# Global runoff partitioning based on Budyko-constrained machine learning

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May 25, 2023

#### Abstract

Understanding the partitioning of runoff into baseflow and quickflow is crucial for informed decision-making in water resources management, guiding the implementation of flood mitigation strategies, and supporting the development of drought resilience measures. Methods that combine the physically-based Budyko framework with machine learning (ML) have shown promise in estimating global runoff. However, such 'hybrid' approaches have not been used for baseflow estimation. Here, we develop a Budyko-constrained ML approach for baseflow estimation by incorporating the Budyko-based baseflow coefficient (BFC) curve as a physical constraint. We estimate the parameters of the original Budyko curve and the newly developed BFC curve based on 13 climatic and physiographic characteristics using boosted regression trees (BRT). BRT models are trained and tested in 1226 catchments worldwide and subsequently applied to the entire global land surface at a 0.25° grid scale. The catchment-trained models exhibit strong performance during the testing phase, with R2 values of 0.96 and 0.88 for runoff and baseflow, respectively. Results reveal that, on average, 30.3% (spatial standard deviation std=26.5%) of the continental precipitation is partitioned into runoff, of which 20.6% (std=22.1%) is baseflow and 9.7% (std=10.3%) is quickflow. Among the 13 climatic and physiographic characteristics, topography and soil-related characteristics generally emerge as the most important drivers, although significant regional variability is observed. Comparisons with previous datasets suggest that global runoff partitioning is still highly uncertain and warrants further research.

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12									
13									
14	Highlights:								
15	1. A Budyko-constrained machine learning approach is developed for								
16	estimating long-term mean runoff and baseflow.								
17	2. The hybrid approach performs well in terms of both the runoff coefficient								
18	$(R^2=0.93)$ and the baseflow coefficient $(R^2=0.84)$ .								
19	3. Globally, 30% of the precipitation is partitioned into runoff, with baseflow								
20	contribution estimated to be twice the quickflow (20.6% vs. 9.7%).								
21	4. Primary drivers of runoff partitioning vary in space with topography and soil								
22	properties as dominant factors.								
23									

24 Abstract: Understanding the partitioning of runoff into baseflow and quickflow 25 is crucial for informed decision-making in water resources management, guiding the 26 implementation of flood mitigation strategies, and supporting the development of 27 drought resilience measures. Methods that combine the physically-based Budyko 28 framework with machine learning (ML) have shown promise in estimating global 29 runoff. However, such 'hybrid' approaches have not been used for baseflow estimation. 30 Here, we develop a Budyko-constrained ML approach for baseflow estimation by 31 incorporating the Budyko-based baseflow coefficient (BFC) curve as a physical 32 constraint. We estimate the parameters of the original Budyko curve and the newly 33 developed BFC curve based on 13 climatic and physiographic characteristics using 34 boosted regression trees (BRT). BRT models are trained and tested in 1226 35 catchments worldwide and subsequently applied to the entire global land surface at a 36 0.25° grid scale. The catchment-trained models exhibit strong performance during the testing phase, with  $R^2$  values of 0.96 and 0.88 for runoff and baseflow, respectively. 37 38 Results reveal that, on average, 30.3% (spatial standard deviation std=26.5%) of the 39 continental precipitation is partitioned into runoff, of which 20.6% (std=22.1%) is 40 baseflow and 9.7% (std=10.3%) is quickflow. Among the 13 climatic and 41 physiographic characteristics, topography and soil-related characteristics generally 42 emerge as the most important drivers, although significant regional variability is 43 observed. Comparisons with previous datasets suggest that global runoff partitioning 44 is still highly uncertain and warrants further research.

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46 Keywords: runoff partitioning, baseflow, quickflow, Budyko, machine learning

47

#### 48 1 Introduction

49 Accurate partitioning of runoff (O) into its main components – baseflow ( $O_b$ ) and 50 quickflow  $(Q_q)$  – is crucial for water management and emergency planning during 51 droughts (Apurv & Cai, 2020) and floods (Roxy et al., 2017). Baseflow, sometimes 52 referred to as 'slow flow', provides most of the water for sustaining river flows during 53 dry periods (Miller et al., 2016). It originates from groundwater and other delayed 54 sources, such as wetlands, lakes, melting of snow and ice (Hall, 1968). Quickflow is 55 directly responsible for flood generation (Yin et al., 2018), and is a result of fast 56 processes such as saturation or infiltration of excess overland flow and fast subsurface 57 flow, i.e., processes where precipitation is not retained in the soil (Beven & Kirkby, 58 1979). Process-based models play an important role in accurately estimating global 59 runoff, quickflow and baseflow; this includes among others land surface models 60 (LSMs) and global hydrological models (GHMs). Nonetheless, LSMs and GHMs 61 struggle with runoff partitioning resulting in poor performances in terms of baseflow 62 index (BFI= $Q_b/Q$ ) – see e.g. Beck et al. (2017).

63 To complement process-oriented models, data-driven machine learning (ML) 64 techniques have been developed to assess runoff partitioning regionally and globally 65 without the biases induced by process-based models. For instance, Huang et al. (2021) 66 adopted a random forest model (RF) and multiple linear regression approach to 67 estimate the baseflow index (BFI =  $Q_b/Q$ ) in the United States. Beck et al. (2013, 2015) achieved satisfactory performance for BFI estimation globally (R<sup>2</sup>=0.65) and 68 69 provided global BFI datasets by using neural networks to relate BFI to 70 climatic/physiographic characteristics. ML has the potential to build effective 71 relationships between inputs and outputs, even if underlying physical processes are 72 unknown. That is why ML has been growing in popularity in hydrological sciences 73 beyond runoff (Xie et al., 2021), being used to predict evaporation (Jung et al., 2010) 74 and precipitation (Sadeghi et al., 2019; Beck et al., 2010) as well. Despite the strength of pure ML models, the major limitation is their "black box" nature, and hence their 75 76 lack of physical constraints and limited interpretability. The combination of 77 physically-based models and ML methods, i.e., 'hybrid' approaches, can retain both of 78 their individual strengths (de Bézenac et al., 2019; Koppa et al., 2022; Kraft et al., 79 2022; Zhao et al., 2019). Hence, these physically-constrained ML methods can 80 potentially improve the realism of the runoff partitioning estimates globally.

81 Previous studies have illustrated the advantage of the Budyko (1961) framework 82 as a physical constraint for pure ML to estimate runoff (Bai et al., 2020; Liu & You, 83 2021), while no such attempt has been made for baseflow estimation yet. Recently, 84 the Budyko framework was expanded by Cheng et al. (2021) to partition baseflow 85 from precipitation with the Budyko-based baseflow coefficient (BFC) curve. This 86 enables the Budyko framework to provide consistent physical constraints for both 87 runoff and baseflow estimation. Both the Budyko and BFC curves depend on the 88 aridity index and use lumped parameters (parameter  $\alpha$  in Fu's equation and  $Q_{b,p}$  in the 89 BFC curve, see Section 2.1) to incorporate climatic and physiographic properties such 90 as vegetation, soil, topography, and human activities (Mianabadi et al., 2020; Potter et 91 al., 2005; Tang & Wang, 2017; Zhang et al., 2001). Zhang et al. (2001) revealed the 92 impact of vegetation change on long-term evaporation and suggested  $\alpha$  equal to 0.5 93 and 2.0 for herbaceous plants and trees, respectively. Besides vegetation, Liu et al. 94 (2018) indicated that climate seasonality also plays an important role on the Budyko 95 parameter  $\alpha$ . More complex relationships have also been proposed for small 96 catchments (Bai et al., 2020). These different relationships between  $\alpha$  and catchment 97 properties indicate that a detailed understanding of the Budyko parameter is yet to be 98 achieved (Padrón et al., 2017). ML models have the strength to achieve better 99 regionalization of the parameters within the Budyko and BFC curves.

100 In this study, we design a framework for the long-term partitioning of global 101 runoff by adopting the Budyko and Budyko-based BFC curves as physical constraints 102 for ML models. The hybrid Budyko-ML approach makes full use of the available 103 data, and enables physical consistency by obeying the Budyko limits of water and 104 energy conservation. The primary objectives are to (1) develop Budyko constrained 105 ML models to estimate individual runoff components globally, (2) assess the accuracy 106 of the different estimated components, (3) analyse their spatial patterns, and (4) 107 identify and quantify the primary drivers of runoff partitioning. The derived dataset 108 includes gridded total runoff (Q), baseflow ( $Q_b$ ), quickflow ( $Q_q$ ), runoff coefficient 109 (RFC=Q/P), baseflow coefficient (BFC= $Q_b/P$ ), and quickflow coefficient 110 (QFC=RFC-BFC) at 0.25° resolution. The structure of the paper is as follows: 111 Section 2 describes the data development process, Section 3 describes the input 112 datasets, and Sections 4 and 5 present the results and discussions, respectively.

#### 113 2 Methods

#### 114 2.1 Budyko curve for runoff estimation

The Budyko framework is a first order approach that partitions long-term mean precipitation into runoff and actual evaporation (Budyko, 1961). According to this framework, both fluxes are limited by the water supply (typically precipitation, P) and the energy demand on evaporation (typically potential evaporation,  $E_p$ ). This framework assumes that long-term soil water storage changes are negligible. Hence, the water balance can be written as:

$$121 P = E_a + Q (1)$$

122 where *P* is precipitation, *Q* is runoff and  $E_a$  is actual evaporation.

As the original Budyko (1961) equation does not consider climatic and physiographic properties, several studies proposed alternative equations that introduce a single parameter to incorporate these properties (Choudhury, 1999; Yang et al., 2007; Zhang et al., 2001). The formulation proposed by Fu (1981) and Zhang et al. (2004) is adopted in this study:

128 
$$\frac{E_a}{P} = 1 + \frac{E_p}{P} - \left[1 + \left(\frac{E_p}{P}\right)^a\right]^{\frac{1}{a}}$$
(2)

By combining Eq.1 and Eq.2, the equation for *Q* estimation can be written as:

130 
$$\frac{Q}{P} = 1 - \frac{E_a}{P} = -\frac{E_p}{P} + \left[1 + \left(\frac{E_p}{P}\right)^a\right]^{\frac{1}{a}}$$
(3)

where  $\alpha$  is a parameter reflecting the secondary controls such as climate variability, vegetation, soil and topography, and can range from 1 to  $\infty$  (Zhang et al., 2004). High  $\alpha$  values result in low runoff and high actual evaporation for specific precipitation and potential evaporation values (Figure 1a). Figures in this study visualise  $P/E_p$  instead of  $E_p/P$  to put more focus on humid regions with larger variability of Q/P.

#### 136 **2.2 BFC curve for baseflow estimation**

137 The BFC curve was developed by Cheng et al. (2021) to estimate long-term 138 mean baseflow ( $Q_b$ ) based on the Budyko framework with suitable modifications (see 139 supplementary material). The BFC equation (Eq. 4) indicates that the baseflow not 140 only depends on P and potential evaporation  $E_p$ , but also on the potential baseflow 141  $(Q_{b,p})$ . This latter parameter is newly introduced in this study and indicates the 142 amount of baseflow that would occur if sufficient water were available. Hence, it is an 143 upper limit for the baseflow, analogous to the concept of  $E_p$  for the case of 144 evaporation. See the supplementary material for the derivation of the equation, which 145 is slightly modified compared to Cheng et al. (2021). The final equation of the BFC 146 curve is as follows:

147 
$$\frac{Q_b}{p} = \frac{Q_{b,p}}{p} + \left[1 + \left(\frac{E_p}{p}\right)^{\alpha}\right]^{\frac{1}{\alpha}} - \left[1 + \left(\frac{E_p}{p} + \frac{Q_{b,p}}{p}\right)^{\alpha}\right]^{\frac{1}{\alpha}}$$
(4)

148 where  $\alpha$  is a parameter (identical to the one in Eq. 3).  $Q_b/P$  increases with increasing 149  $P/E_p$  and  $Q_{b,p}/P$ . High  $Q_{b,p}$  values result in high baseflow and low quickflow for 150 specific precipitation and potential evaporation values (Figure 1b).



151

152 Figure 1. Visualization of the physical constraints for (a) runoff, Budyko curve (Eq. 3), and153 (b) baseflow, BFC curve (Eq. 4).

154 2.3 Calibration of parameters

The Budyko and BFC curves include the following two parameters:  $\alpha$  and  $Q_{b,p}$ . The latter is also parameterized, since its value cannot be determined with any available dataset. For individual catchments, the parameter  $\alpha$  is calibrated first by using the Budyko curve (Eq. 3) and observed long-term mean Q, P, and  $E_p$ . Then,  $Q_{b,p}$  is calibrated using the BFC curve (Eq. 4) and observed long-term mean  $Q_b$ , P,  $E_p$ , and  $\alpha$  (as calibrated in the previous step).

## 161 2.4 Machine learning to relate parameters to climatic and 162 physiographic properties

163 The parameters ( $\alpha$  and  $Q_{b,p}$ ) are regionalized as functions of climatic and 164 physiographic properties using ML. The calibrated  $\alpha$  and  $Q_{b,p}$  in each catchment (see 165 Section 2.3) serve as a benchmark for training ML models. The catchment-trained ML 166 models are then used to regionalize  $\alpha$  and  $Q_{b,p}$  globally at grid scale.

167 This study uses Boosted Regression Trees (BRT), which combines the strengths 168 of a regression tree algorithm and a boosting algorithm (Elith et al., 2008). BRT 169 differs fundamentally from conventional techniques that aim to produce a single "best" 170 parsimonious model, as it constructs multiple regression models in the algorithm 171 (Elith et al., 2008). The process of training a BRT model includes two parts: 172 regression trees and a boosting algorithm. First, multiple regression trees are built by 173 minimizing the prediction errors. Second, the boosting algorithm combines the 174 regression trees to give improved predictive performance. An effective strategy for 175 fitting a single decision tree is to grow a large tree, and then to prune it by collapsing 176 the weakest links as identified through cross-validation (Franklin, 2008). The first 177 regression tree is grown using recursive binary splits, that is, a binary split is 178 repeatedly applied to its own output until the loss function is maximally reduced. The 179 second tree is fitted to the residuals of the first tree, and the second tree can contain 180 quite different variables and split points. Consequently, multiple trees are fitted 181 additively based on the residuals of the previous tree. For multiple fitted trees, the 182 boosting algorithm averages trees to increase model performance. The dominant 183 drivers for the parameters  $\alpha$  and  $Q_{b,p}$  are estimated through method local interpretable 184 model-agnostic explanations (LIME) (Ribeiro et al., 2016).

185 Several hyper-parameters in BRT can be adjusted, including tree complexity (tc), 186 learning rate (lr) and bag fraction (bf). To find the most robust model for our analysis, 187 combinations of the following parameter values are tested using a 10-fold cross-188 validation strategy:  $tc \in \{4, 7, 10, 12\}$ ,  $lr \in \{0.0005, 0.005, 0.01\}$  and  $bf \in \{0.4, 0.5, 0.6, 0.01\}$ 189 (0.8) (Elith et al., 2008). The combination of hyper-parameter values with the highest 190 test performance is tc=12, lr=0.01, and bf=0.50. 10-fold cross-validation strategy is 191 also used for training models. The training is conducted ten times. Each time, 10 192 groups of catchments are randomly formed, of which nine groups are used for training 193 and one for testing. Ten BRT models are finally constructed at catchment scale and 198 then applied at grid scale globally. 10 maps of  $\alpha$  and  $Q_{b,p}$  are produced, and hence 10 199 maps of Q and  $Q_b$ . The mean values of the 10 maps are computed as a final result, 200 with the uncertainty calculated as the standard deviation of the 10 BRT models shown 201 in supplementary Figure S3.

#### 199 2.5 Overview of the modelling process

209 The methods and input datasets used in this study are summarized in Figure 2. 210 Global runoff partitioning maps are developed with the following steps: First, 211 parameters  $\alpha$  and  $Q_{b,p}$  in Eq.3 and Eq.4 are calibrated at catchment level (see Section 212 2.3). This step uses Q,  $Q_b$ , P and  $E_p$  data at the catchment level.  $Q_b$  is extracted from 213 Q using the digital filter method (see Section 3.1). Next, BRT models are developed 214 at the catchment level to relate  $\alpha$  and  $Q_{b,p}$  to various climatic and physiographic 215 properties. This step applies a 10-fold cross-validation strategy, resulting in 10 BRT 216 models. The BRT models are then used to estimate  $\alpha$  and  $Q_{b,p}$  globally at grid scale. 217 Finally, Q and  $Q_b$  are estimated globally using Eq. 3–4, P and  $E_p$  data, and the BRT-218 derived parameters  $\alpha$  and  $Q_{b,p}$  as inputs.



Figure 2. Overview of the modelling process and input datasets. The input datasets required in
each step are indicated by the colored squares; they correspond to the input datasets listed on
the left.

#### 213 3 **Data**

#### 214 3.1 Observed runoff, baseflow and quickflow

215 Observed daily discharge data from 3274 gauge-stations are obtained from the 216 Global Runoff Data Centre (GRDC) dataset together with the corresponding 217 catchment boundaries (https://www.bafg.de/GRDC/). A set of 1314 gauge-stations 218 and their corresponding catchments are selected from the initial dataset based on the 219 following requirements. First, the record length needed to be at least 10 years to allow 220 analyses on long-term mean values. Second, the missing data rate should be smaller 221 than 20% to warrant the representativeness of the mean values. Third, the water balance should close, i.e.,  $\left|\frac{P-E_a-Q}{P}\right| < 0.1$ , to exclude stations with too large data 222 223 uncertainties, or regional groundwater export/import as this is not included in the 224 Budyko framework. The spatial distribution of the selected 1314 catchments is shown 225 in Figure 3c.

226 Daily  $Q_b$  and quickflow  $(Q_q=Q-Q_b)$  are separated from daily Q using a digital 227 filter technique, more specifically the Lyne–Hollick (LH) method (Lyne & Hollick, 228 1979). Different digital filter methods have no significant influence on the long-term 229 estimation of  $Q_b$  and  $Q_s$  (Chen et al., 2023). The LH method has the advantage of 230 being minimally parameterized, and thus is easily applicable to a large sample of 231 catchments. The filter parameter  $f_l$ , also called recession constant, affects the degree 232 of attenuation. The number of passes determines the degree of smoothing, with the 233 backward pass nullifying the phase distortion from the forward pass. Here, the LH 234 method is applied in a conventional way with three passes (forward, backward, and 235 forward again) and the filter parameter  $f_1$  is set to 0.925 (Nathan & McMahon, 1990).

Long-term mean Q,  $Q_b$  and  $Q_q$  are estimated from their daily values and used to estimate the catchment runoff coefficient (RFC=Q/P), baseflow coefficient (BFC= $Q_b/P$ ), and quickflow coefficient (QFC=RFC-BFC). Note that the time period for P,  $E_p$ , Q,  $Q_b$  and  $Q_q$  are consistent within each catchment by selecting their crossing period. The available data lengths of the 1314 catchments vary from 10 to 41 years.

#### 242 **3.2 Climatic and Physiographic Characteristics**

243 Table 1 lists 16 climatic and physiographic variables that are used in this study, 244 including the respective references, original spatial resolution and temporal coverage. 245 In this study, analysis is done at 0.25° resolution; hence, observations are resampled 246 to 0.25° using bilinear interpolation method when needed. Among the 16 variables, 247 precipitation (P), potential evaporation  $(E_p)$  and evaporation  $(E_q)$  are direct inputs in 248 the Budyko and BFC curves (Eq. 3 and 4). The remaining 13 variables are predictors 249 for parameters  $\alpha$  and  $Q_{b,p}$  during the ML step (see Section 2.4). Three of these 250 characteristics are related to climate, four to vegetation, three to topography, two to 251 soil and one is related to human activities.

Table 1. Gridded climatic and physiographic characteristics used directly in the Budyko and

**253** BFC curve  $(P, E_a \text{ and } E_p)$ , or to predict runoff and baseflow with ML (remaining variables).

Subcategory	Data	Description	Data Sources	Original Resolution	Temporal coverage
	Р	Precipitation	MSWEP v1.1 (Beck et al., 2017)	0.25°	-
	$E_p$	Potential Evaporation	TerraClimate (Abatzoglou et al., 2018)	1/24°	
	Ea	Actual evaporation	GLEAM v3.6 (Martens et al., 2017)	0.25°	
Climate	TC	Air temperature	ERA5 (Hersbach et al., 2020)	0.25°	1980–2020
	SAI	Seasonality and asynchrony index	Calculated from daily $P$ and $E_p$ (Liu et al., 2018)	0.25°	
	SWE	Snow water equivalent	GLOBSNOW L3av2 and NSIDC v0.1 (Armstrong, 2005; Luojus et al., 2013)	0.25°	
	NDVI	Normalized difference vegetation index	MODIS (https://modis.gsfc.nasa.gov/)	0.05°	2000–2014
Vegetation	WUE	Water use efficiency			
	LAI	Leaf area index			
	RD	Maximum rooting depth	Fan et al. (2017)	~1km	Static
Topography	CTI	Topographic index	Marthews et al. (2015)	500m	Static
	ELEV	Mean	Yamazaki et al. (2019)	90m	

		elevation			
	SLO	Slope	Amatulli et al. (2018)	1km	
Soil	STHI	Average soil and sedimentary deposit thickness	Pelletier, J.D, et.al, (2016)	lkm	Static
	SPO	Soil porosity	SoilGrids 2.0 (Poggio et al., 2021)	250 m	
Human activities	HFP	Human influence index	Eric W. Sanderson et al. (2002)	1km	1995–2004

254

#### 255 4 Results

#### **4.1 Calibrated parameters at catchment scale**

257 Figure 3 visualises the values of the parameters  $\alpha$  and  $Q_{b,p}$  for all 1314 258 catchments as calibrated with Eq. 3 and 4. Due to the large variability of catchment 259 conditions, the parameter values vary such that their 5% and 95% quantiles range between  $\alpha = 1.94-5.55$  and  $Q_{b,p} = 104-2242$  mm yr<sup>-1</sup>, resulting in different Budyko 260 261 and BFC curves as shown in Figure 3a and b with the purple and orange lines. The 262 median values of the catchment-specific  $\alpha$  and  $Q_{b,p}$  are 2.83 and 547 mm yr<sup>-1</sup>, 263 respectively. The large variability of  $\alpha$  and  $Q_{b,p}$  is spatially shown in Figure 3c and d, 264 respectively. Large  $\alpha$  values (i.e.,  $\alpha > 4$ ) mainly appear in the Great Plains in North 265 America, the east coast of Australia and South America. A mix of low and median  $\alpha$ 266 values (i.e.,  $\alpha < 3$ ) appear in Europe and in the east of the United States. For the 267 spatial distribution of  $Q_{b,p}$ , Australia, southern Africa and the middle of the United 268 States show low  $Q_{b,p}$  values. There are no obvious spatial patterns elsewhere. Of the 269 1314 catchments, 88 stations show extreme parameter values (i.e.,  $\alpha > 6.0$  and 270  $Q_{b,p}$  >3000; see the tails in the density plots in Figure 3c and d). In addition, 38 271 stations of these 88 stations fall outside the Budyko limits (i.e.,  $\alpha \rightarrow \infty$ ) as shown in 272 Figure 3a. These 88 stations with extreme parameter values are considered as outliers 273 and are therefore excluded, such that 1226 stations are left for the remainder of the 274 analysis. These remaining stations are further tested by analysing results during 275 calibration and validation periods (see Figure S1). For each catchment, the first 20 276 years are used to calibrate the parameters  $\alpha$  and  $Q_{b,p}$ , and the remaining years are used for validation. Catchments with less than 30 years of data are not validated. The validated runoff and baseflow show a correlation ( $R^2$ ) of 0.95 and 0.94, respectively. The high validation performance illustrates that the Budyko and BFC curve with the calibrated  $\alpha$  and  $Q_{b,p}$  can reproduce the spatial variability of Q and  $Q_b$  well at the selected catchments.



283

Figure 3. Scatterplots of (a) Q/P and (b)  $Q_b/P$  versus  $P/E_p$ . The lines in panel (a) and (b) are the Budyko and BFC curves, respectively, using the following quantile values for the parameters  $\alpha$  and  $Q_{b,p}$ : 5% (purple), 50% (red), and 95% (orange). Note, that in (b)  $\alpha$  is fixed to its median value of 2.83 to focus on  $Q_{b,p}$  changes. Spatial distribution and density plots of (c)  $\alpha$  and (d)  $Q_{b,p}$ . Extreme values beyond the grey lines in the density plots are considered as outliers and are removed.

#### 289 4.2 Catchment-scale performance of trained models

290 The first row in Figure 4 shows the performances of BRT-derived  $\alpha$ , Q/P and Q291 using Eq.3 and BRT-derived  $\alpha$  (Budyko–ML). During training, all three variables 292 agree well with observations with RMSE for Q/P and Q equal to 0.02 and 17 mm yr<sup>-1</sup>, 293 respectively (Figure 4b and c). During testing, the performances decrease as expected, 294 especially for  $\alpha$ , with  $R^2 = 0.50$ . The performances of Q/P and Q remain high though, 295 with  $R^2 = 0.93$  and 0.96 and RMSE = 0.04 and 46 mm yr<sup>-1</sup>, respectively.

296 Similar to runoff, the second row in Figure 4 shows the performances of BRT-297 derived  $Q_{b,p}$ ,  $Q_b/P$  and  $Q_b$  estimated with Eq. 4 and BRT-derived  $\alpha$  and  $Q_{b,p}$ . The performance for these three variables is high during training, with  $R^2 = 0.92$ , 0.96 and 298 299 0.97, respectively (Figure 4d, e and f). The performance of  $Q_{b,p}$  decreases during the testing phase ( $R^2=0.41$ ). As a result, also  $Q_b/P$  and  $Q_b$  perform slightly worse during 300 testing, but their performances are still acceptable, with  $R^2$  for  $Q_b/P$  and  $Q_b$  equal to 301 302 0.84 and 0.88, respectively. The good performances of runoff and baseflow during the 303 testing phase indicates that the trained ML models for  $\alpha$  and  $Q_{b,p}$  at catchment scale 304 are reliable for estimating runoff and baseflow globally.



Figure 4. Performance of parameters  $\alpha$  and  $Q_{b,p}$  (a and d) from BRT models, Q/P (b),  $Q_b/P$ (e), Q (c) and  $Q_b$  (f) using the Budyko framework and BFC curve at catchment scale. Each point represents a catchment (n=1226 in each panel). The orange and blue lines are linear regression lines and the black lines mark the 1:1 relation.

#### 311 4.3 Global map of runoff partitioning

325 The catchment-trained BRT models are applied globally to estimate parameters  $\alpha$ 326 and  $Q_{b,p}$  on grid-scale. The spatial distribution of  $\alpha$  and  $Q_{b,p}$  is shown in Figure S2. 327 Figure 5a, c and e illustrate the global, Budyko-based Q,  $Q_b$  and  $Q_q$ . This is compared 328 to observations in Figure 5b, d, and f, respectively. The estimated global values show 329 very similar spatial patterns to the observations. High flows appear at medium 330 latitudes near the equator  $(30^{\circ}N-30^{\circ}S)$ , while low flows are located at high latitudes 331 (30°N–90°N and 30°S–60°S). Northern Africa and western Asia are exceptions, as 332 they show low values at medium latitudes. Similarly, exceptions at high latitudes 333 appear in regions near the coast of Chile, Europe and Canada where high runoff is 334 found in the estimated maps (Figure 5a, c and e). The uncertainty for each variable ( $\alpha$ , 335  $Q_{b,p}$ , Q/P,  $Q_b/P$ , Q, and  $Q_b$ ), which is considered equal to the standard deviation in the 336 10 BRT models, is shown in Figure S3. The spatial uncertainty is equal to 0.13 for  $\alpha$ , 114 mm yr<sup>-1</sup> for  $Q_{b,p}$ , 0.009 for Q/P, 0.01 for  $Q_b/P$ , 5.78 mm yr<sup>-1</sup> for Q, and 10.9 mm 337  $yr^{-1}$  for  $Q_b$ . The uncertainty is larger for  $Q_b$  than Q since Q only relies on one 338

parameter ( $\alpha$ ), while  $Q_b$  relies on two parameters ( $\alpha$  and  $Q_{b,p}$ ). Overall, the global, long-term mean annual Q is on average 274 (std=418) mm yr<sup>-1</sup>,  $Q_b$  151 (std=181) mm yr<sup>-1</sup> and  $Q_q$  123 (std=270) mm yr<sup>-1</sup>. The results illustrate that the global river supply relies more on baseflow than quickflow.



Figure 5. Global maps of estimated (a) Q, (c)  $Q_b$  and (e)  $Q_q$ . Station-based observed (b) Q, (d)  $Q_b$  and (f)  $Q_q$ .

332 Figure 6 shows the global map of gridded RFC, BFC, QFC, baseflow index 333  $(BFI=Q_b/Q)$  and quickflow index  $(QFI=Q_a/Q)$ . RFC, BFC and QFC have similar 334 spatial patterns with low values in western America, northern Africa, southern Africa, 335 western Asia, central Asia, and Australia. However, regions with high RFC values, 336 show both high and low BFC and QFC values depending on the region. For example, 337 Q is partitioned more into  $Q_q$  than  $Q_b$  in the Amazon and southeast Asia, while in 338 Canada and Russia, more  $Q_b$  is generated than  $Q_q$ . This is also illustrated with Figure 339 6f-h, which show RFC, BFC and QFC for different quantiles as a function of the 340 latitude. High RFC values are generally located at 60°N-85°N, 5°N-5°S and 45°S-60°S. In these latitudinal intervals, the partitioning of Q into  $Q_b$  and  $Q_q$  differs in 341 342 space. As shown in Figure 6i and j, between  $60^{\circ}N-85^{\circ}N$ , the majority of Q are mostly 343 partitioned into  $Q_b$  (the median values in this latitudinal interval is on average 80.7%), 344 and less  $Q_q$  (19.3%). Between 5°N–5°S and 45°S–60°S, the BFC and QFC are quite

- similar to each other with  $Q_b$  of 42.1% and 54.9%, respectively, and  $Q_q$  of 57.9% and
- 346 45.1%, respectively. Across all latitudes, the mean difference between the 5<sup>th</sup> and 95<sup>th</sup>
- 347 quantiles is larger for RFC (0.50) and BFC (0.35) than for QFC (0.26). The spread of
- 348 QFC is more pronounced near the equator (5°N-5°S) and in the Southern
- Hemisphere high latitudes ( $45^{\circ}S-60^{\circ}S$ ). Overall, average 30.3% (std=26.5%) of P is
- 350 partitioned into Q, of which 20.6% (spatial standard deviation std=22.1%) is  $Q_b$  and
- 351 9.7% (std=10.3%)  $Q_q$ .

352



354

Figure 6. Global map of flow coefficients: (a) runoff coefficient (RFC) estimated with the Budyko curve (Eq. 3), (b) baseflow coefficient (BFC) estimated with the BFC curve (Eq. 4), (c) quickflow coefficient (QFC=RFC-BFC), (d) baseflow index (BFI= $Q_b/Q$ ) and (e) quickflow index (QFI= $Q_q/Q$ ). Subplots (f), (g), (h), (i) and (j) show the median latitudinal variation of the respective variables (in red), and the 5<sup>th</sup> (purple) and 95<sup>th</sup> (blue) percentiles.

#### 359 4.4 Dominant drivers of runoff partitioning

360 The most important drivers for  $\alpha$  and  $Q_{b,p}$  vary across regions (Figure 7). 361 Topography and soil properties are most important for most catchments (75.5% 362 catchments for  $\alpha$ ; 67.0% catchments for  $Q_{b,p}$ , see blue points in Figure 7). Slope (SLO) 363 is identified most frequently as the dominant driver for both  $\alpha$  (48.7% catchments) 364 and  $Q_{b,p}$  (34.1% catchments). The second driver is elevation (ELEV) for  $\alpha$  dominant 365 in 25.6% catchments, and soil thickness (STHI) for  $Q_{b,p}$  in 29.1% catchments. 366 Climate related factors are recognized as the most important driver at a smaller 367 number of catchments (12.4% for  $\alpha$  and 27.3% for  $Q_{b,p}$ ) as also vegetation related factors (12.1% for  $\alpha$  and 5.7% for  $Q_{b,p}$ ). 368

369 The main drivers for the parameters are region specific. This provides another 370 perspective on why there is no universally accepted relationship yet (Padrón et al., 371 2017), besides the complex interaction between the drivers (Ning et al., 2019) and 372 uncertainties in P,  $E_p$ , and Q (Koppa et al., 2021). Previous studies have investigated 373 the main drivers to Budyko parameters. These identified dominant drivers depend on 374 the region of interest and are different from each other. Considering large basins 375 globally, studies illustrated the main dominant property is vegetation (Li et al., 2013; 376 Zhang et al., 2001) or climate seasonality (Liu et al., 2018). In small catchments 377 regionally, the influence of climatic and physiographic properties on  $\alpha$  becomes more 378 variable as other factors need to be considered including soil properties (Shen et al., 379 2017), topography (Shao et al., 2012), human activities (Xing et al., 2018) and a 380 combination of various controls (Yang et al., 2007). According to the regions 381 identified in Figure 7, topography and soil related factors should be first considered 382 for regionalizing  $\alpha$  in most catchments. Climate related factors are important in 383 eastern South America and the coastline of Australia. Vegetation is the most dominant 384 driver in western America and the United Kingdom.



Figure 7. Spatial distribution of the most important driver to: (a) parameter  $\alpha$  in Budyko and BFC curves, and (b) parameter  $Q_{b,p}$  in BFC curve. The explanation of the abbreviations is provided in Table 1.

390

#### 391 5 Discussion

#### 392 **5.1 Comparison to existing global datasets**

The global, gridded baseflow dataset developed in this study is compared to baseflow products from previous studies. This includes the Global Streamflow Characteristics Dataset (GSCD) (Beck et al., 2015) and ERA5-Land dataset (Muñoz Sabater, 2019). The baseflow is directly available in the ERA5-Land dataset, and indirectly with GSDC as only the baseflow index (BFI) and runoff ( $Q_{mean}$ ) are provided. To remain consistent with this study, "BFI1" in the GSCD dataset is selected where the baseflow is also calculated from the digital filter method. The

399 long-term mean baseflow of this study (151 (spatial standard deviation std=181) mm yr<sup>-1</sup>) is smaller than GSCD-based baseflow ( $Q_{b,GSCD} = 241$  (std=321) mm yr<sup>-1</sup>, Figure 400 8a and c), and larger than ERA5-Land-based baseflow ( $Q_{b,ERA5-Land} = 79$  (std=145) 401 mm yr<sup>-1</sup>, Figure 8b and d). The baseflow estimated in this study has a larger spatial 402 correlation with  $Q_{b,GSCD}$  (R<sup>2</sup>=0.84) than  $Q_{b,ERA5-Land}$  (R<sup>2</sup>=0.51), while a smaller RMSE 403 is found relative to  $Q_{b,ERA5-Land}$  (RMSE=143 mm yr<sup>-1</sup>) compared to  $Q_{b,GSCD}$ 404 (RMSE=198 mm yr<sup>-1</sup>). This means the spatial variability of our Budyko-ML-based 405 406 baseflow is more similar to GSCD, while the magnitudes are closer to ERA5-Land 407 values. The baseflow coefficient (BFC= $Q_b/P$ ) is also compared to estimates according 408 to GSCD and ERA5-Land. Figure S4 shows that the correlation of BFC is higher relative to GSCD ( $R^2=0.73$ ) than ERA5-Land ( $R^2=0.07$ ). 409

410 These three datasets are a result of different types of methods with each their 411 strengths and weaknesses: physically constrained ML in this study, pure ML for 412 GSCD and the land surface model H-TESSEL for ERA5 Land. The GSCD dataset is 413 not physically constrained, but available at a higher spatial resolution (0.05°) and 414 based on significantly more catchments (3394). The H-TESSEL used for ERA5 Land 415 is not specifically developed for runoff estimation, but for land-atmosphere 416 interactions. Also, H-TESSEL uses "expert opinion" based parameterization instead 417 of being calibrated. This may be the cause for the poor correlation results and 418 confirms opinions that land surface models such as the H-TESSEL poorly estimate 419 baseflow and groundwater-surface water interactions (Clark et al., 2015, Beck et al., 420 2017).

421 As the baseflow index (BFI= $Q_b/Q$ ) is more sensitive to both baseflow and runoff 422 uncertainties (Gnann et al., 2019), the BFI is only compared to GSCD. As shown in Figure S5, the performance of BFI at catchment scale is acceptable with  $R^2$  of 0.54. 423 However, the performance decreases at global grid scale ( $R^2=0.18$ ). This low 424 425 correlation of BFI may be attributed to several aspects. First, getting accurate BFI 426 estimates from separately estimated Q and  $Q_b$  is difficult (Beck et al., 2017). The 427 spatial variability of the individual variables Q and  $Q_b$  is much larger than the 428 difference between Q and  $Q_b$  within each catchment (BFI). High similarities in the 429 spatial distribution of Q and  $Q_b$  does not guarantee similar BFI values. The BFI is 430 especially sensitive in dry regions since very low Q values (in the denominator) 431 would result in high BFI values. Second, the study period of the GSCD dataset and

437 this study is different. The GSCD dataset adopted average P and  $E_p$  datasets with 438 daily Q datasets, while we kept their period consistent by selecting the crossing period. 439 Third, the different digital filters used, Lyne–Hollick in this study and method from 440 Van Dijk (2010) for GSCD, may cause a slight difference in the observed baseflow 441 used to train models.



438

Figure 8. Estimated global baseflow compared to GSCD (a and c) and ERA5-Land (b and d). Subplots (a) and (d) show the pixel-by-pixel scatter plot with the red lines representing the fitted curve, and the black lines the 1:1 line. Subplots (c) and (d) show the spatial distribution of their difference, calculated as their difference divide by their average (i.e.,  $(Q_{b,this study} -$ 

442  $Q_{b,GSCD}/(0.5 * (Q_{b,this study} + Q_{b,GSCD}))$  for plot (c), and replace  $Q_{b,GSCD}$  with  $Q_{b,ERA5-Land}$  for 443 plot (d).

#### 444 **5.2** Partitioning in northern latitudes

445 The runoff partitioning dataset developed in this study has difficulties in 446 representing high northern latitudes correctly (HNL). First, precipitation datasets tend 447 to be underestimated at latitudes higher than 60 °N (snow-dominant regions) at a 448 long-term scale (Beck et al., 2017). The MSWEP dataset used in this study attempted 449 to correct this underestimation bias by the catch-ratio equation (Goodison et al., 1998). 450 But the precipitation in HNL still has uncertainties for the gauge under-catch. By 451 using the Budyko constrained ML framework, precipitation is a dominant forcing for 452 the runoff and baseflow estimation, such that the uncertainty of precipitation could 453 bring large uncertainties. Second, there are no catchments in HNL when applying the 454 selection criteria as described in Section 3.1, which means relations based on trained 455 ML models may not be accurate there. As a data-oriented method, ML relies on 456 training data sources with all representative data expected to be included (Ma et al., 457 2020). Third, the partitioning of baseflow and quickflow from snow-melt runoff is 458 different from precipitation-generated runoff. Based on the definition of baseflow 459 from Hall (1968), snow-melt runoff is grouped under baseflow. However, this 460 contradicts the digital filter technique that considers high frequency parts as 461 quickflow. Snow-melt runoff can have quickflow features of high frequency and 462 peaks during summer, even generating floods (Benn et al., 2012). As shown in Figure 463 6d and 6i, the baseflow index in high northern latitudes have high values, which 464 means runoff comes more from baseflow rather than quickflow. It makes sense if we 465 consider snow-melt runoff as baseflow following the definition of Hall (1968). 466 However, we recommend further investigation on runoff partitioning in NHL regions.

#### 467 6 **Conclusion**

468 This study extends the Budyko constrained machine learning (Budyko–ML) 469 approach to develop global datasets for the runoff (Q), baseflow  $(Q_b)$ , quickflow  $(Q_q)$ 470 and the respective coefficients relative to the precipitation  $(Q/P, Q_b/P \text{ and } Q_q/P)$  at 471 0.25° resolution. This hybrid approach, combining the Budyko-based framework 472 (Budyko and BFC curve) with ML (BRT), retains the advantage of both the physical 473 part and ML to achieve good performances within physical boundaries. This

advantage is illustrated by the good performance of both Q and  $Q_b$  as they performed 474 475 well compared to field observations during the testing phase with  $R^2=0.96$  and  $R^2=0.88$  for Q and  $Q_b$ , respectively. BRT estimates parameters globally, despite their 476 477 unknown relationship with climatic and physiographic properties. Among the 13 478 climatic and physiographic properties considered, the main drivers are region specific, 479 with topography and soil related factors being predominant in most catchments. 480 Findings indicate that global runoff amounts to 274 (spatial standard deviation 481 std=418) mm yr<sup>-1</sup>, which means 30.3% (std=26.5%) of the precipitation, of which 482 20.6 (std=22.1%) is baseflow and 9.7% (std=10.3%) is quickflow. Our baseflow 483 estimates are lower than GSCD estimates (241 (std=321) mm yr<sup>-1</sup>) but larger than ERA5-Land estimates (79 (std=145) mm yr<sup>-1</sup>). These large differences illustrate the 484 485 large uncertainty that remains in runoff partitioning at global scales, and the required 486 efforts to improve it further.

487

#### 488 **Data Availability Statement**

489 The developed global 0.25° datasets including runoff (Q), baseflow ( $Q_b$ ), runoff 490 coefficient (Q/P), baseflow coefficient ( $Q_b/P$ ) and baseflow index ( $Q_b/Q$ ) are 491 available at <u>Global runoff partitioning based on Budyko-constrained machine learning</u> 492 <u>Zenodo</u>.

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Figure1.



Figure2.











Figure3.



Parameter  $Q_{b,p}^{1000}$  in BFC curve (mm yr<sup>-1</sup>) 2500

<50

>3000

Figure4.







Figure5.







Figure6.









 $\mathsf{BFI}\; Q_{\mathit{b}}/Q$ 





Figure7.

(a) Most important drivers for parameter  $\alpha$ 



(b) Most important drivers for parameter  $Q_{b,p}$ 



Figure8.





# **AGU** PUBLICATIONS

#### [Water Resources Research]

#### Supporting Information for

#### [Global runoff partitioning based on Budyko-constrained machine learning][Shujie Cheng<sup>1,2</sup>, Petra

Hulsman<sup>2</sup>, Akash Koppa<sup>2</sup>, Hylke E. Beck<sup>3</sup>, Lei Cheng<sup>1</sup>, and Diego G. Miralles<sup>2</sup>]

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#### 1 Method

#### Baseflow curve based on limit concept

In general, the water balance can be written as:

$$\frac{dS}{dt} = P - E_a - Q \tag{S1}$$

where S is water stored in underground, P is precipitation,  $E_a$  is actual evaporation, Q is discharge which can be partitioned into  $Q_b$  is baseflow and  $Q_q$  is quick flow ( $Q = Q_b + Q_q$ ).

The basic limit concept of the Budyko framework for estimating  $E_a$  is:  $E_a/P \rightarrow 1 \text{ as } E_p/P \rightarrow \infty$  for very dry conditions, and  $E_a \rightarrow E_p \text{ as } E_p/P \rightarrow 0$  for very wet conditions, where  $E_p$  is potential evaporation. The demand limit of  $E_a$  is  $E_p$  and the supply limit is *P*. Fu (1981) proposed  $E_a$  can be calculated with:

$$\frac{E_a}{P} = 1 + \frac{E_p}{P} - \left[1 + \left(\frac{E_p}{P}\right)^{a_1}\right]^{1/a_1}$$
(S2)

Assuming  $\frac{dS}{dt} \approx 0$  on long term time scales and with the catchment retention defined as

$$CR = E_a + Q_b \tag{S3}$$

Equation S1 can be expressed as:

$$P = CR + Q_q \tag{S4}$$

The demand limit for *CR* is  $CR_0 = E_p + Q_{b,p}$ . The  $E_p$  and  $Q_{b,p}$  are the potential values for *E* and  $Q_b$ , respectively. According to Zhang et al. (2008), the limits concept of Budyko can also be applied to *CR* such that:  $CR/P \rightarrow 1$  as  $CR_0/P \rightarrow \infty$  for very dry conditions, and  $CR \rightarrow CR_0$  as  $CR_0/P \rightarrow 0$  for very wet conditions. Then *CR* can be estimated as:

$$\frac{CR}{P} = 1 + \frac{CR0}{P} - \left[1 + \left(\frac{CR0}{P}\right)^{a_2}\right]^{1/a_2}$$
(S5)

Combining Eq. S2, Eq. S3 and Eq. S5:

$$\frac{Q_b}{P} = \frac{Q_{b,p}}{P} + \left[1 + \left(\frac{E_p}{P}\right)^{a_1}\right]^{1/a_1} - \left[1 + \left(\frac{E_p + Q_{b,p}}{P}\right)^{a_2}\right]^{1/a_2}$$
(S6)

Under very limited storage capacity conditions (for instance an impervious catchment), no/limited water is stored in the subsurface such that the baseflow also approaches zero (i.e.,  $Q_b/P \rightarrow 0$  if  $Q_{b,p}/P \rightarrow 0$ ). Under that condition, Eq. S11 changes to  $0 \approx \left[1 + \left(\frac{E_p}{P}\right)^{a_1}\right]^{1/a_1} - \left[1 + \left(\frac{E_p}{P}\right)^{a_2}\right]^{1/a_2}$ . This equation can only be satisfied if  $a_1 = a_2$ . Thus Eq. S11 can be written as:

$$\frac{Q_b}{P} = \frac{Q_{b,p}}{P} + \left[1 + \left(\frac{E_p}{P}\right)^{\alpha}\right]^{1/\alpha} - \left[1 + \left(\frac{E_p + Q_{b,p}}{P}\right)^{\alpha}\right]^{1/\alpha}$$
(S7)

2 Figures



Figure S1. Performance of (a) Q and (b)  $Q_{b}$  at catchment scale during the calibration (orange) and validation (blue) periods.



Figure S2. Global maps of (a) parameter  $\alpha$  in the Budyko curve (Eq. 3) and BFC curve (Eq. 4), and (b) parameter  $Q_{b,p}$  in BFC curve estimated as the mean of 10 BRT models.



Figure S3. Global map of the uncertainty of (a) parameter  $\alpha$ , (b) parameter  $Q_{b,p}$ , (c) runoff coefficient (RC=Q/P), (d) baseflow coefficient (BFC= $Q_b/P$ ), (e) runoff (Q), and (f) baseflow ( $Q_b$ ). These uncertainty values are equal to the standard deviation of the 10 trained BRT models using the 10-fold cross-validation strategy.



Figure S4. Comparison of the baseflow coefficient  $(Q_b/P)$  from this study with estimates according to (a) GSCD and (b) ERA5-Land.



Figure S5. Comparison of the baseflow index  $(Q_b/Q)$  as estimated in this study with (a) field observations and (b) GSCD estimates.