IMPROVING THE PREDICTABILITY OF HYDROLOGIC INDICES IN ECOHYDROLOGICAL APPLICATIONS

By

Juan Sebastian Hernandez Suarez

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ABSTRACT

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Monitoring freshwater ecosystems allow us to better understand their overall ecohydrological condition within large and diverse watersheds. Due to the significant costs associated with biological monitoring, hydrological modeling is widely used to calculate ecologically relevant hydrologic indices (ERHIs) for stream health characterization in locations with lacking data. However, the reliability and applicability of these models within ecohydrological frameworks are major concerns. Particularly, hydrologic modeling's ability to predict ERHIs is limited, especially when calibrating models by optimizing a single objective function or selecting a single optimal solution. The goal of this research was to develop model calibration strategies based on multi-objective optimization and Bayesian parameter estimation to improve the predictability of ERHIs and the overall representation of the streamflow regime. The research objectives were to (1) evaluate the predictions of ERHIs using different calibration techniques based on widely used performance metrics, (2) develop performance and signature-based calibration strategies explicitly constraining or targeting ERHIs, and (3) quantify the modeling uncertainty of ERHIs using the results from multi-objective model calibration and Bayesian inference. The developed strategies were tested in an agriculture-dominated watershed in Michigan, US, using the Unified Non-dominated Sorting Algorithm III (U-NSGA-III) for multi-objective calibration and the Soil and Water Assessment Tool (SWAT) for hydrological modeling. Performance-based calibration used objective functions based on metrics calculated on streamflow time series, whereas signature-based calibration used ERHIs values for objective

functions’ formulation. For uncertainty quantification purposes, a lumped error model accounting for heteroscedasticity and autocorrelation was considered and the multiple-try Differential Evolution Adaptive Metropolis (ZS) (MT-DREAM$_{(ZS)}$) algorithm was implemented for Markov Chain Monte Carlo (MCMC) sampling. In relation to the first objective, the results showed that using different sets of solutions instead of a single optimal introduces more flexibility in the predictability of various ERHIs. Regarding the second objective, both performance-based and signature-based model calibration strategies were successful in representing most of the selected ERHIs within a ±30% relative error acceptability threshold while yielding consistent runoff predictions. The performance-based strategy was preferred since it showed a lower dispersion of near-optimal Pareto solutions when representing the selected indices and other hydrologic signatures based on water balance and Flow Duration Curve characteristics. Finally, regarding the third objective, using near-optimal Pareto parameter distributions as prior knowledge in Bayesian calibration generally reduced both the bias and variability ranges in ERHIs prediction. In addition, there was no significant loss in the reliability of streamflow predictions when targeting ERHIs, while improving precision and reducing the bias. Moreover, parametric uncertainty drastically shrank when linking multi-objective calibration and Bayesian parameter estimation. Still, the representation of low flow magnitude and timing, rate of change, and duration and frequency of extreme flows were limited. These limitations, expressed in terms of bias and interannual variability, were mainly attributed to the hydrological model’s structural inadequacies. Therefore, future research should involve revising hydrological models to better describe the ecohydrological characteristics of riverine systems.

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KEY TO ABBREVIATIONS

ABC: Approximate Bayesian Computation

AIC: Akaike Information Criterion

ALPHA_BF: Baseflow alpha factor ($days^{-1}$)

ANCOVA: Analysis of Covariance

ANFIS: Adaptive Neuro-Fuzzy Inference Systems

ANN: Artificial Neural Network

AR (1): Autoregressive Model with Lag 1

AUC: Area Under Receiver Operating Characteristic Curve

BBN: Bayesian Belief Networks

BIC: Bayesian Information Criterion

BIOMIX: Biological mixing efficiency

BRT: Boosted Regression Trees

CA: Correspondence Analysis

CANMX: Maximum canopy storage (mm H_2O)

CAR (1): Continuous Autoregressive Model with Lag 1

CART: Classification and Regression Trees

CCA: Canonical Correspondence Analysis

CDF: Cumulative distribution function

CH_K (2): Effective hydraulic conductivity in main channel alluvium (mm hr^{-1})

CH_N (2): Manning's "n" value for the main channel

CN2: Curve Number for moisture condition II

COIN: Computational Optimization and Innovation Laboratory at Michigan State University

d: Index of Agreement

DCA: Detrended Correspondence Analysis

DCCA: Detrended Canonical Correspondence Analysis

DH: High flows duration indices

DH1: Annual maximum daily flow (m^3 s^{-1})

DH2: Annual maximum of 3-day moving average flow (m^3 s^{-1})

DH3: Annual maxima of 7-day means of daily discharge (m^3 s^{-1})

DH4: Annual maxima of 30-day means of daily discharge (m^3 s^{-1})

DH5: Annual maxima of 90-day means of daily discharge (m^3 s^{-1})

DH6: Variability of annual maximum daily average flow

DH7: Variability of annual maximum of 3-day moving average flow

DH8: Variability of annual maximum of 7-day moving average flow

DH9: Variability of annual maximum of 30-day moving average flow

DH10: Variability of annual maximum of 90-day moving average flow

DH15: High flow pulse duration with a threshold equal to the 75th percentile of the entire flow record (days)

DH16: Variability in high flow pulse duration with a threshold equal to the 75th percentile of the entire flow record

DH17: High flow duration with a threshold equal to the median flow (days)

DH19: High flow duration with a threshold equal to 7 times the median flow (days)

DH20: High flow duration with a threshold equal to the 75th percentile value for the median annual flows (days)

DH21: High flow duration with a threshold equal to the 25th percentile value for the median annual flows (days)

DH23: Flood duration with a threshold equal to the flow equivalent for a flood recurrence of 1.67 years (days)

DL: Low flows duration indices

DL1: Annual minimum daily flow (m^3 s^{-1})

DL2: Annual minimum of 3-day moving average flow (m^3 s^{-1})

DL3: Annual minima of 7-day means of daily discharge (m^3 s^{-1})

DL4: Annual minima of 30-day means of daily discharge (m^3 s^{-1})

DL5: Annual minima of 90-day means of daily discharge (m^3 s^{-1})

DL6: Variability of annual minimum daily average flow

DL7: Variability of annual minimum of 3-day moving average flow

DL8: Variability of annual minimum of 7-day moving average flow

DL9: Variability of annual minimum of 30-day moving average flow

DL10: Variability of annual minimum of 90-day moving average flow

DL11: Mean of 1-day minima of daily discharge

DL12: Mean of 3-day minima of daily discharge

DL16: Low flow pulse duration (days)

DREAM: Differential Evolution Adaptive Metropolis

EPCO: Plant uptake compensation factor

ERHI: Ecologically Relevant Hydrologic Index

ESCO: Soil evaporation compensation factor

FDC: Flow Duration Curve

FH: High flows frequency indices

FH1: High flood pulse count with a threshold equal to the 25th percentile of the entire flow record ($year^{-1}$)

FH2: Variability in high flood pulse count with a threshold equal to the 25th percentile of the entire flow record

FH4: High flood pulse count with a threshold equal to 7 times median daily flow ($year^{-1}$)

FH5: Flood frequency with a threshold equal to the median flow ($year^{-1}$)

FH8: Flood frequency with a threshold equal to the 25th percentile of the entire flow record ($year^{-1}$)

FH9: Flood frequency with a threshold equal to the 75th percentile of the entire flow record ($year^{-1}$)

FHV: FDC very-high-segment volume

FL: Low flows frequency indices

FL1: Low flood pulse count ($year^{-1}$)

FL2: Variability in low flood pulse count

FLV: FDC low-segment volume

FMS: FDC midsegment slope

FMV: FDC high-segment volume

GA: Genetic Algorithm

GAM: Generalized Additive Model

GARP: Genetic Algorithm for Rule set Production

GLM: Generalized Linear Model

GLS: Generalized Least-Squares

GRNN: Generalized Regression Neural Network

GW_DELAY: Groundwater delay time (days)

GW_REVAP: Groundwater "revap" coefficient

GWQMN: Threshold depth of water in the shallow aquifer required for return flow to occur (mm H_2O)

HIT: Hydrologic Index Tool

HRU: Hydrologic Response Unit

I-IBI: Macroinvertebrate Index of Biotic Integrity

IBI: Fish Index of Biotic Integrity

ICI: Invertebrate Community Index

IHA: Indices of Hydrologic Alteration

IoA: Index of Agreement

IQR: Interquartile Range

KGE: Kling-Gupta Efficiency

MA: Average flows magnitude indices

MA12: Mean monthly flow for January (m^3 s^{-1})

MA13: Mean monthly flow for February (m^3 s^{-1})

MA14: Mean monthly flow for March (m^3 s^{-1})

MA15: Mean monthly flow for April (m^3 s^{-1})

MA16: Mean monthly flow for May (m^3 s^{-1})

MA17: Mean monthly flow for June (m^3 s^{-1})

MA18: Mean monthly flow for July (m^3 s^{-1})

MA19: Mean monthly flow for August (m^3 s^{-1})

MA20: Mean monthly flow for September (m^3 s^{-1})

MA21: Mean monthly flow for October (m^3 s^{-1})

MA22: Mean monthly flow for November (m^3 s^{-1})

MA23: Mean monthly flow for December (m^3 s^{-1})

MA24: Variability in January flows

MA25: Variability in February flows

MA26: Variability in March flows

MA27: Variability in April flows

MA28: Variability in May flows

MA29: Variability in June flows

MA30: Variability in July flows

MA31: Variability in August flows

MA32: Variability in September flows

MA33: Variability in October flows

MA34: Variability in November flows

MA35: Variability in December flows

MA42: Variability across annual flows

MA44: Variability across annual flows

MA45: Skewness in annual flows

MAG: Magnificent Seven indices

MAG1: First L-moment

MAG2: Second L-moment

MAG3: Third L-moment

MAG4: Fourth L-moment

MAG5: Autoregressive lag-one AR(1) correlation coefficient

MAG6: Amplitude of the seasonal signal

MAG7: Phase of the seasonal signal

MARS: Multivariate Adaptive Regression Splines

MCDM: Multicriteria Decision-Making

MCMC: Markov Chain Monte Carlo

MH: High flows magnitude indices

MH10: Mean maximum October monthly flow ($m^3 s^{-1}$)

MH11: Mean maximum November monthly flow ($m^3 s^{-1}$)

MH21: High flow volume (days)

MH22: High flow volume (days)

MH23: High flow volume (days)

MH6: Mean maximum June monthly flow ($m^3 s^{-1}$)

MH7: Mean maximum July monthly flow ($m^3 s^{-1}$)

MHIT: MATLAB Hydrologic Index Tool

ML: Low flows magnitude indices

ML7: Mean minimum July monthly flow ($m^3 s^{-1}$)

ML8: Mean minimum August monthly flow ($m^3 s^{-1}$)

ML9: Mean minimum September monthly flow ($m^3 s^{-1}$)

ML14: Mean of annual minimum flows

ML15: Low flow index

ML16: Median of annual minimum flows

ML17: Baseflow index based on the seven-day minimum flow

ML18: Baseflow index based on the seven-day minimum flow

ML19: Variability of baseflow index based on the lowest annual daily flow

ML21: Variability across annual minimum flows

ML22: Specific mean annual minimum flows ($m^3 s^{-1} km^{-2}$)

MLP: Multilayer Perceptron

MLR: Multiple Linear Regression

MOEA: Multi-objective evolutionary algorithm

MT-DREAM$_{(ZS)}$: Multiple-try Differential Evolution Adaptive Metropolis (ZS)

NASS: National Agricultural Statistics Service

NCDC: National Climatic Data Center

NCEI: National Centers for Environmental Information

NED: National Elevation Dataset

NMDS: Nonmetric Multidimensional Scaling

NOAA: National Oceanic and Atmospheric Administration

NRCS: Natural Resources Conservation Service

NSE: Nash-Sutcliffe Efficiency

NSE$_{rel}$: Relative NSE

NSE_{sqrt}: Root-squared-transformed NSE

NSGA-II: Non-dominated Sorting Genetic Algorithm II

NSGA-III: Nondominated Sorted Genetic Algorithm III

OF: Objective function

PBIAS: Percent Bias

PCA: Principal Component Analysis

PCoA: Principal Coordinates Analysis

PLSR: Partial Least Squares Regression

PO: Polar Ordination

PQQ: Predictive quantile-quantile plot

Q25: flow exceeded 25% of the time

Q75: flow exceeded 75% of the time

r: Correlation coefficient

R^2: Coefficient of Determination

R4MS4E: Fourth Root Mean Quadrupled Error

RA: Rate of change indices

RA1: Rise rate (m^3 s^{-1} d^{-1})

RA2: Rise rate variability

RA3: Fall rate (m^3 s^{-1} d^{-1})

RA4: Fall rate variability

RA6: Change of flow- increasing (m^3 s^{-1})

RA7: Change of flow - decreasing (m^3 s^{-1})

RA8: Reversals ($year^{-1}$)

RA9: Reversals variability

RCHRG_DP: Deep aquifer percolation fraction

RDA: Redundancy Analysis

REVAPMN: Threshold depth of water in the shallow aquifer for "revap" or percolation to the deep aquifer to occur (mm H_2O)

RF: Random Forests

RIVPACS: River Invertebrate Prediction and Classification System

RMSE: Root Mean Squared Error

RR: Runoff Ratio

SBX: Simulated Binary Crossover

SCS: Soil Conservation Service

SDM: Species Distribution Model

SEM: Structural Equation Modeling

SOL_AWC: Available water capacity of the soil layer (mm H_2O mm^{-1} soil)

SSURGO: Soil Survey Geographic Database

SURLAG: Surface runoff lag coefficient

SVM: Support Vector Machine

SWAT: Soil and Water Assessment Tool

TA: Average flows timing indices

TH: High flows timing indices

TH1: Julian date of annual maximum

TH2: Julian date of annual maximum variability

TL: Low flows timing indices

TL1: Julian date of annual minimum

TL2: Julian date of annual minimum variability

TL4: Seasonal predictability of non-low flow

U-NSGA-III: Unified Non-dominated Sorting Algorithm III

US: United States

USDA: US Department of Agriculture

USEPA: US Environmental Protection Agency

USGS: US Geological Survey

WFG: Walking Fish Group

WWAP-UN: United Nations World Water Assessment Programme

WXGEN: SWAT Stochastic Weather Generator

1 INTRODUCTION

One of the major concerns in the twenty-first century is the increasing pressure on water resources worldwide. Nearly 80% of the global population are exposed to high levels of threat to water security (Vörösmarty et al., 2010). In addition, freshwater ecosystems are deeply fragmented by built infrastructure, with only 23% of rivers longer than 1000 km arriving uninterrupted to the ocean (Grill et al., 2019). Unfortunately, this crisis is not only limited to water quantity but also is expanded to water quality. According to the United Nations World Water Assessment Programme (WWAP-UN), over 80% of global wastewater is discharged to waterbodies without any treatment (WWAP-UN, 2017). Moreover, most agriculture and urban runoff are delivered to freshwater and marine ecosystems without any water quantity and quality control (Eckart et al., 2017; Mateo-Sagasta et al., 2018). Summed to climate change, all these factors have increased the occurrence of waterborne disease. In addition, the resulting biodiversity and ecosystem losses imperil valuable ecosystem services necessary to sustain human societies (Hipsey et al., 2015; Pham et al., 2019).

In the United States, the Clean Water Act was enacted in 1972 to restore and maintain US waters' chemical, physical, and biological integrity. In river systems, chemical integrity can be associated with instream water quality. Meanwhile, physical integrity can be described in terms of water quantity, physical habitat, and stream's geomorphology. Likewise, biological integrity is expressed in terms of abundance, composition, and diversity of freshwater organisms. Since these three components support biotic systems necessary for human and environment well-being, the paradigm comprising these concepts is known as stream or river health (Karr, 1999; Maddock, 1999). Stream health is generally measured using bioassessments, which have gained popularity for supporting water quality management, complementing chemical and microbiological criteria (US EPA, 2011). Particularly, fish and benthic macroinvertebrates are commonly used as biological indicators. Fish are suitable for monitoring broad habitat conditions, streams connectivity, and long-term effects, whereas benthic macroinvertebrates are preferred when assessing local conditions and short-term effects (Herman and Nejadhashemi, 2015).

Stream health monitoring is usually done sparsely in time and space (Einheuser et al., 2012). Knowing the stream health condition of every single stream within a watershed is desirable for environmental management and policymaking. However, extensive biological monitoring is costly, time-consuming, and impractical for large areas. Therefore, modeling techniques have been developed to extend available information to locations with lacking biological data (Woznicki et al., 2016a). Stream health models generally use landscape attributes (e.g., land use/cover, slope, soils, geology) and instream physical and chemical characteristics (e.g., temperature, streamflow, nutrients, sediments, substrate) as explanatory variables to predict instream biological responses (Einheuser et al., 2012; Sowa et al., 2016). Streamflow is considered a master variable that dictates patterns and processes occurring in rivers and streams, including water quality, physical habitat formation, and life cycles of living organisms (Walker et al., 1995). Therefore, by studying the streamflow behavior over time (i.e., streamflow regime), it is possible to approximate the overall stream health condition (Poff et al., 1997; Richter et al., 2003).

The streamflow regime is generally described using metrics or indices related to five major facets: magnitude, duration, frequency, timing, and rate of change of flows (Sofi et al., 2020). *Magnitude* refers to the volume of water passing through a fixed location per unit of time. Based on this facet, streamflow can be classified as high, average, or low flow. Streamflow plays different roles depending on its magnitude (Sofi et al., 2020); for instance, low flows maintain instream water quality conditions, define the longitudinal stream connectivity, enable fish and nutrients to move, and allow natural selection by purging invasive species (Poff et al., 1997). Meanwhile, high flows give shape to streams, flush away pollutants, and maintain lateral connectivity, favoring floodplains, wetlands, and riparian vegetation (Poff et al., 1997). *Duration* is the length of time associated with a flow event being read horizontally in a hydrograph. This facet influences the persistence of aquatic and riparian species and controls fish growth potential and development under flooding events (Bunn and Arthington, 2002). *Frequency* refers to how often a streamflow magnitude occurs over a specific period of time, and it is generally described using Flow Duration Curves (FDC). This facet is important for controlling aquatic and riparian species' life cycles and productivity (Bunn and Arthington, 2002). For example, frequency regulates how often fish can move upstream or to floodplains for migration or reproduction (Poff et al., 1997). *Timing* is the degree to which flow events are temporally autocorrelated, indicating that the system has memory. For instance, certain rivers always experience high flows in spring and low flows in summer. This facet works as a trigger the system needs to start a process (e.g., fish spawning). Additionally, timing helps to maintain species diversity (Bunn and Arthington, 2002). Finally, the *rate of change* describes how fast the system goes up and down. This facet influences species persistence and coexistence and controls the establishment of nonnative species (Poff et al., 1997; Sofi et al., 2020). In summary, there are many indices describing the aforementioned streamflow regime facets (Olden and Poff, 2003), and they are known as ecologically relevant hydrologic indices (ERHIs).

Calibrated hydrological models are used to predict streamflows beyond monitoring stations. Consequently, ERHIs can be estimated in ungauged locations using results obtained