On weighted ensembles of streamflow: bias correct separately and prefer constrained weights for more reliable and predictable outputs

Kallio, Marko[a]

[a] Aalto University, Department of Built Environment, Espoo, Finland

Correspondence to: Marko Kallio (marko.k.kallio@aalto.fi)

Correspondence can also be directed to twitter: @mkkallio

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Abstract

It has become more and more common in hydrology to consider multiple estimates of hydrological variables – ensembles – over single model runs. Ensemble members represent different realisations of various model structures, input data, and/or parametrisations. Improved predictions can be made using weighted ensembles with wide variety of model averaging methods found in the literature, but only a few explicitly discuss constraints to the weights. Here I perform a large sample study of 482 catchments and approximately 440 000 small and large weighted ensembles of streamflow and focus on comparing how constraints to the weights influence overall performance of the weighted ensemble, and their ability to reproduce select hydrological signatures. The results show that constraining the weights is clearly advantageous for they are less sensitive to the composition of the ensemble, they are less sensitive to the size of the ensemble, do not risk negative streamflow predictions, are more reliable in reproducing flow quantiles and variation (but not in daily and weekly dynamics), and their overall performance in terms of KGE is not worse when the weights have no constraints. From the results it is also clear that bias correction should be conducted separately and explicitly, prior to deriving weights for the ensemble. This is necessary for methods which require the weights to sum to 1, but is also advantageous for methods with implicit bias correction where the sum of weights is free, for it limits the magnitude of weights. I recommend that 1) bias correction be applied explicitly prior to deriving the weights, 2) use constrained weights and do not allow an intercept in the weighted ensemble, and 3) choose the method and potential pre-processing technique considering the specific hydrological signatures you wish to target. I also note that the ensemble mean is inferior in reproducing the hydrological signatures compared to weighted ensembles, and that the ensemble mean is best applied for ensembles without transformations. This research is useful for choosing the weighting method particularly when careful testing of alternatives is not possible, for whatever reason.

Highlights

- I explore the influence of constraints on the weights in weighted ensembles
- I consider linear bias correction, and square root and log transformation
- Bias correction should be applied explicitly prior to deriving weights
- Constraining weights is advantageous compared to allowing free weights
- Ensemble mean is inferior to weighted ensembles in hydrological signatures

Keywords: weighted ensembles, hydrological modelling, hydrological signatures, ensemble size, model averaging

1 Introduction

Over the past decades an increasing number of hydrological models have been developed for various purposes (Clark et al., 2011; Horton et al., 2021; Weiler and Beven, 2015). Each model display strengths and weaknesses and it may be difficult to choose a single right model for a specific modelling task, contributing to increased use of ensembles – collections of estimates of some variable. arising from different combinations of models, input data and/or model parameters. A common use case for ensembles is uncertainty quantification and to improve estimates through a weighted combination of the ensemble members (e.g. Diks and Vrugt, 2010; Franz and Hogue, 2011; Gosling et al., 2017; Kallio et al., 2021; Krysanova et al., 2020; McIntyre et al., 2005; Todorović et al., 2022; Vrugt and Robinson, 2007).

A large number of methods have been developed to derive optimal weights, exemplified by the numerous studies comparing the performance of different methods to weight the ensemble. Methods include a wide variety of techniques including the ensemble mean (a simple arithmetic mean of the ensemble members, included in most studies as a benchmark), different flavours of Ordinary Least Squares regression (OLS, Arsenault et al., 2015; Granger and Ramanathan, 1984), Bayesian model averaging (Buckland et al., 1997; Höge et al., 2019; Raftery et al., 2005), weights based on the performance of the ensemble members (Krysanova et al., 2020), weights derived by different optimisation algorithms (e.g. the Shuffled Complex Evolution algorithm; Arsenault et al., 2015; Duan et al., 1992), to complex machine learning approaches such as Gene Expression Programming (Zaherpour et al., 2019) or deep learning (Chen et al., 2023). Several studies pit methods against one another in comparison which usually analyse the overall performance of the weighted ensembles (Arsenault et al., 2015; Diks and Vrugt, 2010; Qi et al., 2021, and many more), and where the overall performance of the compared methods differ relatively little from one another.

Relatively few comparisons of model averaging methods discuss hydrological signatures, although we know from literature that goodness-of-fit assessments focusing on overall timeseries do not necessarily imply well replicated hydrological signatures (e.g. Todorović et al., 2022). General tendency seems to be to consider dry and wet periods within the comparison framework (see e.g. Broderick et al., 2016; Huang et al., 2020; Krysanova et al., 2020; Zaherpour et al., 2019, among others). However, Todorović et al. (2024) compare model averaging methods and their influence on a large number of hydrological signatures and report no improvement in the replication of most hydrological signatures with the tested model averaging methods.

Model averaging methods differ in what kind or restrictions they place on the weights in the weighted ensemble. Hydrological studies comparing model averaging methods sometimes report whether the weighting method result in the so-called *simplex* weights where the weights must be positive, and sum of weights equal to 1 (e.g. Diks and Vrugt, 2010; Todorović et al., 2024), but rarely discuss them at length. One particular study is of interest wrt. constraining weights in model averaging; Lee and Song (2021) compare three methods and five different constraints and conclude that strictly positive weights and weights summing to 1 (simplex) is advantageous in a real world application to water quality data.

Previous research has shown that various methods are applicable to different use cases, but there is no clear guidance in selecting methods particularly focusing on the constraints to the weights. In this research paper I fill in this gap by comparing weighted ensembles of streamflow predictions. To do this, I use a simple linear regression approach with and without restrictions to derive the weights. I further assess how the restrictions affect selected hydrological signatures (flow quantiles, coefficient of variation, and daily and weekly dynamics). In Section 2 I outline the case study methods, data and experimental design. In Section 3 I provide the results, and in Section 4 I discuss the outcomes, and their implications. Section 5 concludes and draws recommendations based on the results and discussion.

2 Case study design

The influence of different common model averaging methods on hydrological signatures is explored in a set of experiments. In Section 2.1 I describe the selected model averaging (optimisation) methods, pre-processing methods, the hydrological signatures, and the evaluation method used in the experiment. Section 2.2 provides a description of the data and methodology I use to evaluate the influence of model averaging on hydrological signatures.

2.1. Methods

2.1.1 Model averaging methods

The methods used to derive weights for the weighted ensemble in this study are all based on linear regression,

$$y = \alpha + \beta \boldsymbol{X} + \varepsilon \qquad (1)$$

with various restrictions, shown in Table 1. Here, α refers to the intercept, β to the regression coefficients, $\boldsymbol{X}$ represents the data matrix (of ensemble members) and ε is the error term, and y is the observed streamflow. Since the coefficients are used as weights in the weighted ensemble, I will call them weights in this paper. The first method, the ensemble mean (EM), does not require observations, and is used as the benchmark which the other methods are compared to (i.e. for a weighted ensemble to be useful, it needs to improve upon the naïve benchmark). I assess three constraints on for the linear regression; 1) whether to include the intercept α, 2) Constrain the weights β strictly positive values, and 3) to require the sum of weights β to equal 1. These correspond to the restrictions considered in Lee and Song (2021) and/or Clarke (2003). Since all of the methods here are based on least squares regression, they all minimise error and do not consider other properties of the timeseries.

Table 1. Linear regression-based model averaging methods compared in this study, starting from the most restrictive to the least restrictive method. Restrictions include the inclusion of intercept, coefficients restricted to strictly positive values, and the sum of coefficients equal to unity. The ensemble mean and the best ensemble member are also included in the table for completeness.

	Coefficient constraints			
Method	$\alpha = 0$	$\beta \geq 0$	$\sum \beta = 1$	Note
EM	-	-	-	Ensemble (arithmetic) mean
Best	-	-	-	Best individual ensemble member (RMSE)
CLS	**Yes**	**Yes**	**Yes**	Constrained Least Squares
NNLS	**Yes**	**Yes**	No	Non-Negative Least Squares
NNLS2	No	**Yes**	No	Non-Negative Least Squares with an intercept
GRB	**Yes**	No	**Yes**	Granger-Ramanathan method B
GRA	**Yes**	No	No	Granger-Ramanathan method A
GRC	No	No	No	Granger-Ramanathan method C (Ordinary Least Squares)

The methods I employ here are simple but serve the purpose of exploring constraints of weights and the potential intercept in weighted ensembles. The constraints lead to important restrictions for the weighted ensembles. Constrained Least Squares (CLS) regression with full constraints results in an optimised weighted ensemble where the streamflow values can never be outside the envelop provided by the ensemble members. With Non-Negative Least Squares (NNLS) regression, weighted ensemble can lead to streamflow beyond the envelope of the ensemble members (since the sum of the weights are not restricted), but where the streamflow values are guaranteed to be positive provided that the ensemble members are strictly positive. Including an intercept in NNLS2, however, may result in negative streamflow if the intercept is negative. And finally, Granger-Ramanathan methods with different flavours (GRA, GRB, and GRC) may result in negative streamflow because negative weights are allowed in the weighted ensemble. It should be also noted that the benchmark method, the ensemble mean, assumes that the ensemble is always identically distributed around the true value.

2.1.2 Pre-processing methods

Three pre-processing methods are employed in this study: (linear) bias correction, log-transformation, and square root-transformation. In linear bias correction, each of the ensemble members are bias corrected so that the mean of the ensemble member matches the mean of observed timeseries,

$$M_{bc} = M \frac{\mu_{obs}}{\mu_M}$$

where M is the ensemble member, M_{bc} stands for bias corrected ensemble member, μ_{obs} is the mean of observed data and μ_M is the mean of the ensemble member timeseries. Linear bias correction only corrects the bias, and retains the dynamics of the timeseries unaltered (Kallio et al., 2022). I always performed bias correction using the untransformed timeseries before other pre-processing methods.

I also test two non-linear transformations with and without bias correction: natural logarithm and square-root transformation. I apply the transformations for all ensemble members and the observed timeseries before deriving weights. I also apply back transformations of the weighted ensemble prediction with the exponential function e^x for natural logarithm and by taking the square x^2 for square root-transformation. All goodness-of-fit and hydrological signature computations are done after back transformations.

2.1.3 Hydrological signatures

I analyse the influence of the ensemble optimisation methods to commonly used hydrological signatures: Low flow quantiles Q95 and Q75, median flow (Q50), and high flow quantiles Q25 and Q5. In addition, I compute 1- and 7-day autocorrelation, describing the day-to-day and weekly dynamics in streamflow. Furthermore, I assess the variability with computing the coefficient of variation, σ/μ, where σ is the standard deviation and μ is the mean of the timeseries. I compute the hydrological signatures for the observed timeseries as well as for each HBV simulation and each weighted ensemble prediction.

2.1.4 Evaluation method

The non-parametric variant of the Kling-Gupta Efficiency (KGE) is used to assess the goodness-of-fit of the output timeseries against observations. KGE is an aggregated metric consisting of three components; variability, bias, and dynamics (Gupta et al., 2009):

$$KGE = 1 - \sqrt{(\alpha - 1)^2 + (\beta - 1)^2 + (r - 1)^2}$$

where α (variability) is ${\sigma_{sim}}/{\sigma_{obs}}$, β (bias) is ${\mu_{sim}}/{\mu_{obs}}$, and r (dynamics) is Pearson correlation coefficient. In the non-parametric variant, Pool et al. (2018) replace the dynamic and variability terms of KGE with Spearman rank correlation coefficient and normalised flow duration curve, respectively. Because KGE can take any value $[-\infty, 1]$, with 1 denoting perfect fit to the observations, I transform the KGE values to bounded KGE$_b$ (Beck et al., 2020; Mathevet et al., 2006),

$$KGE_b = \frac{KGE}{2 - KGE}$$

which is guaranteed to lie in $[-1, 1]$. The bounded KGE$_b$ helps particularly in visualising the results, as many of the weighted ensembles have KGE values much smaller than -1.

To compare the hydrological signatures computed from the observed timeseries to the signatures of weighted ensembles, I compute a relative value $S_{relative}$

$$S_{relative} = \frac{s_{opt}}{s_{obs}}$$

where s_{opt} is the hydrological signature computed for the weighted ensemble, and s_{obs} is the same hydrological signature for the observed timeseries.

Furthermore, I also record the number of negative values in the weighted ensemble streamflow values, as some of the weighting methods may cause negative streamflow values if the intercept or some of the weights are negative. I note here that log or square root transformed timeseries do not contain negative values after back-transform, because e^x for $x < 0$ is a positive number and squaring a negative number result in a positive number. Therefore, for square root transformation, I record the number the number of negative predictions *prior* to back transforming because they may result in streamflow artefacts and impact, in particular, the low flow quantiles where most potential negative values most likely occur.

2.2 Experimental design

I conducted the experiments based on the CARAVAN (version 1.2) large-sample hydrological dataset (Kratzert et al., 2022), and in particular the 482 catchments included from the CAMELS dataset (Addor et al., 2017). The ensemble simulations are based on Beck et al. (2020); a global, regionalised parametrisation of the HBV conceptual hydrological model (Bergström, 1976). Beck et al. provide HBV parameters at a 5 arc-minute grid (approximately 9 km at the equator) in 10 cross-validation folds. The catchments range from 100 km^2 to 1980 km^2 in size with the centroids of 3 to 98 five arc-minute grid cells falling in each catchment. I conduct HBV simulations for all grid cells located at the 482 CAMELS catchments and for all 10 ten cross validation folds from Beck et al. (2020) for a total ensemble sizes between 30 and 980 depending on the catchment size. The total number of HBV simulations is 116 360. The ensemble therefore consists of simulations with parameters that are regionalised from a large set of donor catchments. All simulations were run for the full period of daily climate forcing provided in the CARAVAN dataset (1981-2020) with a 5-year spin-up period to fill the stores. I used the same catchment-specific climate input provided in the CARAVAN dataset for all parametrisations within individual catchments.

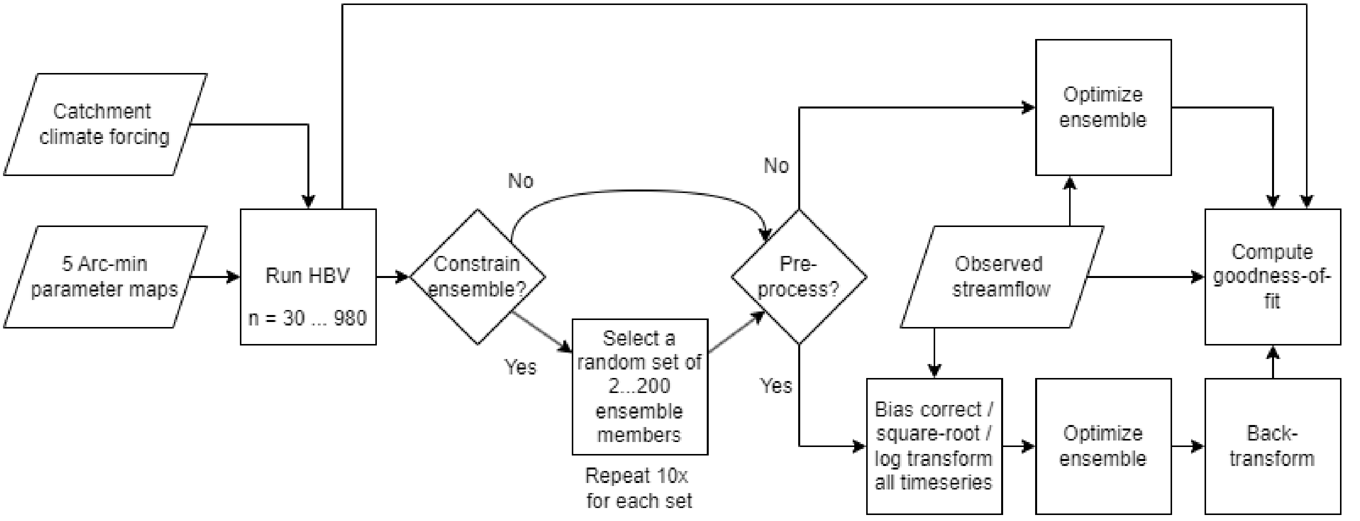

Figure 1. Workflow used in this study. The same workflow was applied for each of the 482 catchments included in this study.

The overall workflow is visualised in Figure 1. The ensembles obtained with the HBV simulations are evaluated for the full ensemble (with sizes ranging from 30 to 980) as well as constrained ensembles of 2, 5, 10, 15, 25, 50, 100, 150, and 200 members. The constrained ensembles consist of a random selection from the full ensemble of each catchment (if possible, given the size of the full ensemble). For each ensemble size and catchment, the process is repeated 10 times. The total number of successful ensemble evaluations with combinations of bias correction, pre-processing, model averaging methods, and ensemble sizes is approximately 440 000.

3 Results

3.1 HBV simulation performance

HBV simulations used as ensemble members show variation in their performance, with the mean KGE_b at 0.07 and the middle 50% (Interquartile range; IQR) of simulations falling between -0.02 and 0.17 (averaged over all catchments and all ensemble members). The poor performance is mainly due to a strong bias: the mean of the variability term is 0.72 (IQR 0.62-0.85) and the mean of the dynamics term is 0.63 (IQR 0.56-0.73). Applying bias correction brings the mean of KGE_b to 0.35 (IQR 0.24-0.46). The Ensemble Mean (EM) performs better than 54% of ensemble members when assessed over the full timeseries. After applying bias correction, the EM is better than 81 % of the members. A way to look at it is, that, when bias correction is applied, the bias term in KGE is always perfect for both the EM and each individual member. Thus, the EM represents variability and dynamics better than 81% of the individual members. When bias correction is not applied, ensemble mean may have stronger biases than any individual member due to some members being considerably more biased than most other members. This is reflected in the smaller number of members beaten by the ensemble mean when no bias correction is applied. The EM is also better than most ensemble members in all hydrological signatures except for Q5 when no bias correction is applied.

An example of the ensemble and the weighted ensembles along with the KGE performance for station 1202500 from the CAMELS dataset is shown in Figure 2. From the figure we can read that the weighted ensembles from CLS, NNLS, NNLS2 result in a highly similar behaviour with minimal differences. The same applies for the methods with less constraints (GRA, GRB, GRC). It is notable that despite having a high KGE, the ensemble mean is clearly inferior to the weighted ensembles, even if the difference in numerical performance is small. We can also note that in this example, the best individual ensemble member is very similar to the methods which constrain weights to be strictly positive.

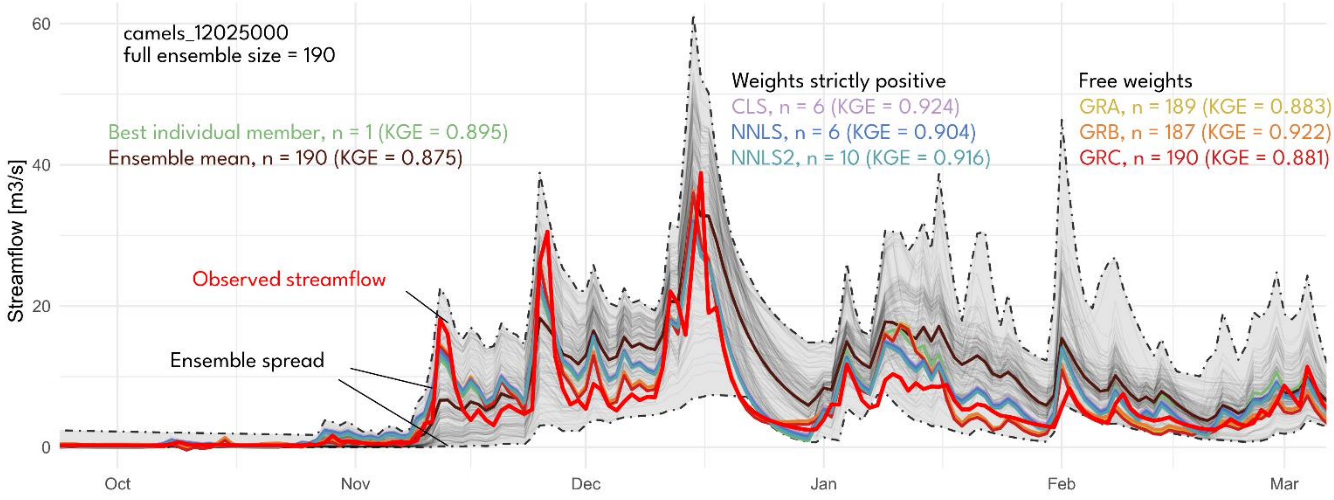

Figure 2. Example of the ensemble and optimised weighted ensembles for station 12025000 for a single time slice. The reported KGE is computed for the full timeseries including timesteps outside what is shown here. The value *n* shows the number of ensemble members which are assigned a significant weight (> 0.01), except for ensemble mean, for it gives equal weight for each observation. The bias corrected ensemble shown here is for one of the stations where the weighted ensembles perform exceptionally well.

3.2 Performance of optimised ensembles

The performance of the optimised ensembles in training and testing periods are shown in Figure 3 for bias corrected and non-bias corrected combinations. From the figure we can learn a few things. First, the methods which do not require the ensemble weights to sum to unity (that is, NNLS, NNLS2, GRA, GRC) are not impacted by bias in the ensemble. We can think that these methods have an implicit bias correction mechanism built into them, whether or not they include an intercept or not. The bias corrective mechanism manifests itself it in the magnitude of assigned weights. We can observe this from the fact that the linear bias correction which I apply in this study does not change the relationships between the ensemble members (Kallio et al., 2022), and therefore the only thing that changes is the magnitude of the weights. Second, the methods which constrain weights to strictly positive (CLS, NNLS and NNLS2) show less overfitting to the training period than methods which allow free weights (GRA, GRB, GRC). Third, CLS, the ensemble mean and the best individual ensemble member are strongly impacted by bias correction, but they all perform consistently in the testing period without overfitting. Since the different methods have relatively similar characteristics in the overall performance assessment, depending on the constraints, I perform the remaining analysis with the ensemble mean (as the benchmark to beat), CLS as the most constrained technique, GRC as the most flexible method, and NNLS2 as the middle ground in terms of constraints.

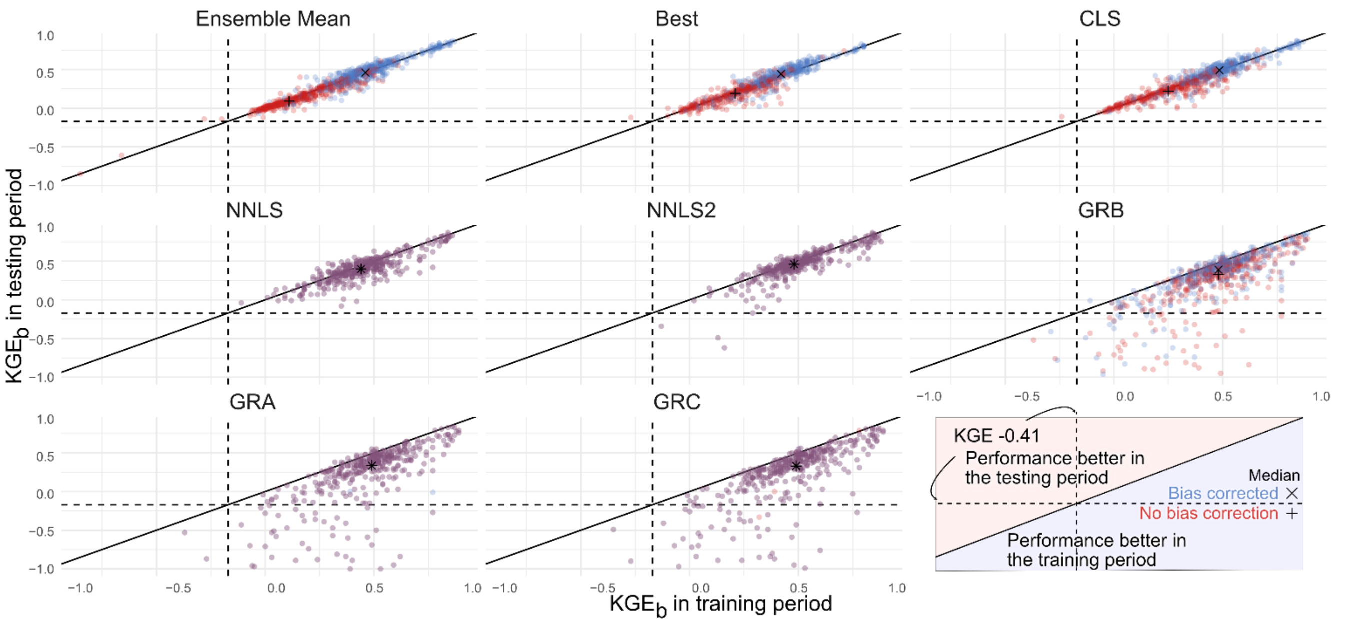

Figure 3. The KGE$_b$ performance of optimised ensembles in the training and testing periods with and without linear bias correction. The data shown here are the full ensembles for each catchment (n=482) with ensemble sizes ranging from 30 to 980.

Figure 4 shows a comparison between observed and ensemble hydrological signatures. As with the overall performance shown in Figure 3, bias correcting the ensemble has little influence for the predicted signatures from NNLS2 and GRC ensembles. And conversely, the predicted signatures from the ensemble mean and CLS are significantly improved with bias correction. NNLS2 results in the best overall correspondence to the observed hydrological signatures. Unexpectedly, GRC, the most flexible of the methods tested, shows the poorest performance in the low-flow quantiles and with CV, performing even worse than the ensemble mean. This is mainly due to a number of stations where the testing period performance is very poor compared to the training period (refer to the outliers in Figure 3 and Figure 4). GRC, however, shows the best correspondence to the observed timeseries in 1- day and 7-day autocorrelation, suggesting that it is the best in reproducing short-term dynamics. CLS performs worse than the ensemble mean at low-flow quantiles, on par at median- to high-flow quantiles, and better at variation and autocorrelation.

Because it is clear at this stage that ensemble mean and CLS are strongly disadvantaged by a lack of bias-corrective properties, I continue the analysis using only bias corrected ensembles.

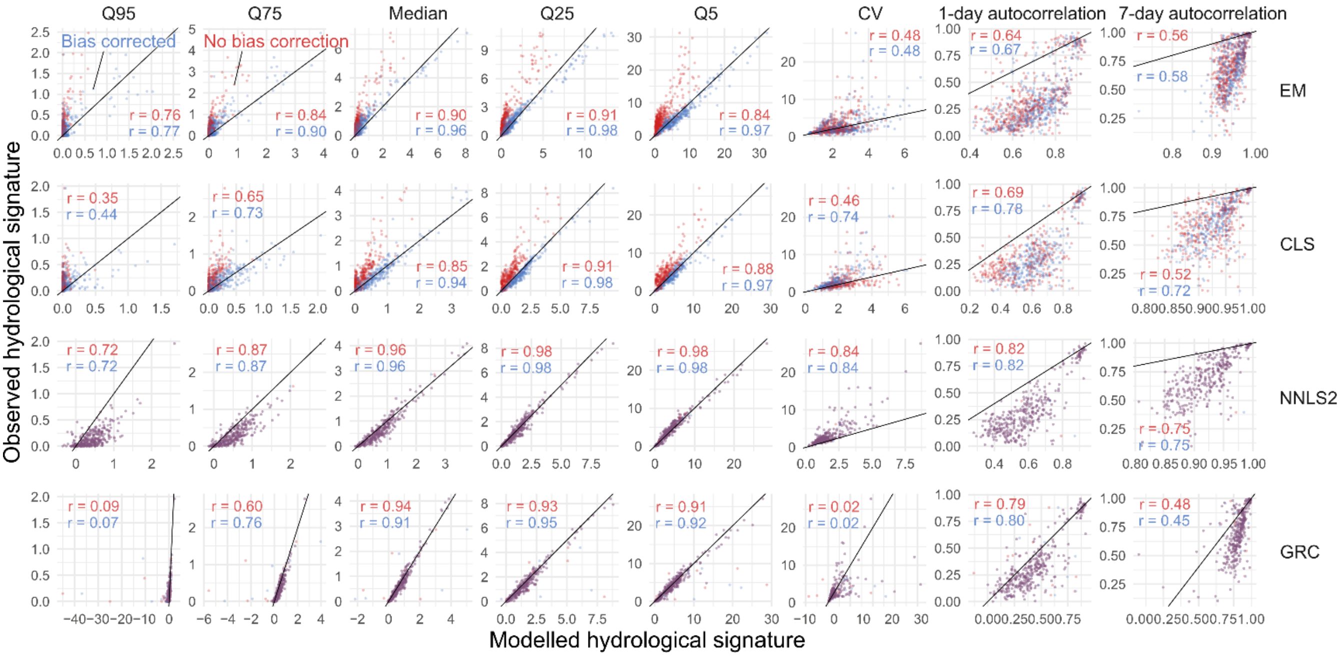

Figure 4. Comparison of modelled and observed hydrological signatures with and without bias correction for the selected ensemble optimisation methods. Pearson correlation coefficient *r* is shown in each facet. The plot does not show 15 datapoints where the coefficient of variation (CV) for GRC exceed the value of 60, but they are included in the computation of Pearson correlation. If excluded from the computation, correlation increases to 0.53 and 0.55 with and without linear bias correction, respectively.

3.3 The influence of transformation depends on the weighting method

Thus far we have looked at weighting the ensembles with untransformed timeseries. The literature on hydrological model calibration, however, tell us that transforming the timeseries prior to calibration has an influence in model performance (e.g. Thirel et al., 2023), and there is no reason to think it wouldn't be the case here as well. Figure 5 shows how the three methods and transformations tested fare benchmarked against the ensemble mean in the overall KGE_b in the testing period. From the figure we can read that log-transformation improves the performance of the ensemble particularly for those stations where the ensemble mean performance is poor, when the weights are derived with CLS or NNLS2. Square-root transformation tends to improve the performance against the ensemble mean when compared to the weighted ensembles without pre-processing, for all the three methods. The figure likewise reveals that GRC generally performs *worse* than the ensemble mean when optimised with log-transformed timeseries or when no transformation is applied. Square root transformation brings the performance on par with (or better than) the ensemble mean.

The performance against the hydrological signatures stays similar or is improved compared to the no-preprocessing case (compare Figure 4 with Supplementary Figures 1 and 2) for all three methods. However, the poor overall performance of GRC may be attributed to the extremely high streamflow in some stations resulting from the log-transformation. The GRC-optimised ensembles also have considerably higher coefficient of variation than CLS, NNLS2, or observations, and it deteriorates the good output of no-preprocessing in autocorrelation. Square root transformation generally always improves the correspondence of the hydrological signatures to observed ones, without such failures as with log-transformation.

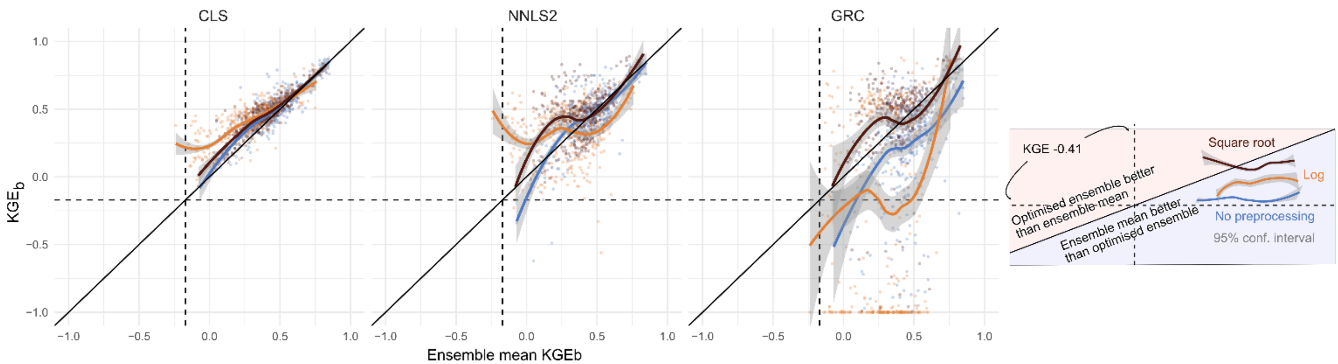

Figure 5. Overall KGE_b performance of CLS, NNLS2 and GRC derived optimal ensembles with transformed timeseries, benchmarked against the performance of the ensemble mean. Shown for full-sized bias corrected ensembles.

3.4 Diminishing returns from ensemble sizes above 15

All of the figures presented above have been computed from full ensembles with sizes varying from 30 to 980. These ensembles are very large, and most practical ensembles tend to be on the smaller size. Figure 6 shows the skill score (wrt. KGE_b) the weighted ensembles have against the ensemble mean benchmark. CLS consistently outperforms the ensemble mean whether the ensemble is bias corrected or not. The ensemble size does not have influence strong influence. For NNLS2, its bias corrective property means that it consistently and significantly outperforms the ensemble mean when the ensemble is not bias corrected. However, there is no clear improvement when the ensemble has no bias. The GRC is again an entirely different case; at ensemble sizes below 300 it improves against the ensemble mean when the ensemble is not bias corrected, but the improvement falls fast as the ensemble sizes increase. When the ensemble is bias corrected (and thus, when GRC loses its advantage being able to bias correct), the ensemble mean is consistently better.

For CLS and ensemble mean the size of the ensemble does not have a large influence for the hydrological signatures after the ensemble reaches 10-15 members in size, as seen in Figure 7. For NNLS2 and GRC the situation is different, however, particularly for the low flows: the low-flow quantiles are very uncertain for the two more flexible methods. The autocorrelation continuously improves for GRC as the ensemble size grows. Notably, for all the methods, high flows are most accurately reproduced hydrological signature.

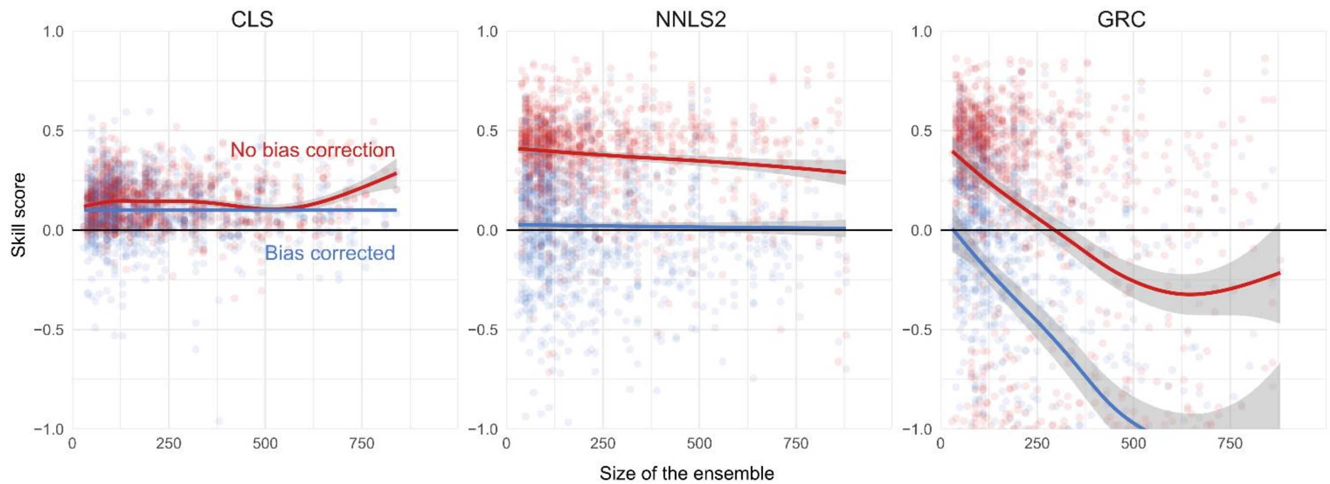

Figure 6. The skill score of CLS, NNLS2 and GRC benchmarked with the ensemble mean for different ensemble sizes. The y-axis is limited to [1, -1] and thus does not show the data points with skill score worse than -1.

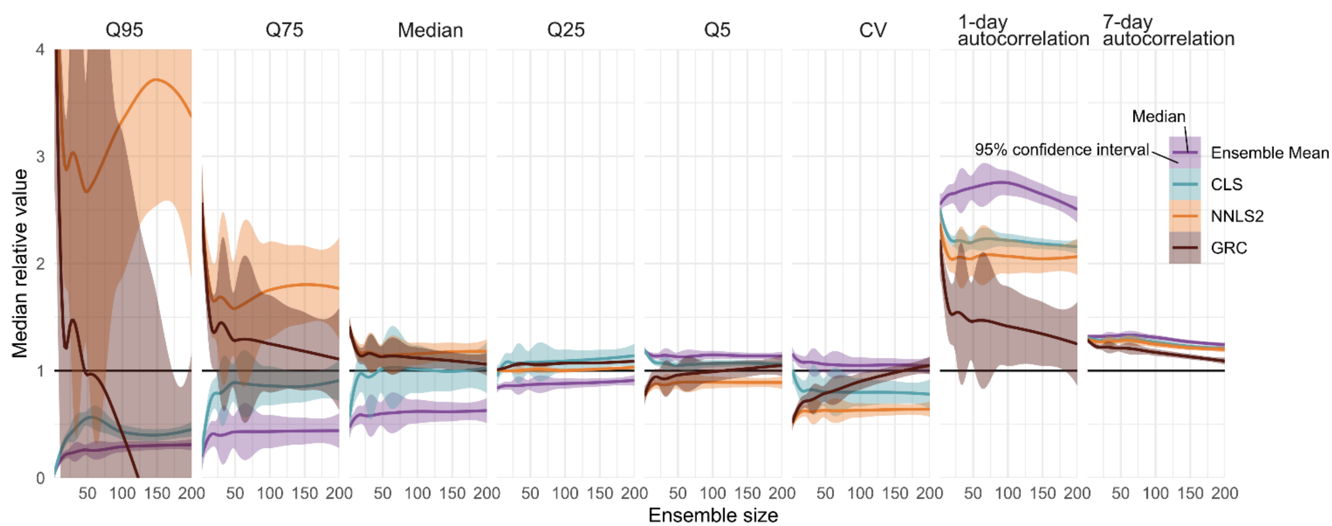

Figure 7. The median relative value of hydrological signature of the optimised ensembles compared to the signature of observed timeseries computed for ensemble sizes varying between 2 and 200. The plot is shown for bias corrected ensembles with no preprocessing. The plot is cropped at [0, 4].

Square root and log preprocessing significantly influence the reproduction of hydrological signatures reported in Figure 7, as shown in Supplementary Figures S3 for square root, and S4 for log preprocessed ensembles. The influence differs with different weighting constraints, and GRC is particularly strongly influenced by the preprocessing. For all weighted ensemble methods, low and median flows are improved or approximately similar to ensembles with no preprocessing using either of the tested preprocessing methods. Log preprocessing in particular is successful with low flows, but high flows are worse than no-or square root preprocessing. Square root preprocessing has a small effect on the coefficient of variance and to short term dynamics. However, GRC particularly fares much less predictable when log preprocessed. As the ensemble size increases, CV sky rockets between ensemble sizes 50 and 100, and both 1-day and 7-day autocorrelation first improve and then deteriorates, both at around ensemble size 100, and never settles. This hints that the optimal ensemble size is around 100 for GRC for these particular ensembles, but since there is constant change with CV and autocorrelation, it is unclear if this translates to other ensembles.

From the experiment with the preprocessing methods, it is also clear that the ensemble mean reproduces the hydrological signatures better when there is no preprocessing applied (apart from bias correction).

4 Discussion

4.1 Negative streamflow

Model averaging methods which allow for negative weights, or an intercept, may result in optimal combinations with negative streamflow values. In general, this is not desired for e.g. streamflow or runoff which, by definition, cannot be negative. Figure 8A shows the proportion of optimised timeseries with more than an 5% of negative values (for we might be tolerant to negative values to a certain extent) for NNLS2 and GRC, and for different ensemble sizes. I observe that the proportion is relatively constant for NNLS2, and it should be noted that since NNLS2 by definition does not allow in negative weights in the weighted ensemble, all negative streamflow are the result of a negative intercept. For GRC, the proportion keeps growing when the ensemble is not transformed, while with square root-transformed ensembles GRC is on par with NNLS2. Figure 8B,C show that, while the proportion keeps growing for non-transformed GRC, the proportion of negative values in the optimal combinations is steadily decreasing. For square root-transformed the number of negative values in the timeseries is relatively constant (Figure 8B,C).

If no negative streamflow values are allowed, up to 17.6% of optimal combinations using NNLS2 (ensemble size 50, no pre-processing) will contain negative values. The proportion is smaller for square root-transformed timeseries, peaking at 8%. For GRC, the proportion of timeseries with negative streamflow values quickly increases being 54% at ensemble size of 5 members, reaching more than 83% at ensemble size 25, and with an ensemble of 200 members, 94% of optimised timeseries contain negative values. Square root-transformation reduces the number of negative streamflow from GRC optimised values to 43% at ensemble size 50 and maxing out at 73% at 200 ensemble members. This means that any method which allows a negative intercept or negative weights needs to be applied carefully and with a pre-defined strategy on what to do for negative streamflow outputs. For large ensemble sizes, one has the option of sampling the ensemble until a solution is found which contain as few negative values as possible. However, if there are significant negative weights, or a negative intercept, applied to the ensemble, there is *no guarantee* that there are no negative values outside the training period, and the issue gets worse with increasing ensemble size.

The negative values from square root-transformation are particularly deceiving, since when back-transforming by squaring, the negative values “disappear”, and require assessment and handling *prior* to back-transforming. In this study, I did not process them in any way other than record when they occurred.

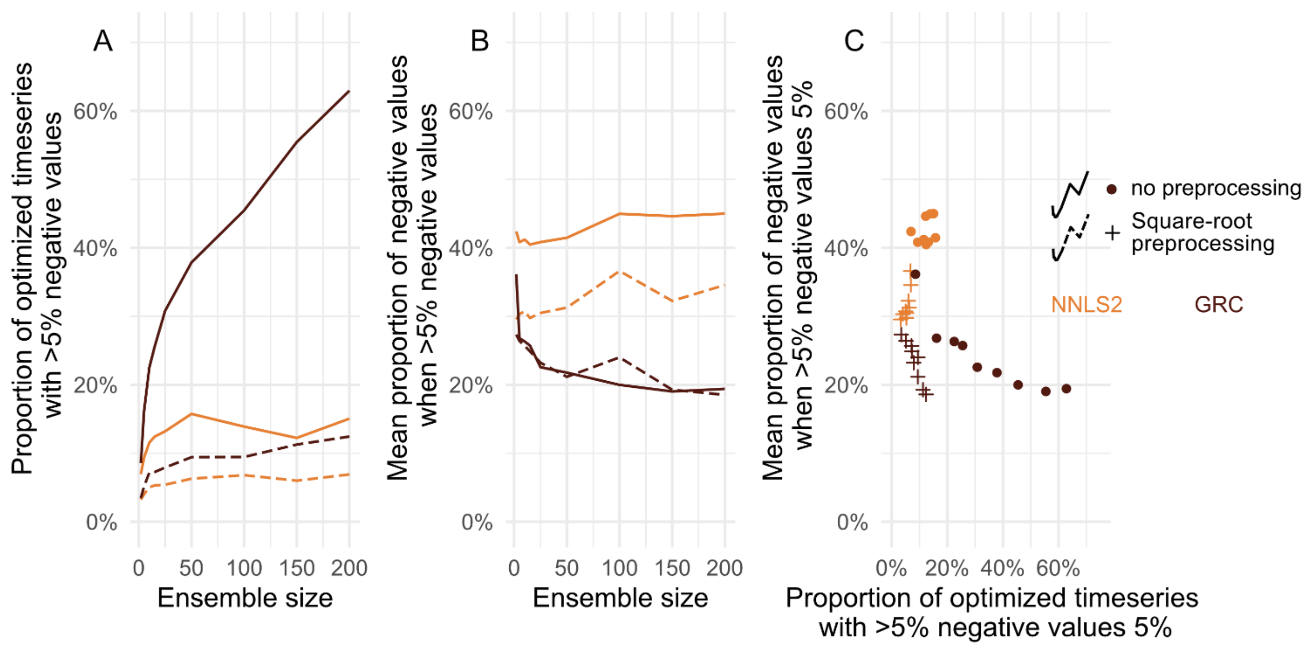

Figure 8. Panel A) shows the proportion of all optimised ensembles with more than 5% of negative streamflow values. Panel B) shows the mean proportion of negative values for those optimised ensembles with more than 5 % negative values. Panel C) shows the two proportions against one another. Optimal combinations with less than 5% negative values are not considered in the plots.

I should note here that many studies successfully apply methods which allow free weights and suggest they work well (e.g. (Arsenault et al., 2015; Todorović et al., 2024; Wan et al., 2021, among others). This suggests that one can apply methods with less constraints on certain situations, and these are likely to vary between variable of interest, ensemble composition, and temporal and spatial scales.

The final remark I make here wrt. to the negative streamflow values is that the absolute magnitude of the streamflow values do not affect the number of negative values in the optimal combination. This is because the weights are dependent on the relationships between the ensemble members, and a consistent linear transformation applied to the ensemble members will not change their relationships and will only lead to a change in the absolute magnitude of the weights.

4.2 Use of ensemble members and the optimal ensemble size

As the ensemble size increases, not all ensemble members necessarily provide useful information for the optimal ensemble combination. Figure 9 shows how the selected methods (GRC, NNLS2, and CLS, without transformation) use the available members for different ensemble sizes. If we assume that an ensemble member has significant weight when the weight is higher than 0.01 (that is, 1% weight) GRC – the unconstrained OLS – tends to use almost every one of the ensemble members for its optimal combination. Thus, even the poorest performing ensemble member has a weight above 0.01, but may be insignificant relative to the sum of weights in the weighted ensemble. For CLS and NNLS2, the number of used weights tends to be around 5 members despite the size of the ensemble, suggesting that the constraints mean that most of the ensemble members do not contribute useful additional information over smaller ensembles. Behaviour of the chosen methods is highly similar for square root transformed ensembles. For all the three shown methods, log-transformed ensembles lead to fewer members with meaningful weights, and where CLS and NNLS2 use only 3-6 ensemble members on average, regardless of ensemble size. For GRC, the number is steadily increasing albeit with a slightly smaller slope for square-root and non-transformed ensembles. Still, log-transformed ensembles with GRC utilise over 90% of the available ensemble members. This result is consistent with, for instance, Wan et al. (2021) who find no improvement with ensemble sizes above 9 members. Figure 2 shows an example of the performance and the number of members with significant weight.

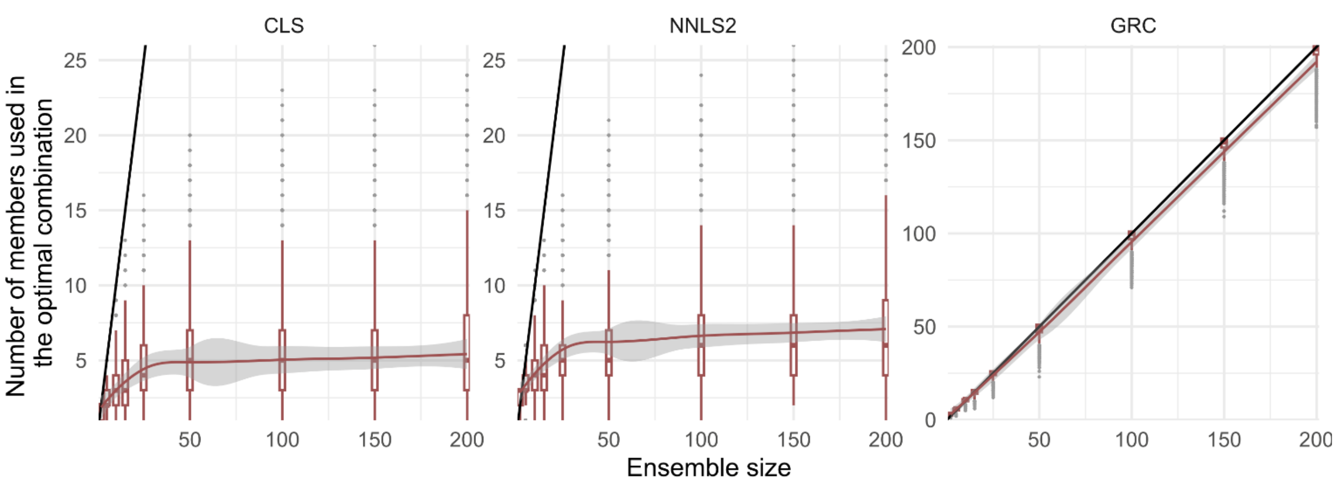

Figure 9. Number of ensemble members with significant weight (> 0.01) for CLS, NNLS2 and GRC. The diagonal black line shows the case where 100% of the ensemble members are assigned significant weight. Shown here for bias corrected ensembles without transformation. The boxes show the inter-quartile range, and the whiskers show 1.5 times the inter-quartile range, and the line shows the mean number of used weights as well as the 95% confidence interval for the mean.

The ensemble size, however, influences the variability of the weighted ensemble. The variability of the resulting timeseries over different ensemble members drops rapidly with increasing ensemble size particularly for CLS, whose variability is the highest with ensemble sizes below 10. NNLS2 has consistently smallest variability over all ensemble sizes. GRC with the most flexibility is the least robust and most sensitive to the ensemble composition for ensemble sizes above 10.

4.3 Alternative weighting methods

The literature on model averaging methods provides plenty of other options for optimising the ensembles. I have excluded them from this research as I think they do not add significantly to the insights shown wrt. ensemble weight constraints. One of the more popular alternatives is the Bayesian Model Averaging (BMA) method, which is often included in different comparisons, so I feel I should say a few words on why I have excluded it here: 1) they are computationally expensive especially for large ensemble sizes (Broderick et al., 2016; Yao et al., 2018), 2) previous research has shown that BMA is not necessarily any better than the regression approach used here in terms of testing period performance (e.g. Arsenault et al., 2015; Broderick et al., 2016; Diks and Vrugt, 2010), 3) in many cases they may fail to converge (in Arsenault et al., 2015, BMA did not converge for 82 out of 429 catchments), and 4) Yao et al. (2018) report that BMA is only appropriate when the true data generating model is within the ensemble, which is not the case here (although, in practise we might choose to disregard this requirement. See the review by Höge et al., 2019 aimed specifically for hydrologists). Clarke (2003) additionally raises concerns on the robustness of BMA.

Furthermore, existing literature also shows that more complex optimisation methods are not clearly better than the simpler regression-based alternatives I use here. See e.g. Zaherpour et al. (2019) for genetic programming, or shuffle-complex evolution in the comparison in Arsenault et al. (2015). It is relatively easy to imagine why it is so when the assessment is done over the entire timeseries (and not individual hydrological signatures): GRC (OLS regression) is the *best linear unbiased estimate* (under the assumptions in Gauss-Markov Theorem). It is hard to beat for any method minimising *error*. However, other methods can lead to improvements over GRC when considering hydrological signatures or alternative objective functions, just as I show here for least squares-approaches with constraints to the weights. I believe that value in using more complex ensemble weighting methods in hydrology should be sought there in the performance on different hydrological signatures or by optimising a more complex objective function than just error.

I would also highlight that if the ensemble is given temporally constant set of weights that do not change over time, it is assumed that the relationship between the ensemble members stay fixed for all parts of the hydrograph, including high and low flow, and through changing environmental and climatic conditions. This is an unreasonable expectation considering, for instance, climate change. The more complex methods would likely be better suited to produce dynamic weights, as is already done by some authors in hydrology (e.g. Chen et al., 2023, or Xia et al., 2014). In ensembles of hydrological models, a natural way forward is to identify the environmental and climatic conditions where each model or parameter set excels and make this the basis of deriving dynamic weights for the ensemble.

4.4 Other types of ensembles

The ensembles here are built with different parametrisations of a single model. However, ensembles are not equal; other types of ensembles compiled using different models, model structures, alternative forcing datasets and modellers may yield in different results. For instance, Velázquez et al. (2011) report that a combination of several hydrological model structures and meteorological ensembles perform better and more reliably than ensembles derived from a single hydrological model. However, in comparing ensembles consisting of different parametrisations against other types, including multi-model ensembles, Doblas-Reyes et al. (2009) find that different types of ensembles may have different strengths, and that differences between ensemble types were small. If the ensemble consists of primarily skilful predictions, the overall performance with any of the methods may be substantially better than for the primarily unskilled ensemble based on regionalised parameters I employ here (see Supplementary Figure S5 for a visualisation on how individual ensemble member fare against the performance of the optimised combination).

5 Conclusion and recommendations

This study performed a large sample study of weighted ensembles of streamflow derived from regression-based model averaging methods with various constraints on the weights. From approximately 440 000 weighted ensembles with sizes ranging from 2 to 980, and with and without linear bias correction, logarithmic transformation and square root transformation, Based on the results and discussion, I derive three main recommendations:

- First, apply bias correction to the ensemble prior to using your method of choice to derive weights for the weighted ensemble. This is critical for any method which only allow so-called simplex weights (strictly positive weights and weights sum to 1) but is also useful for other methods for it limits the magnitude of the resulting weights.
- Second, use constrained weighting schemes, corresponding to the suggestion in Lee and Song (2021), who also recommend using strict simplex constraints. They are more reliable than methods which allow free weights, particularly for low flow hydrological signatures, and the simplex weighting scheme guarantees that the output from the weighted ensemble is within the envelope provided by the ensemble members. Allowing free weights or employing an intercept result in a high risk of negative streamflow in the weighted ensemble, especially when the ensemble is large in size, and are more sensitive to the composition of the ensemble. However, allowing flexibility in the form of free weights will lead to better daily and weekly dynamics than with constrained weighting schemes.

- Third, select the weighting method, including potential pre-processing techniques, aimed at the targeted hydrological signatures and other modelling objectives. For instance, targeting flow quantiles is best done with constraints, but short-term variability is best reproduced with more lax constraints.

In addition to the recommendation, I make note that while the ensemble mean is on par to the performance of the weighted ensembles from the constrained methods with the overall assessment (KGE), the weighted ensembles more reliably reproduce the hydrological signatures. It is also noteworthy that ensemble mean from ensembles with no preprocessing reproduce hydrological signatures better than when preprocessed with square root or log transformation. I therefore suggest that the ensemble mean should only be applied to untransformed ensembles.

The optimal choice of weighting method for your use case is also deeply dependent on the quality of the ensemble (members), the temporal and spatial scale as well as the variable being modelled. This research is useful for choosing a method when deep and thoughtful exploration and testing of alternatives is, for whatever reason, not possible.

Code and data availability

The code to replicate the figures are available from Github at (https://github.com/mkkallio/On_weighted_ensembles) and deposited to Zenodo once the article has been accepted. The CARAVAN Version 1.2 dataset used in the study is available at https://zenodo.org/records/7944025. The regionalised HBV parameter sets used to run HBV are available from https://www.gloh2o.org/hbv/. Since running all the scripts to recompute the data will take a significant amount of time, precomputed data is available from the author on request.

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SUPPLEMENT TO THE ARTICLE:

On weighted ensembles of streamflow: bias correct separately and prefer constrained weights for more reliable and predictable outputs

Kallio, Marko

Correspondence to: Marko Kallio (marko.k.kallio@aalto.fi)

This file includes the Supplementary Figures S1-S5 mentioned in the main text.

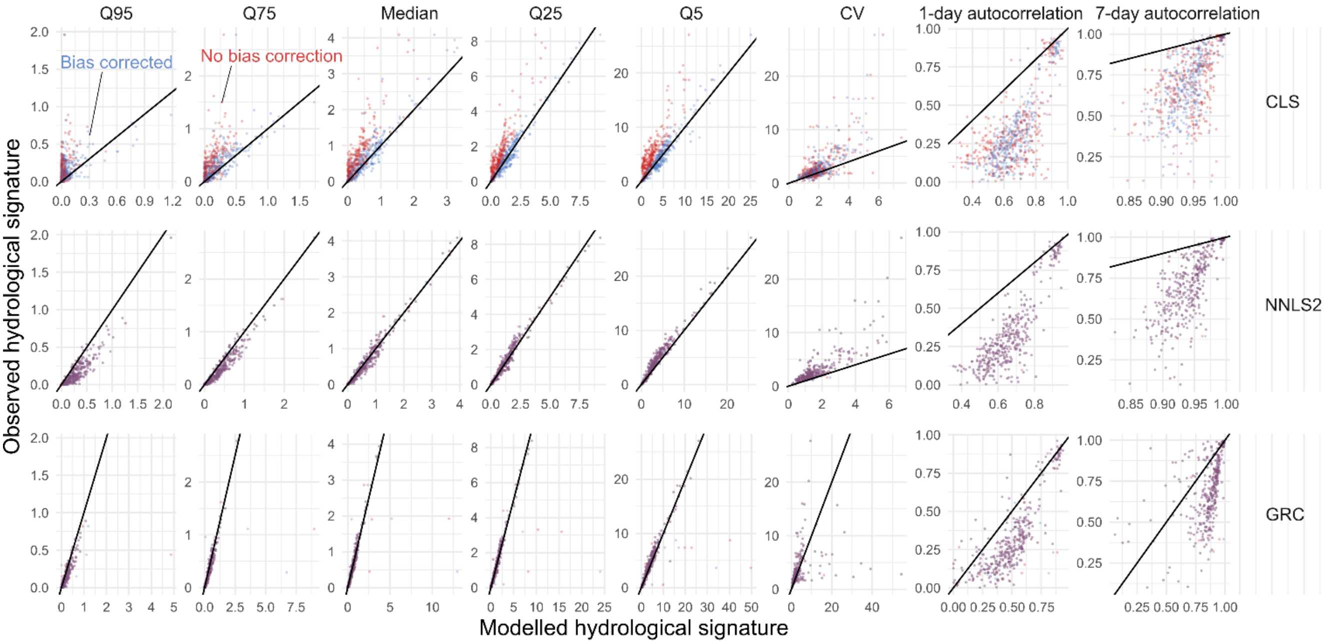

Figure S10. Comparison of modelled and observed hydrological signatures with and without bias correction for the selected ensemble weighting methods with square root preprocessing.

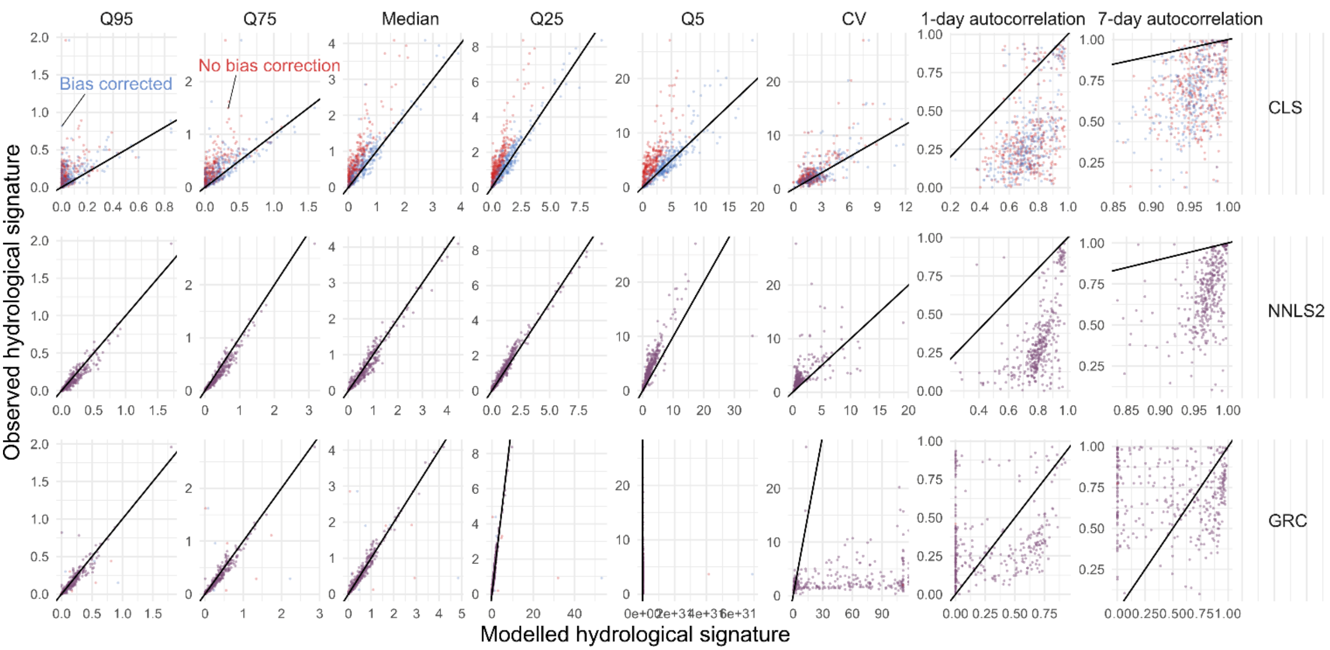

Figure S11. Comparison of modelled and observed hydrological signatures with and without bias correction for the selected ensemble weighting methods with square root preprocessing.

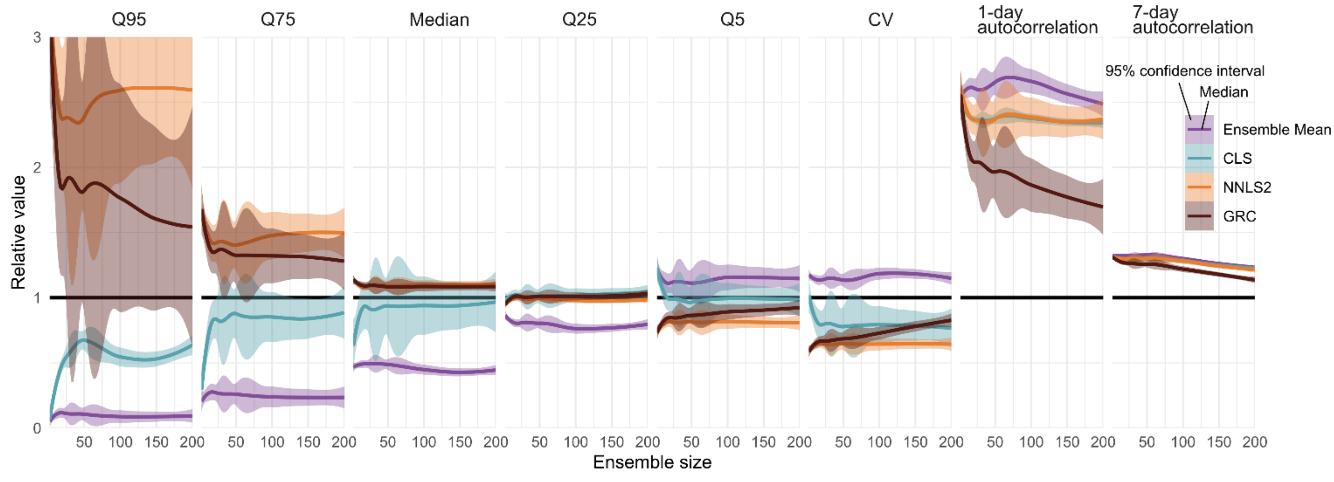

Figure S12. The median relative value of hydrological signature of the optimised ensembles compared to the signature of observed timeseries computed for ensemble sizes varying between 2 and 200. The plot is shown for bias corrected ensembles with square root preprocessing. The plot is cropped at [0, 3].

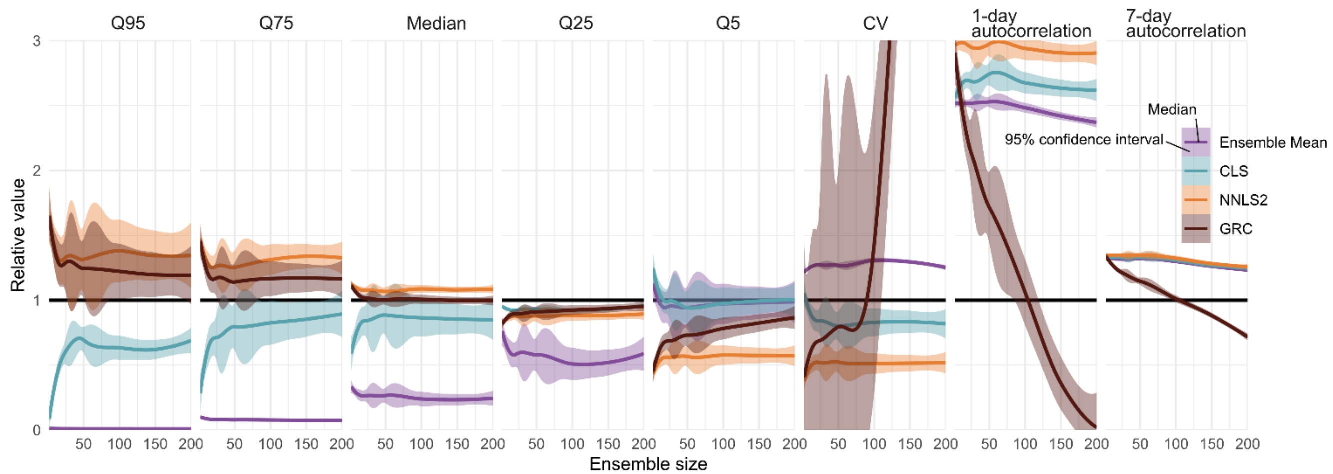

Figure S13. The median relative value of hydrological signature of the optimised ensembles compared to the signature of observed timeseries computed for ensemble sizes varying between 2 and 200. The plot is shown for bias corrected ensembles with log preprocessing. The plot is cropped at [0, 3].

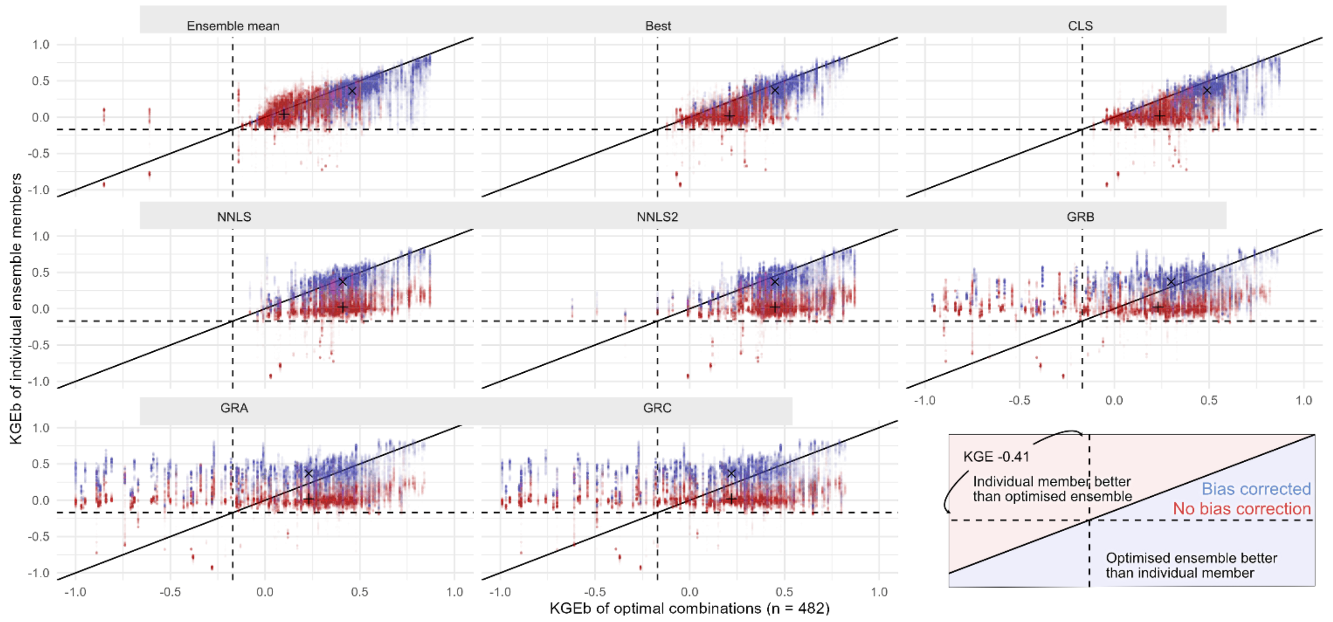

Figure S14. Comparison between the KGE$_b$ of the weighted ensembles, and the KGE$_b$ of each individual ensemble member, shown for full ensembles of size 30 to 980.