Probabilistic forecasting of temperature: comments on the Bayesian Model Averaging approach

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Abstract
A specific implementation of Bayesian model averaging has recently been suggested as a method for the calibration of ensemble temperature forecasts. We point out the similarities between this new approach and an earlier method known as kernel regression. We also argue that the Bayesian model averaging method (as applied) has a number of flaws that would result in forecasts with suboptimally calibrated mean and uncertainty.

1 Introduction
There is significant demand within industry for adequate probabilistic forecasts of temperature. However, this demand has not been met by the meteorological community and such forecasts are not commercially available. A small number of forecast vendors do produce probabilistic forecasts but the calibration methods they use are flawed. A number of academic papers have suggested methods by which such forecasts could be improved but again the methods described are flawed. To attempt to remedy this situation we run a program of research aimed at clarifying the issues involved in the creation of probabilistic temperature forecasts and at developing methods that can be used to produce such forecasts. We are not forecasters ourselves: our hope is that the forecasting community will use the methods we describe to produce forecasts that we can then use in our industrial applications. This article discusses a new method with the name Bayesian model averaging (BMA) that has recently been proposed for the calibration of temperature forecast ensembles (see Raftery et al. (2003)). Our purpose is twofold:

1. To point out the close connections between BMA and earlier methods known as kernel regression (KR) and kernel spread regression (KSR)
2. To describe a number of flaws that we believe that the BMA approach suffers from that render it inappropriate as a method to be used for the calibration of real forecast data

We start by describing the KR and BMA approaches. We then compare the two and point out the problems we see in BMA. Finally, we suggest some further methods that take features from both BMA and KR that could be used to solve the calibration problem that is discussed in Raftery et al. (2003).

2 Kernel Regression
Kernel regression (KR) was described by us in Jewson (2003). It is a method that takes an ensemble forecast and turns it into a probabilistic forecast. The simplest reasonable way to do this is to use linear regression on the ensemble mean. KR is a simple extension of linear regression that allows for the representation of non-normality in the temperature distribution by putting a small kernel of optimum width around each ensemble member. The probability density forecast from KR can be written as:

\[ p(x) = \sum_{i=1}^{M} p_i(x) \]  (1)

where the \( p_i \) are the individual kernels given by

\[ p_i(x) \sim N(x_i, \lambda^2) \]  (2)
where $x_i$ is the $i$’th ensemble member and $\lambda$ is the bandwidth (these equations come from equation 1 in Jewson (2003)).

In addition to applying kernels in this way the mean and the variance of the ensemble members are calibrated using linear regression. We write the complete model as:

$$T_i \sim K(\alpha + \beta m_i, \gamma, \lambda)$$  \hspace{1cm} (3)

KR calibrates the ensemble mean using linear regression (which gives an optimal combination between the ensemble mean and climatology) and fixes the spread and the non-normality using the parameters $\gamma$ and $\lambda$. The parameter $\lambda$ is the bandwidth of the kernels used and controls the smoothness of the final predicted distribution. Small values of $\lambda$ lead to a multimodal distribution while large values of $\lambda$ lead to a unimodal smooth distribution.

The mean of the prediction from KR is given by:

$$E(x) = \alpha + \beta m_i$$  \hspace{1cm} (4)

while the variance of the prediction, which is constant in time for the anomalies, is given by:

$$\text{var}(x) = \chi^2 + \frac{1}{M} \sum_{i=1}^{M} (x_i - \mu)^2$$  \hspace{1cm} (5)

or

$$\text{variance of modelled temperatures} = \lambda^2 + \text{sample variance of calibrated ensemble members}$$  \hspace{1cm} (6)

(this equation is equation 9 in Jewson (2003)).

An extension of KR that allows for the uncertainty to vary in time according to variations in the ensemble spread is also described in Jewson (2003), and can be written as

$$T_i \sim K(\alpha + \beta m_i, \gamma + \delta s_i, \lambda)$$  \hspace{1cm} (7)

This model, known as kernel spread regression (KSR), calibrates the ensemble spread by having separate parameters for the mean and the variance of the spread. This was shown to be necessary in Jewson et al. (2003).

The predicted variance from KSR is:

$$\text{var}(x) = \chi^2 + \frac{1}{M} \sum_{i=1}^{M} (x_i - \mu)^2$$  \hspace{1cm} (8)

or

$$\text{variance of modelled temperatures} = \lambda^2 + (\gamma + \delta s_i)^2$$

\section{Bayesian model averaging}

BMA is a general approach for combining the results from several statistical models using weights (Hoeting et al., 1999). There are a number of ways that BMA could be used in the creation of probabilistic forecasts. We will discuss the particular application of BMA given in Raftery et al. (2003). The conclusions we will draw do not apply to BMA in general, but only to this particular way of using BMA.

The suggestion in Raftery et al. (2003) is that the probability density of future temperatures can be modelled as a weighted sum of a number of probability densities from different sources:

$$p(x) = \sum_{i=1}^{M} w_i g_i(x)$$  \hspace{1cm} (9)

where

$$g_i(x) \sim N(x_i, \sigma_i^2)$$  \hspace{1cm} (10)

where $x_i$ are the ensemble members (these equations are equations 2 and 3 from Raftery et al. (2003), written in our notation).

The variance of the probabilistic forecast is then given by

$$\text{var}(x) = \sum_{i=1}^{M} w_i (x_i - \mu)^2 + \sum_{i=1}^{M} w_i \sigma_i^2$$  \hspace{1cm} (11)

(this is equation 7 from Raftery et al. (2003)).
4 The connection between BMA and KR

We now consider how BMA and KR are related. To see the connection we consider a case where the individual forecasts are statistically identical. BMA also considers the more general case where the forecasts are statistically different although we will argue that since it doesn’t work in the simplest case of identical members it certainly can’t be expected to work in the more complex cases.

If the forecasts are statistically identical then we can assume that the BMA weights and $\sigma_i$’s are equal:

\[ w_i = \frac{1}{M} \quad (12) \]
\[ \sigma_i = \sigma \quad (13) \]

Equation 9 now gives:

\[ p(x) = \sum_{i=1}^{M} \frac{1}{M} g_i(x) \quad (14) \]

and we can see that this agrees with equation 11 if we define $g_i(x) = Mp_i(x)$ i.e. if we normalise the kernels differently. So this part of the two models is the same up to a simple definition of the normalisation.

The BMA predicted mean is just

\[ E(x) = \sum_{i=1}^{M} x_i \quad (15) \]

i.e. the ensemble mean, and the BMA predicted variance is

\[ var(x) = \sum_{i=1}^{M} \frac{1}{M} (x_i - \mu)^2 + \sigma^2 \quad (16) \]

We can now see the similarities and differences between BMA and kernel regression very clearly.

1. By comparing equation 4 with equation 15 we see that BMA predicts the expected temperature using the ensemble mean while KR predicts the expected temperature using an optimum combination of the ensemble mean with climatology.

2. By comparing equations 5 and 8 with equation 16 we see that BMA calibrates the mean level of uncertainty, the variability of the uncertainty and the smoothness of the distribution using a single parameter $\sigma$. KR uses two parameters to calibrate the mean level of uncertainty and the smoothness while KSR uses three parameters to calibrate the mean level of uncertainty, the variability of the uncertainty and the smoothness.

BMA (when applied to the identical members case) is a special case of KSR in which $\beta = 1$, $\gamma = 0$ and $\delta = 1$.

5 The problems with BMA

Unfortunately Bayesian model averaging seems to suffer from a number of flaws as a method for calibrating temperature ensembles. These issues discussed below: the research on which these conclusions are based is summarised in Jewson (2004).

The first problem concerns the calibration of the ensemble mean. In the special case that we are considering BMA predicts the expected temperature using the ensemble mean. However it is well documented (Leith (1974), von Storch and Zwiers (1999), Jewson and Ziehmann (2003)) that the ensemble mean is not the optimal forecast for the expected temperature: a ‘damped’ version of the ensemble mean calculated using linear regression is better. This damping performs an optimal calibration of the ensemble mean with climatology. An undamped ensemble mean such as that produced by BMA does not have the correct variance and will not minimise RMSE.

The second problem concerns the calibration of the uncertainty. To correctly calibrate the uncertainty of a probabilistic forecast one needs to consider (at least) two operations. First, the temporal mean of the uncertainty must be fixed at an appropriate level. There is no information about the temporal mean of the uncertainty in the ensemble itself: this information can only come from past forecast error statistics. Secondly, the amplitude of the variability of the uncertainty must be fixed at an appropriate level. Again,
there is no information about the amplitude of the variability of the uncertainty in the ensemble itself: this must be fitted from past forecast error statistics too. What the ensemble provides is then the relative amplitude and phase of the fluctuations of the uncertainty. The important point is that these two calibration steps (calibrating the mean and the amplitude of the variability of the spread) are independent. To set the mean level of the uncertainty correctly one typically needs to inflate the ensemble spread. However, to set the amplitude of the variations in the uncertainty correctly one may need to reduce the amplitude of the variations in the ensemble spread. A statistical model thus needs at least two parameters in order to calibrate spread correctly. If only one parameter is available, the calibration of the mean and the variability of the uncertainty will be mixed together, and the results will be somewhat arbitrary and very possibly less good than a calibration method that ignores the variability in the ensemble spread altogether. This mixing of different aspects of the calibration is what happens in BMA.

KR, KSR and BMA add another operation in the calibration of the ensemble, which is the smoothing of the ensemble towards or away from a normal distribution. If the bandwidth of the kernel (λ in kernel regression and σ in BMA) is large then the ensemble is smoothed towards a normal while if the bandwidth is small the probability forecast will likely be rather multimodal and will have a shape that depends more strongly on the distribution of the individual ensemble members. This smoothing operation needs a separate parameter to be performed correctly as it is an independent issue from the calibration of the uncertainty. KR and KSR use a separate parameter for this step while BMA uses the same parameter as is used to calibrate the uncertainty.

In summary BMA only has a single free parameter (σ) rather than the three that are required to perform the calibration that is being attempted. Thus the three operations that are being performed (calibration of the mean level of the uncertainty, calibration of the variability of the uncertainty and calibration of the smoothness of the forecast distribution) are mixed together. It is easy to imagine situations in which this would cause problems. For instance it would not be possible for BMA to correctly calibrate an ensemble for which the variability in the ensemble spread contains very little information (requiring a large value of σ) but in which the temporal mean of the ensemble spread is close to the correct level (requiring a small value of σ). Nor would it be possible for BMA to correctly calibrate an ensemble for which the ensemble spread was larger than the actual uncertainty.

6 The solution

The solution to this problem is to use the correct number of free parameters for the calibration that is being attempted. Given only a single parameter the most sensible course of action seems to be to assume a normal distribution, ignore the variations in spread and use the parameter to represent the mean level of uncertainty. Given two parameters one should calibrate the mean and variability of the uncertainty, while still assuming a normal distribution. Finally given three parameters one can calibrate all three of the mean level of uncertainty, the variability of the uncertainty and the smoothness.

7 Weighted kernel regression

In Raftery et al. (2003) BMA was used to combine a number of forecasts that were not statistically identical. We have argued that BMA does not calibrate correctly in the statistically identical case, and so cannot be expected to work in more general cases either. How, then, should the original calibration problem described in Raftery et al. (2003) be solved? The kernel regression models should not be used as is since they assume that the forecasts are statistically identical. One can imagine methods that take the best of the KSR and BMA approaches that might include one or more of the following features:

- the mean is predicted using multiple linear regression on the anomalies
- kernels with different widths are used on each ensemble member
- the kernels could be combined with different weights
- the uncertainty is predicted using some linear function on the weight ensemble spread

1 and to be fair we should note that this problem also arises in other forecast calibration methods that have been suggested in the academic literature such as the methods of Roulston and Smith (2003) and Mylne et al. (2002)
However, our previous experience of calibration suggests to us that much simpler models might perform just as well since the effects of non-normality and the benefit of using the spread may well both be small. In that case multiple linear regression on the anomalies is probably ideal, and whatever method is being used it should be compared with linear regression on the anomalies as an appropriate minimal model.

8 Summary

We have discussed the question of how to produce probabilistic forecasts of temperature. In particular we have dissected the Bayesian model averaging approach of Raftery et al. (2003). This approach is very similar to an earlier approach known as kernel regression (Jewson, 2003). We have argued that BMA does not calibrate temperatures in an appropriate way. Neither the predicted mean nor the predicted variance are constructed accurately. With respect to the predicted mean, the issue of ‘damping’ towards climatology has been omitted. With respect to the variance, BMA mixes the separate functions of calibrating the mean level of uncertainty, the amplitude of the variability of the uncertainty and the smoothness of the forecast distribution into a single factor. We conclude that BMA (as applied in Raftery et al. (2003)) is not a calibration method at all, but simply a method to fit a distribution to a set of ensemble members. As such it is more or less the same as the well known kernel density of classical statistics.

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