In scientific inference problems, the underlying statistical modeling assumptions have a crucial impact on the end results. There exist, however, only a few automatic means for validating these fundamental modelling assumptions. The contribution in this paper is a general criterion to evaluate the consistency of a set of statistical models with respect to observed data. This is achieved by automatically gauging the models’ ability to generate data that is similar to the observed data. Importantly, the criterion follows from the model class itself and is therefore directly applicable to a broad range of inference problems with varying data types. The proposed data consistency criterion is illustrated and evaluated using three synthetic and two real data sets.

Introduction

In many scientific applications, statistical models provide a basis for inferences about real world phenomena. These inferences are typically dependent on the model assumptions being correct. However, there are few automatic means of evaluating these assumptions. In this paper, we address the problem of model validation by developing a method that automatically assesses the consistency of a set of models with respect to the observed data.

Let the observed data set be denoted as

\[ \mathbf{y} = \{ \mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n \}, \quad (1) \]

which consists of \( n \) data blocks of equal dimension, referred to as data points. We describe the mechanism that gave rise to the data by a probability density or mass function \( p_0(\mathbf{y}) \), which is unknown to us. In many applications, the objective of statistical inference is to determine certain properties of the unknown function \( p_0(\mathbf{y}) \). Statistical methods typically specify a family or class of probability distributions that aim to model \( p_0(\mathbf{y}) \). We denote this model class as

\[ \mathcal{P}_0 \triangleq \{ p(\mathbf{y} | \theta) : \theta \in \Theta \}, \]

where each model \( p(\mathbf{y} | \theta) \) is indexed by the parameter vector \( \theta \). Our aim in this paper is to assess whether the models in \( \mathcal{P}_0 \) that best approximate \( p_0(\mathbf{y}) \) are consistent with the observed data \( \mathbf{y} \) or not. The idea behind the proposed data consistency criterion (see below) is that if the best models in \( \mathcal{P}_0 \) fail to generate data sets \( \hat{\mathbf{y}} \) that are ‘similar’ to \( \mathbf{y} \), then \( \mathcal{P}_0 \) can hardly be a valid modelling choice for \( \mathbf{y} \). This notion will be made precise in the subsequent sections.

Past research efforts have mostly focused on comparing model classes, let us say \( \mathcal{P}_0 \) and \( \mathcal{P}_0' \), using tools such as the Akaike or Bayesian information criteria and Bayes factors (Akaike, 1974; Schwartz, 1978; Stoica and Moses, 2004). These criteria typically assume that some model class is well specified, meaning that one of the classes contains the unknown \( p_0(\mathbf{y}) \). While the consistency criterion proposed in this paper also can be used for model comparison, our focus here is rather on validation of one specified model class \( \mathcal{P}_0 \).

One established approach to validation is to use a residual-based criterion which assesses whether there is “any information left” in the data after fitting a model. In the restricted context of linear dynamical systems models, such validation criteria are capable of rejecting model classes that are inconsistent with the data, cf. Ljung and Box (1978) and Söderström and Stoica (1989, Ch. 11). For models with assumption of independent and identical distribution of the data points, classical tests such as Cramér-von Mises, Anderson-Darling and Kolmogornov-Smirnov tests are applicable (Anderson and Darling, 1952; Lehmann, 1975). Those tests are, however, constructed only for a single model, not an entire model class.

In the context of Bayesian modelling, validation of a model class can also be performed using posterior predictive checks which require the user to specify a discrepancy measure, cf. Rubin (1984); Gelman et al. (2014); Box (1980).

Our proposed data consistency criterion (DCC) evaluates the ability of a model to generate data similar to the observed one. In contrast to posterior predictive checks, DCC is automatic and does not require the user to specify any quantities except the model class \( \mathcal{P}_0 \) itself. Furthermore, it applies directly to a broad range of model classes with various data types, e.g., linear regression models, count models, hidden Markov models, autoregressive models, etc. In general, \( p(\mathbf{y} | \theta) \) can be factored as \( p(\mathbf{y} | \theta) = \prod_{i=1}^{n} p(y_i | y_1, \ldots, y_{i-1}, \theta) \). DCC is applicable whenever it is possible to point-wise evaluate \( p(y_i | y_1, \ldots, y_{i-1}, \theta) \) for all \( i \), and simulate new data \( \hat{\mathbf{y}} \) from the model, for any given \( \theta \in \Theta \).

As an introductory application of our approach, we consider a modeling problem in seismology. Then, we explain the principles behind DCC for a single model \( p(\mathbf{y} | \theta) \) and, subsequently, for an entire model class \( \mathcal{P}_0 \). DCC is thereafter applied to the seismological problem as an illustration. We also discuss the implementation of the method as well as illustrate how it can be applied to other model classes, including regression, autoregressive and latent variables models. The source code for all experiments is available online.\(^1\)

Motivating example: Earthquake counts

A standard assumption in earthquake analysis is that earthquakes occur independently as described by a Poisson point process. That is, the number of earthquakes in a certain region during a certain time interval is Poisson distributed. However, it is also well-known that earthquakes tend to be clustered (both in time and space), where each cluster typically has several ‘foreshocks’ and ‘aftershocks’ and one large ‘mainshock’. By modeling the earthquakes within a

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\(^1\)https://github.com/saerdna-se/consistency-criterion
cluster as a branching process, the negative binomial distribution has been suggested for earthquake counts (Kagan, 2013). We consider both model classes, $\mathcal{P}_\Theta = \text{Poisson distribution}$ and $\mathcal{P}_\Theta = \text{negative binomial distribution}$, which have one and two free parameters, respectively. We will use our proposed method to assess whether these model classes are consistent with the data $\mathcal{Y}$ for the given model $\Theta$. By contrast, if both aforementioned

\begin{align*}
\text{Data consistency check for a single model}
\end{align*}

We begin by considering a model class consisting of only a single model, i.e., $\mathcal{P}_\Theta = \{ p(y | \theta) \}$ where $\theta$ is a specified parameter. Let $\hat{y} \sim p(y | \theta)$ denote a sample generated from the model and $\mathbb{P}_{\hat{y}(\theta)}(\cdot)$ the probability of an event under the same model.

Initially, consider the simpler case of models in which the data points $i = 1, \ldots, n$ in (1) are assumed to be independent. Let $\bar{z}_i \triangleq \ln p(\hat{y}_i | \theta)$ denote the log-likelihood for the $i$th generated data point, and let its mean be denoted as $\mathbb{E}[\bar{z}_i]$. For the $i$th observed data point, let $\bar{z}_i \triangleq \ln p(y_i | \theta)$. The observed and generated log-likelihoods, $\bar{z}_i$ and $\bar{z}_i$, form the basis of our criterion. Intuitively, if the deviation of $\bar{z}_i$ from $\mathbb{E}[\bar{z}_i]$ is much larger or much smaller than the deviation of $\bar{z}_i$ from $\mathbb{E}[\bar{z}_i]$, we consider the observed data $\mathcal{Y}$ to be atypical for the given model $p(y | \theta)$. More formally, we define the following statistic

\begin{align*}
T(\mathcal{Y}; \theta) &= \frac{1}{n} \sum_{i=1}^{n} \frac{(\bar{z}_i - \mathbb{E}[\bar{z}_i])^2}{\mathbb{V}[\bar{z}_i]},
\end{align*}

where $\mathbb{V}[\bar{z}_i]$ is variance of $\bar{z}_i$. Similarly, we define the statistic $T(\hat{y}; \theta)$ for generated data by replacing $\mathcal{Y}$ with $\hat{y}$. Let us now define the random event of generating a larger statistic than the observed one:

\begin{align*}
S(\hat{y}, \mathcal{Y}) : T(\hat{y}; \theta) > T(\mathcal{Y}; \theta).
\end{align*}

When the probability of this event $\mathbb{P}_{\hat{y}(\theta)}(S(\hat{y}, \mathcal{Y}))$ is close to 0, it is highly improbable that $\mathcal{Y}$ could have been generated by $p(y | \theta)$ and we deem the model to be inconsistent with the observed data. See Fig. 2a for an illustration. This type of inconsistency is due to under-dispersion of the generated log likelihoods, compared to the observed ones. The probability of the complementary event $\mathbb{P}_{\hat{y}(\theta)}(S(\hat{y}, \mathcal{Y})) = 1 - \mathbb{P}_{\hat{y}(\theta)}(S(\hat{y}, \mathcal{Y}))$ indicates inconsistency as well, see Fig. 2b. Also in this case it is improbable that $\mathcal{Y}$ could have been generated by $p(y | \theta)$. By contrast, if both aforementioned probabilities are significantly different from 0, we do not reject the model as inconsistent, see Fig. 2c.

The criterion above is readily generalized to models in which the data points in (1) are dependent, by extending the definition of $z_i$ to

\begin{align*}
z_i \triangleq \ln p(y_i | y_1, \ldots, y_{i-1}, \theta).
\end{align*}

As above, the same symbols $\mathbb{E}[\bar{z}_i]$ and $\mathbb{V}[\bar{z}_i]$ are used to define the mean and variance of $\bar{z}_i$.

If the model were a match of the unknown data-generating distribution, i.e., $p(y | \theta) = p_0(y)$, then the quantity $\mathbb{P}_{\hat{y}(\theta)}(S(\hat{y}, \mathcal{Y}))$ would be uniformly distributed between 0 and 1 with respect to the observed data $\mathcal{Y}$ see the proof below. In this situation, the probability of falsely rejecting the model due to the generated log likelihoods being under-dispersed would be

\begin{align*}
P_{\text{FA}}(\theta) \triangleq \mathbb{P}_{\hat{y}(\theta)}(S(\hat{y}, \mathcal{Y})).
\end{align*}

Thus, when $p(y | \theta) = p_0(y)$, the probability of $P_{\text{FA}}(\theta)$ to be less than $\rho$, is equal to $\rho$. Symmetrically, the false alarm probability due to over-dispersion is $P_{\text{FA}}(\theta) = 1 - P_{\text{FA}}(\theta)$. If neither $P_{\text{FA}}(\theta)$ nor $P_{\text{FA}}(\theta)$ are small, we cannot reject the model $p(y | \theta)$ on the ground that the observed data $\mathcal{Y}$ is atypical, as discussed above.

This criterion, that neither $P_{\text{FA}}(\theta)$ nor $P_{\text{FA}}(\theta)$ is close to $0$, follows automatically from the specified model class and does not require user choices specific to the application scenario. The false alarm probabilities $P_{\text{FA}}(\theta)$ can be approximated numerically using Monte Carlo methods, as we will detail later.

\begin{align*}
\text{Proof of uniform distribution of PFA}
\end{align*}

Let $\xi \triangleq T(\hat{y}; \theta)$, whose distribution is characterized by a cumulative density function denoted $F_{\xi}(x)$. Further, let $\xi \triangleq T(\hat{y}; \theta)$, which allows us to write

\begin{align*}
\mathbb{P}_{\hat{y}(\theta)}(S(\hat{y}, \mathcal{Y})) = \mathbb{P}_{\hat{y}(\theta)}(\xi < \xi) = F_{\xi}(\xi).
\end{align*}

Now, if $\sim p(y | \theta)$, then also the distribution of $\xi$ is characterized by $F_{\xi}$, implying that $F_{\xi}(\xi) \sim U[0, 1]$ according to the probability integral transform (Casella and Berger, 2002, Thm. 2.1.10).

\begin{align*}
\text{Data consistency check for the best models in a class}
\end{align*}

In most applications, $\theta$ is not given. Instead $\mathcal{P}_\Theta$ may consist of a large number of models, possibly an uncountable number when $\Theta \subseteq \Theta$ is continuous. In such a case, we will aim to evaluate the false alarm probabilities $P_{\text{FA}}(\theta)$ and $P_{\text{FA}}(\theta)$ with respect to the models $p(y | \theta)$ that best approximate $p_0(y)$. A natural measure for quantifying the accuracy of the approximation is the Kullback-Leibler divergence (Kullback, 1959). The best models are then defined as those that minimize the divergence:

\begin{align*}
\theta^* \in \arg \min_{\theta} \mathbb{E}[\ln p_0(y) - \ln p(y | \theta)],
\end{align*}

where the expectation $\mathbb{E}$ is with respect to $y \sim p_0(y)$. In particular, if $\theta^*$ exists such that the model divergence attains the minimum value $0$, it follows that $p(y | \theta^*) = p_0(y)$.

Since $p_0(y)$ is unknown, (7) cannot be used to identify the best models. Consequently we resort to an alternative approach. We assign weights to each model in $\mathcal{P}_\Theta$ so as to average the false alarm probability $P_{\text{FA}}(\theta)$ across those models that are likely to be the best.
Figure 2: Consider a data set \( \mathbf{y} = \{ y_i \} \) containing \( n = 7 \) two-dimensional data points (red triangles, upper panels) and assume a Gaussian i.i.d. model \( p(\mathbf{y} | \mathbf{\theta}) \) = \( \prod_{i=1}^{n} p(y_i | \theta_i) \) (green level curves). The log-likelihoods \( \hat{z}_i = \ln p(y_i | \mathbf{\theta}_i) \) for each data point are shown as red triangles in the lower panels. The generated log-likelihoods \( \tilde{z}_i \) follow the distribution illustrated in green in the same panels. When the deviation of \( \tilde{z}_i \) from \( E[\tilde{z}_i] \) is significantly different from that of \( \hat{z}_i \), it is unlikely that the model could have generated the observed sample. The deviation is quantified by the statistic \( T(\mathbf{y}, \mathbf{\theta}) \). The figure illustrates three cases: two cases of inconsistency (a, b) and a balanced case (c).

(a) The observed data points appear as atypical with respect to the model, since they fall into regions of low probability. We obtain \( T(\mathbf{y}, \mathbf{\theta}_a) = 14 \), and the probability of generating a higher statistic is \( P_0(\theta, (S(\hat{y}, \mathbf{\theta}_a))) = 0.00 \). Thus, the dispersion of \( \tilde{z}_i \) is significantly lower than that of \( \hat{z}_i \) and we reject the model as inconsistent with the observed data.

(b) The observed data points appear as atypical with respect to the model, since they are concentrated asymmetrically. We obtain \( T(\mathbf{y}, \mathbf{\theta}_b) = 0.24 \), and the probability of generating a lower statistic is \( P_0(\theta, (S(\hat{y}, \mathbf{\theta}_b))) = 0.04 \). Thus, the dispersion of \( \tilde{z}_i \) is significantly higher than that of \( \hat{z}_i \), and we reject the model as inconsistent with the observed data.

(c) The observed data points appear to be typical samples from the model. We obtain \( T(\mathbf{y}, \mathbf{\theta}_c) = 0.51 \), and the probability of generating a lower statistic is \( P_0(\theta, (S(\hat{y}, \mathbf{\theta}_c))) = 0.39 \). We do therefore not reject the model as inconsistent.

The averaged false alarm probability due to under-dispersion is given by

\[
\text{PFA}_0^\gamma = \int_{\Theta} \text{PFA}_0(\mathbf{\theta}) w(\mathbf{\theta} | \mathbf{y}) \, d\mathbf{\theta}
\]

where the weights \( w(\mathbf{\theta} | \mathbf{y}) \geq 0 \) are high for models in the neighborhood of \( \mathbf{\theta}_0 \), and integrate to unity. By defining

\[
w(\mathbf{\theta} | \mathbf{y}) \triangleq \frac{w_0(\mathbf{\theta}) p(\mathbf{y} | \mathbf{\theta})}{\int_{\Theta} w_0(\mathbf{\theta}) p(\mathbf{y} | \mathbf{\theta}) d\mathbf{\theta}}.
\]

the weights reflect the uncertainty about the location of \( \mathbf{\theta}_0 \) in the parameter space \( \Theta \) (Casella and Berger, 2002; Bissiri and Walker, 2012). The default choice of the initial weights is \( w_0(\mathbf{\theta}) = 1 \). In certain applications, however, we may have prior information about the location of \( \mathbf{\theta}_0 \) in \( \Theta \). Then the initial weights \( w_0(\mathbf{\theta}) \) can be chosen to describe these prior beliefs. Under certain regularity conditions, the weights in (9) concentrate at \( \mathbf{\theta}_0 \) as \( n \to \infty \) if \( \mathbf{\theta}_0 \) is unique, cf. Ljung and Caines (1979) and Berk (1966).

As before, we still have \( \text{PFA}_0^\gamma = 1 - \text{PFA}_0^\gamma \), and we denote our final criterion

\[
\text{PFA}^* = \min \{ \text{PFA}_0^\gamma, \text{PFA}_c^\gamma \}
\]

In summary, the proposed data consistency criterion (DCC) for the model class \( \mathcal{P}_0 \) is the minimum of \( \text{PFA}_0^\gamma \) and \( \text{PFA}_c^\gamma \) ((8)). A value close to 0 indicates that the observed data \( \mathbf{y} \) is atypical for the best models in \( \mathcal{P}_0 \), and thereby we consider the model class \( \mathcal{P}_0 \) to be inconsistent with \( \mathbf{y} \).

Implementation

The averaged \( \text{PFA}^* \) is available in closed-form only in very few special cases, since there are non-trivial integrals in (5), (8), and (9). However, the integrals can be efficiently approximated by Monte Carlo integration techniques, provided that data \( \mathbf{\hat{y}} \) can be generated from \( p(\mathbf{y} | \mathbf{\theta}) \) and that \( p(y_i | y_1, \ldots, y_{i-1}, \mathbf{\theta}) \) can be evaluated point-wise. We outline such a generic Monte Carlo-based implementation\(^3\) in Algorithm 1, where \( N \) parameters are first drawn using \( w(\mathbf{\theta} | \mathbf{y}) \), and then (for each such draw) \( M + M' \) samples of \( \mathbf{\hat{y}} \) are generated from \( p(\mathbf{y} | \mathbf{\theta}) \), giving a computational complexity on the order of \( N(M + M') \).

The operations needed to execute Algorithm 1 are common in most statistical software packages. The weights \( w(\mathbf{\theta} | \mathbf{y}) \) can be computed (at least approximately) by methods that estimate or learn \( \mathbf{\theta} \). Numerical evaluation of the (incremental) likelihoods \( p(y_i | y_1, \ldots, y_{i-1}, \mathbf{\theta}) \), which in Algorithm 1 has to be performed both for generated data \( \mathbf{\hat{y}} \) (line 5) and observed data \( \mathbf{y} \) (line 6), is possible for many statistical models. If \( n \) is large compared to the number of parameters, it can be justified to use the following weights

\[
w(\mathbf{\theta} | \mathbf{y}) = \begin{cases} 1, & \mathbf{\theta} = \mathbf{\hat{\theta}} \\ 0, & \mathbf{\theta} \neq \mathbf{\hat{\theta}} \end{cases},
\]

where \( \mathbf{\hat{\theta}} \) is the maximum likelihood/maximum a posteriori point estimate (in this case \( N = 1 \)).

\(^3\)Where \( 1[\cdot] \) denotes the indicator function.
Algorithm 1: Monte Carlo implementation of DCC (8)

1. Construct $w(\theta | y)$
2. Draw $N$ samples $\theta^{(j)} \sim w(\theta | y)$, $j = 1, \ldots, N$
3. for $j = 1, \ldots, N$ do
   4. Simulate $M'$ data sets $y^{(k)}$ as (4) for all observed data points $y^{(i)}$
   5. Compute $\bar{z}^{(i)}_{\theta^{(j)}}$ as (4) for all observed data points $y^{(i)}$
   6. Compute $\bar{z}^{(i)}_{\theta^{(j)}}$ as (4) for all generated data points $y^{(i)}$
   7. Simulate $M$ data sets $\tilde{y}^{(i)} \sim \mathcal{N}(\mu, \sigma)$, $i = 1, \ldots, M$
   8. Compute $\bar{z}^{(i)}_{\theta^{(j)}}$ as (4) for all generated data points $\tilde{y}^{(i)}$
   9. Compute $\hat{P}_{FA}^*(i)$ as (4) for all observed data points $\bar{z}^{(i)}_{\theta^{(j)}}$
 10. Compute $\bar{T}(j) = \frac{1}{n} \sum_{i=1}^{n} (\bar{z}^{(i)}_{\theta^{(j)}})^2$
 11. Compute $\bar{P}_{FA}^*(i) = \frac{1}{n} \sum_{i=1}^{n} \bar{T}(j) - \bar{T}(j) \geq 0$
 12. Set $\hat{P}_{FA}^* = \frac{1}{n} \sum_{i=1}^{n} \hat{P}_{FA}^*(i)$ and $\hat{P}_{FA}^* = \min(\hat{P}_{FA}^*, 1 - \hat{P}_{FA}^*)$

Magnitude | Poisson distribution | Negative binomial distribution
--- | --- | ---
$\geq 8$ | $PFA^* = 0.40$ | $PFA^* = 0.39$
$\geq 7$ | $PFA^* = 0.29$ | $PFA^* = 0.38$
$\geq 6$ | $PFA^* = 0.00$ | $PFA^* = 0.30$
$\geq 5$ | $PFA^* = 0.00$ | $PFA^* = 0.13$

Figure 3: Assessment of the two earthquake count models (Poisson and negative binomial) for earthquakes of different magnitudes. The low average false alarm probabilities $PFA^*$ for the Poisson distribution suggests that this model class is not consistent with the observed data for magnitudes $\leq 6$.

Examples

Earthquake counts (cont’d)

To assess whether the Poisson or the negative binomial distribution is best suited for the data (partly) presented in Fig. 1, we are now ready to apply the DCC. We use the Monte Carlo approach in Algorithm 1 with $N = 200$ and $M = M' = 200$, and obtain the results in Table 3. From this table we draw the conclusion that the Poisson distribution and the negative binomial distribution are both consistent with the data for earthquakes with magnitude $\geq 7$. However, only the negative binomial distribution is consistent with the data for smaller magnitudes. This result supports the qualitative reasoning in the literature (Kagan, 2013): the Poisson distribution does not take the clustering effects into account, but since each cluster typically does not contain more than one major earthquake, the number of really big earthquakes can still follow the Poisson distribution.

Synthetic data: Gaussian models

To further illustrate the behavior of $PFA^*$, we conduct a simulation study with two toy model classes $\mathcal{P}_0 = \{\mathcal{N}(0, 1)\}$ and $\mathcal{P}_0' = \{\mathcal{N}(\mu, \sigma) : \sigma^2 > 0\}$ with $\theta = \{\mu, \sigma\}$. Note that $\mathcal{P}_0$ contains only a single model. We consider data sets $y \sim p_0(y)$ of different size $n$ and consider two cases: a standard Gaussian distribution $p_0 = \mathcal{N}(0, 1)$ and a standard uniform distribution $p_0 = U(0, 1)$, respectively. We use $N = 50$ and $M = M' = 100$, and evaluate DCC in 1000 experiments. The results are summarized as histograms in Fig. 4.

In the case when data comes from $p_0 = \mathcal{N}(0, 1)$ (Fig. 4a), both $\mathcal{P}_0$ and $\mathcal{P}_0'$ contain $p_0$. However, only the model in $\mathcal{P}_0$ is $p_0$. Thus the averaged $PFA^*$ is uniformly distributed across experiments (of the proof of uniform distribution for $PFA^*$). By contrast, the weights $w(\theta | y)$ for $\mathcal{P}_0'$ concentrate at the best model $p_0$ only as $n \to \infty$. Thus the averaged $PFA^*$ approaches a uniform distribution only asymptotically. Neither model class is falsely rejected more frequently than the PFA indicates.

In the case when data comes from $p_0 = U(0, 1)$ (Fig. 4b), neither $\mathcal{P}_0$ nor $\mathcal{P}_0'$ contains $p_0$. Unlike $\mathcal{P}_0$, however, the best model in $\mathcal{P}_0'$ matches the mean and variance of $p_0$. The inconsistency of the best model is discernible only for data points generated from the distribution tails. Consequently, it takes more samples $n$ to reject the larger model class $\mathcal{P}_0'$ than the $\mathcal{P}_0$. As $n$ increases, both model classes are clearly rejected.

Synthetic data: Regression models

We illustrate the capability of DCC to reject model classes with an inappropriate model order, using the example of polynomial regression. If the observed data is well described by a high-order polynomial, the best model in $\mathcal{P}_0$, which contains models of lower-order polynomials plus noise, will yield a good fit in the likelihood sense because the noise variance is scaled to match the residuals. Such an example is shown in Fig. 5, where the $\mathcal{P}_0$ contains 1st order polynomial models with independent Gaussian noise. When assessing $\mathcal{P}_0$ using DCC,
we obtain \( PFA^* = 0.01 \) (with \( N = M = M' = 100 \)), which clearly indicates an inconsistency. On the other hand, for the model class containing 3rd order polynomials we obtain \( PFA^* = 0.37 \), which (correctly) indicates no inconsistency.

**Synthetic data: Time-series models**

For the case of time-series data driven by white noise, white noise tests such as the Ljung-Box test (Ljung and Box 1978; see also Stoica 1977) are common validation techniques. The Ljung-Box test constructs a p-value from the fact that the statistic
\[
\sum_{k=1}^h \frac{\hat{r}_k^2}{n-k}
\]
will follow a \( \chi^2_{n-d} \) distribution if the model is correct, with \( \hat{r}_k \) being the lag \( k \) sample correlation of the prediction residuals, and \( d \) the dimension of \( \theta \). We set the upper lag limit \( h \) to \( \lceil \log n \rceil \).

We conduct a simulation study with data from the saturated first order autoregressive model \( y_t = \max(0.7y_{t-1} + e_t, -0.3) \), where \( e_t \sim N(0,1) \). We assume a misspecified model class which consists of first-order linear autoregressive models \( \mathcal{P}_m = \{ p(y | \theta) : y_t = a y_{t-1} + e_t, e_t \sim N(0, \sigma^2) \} \), with unknown parameters \( \theta = \{ a, \sigma^2 \} \). We consider cases where \( X \) contains different amount of data samples \( n \), and use \( N = 200 \) and \( M = M' = 200 \) in Algorithm 1.

The results are shown in Fig. 6. As the amount of data \( n \) grows, both methods correctly reject the misspecified model, with the proposed DCC needing slightly less data to do so than the much more specialized Ljung-Box method.

**Latent-variable models: Evolution of a kangaroo population**

Certain models are too complex to be described using closed-form expressions. Instead these models are often parameterized using latent variables \( \eta \) with a prior distribution \( p(\eta | \theta) \). This includes, e.g., hidden Markov or state-space models, mixed-effect models, latent topic models, etc. Then the data distribution can be written as the integral
\[
p(y | \theta) = \int p(y | \eta, \theta)p(\eta | \theta) d\eta,
\] (11)

Figure 5: Data points from \( p_0 \) (3rd order polynomial, blue dots) and model class \( \mathcal{P}_m = \{ 1st \text{ order polynomial} + \text{Gaussian noise} \} \) where \( \theta \) contains the polynomial coefficients and noise variance. A fitted model is shown with \( \theta \) estimated using the maximum likelihood method (black solid line: estimated polynomial, dashed lines: 2 estimated noise standard deviations). While the estimated noise variance produces a good fit in terms of likelihoods, this model class should ideally be rejected. Using DCC for \( \mathcal{P}_m \), we obtain \( PFA^* = 0.01 \) and can reject \( \mathcal{P}_m \). Similarly, for a model class \( \mathcal{P}_m' \) containing 2nd order polynomials we obtain \( PFA^* = 0.01 \). By contrast, for 3rd order polynomials, \( \mathcal{P}_m'' \), we have \( PFA^* = 0.37 \) and this class is correctly found not to be inconsistent with the data.

If the (incremental) likelihoods \( p(y_t | y_1, \ldots, y_{t-1}, \theta) \) can be evaluated or well approximated, DCC can be computed also for this model class, as we will illustrate in the following.

We consider the dynamics of a population of red kangaroos (Macropus rufus) in New South Wales, Australia. The data \( X \) from Bayliss (1987, Appendix 8.2; available in Fig. 8), is a time series of \( n = 41 \) bi-variate observations from double transect counts at irregular time intervals between 1973 and 1984. In Knape and Valpine (2012) the authors propose three different models for this data. These models are then compared in a pairwise fashion using the Bayes factor. The comparison has recently been repeated in Shao et al. (2017) using the Hyvärinen score. Both Knape and Valpine (2012) and Shao et al. (2017) conclude that among the three different models, the preferred model is the following continuous-time stochastic differential equation
\[
x_1 = LN(0, 5),
\] (12a)
\[
\frac{dx_1}{dt} = \sigma^2 dt + \sigma dW_t,
\] (12b)
\[
y_{1:t}, y_{2:t} | x_t \sim NB \left( \tau, \tau x_t \right),
\] (12c)

where \( LN \) is the log-normal distribution, \( W_t \) is the standard Brownian motion, \( NB \) is the negative binomial distribution, and \( \theta = \{ \sigma, \tau \} \) are unknown parameters. The latent variables are \( \eta = \{ x_t \}_{t \geq 1} \). Note that this model describes a bivariate time-series \( \{ y_t \} \).

While Knape and Valpine (2012) and Shao et al. (2017) favor the model given in (12) over other alternatives, we consider the different question whether the model in (12) is consistent with the observed data \( X \) or not. We first solve (12) analytically to obtain a discrete-time nonlinear state-space model, and use the particle marginal Metropolis-Hastings method (Andrieu et al., 2010) to sample the unknown parameters. A standard particle filter is used to approximate \( p(y_t | y_1, \ldots, y_{t-1}, \theta) \). We use \( N = 1000 \) and \( M = M' = 200 \) and obtain \( PFA^* = 0.28 \). Thus the model in (12) is deemed to be consistent with the observed kangaroo population data (also see Fig. 7 for intuitive support of this conclusion).
Discussion

We have proposed a data consistency criterion (DCC) to assess the consistency of a model class $P_0$ with respect to the observed data $y$. By comparing the observed (incremental) likelihoods $p(y|y_{i-1}, \theta)$ to the ones of generated data $\hat{y}$, DCC rejects a model class for which $y$ is atypical for the best models in the class. The criterion follows automatically from the specification of $P_0$ and does not require additional application-specific choices. It yields an (approximate) false alarm probability $PFA^*$ of erroneously declaring the best models to be inconsistent. When $PFA^*$ falls below some set threshold, there is a sound ground for ruling out the model class $P_0$.

By exploiting properties of the Fisher information matrix of $P_0$, it is possible to construct misspecification tests, cf. White (1982). That is, decide whether $p(y|\theta_0) = p_0(y)$ is true or not. Since all practical models are incomplete in some respect, such tests may not always be relevant. Instead, what matters in many applications is whether the model is accurate or not, and the proposed DCC provides a practically useful criterion in this respect.

Using a Bayesian interpretation of (8), DCC can be understood as a certain posterior predictive check (Rubin, 1984; Gelman et al., 2014; Box, 1980). Posterior predictive checks are, however, not available for plug-and-play since they require the user to specify a ‘discrepancy variable’, in contrast to the fully automatic DCC. The DCC also readily admits a frequentist interpretation in terms of false alarm probability as a sampling property of $p_0(y)$.

The computational cost of the criterion increases indeed with the dimension of $\theta$ and $n$. The operations required are, however, available for many models and well developed in most statistical software packages. DCC could therefore be used as a routine check in existing statistical modeling methods, in order to better guide the end user to well-grounded scientific conclusions.

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## Earthquake Count Example

(a) Data for the earthquake count example: The number of earthquakes above a certain magnitude (left column) in the entire world for 1980-2017, retrieved from the U. S. Geological Survey earthquake catalog.

| Magnitude | 1980 | 1981 | 1982 | 1983 | 1984 | 1985 | 1986 | 1987 | 1988 | 1989 | 1990 | 1991 | 1992 | 1993 | 1994 | 1995 | 1996 | 1997 | 1998 |
|-----------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| ≥8        | 0    | 0    | 0    | 0    | 0    | 2    | 1    | 0    | 0    | 0    | 0    | 0    | 0    | 2    | 2    | 1    | 0    | 1    | 1    |
| ≥7        | 6    | 10   | 7    | 14   | 14   | 15   | 11   | 13   | 11   | 8    | 18   | 17   | 13   | 12   | 20   | 15   | 16   | 12   |
| ≥6        | 96   | 88   | 90   | 139  | 141  | 162  | 140  | 173  | 126  | 139  | 154  | 137  | 179  | 148  | 159  | 201  | 164  | 136  | 121  |
| ≥5        | 1408 | 1265 | 1505 | 1802 | 1683 | 1806 | 1765 | 1572 | 1598 | 1561 | 1765 | 1583 | 1675 | 1564 | 1693 | 1501 | 1373 | 1234 | 1074 |
| Magnitude | 1999 | 2000 | 2001 | 2002 | 2003 | 2004 | 2005 | 2006 | 2007 | 2008 | 2009 | 2010 | 2011 | 2012 | 2013 | 2014 | 2015 | 2016 | 2017 |
| ≥8        | 0    | 0    | 1    | 1    | 0    | 1    | 0    | 1    | 1    | 2    | 2    | 1    | 1    | 0    | 1    | 1    | 1    | 1    | 1    |
| ≥7        | 18   | 15   | 16   | 13   | 15   | 16   | 11   | 11   | 18   | 12   | 17   | 24   | 20   | 20   | 16   | 19   | 12   | 19   | 16   |
| ≥6        | 136  | 160  | 137  | 139  | 156  | 157  | 151  | 153  | 196  | 179  | 161  | 175  | 207  | 133  | 142  | 155  | 146  | 146  | 111  |
| ≥5        | 1192 | 1495 | 1352 | 1309 | 1364 | 1672 | 1843 | 1877 | 2283 | 1965 | 2075 | 2395 | 2692 | 1680 | 1596 | 1729 | 1558 | 1696 | 1560 |

## Kangaroo Population Example

(b) Data for the kangaroo population example, adopted from Bayliss (1987, Appendix 8.2)

| Date       | 1973 Jul | 1973 Oct | 1974 Mar | 1974 Jun | 1974 Sep | 1975 Jan | 1975 Apr | 1975 Jul | 1975 Oct | 1976 Feb | 1976 May | 1976 Aug | 1976 Dec | 1977 Apr |
|------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| Counts     | 267      | 333      | 159      | 145      | 340      | 463      | 305      | 329      | 575      | 227      | 532      | 769      | 526      | 565      |
|            | 326      | 144      | 145      | 138      | 413      | 531      | 331      | 329      | 529      | 318      | 449      | 852      | 332      | 742      |

| Date       | 1977 Jul | 1977 Sep | 1978 Jan | 1978 May | 1978 Aug | 1978 Nov | 1979 Feb | 1979 Aug | 1979 Nov | 1980 Mar | 1980 Jul | 1980 Oct | 1980 Dec | 1981 Mar |
|------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| Counts     | 466      | 494      | 440      | 858      | 599      | 298      | 529      | 912      | 703      | 402      | 669      | 796      | 483      | 700      |
|            | 479      | 620      | 531      | 751      | 442      | 824      | 660      | 834      | 955      | 453      | 953      | 808      | 975      | 627      |

| Date       | 1981 Jul | 1981 Sep | 1981 Dec | 1982 Mar | 1982 Jun | 1982 Sep | 1982 Dec | 1983 Mar | 1983 Jun | 1983 Sep | 1983 Dec | 1984 Mar | 1984 Jun |
|------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| Counts     | 418      | 979      | 757      | 755      | 517      | 710      | 240      | 490      | 497      | 250      | 271      | 303      | 386      |
|            | 851      | 721      | 1112     | 731      | 748      | 675      | 272      | 292      | 389      | 323      | 272      | 248      | 290      |

Figure 8: Complete data sets for the earthquake and kangaroo counting examples.