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Toward a Reliable Prediction of Seasonal Forecast Uncertainty: Addressing Model and Initial Condition Uncertainty with Ensemble Data Assimilation and Sequential Bayesian Combination

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Abstract

Uncertainties are an unfortunate yet inevitable part of any forecasting system. Within the context of seasonal hydrologic predictions, these uncertainties can be attributed to three causes: imperfect characterization of initial conditions, an incomplete knowledge of future climate and errors within computational models. This study proposes a method to account for all three sources of uncertainty, providing a framework to reduce uncertainty and accurately convey persistent predictive uncertainty. In currently available forecast products, only a partial accounting of uncertainty is performed, with the focus primarily on meteorological forcing. For example, the Ensemble Streamflow Prediction (ESP) technique uses meteorological climatology to estimate total uncertainty, thus ignoring initial condition and modeling uncertainty. In order to manage all three sources of uncertainty, this study combines ESP with Ensemble Data Assimilation, to quantify initial condition uncertainty, and Sequential Bayesian Combination, to quantify model errors. This gives a more complete description of seasonal hydrologic forecasting uncertainty. Results from this experiment suggest that the proposed method increases the reliability of probabilistic forecasts, particularly with respect to the tails of the predictive distribution.

Keywords

Streamflow Forecasting, Data Assimilation, Multi-modeling, Ensemble Streamflow Prediction

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1 Introduction

Uncertainty is pervasive throughout hydrologic forecasting. A general lack of information, and skillful modeling frameworks, leads to forecast products that do not have sufficient ability to be relied upon in an entirely deterministic manner. In the specific case of seasonal streamflow, volumetric estimates of runoff are necessary for guidance of an array of water management decisions, yet the accuracy of such estimates is often unsatisfactory (Moradkhani and Meier, 2010). To this end, it should be of high priority to ensure that estimates of forecast uncertainty are statistically reliable. Given that probabilistic estimates of volumetric streamflow are reliable, risk within a reservoir system can be more effectively managed, thus reducing the chance of both flood damages and water shortages concurrently.

Research into probabilistic methods for seasonal forecasts has developed over the past few decades. A first example is the Ensemble Streamflow Prediction (ESP) framework proposed by Twedt et al., (1977) and clarified by Day (1985). ESP works under the assumption that the primary skill in a hydrologic forecast is based on land surface conditions, and as such treats initial conditions as deterministic quantities, while leveraging climatological stochastic forcing to account for poor knowledge of future meteorological conditions. The framework itself has prompted a number of studies to improve seasonal forecasting, including utilizing information from climate indices (Najafi et al., 2012) and climate modeling products (Mo et al., 2013; Yuan and Wood, 2012). Since the literature suggests that some information about seasonal climate is available through both climate modeling and teleconnections, further studies have examined the assumption that skill is primarily derived from initial conditions (Li et al., 2009; Shukla et al., 2013; Wood and Schaake, 2008; Yossef et al., 2012). With an increasing focus on the relative

skill of different aspects of seasonal forecasting, an increasing focus has been placed on determining how best to manage overall uncertainty in the modeling framework.

Interest in probabilistic forecasting is increasing within the hydro-meteorological research and operational communities (Brown et al., 2010; Demargne et al., 2013; Madadgar et al., 2012; Yuan et al., 2013), yet forecast systems rarely approach the uncertainty estimation problem holistically. Primarily, in the seasonal streamflow forecasting realm, these uncertainties arise from meteorological forcing of the model, initial land surface conditions, and model uncertainty. The forecasting community has understandably focused predominantly on the uncertainties relative to future weather conditions, as these uncertainties will become dominant at most forecast lead times (Shukla et al., 2013; Yossef et al., 2012). More specifically, the forecast steadily loses sensitivity to the initial conditions over time, but the forecast will remain sensitive to forcing at all lead times. Though such methods lead to probabilistic flow estimates, these methods generally underestimate the forecasting uncertainty (Wood and Schaake, 2008, Yuan and Wood, 2012). The objective of this study is to develop and test a technique to improve the quantification of uncertainty in probabilistic forecasting of seasonal volumetric streamflow, thus reducing the problem of overconfidence. In order to overcome this overconfidence, this study proposes a movement towards treating the initial land surface states and models as probabilistic values, in addition to meteorological forcing.

Probabilistic estimation of land surface states has proven to be a challenge throughout the land surface modeling community, but great strides are being made in the field of ensemble data assimilation (DA) (Moradkhani, 2008). A number of researchers have been looking into the use of DA methods for improving land surface state prediction (Andreadis and Lettenmaier, 2006; Clark et al., 2008; De Lannoy et al., 2012; Margulis et al., 2002; Reichle et al., 2002) and

examining the ability of stochastic states to estimate uncertainty reliably (DeChant and Moradkhani, 2011a; Leisenring and Moradkhani, 2010; Liu and Gupta, 2007; Moradkhani et al., 2005a,b). The extensive literature on ensemble DA within hydrologic models motivated the use of ensemble DA techniques for probabilistic initial state estimation (ESP-DA) as presented in DeChant and Moradkhani (2011b). Results from this study suggested that accounting for initial condition uncertainty in ESP improves the reliability of seasonal streamflow forecasting, but that results remain overconfident. An important issue that potentially causes this persistent overconfidence is the assumption that model uncertainty is insignificant. Thus model error must also be examined in a seasonal forecasting framework.

An increasingly popular method to account for model uncertainty is through multi-model ensembles (Bohn et al., 2010; Regonda et al., 2006). By having a diverse set of models, a forecast implicitly accounts for the errors related to each individual model. Multi-modeling via Bayesian Model Averaging (BMA) is becoming an increasingly popular technique throughout hydrologic forecasting (Ajami et al., 2007; Duan et al., 2007; Raftery et al., 2005), which has also been extended to estimate the posterior model probability sequentially in time, which is referred to as Sequential Bayesian Combination (SBC) (Hsu et al., 2009). Recently, both BMA and SBC have been shown to be completely compatible with ensemble DA (Parrish et al., 2012), leading the current study to propose the use of model averaging within the previously developed ESP-DA framework to simultaneously account for initial condition and model uncertainty. Through these advancements, it is possible to move hydrologic forecasting towards a more complete accounting of uncertainty (Liu et al., 2012). Thus the hypothesis of this study is that ESP with DA and SBC will lead to more reliable probabilistic forecasts of seasonal streamflow, in comparison to traditional ESP, and the previously examined ESP-DA methodology.

2 Methods

2.1 Study Area

The study examines streamflow forecasting throughout the Upper Colorado River Basin (UCRB), defined here as the entire Colorado River Basin upstream of Lee's Ferry (see Figure 1), which is located just downstream of Lake Powell. The UCRB is located in the southwestern US, covering portions of Wyoming, Utah, Colorado, Arizona and New Mexico. The basin drains an area of roughly 280,000km², with forest covering much of the upper elevations and shrub land covering the valleys. The mean naturalized yearly flow volume at Lee's Ferry is roughly 18 billion cubic meters, providing water to 26 million people with a minimum designated annual flow from Lake Powell set at 9.3 billion cubic meters. In Figure 1, the gauges of the three major sub-basins (Green River, Colorado Headwaters/Gunnison and San Juan) and at Lee's Ferry are identified. These four gauges are used to examine overall forecast reliability, whereas spatial aspects of forecast accuracy are analyzed over 16 smaller sub-basins.

2.2 Hydrologic Models

2.2.1 Variable Infiltration Capacity Model

The VIC model is a physically-based, distributed model that solves the energy and water balance at the land surface, and spatially discretized units are generally placed on a regular grid (Gao et al., 2010; Liang et al., 1994). In order to perform model calculations, VIC requires soil information, vegetation information, elevation bands, precipitation, maximum and minimum temperature, average wind speed, humidity, and incoming shortwave and longwave radiation for each grid cell. Land surface parameters for VIC simulations were gathered from the Natural Resources Conservation Services STATSGO dataset (soil) and the University of Maryland land cover dataset (vegetation). Elevation bands were defined using the USGS National Elevation

Dataset, with information from the Precipitation Regression on Independent Slopes Model (PRISM) yearly precipitation information to aid in the distribution of elevation band precipitation. Readers are referred to section 2.5 for information about the forcing data. Simulations were performed over the entire UCRB at a spatial resolution of 0.25° , which makes 473 model grid cells. Based on the hydrologic fluxes estimated by VIC, excess water is routed to the outlet of the basin with a combination of Nash-Cascade hydrologic routing and Muskingum-Cunge hydraulic routing.

2.2.2 National Weather Service River Forecast Center Models

The SNOW-17 and Sacramento Soil Moisture Accounting (SAC-SMA) models are used by the National Weather Service (NWS) to provide operational streamflow forecasts for flood and water supply monitoring. These models are coupled, with SNOW-17 handling snow accumulation/ablation calculations and SAC-SMA modeling the soil water storage component. Both SNOW-17 and SAC-SMA have a more conceptual nature to model equations than VIC, leading to an increased reliance on calibration, as opposed to soil and vegetation data. Fortunately, the NWS calibrated parameters for each basin within the UCRB have been made available by the Colorado Basin River Forecast Center (CBRFC). The NWS performs simulations from these models with elevation bands for each sub-basin, leading to 409 discretized units. To run SNOW-17 and SAC-SMA, precipitation, average temperature, and potential evapotranspiration (PET) are required. Excess runoff from these models is routed to the outlet with a unit hydrograph for hydrologic routing and Lag/K for hydraulic routing.

2.3 Observations

2.3.1 Passive Microwave Radiance

Passive Microwave (PM) brightness temperature (T_b) from the Advanced Microwave Scanning Radiometer – Earth Observing System (AMSR-E) data was used in this study to perform land surface DA. T_b was chosen for this study as it provides useful information about water stored at the land surface due to its sensitivity to snow water equivalent (SWE) (18.7 and 36.5GHz AMSR-E channels) and soil moisture (6.9 GHz AMSR-E channel). With its sensitivity to both soil moisture and SWE, PM observations provide valuable information about the water storage immediately above and below the land surface. In the presence of snow cover, microwave radiation is a function of snow depth, density, temperature, grain size, and liquid water content (Weismann and Mätzler 1999), and is a function of soil type, temperature and liquid water content in the case of bare soil (Drusch et al., 2001). In order to assimilate T_b , a radiative transfer model (RTM) is used to calculate the microwave radiance from the land/snow surface (Durand and Margulis, 2008; DeChant and Moradkhani, 2011; Montzka et al., 2012, 2013; Andreadis and Lettenmaier, 2012). The RTMs used in this study are described in section 2.4. Passive microwave observations were gathered from the AMSR-E L2A dataset, which was recently shown to have greater information content, with respect to SWE, than the spatially and temporally resampled EASE-Grid products (Li et al., 2012), and distributed to the centroid of each discretized modeling unit through inverse distance squared weighting.

2.3.2 Land Surface Temperature

Land surface temperature (LST) data from the Moderate Resolution Imaging Spectroradiometer (MODIS) were assimilated in conjunction with PM T_b to improve model estimation of surface temperature, and therefore provide more accurate energy balance

estimation and simulations from the RTMs. LST from MODIS is particularly attractive for this study because of the fine resolution observations (1 km by 1 km) and the high frequency (up to 4 observations every 24 hours) of measurements, due to its deployment on both the NASA Aqua and Terra satellites. With high frequency and resolution of the observations, MODIS LST is a powerful source of information about the land surface energy balance. LST from MODIS is estimated through the Generalized Split-Window Algorithm (Wan and Dozier, 1996). This uses the difference between MODIS bands 31 and 32, along with estimated land surface emissivity, to estimate the true temperature of the land surface (Wan and Dozier 1996; Wan et al., 2004). In this study, MODIS LST is aggregated to model resolutions with spatial averaging of observations within each discretized unit.

2.3.3 Naturalized Flow

Naturalized flow data for the UCRB is provided by the United States Bureau of Reclamation (USDOI, 2005). This dataset contains flow reconstructions throughout the entire Colorado Basin, with 20 reconstruction locations in the upper region. Flows are in the form of monthly volumes. For the sake of this study, 16 different flow locations were chosen for verification. In addition, the VIC model was optimized based on the mean square error of monthly flow simulations, for the 10 years prior to the study period, at four locations: the Green River at Green River, Utah, the Colorado River at Cisco, Utah, the San Juan at Bluff, Utah, and Lees Ferry, Arizona, which are shown in Figure 1.

2.4 Radiative Transfer Models

Microwave emission from the land surface is modeled through a combination of the L-Band Microwave Emission Model from the Biosphere (L-MEB) model (Wigneron et al., 2007), for the case of bare soil, the Microwave Emission Model for Layered Snowpack (MEMLS)

(Weismann and Mätzler 1999), when snow cover is present, and vegetation is modeled according to Pullainen et al. (1998). Soil parameters required by the L-MEB model were estimated from the STATSGO dataset, according to suggestions in Wigneron et al. (2007). Although these parameters may be improved through sensitivity analysis (Sabater et al., 2011), calibration (De Llannoy et al., 2013; Drusch et al., 2009) and even the data assimilation itself (Montzka et al., 2013), the default parameters are preferred here to keep the focus on the proposed forecasting technique. In addition to land surface parameters, atmospheric effects are accounted for as described in Durand and Margulis (2008), which allows for comparison with AMSR-E observations. In the VIC model, snow is represented with two layers, a small upper layer and a larger deep layer, whereas SNOW-17 assumes a homogenous snowpack. Both models estimate all snow variables necessary, with the exception of grain size, which is modeled according to DeChant and Moradkhani (2011a). Microwave emission in the 6.9GHz frequency is ignored in the NWS model as the SAC-SMA model does not estimate physical soil moisture. Within the VIC model, assimilation of the 6.9GHz channel is motivated as the soil moisture is expected to affect the forecast for up to one month lead time (Shukla et al., 2013). While SWE is expected to be a much larger factor in the seasonal runoff, the soil moisture is expected to have significant impact on seasonal volumetric runoff.

2.5 Forcing Data

Forcing datasets required for the VIC model are precipitation, maximum and minimum temperature, potential evapotranspiration, wind speed, humidity, and incoming shortwave and longwave radiation. Observed precipitation and temperature data was gathered from the NWS Cooperative Observer Program (COOP) and NRCS SNOTEL sites, and then spatially distributed over the VIC model cells. Distribution of precipitation and temperature was performed with

scaling based on PRISM monthly data (Daly et al., 1994). Wind observations were gathered from the NCEP/NCAR reanalysis dataset (Kalnay et al., 1996), and then scaled to the modeling domain, following the method of Mauer et al., (2002). Humidity is estimated according to Kimball et al., (1997), shortwave radiation is estimated according to Thornton and Running, (1999), and longwave radiation is estimated according to Bras, (1990), all of which are performed internally in the VIC model. The NWS models require precipitation, temperature and PET. All forcing for these models was provided by the CBRFC, where precipitation and temperature are estimated from in-situ observations, and PET is estimated based on pan evaporation rates.

2.6 Error Models

Stochastic estimates of precipitation, temperature, wind, and PET were used to drive the hydrologic models. Precipitation errors are assumed to be heteroschedastic and log-normal with a variance of 25% of the magnitude, temperature errors (PM T_b , LST and Air Temperature) are assumed to be homoschedastic and normal with a standard deviation of 3° C, and both PET and Wind are assumed to have a heteroschedastic normal error with variance equal to 25% of the magnitude. The form and magnitude of these errors follow previous studies (DeChant and Moradkhani 2011a,b, 2012; Parrish et al., 2012). In addition, this study also utilizes spatially and temporally correlated errors as described by Clark and Slater (2006). For application of this method, a correlation length of 100km and temporal correlation of 5 days was used for all inputs, similar to the application in Clark et al. (2008).

3 Experimental Design

3.1 Particle Filtering and Sequential Bayesian Combination

Within a DA framework, the hydrologic model is viewed through the state-space framework as shown in equations (1) and (2).

$$x_{i,t}^- = f(x_{i,t-1}^+, u_{i,t}, \theta) \quad (1)$$

$$y'_{i,t} = h(x_{i,t}^-, \alpha) + v_{i,t} \quad (2)$$

In the above equations, the i^{th} prior states ($x_{i,t}^-$) are estimated through the propagation of the model forward in time, from the i^{th} posterior states at the previous time step ($x_{i,t-1}^+$), utilizing stochastic forcing data ($u_{i,t}$) and static simulation model parameters (θ). Note that model error not added to the states estimated from equation (1), which differs from common representations. The exclusion of model error at this stage is chosen to avoid altering the physical relationship between snow states, which has been found to degrade SWE reconstruction through AMSR-E data assimilation (DeChant and Moradkhani, 2011a). When this error is included, the relationship between snow states (i.e. depth, density, liquid water content, temperature, grain size) is damaged, which leads to errors in future simulations of both the RTM and snow model. From the prior states and static observation model parameters (α), the prediction of the streamflow, LST and T_b ($y'_{i,t}$) is created with the evaluation of an observation operator ($h(\bullet)$) with some predictive error ($v_{i,t}$). For applying DA, the Particle Filter (PF) is utilized in the study presented here. The PF follows sequential Bayes Law (equation 3) to estimate the posterior state distribution.

$$p(x_t | y_{1:t}) = \frac{p(y_t | x_t) p(x_t | y_{1:t-1})}{\int p(y_t | x_t) p(x_t | y_{1:t-1}) dx} \quad (3)$$

Equation 3 mathematically describes the development of a posterior distribution of model predicted states, given all past observations ($y_{1:t}$), by calculating probabilities sequentially in time. Sequential Bayes Law states that the posterior is estimated by the normalized product of the prior distribution, $p(x_t | y_{1:t-1})$, and the likelihood, $p(y_t | x_t)$. In this study, the prior distribution is estimated as the importance density estimated in equation (1), and the likelihood is Gaussian, which is calculated based on the residuals observed and simulated (from equation (2)) PM T_b . This provides a weighted ensemble of states, which represents the posterior distribution. Due to the potential for ensemble members to attain insignificant weight, states are resampled at every observation time step, via the Sampling Importance Resampling (SIR) technique, to develop a probability density with uniform weights. For further details on the implementation of the PF, see Moradkhani and Sorooshian (2008).

Research into streamflow estimation with DA has also highlighted the benefits of parameter estimation for quantifying forecast uncertainty (DeChant and Moradkhani, 2012). This methodology has been rapidly advancing, which has potential for improving uncertainty in streamflow forecasting. Specifically, Moradkhani et al., (2012) introduced a method of parameter estimation using the Variable Variance Multiplier (VVM) (Leisenring and Moradkhani, 2012) methodology for generating proposal parameters, and Metropolis acceptance criteria to ensure that parameters remain within the meaningful regions of the posterior distribution. Through this methodology, parameter estimates are more robust than with previously used PFs. Although parameter estimation is a potential avenue for improving

streamflow predictions, this study assumes calibrated static parameters to focus on the benefits of combining of DA and model averaging.

BMA was introduced to the climate forecasting community by Raftery et al. (2005) and later applied to hydrologic modeling (Ajami et al., 2007; Duan et al., 2007). BMA extends the application of Bayes Law to the case of multiple possible models, where it is assumed that the varying model behavior represents uncertainty. The theory behind this method is described briefly in equation (4) and (5), but the reader is referred to previous applications for additional details.

$$p(M_k | D) = \frac{p(D | M_k)p(M_k)}{p(D)} \quad (4)$$

$$p(y' | M_{1:K}, D) = \sum_{k=1}^K p(y' | M_k, D)p(M_k | D) \quad (5)$$

In equation (4), M_k represents the k^{th} model, D is the training data, $p(M_k | D)$ is the posterior model probability and $p(y' | M_{1:K}, D)$ is the probability of the model prediction based on all K models. In this study, the SBC approach proposed by Hsu et al. (2009) is utilized to weight all models. In this approach, model weights are calculated sequentially, similar to the PF, as shown in equation (6).

$$p(M_k | y_{1:t}) = \frac{p(y_t | M_k)p(M_k | y_{1:t-1})}{\int p(y_t | M_k)p(M_k | y_{1:t-1})dM} \quad (6)$$

In equation (6), the prior distribution ($p(M_k | y_{1:t-1})$) is equal to the posterior probability at the previous time step, and the likelihood ($p(y_t | M_k)$) is estimated with a kernel density smoother (Wilks, 2006) of the ensemble streamflow estimate from the PF.

Parrish et al., (2012) recently showed that the PF and SBC are completely compatible, and often advantageous when used in conjunction. Instead of making the assumption that model errors are normally distributed, as is typically done in SBC and BMA, the PF can be utilized to

develop a probabilistic prediction that is not bound by distributional parameters. Further, the SBC method is preferred over non-Bayesian model averaging methods (Diks and Vrugt, 2010) to remain consistent with the theoretical framework of the PF. With the posterior distribution from filtering of each model, $p(y'_t | M_k, y_{1:t})$, and the weights of each model, $p(M_k | y_{1:t})$, a probability distribution of forecasts from all models can be estimated according to equation (7). In the application here, each model probability is estimated based on the volumetric monthly flows described in section 2.4.1. This is assumed to be a reasonable weighting scheme for the seasonal volumetric flow forecasts analyzed here, but the effects the weighting time scale should be addressed when moving to different forecast lead times (e.g. weekly or annual forecasts).

$$p(y'_t | M_{1:K}, y_{1:t}) = \sum_{k=1}^K p(y'_t | M_k, y_{1:t}) p(M_k | y_{1:t}) \quad (7)$$

3.2 Ensemble Streamflow Prediction with PF-SBC

ESP is a method used by the National Weather Service River Forecast System to create probabilistic forecasts of seasonal streamflow volumes. This method leverages stochastic meteorological data to generate a Monte Carlo sample of streamflow predictions to represent the uncertainty of future streamflow estimates. As described in equation (8), the ESP technique creates a density of streamflow simulations over the forecast period, with each individual simulation referred to as a “trace”, generated from the deterministic states, x_t , resampled historical forcing, $u_{1:Y-1,t}$ (Y represents the current year), and some hydrologic model M , from the initial forecast time t , to estimate the probability of forecast, where $\tilde{y}_t$ refers to forecasted seasonal flow volumes, as opposed to $y'_{i,t}$, which are the predictions during the spin-up period.

$$p(\tilde{y}_t | x_t, u_{1:Y-1}, M) = \sum_{y=1}^{Y-1} p(\tilde{y}_t | x_t, u_{y,t}, M) \approx \sum_{y=1}^{Y-1} \delta(\tilde{y}_t - M(x_t, u_{y,t}, \theta, \alpha)) w_{y,t} \quad (8)$$

Where δ is the Dirac delta function, $M(x_t, u_{y,t}, \theta, \alpha)$ represents the combined hydrologic model (f) and routing function (h), which forecasts streamflow, following the description in section 3.1, and $w_{y,t}$ is the weight of each trace at initial forecast time t , which is uniformly set to $\frac{1}{Y-1}$. While the common practice is to give each trace equal weight, these weights may be estimated with additional climate information (Najafi et al., 2012).

Initial model states are produced by running the model with observed input data up to the initial forecast time-step, which is referred to as a “spin-up”. Starting at this point, the model is forced with resampled historical forcing ($u_{1:Y-1,t}$), beginning at the initial forecast date, for each historical observation year, to estimate meteorological climatology, thus producing a stochastic streamflow forecast. By generating a stochastic streamflow forecast through ESP, it is assumed that the initial state estimates are perfect, the resampled historical forcing represents the future uncertainty, which inherently assumes climate stationarity, and the model has no error. Given that the assumptions of climate stationarity, accurate model initial state estimates and accurate model structure are not significantly violated, ESP will provide a reliable probabilistic prediction of seasonal streamflow.

In any real application of ESP, the assumptions of perfect initial states and model simulations will be violated, necessitating a methodology to account for errors in the states and model, which is performed here with a combination of the PF and SBC (referred to here as PF-SBC). Application of PF-SBC to the ESP framework requires two steps, which are outlined in Figure 2. First, DA is performed in each model during the spin-up period to produce stochastic initial states at each initial forecast date ($x_{1:N,t}$), following the application by DeChant and

Moradkhani (2011b). This ensemble of land surface states represents the uncertainty at the initial forecast date, and a resulting distribution of streamflow forecasts from these states is shown in equation (9), where $p(x_{i,t} | y_{1:t})$ is the posterior distribution from the PF and the weights $w_{i,t}$ are uniform due to the application of SIR. This is the single model ESP-DA forecast.

$$p(\tilde{y}_t | x_{1:N,t}, u_{1:Y-1}, M, y_{1:t}) = \sum_{y=1}^{Y-1} \sum_{i=1}^N p(\tilde{y}_t | x_{i,t}, u_{y,t}, M) p(x_{i,t} | y_{1:t})$$

$$\approx \sum_{y=1}^{Y-1} \sum_{i=1}^N \delta(\tilde{y}_t - M(x_{i,t}, u_{y,t}, \theta, \alpha)) w_{y,t} w_{i,t}$$
(9)

A second step is performing the ESP-DA with all models, and then applying the weights to each ensemble member. In this step, each model and initial state ensemble member is propagated forward with the ESP framework, providing a multi-model ensemble forecast, creating $N * (Y - 1) * K$ streamflow traces. At this point, a stochastic multi-model forecast is available, represented by $p(\tilde{y}_t | x_{1:N,t}, u_{1:Y-1}, M_{1:K})$, but this does not account for the relative accuracy of each model, thus creating an overly uncertain forecast. In order to reduce this uncertainty, each model is averaged according to PF-SBC, based on weights estimated from the observations during the spin up period ($y_{1:t}$). The proposed methodology estimates the probability distribution of $\tilde{y}_t$ based on resampled historical forcing, stochastic states and multiple weighted models, as represented in equation (10). In the application presented here, both $w_{i,t}$ and $w_{y,t}$ are uniform, and therefore their product is equal to $1/(N * (Y - 1))$, making the weight of each trace estimated by equation (11). Although this study produces a weighted ensemble, a uniformly weighted ensemble forecast may be preferred in operational applications to be more consistent with the conventional ESP methodology. In order to overcome this issue, forecast ensemble members may be resampled, similar to the SIR, therefore producing an ensemble forecast with equally

weighted members. Note that this resampling of ensemble forecasts was not performed here, but such a discussion is provided to explain the potential use in an operational setting.

$$p(\tilde{y}_t | x_{1:N,t}, u_{1:Y-1}, M_{1:K}, y_{1:t}) = \sum_{y=1}^{Y-1} \sum_{i=1}^N \sum_{k=1}^K p(\tilde{y}_t | x_{i,t}, u_y, M_k) p(M_k | y_{1:t}) p(x_{i,t} | y_{1:t})$$

$$\approx \sum_{y=1}^{Y-1} \sum_{i=1}^N \sum_{k=1}^K \delta(\tilde{y}_t - M_k(x_{i,t}, u_{y,t}, \theta, \alpha)) w_{y,t} w_{i,t} w_{k,t}$$

$$w_{k,i,y,t} = w_{y,t} w_{i,t} w_{k,t} = \frac{1}{N * (Y-1)} p(M_k | y_{1:t})$$

3.3 Performance Metrics

The proposed forecasting framework is intended to improve the reliability of probabilistic seasonal streamflow forecasts, as currently available techniques are typically overconfident. In order to test the proposed methodology, this study requires the use of probabilistic verification methods that quantify the reliability. Many techniques are available for probabilistic verification, with the most commonly used methods in hydro-meteorological forecasting being the Brier Score (binary or categorical events) or the Continuous Rank Probability Score (continuous predictands), for quantitative assessment, and the Rank Histogram for visual assessment (Wilks, 2006; Jolliffe and Stephenson, 2003). Although the quantitative methods are commonly used, they are not necessarily prudent in this application. Since the focus here is solely on forecast reliability, and the Brier Score and Continuous Rank Probability Score both have aspects of reliability, resolution, uncertainty and sharpness (Murphy, 1973; Hersbach, 2000), other quantitative metrics are preferred.

The first quantitative measure is the Exceedance Ratio (ER) (Moradkhani et al., 2006; Moradkhani and Meskele, 2009). This measure can be applied to any predictive quantile range desired, but here it is used to analyze the tails of the distribution (99%, 95% and 90%).

Calculation of the ER of a given quantile range is performed according to equations (12), (13), and (14). In these equations, the cumulative probability of each observation, given its respective forecast, is represented by z_t . This vector z can then be analyzed at any predictive bound P desired, as shown in equation (13). Then the ER is estimated as the percentage of observations that fall outside this quantile range, which should be equal to $1 - P$. Since the ER is used to examine the tails of the distribution, a metric is also necessary to examine the whole probabilistic forecast. The reliability (R) is used here to examine the entire predictive distribution. This measure is based on the assumption that over a large enough sample of observations, the probabilities of those observations given their respective probabilistic forecast ($p(y_t | y'_{1:N,t})$) will be uniformly distributed, which indicates that each quantile contains the statistically correct portion of observations (e.g. 50% of the observations fall within the interquartile range). This is described in equations (12), (15), and (16). Similar to the ER, a vector z is calculated, but here they are sorted in ascending order, as noted in equation (15). The reliability can then be calculated according to equation (16), where the $\hat{z}$ are compared against the uniform cumulative density to determine the accuracy of the probabilistic forecast. A value of 1 equals a perfect forecast and a value of 0 is the mathematically worst forecast.

$$z_t = \sum_{k=1}^K \sum_{i=1}^N \sum_{y=1}^{Y-1} \chi_{k,i,y,t} \quad \chi_{k,i,y,t} = \begin{cases} w_{k,i,y,t} & y_t > \tilde{y}_{k,i,y,t} \\ 0 & y_t < \tilde{y}_{k,i,y,t} \end{cases} \quad (12)$$

$$\varepsilon'_t = \begin{cases} 1 & \text{if } z_t > 1 - \frac{1-P}{2} \text{ or } z_t < \frac{1-P}{2} \\ 0 & \text{otherwise} \end{cases} \quad (13)$$

$$ER = 100 \times \sum_{t=1}^T \frac{\varepsilon'_t}{T} \quad (14)$$

$$\hat{z} = \text{sort}(z_{1:t}) \quad (15)$$

$$R = 1 - 2 \sum_{t=1}^T \left| \hat{z}_t - \frac{t}{T} \right| \quad (16)$$

The predictive Quantile-Quantile (QQ) plot is used as a visual method to diagnose errors in the forecast distribution (DeChant and Moradkhani, 2011b). This diagram presents nearly identical information to the more commonly used Rank Histogram, but the predictive QQ plot is preferred here, as multiple forecasts may be evaluated on the same plot. This plot compares the $\hat{z}$ vector on the x-axis and the uniform distribution on the y-axis to examine the reliability of the forecast distribution. Given that the plot follows a 1:1 line, this forecast is perfectly reliable ($R=1$). If the predictive QQ line falls above the 1:1 line, the forecast has a high bias (observations have a tendency to fall too low in the forecast distribution) and a predictive QQ line falling below the 1:1 line indicates a low bias. In addition to bias, the over/underconfidence of a forecast distribution can be diagnosed with this plot. If the predictive QQ line falls above the left side of the 1:1 line and crosses the 1:1 line in the middle, the forecast is overconfident (a disproportionately high number of observations being captured by the outer quantiles) and the reverse indicates underconfidence. For a more complete explanation of this plot, see Laio and Tamea (2007).

3.4 Experiments

In this study, seasonal ensemble forecasts are examined from seven different modeling scenarios. The first two forecast experiments are the standard ESP method, referred to as “open loop”. The first open loop experiment is performed with the NWS models, and the second open loop experiment is performed with the VIC model. Each open loop experiment performs a spin up to an initial forecast date, and then 29 separate forcing years are resampled between 1981 and 2010 to represent climatology (the forecast year is excluded leaving only 29 of the 30 years

used). Four more experiments are performed with DA as a spin up. Each model (VIC and NWS) has a spin up with T_b only and T_b /LST DA. Each DA experiment uses 100 ensemble members, leading to 100 initial condition estimates at each forecast time step, from October 1st, 2002 through September 30th, 2008. Within the PF-SBC algorithm, all streamflow observations are utilized for model weighting, up to the initial forecast date, which makes the minimum length of training data 3 months, and is deemed reasonable based on the findings in Parrish et al., (2012). In the VIC model, it is infeasible to perform all 2900 combinations of initial condition ensemble members and historical forcing years due to computational constraints, and therefore 500 combinations were sampled uniformly from those 2900. Computational demand in the NWS models is significantly lower, and therefore all 2900 combinations are performed. The final experiment is a model averaging experiment of all 6 prior modeling scenarios. All traces are weighted according to the equations in section 3.2 and Figure 2, and the weighted ensemble is evaluated. Each forecasting experiment estimates 3 month volumetric flow from start dates on the 1st and 15th of January through June, in the years 2003 through 2008. This leads to a total of 72 seasonal forecasts from each modeling scenario.

4 Results

A first assessment of the results from this study is provided with the weights of each model in Figure 3. This figure shows the average model weights from each forecast month, as estimated through the PF-SBC algorithm. In general, the NWS models appear to have the highest weights, indicating a higher accuracy in monthly probabilistic streamflow volume estimation, and more reliable estimation of streamflow uncertainty, than the VIC model. However, the VIC model cases were assigned high enough weights to provide a significant contribution in the model averaging framework. In comparing the DA and open loop cases, both DA cases in the

NWS models received higher weight than the open loop model, yet the VIC model with DA received an overall lower weight than the open loop case. A general expectation is for the VIC model, which explicitly solves the energy balance, to be more effective in estimating inputs to the radiative transfer model and land surface temperature, yet the application here does not support this hypothesis. Although the results suggest VIC is less effective for T_b and LST DA than the NWS models, this is not a conclusion that should be drawn here due to the differing spatial discretization and calibration schemes. Another important note is the difference in performance of the two DA cases for each model. In the VIC model, the case of combined LST and T_b DA outperforms the T_b only DA case, but the NWS models perform best without the DA of LST. This is not surprising, as the VIC model explicitly solves for LST, whereas the SNOW-17 model only estimates average pack temperature, thus the VIC model should more accurately estimate LST. Figure 3 also highlights an important temporal aspect to the performance of these modeling cases. In the DA cases, weights tend to be highest during the snow accumulation season (January, February, and March) and have lower weights into the ablation season (May, June). The reverse is true for the open loop cases. This finding is not surprising, due to the poorer sensitivity of microwave T_b to SWE in deeper snowpacks with high liquid water content (DeChant and Moradkhani, 2011a). During the ablation season, the liquid water content in the snowpack remains high, reducing the ability of T_b DA to accurately construct SWE. Such temporal variation in DA performance necessitates the use of the PF-SBC methodology, as opposed to batch framework, to allow for dynamic weights, thus providing more accurate weights at each forecast initial condition.

During the forecast phase, the ability of each modeling case to reliably estimate seasonal runoff volumes is assessed. From a risk management perspective, it is important to examine the

accuracy of the tails of the forecast distributions, which may be used as maximum or minimum expected flows. In order to assess the tails of the forecast distributions, the 99%, 95% and 90% predictive bounds from each method are examined, with their respective ERs, in Figure 4. This figure suggests that every modeling scenario is overconfident at every predictive bound (each predictive bound is exceeded at a frequency higher than optimal). At the 99% predictive bound, each DA case reduces the overconfidence, highlighting the importance of initial condition uncertainty, and PF-SBC further reduces the ER to about 3%. This still remains slightly overconfident, yet is a significant improvement over the other modeling cases (the best ESP-DA case had 14.9% ER), thus highlighting the importance of accounting for model errors. At the 95% and 90% ERs, DA continues to improve overconfidence, with the exception of VIC with T_b only DA, and PF-SBC again performs best overall. These results suggest that across the entire basin, both ESP-DA and ESP-PF-SBC improve the reliability of the tails of the forecast distributions, but gives no assessment of the performance spatially. In order to examine the performance of the methods across several sub-basins, Figure 5 shows the 99% ER of 16 different sub-basins within the UCRB.

The accuracy of the 99% predictive bounds varies spatially throughout the UCRB. In the VIC open loop model, the San Juan is the only basin that has an ER of lower than 50% (optimal is 1%), which shows that the probabilistic forecasts does not convey the proper uncertainty for this model. In the DA cases, a reduction in the 99% ER is observed in every sub-basin outside of the Colorado River headwater region. In this region, DA appears to struggle in improving the accuracy of initial conditions, which is an observation that will be discussed further in relation to later results. The NWS models perform much more consistently throughout the UCRB, with ERs generally around 50%, and greater variability in the Rocky Mountains. In the DA cases, the ER

is reduced in all basins, suggesting generally more reliable forecasting of low probability events. DA in these models appears to be more consistently effective than in VIC, which is attributed to the differing spatial discretization, as mentioned in respect to model weights from Figure 3. Finally, PF-SBC further reduces the ER, from which values are consistently below 10%, with the exception of the Dolores River Basin (southwestern sub-basin of the Colorado River headwater region) at around 20%. Overall this shows that DA tends to improve probabilistic prediction, highlighting the importance of initial condition errors, and further improvements are made through PF-SBC, showing the importance of the model error component. Though the results here are encouraging, it is important to also look at the overall reliability of the forecast distributions to ensure that reliability of the entire forecast distribution is improved. This is performed with the R metric and is shown spatially in Figure 6.

In the VIC open loop case, reliability is low in the Green River Basin and in the Colorado Headwaters, with better performance in the San Juan and at Lee's Ferry, which suggests a more accurate reconstruction of initial states in the San Juan than the other sub-basins. In the two DA cases, reliability is improved in both the Green and San Juan basins, but the headwater basins performs worse, similar to the results of the 99% ER. Both DA cases improved the initial condition distribution in the Green and San Juan basins, yet struggled in the Colorado River headwaters. In contrast to the VIC model, the NWS models have less variation in reliability, and no identifiable pattern in performance. Also, the DA cases only show improvements in the San Juan River basin, with slightly worse performance in many other basins. This observation is unexpected in light of the improvements shown in figures 4 and 5. Such an observation suggests that this method is unable to improve the central portions of the predictive distribution. Despite an improvement in the tails for the forecast distributions from the DA cases, the mode of the

distribution is not shifted enough to observe general improvements in reliability. Results from the PF-SBC experiment show that the model averaging scenario is superior to all other cases in the majority of basins, though exceptions are present in the upper Green river basin and central Gunnison river basin (south-central portion of the Colorado River headwaters). The superior results from PF-SBC over the entire forecast distribution, in conjunction with unimproved reliability from DA, suggests that model errors are persistent in the central portion of the forecast distribution. While the initial condition errors were important in estimating the low probability events, it is essential to manage model error for accurate prediction of the mode of the forecast distribution.

The conflicting results regionally, and within different portions of the forecast distributions, requires further examination of the regional forecast distributions. The causes of conflicting information from previous results are diagnosed with the predictive QQ plot from each of the four gauges shown in Figure 1, which are provided in Figure 7. In the upper left plot of Figure 7, it appears that both the NWS models and the VIC model have significant biases, with the NWS models showing a generally high bias (observations primarily falling in the lower portions of the forecast distributions) and the VIC model having a generally low bias (observations primarily falling in the higher portions of the forecast distributions). In the NWS models, DA does not change the bias, though it does move the tails of the distribution to encompass more observations, but the VIC model has increasingly low bias with DA. These differing results highlight the effects of spatial resolution on T_b DA in regions of highly complex topography and thick vegetation. From Figure 1, it is apparent that the Colorado River headwaters is the most topographically rough sub-basin and has the densest forest cover of all regions, causing greater problems for DA in the VIC model. Since the NWS models are

distributed based on topography, the basins in this region are much smaller than in the VIC model, and thus the spatial heterogeneity is more effectively modeled. Conversely, in the Green River, the bias in the VIC model was reduced through DA, but again only little change was observed in the NWS bias in the DA case. In the San Juan, which has the lowest density of forest cover and driest climate, the bias in both models is reduced, showing the ability of T_b DA to reduce SWE errors in regions of thin vegetation and dry climates. With respect to the PF-SBC case, the forecasts in the headwaters have a high bias, generally following the NWS model forecasts, but in the Green and San Juan basins, PF-SBC provides a significant reduction in model bias. In basins where both models provide sufficiently accurate forecasts, PF-SBC is capable of effectively leveraging information from multiple model structures to improve forecasts, but the poor forecasts from VIC in the headwaters forces PF-SBC to rely primarily on the NWS modeling cases. Results at Lee's Ferry indicate the strong influence of the Colorado River headwaters in flow at the outlet (on average it provides 45% of the runoff at Lee's Ferry), which is unfortunate because forecasts for the headwaters are the least skillful, and show the least sensitivity to the remotely sensed observations. Overall it appears that the tails of the forecast distributions at Lee's Ferry are most accurate when using the ESP combined with PF-SBC, but this framework is unable to provide much improvement in the mode of the forecast distributions.

5 Discussion and Conclusion

This study examined a number of modeling scenarios in attempts of improve the characterization of errors in seasonal hydrologic forecasting. Based on the operational ESP framework, the VIC and NWS models were used to generate probabilistic seasonal streamflow forecasts. Each model had an open loop case, two DA cases (T_b only and T_b with LST DA), and

a model averaging case of all six prior scenarios was performed with PF-SBC. DA was implemented to account for initial condition uncertainty, and PF-SBC is used to account for uncertainty. Such an experiment is expected to improve the reliability of forecast distributions from ESP, as ESP tends to produce overconfident results.

A first comparison of the modeling scenarios was provided with the relative performance of each during the spin up period. During this time, the NWS models with T_b only DA provided the best overall probabilistic prediction, highlighting the effectiveness of the NWS forecasting system, and the sensitivity of passive microwave T_b to snowpack states. In addition, the relative accuracy of the models with and without DA over the course of the accumulation and ablation season highlights the temporal characteristics of T_b DA performance. In the accumulation season, DA is more effective as the snow tends to be drier, but the open loop models perform better in the ablation season as T_b becomes less sensitive to SWE. Relative model weights also suggest that VIC is more efficient in assimilating LST, which was expected as the VIC model explicitly solves for LST, whereas the SNOW-17 model only estimates average pack temperature.

Forecast reliability was shown to have a strong spatial component in figures 5 and 6. The VIC model produced forecasts with lower reliability than the NWS models, with the exception of the San Juan basin, over the UCRB. Both VIC DA cases were capable of improving the forecast reliability in the Green and San Juan basins, suggesting improvements in initial conditions, but produced worse forecasts in the Colorado River headwaters. While the VIC model performed worse with DA in the headwaters, the NWS models improved. This is counterintuitive as the VIC model is expected to more accurately reconstruct the land surface states, but this result is attributed to the coarser resolution of the VIC model, with respect to the NWS models in this

region. In addition, DA in the NWS models provided the least improvement in this region, in comparison to other regions, which highlights the difficulty of utilizing remotely sensed information to reconstruct land surface states in regions of thick forest cover. This is unfortunate as forest thickness is generally correlated with precipitation quantity, and thus more important from a water supply perspective. Since the most densely forested region in a basin will tend to be the most important from a water supply perspective, it is imperative that the accuracy of land surface state estimation and observation, and therefore the combination of both through DA, be improved in these regions, which is a great challenge for land surface hydrologist.

A final conclusion from this paper relates to the performance of different portions of the forecast distributions. In general, the improvements were stronger in the tails of the distributions than in the central portions, with the exception of the PF-SBC case in the Green and San Juan basins. Since DA improved the tails of the distribution in nearly all basins/cases, yet did not consistently improve total reliability, initial condition uncertainty is shown to have stronger control over the reliability of predicting low probability events. Alternatively, PF-SBC improved the overall reliability in nearly all basins, suggesting that model error strongly controls uncertainty in the forecast distribution mode. Overall, this highlights that both initial condition and model error are important factors in seasonal prediction.

The presented methodology shows promise for improving the reliability of seasonal forecasting, by accounting for all sources of forecast uncertainty, but the results from the application here clearly show room for improvement. It is suggested that these improvements will come from advancements in land surface DA and improved multi-modeling to more effectively manage forecast uncertainty. By developing more effective DA systems, the proposed framework will have more accurate and reliable prediction of initial land surface conditions,

which were shown to have significant contribution to probabilistic streamflow forecasting. In addition, the inclusion of a greater variety of model structures will more effectively manage model error, thus leading to more reliable forecast uncertainty quantification. Beyond simply adding more models, the methodology may also benefit from more complex weighting schemes, which focuses on different flow regimes (Georgakakos et al. 2004, Parrish et al., 2012) and different forecast training window lengths (Parrish et al., 2012). A further advancement in quantifying forecast uncertainty may also come from the use of state-parameter estimation within the DA framework (DeChant and Moradkhani, 2012), which is becoming increasingly effective and efficient (Moradkhani et al., 2012), and therefore more applicable to the spatial extents considered here.

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- 815

Upper Colorado River Basin

Western USA

Legend

Headwaters

Green

San Juan

Lee's Ferry

Rivers

Vegetation Type

Open Shrubland

Dense Forest

Streamflow Gauges

0 125 250 500 750 km

Figure 1. Map of the upper Colorado River Basin, with major sub-basins highlighted, and vegetation density overlying shaded relief.

Figure 2. Flowchart describing the application of the PF-SBC algorithm to streamflow forecasting with ESP.

Figure 3. 3-dimensional bar plot of the average weights for each modeling scenario and forecast month, as estimated during the spin-up period.

Figure 4. Histogram of the 99%, 95% and 90% exceedance ratios of each modeling scenario, for all seasonal forecasting experiments. The optimal exceedance ratio is on the far right of this figure.

Figure 5. 99% exceedance ratio over 16 sub-basins within the upper Colorado River Basin, for all volumetric streamflow forecasts.

Figure 6. Reliability over 16 sub-basins within the upper Colorado River Basin, for all volumetric streamflow forecasts.

Figure 7. Predictive QQ plot of the volumetric seasonal forecasts from the four major sub-basins of the upper Colorado River Basin.

Highlights

- Data Assimilation and Sequential Bayesian Combination reduces overconfidence in ESP
- Initial condition uncertainties have strongest effects on the tails of the forecast distribution
- Model structural errors have strongest effect on the medial portions of the forecast distribution
- Data Assimilation appears to be necessary to maximize the reliability of seasonal forecasts