



## Forecast Verification Methods Implemented in the R package **SpecsVerification**: Ensemble Scores, Comparative Verification, and Uncertainty Quantification

Stefan Siegert  
University of Exeter

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### Abstract

WRITE ABSTRACT

*Keywords:* keywords, comma-separated, not capitalized, R.

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### Note to editor and reviewers

A package called **SpecsVerification** is currently available on CRAN. The package documented in this paper is an updated, yet unpublished version of **SpecsVerification**, documenting new and rewritten functions that are not currently available.

## 1. Introduction

**Ensemble forecasting general** An ensemble forecast is a collection of forecasts for the same target. The ensemble members usually differ in the initial conditions, boundary conditions, model physics and background information. Ensemble forecasting is today operationally used to quantify forecast uncertainty. Since ensembles are composed of multiple runs of deterministic models, but are used to provide uncertainty information, they can be regarded as a hybrid of deterministic and probabilistic forecasts. To evaluate the quality of ensemble forecasts, the forecasts have to be compared to their verifying observations of the real world.

**Forecast verification general** The comparison of forecasts with their verifying observations is commonly referred to as forecast verification (Jolliffe and Stephenson 2012). A verification

measure is thus a function that depends on the collection  $D = \{x_t, y_t\}_{t=1}^N$  of past forecasts  $x_t$  and verifying observations  $y_t$ . The collection  $D$  is also called a hindcast data set. A scoring rule is a function  $s(x_t, y_t)$  that assigns a real number to a forecast-observation pair. A general convention that the best possible forecast achieves a score of zero, and lower scores indicate “better” forecasts. The empirical score  $1/N \sum_t s(x_t, y_t)$  can be used as a verification measure. There are verification measures that are not scoring rules; examples include the correlation coefficient, and the area under the ROC curve. There are different scoring rules and verification measures for deterministic forecasts and probabilistic forecasts. Since ensembles are interpreted as a hybrid, both types of verification measures can be applied to ensembles.

**Finite size effect in ensemble verification** It is known that verification measures can depend on the ensemble size. In general, large ensembles achieve better average verification scores than small ensembles, when both ensembles come from the same ensemble forecasting system (Buizza and Palmer 1998). In hindcast experiments it is often desirable to estimate the finite-ensemble effect on the verification score. For example, an experimental model configuration might be run at a small ensemble size to save computational resources. The skill calculated for the hindcast experiment is not representative of the skill that an operational ensemble with many members would achieve. A number of verification scores have been proposed in the past to estimate the finite ensemble effect, and correct it. These will be summarised in the present paper, and are implemented as R functions in the package **SpecsVerification**.

**Comparative verification** The value of a verification score is often of little interest by itself. If the value of the score is not zero, we know that the forecast was not perfect. But a score different from zero is often difficult to interpret without a reference point. For this reason, forecasts should be evaluated in a comparative way, by subjecting the forecast of interest to a simple reference forecast, such as the climatological average, or a simple time-series model. If the forecast is able to achieve a better score than the reference forecast, there is non-trivial information in the forecast. Forecast verification therefore often includes comparative measures of forecast performance. The package **SpecsVerification** includes functions to compare forecast verification scores.

**Uncertainty quantification** If the score was calculated from a finite number of forecast-observation pairs, the value of a verification score is of little use without a measure of uncertainty.

## 2. Short description and applications of SpecsVerification functions

Function	Long name	Applies to:
<code>AbsErr</code>	Absolute error Score*	Deterministic forecasts of continuous observations
<code>Auc</code>	Area under the ROC curve	Probability forecasts of binary observations
<code>AucDiff</code>	Difference between two areas under the ROC curve	Two competing probability forecasts for the same binary observations
<code>ClimEns</code>	Climatological ensemble	n/a
<code>Corr</code>	Correlation coefficient	Deterministic forecasts of continuous observations
<code>CorrDiff</code>	Difference between two correlation coefficients	Two competing deterministic forecasts for the same continuous observations
<code>EnsBrier</code>	Ensemble-adjusted Brier score*	Ensemble forecast of binary observations
<code>EnsCrps</code>	Ensemble-adjusted continuous ranked probability score*	Ensemble forecasts of continuous observations
<code>EnsRps</code>	Ensemble-adjusted ranked probability score*	Ensemble forecasts of categorical observations
<code>EnsQs</code>	Ensemble-adjusted quadratic score*	Ensemble forecasts of categorical observations
<code>GaussCrps</code>	Continuous ranked probability score for Normal distributions*	Probability forecasts of continuous observations
<code>PlotRankhist</code>	Plot a rank histogram	n/a
<code>Rankhist</code>	Calculate a rank histogram	Ensemble forecasts of continuous observations
<code>ReliabilityDiagram</code>	Calculate and plot a reliability diagram	Probability forecasts of binary observations
<code>ScoreDiff</code>	Calculate a score difference and assess uncertainty	All scores marked with a *
<code>SkillScore</code>	Calculate a skill score and assess uncertainty	All scores marked with a *
<code>TestRankhist</code>	Statistical tests of a rank histogram	n/a
<code>SqErr</code>	Squared error score*	Deterministic forecasts of continuous observations

## 3. Forecast and observation data

Included in **SpecsVerification** is a data set `eurotempforecast` of seasonal temperature ensemble forecasts and verifying observations. The forecasts 24-member ensembles of near-surface air temperatures produced by the NCEP climate forecast system version 2 (Saha, Moorthi, Wu, Wang, Nadiga, Tripp, Behringer, Hou, Chuang, Iredell, and Coauthors 2014), initialised between 11 April and 6 May each year from 1983–2009 ( $N = 27$ ), and averaged over the region limited by latitudes 30°N – 75°N and longitudes 12.5°W – 42.5°E, and over the months

```
par(las=1, cex=0.7, mgp=c(3, 1, 0), mar=c(2,4,1,1))
matplot(yrs, ens, ylab="temp [C]", pch=1, col=gray(.5))
points(yrs, obs, pch=15, cex=1.5)
```

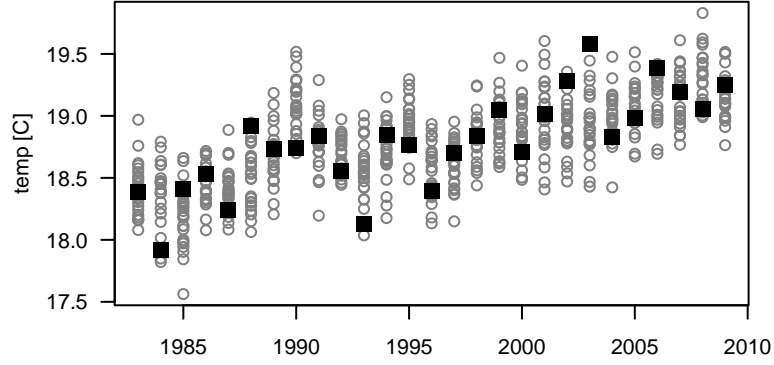


Figure 1: Seasonal European temperature ensemble forecasts (circles) and verifying observations (squares).

June-July-August, i.e., the lead time is about 1–3 months. Data from the NCEP climate forecast system reanalysis (Saha, Moorthi, Pan, Wu, Wang, Nadiga, Tripp, Kistler, Woollen, Behringer, and Coauthors 2010) was taken as verifying observations. All data was downloaded through the ECOMS user data gateway R-interface (Santander Meteorology Group 2015). Ensemble members and observation data are plotted as time series in Figure 1.

```
data(eurotempforecast)
R <- ncol(ens)
yrs <- as.numeric(names(obs))
N <- length(obs)
```

All functions in **SpecsVerification** that analyse ensemble forecast data, assume that archives of  $N$  instances of  $R$ -member ensemble forecasts, are represented by  $N \times R$  matrices. The data shown in Figure 1 depicts 27 years or 24-member ensemble forecasts, and is thus a R matrix with 27 rows and 24 columns.

In addition to the real-valued forecasts (matrix `ens`) and real-valued observations (vector `obs`), binary and categorical forecasts and observations are provided, saved in the variables `ens.bin`, `obs.bin`, `ens.cat`, and `obs.cat`. The binary forecasts, saved in matrix `ens.bin` were generated by considering the question "Will this year's summer be warmer than last year's"? The binary observation at index  $t$  is equal to one if the temperature in the corresponding year exceeds the temperature of the previous year, and the binary observation is zero otherwise. The individual ensemble members were transformed equivalently, by comparing the  $r$ th ensemble member in year  $t$  to the observation in year  $t - 1$ . Categorical forecasts and observations were generated by addressing the question "Will this year's temperature be similar to last year's temperature (within a 0.5K range), colder, or warmer?" Each ensemble member and the observation thus falls into one of 3-categories: Category 1 indicates a temperature that is less than 0.25K colder than the previous year's observed temperature, category

2 indicates a temperature that is within  $\pm 0.25K$  of the previous year's temperature, and category 3 indicates more than  $0.25K$  warmer. In addition, the vector `obs.lag` is provided with 1-year lagged observations.

As an example, the observation in the year 2000, i.e., the lagged observation for year 2001, is

```
obs.lag["2001"]
```

```
## 2001
## 18.71
```

The continuous observation and forecasts, and the derived binary and categorical observations and forecasts for the year 2001 are thus

```
rbind(
  continuous = c(obs=obs["2001"], ens["2001", 1:5]),
  binary      = c(obs=obs.bin["2001"], ens.bin["2001", 1:5]),
  categorical  = c(obs=obs.cat["2001"], ens.cat["2001", 1:5]))

##          obs.2001 Member_1 Member_2 Member_3 Member_4 Member_5
## continuous    19.01    18.65    18.96    19.23    18.41    18.81
## binary         1.00     0.00     1.00     1.00     0.00     1.00
## categorical     3.00     2.00     3.00     3.00     1.00     2.00
```

## 4. Ensemble-adjusted verification scores

### 4.1. Binary ensemble forecasts

This section outlines the theory behind ensemble-adjusted verification scores, using probabilistic forecasts of binary events for illustration.

One of the most common verification measures for probabilistic forecasts of binary events is the Brier score (Brier 1950). Suppose a probability forecast  $p_t \in [0, 1]$  is issued at time  $t$  for a binary (yes/no) event. The occurrence or non-occurrence of the event is coded as  $y_t = 1$  or  $y_t = 0$ , respectively. The Brier score is given by the squared difference between forecast and observation:

$$s_B(p_t, y_t) = (p_t - y_t)^2 \quad (1)$$

The Brier score is negatively oriented - lower scores indicate better forecasts. The Brier score is a strictly proper verification score, meaning that the expected score obtains its minimum value if and only if the observation  $y_t$  is a random draw from  $p_t$  (Gneiting and Raftery 2007).

Assume next that instead of predicting the probability  $p_t$ , we make a prediction based on an ensemble forecast of size  $R$ , whose members were sampled identically and independently with probability  $p_t$ . That is, each of the  $R$  ensemble members is an independent Bernoulli trial with success probability  $p_t$ . An unbiased estimator of the success probability  $p_t$  is given by

the fraction  $i_t/R$ , where  $i_t$  is the number of successes, i.e. the number of ensemble members that predict the event  $y_t = 1$ . The Brier score of the estimated probability is equal to

$$s_B\left(\frac{i_t}{R}, y_t\right) = \left(\frac{i_t}{R} - y_t\right)^2 \quad (2)$$

Taking expectation over the random variable  $i_t \sim \text{Binomial}(p_t, R)$ , it is shown that (Ferro, Richardson, and Weigel 2008)

$$E\left[s_B\left(\frac{i_t}{R}, y_t\right)\right] = s_B(p_t, y_t) + \frac{p_t(1-p_t)}{R} \quad (3)$$

That is, even though the fraction  $i_t/R$  is an unbiased estimator of the event probability  $p_t$ , the Brier score of  $i_t/R$  is not an unbiased estimator of the Brier score of  $p_t$ . The Brier score of  $i_t/R$  is in general larger than the Brier score of  $p_t$ . The bias, given by the additional positive term on the rhs of Equation 3, depends on the ensemble size and vanishes for  $R \rightarrow \infty$ . The bias can thus be interpreted as a finite-ensemble penalty: If two ensembles sample their members from the same probability  $p_t$ , the one with the larger ensemble size obtains the lower (i.e. better) Brier score on average. This is reasonable since more ensemble members allow for more robust estimation of the “true” probability  $p_t$ . But in the analysis of ensemble hindcasts it is sometimes desirable to correct the finite-ensemble bias. For example, if the hindcast ensemble has  $R$  members, and future operational forecasts will be made with  $R^* > R$  ensemble members, the score calculated for the  $R$ -member hindcast ensemble will be a too pessimistic estimate of the score of the  $R^*$ -member forecast ensemble.

The ensemble-adjusted Brier score, given by (Ferro *et al.* 2008)

$$s_B^*(i_t, R, R^*, y_t) = \left(\frac{i_t}{R} - y_t\right)^2 - \frac{i_t(R - i_t)}{R(R - 1)} \left(\frac{1}{R} - \frac{1}{R^*}\right) \quad (4)$$

allows to correct the finite-ensemble bias. The ensemble-adjusted Brier score is in expectation equal to the Brier score that would be achieved by an ensemble with  $R^*$  members sampled from the same probability  $p_t$ , i.e.,

$$E[s_B^*(i_t, R, R^*, y_t)] = (p_t - y_t)^2 + \frac{p_t(1-p_t)}{R^*}. \quad (5)$$

Note that, trivially,  $s_B^*(i_t, R, R, y_t) = s_B(i_t/R, y_t)$ . Note further that setting  $R^* = \infty$  yields the fair Brier score (Ferro 2013) which estimates the score of the underlying probability  $p_t$ . The ensemble-adjusted Brier score can be used to compare ensemble forecasting systems with different numbers of members. It further allows for the extrapolation of the average score of an ensemble forecast system to larger ensemble sizes.

The **SpecsVerification** function **EnsBrier** calculates the ensemble-adjusted Brier scores of a collection of  $N$  ensemble forecasts and their corresponding binary observations. The argument **R.new** allows for estimation of the score of an arbitrary ensemble size, including **R.new=Inf**.

To illustrate the finite ensemble effect and highlight the benefit of the finite-ensemble adjustment, we randomly split the 24-member forecast ensemble into a small 5-member ensemble and a larger 19-member ensemble. We then calculate their unadjusted Brier scores:

```
i.small <- sample(1:R, 5)
i.large <- setdiff(1:R, i.small)
c(small.ens=mean(EnsBrier(ens.bin[, i.small], obs.bin)),
  large.ens=mean(EnsBrier(ens.bin[, i.large], obs.bin)))

## small.ens large.ens
##      0.1689      0.1465
```

As expected, the large ensemble obtains a better score than the large ensemble. We next adjust the Brier score for the finite ensemble size, by calculating  $s_B^*$  using  $R^* = 20$  for both ensembles:

```
c(small.ens=mean(EnsBrier(ens.bin[, i.small], obs.bin, R.new=19)),
  large.ens=mean(EnsBrier(ens.bin[, i.large], obs.bin, R.new=19)))

## small.ens large.ens
##      0.1454      0.1465
```

The scores are very similar thus confirming that it is possible to estimate the score of the 19-member ensemble, using only a 5-member ensemble. How big is the estimated improvement if we could further increase the ensemble size? We show this in Figure 2, where we plot the ensemble adjusted Brier score over the adjusted ensemble size  $R^*$ . The Brier score estimated for  $R^* = \infty$  is

```
mean(EnsBrier(ens.bin, obs.bin, R.new=Inf))

## [1] 0.1316
```

## 4.2. Categorical ensemble forecasts

Assume the ensemble forecasting system produces an ensemble of categorical rather than binary forecasts. That is, each ensemble members and the verifying observation falls into one of  $K$  classes. Two types of categorical forecasts can be distinguished: Disjoint categories and nested categories.

Assume the observation assumes on of  $K$  possible values, or classes, and a probabilistic forecast  $\mathbf{p}_t = (p_{t,1}, \dots, p_{t,K})$ , is issued. The verifying observation is vector-valued  $\mathbf{y}_t$ , where the  $k$ -th element of  $\mathbf{y}_t$  is  $y_{t,k} = 1$  if the  $k$ -th class is observed, and  $y_{t,k} = 0$  otherwise. The quadratic score for such a probability forecast is given by

$$s_Q(\mathbf{p}_t, \mathbf{y}_t) = \sum_{k=1}^K (p_{t,k} - y_{t,k})^2 \quad (6)$$

The quadratic score is simply the sum of Brier scores for the individual categories. Or stated differently, the Brier score is one-half the quadratic score of a 2-class categorical forecast.

Now assume an  $R$ -member categorical ensemble forecast  $\mathbf{i}_t$  is issued at time  $t$ , indicating that  $i_{t,k}$  out of  $R$  ensemble members have predicted the  $k$ -th category, for  $k = 1, \dots, K$ . Using

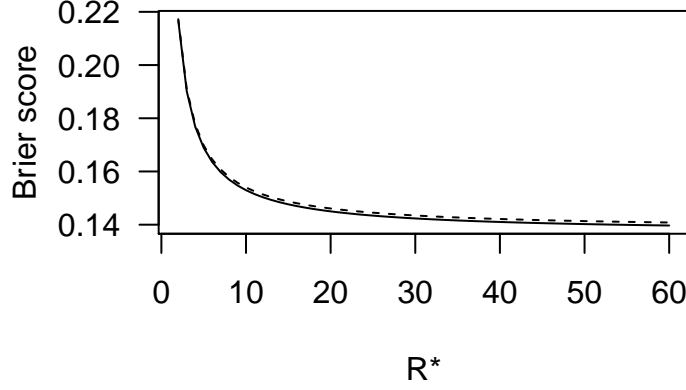


Figure 2: Ensemble-adjusted Brier score as a function of the adjusted ensemble size, calculated from a small 5-member ensemble (solid line) and a larger 19-member ensemble (dashed line), produced by the same forecasting system.

results obtained for the ensemble-adjusted Brier score, the ensemble-adjusted quadratic score is seen to be

$$s_Q^*(\mathbf{i}_t, R, R^*, \mathbf{y}_t) = \sum_{k=1}^K \left\{ \left( \frac{i_{t,k}}{R} - y_{t,k} \right)^2 - \left( \frac{1}{R} - \frac{1}{R^*} \right) \frac{i_{t,k}(R - i_{t,k})}{R(R-1)} \right\} \quad (7)$$

The ensemble adjusted quadratic score is implemented as the function `EnsQs` in **SpecsVerification**.

The quadratic score is insensitive to relabelling the  $K$  categories. Sometimes this is undesired in categorical forecasting problems. The forecast categories might have a natural ordering, such as low/medium/high intensity of precipitation. In that case, an order-sensitive score might be desired that penalises forecasts that assign most probability to the “high” category more than it penalises forecasts that assign most probability to the “medium” category, if the low category verifies. A lot of probability in the “medium” category can be considered closer to the observation than a lot of probability in the “high” category, such that the former forecast can be considered “better”. An order-sensitive score is also desired if the forecast categories are nested within one another, e.g., for precipitation amounts categorised into  $<1\text{mm}/<5\text{mm}/<20\text{mm}/<\infty$ . In that case, a high probability assigned to the  $<5\text{mm}$  category should receive less penalty than a high probability assigned to the  $<20\text{mm}$  category, if the actual amount is  $<1\text{mm}$ .

The ranked probability score (RPS) is an order-sensitive quadratic score for categorical probability forecasts. The forecast vector  $\mathbf{i}_t$  is transformed to the  $K$ -element cumulated forecast vector  $\mathbf{j}_t$ , with  $k$ -th element equal to  $j_{t,k} = \sum_{l=1}^k i_{t,l}$ . Likewise, the cumulated observation vector  $\mathbf{z}_t$  has its  $k$ -th element equal to  $z_{t,k} = \sum_{l=1}^k y_{t,l}$ . The RPS is the quadratic score achieved by the cumulative forecast  $\mathbf{j}_t$  for the cumulative observation  $\mathbf{z}_t$ . Accumulating the



elements of  $\mathbf{i}_t$  and  $\mathbf{y}_t$  nests the  $K$  forecast categories within each other. The forecast is transformed from “ $i_{t,k}$  out of  $R$  ensemble members predict category  $k$ ” to the forecast “ $j_{t,k}$  out of  $R$  ensemble members forecast category  $k$  or less”. The nesting of forecast categories ensures order-sensitivity of the score. Using results from the previous section, we get the ensemble-adjusted RPS

$$s_R^*(\mathbf{i}_t, R, R^*, \mathbf{y}_t) = \sum_{k=1}^K \left\{ \left( \frac{j_{t,k}}{R} - z_{t,k} \right)^2 - \left( \frac{1}{R} - \frac{1}{R^*} \right) \frac{j_{t,k}(R - j_{t,k})}{R(R-1)} \right\} \quad (8)$$

The ensemble adjusted RPS is implemented as the function `EnsRps` in **SpecsVerification**. Note that the ensemble forecast vector  $\mathbf{i}_t$  in the above equations is assumed to be a histogram, indicating the number of ensemble members that forecast each class. The functions `EnsQs` and `EnsRps` assume as inputs true categorical ensemble forecasts, i.e. vectors of length  $R$  (ensemble size), with entries indicating which class label the ensemble predicts.

To illustrate the finite-ensemble effect and its adjustment, we randomly split the entire ensemble into a small 5-member ensemble and a larger 19-member ensemble. We then evaluate the unadjusted quadratic score of the full 24-member ensemble, the unadjusted scores of the small and large sub-ensembles, as well as the quadratic scores of the two sub-ensembles adjusted for the size of the full ensemble:

```
i.small <- sample(1:R, 5)
i.large <- setdiff(1:R, i.small)
rbind(
  ens      = mean(EnsQs(ens.cat,      obs.cat)),
  small.ens = mean(EnsQs(ens.cat[, i.small], obs.cat)),
  large.ens = mean(EnsQs(ens.cat[, i.large], obs.cat)),
  small.ens.adj = mean(EnsQs(ens.cat[, i.small], obs.cat, R.new=24)),
  large.ens.adj = mean(EnsQs(ens.cat[, i.large], obs.cat, R.new=24)))

##           [,1]
## ens          0.5782
## small.ens     0.6519
## large.ens     0.5856
## small.ens.adj 0.5815
## large.ens.adj 0.5810
```

The full-ensemble obtains a better score than either of the sub-ensembles. The large sub-ensemble performs better than the small sub-ensemble. When adjusting scores of the sub-ensembles to  $R^* = 24$  the scores of the sub-ensembles agree, and are close to the score of the full ensemble.

Repeating the evaluation with the ranked probability score, we obtain

```
rbind(
  ens      = mean(EnsRps(ens.cat,      obs.cat)),
  small.ens = mean(EnsRps(ens.cat[, i.small], obs.cat)),
  large.ens = mean(EnsRps(ens.cat[, i.large], obs.cat)),
```

```

small.ens.adj = mean(EnsRps(ens.cat[, i.small], obs.cat, R.new=24)),
large.ens.adj = mean(EnsRps(ens.cat[, i.large], obs.cat, R.new=24))

##           [,1]
## ens       0.3344
## small.ens  0.3719
## large.ens  0.3386
## small.ens.adj 0.3597
## large.ens.adj 0.3378

```

Again, the full ensemble outperforms both sub-ensembles, and the large sub-ensemble outperforms the small sub-ensemble. In this analysis, the scores do not agree that well after adjusting to  $R^* = 24$ . Recall that the equality of ensemble-adjusted scores is only in expectation, and empirical averages over finite hindcast data sets should be expected to differ.

### 4.3. Continuous ensemble forecasts

If the forecast target is a continuous variable, such as temperature or pressure, the continuous ranked probability score ([Matheson and Winkler 1976](#)) can be used for forecast verification. If the forecast for the continuous target  $y_t$  is given as a cumulative distribution function  $F_t(x)$ , the CRPS is given by

$$s_C(F_t, y_t) = \int_{-\infty}^{\infty} dz |F_t(z) - H(z - y_t)|^2 \quad (9)$$

where  $H(x)$  is the Heaviside step-function, satisfying  $H(x) = 1$  for all  $x \geq 0$  and  $H(x) = 0$  otherwise. Suppose an ensemble forecast  $x_t$  with  $R$  real-valued members  $x_t = \{x_{t,1}, x_{t,2}, \dots, x_{t,R}\}$  is issued for the real-valued verifying observation  $y_t$ . The ensemble can be transformed into a cdf by taking the empirical distribution function given by

$$\hat{F}_t(z) = \frac{1}{R} \sum_{r=1}^R H(z - x_{t,r}). \quad (10)$$

Using properties of the Heaviside function, it is straightforward to show that the CRPS of the empirical distribution  $\hat{F}$  is given by

$$s_C(\hat{F}_t, y_t) = \frac{1}{R} |x_{t,r} - y_t| - \frac{1}{2R^2} \sum_{r=1}^R \sum_{r'=1}^R |x_{t,r} - x_{t,r'}|. \quad (11)$$

[Fricker, Ferro, and Stephenson \(2013\)](#) show that the CRPS is sensitive to the ensemble size, and propose the ensemble-adjusted CRPS

$$s_C^*(x_t, R, R^*, y_t) = \frac{1}{R} \sum_{r=1}^R |x_{t,r} - y_t| - \frac{1}{2R(R-1)} \left(1 - \frac{1}{R^*}\right) \sum_{r=1}^R \sum_{r'=1}^R |x_{t,r} - x_{t,r'}|. \quad (12)$$

The ensemble-adjusted CRPS is, in expectation, equal to the CRPS that the empirical distribution function calculated from an ensemble of size  $R^*$  would achieve. This includes the case  $R^* = \infty$ , for which the fair CRPS is obtained. The ensemble-adjusted CRPS is implemented in the **SpecsVerification** function `EnsCrps`.

```

rbind(
  unadjusted = mean(EnsCrps(ens, obs)),
  fair       = mean(EnsCrps(ens, obs, R.new=Inf))
)

##           [,1]
## unadjusted 0.1381
## fair       0.1329

```

## 5. Comparative verification and uncertainty quantification

### 5.1. Reference forecast

The value of a verification score by itself is meaningless. In order to evaluate the skill of a forecast, its verification score has to be compared to the score achieved by a reference forecast. For example, if the skill of a state-of-the-art high resolution climate model is evaluated, it is reasonable to compare its verification score to the score achieved by an older climate model, possibly with lower resolution and less physical detail.

In the absence of a dynamical climate model to which the score can be compared, simple statistical benchmark predictions can be used. A popular simple reference forecast is the climatological forecast, which is only based on the known record of observations, without reference to any numerical forecast model. **SpecsVerification** includes the function **ClimEns** which transforms a vector of observations into a matrix of climatological ensemble forecasts, including the possibility to leave out the  $t$ -th observation in the  $t$ -th climatological ensemble:

```

ens.ref      <- ClimEns(obs,      leave.one.out=TRUE)
ens.cat.ref  <- ClimEns(obs.cat,  leave.one.out=TRUE)
ens.bin.ref  <- ClimEns(obs.bin,  leave.one.out=TRUE)

```

The new data set of climatological ensembles can be used as a reference ensemble to which the numerical forecast ensemble can be compared. We recommend also considering statistical reference forecasts such as a linear trend or an auto-regressive model, which might be more suitable than the climatological forecast.

### 5.2. Score differences

Suppose we have calculated two time series  $\{s_{1,1}, s_{1,2}, \dots, s_{1,N}\}$  and  $\{s_{2,1}, s_{2,2}, \dots, s_{2,N}\}$  of verification scores for two competing forecast systems for the same observation. [Diebold and Mariano \(1995\)](#) suggest to test the null-hypothesis of equal forecast accuracy using the time series  $d_1, \dots, d_N$  of loss differentials  $d_t = s_{1,t} - s_{2,t}$ . Define  $\bar{d}$  to be the empirical average over  $d_1, d_2, \dots$ . Under the assumption of temporal independence of  $d_t$ , and zero mean of the loss-differential, the test statistic

$$T = \bar{d} \sqrt{\frac{N}{\text{var}(d_t)}} \quad (13)$$

is asymptotically Normally distributed with mean zero and variance one. This test is implemented in **SpecsVerification** in the function `ScoreDiff`. The function includes the option to account for autocorrelation of the loss-differential by specifying an effective sample size `N.eff`.

```

rbind(
  brier = ScoreDiff(EnsBrier(ens.bin,      obs.bin),
                    EnsBrier(ens.bin.ref, obs.bin)),
  qs    = ScoreDiff(EnsQs(  ens.cat,      obs.cat),
                    EnsQs(  ens.cat.ref, obs.cat)),
  rps   = ScoreDiff(EnsRps(  ens.cat,      obs.cat),
                    EnsRps(  ens.cat.ref, obs.cat)),
  crps  = ScoreDiff(EnsCrps( ens,          obs),
                    EnsCrps( ens.ref,      obs))
)

##      score.diff score.diff.sd   p.value      L      U
## brier    0.12185      0.04217 0.00192772  0.03921 0.2045
## qs       0.12004      0.08972 0.09046758 -0.05581 0.2959
## rps      0.09753      0.06438 0.06491317 -0.02866 0.2237
## crps     0.09391      0.02400 0.00004543  0.04688 0.1409

```

### 5.3. Skill scores

It is common practice to compare scores of competing forecasts by a so-called skill score, which is a normalised mean score difference (Wilks 2011). Denote by  $S$  the mean score of the forecast under evaluation, by  $S_{ref}$  the mean score of a reference forecast, and by  $S_{perf}$  the mean score that would be achieved by the perfect forecaster. The skill score is then given by the score difference between the reference forecast and the evaluated forecast, normalised by the difference between the reference forecast and the perfect forecast:

$$SS = \frac{S_{ref} - S}{S_{ref} - S_{perf}} \quad (14)$$

The variance of the skill score can be estimated by error propagation as follows

$$var(SS) \approx \frac{1}{(S_{ref} - S_{perf})^2} var(S) + \frac{(S - S_{perf})^2}{(S_{ref} - S_{perf})^2} var(S_{ref}) - 2 \frac{S - S_{perf}}{(S_{ref} - S_{perf})^3} cov(S, S_{ref}) \quad (15)$$

where the variances and covariances of the mean scores  $S$  and  $S_{ref}$  are approximated by the variances and covariances calculated for the individual scores, divided by the sample size. The skill score is implemented in **SpecsVerification** in the function `SkillScore`, which takes as inputs two vectors of verification scores of the evaluated and the reference forecast, the constant score achieved by a perfect forecaster, as well as a possibly user-defined effective sample size.

```

rbind(
  brier = SkillScore(EnsBrier(ens.bin, obs.bin),
                     EnsBrier(ens.bin.ref, obs.bin)),
  qs    = SkillScore(EnsQs(ens.cat, obs.cat),
                     EnsQs(ens.cat.ref, obs.cat)),
  rps   = SkillScore(EnsRps(ens.cat, obs.cat),
                     EnsRps(ens.cat.ref, obs.cat)),
  crps  = SkillScore(EnsCrps(ens, obs),
                     EnsCrps(ens.ref, obs))
)

##      skillscore skillscore.sd
## brier      0.4680      0.14973
## qs         0.1719      0.13042
## rps        0.2258      0.14624
## crps       0.4048      0.07343

```

#### 5.4. Correlation and correlation difference

The Pearson (product-moment) correlation coefficient is one of the most popular verification criteria, and can be calculated with the built-in R function `cor`. Since uncertainty quantification is often of interest in forecast verification, **SpecsVerification** provides the function `Corr`, which returns the sample correlation coefficient  $r_{xy}$ , a one-sided p-value and a confidence interval. The p-value is calculated based on the test statistic

$$T_{cor} = \sqrt{(N-2) \frac{r_{xy}^2}{1-r_{xy}^2}} \quad (16)$$

which has a Student's t-distribution with  $N-2$  degrees of freedom under the null-hypothesis of zero correlation in the population. The confidence interval  $[L, U]$  with a user-defined confidence coefficient  $1-\alpha$ , calculated by

$$[L, U] = \left[ \tanh \left( z_{xy} + \frac{Z_{\alpha/2}}{\sqrt{N-3}} \right), \tanh \left( z_{xy} + \frac{Z_{1-\alpha/2}}{\sqrt{N-3}} \right) \right] \quad (17)$$

where  $z_{xy} = \text{atanh}(r_{xy})$  is the Fisher transformation of the correlation coefficient, and  $Z_p$  is the  $p$ -quantile of the standard Normal distribution. An effective sample size to account for possible auto-correlation can be specified.

```

ens.mean <- rowMeans(ens)
Corr(ens.mean, obs, conf.level=0.95)

##      corr      p.value      L      U
## 0.757095576 0.000002427 0.529391069 0.883049977

```

It is often of interest to compare the correlation coefficients between two forecasts for the same observation by calculating the correlation difference. **SpecsVerification** implements the

function `CorrDiff` that returns the difference between the correlation  $r_{by}$  of the forecast B and the correlation  $r_{ay}$  of a reference forecast A, both of which were issued for the same observation Y. The function calculates a one-sided p-value using the test by [Steiger \(1980\)](#): Denote by  $r_{ab}$  the correlation between forecast A and forecast B. The determinant of the sample correlation matrix of the two forecasts and the observation is calculated:

$$R = (1 - r_{ay}^2 - r_{by}^2 - r_{ab}^2) + (2r_{ay}r_{by}r_{ab}) \quad (18)$$

The test statistic

$$T_{cordiff} = (r_{by} - r_{ay}) \sqrt{\frac{(N-1)(1+r_{ab})}{2\left(\frac{N-1}{N-3}\right)R + \frac{1}{4}(r_{ay} + r_{by})^2(1-r_{ab})^3}} \quad (19)$$

has a Student's  $t$ -distribution with  $N - 3$  degrees of freedom under the null-hypothesis that A and B have equal correlations. Furthermore, a confidence interval based on [Zou \(2007\)](#) is calculated. First estimate the correlation between the correlation coefficients  $r_{ay}$  and  $r_{by}$  by

$$c_{ab} = \frac{(r_{ab} - \frac{1}{2}r_{ay}r_{by}) \left(1 - r_{ay}^2 - r_{by}^2 - r_{ab}^2\right) + r_{ab}^3}{(1 - r_{ay}^2)(1 - r_{by}^2)}, \quad (20)$$

Then calculate  $(1 - \alpha) \times 100\%$  confidence intervals  $(l_a, u_a)$  for  $r_{ay}$  and  $(l_b, u_b)$  for  $r_{by}$ , using the Fisher transformation as in eq. 17. An approximate  $(1 - \alpha) \times 100\%$  confidence interval  $(L, U)$  for the correlation difference  $r_{by} - r_{ay}$  is then given by

$$\begin{aligned} L &= (r_{by} - r_{ay}) - \sqrt{(r_{by} - l_b)^2 + (u_a - r_{ay})^2 - 2c_{ab}(r_{by} - l_b)(u_a - r_{ay})}, \\ U &= (r_{by} - r_{ay}) + \sqrt{(u_b - r_{by})^2 + (r_{ay} - l_a)^2 - 2c_{ab}(u_b - r_{by})(r_{ay} - l_a)}. \end{aligned} \quad (21)$$

For illustration, we evaluate the difference in correlation between the ensemble mean forecast and the persistence forecast:

```
CorrDiff(fcst=ens.mean, fcst.ref=obs.lag, obs=obs, conf.level=0.95)
```

```
## corr.diff    p.value        L        U
##  0.179021    0.029082 -0.005417  0.440518
```

The one-sided p-value is small and the value of zero correlation is close to the boundary of the 95% confidence interval, which provides ample evidence that the seasonal forecast has higher correlation skill than the persistence forecast.

## 5.5. Area under the curve (AUC) and AUC differences

Relative operating characteristics (ROC, [Mason and Graham 2002](#), and references therein) analysis is a method from signal detection theory to evaluate the quality of forecasts for binary events. Consider the two competing forecasts  $x_t^{(1)}$  and  $x_t^{(2)}$  for the same binary observations  $y_t \in \{0, 1\}$  for  $t = 1, \dots, N$ . (The forecasts are allowed to take values on the real line, and need not be probabilities.) For ROC analysis, the forecasts are grouped into two sets:  $C_0^{(r)}$

contains all forecasts  $x^{(r)}$  for which an event did not happen ( $y_t = 0$ ), and  $C_1^{(r)}$  contains all forecasts for which an event did happen ( $y_t = 1$ ). The area under the ROC curve (AUC) for the  $r$ th forecast ( $r = 1, 2$ ) is equal to the probability that a randomly drawn forecast from  $C_1^{(r)}$  is larger than a randomly drawn forecast from  $C_0^{(r)}$ . The AUC is thus a measure of the ability of the forecasts to distinguish events from non-events.

DeLong, DeLong, and Clarke-Pearson (1988) suggest a nonparametric method to estimate the variance of AUC and of differences in AUC. Denote by  $X_i^{(r)}$ ,  $i = 1, \dots, m$  the elements of  $C_1^{(r)}$  and by  $Y_j^{(r)}$ ,  $j = 1, \dots, n$  the members of  $C_0^{(r)}$ . Define the function  $\Psi$  as

$$\Psi(x, y) = \mathbb{1}(x > y) + \frac{1}{2}\mathbb{1}(x = y) \quad (22)$$

where  $\mathbb{1}(\cdot)$  is the indicator function which equals one if its argument is true, and zero otherwise. The AUC of the  $r$ th forecast is estimated by

$$\hat{\theta}^{(r)} = \frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n \Psi(X_i^{(r)}, Y_j^{(r)}) \quad (23)$$

For variance estimation, first define the quantities  $V_i^{(r)}$  and  $W_j^{(r)}$  by

$$V_i^{(r)} = \frac{1}{n} \sum_{j=1}^n \Psi(X_i^{(r)}, Y_j^{(r)}) \quad \text{and} \quad W_j^{(r)} = \frac{1}{m} \sum_{i=1}^m \Psi(X_i^{(r)}, Y_j^{(r)}). \quad (24)$$

and  $v_{r,s}$  and  $w_{r,s}$  by

$$v_{r,s} = \frac{1}{m-1} \sum_{i=1}^m [V_i^{(r)} - \hat{\theta}^{(r)}][V_i^{(s)} - \hat{\theta}^{(s)}] \quad (25)$$

$$w_{r,s} = \frac{1}{n-1} \sum_{j=1}^n [W_j^{(r)} - \hat{\theta}^{(r)}][W_j^{(s)} - \hat{\theta}^{(s)}] \quad (26)$$

where  $r = 1, 2$  and  $s = 1, 2$ . Finally, the estimated variance of the  $r$ th AUC estimate  $\hat{\theta}^{(r)}$  is given by

$$\text{var}(\hat{\theta}^{(r)}) = \frac{1}{m} v_{r,r} + \frac{1}{n} w_{r,r} \quad (27)$$

and the variance of the AUC difference  $\theta^{(2)} - \theta^{(1)}$  is given by

$$\text{var}(\hat{\theta}^{(2)} - \hat{\theta}^{(1)}) = \frac{1}{m} (v_{1,1} + v_{2,2} - 2v_{1,2}) + \frac{1}{n} (w_{1,1} + w_{2,2} - 2w_{1,2}). \quad (28)$$

Note that the AUC is asymptotically Normally distributed. The estimated variance can therefore be used to construct a confidence interval, i.e.,  $\hat{\theta} \pm 1.96\sqrt{\text{var}(\hat{\theta})}$  is a central 95% confidence interval.

**SpecsVerification** provides the functions `Auc` and `AucDiff` that implement calculation of AUC and AUC differences and the corresponding variance estimates. The following calculates AUCs for the ensemble mean of the binary ensemble, using a large and a small subensemble:

```

rbind(
  large.ens = Auc(rowMeans(ens.bin[, i.large]), obs.bin),
  small.ens = Auc(rowMeans(ens.bin[, i.small]), obs.bin)
)

##           auc  auc.sd
## large.ens 0.8892 0.06944
## small.ens 0.8523 0.07179

```

The AUC of both ensembles is significantly larger than 0.5, which is a sign of forecast skill. The large subensemble has a slightly higher AUC than the small subensemble. The following evaluates the AUC difference between the large and a small ensemble:

```

AucDiff(rowMeans(ens.bin[, i.large]), rowMeans(ens.bin[, i.small]), obs.bin)

##      auc.diff auc.diff.sd
##      0.03693      0.06346

```

The AUC difference is within sampling variability, and we remain uncertain about whether the larger ensemble improves the AUC. In general, we expect ensemble size to effect AUC, but we are not aware of published ensemble-adjustments for the AUC.

## 6. Rank histogram analysis for ensemble forecasts

The verification rank histogram (Hamill 2001) is a non-parametric graphical tool to assess the reliability of an ensemble forecasting system. For each pair of ensemble forecast and verifying observation, the rank of the observation among the ordered ensemble members is calculated. In a  $R$ -member ensemble, the rank is between 1 and  $R + 1$ . If the ensemble is a reliable representation of the uncertainty in the observation, the observation should statistically behave like “just another ensemble member”. Each verification rank should therefore be equally likely on average, and the histogram over verification ranks should be flat. **SpecsVerification** contains the function `Rankhist` to calculate the verification rank counts for an archive of ensembles and observations.

```

rh <- Rankhist(ens, obs)
rh

## [1] 0 2 1 0 2 4 1 1 0 0 0 0 1 2 2 1 3 1 1 0 1 1 0 2 1

```

The function `PlotRankhist` plots the rank histogram. Two plotting modes are available: `mode="raw"` simply plots the rank counts as a bar plot histogram. `mode="prob.paper"` plots the rank counts on probability paper following Bröcker (2008). Assuming that each rank count has a binomial distribution with success probability  $1/(R + 1)$  and sample size  $N$ . The observed rank count  $c_i$  is transformed to the cumulative probability  $\nu_i$  under the Binomial distribution. To test the null-hypothesis of a flat rank histogram, 90-, 95-, and 99-percent



```
PlotRankhist(rh, mode="raw")
```

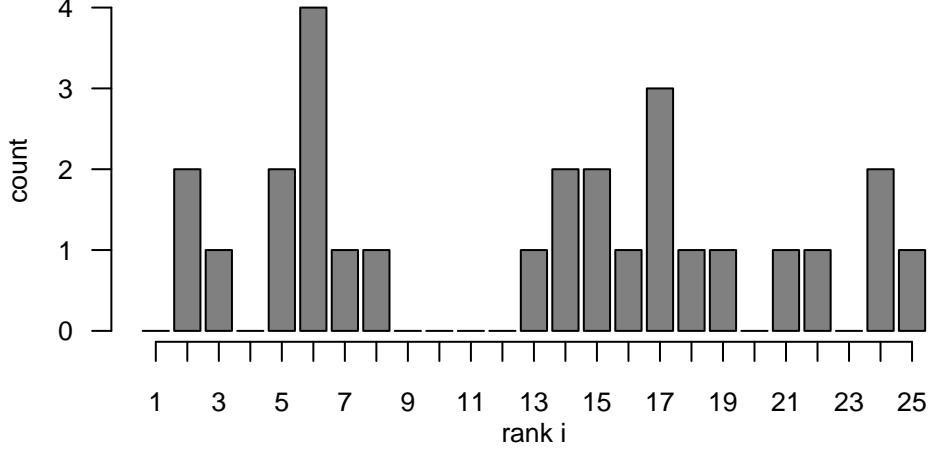


Figure 3: Rank histogram

prediction intervals are included, corrected for multiple testing. The interpretation is, given that the null-hypothesis is true, on average 9 out of 10 rank histograms should lie completely inside the 90% prediction interval.

The function `TestRankhist` implements different statistical tests of the null-hypothesis of flat rank histogram. Flatness of the rank histogram can be assessed by a Pearson  $\chi^2$ -test (Pearson 1900). Suppose rank  $i$  was observed  $r_i$  times for  $i = 1, \dots, R+1$ , and define  $e_i = N/(R+1) \forall i$  the expected number of counts if each verification rank were equally likely. Define further

$$x_i = \frac{r_i - e_i}{\sqrt{e_i}}. \quad (29)$$

Under the null-hypothesis of equally likely verification ranks, the test statistic

$$\chi^2 = \sum_{i=1}^{R+1} x_i^2 \quad (30)$$

has a  $\chi^2$ -distribution with  $R$  degrees of freedom.

Hamill (2001) showed that certain types of violation of ensemble reliability are visible as different patterns in the rank histogram. In particular, a systematic bias of the ensemble mean produces sloped rank histograms, and ensembles with insufficient (excessive) ensemble spread produce U-shaped ( $\cap$ -shaped) rank histogram. Jolliffe and Primo (2008) showed that the  $\chi^2$ -test statistic can be decomposed to test for sloped and convex rank histograms specifically, thus increasing the power of the test. The test requires the definition of suitable contrast vectors  $\mathbf{c}$  of length  $R+1$ , that satisfy  $\sum_i c_i = 0$ ,  $\sum_i c_i^2 = 1$ , and  $\sum_i c_i c'_i = 0$  for every pair of contrasts  $\mathbf{c}$  and  $\mathbf{c}'$ . Assuming a number of up to  $R$  contrast vectors  $\mathbf{c}^{(1)}, \mathbf{c}^{(2)}, \dots$ , the test statistics  $(\sum_i c_i^{(k)} x_i)^2$  are independently  $\chi^2$  distributed with one d.o.f. The function `TestRankhist` applies this test, using a linear and a squared contrast. Defining  $J = R+1$ ,

```
PlotRankhist(rh, mode="prob.paper")
```

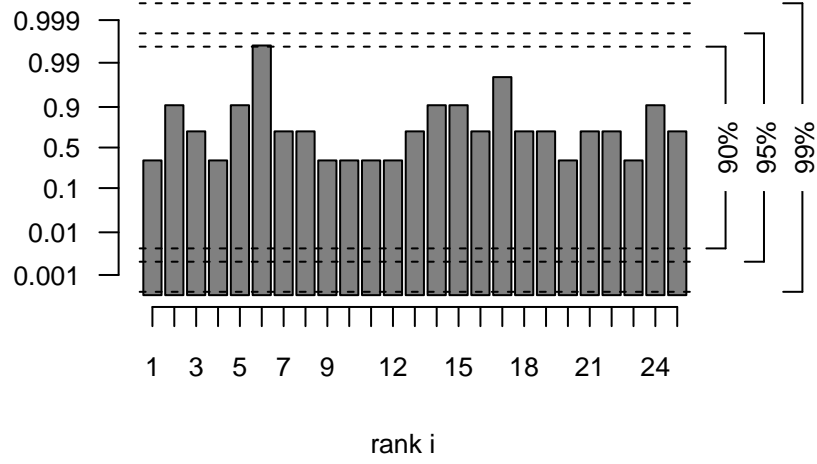


Figure 4: Rank histogram on probability paper

the  $i$ -th element of the contrast vectors  $\mathbf{c}^{(lin)}$  and  $\mathbf{c}^{(sq)}$ , for  $i = 1, \dots, J$  are given by

$$c_i^{(lin)} = -\sqrt{\frac{3(J+1)}{J(J-1)}} + i\sqrt{\frac{12}{J^3 - J}}, \text{ and} \quad (31)$$

$$c_i^{(sq)} = -\frac{\sqrt{5}J^2 - \sqrt{5}}{\sqrt{4(J-2)(J-1)J(J+1)(J+2)}} + \left(i - \frac{J+1}{2}\right)^2 \sqrt{\frac{180}{J^5 - 5J^3 + 4J}}. \quad (32)$$

The  $\chi^2$  test using the linear contrast is sensitive to sloped rank histograms, i.e. biased ensembles, while the  $\chi^2$  based on the squared contrast is sensitive to convex rank histograms, i.e. over- or under-dispersed ensembles. `TestRankhist` returns the test-statistics and one-sided p-values of the Pearson  $\chi^2$  test, and of the two tests based on the contrasts  $\mathbf{c}^{(lin)}$  and  $\mathbf{c}^{(sq)}$ :

```
TestRankhist(rh)
```

```
##                pearson.chi2  jp.slope  jp.convex
## test.statistic      23.9259    0.0114   0.005574
## p.value             0.4658    0.9150   0.940485
```

The rank histogram of the temperature ensemble forecast provides no evidence against the null-hypothesis of a reliable ensemble.

## 7. Reliability diagrams for probability forecasts

The reliability diagram is a classical tool to compare probability forecasts of binary events to the verifying binary observations (Jolliffe and Stephenson 2012). The reliability diagram compares the forecast probability to the conditional frequency of the observation, given the forecast. A forecast is reliable if the forecast probability and conditional event frequency coincide. Forecast reliability is a reasonable criterion that probability forecasts should satisfy; over all instances that the forecast issued a probability  $p$ , the event should happen  $p \times 100\%$  of the time.

If the forecast issues probabilities that take any value on the unit interval, most forecast probabilities will be issued only once. To estimate the conditional event frequency in this case the forecasts can be grouped into a finite number of non-overlapping bins. The average event frequency taken over all instances where the forecast is in a given bin is then taken as an average of the conditional event frequency. The reliability diagram is a plot of the conditional event frequency over the in-bin average of the forecast probabilities. **SpecsVerification** provides the function `ReliabilityDiagram` that takes as inputs a collection of probability forecasts and binary verifying observations, and calculates the reliability diagram for a specified number of equidistant bins, or a user-defined non-equidistant binning. The consistency resampling method proposed by Bröcker and Smith (2007) is used to estimate the likely spread of the reliability diagrams around the diagonal if the given forecast were, in fact, reliable.

If the `plot` argument is set to `FALSE`, the `ReliabilityDiagram` function returns the quantities necessary to plot the reliability diagram.

```
p.bin <- rowMeans(ens.bin)
ReliabilityDiagram(p.bin, obs.bin, plot=FALSE, bins=3)
```

##	p.avg	cond.probs	cbar.lo	cbar.hi	p.counts	bin.lower	bin.upper
## 1	0.1713	0.2222	0.0000	0.4784	9	0.0000	0.3333
## 2	0.5833	0.4286	0.1667	1.0000	7	0.3333	0.6667
## 3	0.8447	1.0000	0.6000	1.0000	11	0.6667	1.0000

If the argument `plot=TRUE` the reliability diagram is plotted, as shown in Figure 5. The logical argument `plot.refin` controls the refinement diagram, i.e. the histogram over the forecast probabilities. The logical argument `attributes` controls plotting of the polygon defined by the vertical no-resolution line at  $\bar{y} = 1/n \sum_t y_t$ , where  $y_t$  is the binary observation at time  $t$ , and the no-skill line defined by the linear equation  $f(x) = (x + \bar{y})/2$ , to produce the attributes diagram (Hsu and Murphy 1986). Points that fall into the shaded area of the attributes diagram contribute positively to forecast skill (defined by the Brier skill score).

## 8. Additional functions

The focus of **SpecsVerification**, and of the present paper, is on verification functions for ensemble and probability forecasts, uncertainty quantification, and graphical display. **SpecsVerification** includes a number of additional functions for recalibration and verification of forecasts. For verification of deterministic forecasts  $x_t$ , e.g. the ensemble mean forecast, the squared error score  $(x_t - y_t)^2$  (function `SqErr`), and the Absolute Error score  $|x_t - y_t|$  (function `AbsErr`)

```
rd <- ReliabilityDiagram(p.bin, obs.bin, plot=TRUE, bins=3, attributes=TRUE)
```

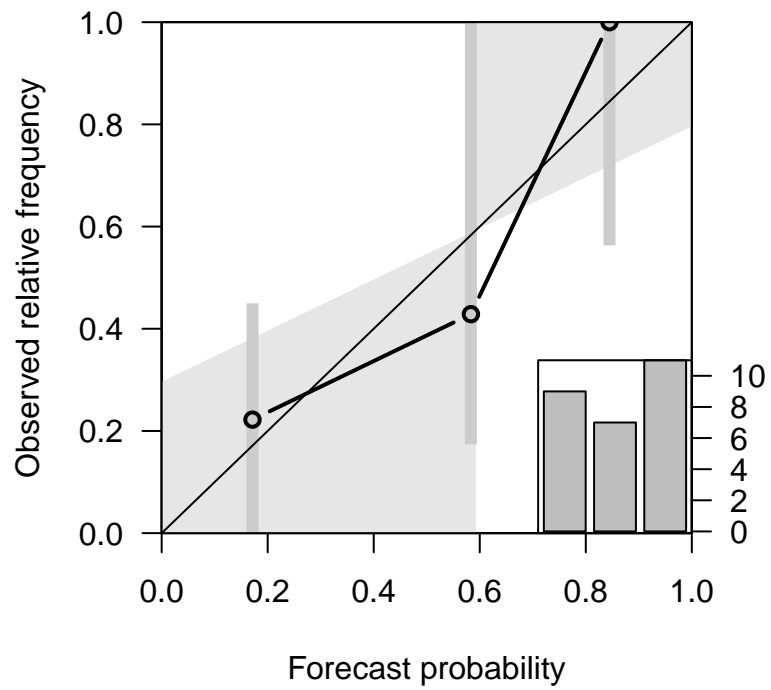


Figure 5: Reliability diagram

have been implemented, and can be analysed by the functions `ScoreDiff` and `SkillScore`. The function `GaussCrps` calculates the CRPS (eq. 9) where the forecast cdf  $F_t(x)$  is a Normal distribution with mean  $\mu_t$  and standard deviation  $\sigma_t^2$ . The CRPS integral can then be solved analytically (Gneiting, Raftery, Westveld, and Goldman 2005) thus eliminating the need for expensive numerical integration.

## 9. Conclusion

## Acknowledgments

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**Affiliation:**

Stefan Siegert  
Exeter Climate Systems  
College for Engineering, Mathematics, and Physical Sciences  
University of Exeter  
Exeter, EX4 4QF, United Kingdom  
E-mail: [Stefan.Siegert@exeter.ac.uk](mailto:Stefan.Siegert@exeter.ac.uk)  
URL: <http://emps.exeter.ac.uk/mathematics/staff/ss610>