# Multi-Proxy, Multi-Season Streamflow Reconstruction with Mass Balance Adjustment

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#### Abstract

Despite having offered important hydroclimatic insights, streamflow reconstructions still see limited use in water resources operations, because annual reconstructions are not suitable for decisions at finer time scales. Attempts towards sub-annual reconstructions have relied on statistical disaggregation, which uses none or little proxy information. Here, we develop a novel framework that optimizes proxy combinations to simultaneously produce seasonal and annual reconstructions. Importantly, the framework ensures that total seasonal flow matches annual flow closely. This mass balance criterion is necessary to avoid misguiding water management decisions, such as water allocation. Using the framework, and leveraging a multi-species network of ring width and cellulose  $\delta 180$  in Southeast Asia, we reconstruct seasonal and annual inflow to Thailand's largest reservoir. The reconstructions are statistically skillful. This work is one step closer towards operational usability of streamflow reconstruction in water resources management.

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#### **9 Key Points:**

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10	•	Ring width and $\delta^{18} O$ are combined to reconstruct dry season, wet season, and an-
11		nual streamflow
12	•	Optimal proxy combinations are found with an automatic input selection scheme
13	•	Mass-balance adjustment improves the agreement between seasonal and annual
14		reconstructions

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#### 15 Abstract

Despite having offered important hydroclimatic insights, streamflow reconstructions still 16 see limited use in water resources operations, because annual reconstructions are not suit-17 able for decisions at finer time scales. Attempts towards sub-annual reconstructions have 18 relied on statistical disaggregation, which uses none or little proxy information. Here, 19 we develop a novel framework that optimizes proxy combinations to simultaneously pro-20 duce seasonal and annual reconstructions. Importantly, the framework ensures that to-21 tal seasonal flow matches annual flow closely. This mass balance criterion is necessary 22 to avoid misguiding water management decisions, such as water allocation. Using the 23 framework, and leveraging a multi-species network of ring width and cellulose  $\delta^{18}$ O in 24 Southeast Asia, we reconstruct seasonal and annual inflow to Thailand's largest reser-25 voir. The reconstructions are statistically skillful. This work is one step closer towards 26 operational usability of streamflow reconstruction in water resources management. 27

#### <sup>28</sup> Plain Language Summary

Long history of river discharge, or streamflow, can be reconstructed from tree rings. 29 These reconstructions help us understand the water cycle in the past, but they have not 30 been widely used in water resources operations. This is because reconstructions are of-31 ten annual (having only one data point per year). By combining different tree species 32 and different features of tree rings (for example, ring width and stable isotope ratio), it 33 is possible to reconstruct seasonal streamflow in addition to the annual one, and that 34 is our first goal. But a major challenge arises: how do we ensure that the total flow vol-35 ume of the seasonal reconstructions closely matches the annual one? This criterion is called 36 mass balance, and it is important to avoid misguiding water management decisions such 37 as allocating water to different sectors. We develop a novel method to reconstruct sea-38 sonal and annual streamflow while accounting for mass balance at the same time. Our 39 work is thus a step closer towards operational usability of streamflow reconstructions in 40 water resources management. 41

#### 42 **1** Introduction

Dendrohydrology, the study of past hydroclimate using tree rings, has been largely 43 motivated by water resources management. The field traces back to Hardman and Reil 44 (1936), who recognized that instrumental records were too short to understand drought 45 trends, and demonstrated that better understanding could be gained from exploring the 46 links between tree rings and streamflow. Their work was motivated by contemporary droughts 47 that affected irrigation. Also to understand droughts, Schulman (1945) established a tree 48 ring chronology for the Colorado River Basin, this time motivated by the war effort-49 to examine Hoover Dam's hydropower production reliability to meet wartime demand. 50 While these early works stopped at studying tree ring indices, dendrohydrology took a 51 big step when Stockton (1971), leveraging advanced multivariate techniques (Fritts et 52 al., 1971), showed that reconstructing streamflow record back in time was feasible—long 53 term surface water availability could now be quantified directly. Soon, multiple stream-54 flow reconstructions were developed across the Colorado River Basin (Stockton & Ja-55 coby, 1976), revealing the shortcomings of the Colorado River Compacts (Woodhouse 56 et al., 2006), and providing insights about long term hydrology of Lake Powell, the United 57 States' second largest reservoir. 58

Streamflow reconstruction has become "an important planning and research tool" 59 in water resources management (Meko & Woodhouse, 2011). Yet, its use in practical, 60 operational aspects of water management is still limited. That is because reconstructions 61 often target specific components of the hydrograph that best correlated with tree ring 62 proxies. Perhaps most commonly, reconstructions from ring width often target the growth 63 season (e.g., D'Arrigo, Abram, et al., 2011; Güner et al., 2017). Another example is given 64 by reconstructions targeting peak flow using tree ring cellulose stable oxygen isotope ra-65 tio ( $\delta^{18}$ O) (C. Xu et al., 2019). These reconstructions reveal important insights about 66 the hydroclimate, but do not provide the total annual surface water availability. Other 67 works target the annual flow (e.g., Rao et al., 2018; Nguyen & Galelli, 2018), but even 68 so, the annual resolution is not suitable for making operational decisions at finer time 69 scales—crop planning, for instance, is often based on seasonal flow; reservoir releases are 70 determined at monthly or even weekly time steps. 71

The water resources community recognizes the need for sub-annual reconstructions. 72 Attempts towards this goal have relied on statistical disaggregation, assuming some sta-73 tistical relationships between the sub-annual and annual flows (Prairie et al., 2008; Sauchyn 74 & Ilich, 2017). These assumptions are reasonable but not always valid (Figure S1). More 75 importantly, paleoclimatic proxies are not used in these methods, and their rich infor-76 mation are not utilized. Recent progress was made by Stagge et al. (2018), who used multi-77 species chronologies as additional inputs to disaggregation, showing that these inputs 78 can be weighted differently for each month to improve the monthly reconstructions. 79

The works of Stagge et al. (2018), C. Xu et al. (2019), and others discussed above suggest that different proxies have different seasonal sensitivities. Therefore, instead of disaggregation, we propose to use multiple proxies to simultaneously reconstruct subannual (e.g., seasonal) and annual flows. Two challenges arise. How to combine prox-

- ies optimally for different targets? And how to ensure that the seasonal flows add up to
- the annual flow, i.e., how to account for mass balance? We develop a unified framework
- to address both challenges. Mass balance is accounted for by a term in the regression
- <sup>87</sup> formulation that penalizes the differences between total seasonal flow and annual flow
- (Section 3.1), and proxy combination is optimized with an automatic input selection scheme
- (Section 3.2). We test the framework with a case study in the Chao Phraya River Basin,
- <sup>90</sup> Thailand, pooling together a multi-species network of ring width and cellulose  $\delta^{18}$ O chronolo-
- gies from Southeast Asia (Section 2). This work is one step closer towards operational
- <sup>92</sup> usability of streamflow reconstruction in water resources management.

#### <sup>93</sup> 2 Study Site and Data

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#### 2.1 The Southeast Asian Dendrochronology Network

Over the past three decades, an extensive network of tree ring chronologies have 95 been developed in Southeast Asia. This network has been instrumental in improving our 96 understanding of Southeast Asia's hydroclimate and history. Tree ring data from Thai-97 land and northern Vietnam (Buckley, Palakit, et al., 2007; Sano et al., 2009) revealed 98 a multidecadal drought, what is later known as the Strange Parallel Droughts (E. R. Cook 99 et al., 2010), which coincided with a tumultuous period of Southeast Asian history (Lieberman, 100 2003; Lieberman & Buckley, 2012). Further back in time, tree ring data from southern 101 Vietnam linked megadroughts in the 14<sup>th</sup> and 15<sup>th</sup> centuries to the demise of the Angkor 102 Civilization (Buckley et al., 2010, 2014). These findings are among many insights that 103 the Southeast Asian Dendrochronology Network has brought forth. 104

In this work, we use twenty tree ring chronologies from Vietnam, Laos, Cambodia, 105 Thailand, and Myanmar (Figure 1). The chronologies at Kirirom, Petchaburi, Pha Taem, 106 and Wiang Haeng are published here for the first time. The metadata of the chronolo-107 gies are provided in Table 1. The common period of most chronologies in our network 108 is 1748–2005 (Figure S6), and is the same as the time span of our  $\delta^{18}$ O network. Sev-109 eral chronologies are some decades shorter. Following Stagge et al. (2018), we imputed 110 the missing years using the R package missMDA (Josse & Husson, 2016) (see Figure S7). 111 We imputed the tree ring data instead of building nested models because nesting is not 112 applicable in our reconstruction framework. As we shall explain in Section 3.1, the frame-113 work is designed to account for mass balance, tuning the regression parameters such that 114 the total sub-annual flow matches the annual flow closely. With nesting, the final vari-115 ance correction can disrupt the mass balance. 116

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#### 2.2 Cellulose $\delta^{18}O$

<sup>118</sup> We use four chronologies of tree ring cellulose stable oxygen isotope ratio ( $\delta^{18}$ O) <sup>119</sup> that were developed in Laos, Thailand, and Vietnam over the past decade (Figure 1 and <sup>120</sup> Table 2).  $\delta^{18}$ O exhibits strong mechanical and statistical relationship with the hydro-<sup>121</sup> climate (C. Xu et al., 2011; Sano et al., 2012), and has been used to reconstruct wet sea-<sup>122</sup> son precipitation in the region (C. Xu et al., 2015, 2018).  $\delta^{18}$ O in Laos was also found



**Figure 1.** Map of the study region, showing the Chao Phraya River, the proxy network, and the target streamflow station.

<sup>123</sup> to have significant negative correlation with Mekong River water level (C. Xu et al., 2013), <sup>124</sup> suggesting promising hydrological applications. Finally, three  $\delta^{18}$ O chronologies were used <sup>125</sup> to reconstruct Chao Phraya River peak season flow (C. Xu et al., 2019). These works <sup>126</sup> support recent literature (Treydte et al., 2006; G. Xu et al., 2019) that  $\delta^{18}$ O has indeed <sup>127</sup> moved beyond "potential" (Gagen et al., 2011), and earned its place as a practical, valu-<sup>128</sup> able paleoclimate proxy.

#### 129 **2.3 Streamflow**

The Chao Phraya River Basin covers 30% of Thailand's area, and is home to about 25 million people. Thailand's largest reservoir, the Bhumibol (active capacity 9.7 km<sup>3</sup>), lies on the Ping River tributary. Reliable operations of this reservoir require accurate assessment of inflow availability, on both inter- and intra-annual scales.

Streamflow station P.1 is located upstream of Bhumibol Reservoir. P.1 has the longest and most complete record in Thailand: daily data are available from April 1921–present. Since 1985, the river upstream of P.1 has been impounded by the Mae Ngat Dam, which, at full capacity, stores about 14% of P.1's mean annual flow. Dam operations modify the seasonal streamflow patterns, thereby interfering with the proxy-streamflow relationship. Therefore, we naturalized the streamflow data from 1985. The naturalization process is

Site	Longitude	Latitude	Species	References
Bidoup	108.45	11.97	Fokienia hodginsii	Buckley et al. (2010)
Chin Hills	93.50	22.17	Pinus kesiya	Rao (2020)
Kim Hy	106.04	22.25	$Pseudotsuga\ sinensis$	Hansen et al. (2017)
Kirirom	104.10	11.95	Pinus merkusii	This study <sup>a</sup>
Kon Ka Kinh	108.18	14.91	Fokienia hodginsii	Buckley et al. (2019)
Mae Hong Son	98.93	19.28	Tectona grandis	Buckley, Palakit, et al. (2007)
Maingtha	96.20	23.20	Tectona grandis	D'Arrigo, Palmer, et al. (2011)
Mu Cang Chai	104.06	21.40	Fokienia hodginsii	Sano et al. (2009)
Nam Nao	101.57	16.73	Pinus merkusii	Buckley et al. (1995)
Petchaburi	99.56	12.96	Pinus merkusii	This study
Pha Taem	105.00	15.70	Pinus merkusii	This study
Phou Khao Khouay	102.79	18.32	Pinus merkusii	Buckley, Duangsathaporn, et al. (2007)
Phu Kradung	101.88	16.90	Pinus merkusii	D'Arrigo et al. (1997)
Phu Toei	99.43	14.98	Pinus merkusii	E. R. Cook et al. (2010)
Pu Mat	104.85	19.06	Fokienia hodginsii	Buckley et al. (2019)
Quang Nam	107.33	15.81	Fokienia hodginsii	Buckley et al. (2017)
Salaeng Luang	100.55	16.75	Pinus merkusii	Buckley et al. (1995)
San Luang	97.93	19.10	Pinus merkusii	E. R. Cook et al. (2010)
Wat Chan	98.23	19.02	Pinus merkusii	Buckley et al. (1995)
Wiang Haeng	98.64	19.56	Pinus merkusii	This study

 Table 1.
 Metadata of tree ring width chronologies.

<sup>a</sup> Several cores from this site were analyzed by Zhu et al. (2012) for  $\delta^{18}$ O but the ring width chronology has not been published until now.

Site	Longitude	Latitude	Species	References
Mae Hong Son	98.93	19.28	Pinus merkusii	C. Xu et al. (2015)
Mu Cang Chai	104.06	21.40	Fokienia hodginsii	Sano et al. $(2012)$
Phou Khao Khouay	102.79	18.32	Pinus merkusii	C. Xu et al. (2019)
Umpang	98.87	16.09	Pinus merkusii	C. Xu et al. (2018)

Table 2. Metadata of  $\delta^{18}O$  chronologies.

described in Text S3. After naturalization, we aggregated daily data into dry season (November–

June), wet season (July–October), and water year (November–October). The season de-

lineation was determined by the method of B. I. Cook and Buckley (2009) (Text S2). To

match the proxies' time span, we finally used the streamflow data from November 1921

144 to October 2005.

#### <sup>145</sup> 2.4 Proxy–Streamflow Correlations

As a preliminary investigation, we performed correlation analyses between stream-146 flow and proxy data. Correlations are calculated at different lags: l = -2 to +2 years. 147 Negative lags account for the case when trees use stored carbon from previous years, and 148 positive lags for the case when the catchment's runoff processes are slower than precip-149 itation inputs (Stockton & Jacoby, 1976; Meko et al., 2007). For robustness, we repeated 150 the correlation analysis 1,000 times using the stationary bootstrap (Politis & Romano, 151 1994). In the following discussion we refer to the median bootstrap correlations (Figure 152 2).153

Among the ring width sites, there are multiple correlation patterns (Figure 2a): some sites such as Chin Hills and Phu Toei correlate positively, while others (e.g., Phou Khao Khouay) correlate negatively. Peculiarly, the Mae Hong Son site displays significant negative correlation at l = -2 but significant positive correlations at l = 0 and l = 2. Five sites do not correlate with streamflow at all. These various patterns suggest that the ring width-streamflow relationship is complex and "noisy". A large number of sites are thus required to extract the strongest signals.

<sup>161</sup> Unlike ring width,  $\delta^{18}$ O displays more consistent correlation patterns (Figure 2b): <sup>162</sup> all significant correlations are negative, and the strongest correlations are often observed <sup>163</sup> at l = 0. Some correlations have magnitudes larger than 0.5, while the largest corre-<sup>164</sup> lation magnitude in ring width is only 0.36. These observations corroborate that  $\delta^{18}$ O <sup>165</sup> chronologies may contain stronger climate signals than do ring width chronologies (C. Xu <sup>166</sup> et al., 2019; Gagen et al., 2011).

In general, we observe that ring width tends to correlate more strongly with dry season flow than with wet season flow. Conversely,  $\delta^{18}$ O tends to correlate more strongly with wet season flow than with dry season flow. Both proxies correlate well with annual flow. The proxy-streamflow correlations observed here are also in agreement with the proxy-precipitation correlation analysis (Text S5). Both analyses show that tree ring proxies have different strength and sensitivity to different parts of the hydrograph, and have the potential to be combined for better seasonal reconstructions.

#### **3** Reconstruction Framework

The correlation analysis shows diverse seasonal sensitivity among proxy chronologies and at different lags. To build reconstruction models, we define an *input* as a chronologylag combination that significantly correlates with streamflow. For instance, some inputs for the annual reconstruction are Chin Hills ring-width at lag -2, and Umpang  $\delta^{18}$ O at lag 0 (Figure 2).

The reconstruction framework consists of two main modules: Regression and Input Selection. In Regression (Section 3.1), the selected inputs for each target are given, and we find the regression coefficients that best match the targets while accounting for mass balance simultaneously, using a *penalized least squares* formulation. In Input Selection (Section 3.2), we find the best subset of inputs that minimizes the penalized least



#### a) Correlations between ring width and instrumental + naturalized streamflow

Figure 2. Streamflow-proxy correlations. The error bars show the  $5^{\text{th}}-95^{\text{th}}$  bootstrapped empirical quantiles obtained from 1,000 replicates, using the stationary bootstrap (Politis & Romano, 1994). The dots indicate the medians. Lag *l* denotes correlations between proxy at year *t* and streamflow at year t + l.

squares. The two modules are unified in a nested optimization framework that includes a rigorous cross-validation scheme to assess reconstruction skills (Section 3.3).

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#### 3.1 Mass-balance-adjusted Regression

Assume that we have a matrix  $U_d$  whose columns contain the selected inputs for the dry season. We first need to remove multicollinearity within  $U_d$ . A common approach in dendrohydrology is to perform Principal Component Analysis (PCA) on  $U_d$ , then reduce the set of principal components (PCs) to a parsimonious subset that is most relevant to the streamflow target (Hidalgo et al., 2000; Coulthard et al., 2016). Here, we use a backward stepwise PC selection routine (Woodhouse et al., 2006). This transformation from the selected inputs to the selected PCs is denoted as the function g(.):

$$\mathbf{X}_{\mathbf{d}} = g(\mathbf{U}_{\mathbf{d}}) \tag{1}$$

Similarly, given the selected inputs  $\mathbf{U}_{\mathbf{w}}$  for the wet season and  $\mathbf{U}_{\mathbf{q}}$  for the water year, we apply g(.) to get

$$\mathbf{X}_{\mathbf{w}} = g(\mathbf{U}_{\mathbf{w}}) \tag{2}$$

$$\mathbf{X}_{\mathbf{q}} = g(\mathbf{U}_{\mathbf{q}}) \tag{3}$$

Now, let  $y_d, y_w$ , and  $y_q$  be the target time series of dry season, wet season, and annual streamflow, respectively (these targets can be log-transformed when necessary). Reconstructing streamflow for the three targets means solving the following regression equations:

$$\mathbf{y}_{\mathbf{d}} = \mathbf{X}_{\mathbf{d}} \boldsymbol{\beta}_{\mathbf{d}} + \boldsymbol{\varepsilon}_{\mathbf{d}}$$
(4)

$$\mathbf{y}_{\mathbf{w}} = \mathbf{X}_{\mathbf{w}} \boldsymbol{\beta}_{\boldsymbol{w}} + \boldsymbol{\varepsilon}_{\boldsymbol{w}} \tag{5}$$

$$\mathbf{y}_{\mathbf{q}} = \mathbf{X}_{\mathbf{q}} \boldsymbol{\beta}_{\boldsymbol{q}} + \boldsymbol{\varepsilon}_{\boldsymbol{q}} \tag{6}$$

where  $\beta_d$ ,  $\beta_w$ , and  $\beta_q$  are the corresponding regression coefficients; and  $\varepsilon_d$ ,  $\varepsilon_w$ , and  $\varepsilon_q$ are white noise.

<sup>10</sup> 
$$\mathbf{y} = \begin{bmatrix} \mathbf{y}_{\mathbf{d}} \\ \mathbf{y}_{\mathbf{w}} \\ \mathbf{y}_{\mathbf{q}} \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} \mathbf{X}_{\mathbf{d}} & & \\ & \mathbf{X}_{\mathbf{w}} \\ & & \mathbf{X}_{\mathbf{q}} \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \boldsymbol{\beta}_{d} \\ \boldsymbol{\beta}_{w} \\ \boldsymbol{\beta}_{q} \end{bmatrix}, \quad \text{and} \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \boldsymbol{\varepsilon}_{d} \\ \boldsymbol{\varepsilon}_{w} \\ \boldsymbol{\varepsilon}_{q} \end{bmatrix}.$$
 (7)

Equations 4–6 can then be converted to a more compact form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}.$$
 (8)

Equation 8 has the canonical form of linear regression. It can be solved as a least-squares problem:

$$\min_{\boldsymbol{\beta}} \quad J_1 = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}), \tag{9}$$

216 yielding the solution

$$\boldsymbol{\beta} = \left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{X}'\mathbf{y}.$$
(10)

Solving Equation 8 is equivalent to solving Equations 4–6 simultaneously. The three re-

gression problems in Equations 4–6 are independent of one another, and the above for-

mulation places no constraints to match the sum of the seasonal flows to the annual flow.

Therefore, such formulation can yield large differences in the annual mass balance. As

we shall see later, this happens at station P.1.

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To account for mass balance, it is tempting to impose a constraint,

$$\mathbf{X}_{\mathbf{d}}\boldsymbol{\beta}_{\boldsymbol{d}} + \mathbf{X}_{\mathbf{w}}\boldsymbol{\beta}_{\boldsymbol{w}} = \mathbf{X}_{\mathbf{q}}\boldsymbol{\beta}_{\boldsymbol{q}}.$$
 (11)

But, Equation 11 is often overdetermined: it is a system of T equations, one for each year, and we almost always have more equations than unknowns in a regression problem. Instead, we can add to the objective function in Equation 9 a penalty term that is based on the differences ( $\delta$ ) between the LHS and the RHS of Equation 11.

$$\delta = \mathbf{X}_{\mathbf{d}}\boldsymbol{\beta}_{\boldsymbol{d}} + \mathbf{X}_{\mathbf{w}}\boldsymbol{\beta}_{\boldsymbol{w}} - \mathbf{X}_{\mathbf{q}}\boldsymbol{\beta}_{\boldsymbol{q}}.$$
 (12)

<sup>230</sup> If the reconstructions involve log-transformed flows, the mass difference is

$$\delta_t = \log \left( \exp(\mathbf{x}_{\mathbf{d},t} \boldsymbol{\beta}_{\mathbf{d}}) + \exp(\mathbf{x}_{\mathbf{w},t} \boldsymbol{\beta}_{\mathbf{w}}) \right) - \mathbf{x}_{\mathbf{q},t} \boldsymbol{\beta}_{\mathbf{q}} \qquad \forall t = 1, ..., T.$$
(13)

Just as we minimize the squared differences between prediction and observation, we also minimize the squared mass differences. Finally, we add a weight  $\lambda$  to represent the importance of the penalty term, and obtain a new objective function

 $\min_{\boldsymbol{\beta}} \quad J_2 = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) + \lambda \boldsymbol{\delta}' \boldsymbol{\delta}$ (14)

We call this the *penalized least squares* problem. Observe that when  $\lambda = 0$ , the penalty term disappears, and the penalized least squares problem becomes the canonical least squares problem. The higher  $\lambda$  is, the more important the penalty becomes.

<sup>239</sup> Without flow transformation,  $\delta$  is linear (Equations 12), so  $J_2$  is quadratic. We can <sup>240</sup> solve Equation 14 analytically to get

 $\boldsymbol{\beta} = (\mathbf{X}'\mathbf{X} + \lambda \mathbf{A}'\mathbf{A})^{-1}\mathbf{X}'\mathbf{y}$ (15)

where  $\mathbf{A} = [\mathbf{X}_{\mathbf{d}} \quad \mathbf{X}_{\mathbf{w}} \quad -\mathbf{X}_{\mathbf{q}}]$ . The proof is provided in Text S6.

<sup>243</sup> When log-transformations are involved,  $\delta$  is not linear, and Equation 14 cannot be <sup>244</sup> solved analytically. But it can be solved numerically using any nonlinear solver. Here, <sup>245</sup> we use an efficient quasi-Newton method called L-BFGS-B (Byrd et al., 1995), available <sup>246</sup> in the R function optim(). We have implemented the mass-balance-adjusted regression <sup>247</sup> procedure in the R package mbr, currently available on GitHub at github.com/ntthung/ <sup>248</sup> mbr.

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#### 3.2 Optimal Input Selection

A consolidated approach to input selection in the literature is to use Branch and Bound algorithms, such as Leaps and Bounds (Furnival & Wilson, 1974) or its more recent variants (Duarte Silva, 2001, 2002). These algorithms are conceived to balance goodnessof-fit with model simplicity. In this work however, we also need to account for mass balance besides goodness-of-fit. Therefore, the input selection routine must explicitly account for the penalized least squares objective (Equation 14). If the number of inputs is small, we can exhaustively search all possible subsets and choose the one that yields the minimum penalized least square value (PLSV). However, this method quickly becomes infeasible with increasing input size: there are  $2^n$  subsets of n inputs (for station P.1, n = 19, 28, and 30). A computationally tractable optimization is necessary (Galelli et al., 2014).

We formulate input selection as a binary optimization problem. Each input has an index, and a binary vector  $\mathbf{p}$  encodes input selection:  $p_i = 1$  means the *i*<sup>th</sup> input is selected. For any given  $\mathbf{p}$ , i.e., for any given input subset, we can solve the mass-balanceadjusted regression problem to obtain a PLSV. Our goal then is to find  $\mathbf{p}$  that has the best PLSV over all  $\mathbf{p}$ 's.

Note that  $\mathbf{p}$  has three components:  $\mathbf{p} = [\mathbf{d} \ \mathbf{w} \ \mathbf{q}]'$ . Component  $\mathbf{d}$  represents the dry season:

$$d_i = \begin{cases} 1 & \text{if proxy } i \text{ is used for the dry season} \\ 0 & \text{otherwise} \end{cases} \qquad i = 1, ..., n_d. \tag{16}$$

(17)

So, where  $d_i = 1$ , we take the *i*<sup>th</sup> inputs and place into the matrix  $\mathbf{U}_{\mathbf{d}}$ . Similarly, we create  $\mathbf{U}_{\mathbf{w}}$  from  $\mathbf{w}$  and  $\mathbf{U}_{\mathbf{q}}$  from  $\mathbf{q}$ . Once we have  $\mathbf{U}_{\mathbf{d}}$ ,  $\mathbf{U}_{\mathbf{w}}$ , and  $\mathbf{U}_{\mathbf{q}}$ , the mass-balanceadjusted regression procedure can be applied. To improve the robustness of the input selection, the regression is cross-validated 50 times (Section 3.3), each yields one PLSV estimate. The average of all runs, denoted  $f(\mathbf{p})$ , is used as the final PLSV for  $\mathbf{p}$ .

274 The remaining task is to solve

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$$\min_{\mathbf{p}} f(\mathbf{p}).$$

We solve Equation 17 with Genetic Algorithm (Holland, 1975), a metaheuristic optimization technique that allows us to treat the underlying regression as a black-box while searching for the best subset of inputs (Kohavi & John, 1997), and is well suited for binary optimization (Whitley, 1994). We use the R package GA (Scrucca, 2013). Details about the implementations are provided in Text S8.

3.3 Model Assessment

We set up a reconstruction experiment involving two models: Model 0 runs without the mass balance adjustment ( $\lambda = 0$  in Equation 14) and Model 1 has the adjustment ( $\lambda = 1$ ). Other than the different values for  $\lambda$ , both models are trained exactly the same way, following Sections 3.1 and 3.3.

During optimization, multiple reconstructions are created while the optimal  $\mathbf{p}$  is sought for each model. These reconstructions are assessed with the PLSV. The final reconstructions, created with the optimal inputs, are further assessed post hoc with the commonly used metrics: coefficient of determination ( $\mathbb{R}^2$ ), reduction of error ( $\mathbb{R}E$ ), and coefficient of efficiency (CE) (Nash & Sutcliffe, 1970; Fritts, 1976). All metrics are calculated over 50 cross-validation runs.

Following Nguyen et al. (2020), we adopt a leave-25%-out cross-validation scheme, where each hold-out chunk is contiguous. The contiguous chunks aim to test whether

the reconstruction can capture regimes in the time series, in line with the traditional split-294

sample scheme. The 50 repetitions provide a distribution for each skill metric, allowing 295

more robust estimation of the mean skill score. More importantly, the distributions en-296

able us to assess the statistical significance of skills. For example, a reconstruction is con-297

- sidered statistically skillful with respect to CE at  $\alpha = 0.1$  if the probability of nega-298
- tive CE is less than 0.1. 299

#### 4 Results 300

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## 4.1 Reconstructions

For Model 0's dry season and annual reconstructions, all metrics are at least 0.40, 302 and the reconstructions match their targets closely (Figure 3a). Furthermore, these re-303 constructions are statistically skillful at  $\alpha = 0.1$ . Conversely, Model 0's wet season re-304 construction is not statistically skillful. Although the mean RE and CE are positive (RE 305 = 0.35, CE = 0.23), these scores vary widely over the cross-validation runs (Figure S12), 306 suggesting that the wet season reconstruction is sensitive to training data. The large vari-307 ability of skills is also consistent with the high variability of streamflow (Figure S5). These 308 observations suggest that there may be nonlinearity in the streamflow-proxy relation-309 ships at the extremes. In future studies, nonlinear reconstruction models (e.g., Nguyen 310 & Galelli, 2018) could be incorporated to address this problem. 311

Model 1, with the penalty term, makes visible adjustments to the seasonal recon-312 structions but minimal changes to the annual one for the instrumental period (Figure 313 3a). Dry season skills slightly decrease, wet season's RE and CE increase, and annual 314 skills remain almost the same. While the mean skill scores of both models are similar, 315 Model 1 produces notably narrower distributions of RE and CE for the wet season (Fig-316 ure S12). Consequently, Model 1's wet season reconstruction becomes statistically skill-317 ful. Overall, Model 1 is more robust. 318

To understand Model 1's robustness, let us recall the models' formulation. Model 319 0 reconstructs the dry season, wet season, and annual flows independently. Each recon-320 struction is geared towards its own target, and can become sensitive to training data— 321 the wet season reconstruction does. Contrarily, Model 1 links all three reconstructions 322 together via the penalty term (Equations 12–14). This link provides each reconstruction 323 with additional information from the other two, thus preventing each reconstruction from 324 overfitting to its own target. In our case, the wet season reconstruction benefited sig-325 nificantly from this additional information to become statistically skillful, with minimal 326 trade-off from the other two reconstructions. 327

The selected input subsets by both models provide further insights into their sim-328 ilarities and differences. Both models use similar input subsets, with identical ones for 329 the water year. However, Model 1 uses fewer inputs than does Model 0 for the wet and 330 dry seasons (Figure 4). Therefore, the models behave similarly, but Model 1 is more par-331 simonious. 332



Figure 3. (a) Reconstruction skills and time series for the instrumental period, produced using two models: without mass balance penalty ( $\lambda = 0$ ) and with penalty ( $\lambda = 1$ ) in the regression problem (Equation 14). Grey lines show naturalized observations. Underlined scores show where the reconstruction is not statistically skillful at  $\alpha = 0.1$ . (b) Full reconstructions with  $\lambda = 1$ .



Figure 4. Selected inputs for each streamflow target (columns) in each models (panels). Only inputs that were selected at least once are shown. The stable oxygen isotope (OX) inputs are marked in dark red. Bold numbers at the bottom row of the x-axis are the number of selected inputs in each column.

Surprisingly, the Mu Cang Chai and Mae Hong Son  $\delta^{18}$ O chronologies were con-333 sistently selected by both models for all reconstructions, including the dry season recon-334 structions where we expected ring width chronologies to dominate, based on the observed 335 tendencies of ring width to correlate more with wet season flow and  $\delta^{18}$ O to correlate 336 more with dry season flow. Upon closer examinations of the correlation analysis (Fig-337 ure 2), the puzzle is solved. First, the  $\delta^{18}$ O chronologies are intercorrelated (C. Xu et 338 al., 2019), and the input selection algorithm correctly selected the two sites that exhibit 339 the strongest correlations. Second, while these  $\delta^{18}$ O chronologies correlate less with dry 340

season flow than they do with wet season flow, the correlations are still stronger than
 those observed at many ring width sites.

Over the whole study horizon, we observe similar results to those of the instrumental period (Figure S13). The two models agree with each other. Model 1's adjustments are generally small. The largest adjustments are in the wet season ( $\pm 400 \text{ Mm}^3$ ); smaller but notable adjustments are seen in the dry season ( $\pm 200 \text{ Mm}^3$ ), and minute adjustments (< 90 Mm<sup>3</sup>) are seen in the annual reconstruction. We will examine the effects of these adjustments in Section 4.2.

The reconstructions provide some interesting insights into the inter- and intra-annual 349 variability of the river (Figure 3b). Between 1825–1855, sustained low flow was observed 350 in the wet season and water year reconstructions. However, in the dry season, the low 351 flow period ended 15 years earlier, around 1840. Conversely, a period of sustained high 352 flow was observed in all three reconstructions between 1790–1820, especially for the dry 353 season. Most notably, dry season flow in 1815 was so high that it accounted for more than 354 50% of the annual flow—a rare event that occurred in only 8 of 254 years (Figure S14, 355 see also Text S9). 356

357

#### 4.2 Annual Mass Balance

For each model, we compare the total seasonal flow with the annual flow. To pre-358 serve the annual mass balance, these two time series should ideally be the same. How-359 ever, for Model 0, large discrepancies are seen between the two time series (Figure 5a). 360 For Model 1, the two time series agree with each other better. As each time series pro-361 vides an estimate of the annual water budget, we are also interested in their distribu-362 tions. We observe that the distributions produced by Model 0 are notably different from 363 each other, but those produced by Model 1 are almost identical (Figure 5b). This im-364 plies that the distributions derived from Model 1 are more reliable. Using the same anal-365 ysis, we show that Model 1 also produces more reliable distributions of the dry and wet 366 season's water budget than does Model 0 (Figure S15). 367

Next, for each model, we calculate the mass difference,  $\Delta Q$ , between the total sea-368 sonal flow and the annual flow, then examine its trajectory and distribution (Figures 5c 369 and 5d). The mass difference for Model 0 ranges from  $-640 \text{ Mm}^3$  to  $600 \text{ Mm}^3$ , while that 370 range for Model 1 is  $-270 \text{ Mm}^3$  to  $370 \text{ Mm}^3$ ; a 50% reduction in range. Moreover, Model 371 0 yields a mass difference outside the interval  $\pm 190 \text{ Mm}^3$  ( $\pm 10\%$  of the mean annual flow; 372 shaded region in Figure 5d) in 28% of the years. That figure for Model 1 is only 11%. 373 By these metrics, Model 1 is twice better than Model 0 in terms of preserving mass bal-374 ance. 375

### <sup>376</sup> 5 Discussion and Conclusions

In Section 4.1, we showed that the optimal input selection procedure yields good reconstruction skills for both model setups, and that Model 1, by imposing a mass balance adjustment, produces more robust reconstructions than does Model 0. More im-



Figure 5. (a) Comparison between the total seasonal flow (TSF; Wet + Dry) and the annual flow (AF; Water year) for Model 0 ( $\lambda = 0$ ) and Model 1 ( $\lambda = 1$ ). (b) Distributions of the annual water budget, estimated by either the TSF or the AF for both models. (c) The differences,  $\Delta Q$ , between the TSF and the AF. (d) Distributions of  $\Delta Q$ . The shaded region denotes the ±190 Mm<sup>3</sup> range, equivalent to ±10% of the mean annual flow.

portantly, the adjustment significantly reduces the differences between the total seasonal flow and the annual flow (Section 4.2). Without the adjustment, the mass difference can be as large as 640 Mm<sup>3</sup>, or about 30% of the mean annual flow. It amounts to 90% of the irrigation demand from the Ping River downstream of Bhumibol Reservoir (Divakar et al., 2011). Such a discrepancy may lead to water allocation disputes. With the adjustment, both the frequency and magnitude of discrepancies are reduced—this is cru-

cial for water availability assessment, a major goal of dendrohydrology.

We also showed that the mass-balanced-adjusted regression produces reliable dis-387 tributions of the seasonal and annual streamflow. These distributions can be used for 388 probabilistic studies in water resources applications. For example, sub-annual stochas-389 tic time series can be generated from the distributions to be used in bottom-up vulner-390 ability assessments of water systems (Pielke et al., 2012; Herman et al., 2016). In Text 391 S10 we illustrate one simple way to do so (by sampling from a bivariate distribution fit-392 ted to the seasonal reconstructions), but more advanced methods are available (e.g., Bor-393 gomeo, Farmer, & Hall, 2015; Borgomeo, Pflug, et al., 2015). 394

The framework that we proposed here can be reapplied and expanded in several 395 ways. First, analysts adopting our framework have the choice to tune  $\lambda$ , depending on 396 how important it is to preserve mass balance in their applications. In this case, a sen-397 sitivity analysis with respect to  $\lambda$  may be informative. Second, the mass balance formu-398 lation is applicable to other climate variables such as precipitation, and to other contexts 399 where a penalty term in the regression equation is desirable. For example, if one wishes 400 to reconstruct streamflow at two tributaries as well as the main stream of a river, the 401 mass balance adjustment should be used to minimize the difference between the total 402 flow of the tributaries and the flow on the main stream. Finally, the mass balance for-403 mulation is readily extendable to higher resolutions, e.g., quarterly or monthly (Text S7), 404 as long as the proxy network is sensitive enough to the higher resolution targets. These 405 directions can help dendrohydrology realize its value in operational water management, 406 an area where annual, unconstrained streamflow reconstructions have had limited suc-407 cess. 408

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