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Corresponding Author: Dr. Douglas James Booker, Ph.D.

Corresponding Author's Institution: National Institute of Water and Atmospheric Research

First Author: Douglas James Booker, Ph.D.

Order of Authors: Douglas James Booker, Ph.D.; Ross A Woods, Ph.D.

Suggested Reviewers: Neil Viney PhD Principal Research Scientist, Modelling catchment hydrology, CSIRO Neil.Viney@csiro.au Expertise in hydrological modelling, prediction in ungauged basins and ensemble modelling.

David Post PhD Senior Research Scientist, Land and Water, CSIRO David.Post@csiro.au Expertise in catchment-scale hydrology, regionalisation to ungauged catchments, land use and climate change impacts on hydrology.

Parajka Juraj PhD Research and Lecturer, Centre for Water Resource Systems, Institute of Hydraulic Engineering and Water, Vienna University of Technology parajka@hydro.tuwien.ac.at Expertise in Experimental Hydrology, Hydrology, Snow modelling and water balance modelling.

Stacey Archfield PhD Research Hydrologist, Massachusetts-Rhode Island Water Science Center, USGS sarch@usgs.gov Expertise in flood prediction in ungauged catchments, environmental flow setting, hydrological regionalisation

Mike Acreman PhD Senior scientist, Ecohydrological processes, entre for Ecology and Hydrolgy, UK man@ceh.ac.uk Expertise in water resource assessment, environmental flow setting and flow duration curve analysis

Highlights for "Comparing and combining physically-based and empirically-based approaches for estimating the hydrology of ungauged catchments" by Booker and Woods

- Methods for estimating various hydrological indices at ungauged sites were compared.
- Methods included a TopNet rainfall-runoff model and a Random Forest empirical model.
- TopNet estimates were improved through correction using Random Forest estimates.
- Random Forests provided the best estimates of all indices except mean flow.
- Mean flow was best estimated using an already published empirical method.

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5	estimating the hydrology of ungauged catchments.
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8	Booker, D.J. ^{a*} , Woods, R.A. ^b
9	
10	^a National Institute of Water and Atmospheric Research,
11	P O Box 8602
12	Riccarton,
13	Christchurch,
14	New Zealand
15	Email address: d.booker@niwa.co.nz
16	Phone: +64 (0)3 348 8987
17	Fax: +64 (0)3 348 7891
18	
19	^b Department of Civil Engineering
20	University of Bristol,
21	Bristol,
22	UK
23	Email address: ross.woods@bristol.ac.uk
24	
25	*Corresponding author
26	
27	Short title: hydrological estimates for ungauged catchments
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29

Abstract

30 Predictions of hydrological regimes at ungauged sites are required for various 31 purposes such as setting environmental flows, assessing availability of water resources or 32 predicting the probability of floods or droughts. Four contrasting methods for estimating 33 mean flow, proportion of flow in February, 7-day mean annual low flow, mean annual high 34 flow, the all-time flow duration curve and the February flow duration curve at ungauged sites 35 across New Zealand were compared. The four methods comprised: 1) an uncalibrated 36 national-coverage physically-based rainfall-runoff model (TopNet); 2) data-driven empirical 37 approaches informed by hydrological theory (Hydrology of Ungauged Catchments); 3) a 38 purely empirically-based machine learning regression model (Random Forests); and 4) 39 correction of the TopNet estimates using flow duration curves estimated using Random 40 Forests. Model performance was assessed through comparison with observed data from 485 41 gauging stations located across New Zealand. Three model performance metrics were 42 calculated: Nash-Sutcliffe Efficiency, a normalised error index statistic (the ratio of the root 43 mean square error to the standard deviation of observed data) and the percentage bias. Results 44 showed that considerable gains in TopNet model performance could be made when TopNet 45 time-series were corrected using flow duration curves estimated from Random Forests. This 46 improvement in TopNet performance occurred regardless of two different parameterisations 47 of the TopNet model. The Random Forests method provided the best estimates of the flow 48 duration curves and all hydrological indices except mean flow. Mean flow was best estimated 49 using the already published Hydrology of Ungauged Catchments method.

50

51 Key words: hydrological indices; flow duration curves; ungauged sites; rainfall-runoff model;
52 random forests.

54 1. Introduction

55 River water provides a valuable resource for out-of-stream water use as well as for supporting in-stream environmental values. Alteration of natural river flow regimes is 56 57 increasing globally as water is taken for human, agricultural and industrial use and power production, threatening both river biodiversity and security of human water use (Vörösmarty 58 59 et al., 2010). Globally, this has led to a variety of legislative processes aimed at promoting 60 prudent and rational use of natural water resources which seek to judge the trade-off between 61 economic development and impact to the natural environment (e.g. EC, 2000; New Zealand 62 Government, 2011). For example, default limits to water resource use for all rivers in New 63 Zealand must comprise at least a minimum flow (the flow below which no water can be 64 abstracted) and an allocation limit (a limit on the amount of abstraction taken from the 65 resource) (New Zealand Government, 2011; Snelder et al., 2013).

66 Information summarising natural flow regimes is therefore required to assess both the 67 in-stream environmental and out-of-stream economic effects of potential alterations to flow 68 regimes. This information may take the form of various hydrological indices describing 69 different aspects of the flow regime such as low flows, high flows or flow variability (Olden 70 and Poff, 2003; Poff et al., 2010). Flow duration curves (FDCs) may also be utilised for 71 various purposes including low flow analysis (Smakhtin, 2001), quantifying reliability of 72 water supply (Snelder et al., 2011) and quantifying alterations to hydrological regimes (Vogel 73 et al., 2007). This type of hydrological information is ideally derived from observed flow 74 time-series at the site, or sites, of interest. However, flow time-series are only available at a small number of locations where flow gauges have been maintained and operated. 75 76 Hydrological estimates are therefore often required at ungauged sites across a catchment or 77 landscape (Sivapalan et al., 2003).

78 A variety of approaches can be used to provide estimates of hydrological indices at 79 ungauged sites. In theory, these approaches range from purely physically-based to purely 80 empirically-based. Physically-based approaches have also been referred to as deterministic 81 (Chow et al., 1988), distributed (Beven and Binley, 1992), physics-based (Pechlivanidis et 82 al., 2011), process-based or Newtonian (Yaeger et al., 2012). Empirically-based approaches 83 have also been referred to as stochastic (Chow et al., 1988), metric (Pechlivanidis et al., 84 2011) data-based or Darwinian (Yaeger et al., 2012). Physically-based approaches are those 85 that aim to estimate streamflow by utilising a conceptual understanding of the physics 86 describing various parts of the hydrological cycle by approximating physical processes such 87 as interception, evaporation, and storage (e.g. Beven and Kirkby, 1979; Clark et al., 2008). However, assumptions about physical processes are necessarily required to apply this 88 89 understanding (Beven, 1997). For example, assumptions about continuity of volumes, 90 discretisation of governing equations and some form of spatial averaging may be required for 91 a physically-based approach to be spatially-distributed (Beven, 1989; Bloschl and Sivapalan, 92 1995; Singh and Frevert, 2006). Similarly, time dependence must be represented by updating 93 state variables through a sequence of time steps (Singh, 1995). Physically-based approaches 94 may also require spatially distributed input data such as information on soil characteristics 95 such as water holding capacity, rainfall time-series or temperature time-series (e.g. Clark et 96 al., 2008). This has led to much analysis and debate relating to data needs, parameter 97 calibration and uncertainty in physically-based hydrological models (Beven, 1997; Beven, 98 1989; Singh and Woolhiser, 2002; Gupta et al., 2006). 99 Empirically-based approaches are those that seek to estimate hydrological indices by 100 quantifying patterns between observed hydrological indices and catchment characteristics. 101 These patterns can be quantified using a variety of techniques including linear regression

102 (e.g. Engeland and Hisdal, 2009), or machine learning techniques (e.g. Booker and Snelder,

2012). One advantage of empirically-based approaches is that their relative simplicity has
allowed them to be transferred to ungauged catchments by way of regionalisation (e.g.
Castellarin et al., 2004), generalisation or dissimilarity modelling (e.g. Booker and Snelder,
2012).

In practice, many physically-based models have empirical components and many 107 108 empirical models incorporate some level of knowledge about physical processes. A balance 109 between model complexity and data availability must be found for both physically-based 110 (Fenicia et al., 2008) and empirically-based (Jakeman and Hornberger, 1993) approaches. All 111 physically-based approaches require some parameterisation, and are known to perform best 112 when calibrated against observed data (e.g. Clark et al., 2008; McMillan et al., 2013). 113 Similarly, the independent variables used in empirically-based approaches are often chosen 114 after consideration of physical principles and the form of fitted empirical relationships can 115 also be interrogated to ensure consistency with physical principles (e.g. Booker and Snelder, 116 2012). Hybrid metric-conceptual models are those that seek to combine the strengths of 117 empirically-based and physically-based conceptual models (Pechlivanidis et al., 2011). 118 Despite the variety of approaches available for estimating hydrological conditions at 119 ungauged sites, few studies have compared estimates calculated using contrasting 120 approaches. The aim of this work was to compare a variety of available methods for 121 estimating several hydrological indices and flow duration curves at ungauged catchments 122 across New Zealand. These methods employed a range of approaches from a physically-123 based rainfall-runoff model to empirically-based regressions. The primary aim was to objectively judge which method was best able to estimate several hydrological indices across 124 125 New Zealand given current climatic and landcover conditions. The secondary aim was to 126 assess the advantages of combining two approaches by correcting physically-based estimated 127 time-series using empirically-based estimated FDCs.

128 **2. Data Description**

129 *a.* Flow time-series

130 A flow time-series database was collated that comprised mean daily flows observed at 131 485 gauging stations with available records of 5 full years or longer. Available mean daily flow time-series from the National Institute of Water and Atmospheric Research's (NIWA) 132 133 national database were collated alongside data supplied by particular regional councils 134 (Northland Regional Council, Auckland Council, Waikato Regional Council, Greater 135 Wellington Regional Council, and Environment Canterbury). The time-series database 136 contained only sites that were not affected by large engineering projects such as dams, 137 diversions or substantial abstractions, according to information given by each data provider. 138 See Snelder et al. (2005) and Booker (in press) for further details on gauging station 139 selection. These gauging stations were located throughout New Zealand (Figure 1) and 140 represented a wide range of hydrological conditions (Table 1). The observed time-series did 141 not all cover the same time periods.

142 It is known that hydrological regimes may not be stationary (constant mean and 143 constant variance through time; Hamilton, 1994) due to the presence of trends and temporal 144 autocorrelations (Milly et al., 2008). This is because hydrological regimes may be influenced 145 by a variety of factors including land cover change (e.g. Fahey & Jackson, 1997), inter-146 decadal climatic patterns (e.g. Kiem et al., 2003) and longer-term climate shifts (Parry et al., 147 2007). However, the purpose of this study was to compare the ability of various approaches 148 to characterise differences in flow regimes between sites across New Zealand given current 149 climatic and land cover conditions rather than to characterise differences through time. For 150 empirically-based methods it was therefore assumed that differences in hydrological regimes 151 between sites far exceeded any differences in hydrological regimes that may have occurred 152 due to differences in observation periods (which were different for each observed time-series)

despite some evidence for inter-decadal patterns in some, but not all, indices for particular
regions of New Zealand but not others (e.g. McKerchar and Henderson, 2003; Booker, in
press).

156 b. Observed hydrological indices

Several hydrological indices were calculated for each observed flow time-series 157 158 (Table 2). These indices were chosen because they represent a range of hydrological 159 conditions including floods and droughts, can be used to estimate water resource availability, 160 and are used in environmental flow setting procedures. Mean flow, Q_{bar}, represents total 161 potential water availability, is used for scaling of dimensionless metrics such as standardised 162 flow duration curves (e.g. Booker and Snelder, 2012) and may be used when comparing sites 163 for ecological studies (e.g. Leathwick et al., 2005). The proportion of flow in each month 164 may be of interest when investigating seasonality of flow. The proportion of flow in 165 February, Q_{Feb}, was chosen as an example because the mid-summer month of February 166 represents a generally dry month in which both irrigation demand (the largest consumptive 167 water use in New Zealand) and ecological stress are likely to be high. The 7-day mean annual 168 low flow, Q_{MALF}, is often used as an indicator of low flow in ecological studies (e.g. Caruso, 169 2002; Suren and Jowett, 2006) and to represent one component of the flow regime in 170 environmental flow assessments (e.g. Richter et al., 1997; Poff et al., 1997). Since limits to 171 water resource use may be expressed as proportions of Q_{MALF}, this index is of particular 172 interest in New Zealand (MFE, 2008). Mean annual flood, Q_F, may be used for flood risk 173 assessment and flood design, but may also be used as a surrogate for physical disturbance 174 (e.g. Poff and Ward, 1989; Poff, 1996) especially when compared to geomorphological 175 characteristics such as sediment grain size and channel slope (Clausen and Plew, 2004). All four of these hydrological indices may also be used for data driven environmental 176 177 classifications (e.g. Snelder and Booker, 2012). Many further hydrological indices could have

been compared, but it was desirable to provide an expedient analysis and there is known to be
a high degree of covariance within sets of these indices (Clausen and Biggs, 1997; Olden and
Poff, 2003).

In order to minimise the likelihood of low flow periods crossing years, each day in each observed time-series was assigned to a water year starting on the 1st of October. Water years with more than 30 days of missing data were excluded from the analysis. Calculations of (Q_{MALF}) , and mean annual flood (Q_F) were based on water years. Q_{MALF} was calculated as being the mean of the 7-day running average annual low flow in each water year.

Many hydrological indices are scale-dependent; bigger catchments have larger values of Q₅, Q_{MALF}, Q_F and Q_{bar} than smaller catchments. The values for these indices were therefore standardised by dividing by catchment area. Further transformations were then applied in order to more closely approximate normal distributions (Table 2).

190 *c. Flow duration curves*

FDCs represent the relationship between magnitude and frequency of flow by 191 192 defining the proportion of time for which any discharge is equalled or exceeded (Vogel and 193 Fennessey, 1994; Vogel and Fennessey, 1995). Flow duration curves are a useful tool for 194 quantifying flow regimes for both resource availability (Snelder et al., 2011) and for 195 departure from a reference state (Vogel et al., 2007). For each flow time-series two observed 196 FDCs were calculated from mean daily flows. FDCs were calculated from: a) mean daily 197 flows in all months of the year; and b) mean daily flows in February. These two FDCs 198 represent the probability distribution of flow over all-time and the probability distribution of 199 flow for the month of February over all years. As above, February was chosen to represent a 200 dry month in which both irrigation demand and ecological stress are likely to be high. 201 For calculation of each FDC, mean daily flows for each gauging station were sorted 202 lowest to highest and then interpolated onto percentile values from 0 to 100 in intervals of 1

to determine the proportion of the time that each flow was not exceeded. Each FDC was
therefore characterised using the same number of data points (101), providing for a balanced
study design in further statistical analysis. All daily flows were divided by catchment area to
allow modelling of differences in mean flow whilst standardising for differences in catchment
size. This was in contrast to the method of Booker and Snelder (2012) which investigated
only the shapes of FDCs after having standardised by Q_{bar}.

209 *d.* Catchment characteristics

210 A GIS representation of the New Zealand river network comprising 550,000 segments, their 211 unique upstream catchments and an associated database of catchment characteristics were 212 used to provide information for each gauging station. The catchment characteristics include a 213 range of categorical and continuous variables (Snelder and Biggs, 2002; Snelder et al., 2004; 214 Leathwick et al., 2011). The GIS river network and associated databases have previously been used to define a hierarchical classification of New Zealand's rivers called the River 215 216 Environment Classification (REC; Snelder and Biggs 2002). These databases provide 217 inventories for river resource analysis and management purposes (Snelder and Hughey, 2005; 218 Leathwick et al., 2011; Clapcott et al., 2010; Clapcott et al., 2011). They have also been used 219 to create nationwide models for estimating flow statistics such as flood flows (Pearson and 220 McKerchar, 1989), low flows (Pearson, 1995), mean flow (Woods et al., 2006) and shapes of 221 FDCs (Booker and Snelder, 2012) at ungauged sites using relationships between these 222 hydrological metrics and catchment characteristics. Snelder et al. (2005) showed that 223 grouping river segments by nested categorical subdivisions of climate and topography, 224 known as the Source-of-Flow grouping factor (Table 3), provided an a priori hydrological 225 regionalisation.

226

3. **Estimation methods**

227 For this study four methods for calculating hydrological indices and FDCs at 228 ungauged locations were compared (Figure 2). Method 1 used a physically-based approach. 229 Method 2 used a data-driven empirical approach that was informed by hydrological theory to 230 estimate each hydrological index separately. Method 2 can be classified as being a hybrid 231 metric-conceptual approach under the classification proposed by (Pechlivanidis et al., 2011). 232 Method 2 was named after a sequence of projects collectively known as the Hydrology of 233 Ungauged Catchments (HUC) projects. Method 3 used an empirically-based regression 234 approach. Method 4 combined a physically-based and empirically-based approach. All 235 methods were able to produce estimates for all reaches that comprise the NZ river network 236 and were therefore applicable to ungauged sites across New Zealand.

237

a. Method 1 TopNet

238 Topnet is a spatially distributed time-stepping hydrological model which combines 239 TOPMODEL concepts of sub-surface storage controlling the dynamics of the saturated 240 contributing area and baseflow recession (Beven and Kirkby, 1979; Beven et al., 1995) with 241 submodels for snow and plant canopies, and a kinematic wave channel routing algorithm 242 (Goring, 1994). See McMillan et al. (2013) for further detailed description and Clark et al. 243 (2008) for complete model equations.

244 TopNet has two fundamental components: (i) simulating the water balance over sub-245 catchments throughout a river basin, and (ii) routing streamflow from each sub-catchment to 246 the basin outlet. The water balance model includes simulating the storages and fluxes of 247 water in the canopy, snowpack, unsaturated and saturated soil zone. TopNet also accounts for 248 time delay due to flow routing within each sub-basin. Runoff from each sub-basin flows into 249 a digital stream network and is routed through the river network. For this application TopNet 250 models used daily precipitation and temperature data from the New Zealand Virtual Climate

Station Network (Tait, 2008, Tait et al., 2006), which was then disaggregated to hourly
resolution using stochastic disaggregation for precipitation (Rupp et al., 2009). Additional
model boundary conditions were estimated directly from GIS data on topography, soil and
vegetation (Clark et al., 2008; McMillan et al., 2013).

For catchment specific applications TopNet parameters can be calibrated to optimise 255 256 model performance (e.g. Bandaragoda et al., 2004; McMillan et al. 2013). However, in this 257 case uncalibrated national TopNet models of New Zealand (Henderson et al., 2011) were run 258 using an hourly timestep over the period 1973-2010. Two different versions of TopNet were 259 available. National TopNet Version 0 was discretised using Strahler-1 sub-catchments from the REC. The typical catchment area of a Strahler-1 catchment is 0.7 km². This version had a 260 261 spatially uniform value for the parameter, f, which represents the decline in saturated 262 hydraulic conductivity of the soil with depth (Clark et al., 2008). This parameter effectively 263 controls responsiveness of river flow to rainfall. National TopNet Version 1 was discretised using Strahler-3 sub-catchments from the REC. This version had a spatially distributed set of 264 265 values for f. The f parameter took different values according to the hydrological regionalisation described by Toebes and Palmer (1969), ranging from values more than 8 m⁻¹ 266 for steep catchments in the Southern Alps to less than 1 m⁻¹ in flat catchments on the volcanic 267 268 plateau in the central North Island (see Figure 1 for place names). Where flow time-series 269 were required for Strahler-1 and Strahler-2 catchments flow data were downscaled by 270 multiplying flows from the nearest available Strahler-3 node in the REC network by the ratio 271 of the catchment area of the required location with that of the substitute location. For both 272 Version 0 and Version 1 hourly data for the river reach in which each gauging station was 273 located were averaged over each calendar day to obtained mean daily flow time-series. 274 Hydrological indices were then calculated using the same algorithms as were applied to the 275 observed flow time-series.

276 Ideally both observed and estimated time-series would be available for a very long 277 period (e.g. 100 years). However, the available observed flow time-series did not all cover the 278 same period, and TopNet data were available for a uniform time period (1973-2010). This 279 provided the opportunity to test the sensitivity of correspondence between observed and 280 estimated hydrological indices to synchronisation of the observed and TopNet estimated 281 time-series. Observed and TopNet Version 1 estimated indices were compared using two 282 different procedures. For the first procedure, indices calculated from all available observed 283 flows (5 years or more) were compared with those calculated from all available TopNet 284 Version 1 estimated flows (1973-2010). Essentially this procedure assumed that, when 285 averaged over time, both the observed and TopNet estimated time-series represented the long 286 term hydrological conditions (i.e. that both observed and TopNet estimated time-series were 287 stationary and that records were sufficiently long to characterise long term conditions). For 288 the second procedure only the time period for which both observed flows and TopNet 289 estimated flows were available was identified for each gauging station. Observed indices for 290 this period were then compared with TopNet Version 1 estimated indices for the same period 291 at each gauged location. Better fit between synchronised observed and estimated values (the 292 second procedure) in comparison to non-synchronised (the first procedure) would indicate 293 non-stationarities in the observed hydrological regimes that were detectable in the TopNet 294 time-series. Some observed time-series fell completely outside of the TopNet time-series. 295 This reduced the number of time-series available for the second procedure compared to the 296 first.

b. Method 2 *HUC*

The approach used to estimate Q_{bar} for Method 2 (HUC) is described in Woods et al. (2006). Woods et al. (2006) evaluated four simple models of mean annual runoff throughout New Zealand, predominantly based on precipitation information and estimated

evapotranspiration. Model results were compared to observed data and synthesised estimates
of catchment runoff. The preferred model of Woods et al. (2006) subtracts an estimate of
annual actual evapotranspiration from a precipitation surface. Annual actual
evapotranspiration is estimated according to the ratios of potential evapotranspiration with
annual precipitation, and a single water balance parameter which is estimated by independent
calibration. This method applies a regional bias correction to the results of a previously
uncorrected model.

The approach used to estimate Q_{Feb} for Method 2 was to employ a regionalisation of Q_{Feb} based on Source-of-Flow groupings in the REC and New Zealand island (i.e. North Island or South Island, Figure 1), where Source-of-Flow is a combination of the climate and topography classes of a catchment (Table 3). For each region Q_{Feb} was the mean of the Q_{Feb} for all observed flow records that belong to that class in that island. For cases where no measured flow was available, expert judgement was applied to make use of data from other classes.

315 The approach used to estimate Q_{MALF} for Method 2 is described in Henderson et al. 316 (2004). Figure 3 shows a schematic description of the model and its parameters. These fall 317 into three categories: a) climate parameters (T the average length of a dry season, N the 318 number of rain events in that season, P the amount of rain in the dry season); b) flow 319 parameters (Q_{mean} the mean flow, Q_0 the average flow at the start of the dry season, α the 320 fraction of that rain that affects the streamflow); and c) catchment parameters that describe 321 the way in which water is released from catchments during the dry season (b and T*). 322 Estimates of all these input parameters have previously been developed for all of New 323 Zealand (Henderson et al, 2004). The parameter Q_0 corresponds to the average flow at the 324 start of the dry season. The predictions are most sensitive to the value of the b parameter, 325 which describes the type of river flow recession. For example, catchments in dry catchments

typically have b values near 1, hill country catchments typically have b values near 2, andcatchments with volcanic geology typically have b values of 3 or larger.

The approach used to estimate Q_F for Method 2 is described in Pearson and McKerchar (1989) and McKerchar and Pearson (1989). Essentially, these estimates are gained from interpolation onto ungauged sites from a contour map of Q_F which was itself derived from a spatial interpolation of observed data. Since this approach used instantaneous flow data to calculate Q_F , rather than mean daily values, it was anticipated that the approach would overestimate Q_F in comparison to observed values derived from mean daily values. However, the estimates were still included in the analysis.

335 The approach used to estimate FDCs for Method 2 was to assume a log-normal

336 probability distribution as a model of the flow duration curves. This is a log transformation of

337
$$g(x, \theta) = (1/\sqrt{2\pi}\theta_2) \exp[-1/2((x-\theta_1)/\theta_2)^2],$$
 Equation 1

which has two parameters, θ_1 and θ_2 . It was further assumed that θ_1 could be estimated as the mean flow (Q_{bar} from Method 2) and that θ_2 would be estimated as a linear function of the b parameter, which was also used to calculate Q_{MALF} for Method 2. The approach used to estimate FDC_{Feb} was to scale the estimated FDC for Method 2 by the estimated Q_{Feb} for Method 2.

343 c. Method 3 Random Forests

A regression technique called Random Forests was used to apply a regression of each observed hydrological index (Table 2) and each of the three parameters describing a GEV distribution of the all-time FDC and the FDC for February as a function of available catchment characteristics (Table 4). This method uses machine-learning by combining many regression trees into an ensemble to produce more accurate regressions by drawing several bootstrap samples from the original training data and fitting a tree to each sample (Breiman, 2001; Cutler et al., 2007). Random forest models fitted using catchment characteristics have 351 previously been shown to be able to explain variation in hydrological patterns such as 352 parameters describing FDCs (Booker and Snelder, 2012), the frequency of events that exceed 353 three time the median flow (Booker, in press) and various other hydrological indices (Snelder 354 and Booker, 2012). Each random forest was developed by growing 500 trees. As the number 355 of trees (k) increases the generalisation error always converges and it was assumed that use of 356 500 trees was sufficiently high to ensure convergence.

357 The predictions from random forest models were tested using a leave-one-out cross 358 validation procedure referred to here as jack-knifing (Efron, 1982; Booker and Snelder, 359 2012). This cross-validation procedure was applied by leaving out all data associated with 360 each of the 485 sites and then estimating each hydrological index for the left-out site from all 361 remaining sites. The results from this procedure produced estimates as if each site were 362 ungauged (Ganora et al., 2009). Comparison between observed and jack-knifed values 363 allowed an assessment of both the robustness and reliability for estimation at ungauged sites 364 (Castellarin et al., 2004).

365

For each time-series, the parameters describing a GEV distribution,

366

 $G(x, \mathcal{G}) = \exp\left[-(1 - (\mathcal{G}_3(x - \mathcal{G}_1))/\mathcal{G}_2)^{1/\mathcal{G}_1}\right],$ Equation 2

were fitted to all observed mean daily flows and all observed mean daily flows in February.
In both cases observed mean daily flows were divided by catchment area for each gauging
station prior to fitting the GEV parameters. The GEV distribution is described by three
parameters and has shown to represent the range of shapes of standardised FDCs found
across New Zealand. See Booker and Snelder (2012) for further discussion of estimating
standardised FDCs at ungauged sites across New Zealand using various statistical techniques
to generalise parameters describing various probability distributions.

d. Method 4 TopNet Corrected

FDCs calculated using the jack-knifed Random Forests method represent a unique FDC at any location in the New Zealand river network as if each location were ungauged. This provided the opportunity to correct for bias in the TopNet estimated FDCs using the Random Forests estimated FDC at each site as if it were an observed FDC. Therefore the jack-knifed Random Forests FDCs were used to calculate a correction factor for each percentile, *i*, of the TopNet FDC for each site, *j*.

381TopNet Corrected_{ij} = TopNet_{ij} * (Random Forest_{ij} / TopNet_{ij})Equation 3382Since the exceedance percentile of each datum in each TopNet time-series was known, these383corrections could also be applied to each TopNet time-series. This allowed re-calculation of384each hydrological index from each corrected time-series. This procedure was repeated385separately for TopNet Version 0 FDCs and TopNet Version 1 FDCs.

386

4. Observed versus predicted values

Scatterplots of observed versus predicted values after having standardised and 387 388 transformed each index (Table 2) were plotted for each index for each method. These 389 scatterplots were overlaid with a linear regression with observed values on the y-axis as 390 recommended by Piñeiro et al. (2008). Following the suggestion of Moriasi et al. (2007), 391 three model performance metrics were calculated for each set of observed versus predicted 392 values: Nash-Sutcliffe efficiency (NSE); percent bias (pbias); and ratio of the root mean 393 square error to the standard deviation of observed data (RSR). NSE is a dimensionless metric 394 that determines the relative magnitude of the residual variance ("noise") compared to the 395 observed data variance ("information") (Nash and Sutcliffe, 1970). NSE values of 1 indicate 396 a perfect match between estimates and observations, whereas values of 0 indicate 397 performance equal to estimating the mean observed value across all observations. pbias 398 measures the average tendency of the simulated data to be larger or smaller than their

observed counterparts (Gupta et al., 1999). Negative pbias values represent overestimation 399 400 and positive values indicate underestimation. RSR standardises RMSE using the observations 401 standard deviation, and it combines both an error index and the additional information 402 recommended by Legates and McCabe (1999). Lower RSR values indicate better model 403 performance, with 0 indicating perfect correspondence between estimates and observations. 404 See Moriasi et al. (2007) and references therein for full details of these performance 405 evaluation metrics. The same metrics were applied to 101 points representing log specific 406 (flow per unit catchment area) FDCs for each site for each method for the February and all-407 time FDCs separately.

408 **5. Results**

409

a. Hydrological indices

410 Synchronisation of TopNet Version 1 with the observed time-series made little impact 411 on the performance metrics (NSE, RSR and pbias) when compared to using the full TopNet 412 time-series (Table 5). This was especially the case for Q_{bar}, Q_{MALF} and Q_F. For Q_{bar}, 413 synchronisation marginally reduced an overestimation bias, but also resulted in a small 414 reduction in performance in terms of NSE and RSR (reduced NSE, increased RSR). For Q_{MALF}, synchronisation resulted in increased overprediction bias, but marginally improved 415 416 performance in terms of NSE and RSR. The process of synchronisation did alter performance 417 for Q_F as synchronisation improved performance in terms of NES and RSR, but substituted 418 an overprediction bias with an underprediction bias of the same magnitude. These results 419 indicate that it was not the case that there were non-stationarities in observed hydrological 420 regimes that were generally detectable in the TopNet time-series for Q_{bar}, Q_{MALF} or Q_F. This 421 may not have been the case for Q_{Feb}. This is an understandable result as Q_{bar}, Q_{MALF} and Q_F 422 will be less sensitive to inter-annual variability than Q_{Feb}. This is because Q_{bar} is an average 423 calculated over all the record, and both Q_{MALF} and Q_F are both averages of indices calculated

for each year of record, whereas Q_{Feb} is calculated over a smaller time-window in each year
of record.

Overall there was more difference in performance between TopNet Version 0 and TopNet Version 1 than there were differences between synchronisation and nonsynchronisation of TopNet Version 1. This indicates that TopNet results are more sensitive to changes to the TopNet *f* parameter than to either the assumption that the 1973-2010 timeseries represent the long-term flow regime, or any non-stationarities combined with relatively short records in the observed time-series.

432 When compared to TopNet Version 0, TopNet Version 1 reduced an overestimation of Q_{bar}, but reduced performance in terms of NSE and RSR. For Q_{Feb}, TopNet Version 1 433 434 marginally improved NSE, reduced an overestimation pbias, but increased RSR. For Q_{MALF}, 435 TopNet Version 1 dramatically improved NSE, improved RSR and replaced a large 436 overestimation with an underestimation of lesser magnitude. For Q_F, TopNet Version 1 437 reduced performance of all metrics when compared to TopNet Version 0. This indicates that 438 high flows were not better predicted following the regionalisation of the TopNet f parameter. 439 However, over all four indices there were greater differences between methods (TopNet, 440 HUC and Random Forests) than there was between the two TopNet versions (Table 5, Figure 441 4).

442 The TopNet time-series was corrected using the jack-knifed Random Forests FDC 443 estimates and then used to estimate the hydrological indices. For all indices and both TopNet 444 versions, corrected estimates improved performance in terms of NSE and RSR when 445 compared to the uncorrected TopNet estimates. Corrected estimates produced less bias as 446 indicated by smaller magnitude pbias when compared to uncorrected estimates from both 447 TopNet versions for all indices except Q_{Feb} for Version 1 and Q_F for version 0. Correction of 448 TopNet Version 1 caused an increase in overprediction of Q_{Feb} . Correction of TopNet

Version 0 caused an overprediction to change to an underprediction of greater magnitude.
Overall, correction greatly reduced differences in performance between the two TopNet
versions (Table 5, Figure 4).

For Q_{bar} and Q_{Feb} there was more difference between TopNet Version 0 and TopNet Version 1 than there was between TopNet Version 1 and TopNet 1 Corrected. After correction, the performance of Q_{bar} estimated from both TopNet versions matched the performance of those estimated using Random Forests. This was because the correction procedure forced the TopNet corrected estimated FDCs to match jack-knifed Random Forests estimated FDCs and therefore TopNet corrected Q_{bar} matched jack-knifed Random Forests estimated Q_{bar}.

459 NSE was positive (negative values indicate that the mean observed value is a better 460 predictor than the simulated value) for all indices for all methods except Q_F for Method 2 461 HUC (Table 5). This indicates that, except for Q_F from the HUC method, all methods 462 provided some degree of useful information about patterns in the estimated values. In this 463 comparison HUC estimates of instantaneous Q_F were compared with observed Q_F calculated 464 from mean daily flow data. Poor performance and, in particular, overestimation of Q_F for 465 Method 2 HUC was therefore not surprising. In fact, McKerchar and Pearson (1989) previously showed that the method was able to explain a substantial fraction of the observed 466 467 variation in Q_F when compared to observed values calculated from instantaneous flow data. 468 For Q_{bar} the HUC method performed best in terms of both NSE and RSR. This is the method already recommended by Woods, et al. (2006). For Q_{MALF}, Q_F and Q_{Feb} the Random 469 470 Forests method performed best in terms of both NSE and RSR. The Random Forests method 471 also gave the lowest magnitude pbias for Q_F and Q_{Feb} but not for Q_{MALF} (Table 5). These findings correspond well with visual inspection of observed against predicted values, which 472

473 indicated that the Random Forests method reduced scatter and produced unbaised estimates
474 for all four indices but was out-performed by Method 2 HUC for Q_{bar} (Figure 4).

475 *b.* Flow duration curves

476 More sites had better performance as indicated by higher NSE values, lower RSR values and lower magnitude pbias for all-time FDCs compared to February FDCs regardless 477 478 of estimation method (Figure 5). This indicates greater uncertainties associated with estimation of February FDCs compared to all-time FDCs. More sites had better performance 479 480 in terms of NSE, RSR and pbias for TopNet Version 1 in comparison to TopNet Version 0 481 for the all-time FDC and the February FDC in particular. Negative pbias values for many 482 TopNet Version 0 estimated February FDCs indicated consistent underestimation. This 483 consistent underestimation was not present for TopNet Version 1, which showed an equal 484 likelihood for either underestimation or overestimation of the February FDC. This indicated 485 that regionalisation of the TopNet *f* parameter improved flow estimation, particularly in 486 February.

Both the HUC and the Random Forests methods performed better than either of the uncorrected TopNet methods for both the all-time and February FDCs. Both all-time and February FDCs had more sites with higher NSE, lower RSR and lower magnitude pbias when estimated using the Random Forests method compared to the other methods. Since the TopNet 1 Corrected estimated all-time FDC was corrected using the jack-knifed Random Forests estimated FDC, performance of the TopNet 1 Corrected estimated all-time FDC was the same as the jack-knifed Random Forests estimated FDC.

494 *c. National estimates for New Zealand*

495 All methods were able to provide predictions for ungauged sites across New Zealand 496 which reproduced the major regional variations in observed Q_{MALF} (Figure 6). These 497 geographical patterns included a strong east-west gradient in the South Island as well as the

498 influence of the Southern Alps (see Figure 1 for place names). As they cross the eastern 499 plains of the South Island, large mountain-fed rivers with markedly higher Q_{MALF} stand out 500 against a background of comparatively lower-yielding lowland streams. To the northeast of 501 the central North Island, the rivers draining a volcanic plateau have relatively high Q_{MALF}. 502 with large storage capacity in the thick pumice and ash layers sustaining low flows (Mosley 503 and Pearson, 1997). Both Random Forests (Figure 6c) and TopNet (Figure 6d) predicted 504 lower values of Q_{MALF} than HUC (Figure 6b) for the south west coast of the South Island, but 505 predicted slightly higher Q_{MALF} for most other locations in comparison with HUC. It should 506 be noted that none of the methods were designed to take account of large engineering 507 schemes such as those currently in place on several of New Zealand's large rivers (e.g. the 508 Waikato, Rangitata, Waitaki, Clutha and Waiau rivers).

509 **6. Discussion**

510 A limited set of hydrological indices along with both the all-time and February FDCs 511 were investigated (Table 2). This set of hydrological indices included those representing both 512 high and low flow extremes as well as an aspect of seasonality. These indices are commonly 513 used for water resource planning in New Zealand, however not all aspects of the flow regime, 514 such as the frequency of mid-range flows, were represented. This aspect of the flow regime 515 could have been included by calculating various additional indices such as the number of 516 events exceeding three times the long-term median flow (FRE3; Biggs 2000), but no HUC 517 method was available for estimating this index. National estimates of FRE3 using random 518 forests, including comparison with observed values, were calculated and compared with 519 observations by Booker (in press).

520 For the Random Forests method FDCs were described using the three parameter GEV 521 distribution. Other distributions could have been used including log Pearson Type III (LP3; 522 Ganora et al., 2009) or a mixed gamma distribution (Cheng et al., 2012). Booker and Snelder

(2012) showed that, although the LP3 distribution may provide better fits to observed FDCs
when standardised by mean flow, uncertainties in generalising the LP3 parameters from
catchment characteristics meant that a method using the GEV distribution to parameterise the
shape of the FDC gave better performance for prediction at ungauged locations.

527 The same set of independent variables was used to model all four hydrological 528 indices. Procedures designed to optimise the set of independent variables such as the Model 529 Improvement Ratio (Murphy et al. 2010) were not employed to optimise the predictor data 530 set. This approach may not have provided optimal Random Forest models in all cases as one 531 would expect different sets and different numbers of independent variables to best predict 532 each dependent variable. For example, summer temperature might be expected to be related 533 to low flows, but not flood flows. Despite this the Random Forests method still outperformed 534 the other methods even when a leave-one-out cross validation procedure was applied to allow 535 for independent assessment of estimation performance against observed data.

Although many performance metrics are available to assess model performance, NSE, RSR and pbias were used as recommended by Moriasi et al., (2007). Although these three metrics are designed to quantify different aspects of model performance, they often gave consistent information regarding model performance.

540 The aim of this work was to assess the ability of various methods to estimate 541 hydrological conditions for ungauged catchments in the absence of major hydrological 542 alterations such as that caused by abstraction, storage or diversion. The ability to estimate the 543 effects of either climate change or land cover change were not assessed. It may be necessary to assess the potential effects of climate change (Zemansky et al., 2012; Earman and 544 545 Dettinger 2011), land use change (Scanlon et al., 2007) or their combined effects (Brekke et 546 al., 2004) on flow regimes to develop rational management strategies. Both TopNet and the 547 Random Forests models described above have inputs that could be changed to assess the

548 impacts of climate change. However, the validity of this approach was not tested here. It 549 should be noted that there are several issues relating to model structure and parameterisation 550 that would need to be resolved when using physically-based models to predict the 551 hydrological impacts of environmental change (Wagener, 2007). Similarly, when using 552 flexible empirically-based models such as Random Forests to predict outside of the fitted 553 model domain it is important to understand how the algorithms perform when projected into 554 the new environmental conditions (Elith and Graham, 2009).

555 These results indicate that Random Forests outperformed both TopNet versions for all 556 four hydrological indices as well as for FDCs. This finding corresponds well with the 557 findings of others. For example, Parkin et al. (1996) found that streamflow predictions from 558 an a priori parameterised physically-based model contained considerable uncertainty. It 559 should be noted that, although TopNet Version 1 arguably represents the best currently 560 available physically-based approach for application to ungauged sites across New Zealand, 561 this method was uncalibrated. It is known that calibration of TopNet parameters can 562 significantly improve estimation performance by optimising model performance against observed flows (e.g. Bandaragoda et al., 2004; McMillan et al., 2013). Calibration procedures 563 are only possible for catchment specific applications with available flow data. It is possible to 564 565 transfer calibrated parameter sets to ungauged sites (e.g. Yu and Yang, 2000) given a suitable 566 regionalisation procedure (McDonnell and Woods, 2004; Li et al., 2010; Olden et al., 2012; 567 Coopersmith et al., 2012). Although calibration procedures have been applied to TopNet for 568 several catchments (Bandaragoda et al., 2004; Clark et al., 2008; McMillan et al. 2013), a 569 procedure to regionalise the calibrated parameter values is not currently available. Such 570 procedures can be hampered by issues such as equifinality within the calibration parameter 571 sets (Beven 2006; Bárdossy, 2007).

572 The Random Forests method can be used to estimate a unique FDC at any location in 573 the New Zealand river network. These estimated FDCs could be used to provide a more 574 reliable regionalisation than would be the case using data from observed locations alone 575 because they represent variability across all of New Zealand rather than a sample of observed FDCs (Snelder and Booker, 2012). Furthermore, the Random Forests estimated FDC's at 576 577 ungauged locations could provide the opportunity to calibrate TopNet parameters against an 578 estimated FDC for ungauged locations in the New Zealand river network. This would require 579 a method that allowed calibration against an observed (or estimated) FDC (e.g. Yu and Yang 580 2000; Yadav et al., 2007; Westerberg et al., 2011). Such a method may be developed as part 581 of future work. However, considerable improvements in performance were gained when both 582 TopNet versions were corrected using the jack-knifed estimated FDCs from Random Forests. 583 This indicates that TopNet performance can be increased considerably without automated 584 parameter set calibration procedures (Yu and Yang, 2000) or increased understanding of 585 hydrological processes controlling variability of FDCs across catchments (Yaeger et al., 586 2012). Furthermore, the correction procedure reduced differences in performance between TopNet Version 0 and TopNet Version 1. 587

588 The TopNet correction procedure tested here represents one relatively crude method 589 of combining a process-based approach with a data-based approach. The procedure provides 590 estimates calculated using a data-based approach to correct for bias within FDCs calculated 591 using a process-based approach. This contrasts with alternative approaches which have 592 augmented stochastic approaches with more process-based approaches by incorporating 593 different components of catchment dynamic responses into stochastic models (e.g. Botter et 594 al., 2007a, 2007b, 2009; Muneepeerakul et al., 2010; Cheng et al., 2012) or by applying a 595 water balance modelling framework to divide the FDC into three parts (Yokoo and Sivapalan, 596 2011).

597 The TopNet correction procedure provided results that matched the performance of 598 Random Forests for Q_{bar} and the all-time FDC, but not for Q_{Feb} , Q_{MALF} or Q_F . It should be 599 noted that this procedure allowed improved estimation of the entire time-series of flows using 600 both TopNet versions. This method has a major advantage over the Random Forest method 601 because any required hydrological indices can be calculated from the estimated time-series. 602 In contrast, the Random Forests method requires fitting of new models to any newly 603 calculated indices prior to estimation of these new indices at ungauged sites.

604 **7.** Conclusion

Results showed the Random Forests method provided the best estimates of both FDCs and all four hydrological indices except mean flow. Mean flow was best estimated using the already published HUC method (Woods et al., 2006). Results also showed that considerable gains in estimation performance can be made by correcting estimates calculated using physically-based models with estimated values calculated using empirically-based models.

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Tables Table 1. Codes, descriptions and numbers of sites used in the analysis. See Snelder and Biggs (2002) and Snelder and Hughey (2005) for full descriptions of codes. Table 2. Hydrological Indices derived from observed mean daily flows. Table 3. Summary of the defining characteristics, categories and category membership criteria that combine to define Source-of-Flow groupings within the REC. Table 4. Codes and descriptions of independent variables used to fit regression models. See Leathwick et al., (2011) for full descriptions. Table 5. Various metrics quantifying correspondence between observed and predicted values for four hydrological indices (Table 2) using various estimation methods.

909	Figures
910	
911	Figure 1. Map showing the locations of the gauging stations used in this study.
912	
913	Figure 2. Schematic showing different methods used to estimate hydrological indices and
914	flow duration curves (FDCs).
915	
916	Figure 3. Hydrology of ungauged catchments (HUC) low flow model and parameters.
917	
918	Figure 4. Observed against calculated values for each index for each method ($n = 485$). Grey
919	dashed line is linear regression. Black line is 1:1 such that x-limits are equal to y-limits for all
920	plots. Qbar is mean flow. QFeb is proportion of flow in February. QMALF is 7-day mean
921	annual low flow. QF is mean annual flood.
922	
923	Figure 5. Box and whisker plots of Nash-Sutcliffe efficiency, RSR (ratio of the root mean
924	square error to the standard deviation of observed data) and pbias (average tendency of the
925	calculated data to be larger or smaller than their observed counterparts) at each site for all-
926	time and February flow duration curves for each method ($n = 101$ points at each of 485sites).
927	
928	Figure 6. All observations and for each method predictions of 7-day mean annual low flow
929	(MALF) for all rivers of Strahler order greater than three. TopNet results are for uncorrected
930	TopNet Version 1.

Figures

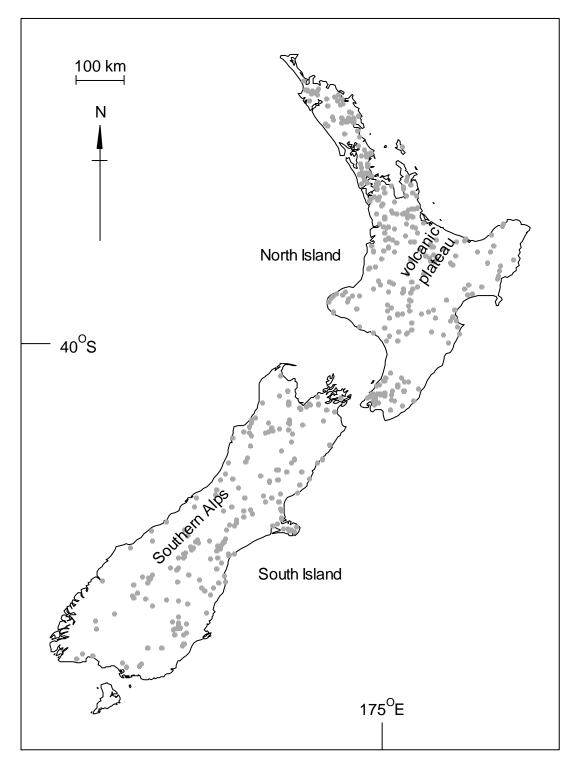


Figure 1. Map showing the locations of the gauging stations used in this study.

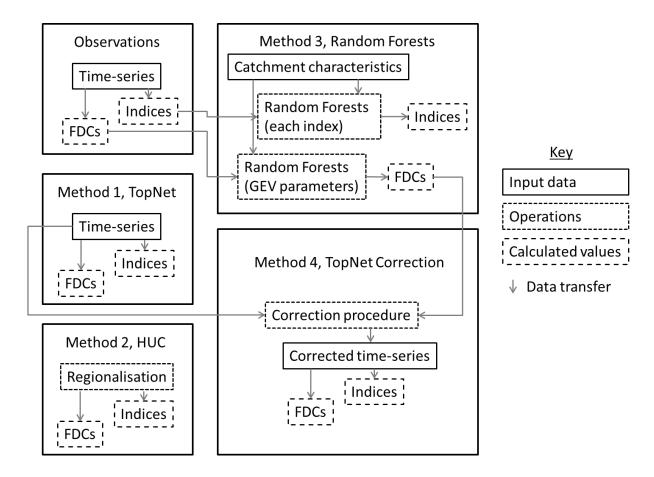


Figure 2. Schematic showing different methods used to estimate hydrological indices and flow duration curves (FDCs).

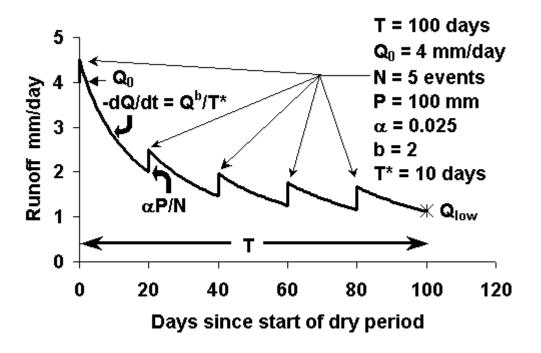


Figure 3. Hydrology of ungauged catchments (HUC) low flow model and parameters.

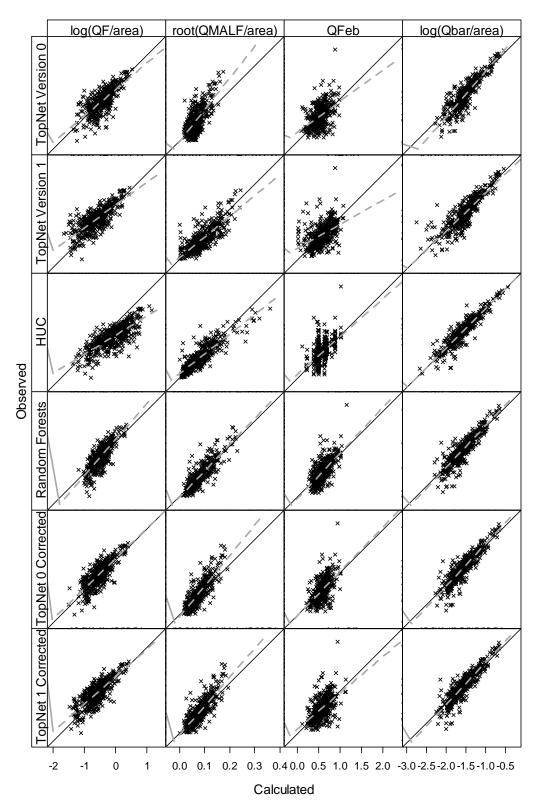


Figure 4. Observed against calculated values for each index for each method (n = 485). Grey dashed line is linear regression. Black line is 1:1 such that x-limits are equal to y-limits for all plots. Qbar is mean flow. QFeb is proportion of flow in February. QMALF is 7-day mean annual low flow. QF is mean annual flood.

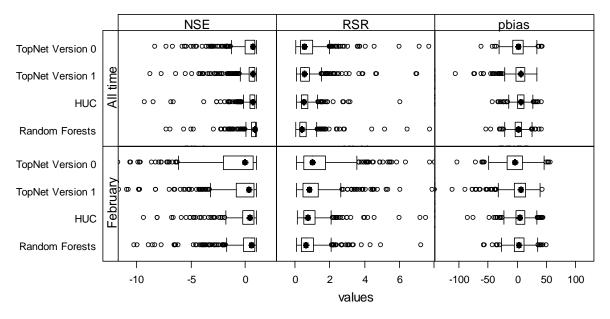


Figure 5. Box and whisker plots of Nash-Sutcliffe efficiency, RSR (ratio of the root mean square error to the standard deviation of observed data) and pbias (average tendency of the calculated data to be larger or smaller than their observed counterparts) at each site for all-time and February flow duration curves for each method (n = 101 points at each of 485sites).

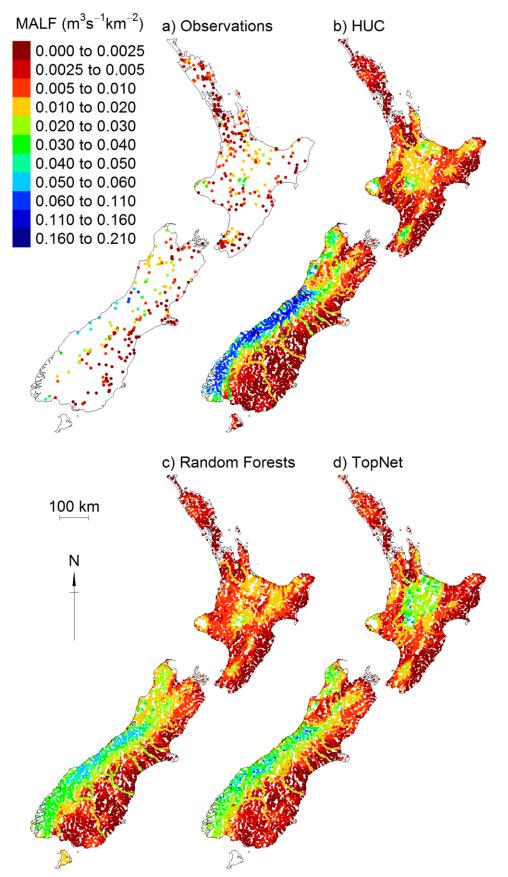


Figure 6. All observations and for each method predictions of 7-day mean annual low flow (MALF) for all rivers of Strahler order greater than three. TopNet results are for uncorrected TopNet Version 1.

Tables

Table 1. Codes, descriptions and numbers of sites used in the analysis. See Snelder and Biggs (2002) and Snelder and Hughey (2005) for full descriptions of codes.

Code	Description	Number of sites, total
Island	•	, ,
Ν	North Island	289
S	South Island	196
Climate		
WD	Warm-dry	18
WW	Warm-wet	152
WX	Warm-extremely wet	4
CD	Cool-dry	75
CW	Cool-wet	154
CX	Cool-extremely wet	82
Topographic source of flow		
GM	Glacial mountain	10
Н	Hill	167
L	Low elevation	241
Lk	Lake	19
М	Mountain	48
Land cover		
В	Bare	16
EF	Exotic-Forest	22
IF	Indigenous-Forest	105
Р	Pastoral	247
S	Scrub	17
т	Tussock	63
U	Urban	15

Index	Description	Calculation	Standardisation	Transformation
Q _{bar}	Mean flow over all time	Mean of all daily flows	Divide by catchment area to get specific mean flow (m ³ s ⁻¹ km ⁻²)	Log base 10
Q _{Feb}	Proportion of flow in February	Mean of all daily flows for each calendar month after having divided by the overall mean flow	Divide by mean flow over entire record to get proportion of flow in February (unitless)	None
Q _{MALF}	Mean of minimum 7-day flow in each year	Mean of minimum flow for each water year after having applied a running 7-day mean to the daily flows	Divide by catchment area to get specific QMALF (m ³ s ⁻¹ km ⁻²)	Square root
Q _F	Mean of maximum flow in each year	Mean of maximum flow for each water year	Divide by catchment area to get specific QF ($m^3 s^{-1} km^{-2}$)	Log base 10
FDC	Probability distribution of daily flow	Interpolation of the cumulative frequency distribution of daily flows on to 101 points (0 to 100 in steps of 1)	Divide by catchment area to get specific FDC (m ³ s ⁻¹ km ⁻²)	Log base 10
FDC _{Feb}	Probability distribution of daily flow for February	Interpolation of the cumulative frequency distribution of daily flows for each calendar month on to 101 points (0 to 100 in steps of 1)	Divide by catchment area to get specific FDC (m ³ s ⁻¹ km ⁻²)	Log base 10

Table 2. Hydrological Indices derived from observed mean daily flows.

Table 3. Summary of the defining characteristics, categories and category membership criteria that combine to define Source-of-Flow groupings within the REC.

Defining characteristic	Categories	Notation	Category membership criteria
Climate	Warm-extremely-wet	WX	Warm: mean annual temperature > 12°C
	Warm-wet	WW	Cool: mean annual temperature < 12°C
	Warm-dry	WD	Extremely Wet: mean annual effective precipitation ^a > 1500 mm
	Cool-extremely-wet	СХ	Wet: mean annual effective precipitation > 500 and < 1500 mm
	Cool-wet	CW	Dry: mean annual effective precipitation \leq 500 mm
	Cool-dry	CD	
Topography	Glacial-mountain	GM	GM: M and % permanent ice > 1.5%
	Mountain	М	M: > 50% annual rainfall volume above 1000 m ASL
	Hill	Н	H: 50% rainfall volume between 400 and 1000 m ASL
	Low-elevation	L	L: 50% rainfall below 400 m ASL
	Lake	Lk	Lk: Lake influence index ^b > 0.033

a. Effective precipitation = annual rainfall - annual potential evapotranspiration

b. See Snelder and Biggs (2002) for a description.

 Table 4. Codes and descriptions of independent variables used to fit regression models. See Leathwick et al., (2011) for full descriptions.

Variable name	Description
usPET_Q	Annual potential evapotranspiration of catchment (mm)
usRainDays10_Q	Catchment rain days, greater than 10 mm/month (days/year)
usAnRainVar_Q	Coefficient of variation of annual catchment rainfall (m)
usSteep_Q	% annual runoff volume from area of catchment with slope > 30° (%)
usCatElev	Average elevation in the upstream catchment (m)
usParticleSize_Q	Catchment average of particle size (ordinal scale)

Index	Method	n	NSE	pbias	RSR	
log(Q _{bar} /area)						
	TopNet_0	485	0.73	4.050	0.523	
	TopNet_1 Sync	456	0.70	3.138	0.552	
	TopNet_1	485	0.71	3.469	0.537	
	HUC	485	0.87	0.298	0.363	
	RFjacked	485	0.80	-0.241	0.446	
	TopNet_0 Corrected	485	0.80	-0.410	0.447	
	TopNet_1 Corrected	485	0.80	-0.433	0.447	
Q _{Feb}						
	TopNet_0	485	0.09	11.733	0.955	
	TopNet_1 Sync	456	0.29	-2.420	0.843	
	TopNet_1	485	0.08	2.499	0.960	
	HUC	485	0.22	5.354	0.884	
	RFjacked	485	0.44	0.216	0.748	
	TopNet_0 Corrected	485	0.31	2.872	0.828	
	TopNet_1 Corrected	485	0.27	3.020	0.853	
root(Q _{MALF} /area)						
	TopNet_0	485	0.36	17.496	0.797	
	TopNet_1 Sync	454	0.59	-11.031	0.643	
	TopNet_1	485	0.58	-10.739	0.646	
	HUC	485	0.71	-0.506	0.540	
	RFjacked	485	0.75	0.157	0.499	
	TopNet_0 Corrected	485	0.66	9.132	0.587	
	TopNet_1 Corrected	485	0.67	5.923	0.571	
log(Q _F /area)						
	TopNet_0	485	0.50	7.523	0.704	
	TopNet_1 Sync	456	0.30	-36.797	0.837	
	TopNet_1	485	0.31	-34.958	0.832	
	HUC*	485	-0.45	73.012	1.206	
	RFjacked	485	0.63	-0.674	0.609	
	TopNet_0 Corrected	485	0.55	-16.521	0.668	
	TopNet_1 Corrected	485	0.46	-31.733	0.734	

 Table 5. Various metrics quantifying correspondence between observed and predicted values for four hydrological indices (Table 2) using various estimation methods.

 * Table footnote: In this comparison HUC estimates of instantaneous Q_F were compared with observed Q_F calculated from mean daily flow data.