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Dormann, Carsten F., Calabrese, Justin M., Guillera-Arroita, Gurutzeta et al. (20 more authors) (2018) Model averaging in ecology::a review of Bayesian, information-theoretic and tactical approaches for predictive inference. Ecological Monographs. pp. 485-504. ISSN 0012-9615

https://doi.org/10.1002/ecm.1309

Model averaging in ecology: a review of Bayesian, information-theoretic and tactical approaches

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December 6, 2017

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Keywords: AIC-weights, ensemble, model combination, model averaging, nominal coverage, prediction averaging, uncertainty

Abstract

In ecology, the true causal structure for a given problem is often not known, and several plausible models exist. It has been claimed that using weighted averages of these models can reduce prediction error, as well as better reflect model selection uncertainty. However, a large range of different model averaging methods exists, raising the question of how they differ regarding these goals. A core question for an analyst is thus to understand under which circumstances model averaging can improve predictions and their uncertainty estimates.

Here we review the mathematical foundations of model averaging along with the diversity of approaches available. The terms contributing to error in model-averaged predictions are each model's bias (i.e. the deviation of each model prediction from the

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unknown truth), variance of, and covariance among, model predictions, and uncertainty of model weights.

If bias of contributing model predictions is substantially larger than their variance, the advantage of reduced variance through weighted averages is greatly reduced. For noisy data, which predominate in ecology, variance is probably often larger than bias and model averaging becomes an option to reduce prediction error. Correlation between model predictions also reduces the effect of model averaging, and to counteract this effect, model weights could be adjusted to maximise the variance reduction.

Model-averaging weights have to be estimated from the data, and this estimation process carries some uncertainty, so that "optimised" model weights may not be better than the use of arbitrary weights, such as equal weights for all models. In the presence of inadequate models, however, estimating model weights is still likely to be superior to equal weights. Many different methods to derive averaging weights exist, from Bayesian over information-theoretical to optimised and resampling approaches, as reviewed here.

We also investigate the coverage of the confidence interval of the prediction for different ways to combine model prediction distributions, showing that they differ greatly, and that the full model has very good coverage properties. Our overall recommendations stress the importance of validation-based approaches and of uncertainty quantification to avoid unreflected use of model averaging.

1 Introduction

Models are an integral part of ecological research, representing alternative, possibly overlapping, hypotheses (Chamberlin, 1890). They are also the key approach to making

predictions about ecological systems (Mouquet et al., 2015). In many cases it is not possible to clearly identify a single most-appropriate model. For instance, process-based models may differ in the specific ways they represent ecological mechanisms, but several different process models may accord with our ecological understanding. Statistical models are limited in their complexity by the amount of data available for fitting, making several combinations of predictors plausible, and different modelling approaches are available for statistical analysis (e.g. Hastie et al., 2009; Kuhn and Johnson, 2013).

Model averaging, as the weighted sum of predictions from several candidate models, provides a potential avenue to avoid selecting a single model over others similarly plausible. Scientists average model predictions for different reasons, most prominently: (a) reducing prediction error through reduced variance, and partially by (b) reducing prediction bias (based on arguments described in Madigan and Raftery, 1994), and (c) accommodating/quantifying uncertainty about model parametrisation and structure (Wintle et al., 2003, see also section 2.3).

Here we focus on averaging sets of models that differ in structure, as opposed to mere differences in initial conditions or parameter values (Gibbs, 1902; Johnson and Bowler, 2009). The latter case in the statistical and physical literature is called "ensemble", while in ecology that term is used more loosely. For some ecological examples of model averaging see Wintle et al. (2003); Thuiller (2004); Richards (2005); Brook and Bradshaw (2006); Dormann et al. (2008); Diniz-Filho et al. (2009); Le Lay et al. (2010); Garcia et al. (2012); Cariveau et al. (2013); Meller et al. (2014), and Lauzeral et al. (2015).

Several previous publications have reviewed model averaging in ecology and evolution, focussing exclusively on 'information-theoretical model averaging' (Johnson and Omland, 2004; Hobbs and Hilborn, 2006; Burnham et al., 2011; Freckleton,

2011; Grueber et al., 2011; Nakagawa and Freckleton, 2011; Richards et al., 2011; Symonds and Moussalli, 2011), probably under the influence of the AIC-weighted averaging popularised by Burnham & Anderson (2002; Posada and Buckley 2004). *Bayesian* model averaging has been treated less frequently in ecology (for an example see Corani and Mignatti, 2015), but for an excellent recent review of this topic in the context of Bayesian model selection see Hooten and Hobbs (2015, see also Hoeting et al. 1999; Ellison 2004; Link and Barker 2006). However, none of the above is a comprehensive review of the state of knowledge across the available model averaging approaches.

Our aim is to provide such a comprehensive review in the light of developments over the last 20 or so years, summarising the actual mathematical reasoning and offering an intuitive as well as technical entry, illustrated by case studies. We primarily address averaging of predictions from correlative models, although most of the points will similarly apply to mechanistic/process-based models (see, e.g., Knutti et al., 2010; Diks and Vrugt, 2010, for a review in the context of climate and hydrological models, respectively). We do not concentrate on averaging model parameters, because we agree with the criticism summarised in Banner and Higgs (2017): parameters are estimated conditional on the model structure; as the model structure changes, parameters may become incommensurable (see Posada and Buckley, 2004; Cade, 2015; Banner and Higgs, 2017, and Appendix S1 for short review of the parameter-averaging literature).

This review is divided into two parts: theoretical and practical. In the first we present the mathematical logic behind model averaging, and why this alone puts severe constraints on *how* we do model averaging. Then, in the second part, we review the different ways model-averaging weights can be derived, comparing Bayesian, information-theoretic and other tactical perspectives (i.e. those not derived from statistical theory but still with a clear objective). This is followed by a brief exploration

of how to quantify model-averaged prediction uncertainty. We briefly illustrate model averaging with two case studies, before closing with unresolved challenges and recommendations.

2 The mathematics behind model averaging

Model averaging refers to the computation of a weighted-average prediction $\widetilde{Y}$ based on the predictions of several (M) contributing models, $\widehat{Y}_1, \widehat{Y}_2, \ldots, \widehat{Y}_M$:

$$\widetilde{Y} = \sum_{m=1}^{M} w_m \widehat{Y}_m \ , \quad \text{with} \ \sum_{m=1}^{M} w_m = 1. \tag{1}$$

Conceptually, the role of weights w_m is to adjust predictions such that the average prediction has improved properties over selecting a single among a number of candidate models (for example, less bias, lower variance or closer-to-nominal coverage). In accordance with virtually all applications of model averaging we encountered, we first focus on how model averaging reduces prediction error, here quantified as mean squared error (MSE) of a prediction $\widehat{Y}_m$ of model m, which is composed of prediction bias and prediction variance:

$$\text{MSE}(\widehat{Y}_m) = \left\{\text{bias}(\widehat{Y}_m)\right\}^2 + \text{var}(\widehat{Y}_m). \tag{2}$$

We shall now decompose this equation to understand what contributes to prediction error in the context of model averaging.

Bias, i.e. the difference between the prediction expectation and the truth (y^*), will depend directly on the bias of the contributing models, as well as their weights (eqn 1). As the truth is unknown (except in simulations), the statistical model-averaging literature typically makes the assumption that individual models have no bias (Bates and Granger, 1969; Buckland et al., 1997; Burnham and Anderson, 2002). In contrast, the focus of averaging process models is primarily on removing bias (e.g. Solomon et al., 2007; Gibbons et al., 2008; Dietze, 2017).

Prediction variance (arising from n hypothetical repeated samplings) is composed of two terms, the variance of each contributing model's prediction,

$$\text{var}(\widehat{Y}_m) = \frac{1}{n-1}\sum_{i=1}^{n}(\overline{\widehat{Y}}_m - \widehat{Y}_m^i)^2,$$

and the covariances between predictions of model m and m':

$$\text{cov}(\widehat{Y}_m, \widehat{Y}_{m'}) = \frac{1}{n-1}\sum_{i=1}^{n}(\overline{\widehat{Y}}_m - \widehat{Y}_m^i)(\overline{\widehat{Y}}_{m'} - \widehat{Y}_{m'}^i).$$

For the average of two predictions, $\widehat{Y}_1$ and $\widehat{Y}_2$, we have:

$$\text{var}(\widetilde{Y}) = w_1^2\text{var}(\widehat{Y}_1) + w_2^2\text{var}(\widehat{Y}_2) + 2w_1w_2\text{cov}(\widehat{Y}_1, \widehat{Y}_2). \tag{3}$$

When averaging several models, we expand eqn (3) to:

$$\begin{aligned}\text{var}(\widetilde{Y}) &= \text{var}\left(\sum_{m=1}^{M} w_m\widehat{Y}_m\right) = \sum_{m=1}^{M} w_m^2\text{var}(\widehat{Y}_m) + \sum_{m=1}^{M}\sum_{m'\neq m} w_m w_{m'}\text{cov}(\widehat{Y}_m, \widehat{Y}_{m'}) \\ &= \sum_{m=1}^{M}\sum_{m'=1}^{M} w_m w_{m'}\text{cov}(\widehat{Y}_m, \widehat{Y}_{m'}) = \sum_{m=1}^{M}\sum_{m'=1}^{M} w_m w_{m'}\rho_{mm'}\text{var}(\widehat{Y}_m)\text{var}(\widehat{Y}_{m'}),\end{aligned} \tag{4}$$

where $\rho_{mm'}$ is the correlation between $\widehat{Y}_m$ and $\widehat{Y}_{m'}$.

Putting eqns 2 and 3 together we get:

$$\text{MSE}(\widetilde{Y}) = \left(\sum_{m=1}^{M} w_m\left(E(\widehat{Y}_m) - y^*\right)\right)^2 + \sum_{m=1}^{M}\sum_{n=1}^{M} w_m w_{m'}\rho_{mn}\text{var}(\widehat{Y}_m)\text{var}(\widehat{Y}_{m'}), \tag{5}$$

where $E(\widehat{Y}_m) - y^* = \text{bias}(\widehat{Y}_m)$ represents model misspecification bias.

2.1 Influences on the error of model-averaged prediction

Equation 5 allows us to make a number of statements about the potential benefits of model averaging. Firstly, bias will typically remain unknown, as truth y^* is unknown, but it can be estimated through (cross-)validation, and hence also the relative importance of bias to variability of predictions can be quantified (Fig. 1). When each model produces a distinct prediction, with variances substantially lower than

differences between models, then bias dominates (Fig. 1 top). As variance increases (or bias decreases), the different model predictions overlap more and more, until bias is small relative to variance (Fig. 1 bottom). Predictions from any model will now typically have higher variance than the averaged prediction. Also, averaging can reduce bias, if predictions scatter around the truth, but not unidirectional bias, that is if all (most) model predictions err on the same side (see also Fig. 2 top row). However, if predictions scatter around the truth, bias can be reduced by averaging.

[Fig. 1 approximately here.]

We thus conclude that as bias becomes large relative to prediction variance, model averaging is less and less likely to be useful for reducing variance – it may still be useful for reducing bias (under the condition of bidirectional bias: Fig. 2, lower row).

[Fig. 2 approximately here.]

Downweighting of variances is the mathematical reason how model averaging reduces the variance over single model predictions. In the unlikely, but didactically important case that predictions are independent, their covariance is 0 and the correlation matrix ρ_{mn} of eqn 5 becomes the identity matrix (or, equivalently, the covariance term of eqn 4 vanishes). If we also assume both predictions have equal variances ($\text{var}(\widehat{Y}_1) = \text{var}(\widehat{Y}_2) = \text{var}(\widehat{Y})$), and since $w_2 = 1 - w_1$, the above equation simplifies to $\text{var}(\widetilde{Y}) = (2w_1^2 - 2w_1 + 1)\text{var}(\widehat{Y})$. If one model gets all the weight, we have $\text{var}(\widetilde{Y}) = \text{var}(\widehat{Y})$. If the two models receive equal weight, we have $\text{var}(\widetilde{Y}) = (2 \cdot (0.5)^2 - 2 \cdot 0.5 + 1)\text{var}(\widehat{Y}) = 0.5\text{var}(\widehat{Y})$, a considerable improvement in prediction variance (and the minimum of this equation). Other weights fall in-between these values. More generally, Bates and Granger (1969) showed that for unbiased models with uncorrelated predictions, the variance in the average is never greater than the smaller of the individual predictions (making the important assumption that the weights are known, which will be discussed below). In other

words, model averaging can reduce prediction error because weights enter as quadratic terms in eqn 3, rather than linearly.

The correlation between model predictions, i.e. the matrix $(\rho_{ij}) \in \mathbb{R}^{M \times M}$, substantially affects the benefit of model averaging (see also Fig. 3 and interactive tool in the Appendix Data S2). In the best case, correlations between model predictions are negative or at least absent, and the second term of eqn (5) is negative or vanishes. Here, the variance in the average is dominated by individual models' prediction variances. As correlation between predictions increases, the covariance-term contributes more and more to the overall prediction error, making the averaging of perfectly correlated predictions exactly outweigh the benefit gained by the quadratic weights-effect for the variances.

[Fig. 3 approximately here.]

This point provides some important insights about why some machine learning methods that average a large number of bad models work so well. When averaging *poor* models, e.g. trees in a randomForest, covariance is negligible, but the variance of each model prediction is high. Because w_m becomes very small with hundreds of models (around $1/M$), the variance of many averaged poor models (with similar variance) tends to be low: $\text{var}(\widetilde{Y}) = \sum_{m=1}^{M} \frac{1}{M^2} \text{var}(\widehat{Y}_m) + \frac{1}{M^2} \sum_{m=1}^{M} \sum_{m \neq n} \text{cov}(\widehat{Y}_m, \widehat{Y}_n) \approx M \frac{1}{M^2} \text{var}(\widehat{Y}) = \frac{1}{M} \text{var}(\widehat{Y})$, where the second term disappears due to lack of correlations among predictions. We may speculate that poor models typically also exhibit substantial but undirected bias, which again would be reduced by averaging.

The effect of correlations in the potential reduction of prediction error is rather intuitive. If a prediction from a given model is extreme (e.g. on the high end of the distribution), negative correlation will tend to balance out, while positive correlation will accentuate total variance (e.g. Bohn et al., 2010). Ecologists know an analogous effect from biodiversity studies, where it is called the 'portfolio effect'

(e.g. Thibaut and Connolly, 2013). It states that the fluctuation in biomass of a community is less than the fluctuations of biomass of its members, because the species respond to the environment differently. This asynchrony in response is analogous to negative covariance in community members' biomass, buffering the *sum* of their biomasses.

Putting bias, variance and correlation together (Fig. 2), we note that model averaging will deliver smaller prediction error when bias is "bidirectional" (i.e. model predictions over- and underestimate the true value: bottom row of Fig. 2) and predictions are negatively correlated (Fig. 2 bottom right). Uni-directional bias will remain problematic (top row of Fig. 2), irrespective of covariances among predictions.

Thus, for a given set of weights, the prediction error of model-averaged predictions depends on three things: the bias of the model average, the individual model prediction variances, and the correlation between individual model predictions.

2.2 Estimating weights can thwart the benefit of model averaging

Equation 5 assumes that the values of the weights are set a priori, and thus there is no uncertainty about them. However, that would imply that an arbitrary set of weights is used. Instead, the aim of optimising predictive performance suggests weights need to be estimated from the data. But estimation brings associated uncertainty with it, and this has implications for the actual benefits of model averaging: estimated "optimal" weights will be suboptimal (Nguefack-Tsague, 2014), so the averaged prediction even for only mildly correlated predictions will more likely be biased than if the (unknown) truly optimal weights were used (Claeskens et al., 2016). It may in fact be often no better than one obtained using some arbitrary weights, e.g. equal weights (Clemen,

1989; Smith et al., 2009; Graefe et al., 2014, 2015). The "simple theoretical explanation" provided by Claeskens et al. (2016) demonstrates that estimating weights introduces additional variance into the prediction. As a consequence, the predictions averaged with estimated weights may be worse than that of a single model (in contrast to the assertion of Bates and Granger 1969; see Claeskens et al. 2016 for an example).

Finding optimal weights now becomes far more involved, and currently no closed solution is available, not even for linear models (Liang et al., 2011). The interactive tool we provide (Fig. 3) allows readers to explore this issue in a simple 2-model case. It shows that, in this simple case, estimating weights substantially reduces the parameter space where model averaging is superior to the best single model.

The performance reduction does not however imply that estimated weights are of no use, or that the use of arbitrary weights (e.g. equal weights) is generally superior. While uncertainty in estimated weights increases prediction error, the ability to downweight or wholly remove unsuitable models from the prediction set is a substantial benefit. In Claeskens et al. (2016) and similar simulations, all models considered are "alright" (bias-free and with similar prediction variance), which obviously need not be the case. Model weights are a measure of suitability for prediction, which can be derived most logically from validation on (semi-)independent data (see section 3 for details). If the unknown optimal model weights deviate strongly from $1/m$, their estimation uncertainty is then a price worth paying.

2.3 Model averaging (typically) reduces prediction errors

The majority of studies we encountered (as random draws from the results of a systematic literature search: see Appendix S7) used an empirical approach to assess predictive performance, i.e. forecasting, hindcasting or cross-validation to observed data (e.g. Namata et al., 2008; Marmion et al., 2009*a*,*b*; Grenouillet et al., 2010;

Montgomery et al., 2012; Smith et al., 2013; Engler et al., 2013; Edeling et al., 2014; Trolle et al., 2014). Across the 180 studies we examined, model averaging generally yielded lower prediction errors than the individual contributing models. Most of these studies used test datasets to estimate predictive success, and rely critically on the assumption of independence between test and training datasets (Roberts et al., 2017). Few studies used simulated data to examine the performance of model averaging under specific conditions (e.g. small sample size, model structure uncertainty, missing data: Ghosh and Yuan, 2009; Schomaker, 2012). Very few studies provide mathematical analyses (Shen and Huang, 2006; Potempski and Galmarini, 2009; Chen et al., 2012; Zhang et al., 2013).

Summarising section 2 so far, we observe that

1. model averaging reduces prediction error by reducing prediction variance and bias;
2. the more positively correlated predictions are, the smaller is the benefit gained from averaging them;
3. when bias is large relative to the prediction variance of individual models, the least-biased model will be a better choice than the model average; and
4. estimating weights introduces additional variance, outweighing, in some situations, the benefits of model averaging.

2.4 Quantifying uncertainty of model-averaged predictions

In random sampling, in addition to a statistic of interest, say a point prediction, we are typically interested in the uncertainty of this statistic, e.g. as quantified by its variance (goal 2 at the beginning of the paper). A relevant question is whether the associated

confidence intervals have nominal coverage, i.e. whether the true value is in the 95%-CI indeed 95% of the time in repeated experiments.

If we attempt an analogy between random sampling and model averaging, the first catch is that predictions from different models will be non-independent. In this case the standard deviation does not decrease as square root of n, but more slowly. The second catch is that models are almost certainly not random draws from the population of models (if we just think of all the models which we did *not* include). Non-random draws from a distribution are almost certain to yield biased estimates of that distribution's parameters.

The first catch can be taken care of by taking into account the variance-covariance matrix of model predictions (see section 2, eqns 3-5). The second catch (models are non-random draws) is harder and the severity of this problem depends on whether model predictions are biased in the same direction (the "unidirectional bias" in Fig. 2) or in different ways. Model averaging can only successfully unite diverging biased predictions when they are biased in different directions. The approaches to computing prediction variance below rely on the assumption that model predictions in fact do scatter around the truth, and that the (weighted) average of model predictions is unbiased. Since truth is unknown, this assumption cannot be tested. When models share their fundamental structure (e.g. process models relying on the same equations), it is more likely that they are unidirectionally biased.

2.4.1 Simplified error propagation in model-averaged predictions

To approximate the predictive variance of model-averaged predictions, Buckland et al. (1997) proposed a simplification of eqn (5) (for derivation see Burnham and Anderson,

2002, p. 159-162):

$$\mathrm{var}(\widetilde{Y}) = \left(\sum_{m=1}^{M} w_m \sqrt{\mathrm{var}(\widehat{Y}_m) + \gamma_m^2} \right)^2 . \quad (6)$$

Misspecification bias of model m is computed as $\gamma_m = \widehat{Y}_m - \widetilde{Y}$, thus assuming (explicitly on page 604 of Buckland et al. 1997) that the averaged point estimate $\widetilde{Y}$ is unbiased and can hence be used to compute the bias of the individual predictions. This assumption can be visualised in Fig. 2 as the situation where the empty triangles always sit right on top of 'truth'. This assumption is problematic as it cannot be met by unidirectionally biased model predictions, nor when weights w_m fail to get the weighting *exactly* right and thus $\widetilde{Y}$ remains biased. Less problematically, Buckland et al. (1997) also assumed that predictions from different models are *perfectly* correlated, making the covariance-term as large as possible, and variance estimation conservative. The distribution theory behind this approach has been criticised as "not (even approximately) correct" (Claeskens and Hjort, 2008, p. 207), but shown to work well in simulations (Lukacs et al., 2010; Fletcher and Dillingham, 2011).

Improving on eqn (6) requires knowledge of the correlation matrix ρ_{mn} of eqn (5). The key problem is that there is no analytical way to compute the correlation of model predictions. While bootstrapping models and their prediction can provide an estimate of ρ_{mn}, it can more directly provide an estimate of $\mathrm{var}(\widetilde{Y})$, rendering the indirect route via eqn (6) unnecessary.

2.4.2 Coverage of the model-averaged prediction

Predictions from a selected single-best model *always* underestimate the true prediction error (e.g. Namata et al., 2008; Fletcher and Turek, 2012; Turek and Fletcher, 2012). The reason is that the uncertainty about which model is correct is not included in this final prediction: we predict as if we had not carried out model selection but had known from the beginning which model would be the best (as if the model had been "prescribed":

Harrell, 2001). Thus, even if we were able to choose, from our model set M, the model closest to truth, we would still need to adjust the confidence distribution for model selection; however, a perfect adjustment was analytically shown not to exist (Kabaila et al., 2015).

For statistical models, it is less clear whether the full model (i.e. prior to any model selection; see Appendix S3) or model averaging computes the uncertainty intervals correctly. Simulations suggest that model averaging may improve coverage (Namata et al., 2008; Wintle et al., 2003; Zhao et al., 2013, none of who tested the full model), which can be understood to happen because the process of averaging allows us to take into account model uncertainty (Liang et al., 2011). Given that model averages need not be normal (at the link scale), Fletcher and Turek (2012) and Turek and Fletcher (2012) explore how to improve the tail areas of the confidence distribution, albeit under the assumption that the true model is in the model set. Their approach was re-analysed by Kabaila et al. (2015) under model selection. The key finding of this latter study is that the full model coverage was still superior to all other model averaging approaches, suggesting that the full model should currently be kept in mind, both for inference, minimal bias and correct prediction intervals (see also Harrell, 2001, p. 59). Such findings sit uncomfortably with the bias-variance trade-off (Hastie et al., 2009), which states that overly complex models have poor predictive performance; and indeed the full model has high prediction variance. However, our statements are about the confidence intervals, rather than the point predictions, and those will be incorrectly narrow for model selection without selection-correction. Regrettably, such reasoning cannot be extended in an obvious way to models that do not have a "full model" (non-nested models, process models, or machine learning models). Here model averaging provides a way forward in representing prediction coverage more fairly.

Given the diversity of approaches to computing model weights encountered in

section 3, these studies cannot be seen as conclusive, only as suggestive, for the improvement of nominal coverage using model averaging.

In a different approach to characterising the uncertainty in model predictions, model averaging can be interpreted as computing the distribution of a random variable that is derived from a collection of random variables (the model predictions), also known as a **mixture distribution** (Claeskens and Hjort, 2008, p. 217). In a two-step process, the model weights determine the probability of choosing the model, and then the model prediction is drawn from its confidence distribution. If predictions are unbiased, they stack up high around the mean, and yield the same value as the equation for the standard error of the mean. If predictions differ widely, e.g. due to bias, the mixed confidence distribution will be much wider and possibly multi-modal. Mixing distributions assumes their independence, i.e. the random draw of a value from one model prediction is uncorrelated with the next draw of model and prediction. As model predictions are likely to be positively correlated, assuming (conditional) independence will *underestimate* variance (i.e. correlated draws would yield wider confidence distributions).

Overall, this leaves us with the following options for computing the confidence intervals of averaged predictions (which we will compute for a set of simple linear regressions in Fig. 5):

1. Make the assumption that model-averaged predictions are unbiased (i.e. that y^* can be estimated as $\widetilde{Y}$). Use bootstrapping to estimate covariances of predictions for each model. From these estimates, compute prediction variance according to eqn (5). This solution is computer-intensive, but it takes into account covariance of model predictions. (Note that simply averaging predictions from bootstrapped models is not correct, as it does not incorporate model misspecification bias.)

2. Make again the assumption that model-averaged predictions are unbiased. Use Buckland et al. (1997)'s approach (eqn 6). This will yield wider estimates than option 1, because assuming perfect correlation is conservative.
3. Make the assumption that predictions from different models are effectively uncorrelated. Use model mixing to compute the confidence distribution of the average.
4. Fit the full model (if available) and use its confidence distribution, which can rarely be improved on (Kabaila et al., 2015).

[Figure 5 approximately here.]

When averaging models with largely independent (i.e. uncorrelated) predictions, only the bootstrap-estimated covariance matrix (option 1 above) will also compute lower variances (according to eqn 4). In our illustration (Fig. 5, see Appendix S8), the first three options ("propagation", "Buckland" and "mixing") hardly differ, while the full model has a different location and is wider. The coverage of the 95% confidence interval, computed through 1000 simulations, is best matched by the full model, while the propagation approach is overly conservative. Buckland's equation and mixing have slightly too low coverage.

3 Approaches to estimating model-averaging weights

When faced with predictions from very different models, estimating weights aims at abating poorly, and elevating well predicting ones. For the resulting averaged predictions, the actual method for estimating weights has obvious fundamental importance. We now review approaches to estimate model-averaging weights and

elucidate on their interconnections (Table 1). Different perspectives on model-averaging weights have emerged, which we present in somewhat arbitrary four categories of decreasing probabilistic interpretability:

1. In the Bayesian perspective, model weights are probabilities that model M_i is the 'true' model (e.g. Link and Barker, 2006; Congdon, 2007).
2. In the information-theoretic framework, model weights are measures of how closely the proposed models approximate the true model as measured by the Kullback-Leibler divergence, relative to other models.
3. In a 'tactical' perspective, model weights are parameters to be chosen in such a way as to achieve best predictive performance of the average. No specific interpretation of the model is attached to the weights; they only have to work.
4. Assigning fixed, equal weights to all predictions can be seen as a reference naïve approach, representing the situation without adjusting for differences in models' predictive abilities.

We shall address these four perspectives in turn, also hinting at relationships between them.

[Table 1 approximately here.]

3.1 Bayesian model weights

Our outline of Bayesian model weights follows that of Wasserman (2000), paying attention to recent computational advances in the field.

Theory Bayes' formula can be applied to models in much the same way as to parameters. Hence, to perform inference with multiple models, one can write down the joint posterior probability $P(M_i, \Theta_i|D)$ of model M_i with parameter vectors Θ_i, given the observed data D, as

$$P(M_i, \Theta_i|D) \propto L(D|M_i, \Theta_i) \cdot p(\Theta_i) \cdot p(M_i), \tag{7}$$

where $L(D|M_i, \Theta_i)$ is the likelihood of model M_i, $p(\Theta_i)$ is the prior distribution of the parameters of the respective model M_i, and $p(M_i)$ is the prior weight on model M_i.

The joint distribution provides all information necessary for inference. Often, in practice, we want to extract some simplified statistics from this distribution such as the model with the highest posterior model probability, or the distribution of a parameter or prediction including model selection uncertainty. To obtain this information, we can marginalise (average, integrate) over parameter space, or marginalise over model space.

If we marginalise over parameter space, we obtain model weights (whilst marginalising over model space yields averaged parameters, which we shall not address here). The first step is to calculate the marginal likelihood, defined as the average of eqn (7) across all k parameters for any given model:

$$P(D|M_i) \propto \int_{\Theta_1} \cdots \int_{\Theta_k} L(D|M_i, \Theta_i) p(\Theta_i) d\Theta_1 \cdots d\Theta_k \tag{8}$$

From the marginal likelihood, we can compare models via the **Bayes factor**, defined as the ratio of their marginal likelihoods (e.g. Kass and Raftery, 1995):

$$\text{BF}_{i,j} = \frac{P(D|M_i)}{P(D|M_j)} = \frac{\int L(D|M_i, \Theta_i) p(\Theta_i) d\Theta_i}{\int L(D|M_j, \Theta_j) p(\Theta_j) d\Theta_j}. \tag{9}$$

with the multiple integral now pulled together for notational convenience. For more than two models, however, it is more useful to standardise this quantity across all models in question, calculating a Bayesian posterior model weight $p(M_i|D)$ (including model priors $p(M_i)$: Kass and Raftery, 1995,) as

$$\text{posterior model weight}_i = \; p(M_i|D) = \frac{P(D|M_i)\; p(M_i)}{\sum_j P(D|M_j) p(M_j)} \tag{10}$$

Estimation in practice While the definition of Bayesian model weights and averaged parameters is straightforward, the estimation of these quantities can be

challenging. In practice, there are two options to numerically estimate the quantities defined above, both with caveats.

The first option is to sample directly from the joint posterior (eqn (7)) of the models and the parameters. Basic algorithms such as rejection sampling can do that without any modification (e.g. Toni et al., 2009), but they are inefficient for higher-dimensional parameter spaces. More sophisticated algorithms such as MCMC and SMC (see Hartig et al., 2011, for a basic review) require modifications to deal with the issue of different number of parameters when changing between models. Such modifications (mostly the reversible-jump MCMCs, **rjMCMC**: Green, 1995, see Appendix S5.1.1) are often difficult to program, tune and generalise, which is the reason why they are typically only applied in specialised, well-defined settings. The posterior model probabilities of the rjMCMC are estimated as the proportion of time the algorithm spent with each model, measured as the number of iterations the algorithm drew a particular model divided by the total number of iterations.

The second option is to approximate the marginal likelihood in eqn (8) of each model independently e.g. compute the maximum a posteriori model probability, renormalise that into weights, and then average predictions based on these weights. The challenge here is to get a stable approximation of the marginal likelihood, which can be very problematic (Weinberg, 2012, see Appendix S5.1.2). Because of the relatively simple implementation, this approach is a more common choice than rjMCMC (e.g. Brandon and Wade, 2006).

Influence of priors A problem for the computation of model weights when performing Bayesian inference across multiple models, is the influence of the choice of *parameter priors*, especially "uninformative" ones (see section 5 in Hoeting et al., 1999; Chickering and Heckerman, 1997).

The challenge arises because in eqns (8) and (9) the prior density $p(\theta_i)$ enters the marginal likelihood and hence the Bayes factor multiplicatively. This has the somewhat unintuitive consequence that increasing the width of an uninformative parameter prior will linearly decrease the model's marginal likelihood (e.g. Link and Barker, 2006). That Bayesian model weights are strongly dependent on the width of the prior choice has sparked discussion of the appropriateness of this approach in situations with uninformative priors. For example, in situations where multiple nested models are compared, the width of the uninformative prior may completely determine the complexity of models that are being selected. One suggestion that has been made is to *not* perform multi-model inference *at all* with uninformative priors, or that at least additional corrections are necessary to apply Bayes factors weights (O'Hagan, 1995; Berger and Pericchi, 1996). One such correction is to calibrate the model on a part of the data first, use the result as new priors and then perform the analysis described above (intrinsic Bayes factor: Berger and Pericchi 1996, fractional Bayes factor: O'Hagan 1995). If sufficient data are available so that the likelihood is sufficiently peaked strongly during the calibration step, this approach should eliminate any complication resulting from the prior choice (for an ecological example see van Oijen et al., 2013).

Bayesian variations In a set of influential publications, Raftery et al. (1997), Hoeting et al. (1999) and Raftery et al. (2005) introduced *post-hoc* Bayesian model averaging, i.e. for vectors of predictions from already fitted models. The key idea is to iteratively estimate the proportion of times a model would yield the highest likelihood within the set of models (through expectation maximisation, see Appendix S5.2 for details), and use this proportion as model weight. In the spirit of the inventors, we refer to this approach as **Bayesian model averaging using Expectation-Maximisation** (BMA-EM), but place it closer to a frequentist than a Bayesian approach, as the models

were not necessarily (and in none of their examples) fitted within the Bayesian framework. It has been used regularly, often for process models (e.g. Gneiting et al., 2005; Zhang et al., 2009), where a rjMCMC-procedure would require substantial programming work at little perceived benefit, but also in data-poor situations in the political sciences (Montgomery et al., 2012).

Chickering and Heckerman (1997) investigate approximations of the marginal likelihood in eqn (9), such as the **Bayesian Information Criterion** (BIC, as defined in the next section; see also Appendix S5.3) and find them to work well for model selection, but *not* for model averaging. In contrast, Kass and Raftery (1995) state (on p. 778) that $\mathbf{e}^{\mathbf{BIC}}$ is an acceptable approximation of the Bayes factor, and hence suitable for model averaging, despite being biased even for large sample sizes. These approximations may be improved when using more complex versions of BIC (SPBIC and IBIC: Bollen et al., 2012).

The "widely applicable information criterion" **WAIC** (Watanabe 2010 and an equivalent **WBIC**: Watanabe 2013) are motivated and actually analytically derived in a Bayesian framework (Gelman et al., 2014). Its uninformative prior implementation should be seen as a variation of AIC (see next section), while the implementation with model priors is based on posterior distribution of parameter estimates, and computed, for each model, from two terms (Gelman et al., 2014): (1) the log pointwise predicted density (lppd) across the posterior simulations for each of the n predicted values, defined as $\text{lppd} = \log \prod_{i=1}^{n} p_{\text{posterior}}(y_i)$; and (2) a bias-correction term $p_{\text{WAIC}} = \sum_{i=1}^{n} \text{var}(\log(p(y_i|\theta_s)))$, where var is the *sample* variance over all S samples of the posterior distributions of parameters θ. Then the WAIC is defined as $\text{WAIC} = -2\,\text{lppd} + 2\,p_{\text{WAIC}}$. In words, the WAIC is the likelihood of observing the data under the posterior parameter distributions, corrected by a penalty of model complexity proportional to the variance of these likelihoods across the MCMC samples.

Model weights are computed from WAIC analogously to equation 11 below.

3.2 Information-theoretic model weights

In the *information-theoretic* perspective, models closer to the data, as measured by the Kullback-Leibler divergence, should receive more weight than those further away.

There are several approximations of the KL-divergence, most famously Akaike's Information Criterion (AIC: Akaike, 1973; Burnham and Anderson, 2002). AIC and related indices can be computed only for likelihood-based models with known number of parameters (p_m), restricting the information-theoretic approach to GLM-like models (incl. GAM):

$$\text{AIC}_m = -2\ell_m + 2p_m \quad \text{and} \quad w_m = \frac{e^{-0.5(\text{AIC}_m - \text{AIC}_{\min})}}{\sum_{i \in \mathcal{M}} e^{-0.5(\text{AIC}_i - \text{AIC}_{\min})}}, \tag{11}$$

where ℓ_m is the log-likelihood of model m.

In the ecological literature, AIC (and its sample-size corrected version AICc, and its adaptations to quasi-likelihood models such as QIC: Pan 2001; Claeskens and Hjort 2008) is by far the most common approach to determine model weights (for recent examples see, e.g., Dwyer et al., 2014; Rovai et al., 2015). **AIC-weights** (eqn (11)) have been interpreted as Bayesian model probabilities (Burnham and Anderson 2002, p. 75; Link and Barker 2006), although we are not aware of a convincing theoretical justification. An alternative interpretation is the proportion of times a model would be chosen as the best model under repeated sampling (Hobbs and Hilborn, 2006), but such an interpretation is contentious (Richards, 2005; Bolker, 2008; Claeskens and Hjort, 2008). In an anecdotal comparison, Burnham and Anderson (2002, p. 178) showed that AIC-weights are substantially different from **bootstrapped model weights**. The latter were proposed by Buckland et al. (1997) and represent the proportion of bootstraps a model is performing best in terms of AIC: see case study 1 below. In

simulations, AIC-weights did not reliably identify the model with the known lowest KL-divergence or prediction error (Richards, 2005; Richards et al., 2011). Instead, **Mallows' model averaging** (MMA) has been shown to yield the lowest mean squared error for *linear* models (Hansen, 2007; Schomaker et al., 2010). Mallows' C_p penalises model complexity equivalent to $-2\ell_m - n + 2p_m$ (for n data points; rather than AIC's $-2\ell_m + 2p_m$, eqn 11).

Other approximations of the KL-divergence include Schwartz' Bayesian Information Criterion (see previous section), which was designed to find the most probable model given the data (Schwartz, 1978; Shmueli, 2010), equivalent to having the largest Bayes factor (see previous section). **BIC** uses $\log(n)$ rather than AIC's "2" as penalisation factor for model complexity (Appendix S5.3). A particularly noteworthy modification of the AIC exist, where the model fit is assessed with respect to a focal predictor value, e.g. a specific age or temperature range, yielding the Focussed Information Criterion (FIC: Claeskens and Hjort 2008). We are not aware of a systematic simulation study comparing the performance of these model averaging weights, but AIC's dominance should not indicate its superiority (see also case study 1 below).

The weighting procedure can additionally be wrapped into a cross-validation and model pre-selection, which leads to the ARMS-procedure (**Adaptive Regression by Mixing with model Screening**: Yang, 2001; Yuan and Yang, 2005; Yuan and Ghosh, 2008). We shall not present details on ARMS here (for cross-validation see next section), because we regard model pre-selection as an unresolved issue (see section 5.3).

3.3 Tactical approaches to computing model weights

Methods covered in this section share the "tactical" goal of choosing weights to optimise prediction (e.g. reduce prediction error). These weighting schemes are not

explicitly building on Bayes or information theory thus most general in application.

Cross-validation approximates a model's predictive performance on new data by predicting to a hold-out part of the data (typically between 5 and 20 folds).

Leave-one-out cross-validation disturbs the data least, omitting each single data point in turn. The fit to the hold-out can be quantified in different ways. If the data can be reasonably well described by a specific distribution with log-likelihood function ℓ (even if the model algorithm itself is non-parametric), the log-likelihood of the data in the k folds can be computed and summed (van der Laan et al., 2004; Wood, 2015, p. 36):

$$\ell^m_{CV} = \sum_{i=1}^{k} \ell(y_{[i]}|\hat{\theta}^m_{y_{[-i]}}), \tag{12}$$

where the index $[-i]$ indicates that the data $y_{[i]}$ in fold i were not used for fitting model m and estimating model parameters $\hat{\theta}^m_{y_{[-i]}}$. *Cross-validation log-likelihood*, specifically leave-one-out cross-validation, is asymptotically equivalent to AIC and thus KL-distance (Stone, 1977), albeit at a higher computational cost. The use of hold-out data in cross-validation implicitly penalises overfitting, and we can hence compute model weights w^m_{CV} in the same way as AIC-weights (Hauenstein et al., 2017):

$$w^m_{\text{CV}} = \frac{e^{\ell^m_{\text{CV}}}}{\sum_{i\in\mathcal{M}} e^{\ell^i_{\text{CV}}}}\,. \tag{13}$$

Other measures of model fit to the hold-out folds have been used, largely as *ad hoc* proxies for a likelihood function (e.g. in likelihood-free models): pseudo-R^2 (e.g Nagelkerke, 1991; Nakagawa and Schielzeth, 2013), area under the ROC-curve (AUC: Marmion et al., 2009*a*; Ordonez and Williams, 2013; Hannemann et al., 2015), or True Skill Statistic (Diniz-Filho et al., 2009; Garcia et al., 2012; Engler et al., 2013; Meller et al., 2014). In these cases, weights were computed by substituting ℓ_{CV} in eqn (13) by the respective measure, or given a value of $1/S$ for a somewhat arbitrarily defined subset of S (out of M) models, e.g. those above an arbitrary threshold considered minimal satisfactory performance (Crossman and Bass, 2008; Crimmins et al., 2013;

Ordonez and Williams, 2013).

Largely ignored by the ecological literature are two other non-parametric approaches to compute model weights: *stacking* and *jackknife model averaging* (see Appendix S4 for discussion of averaging *within* machine-learning algorithms). Both are cross-validation based, and both optimise model weights on hold-out data. **Stacking** (Wolpert, 1992; Smyth and Wolpert, 1998; Ting and Witten, 1999) finds the optimised model weights to reduce prediction error (or maximise likelihood) on a test hold-out of size H. This is, for RMSE and likelihood, respectively:

$$\arg\min_{w_m} \left\{ \sqrt{\frac{1}{H}\sum_{i=1}^{H}\left(y_{[i]} - \sum_{m=1}^{M} w_m \hat{f}\left(X_i \left| \hat{\theta}^m_{[-i]}\right.\right)\right)^2} \right\}$$

(Hastie et al., 2009) and

$$\arg\max_{w_m} \left\{ \ell\left(y_{[i]} \left| \sum_{m=1}^{M} w_m \hat{f}\left(X_i \left| \hat{\theta}^m_{[-i]}\right.\right)\right.\right) \right\},$$

where $\hat{f}(X_i|\hat{\theta}^m_{[-i]})$ is the prediction of model m, fitted without using data i, to data i. This procedure is repeated many times, each time yielding a vector of optimised model weights, w_m, which are then averaged across repetitions and rescaled to sum to 1. Smyth and Wolpert (1998) and Clarke (2003) reports stacking to generally outperform the cross-validation approach from two paragraphs earlier, and Bayesian model averaging, respectively (see also the case studies in section 4 and Appendix S5).

In **Jackknife Model Averaging** (JMA: Hansen and Racine, 2012), each data point is omitted in turn from fitting and then predicted to (thus actually a leave-one-out cross-validation rather than a "jackknife"). Then, weights are optimised so as to minimise RMSE (or maximise likelihood) between the observed and the fitted value across all "jackknife" samples. The optimisation function is the same as for stacking, except that $H = N$. Thus, in stacking, weights are optimised once for each run, while for the jackknife only one optimisation over all N leave-one-out-cross-validations is required (further details and examples with R-code are given in Appendix S5.6).

The forecasting (i.e. time-predictions) literature (reviewed in Armstrong, 2001; Stock and Watson, 2001; Timmermann, 2006) offers two further approaches. Bates and Granger (1969)'s **minimal variance** approach attributes more weight to models with low-variance predictions. More precisely, it uses the inverse of the variance-covariance matrix of predictions, $\mathbf{\Sigma}^{-1}$, to compute model weights. In the multi-model generalisation (Newbold and Granger, 1974) the weights-vector w is calculated as:

$$w_{\text{minimal variance}} = (\mathbf{1}'\mathbf{\Sigma}^{-1}\mathbf{1})^{-1}\mathbf{1}\mathbf{\Sigma}^{-1}, \tag{14}$$

where $\mathbf{1}$ is an M-length vector of ones. This is the analytical solution of eqn 5, assuming no bias and ignoring the problem that weights are random variates, under the weights-sum-to-one constraint. Equation 14 does not ensure all-positive weights, nor is it obvious how to estimate $\mathbf{\Sigma}$. One option (used in our case studies) is to base $\mathbf{\Sigma}$ on the deviation from a prediction to test data in lieu of measure of past performance (following recommendation of Bates and Granger, 1969).

Finally, Garthwaite and Mubwandarikwa (2010) devised a rarely used method, called the "**cos-squared weighting** scheme", designed to adjust for correlation in predictions by different models. It was motivated by (i) giving lower weight to models highly correlated with others (thereby reducing the prediction variance contributed through covariances in eqn 5), (ii) division of weights when a new, near-identical model prediction is added to the set, and (iii) reducing all weights when more models are added to the set. Weights are computed as proportional to the amount of rotation the predictions would require to make them orthogonal in prediction space, hence the trigonometric name of their approach.

Model-based model combination: varying weights

Combining model predictions using statistical models, an approach we term "model-based model combinations" (**MBMC**, also called "superensemble modelling")

was first proposed by Granger and Ramanathan (1984). Here a statistical model f is used to combine the predictions from different models, as if they were predictors in a regression: $\widetilde{Y} \sim f(\widehat{Y}_1, \widehat{Y}_2, \ldots, \widehat{Y}_m)$ (see Fig. 4 left). The regression-type model f can be of any type, such as a linear model or a neural network. We call this regression the "supra-model" in order to distinguish between different modelling levels.

A very simple supra-model would compute the **median of predictions** for each point $\mathbf{X}_i$ (e.g. Marmion et al., 2009*a*). Different models are used in the "average" without requiring any additional parameter estimation. Median predictions imply varying weights, as the one or two models considered for computing the median may change between different $\mathbf{X}_i$.

An ideal model combination could switch, or gently transition, between models (such as manually constructed by Crisci et al., 2017). Since the predictions are combined more or less freely in model-based model combinations to yield the best possible fit to the observed data, MBMC should be superior to any constant-weight-per-model approach (see Fig. 4 right), as was indeed found by Diks and Vrugt (2010). This advantage comes with a severe drawback: a high proclivity to overfitting, as we fit the same data twice (once to each model, then again to their prediction regression).

[Fig. 4 approximately here.]

This does not seem to be recognised as a problem (despite being a key message of Hastie et al., 2009), as all studies we found incorrectly cross-validate the supra-model only, not the *entire* workflow (if at all; e.g. Krishnamurti et al., 1999; Thomson et al., 2006; Diks and Vrugt, 2010; Breiner et al., 2015; Romero et al., 2016). To correctly cross-validate MBMCs, one has to produce hold-outs *before* fitting the contributing models, and evaluate the MBMC prediction on this hold-out (Fig. 4, Appendix S5.9 and case studies).

Note that supra-models may differ substantially in their ability to harness the

contributing models. As it is a yet fairly unexplored field in model averaging, analysts are advised to try different supra-model types (Fig. 4).

3.4 Equal weights

In many fields of science (climate modelling, economics, political sciences), model averaging proceeds with giving the structurally different models equal weight, i.e. $1/M$ (e.g. Johnson and Bowler, 2009; Knutti et al., 2010; Graefe et al., 2014; Rougier, 2016). In ecology, studies analysing species distributions reported equal weights to be a very good choice when assessed using cross-validation (Crossman and Bass, 2008; Marmion et al., 2009*a*; Rapacciuolo et al., 2012), but no better than the single models on validation with independent data (Crimmins et al., 2013). Equal weights may serve as a reference approach to see whether estimating weights reduces prediction error for this specific set of models. In that sense, we may argue, all the above weight estimation approaches only serve to separate the wheat from the chaff; once a set of reasonable models has been identified, equal weights are apparently a good approach.

4 Case studies

All methods discussed above can be applied to simple regression models, while some explicitly rely on a model's likelihood and can thus not be used for non-parametric approaches. We therefore devised two case studies, the first being a rather simple example to illustrate the use of all methods in Table 1, and the second a more complicated species distribution case study based on a reduced set of methods. Note that we do not include adaptive regression by mixing with model screening (ARMS: Yang, 2001) because its more sophisticated variations (Yuan and Yang, 2005) are not implemented, and the basic ARMS is barely different from AIC-model averaging for a

preselected set of models.

4.1 Case study 1: Simulation with Gaussian response, many models and few data points

In this first, simulation-based case study, we explore the variability of model-averaging approaches in the common case where several partially nested models are fit (see Appendix S9 for details and code). The simulation was set up so that several of the fitted models have similar support as explanations for the data. This was achieved by generating the response differently in each of two groups (using similar, but not identical predictors). We simulated 70 data points with 4 predictors yielding $2^4 = 16$ candidate models, and another 70 for validation. We computed model weights in 19 different ways (Table 1) and compared the prediction error of weighted averages as well as the individual models to the validation data points. Simulation and analyses were repeated 100 times.

Two results emerged from this simulation that are worth reporting. First, prediction error (quantified as RMSE) was similar across the 19 weight-computing approaches, with a few noticeable exceptions, and most were no better than those of the best nine single model predictions (the two MBMC approaches, minimal variance and the cos-squared scheme: Fig. 6). Second, most averaging approaches gave some weight ($w > 0.01$) to ten or more models (Table 2), despite models being overlapping and partially nested, so that we have actually only five (more or less) independent models (those containing only one predictor: m2, m3, m5, m9 and intercept-only m1). In real data sets, such spreading of weight is the result of data sparseness or extreme noise, making important effects stand out less; indeed, half of our candidate models are not hugely different, i.e. within $\Delta\text{AIC} < 4$.

[Figure 6 approximately here.]

[Table 2 approximately here.]

4.2 Case study 2: Real species presence-absence data, many data points and a moderate number of predictors

In the second case study we use data on the real distribution of short-finned eel (*Anguilla australis*) in New Zealand (from Elith et al., 2008). The data are provided in the R-package dismo, already split into a 1000-rows training and a 500-rows test data set, and featuring 10 predictors. We ran four different model types (GAM, randomForest-rF, artificial neural network-ANN, support vector machine-SVM), along with two variations of the GLM (best models selected by AIC and BIC). For details see Appendix S10.

The number of averaging approaches that can be used to compute model weights is smaller than in the previous case study, as three of the six models do not report a likelihood or the number of parameters, precluding the use of rjMCMC, Bayes factor, (W)AIC, BIC, and Mallows' Cp. In addition, because we do not know the underlying data-generating model, we evaluate the models on the randomly pre-selected test data provided.

[Table 3 approximately here.]

One interesting result is that model averaging was effectively a model selection tool in several cases (Table 3). Stacking, bootstrapping, JMA, and to a lesser degree minimal variance, BMA-EM and the model-based model combinations yielded non-zero weights for only 1 (or 2) models. Apparently, these approaches yielded sub-optimal model weights, as these "model selection"-outcomes of model averaging fared worse than those that kept all models in the set (equal weight, leave-one-out and cos-squared).

Secondly, the best two model averaging algorithms in this case study, apart from the median where varying weights are used, identified an approximately equal weighting as optimal strategy. That is somewhat surprising, given that SVM performed relatively poorly (and was excluded by BMA-EM, but favoured by cos-squared as a more independent contribution). The likely reason of high weights for the poor SVM is that averaging-in less correlated predictions reduces covariances in eqn (5).

The good performance of the median in both case studies suggests that using the central value of *each prediction*, rather than give constant weights to the model itself, may be even more effective in reducing variance and thus prediction error.

5 Recommendations

Despite setting out to review the field of model averaging for ecologists, the complexity of the topic prevents us from providing final answers. The recent mathematical explanation why estimating optimal weights makes the averaged predictions perform poorly (Claeskens et al., 2016) is an example for fundamental limitations of model averaging. Many issues seem to be statistically unresolved, or addressed by quick-fixes and even fundamental questions remain open, which we will discuss in the final section.

It is unsatisfactory to see the large variance in weights and performance of the different averaging approaches in our case studies. Also the literature provides too few comparisons of model weights to provide robust advice. In general, our recommendations are thus guided by reducing harm, rather than suggesting an optimal solution.

5.1 Averaged prediction should be accompanied by uncertainty estimates

Just like any other statistical approach, model averaging can also be misapplied. Focussing entirely on the predictions rather than their spread can mislead, as Knutti et al. (2010) showed for combining precipitation predictions: spatial heterogeneity cancelled out across models, giving the erroneous impression of little change when in fact all models predict large changes (albeit in different regions). Similarly, King et al. (2008) found that averaging parameters from two competing models led to no effect of two hypothesised impacts, although in both models a (different) driver was very influential. We thus strongly encourage including at least model-averaged confidence intervals alongside any prediction, possibly in addition to the individual model predictions, to prevent erroneous interpretation of averaged predictions. Also, more attention should be paid to the full model. It has many desirable properties (unbiased parameter estimates, very good coverage), but suffers from violation of the parsimony principle ("Occam's razor") and requires more consideration in which form covariates should be fit. Its larger prediction error, compared to the over-optimistic single-best partial model, is the reason for correct confidence intervals.

5.2 Dependencies among model predictions should be addressed

Statistical models, which aim to describe the data to which they are fitted, will often have correlated parameters and fits; process models may overlap in modelled processes. Having highly similar models in the model set will inflate the cumulative weight given to them (as illustrated in Appendix S6) . One way to handle inflation of weights by highly-related models is to assign prior model probabilities in a Bayesian framework.

Another approach would be to pre-select models of different types (see next point). Alternatively, the cos-square scheme of Garthwaite and Mubwandarikwa (2010) uses the correlation matrix of model projections to appropriately change weights of correlated models. It is the only approach currently doing so, and, while the jury is still out on this method, our case study results look only mildly promising (Fig. 6, Tables 2 and 3).

5.3 Validation-based weighting or validation-based pre-selection of models

Madigan and Raftery (1994), Draper (1995) and more recently Yuan and Yang (2005) and Ghosh and Yuan (2009), have argued that only "good" models should be averaged. Different ways of combining model averaging with a model screening step have been proposed (Augustin et al., 2005; Yuan and Yang, 2005; Ghosh and Yuan, 2009), in which , model selection precedes averaging (pre-selection). This will happen implicitly, and in a single step, if any of the model weight algorithms discussed above attributes a weight of effectively zero to a model, as happened in case study 2. How prevalent this effect is in real world studies is unclear, as weights are rarely reported.

In contrast, some studies select models *after* the predictions are made (e.g. Thuiller, 2004; Forester et al., 2013). These studies have averaged models which predict in the same direction (along the "consensus axis": Grenouillet et al. 2010), which are the best 50% in the set (Marmion et al., 2009*a*), or however many one should combine to minimise prediction error. Such approaches necessitate addressing the challenge of using data twice (Lauzeral et al., 2015). Post-selection reduces the ability of "dissenting voices" (i.e. less correlated predictions) to reduce prediction error and instead reinforce the trend of the model type most represented in the set. As a consequence, their

uncertainty estimation will be overly optimistic. We do not advocate their use.

We suggest to employ **validation-based methods of model averaging** rather than relying on model-based estimates of error, i.e. (leave-one out) cross-validation and stacking rather than AIC. On account of us rarely believing our models in ecology, test data give us some capacity to make allowances for predictive bias. It is probably of little practical relevance whether models are pre-selected by validation-based estimates of error and then averaged with equal weights or weighted by validation-based estimates of error without pre-selection.

5.4 Process models are no different

In fishery science, averaging process models is relatively common (Brodziak and Piner, 2010), as it is in weather and climate science (Krishnamurti et al., 1999; Knutti et al., 2010; Bauer et al., 2015). There are at least two connected challenges such enterprises face: validation and weighting. Often process models are tuned/calibrated on all sets of data available, in the logical attempt to describe all relevant processes in the best possible way. That means, however, that no independent validation data are available, so that we cannot use the prediction accuracy of different models to compute model weights. Consequently, all models receive the same weight (e.g. in IPCC reports, or for economic models), or some reasonable but statistically ad-hoc construction of weights is employed (e.g. Giorgi and Mearns, 2002). In recent years, hind-casting has gained in popularity, i.e. evaluating models by predicting to past data. This will only be a useful approach if historic data were not used already to derive or tune model parameters, and if hindcasting success is related to prediction success (which it need not be, if processes or drivers change).

Cross-validation is often infeasible for large models, as run-times are prohibitively long. However, the greatest obstacle to averaging process models is the absence of truly

equivalent alternative models, which predict the same state variable. Fishery science is one of the few areas of ecology in which commensurable models exist and are being averaged in a variety of ways (e.g. Stanley and Burnham, 1998; Brodziak and Legault, 2005; Brandon and Wade, 2006; Katsanevakis, 2006; Hill et al., 2007; Katsanevakis and Maravelias, 2008; Jiao et al., 2009; Hollowed et al., 2009; Brodziak and Piner, 2010). Carbon and biomass assessments are also moving in that direction (Hanson et al., 2004; Butler et al., 2009; Wang et al., 2009; Picard et al., 2012). These fields would profit from averaging methods such as minimal variance and cos-squared, which do not require cross-validation and may perform better than either equal weights or BMA-EM, and probably better than MBMC's potentially overfitted supra-models.

Finally, irrespective of the approach chosen, model averaging studies should report model weights, and predictions should be accompanied by estimates of prediction uncertainty.

Acknowledgements

We like to thank the German Science Foundation (DFG) for funding the workshop "Model averaging in Ecology", held in Freiburg 2-6 March 2015 (DO 786/9-1). Part of this work was carried out during a research stay of CFD at the University of Melbourne, co-funded by the DFG (DO 786/10-1). BS is supported by the DFG (SCHR1000/6-2 and SCHR1000/8-2). DIW is supported by an Australian Research Council (ARC) Future Fellowship (grant number FT120100501). DRR is supported by the Alexander von Humboldt Foundation through the German Federal Ministry of Education and Research. GGA is the recipient of a Discovery Early Career Research Award from the Australian Research Council (project DE160100904). JE is supported by ARC's FT0991640 and DP160101003. JJLM is supported by Australia's National Environmental

Research Program (NERP) Environmental Decisions Hub and ARC DP160101003. KG is supported by the German Federal Ministry of Education and Research (BMBF 01LL0901A). WT received funding from the European Research Council under the European Community's FP7/2007-2013 Grant Agreement no. 281422 (TEEMBIO).

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Table 1: Approaches to model averaging, in particular to deriving model weights, their computational speed, likelihood/number of parameter requirements, as well as references to implementation in R.

Model averaging approach	speed	likelihood value $\|p_m$ required?[1]	comments (R-package)[2]
Reversible jump MCMC	slow	yes|no	Requires individual coding of each model. (rjmcmc)
Bayes factor	slow	yes|no	Requires specification of priors. (BayesianTools, BayesVarSel)
Bayesian model averaging using expectation maximisation (BMA-EM)	moderate	yes|no	Requires validation step. (BMA, EBMAforecast)
Fit-based weights	rapid-slow	yes|yes[3]	AIC, BIC and Cp can be easily computed from fitted models (stats, MuMIn). (LOO-CV as option in MuMIn,[4] also in loo, cvTools, caret, crossval). DIC & WAIC should be implemented in a Bayesian approach for full benefit. (BayesianTools)
Adaptive regression by mixing with model screening (ARMS)	moderate	yes|yes	No up-to-date implementation. (ARMS[5])
Bootstrapped model weights	slow	no|no	(MuMIn,[4] boot, resample)
Stacking	slow	no|no	Requires validation step. (MuMIn[4])
Jackknife model averaging (JMA)	slow	no|no	Computation time increases linearly with n. (MuMIn,[4] boot, resample)
Minimal variance	rapid	no|no	Based only on predictions. (MuMIn[4])
Cos-squared	rapid	no|no	Based only on predictions. (MuMIn[4])
Model-based model combinations	moderate	no|no	Requires setting up regression-type analysis with model predictions, plus validation step. ([2])
$1/M$	rapid	no|no	M is number of models considered.

[1] Does this method require a maximum-likelihood fit and/or number of parameters (p_m of the model? Typically these two are linked, since maximum-likelihood approaches typically employ the GLM, which provides both information.

[2] See also appendix for details and case studies for examples of implementation in R.

[3] While non-parametric models have no readily extractable number of parameters, a Generalised Degrees of Freedom-approach could be used to compute them (Ye, 1998). Similarly, but more efficiently, cross-validation can be used to estimate the effective number of parameters (Hauenstein et al., 2017).

[4] Implemented in MuMIn as part of this publication.

[5] `http://users.stat.umn.edu/~sandy/courses/8053/handouts/Aaron/ARMS/`

Table 2: Model weights (averaged across 100 repetitions) given to the 16 linear regression models of case study 1 by different weighting methods (see Table 1 for abbreviations), arranged by increasing prediction error (last column, median across replications). Only the best (m10) and the full model are shown from the 16 candidate models. LOO-CV: leave-one-out cross-validation using R^2 or RMSE as measure of model performance. For code see case study Appendix S9.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	RMSE
rjMCMC median	0.00	0.01	0.00	0.11	0.00	0.00	0.08	0.11	0.00	0.14	0.00	0.09	0.14	0.13	0.10	0.09	1.069
BIC	0.00	0.01	0.00	0.18	0.00	0.03	0.17	0.04	0.00	0.19	0.00	0.04	0.24	0.05	0.05	0.01	1.074
median[1]	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	1.075
m10[2]	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1.076
rjMCMC weights	0.00	0.01	0.00	0.11	0.00	0.00	0.08	0.11	0.00	0.14	0.00	0.09	0.14	0.13	0.10	0.09	1.076
boot	0.00	0.01	0.00	0.15	0.00	0.04	0.17	0.03	0.00	0.16	0.00	0.08	0.22	0.04	0.07	0.03	1.076
AIC	0.00	0.00	0.00	0.13	0.00	0.02	0.13	0.08	0.00	0.14	0.00	0.08	0.18	0.09	0.09	0.05	1.077
WAIC	0.00	0.00	0.00	0.13	0.00	0.02	0.11	0.09	0.00	0.14	0.00	0.08	0.16	0.10	0.11	0.06	1.078
MMA	0.00	0.00	0.00	0.13	0.00	0.02	0.12	0.08	0.00	0.14	0.00	0.09	0.18	0.10	0.10	0.06	1.078
stacking	0.00	0.07	0.02	0.08	0.04	0.06	0.13	0.07	0.04	0.06	0.06	0.07	0.11	0.07	0.08	0.04	1.079
JMA	0.00	0.01	0.00	0.16	0.00	0.05	0.22	0.01	0.00	0.19	0.03	0.01	0.29	0.02	0.02	0.00	1.079
full[2]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1.086
BMA-EM	0.00	0.08	0.01	0.08	0.02	0.07	0.14	0.06	0.03	0.08	0.10	0.04	0.15	0.06	0.06	0.03	1.104
BayesFactor	0.07	0.06	0.06	0.07	0.06	0.06	0.06	0.06	0.06	0.06	0.07	0.06	0.06	0.06	0.06	0.06	1.109
1/M	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	1.110
LOO-CV (R^2)	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	1.110
LOO-CV (RMSE)	0.09	0.06	0.08	0.06	0.07	0.06	0.06	0.06	0.07	0.06	0.06	0.06	0.06	0.06	0.06	0.06	1.123
MBMC (LM)[3]	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	1.135
MBMC (rF)[3]	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	1.181
minimal variance	−1.15	0.42	0.19	0.00	0.64	0.00	0.00	0.00	0.91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.208
cos-squared	0.00	0.00	0.30	0.00	0.21	0.21	0.02	0.01	0.00	0.00	0.24	0.00	0.00	0.00	0.01	0.00	1.209

[1] Weights not available, as different models contribute to the median at each replication.

[2] Prediction from individual model.

[3] Weights are variable. LM and rF refer to a linear model and a randomForest as supra-model, respectively,

Table 3: Model weights given to the six model types of case study 2 (GLM, GAM, randomForest, artificial neural networks and support vector machine) by different weighting methods (see Table 1 for abbreviations), arranged by decreasing fit of the averaged predictions to test data, assessed as log-likelihood (ℓ) (last column). LOO-CV: leave-one-out cross-validation using R^2 or RMSE as measure of model performance. For code see case study Appendix S10.

Method	GLM_{AIC}	GLM_{BIC}	GAM	rF	ANN	SVM	ℓ
median [1]	(0.176)	(0.216)	(0.212)	(0.162)	(0.146)	(0.088)	−182.84
LOO-CV	0.168	0.168	0.166	0.169	0.165	0.164	−184.82
equal weight	0.167	0.167	0.167	0.167	0.167	0.167	−184.86
cos-squared	0.122	0.104	0.178	0.188	0.186	0.221	−185.02
BMA-EM	0.388	0.192	0.000	0.420	0.000	0.000	−185.24
stacking	0.000	0.000	0.000	1.000	0.000	0.000	−186.82
bootstrap	0.000	0.000	0.000	1.000	0.000	0.000	−186.83
minimal variance	0.155	0.469	−0.036	0.58	−0.026	−0.141	−188.45
MBMC (GAM) [3]	–	–	*	*	–	–	−198.23
MBMC (rF) [3]	–	–	–	–	–	–	−200.20
JMA	0.000	0.000	0.000	0.000	0.000	1.000	−214.68
MBMC (GLM) [3]	–	–	*	*	–	–	−268.52
rF [2]	0	0	0	1	0	0	−186.83
GAM [2]	0	0	1	0	0	0	−193.40
ANN [2]	0	0	0	0	1	0	−194.28
GLM_{AIC} [2]	1	0	0	0	0	0	−197.48
GLM_{BIC} [2]	0	1	0	0	0	0	−197.73
SVM [2]	0	0	0	0	0	1	−214.68

[1] Weights are proportion of times this model was actually used to compute the median value divided by two.

[2] Prediction from individual model.

[3] Weights are variable. Asterisk indicates that a model's prediction was a significant term in the supra-model. GAM, rF and GLM refer to three different types of supra-model: a generalised additive model, a randomForest, and a generalised linear model.

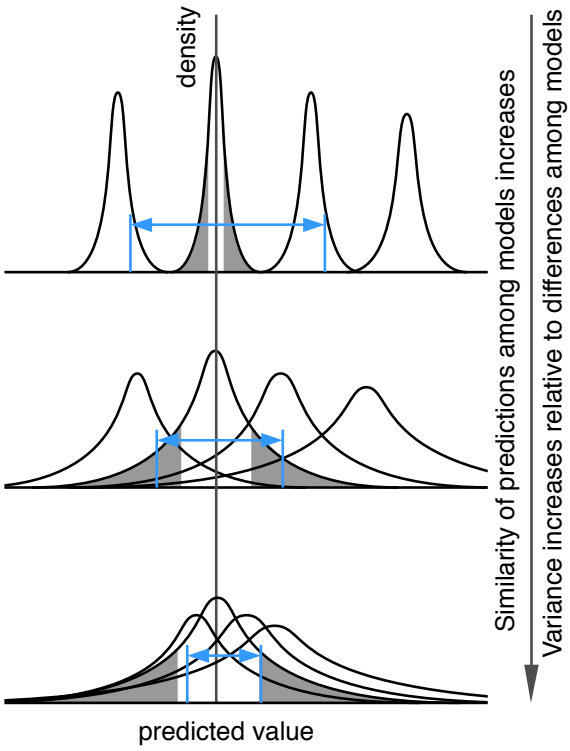

Figure 1: Conceptual depiction of 50% model averaging uncertainty intervals (blue) for different cases of bias and variance in four models (using equal weights). Distributions are the sampling distribution of a prediction from the four models. Truth is indicated by a vertical line. Shaded areas are outer 50% predictions of the best model, illustrating that the best model increasingly predicts to outside the model average's interval as variance becomes large relative to bias. From top to bottom, the source of error morphs from between-model variance to within-model variance. Accordingly, model selection would be more appropriate in the top situation, while model averaging would be superior in the lower situation.

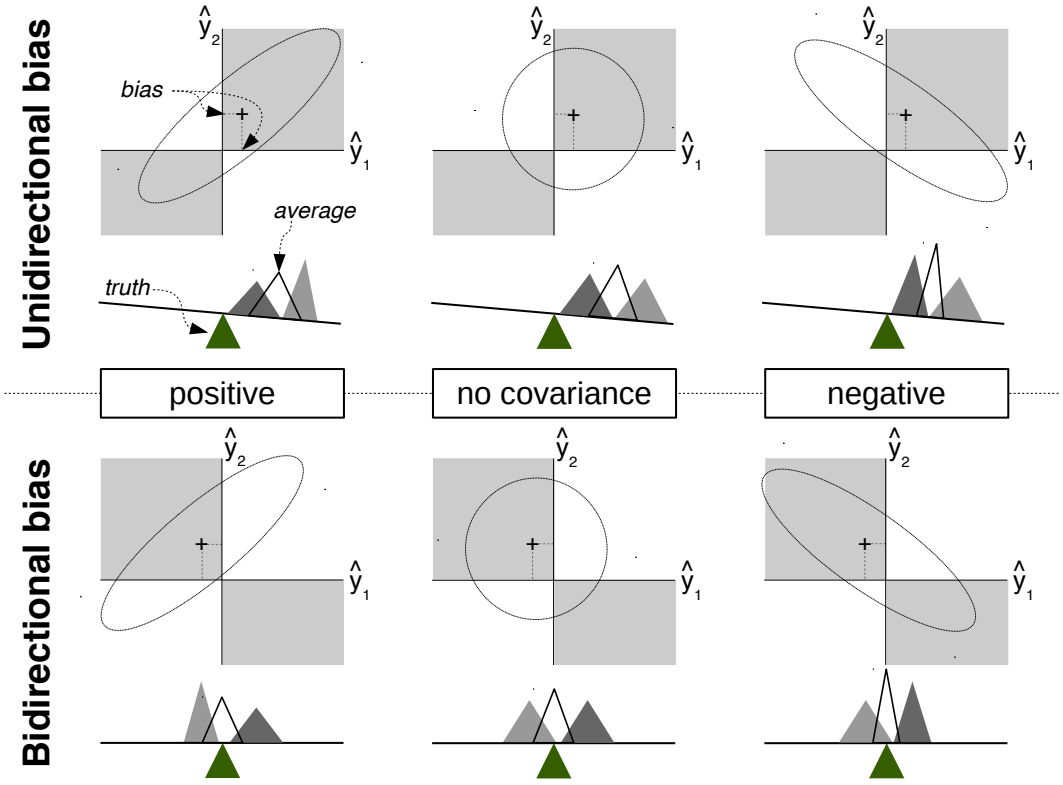

Figure 2: Conceptualised outcomes of model averaging. Sampling distributions of model predictions are depicted as stylised empty triangle on the see-saw (taller means less uncertain). Filled triangles represent the model predictions with unidirectionally bias (top row) or straddling truth (bottom row), and positive, no, or negative covariances among model predictions in columns. In the top row, grey shaded quadrants indicate model combinations with bias in the same direction, leading to a biased average (tilted see-saw). In the bottom row, grey shaded quadrants indicate opposite biases, which *may* lead to less biased averaged prediction, assuming optimal model weights were found. Changes in the covariance (columns) affect the uncertainty of the average, with negatively correlated predictions (right) yielding lowest uncertainty.

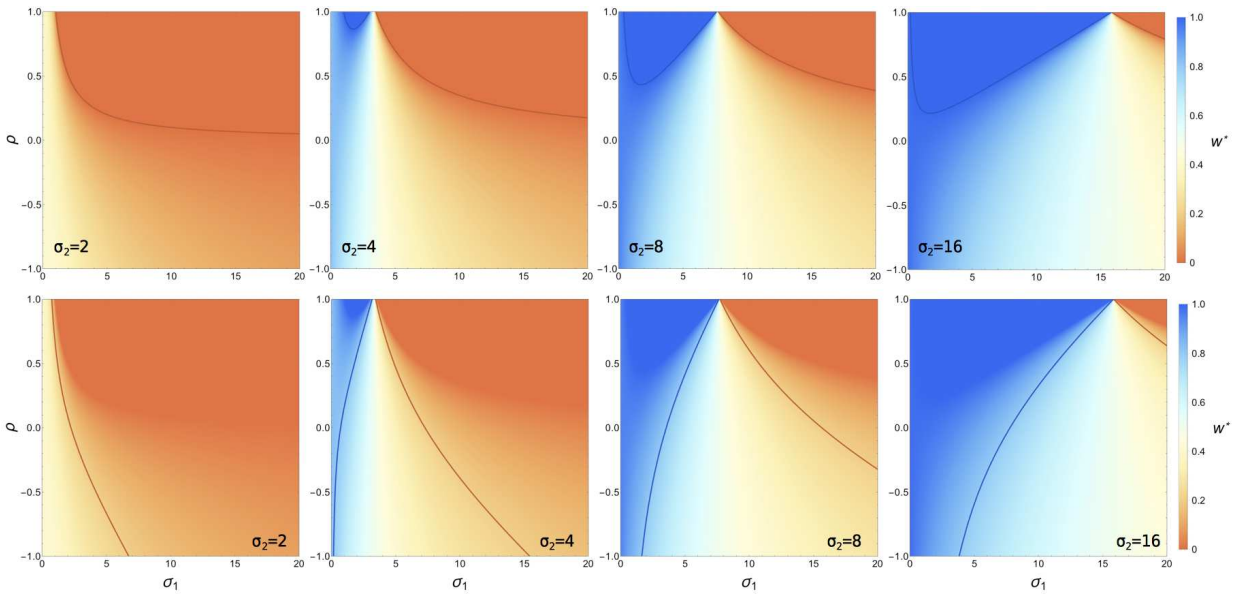

Figure 3: When to average, in the simplest case of two models that make correlated Gaussian predictions. The models are here described by their biases (b_1, b_2, not shown), their standard deviations (σ_1, σ_2), and by the correlation (ρ) between them. Each panel shows the regions in the (σ_1, ρ) plane where model 1 is best (blue shading and contour line), model 2 is best (orange shading and contour line), and where the optimal average is best (colour gradient between blue and orange). Top row represents the case where weights are known (i.e. without error: $\sigma_w = 0$), while the second row represents exactly the same settings, but with estimated weights (with uncertainty $\sigma_w = 0.2$). Notice that when w is estimated with uncertainty, the contours marking the transition between each single model and the average move into the washed-out colours, i.e. deviate from the fixed w situation in the upper panels. These curves now represent a level set at the values $\bar{w}_1^* = 1 - \sigma_w$ (blue curve) and $\bar{w}_2^* = \sigma_w$ (orange curve). As a consequence, the area where model averaging with estimated weights is superior to the better single model decreases substantially relative to the fixed w case, and disappears completely for $\sigma_w \geq 0.5$. Formal derivations for the contours and the critical weights is given in Appendix S2, the interactive tool itself in Data S1. Biases are set to $b_1 = 3$ and $b_2 = 2$.

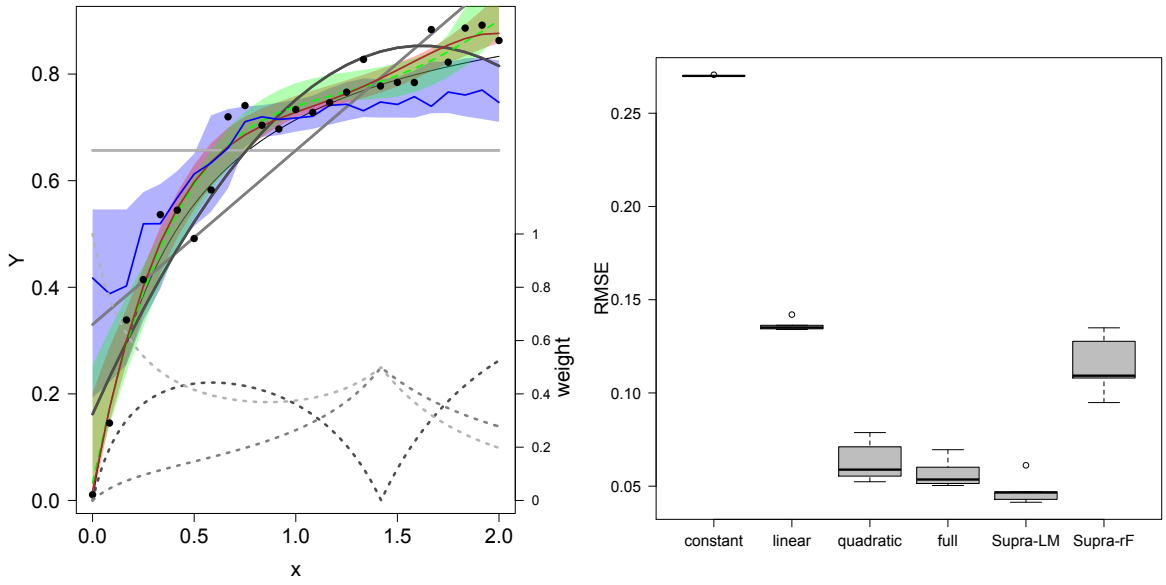

Figure 4: A simple *model-based model combination* example. *Left*: Three models (solid grey lines: constant, linear and quadratic) fitted separately to a data set (points, following the thin black line). Using a linear model (with quadratic terms: red) to combine the three models' fits may improve fit, even more so than the full model (green), and with narrower confidence intervals. Dotted lines indicate the weight that each model receives at each point in the linear model. Such MBMC did not necessarily improve fit, as randomForest-based model combinations showed (blue). *Right*: Using 5-fold cross-validation around the entire workflow shows that the linear supra-model (Supra-LM) indeed improved prediction (decreased root mean squared prediction error), while the randomForest-supra-model (Supra-rF) did not. The full model (as reference) comprised all terms present in Supra-LM, but was fitted directly.

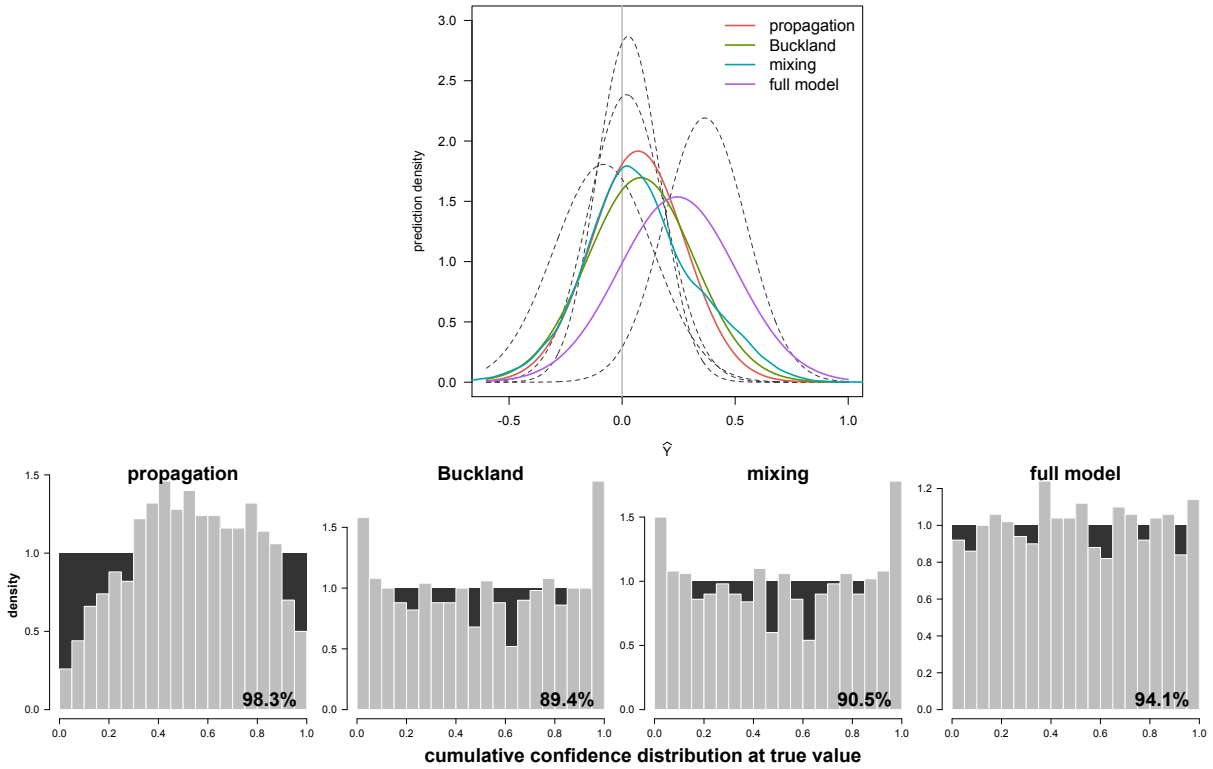

Figure 5: A comparison of different approaches to quantifying uncertainty when combining predictions from four linear models (dashed curves) with equal weights. *Top*: Truth is indicated by the vertical line. Error propagation based on bootstrapped estimates for eqn (5), Buckland et al.'s correction and model mixing yield similar averaged confidence distributions, while the full model is shifted. *Bottom*: Histograms of Bayesian p-values (the quantile of the true value in the posterior distribution across 1000 simulations) for each of the four methods , which should be uniform (black background). Number gives actual coverage for the 95% confidence interval. The error propagation estimate is too conservative with coverage close to 100%. Coverage of the approach of Buckland et al. and mixing are slightly too low in this example.

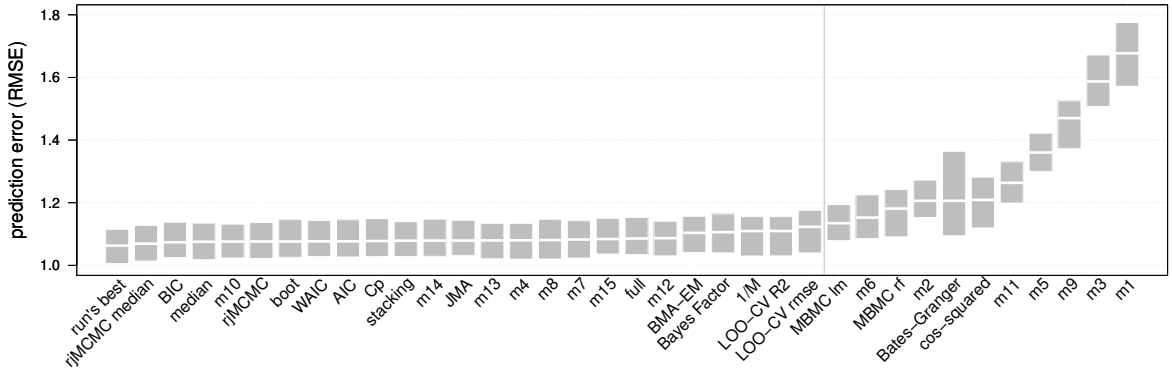

Figure 6: Prediction error of different model averaging approaches (100 repetitions) for case study 1. Box represents quartiles, white line the median. Approaches to the left of the vertical line are very similar, and no better than nine of the candidate models. See Table 1 for list of approaches, and Appendix S9 for list and fits of the individual models.