margin Classifiers, pp. 61–74.

Polson, N. G. and Sokolov, V. (2017). Deep learning: A Bayesian perspective, Bayesian Analysis 12(4): 1275–1304.

Price, L. F., Drovandi, C. C., Lee, A. C. and Nott, D. J. (2018). Bayesian synthetic likelihood, Journal of Computational and Graphical Statistics 27(1): 1–11.

Probst, P., Wright, M. and Boulesteix, A.-L. (2018). Hyperparameters and tuning strategies for random forest, Wiley Interdisciplinary Reviews: Data Mining & Knowledge Discovery.

Raynal, L., Marin, J.-M., Pudlo, P., Ribatet, M., Robert, C. P. and Estoup, A. (2018). ABC random forests for Bayesian parameter inference, Bioinformatics 35(10): 1720–1728.

Rigby, R. A. and Stasinopoulos, D. M. (2005). Generalized additive models for location, scale and shape, Journal of the Royal Statistical Society Series C 54(3): 507–554.

Rodrigues, F. and Pereira, F. C. (2018). Beyond expectation: Deep joint mean and quantile regression for spatio-temporal problems, https://arxiv.org/abs/1808.08798.

Shimazaki, H. and Shinomoto, S. (2010). Kernel bandwidth optimization in spike rate estimation, Journal of Computational Neuroscience 29(1-2): 171–182.
Sisson, S. A., Fan, Y. and Beaumont, M. (2018). *Handbook of Approximate Bayesian Computation*, Chapman & Hall/CRC, New York.

Sklar, A. (1959). Fonctions de repartition a n dimensions et leur marges, *Publ. Inst. Statist. Univ. Paris* 8, 229231 8: 229–231.

Smith, M. S. and Klein, N. (2019). Bayesian inference for regression copulas, *arXiv preprint arXiv:1907.04529*.

Song, P. (2000). Multivariate dispersion models generated from Gaussian copula, *Scandinavian Journal of Statistics* 27(2): 305–320.

Tagasovska, N. and Lopez-Paz, D. (2018). Frequentist uncertainty estimates for deep learning, *arXiv preprint arXiv:1811.00908*.

Teye, M., Azizpour, H. and Smith, K. (2018). Bayesian uncertainty estimation for batch normalized deep networks, *Proceedings of the 35th International Conference on Machine Learning, ICML 2018, Stockholmsmässan, Stockholm, Sweden, July 10-15, 2018*, pp. 4914–4923.

Tran, M.-N., Nguyen, N., Nott, D. and Kohn, R. (2019). Bayesian deep net GLM and GLMM, *Journal of Computational and Graphical Statistics* (To appear).

Turchin, P. and Ellner, S. P. (2000). Living on the edge of chaos: Population dynamics of fennoscandian voles, *Ecology* 81(11): 3099–3116.

Umlauf, N., Klein, N. and Zeileis, A. (2018). BAMLSS: Bayesian additive models for location, scale, and shape (and beyond), *Journal of Computational and Graphical Statistics* 27(3): 612–627.

Uria, B., Murray, I. and Larochelle, H. (2013). RNADE: The real-valued neural autoregressive density-estimator, in C. J. C. Burges, L. Bottou, M. Welling, Z. Ghahramani and K. Q. Weinberger (eds), *Advances in Neural Information Processing Systems 26*, Curran Associates, Inc., pp. 2175–2183.

Wood, S. N. (2010). Statistical inference for noisy nonlinear ecological dynamic systems, *Nature* 466(7310): 1102–1104.

Wood, S. N., Pya, N. and Säfken, B. (2016). Smoothing parameter and model selection for general smooth models, *Journal of the American Statistical Association* 111(516): 1548–1563.

Zhang, D. and Davidian, M. (2001). Linear mixed models with flexible distributions of random effects for longitudinal data, *Biometrics* 57(3): 795–802.
Table 1: Mean logarithmic predictive scores for Boston and Cholesterol datasets.

| Dataset     | DNN ridge | DNN recalibrated | DNNC ridge | DNNC horseshoe |
|-------------|-----------|------------------|------------|----------------|
|             | In-sample log-scores |          |            |                |
| Boston      | -2.7380   | -2.6345          | -2.4933    | **-2.3496**    |
| Cholesterol | -5.1307   | -5.1108          | -4.8332    | **-4.8044**    |
|             | Predictive log-scores |          |            |                |
| Boston      | -2.8612   | -2.6313          | -2.6689    | **-2.5954**    |
| Cholesterol | -5.1642   | -5.0767          | -4.8929    | **-4.8864**    |

Scores are given for all four regression models in columns, and for both in-sample (top half) and out-of-sample (bottom half) predictions. The latter are constructed using ten-fold cross-validation, as discussed in the text. Higher values correspond to more accurate predictive densities, with the highest values for each case in bold.

Table 2: Priors for the parameters of the Blowfly model.

| Parameter | $\delta$ | $P$ | $n_0$ | $\sigma_p^2$ | $\tau$ | $\sigma_d^2$ |
|-----------|----------|-----|-------|---------------|--------|--------------|
| Prior     | U(0.02, 1) | U(3, 30) | U(10, 1000) | U(0.01, 5) | N($\mu = 14$, $\sigma = 5$) | U(0.01, 5) |

Table 3: Priors for the parameters of the Voles model.

| Parameter | Prior           |
|-----------|-----------------|
| $r$       | N($\mu = 5$, $\sigma = 1$) |
| $e$       | N($\mu = 1$, $\sigma = 1$) |
| $g$       | Exp($\lambda = 7$) |
| $h$       | Ga($\kappa = 4$, $\theta = 40$) |
| $a$       | N($\mu = 15$, $\sigma = 15$) |
| $\delta$  | N($\mu = 0.04$, $\sigma = 0.04$) |
| $s$       | N($\mu = 15.5$, $\sigma = 0.5$) |
| $\sigma$  | U(0.5, 30) |
| $\phi$    | U(0.5, 300) |

Table 4: Hyperparameters for ABCrf obtained via the package `tuneRanger` for the Blowfly data.

| Parameter | $\delta$ | $P$ | $n_0$ | $\sigma_p^2$ | $\tau$ | $\sigma_d^2$ |
|-----------|----------|-----|-------|---------------|--------|--------------|
| mtry      | 14       | 21  | 20    | 12            | 6      | 14           |
| min.node.size | 2        | 2   | 4     | 3             | 2      | 2            |
| sample.fraction | 0.86     | 0.61 | 0.58  | 0.58          | 0.80   | 0.62         |
Table 5: Hyperparameters for ABCrf obtained via the package `tuneRanger` for the Voles data.

| Parameter          | r | e | g | h | a | δ | s | σ | φ |
|-------------------|---|---|---|---|---|---|---|---|---|
| mtry              | 5 | 4 | 15| 4 | 16| 14| 11| 8 | 13|
| min.node.size     | 5 | 2 | 118| 105| 6 | 3 | 2 | 8 | 4 |
| sample.fraction   | 0.44| 0.76| 0.21| 0.21| 0.47| 0.24| 0.45| 0.71| 0.45|

Table 6: Simulation results for the Blowfly data

|     | ABC | ABCrf | DNN | DNNC |
|-----|-----|-------|-----|------|
| δ   | 1.35 (0.50) | 1.30 (0.48) | 1.21 (0.62) | 1.02 (0.75) |
| P   | 0.48 (0.82) | 0.50 (0.77) | 0.41 (0.87) | 0.33 (0.89) |
| n₀  | 1.38 (0.54) | 1.41 (0.44) | 1.33 (0.77) | 0.80 (0.95) |
| σ²_p| 1.44 (0.74) | 1.54 (0.67) | 1.05 (0.90) | 0.96 (0.94) |
| τ   | 0.29 (0.70) | 0.31 (0.66) | 0.20 (0.92) | 0.21 (0.96) |
| σ²_d| 1.11 (0.87) | 1.14 (0.86) | 0.92 (0.95) | 0.88 (0.95) |

Each cell gives the mean squared error value, along with coverage of the 95% credible interval in parentheses, of the logarithm of the parameters from the simulated Blowfly test data sets. Each row corresponds to a different parameter, and the columns give results for the ABC, ABCrf, DNN and DNNC methods.

Table 7: Simulation results for the Voles data

|     | ABC | ABCrf | DNN | DNNC |
|-----|-----|-------|-----|------|
| r   | 0.04 (0.94) | 0.02 (0.99) | 0.03 (0.92) | 0.03 (0.94) |
| e   | 0.81 (0.95) | 0.16 (0.99) | 0.24 (0.93) | 0.19 (0.94) |
| g   | 1.56 (0.95) | 1.36 (0.97) | 1.23 (0.94) | 1.17 (0.95) |
| h   | 0.27 (0.95) | 0.25 (0.96) | 0.23 (0.94) | 0.22 (0.95) |
| a   | 0.92 (0.95) | 0.39 (0.99) | 0.39 (0.93) | 0.36 (0.95) |
| δ   | 0.60 (0.95) | 0.32 (0.98) | 0.33 (0.92) | 0.32 (0.94) |
| s   | 0.59 (0.94) | 0.19 (0.98) | 0.19 (0.94) | 0.17 (0.95) |
| σ   | 0.72 (0.94) | 0.21 (0.99) | 0.30 (0.96) | 0.26 (0.93) |
| φ   | 0.32 (0.95) | 0.36 (0.99) | 0.41 (0.97) | 0.34 (0.95) |

Each cell gives the mean squared error value, along with coverage of the 95% credible interval in parentheses, of the logarithm of the parameters from the simulated Voles test data sets. Each row corresponds to a different parameter, and the columns give results for the ABC, ABCrf, DNN and DNNC methods.
Table 8: Composite logarithmic scores and negative energy scores for the Blowfly and Voles datasets.

| Score       | BSL  | semiBSL | ABC   | ABCrf | DNN   | DNNC  |
|-------------|------|---------|-------|-------|-------|-------|
| **Blowfly data** |      |         |       |       |       |       |
| Log-score   | -16.58 | -16.63  | -16.84 | -16.61 | -16.93 | -16.65 |
| neg. energy score | -1967.97 | -1989.98 | -2409.92 | **-1911.50** | -2310.61 | -1923.89 |
| **Voles data** |      |         |       |       |       |       |
| Log-score   | -10.94 | -10.89  | **-10.37** | -11.00 | -14.56 | -10.73 |
| neg. energy score | -48.38 | -50.21  | -46.04 | -45.55 | -66.62 | **-42.26** |

Composite scores are shown for all six regression model in the columns and for both data sets. Higher values correspond to more accurate predictive results with the highest values for each case in bold.
Figure 1: Predictive densities for the Boston housing data.

Results are given for (a) DNN, (b) DNN-recalibrated, (c) DNNC-ridge, and (d) DNNC-horseshoe. Each panel depicts predictive densities $\hat{p}_i(y|x_i)$ (grey lines) for approximately 100 of the $n = 506$ observations. These are selected to correspond to every fifth of the ordered response values. Also shown are a histogram (blue) and KDE (red line) of the response, and the average predictive density $\hat{p}_{\text{marg},n}(y)$ (yellow). Accurate marginal calibration results in the red and yellow lines being very close.
Figure 2: Predictive densities for the Cholesterol data.

Results are given for (a) DNN, (b) DNN-recalibrated, (c) DNNC-ridge, and (d) DNNC-horseshoe. Each panel depicts predictive densities $\hat{p}_i(y|x_i)$ (grey lines) for approximately 100 of the $n = 1,044$ observations. These are selected to correspond to every tenth of the ordered response values. Also shown are a histogram (blue) and KDE (red line) of the response, and the average predictive density $\hat{p}_{\text{marg},n}(y)$ (yellow). Accurate marginal calibration results in the red and yellow lines being very close.
Figure 3: Calibration plots for the Boston housing data.

Panel (a) gives the probability calibration plot, and panel (b) the marginal calibration plot. Results are provided for the DNN (yellow line), DNNC-ridge (blue line), DNNC-horseshoe (red line) and DNN-recalibrated (violet line). Also shown in (b) is the kernel density estimate (grey line) and histogram (grey) of the response.

Figure 4: Calibration plots for the Cholesterol data.

Panel (a) gives the probability calibration plot, and panel (b) the marginal calibration plot. Results are provided for the DNN (yellow line), DNNC-Ridge (blue line), DNNC-Horseshoe (red line) and DNN-Recalibrated (violet line). Also shown in (b) is the kernel density estimate (grey line) and histogram (grey) of the response.
Figure 5: Predictive marginal log-posteriors for the simulated test data from the Blowfly model.

Panels (a) to (f) show the average marginal predictive densities for the four methods ABC (violet line), ABCrf (gray line), DNN (yellow line), DNNC (red line). Also shown in blue is a histogram of the simulated test data.
Figure 6: Predictive marginal log-posteriors for the simulated test data from the Voles model.

Panels (a) to (f) show the average marginal predictive densities for the four methods ABC (violet line), ABCrf (gray line), DNN (yellow line), DNNC (red line). Also shown in blue is a histogram of the simulated test data.
Figure 7: Predictive marginal log-posteriors for the observed test data from the Blowfly model.

Shown are the marginal log-posteriors (averages) of log-parameters for the observed Blowfly data (80% of the series) for the six methods: BSL (green line), semiBSL (blue line), ABC (purple line), ABCrf (gray line), DNN (yellow line), DNNC (red line).
Figure 8: Predictive marginal log-posteriors for the observed test data from the Voles model.

Shown are the marginal log-posteriors (averages) of log-parameters for the observed Blowfly data (80% of the series) for the six methods: BSL (green line), semiBSL (blue line), ABC (purple line), ABCrf (gray line), DNN (yellow line), DNNC (red line).