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Extending Extended Logistic Regression to Effectively Utilize the Ensemble Spread

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Abstract

To achieve well calibrated probabilistic forecasts, ensemble forecasts often need to be statistically post-processed. One recent ensemble-calibration method is extended logistic regression which extends the popular logistic regression to yield full probability distribution forecasts. Although the purpose of this method is to post-process ensemble forecasts, mostly only the ensemble mean is used as predictor variable, whereas the ensemble spread is neglected because it does not improve the forecasts. In this study we show that when simply used as ordinary predictor variable in extended logistic regression, the ensemble spread only affects the location but not the variance of the predictive distribution. Uncertainty information contained in the ensemble spread is therefore not utilized appropriately. To solve this drawback we propose a simple new approach where the ensemble spread is directly used to predict the dispersion of the predictive distribution. With wind speed data and ensemble forecasts from the European Centre for Medium-Range Weather Forecasts (ECMWF) we show that using this approach, the ensemble spread can be used effectively to improve forecasts from extended logistic regression.

Keywords: probabilistic forecasting, extended logistic regression, heteroskedasticity, ensemble spread.

1. Introduction

Weather forecasts are very important for many parts of social and economic life. For example they are used for severe weather warnings, for decision making in agriculture and industry, or for planning of leisure activities. Generally these forecasts are based on numerical weather prediction (NWP) models. Unfortunately, because of uncertainties in the initial conditions and unknown or unresolved atmospheric processes these models are always subject to error. Luckily some of these errors are systematic and can be corrected with statistical post-processing, often also referred to as model output statistics (MOS; Glahn and Lowry 1972). However, not all errors can be corrected and for many customers it is important to get additional information about the remaining forecast uncertainty. For this purpose many forecasting centers provide ensemble forecasts. These are multiple NWP forecasts with slightly perturbed initial conditions and sometimes also different model formulations. The idea is that these different forecasts should represent the range of possible outcomes (Lorenz 1996). Large ensemble spreads are then associated with high forecast uncertainties and small spreads signify low uncertainties. However, due to limited computer power only a relatively small number of different forecasts can be computed, which are insufficient to span the whole range of possible outcomes. Thus, to achieve calibrated uncertainty forecasts, statistical post-processing is needed.

In the past decade much research has gone into finding appropriate methods to post-process ensemble forecasts. For example, Roulston and Smith (2003) proposed dressing the ensemble members with historical model errors and Raftery, Gneiting, Balabdaoui, and Polakowski (2005) suggested Bayesian model averaging for this purpose. Gneiting, Raftery, Westveld, and Goldman (2005) proposed to use linear regression with error variances depending on the ensemble spread, and for binary predictands Hamill, Whitaker, and Wei (2004) proposed to use logistic regression. Comparisons of these and other methods (Wilks 2006a; Wilks and Hamill 2007) showed that logistic regression is one of the better approaches. A very promising extension of logistic regression has been proposed recently (Wilks 2009). By including the predictand threshold in the regression equations this extended logistic regression allows derivation of full predictive distributions. The extended logistic regression method has been used in several studies for probabilistic precipitation forecasts (Schmeits and Kok 2010; Ruiz and Saulo 2012; Roulin and Vannitsem 2012; Hamill 2012; Ben Bouallègue 2013) and it was shown that it performs very well compared to standard logistic regression (Wilks 2009; Ruiz and Saulo 2012) and other ensemble post-processing methods (Schmeits and Kok 2010; Ruiz and Saulo 2012). In all of these studies, extended logistic regression is used to post-process ensemble forecasts, but mostly the ensemble mean was used as the only predictor variable. There were also several attempts to additionally include the ensemble spread but with the exception of Hamill (2012) it was always disregarded because it did not improve the forecasts.

In this study we show that the predictive distribution of the transformed predictand is logistic and that the predictor variables only affect the location (mean) but not the dispersion (variance) of this logistic distribution. So far the ensemble spread was always included as ordinary predictor variable in extended logistic regression so that its information was only used to predict the location but not the dispersion of the forecast distribution. However, the ensemble spread is generally expected to mainly contain information about the forecast uncertainty which in turn should be directly related to the dispersion of the predictive distribution. Hence, the uncertainty information contained in the ensemble spread cannot be utilized properly by extended logistic regression so that it is not surprising that no improvements could be found.

To solve this drawback of extended logistic regression, we therefore propose a simple new approach in which the ensemble spread can be directly used as predictor for the dispersion of the forecast probability distribution. To illustrate our findings and test if improvements can be achieved with this new approach, we compare different approaches to include the ensemble spread in extended logistic regression. We use approximately 3 years of wind speed data from an Austrian weather station and ensemble forecasts from the European Centre for Medium Range Weather Forecasts (ECMWF).

The remainder of the paper is organized as follows: In Section 2 we describe the extended logistic regression model and show the problems when including the ensemble spread as ordinary predictor variable. Our new approach is introduced in Section 3. Results from the case study are shown in Section 4 and a summary and conclusion can be found in Section 5.

2. Extended logistic regression

Originally, logistic regression is a regression model from the generalized linear model framework (Nelder and Wedderburn 1972) to model the conditional probability of binary events. As such it is also a well-suited MOS method for binary predictands (Hamill *et al.* 2004). For example, the probability of a continuous variable y to fall below a certain threshold q can be predicted with:

$$P(y < q|\mathbf{x}) = \frac{\exp(\mathbf{x}^\top \beta)}{1 + \exp(\mathbf{x}^\top \beta)} = \Lambda(\mathbf{x}^\top \beta) \tag{1}$$

where $\mathbf{x}$ is a vector of predictor variables (e.g., NWP forecasts; $\mathbf{x} = (1, x_1, x_2, ...)^\top$) and β is a vector of regression coefficients ($\beta = (\beta_0, \beta_1, \beta_2, ...)^\top$) that is generally estimated with maximum likelihood estimation (see Appendix). The regression function has the same mathematical form as the cumulative distribution function of the standard logistic distribution (Λ) which is indicated by the final equality in Equation 1.

Often more than one threshold is of interest and separate logistic regressions are fitted for each of these thresholds. This approach has the disadvantage that the predicted probabilities are not constrained to be mutually consistent. In other words, for two thresholds q_a and q_b with $q_a < q_b$ it can occur that $P(y < q_a|\mathbf{x}) > P(y < q_b|\mathbf{x})$ which would imply nonsense negative probabilities for $P(q_a < y < q_b|\mathbf{x})$.

To avoid these inconsistencies, Wilks (2009) extended logistic regression by including (a transformation of) the thresholds q_j as additional predictor variable.

$$P(y < q_j|\mathbf{x}) = \Lambda(\alpha g(q_j) + \mathbf{x}^\top \beta) \tag{2}$$

Here $g(q_j)$ is a nondecreasing function of q_j and α is an additional coefficient that has to be estimated. In addition to avoiding negative probabilities, this extended logistic regression has the advantage that fewer coefficients have to be estimated (instead of different vectors β for each threshold α and β are the same for all thresholds), which is especially advantageous for small training data sets (Wilks 2009). Furthermore, the probability to fall below any arbitrary value Q can be easily computed by replacing q_j with Q:

$$P(y < Q|\mathbf{x}) = \Lambda(\alpha g(Q) + \mathbf{x}^\top \beta) \tag{3}$$

Equation 3 can also be interpreted as continuous cumulative distribution function which implies that full continuous probability distributions can be provided.

Since $g()$ has to be a nondecreasing function, the equation

$$P(y < Q|\mathbf{x}) = P(g(y) < g(Q)|\mathbf{x}) \tag{4}$$

is always fulfilled. With Equation 4 and some rearrangements, Equation 3 can also be written as

$$P(g(y) < g(Q)|\mathbf{x}) = \Lambda\left(\frac{g(Q) + \mathbf{x}^\top \beta/\alpha}{1/\alpha}\right) \tag{5}$$

and upon setting $\mu = -\mathbf{x}^\top \beta/\alpha$ and $\sigma = 1/\alpha$ we obtain

$$P(g(y) < g(Q)|\mathbf{x}) = \Lambda\left(\frac{g(Q) - \mu}{\sigma}\right) \tag{6}$$

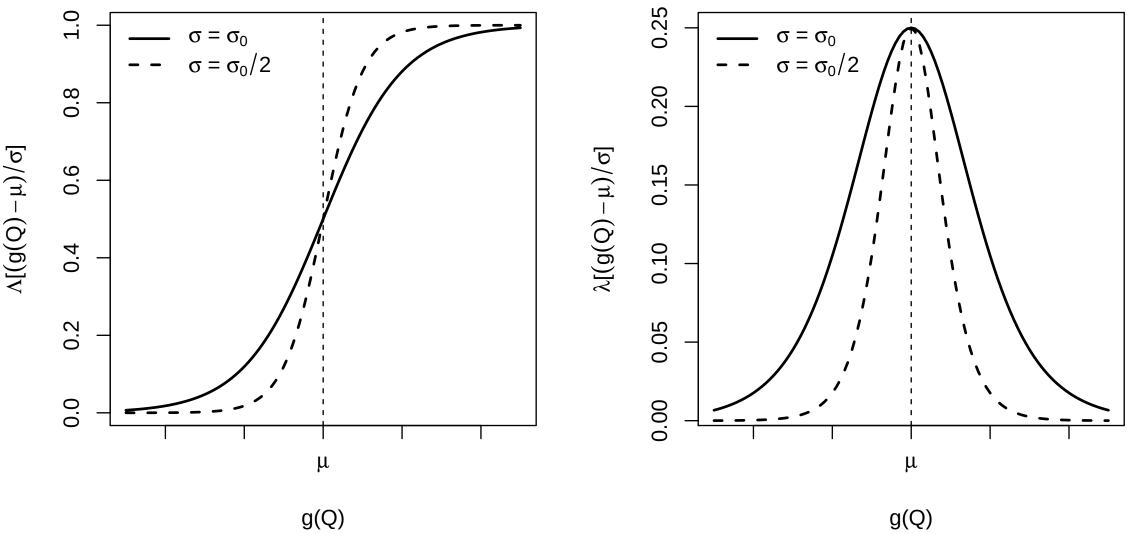

Figure 1: Cumulative distribution function (left) and probability density function (right) of the logistic distribution for different values of σ. Here $\lambda(x) = \frac{d\Lambda(x)}{dx}$ is the probability density function of the standard logistic distribution.

This notation allows one to easily see that the conditional probability distribution of the transformed predictand $g(y)$ given the predictor variables $\mathbf{x}$ is a logistic distribution with location parameter μ and scale parameter σ. Cumulative distribution functions and probability density functions of this distribution with different scale parameters σ are shown in Figure 1. The shape of the logistic distribution is very similar to that of the normal distribution but with somewhat heavier tails. The mean of this distribution is μ and in terms of the scale parameter the variance is $\sigma^2\pi^2/3$ (Johnson, Kotz, and Balakrishnan 1995).

Note that the scale parameter $\sigma = 1/\alpha$ is constant so that the predictor variables in $\mathbf{x}$ only affect the mean but not the variance of the logistic predictive distribution. Hence, when included as additional predictor variable in $\mathbf{x}$, the ensemble spread has no effect on the dispersion of the predictive distribution. However, usually large ensemble spreads are associated with high forecast uncertainties, which in turn should be related to wider predictive distributions. In contrast the level of uncertainty should generally have no effect on the location of the forecast probability distribution. Thus when just including the ensemble spread as additional predictor variable in $\mathbf{x}$ this uncertainty information is not utilized properly by extended logistic regression.

3. Heteroscedastic extended logistic regression

In the previous section we showed that when using the ensemble spread as an ordinary predictor variable in extended logistic regression, uncertainty information is not utilized appropriately. As a more effective approach we therefore propose to use the ensemble spread directly

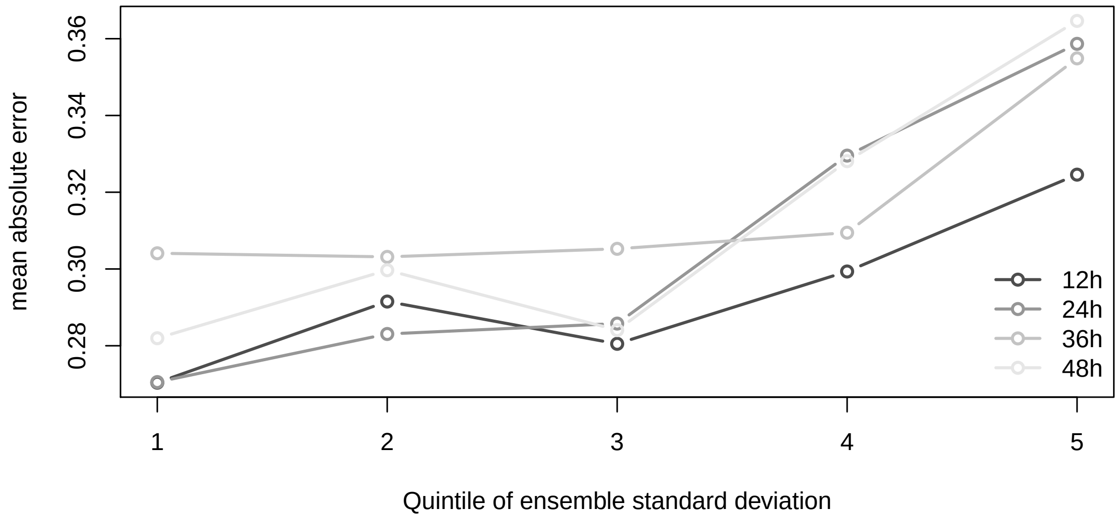

Figure 2: Mean absolute error of ensemble median for different ensemble standard deviations and lead times computed for *Wien – Hohe Warte* (23 months of data). Quintiles are used to divide the ensemble standard deviation into different levels. Note that for this plot all wind speeds are square-root transformed.

as predictor for the *dispersion* of the predictive distribution. Therefore we simply replace μ and σ in Equation 6 with

$$\mu = \mathbf{x}^\top \gamma \tag{7}$$

and

$$\sigma = \exp(\mathbf{z}^\top \delta) \tag{8}$$

respectively. Here $\mathbf{z}$ is an additional vector of input variables (i.e., the ensemble spread) and γ and δ are coefficient vectors that have to be estimated. The exponential function is used here as a simple method to ensure positive values for σ.

Note that with $\mathbf{z} = 1$ this model is completely equivalent to the original extended logistic regression (Equation 2) with $\alpha = 1/\exp(\delta)$ and $\beta = -\gamma/\exp(\delta)$.

The idea of using the ensemble spread as predictor for the dispersion of the predictive distribution is not completely new here. For Gaussian linear regression models, Gneiting *et al.* (2005) proposed a similar approach, which has been proven to perform well in several studies (e.g., Wilks 2006a; Wilks and Hamill 2007).

4. Case study

In this section, we apply the findings from the previous sections on real data in a case study. We use wind speed data from the Austrian automatic weather station *Wien – Hohe Warte* (48.249 N, 16.356 E) from April 2010 to December 2012. As NWP forecasts we use ensemble

Model		$\mathbf{x}$	$\mathbf{z}$
XLR	Extended logistic regression	$(1, M)^\top$	1
XLR:S	Extended logistic regression	$(1, M, S)^\top$	1
XLR:SM	Extended logistic regression	$(1, M, S * M)^\top$	1
HXLR	Heteroscedastic extended log. reg.	$(1, M)^\top$,	$(1, S)^\top$
HXLR:S	Heteroscedastic extended log. reg.	$(1, M, S)^\top$,	$(1, S)^\top$

Table 1: List of different extended logistic regression models. $\mathbf{x}$ and $\mathbf{z}$ are vectors of predictor variables for the location and scale of the predictive distribution respectively. M and S are the mean and standard deviation of square root transformed wind speed ensemble forecasts respectively.

wind speed forecasts interpolated to the instrument location from the European Centre for Medium Range Weather Forecasts (ECMWF; Molteni, Buizza, Palmer, and Petroliagis 1996), initialized at 00 UTC for the lead times 12, 24, 36, and 48 hours. As can be seen in Figure 2, there is a clear positive correlation between ensemble spread and forecast error for these data. This positive spread-skill relationship suggests that the ensemble spread contains potentially useful uncertainty information. To investigate how this information might be used most effectively, we compare different extended logistic regression models.

For all models we use the square root function for $g(\cdot) = \sqrt{\cdot}$. This function gave good results for precipitation forecasts in several studies and also improves our wind speed forecasts compared to the identity function. As potential regressors we use the ensemble mean (M) and standard deviation (S) of the square-root-transformed ensemble wind speed forecasts. Furthermore we selected $J = 9$ climatological quantiles with probabilities 1/10, 2/10, ... 9/10 as thresholds q_j (1.2, 1.7, 2.2, 2.7, 3.2, 3.8, 4.4, 5.2, and 6.4 m/s).

Table 1 lists the models that are used in the following. In addition to the extended logistic regression model with the ensemble mean as single predictor variable (*XLR*) there are 4 models which use the ensemble standard deviation. The models *XLR:S* and *XLR:SM* are standard extended logistic regression models with the ensemble standard deviation as additional predictor variable, either alone (*XLR:S*) or multiplied with the ensemble mean (*XLR:SM*). In the heteroscedastic extended logistic regression model *HXLR* the ensemble standard deviation is only included as predictor variable for the scale and in *HXLR:S* it is additionally also used as predictor variable for the location of the predictive distribution.

Before reporting the forecast quality of these different models it is interesting to investigate the effect of the ensemble spread on the predicted probability distributions. Figure 3 shows predicted probability density functions of the *XLR:S* and *HXLR* model for different ensemble standard deviations. For the *XLR:S* model it can be seen that contrary to the desired effect, larger ensemble standard deviations are related to slightly sharper distributions. In contrast, the *HXLR* model uses the ensemble standard deviation more appropriately and larger ensemble standard deviations are clearly related to wider distributions.

Next we compare the performance of the different models. Since extended logistic regression can provide multi-categorical probabilistic forecasts, the ranked probability score (Epstein 1969; Wilks 2006b) is a well-suited measure of forecast quality.

$$RPS = \sum_{j=1}^{J} (P(y < q_j|\mathbf{x}) - I(y < q_j))^2 \tag{9}$$

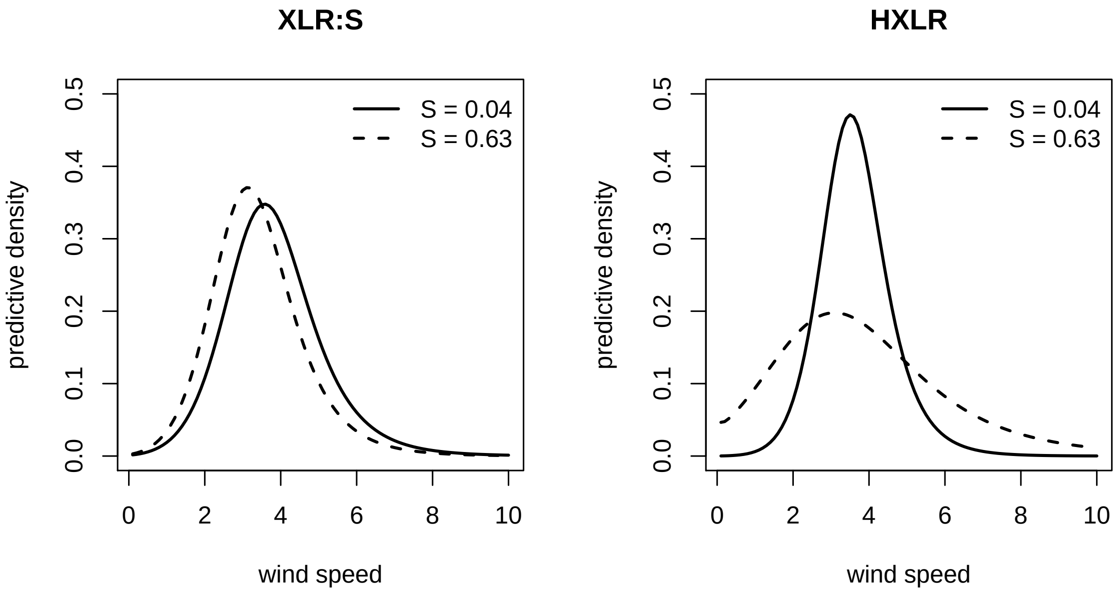

Figure 3: Predicted probability density functions of *XLR:S* (left) and *HXLR* (right) for small and large ensemble standard deviations respectively. The models (see Table 1 for details) are fitted for 36 hours lead time. For all curves the ensemble mean $M = 2$ which is approximately the mean ensemble mean in the data set. The ensemble standard deviations 0.04 and 0.63 are approximately the minimum and maximum ensemble standard deviation in the data set respectively.

Here $J = 9$ is the number of thresholds and $I(\cdot) = 1$ if the argument in brackets is true and 0 if it is not. To get independent training and test data sets we estimate and verify the models with tenfold cross validation. With this cross validation we get one RPS value for each event in the dataset. From these individual RPS, 250 estimates of the mean ($\overline{RPS}$) are computed on 250 bootstrap samples. This is all done separately for each model and lead time. Since we are mainly interested in the improvements that can be achieved with the ensemble standard deviation we finally compute skill scores ($RPSS$) with the standard extended logistic regression model (XLR) as reference.

$$RPSS = 1 - \frac{\overline{RPS}}{\overline{RPS}_{XLR}} \tag{10}$$

Note that here positive values signify improvements over the standard extended logistic regression model.

The $RPSS$ of the different models and lead times are shown in Figure 4. It can be seen that including the ensemble standard deviation simply as ordinary predictor variable (*XLR:S*, *XLR:SM*) deteriorates the forecast quality of extended logistic regression. However, the reason is not the absence of predictive information in the ensemble standard deviation since using it with our new approach ($HXLR$) clearly improves the forecast quality. Since the ensemble standard deviation obviously does not contain any predictive information on the location it is also not advantageous to include it additionally as predictor variable for the

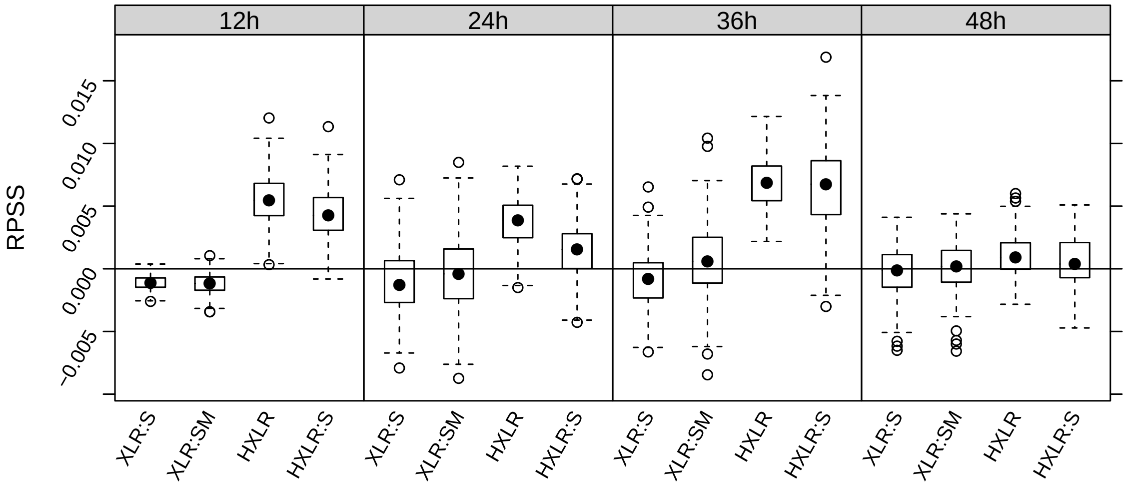

Figure 4: Ranked probability skill score (*RPSS*) relative to extended logistic regression (*XLR*) for different lead times and models (see Table 1 for details) using 9 climatological quantiles as thresholds. Positive values indicate improvements over *XLR*. The boxes indicate the interquartile ranges of the 250 values from the bootstrapping approach, the whiskers show the most extreme values that are less than 1.5 times the length of the box away from the box, and points are plotted for values that are outside the whiskers.

location (*HXLR:S*).

5. Summary and conclusion

The inclusion of the ensemble spread in extended logistic regression has been shown in several studies not to improve the forecast skill. As we have shown in this paper this is not surprising because when the ensemble spread is included as ordinary predictor variable it modifies only the location but not the dispersion of the forecast distribution. Uncertainty information contained in the ensemble spread is therefore not used appropriately. To solve this problem we proposed a simple new approach where the ensemble spread is directly used as predictor for the *scale* of the predictive distribution.

To illustrate the advantages of this new approach we used wind speed data from an automatic weather station in Austria and ensemble forecasts from ECMWF. Consistent with our findings and results from previous studies, the inclusion of the ensemble standard deviation as an ordinary predictor variable has no positive effects on forecast quality. In contrast, with our new approach the uncertainty information in the ensemble standard deviation is used effectively to achieve clear improvements.

Contrary to our results, Hamill (2012) got better forecasts when using the ensemble variance multiplied with the ensemble mean as additional predictor variable. This suggests that in his data the ensemble spread also contained some predictive information on the location. For non-negative predictands like precipitation and wind speed, large observed values are generally related to large ensemble spreads. Therefore it is indeed conceivable that the ensemble spread contained some predictive information on the location that was not yet covered by the ensemble mean. However, probably additional improvements could be achieved when including the ensemble spread also as predictor for the scale of the distribution.

Extended logistic regression has been shown in several studies to perform well compared to other ensemble post-processing algorithms (e.g., Schmeits and Kok 2010; Ruiz and Saulo 2012). However, a major drawback of this method was that uncertainty information contained in the ensemble spread could not be utilized effectively. Our new approach is therefore a very attractive extension of extended logistic regression to further enhance its competitiveness.

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A. Likelihood function

To estimate the coefficients α and β (extended logistic regression) or γ and δ (heteroscedastic extended logistic regression) maximum likelihood estimation is used. The general log-likelihood function for logistic regression models is

$$l = \sum_{i=1}^{N} \log\left(\pi_i\right) \tag{11}$$

where N is the length of the training data set and π_i is the predicted probability for the i-th observed outcome. For binary logistic regression there are two possible outcomes, so that

$$\pi_i = \begin{cases} P(y_i < q|\mathbf{x}_i) & y_i < q \\ 1 - P(y_i < q|\mathbf{x}_i) & y_i \geq q \end{cases} \tag{12}$$

In previous studies the sum of this binary log-likelihood over all thresholds is used as objective function that is maximized to estimate the regression coefficients. However, the predicted probability of the i-th outcome actually is

$$\pi_i = \begin{cases} P(y_i < q_1|\mathbf{x}_i) & y_i < q_1 \\ P(y_i < q_j|\mathbf{x}_i) - P(y_i < q_{j-1}|\mathbf{x}_i) & q_{j-1} \leq y_i < q_j \\ 1 - P(y_i < q_M|\mathbf{x}_i) & y_i \geq q_M \end{cases} \tag{13}$$

so that the correct maximum likelihood estimator is given by the maximization of Equations 11 and 13. In this study we employ this maximum likelihood estimator to take advantage of all standard asymptotic inference in the maximum likelihood framework. However, the concepts presented in this paper do not depend on the objective function and results should also not differ significantly when using the sum of binary log-likelihoods (Equation 12) to estimate the coefficients.

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Extending extended logistic regression to effectively utilize the ensemble spread

Abstract
To achieve well calibrated probabilistic forecasts, ensemble forecasts often need to be statistically post-processed. One recent ensemble-calibration method is extended logistic regression which extends the popular logistic regression to yield full probability distribution forecasts. Although the purpose of this method is to post-process ensemble forecasts, mostly only the ensemble mean is used as predictor variable, whereas the ensemble spread is neglected because it does not improve the forecasts. In this study we show that when simply used as ordinary predictor variable in extended logistic regression, the ensemble spread only affects the location but not the variance of the predictive distribution. Uncertainty information contained in the ensemble spread is therefore not utilized appropriately. To solve this drawback we propose a simple new approach where the ensemble spread is directly used to predict the dispersion of the predictive distribution. With wind speed data and ensemble forecasts from the European Centre for Medium-Range Weather Forecasts (ECMWF) we show that using this approach, the ensemble spread can be used effectively to improve forecasts from extended logistic regression.

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