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The Use of Entropy as a Model Diagnostic in Rainfall-Runoff Modelling

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Abstract: Recent papers have called for the development of robust model diagnostics (in addition to traditional "measures of fit") that provide insights on where model structural components and/or data may be insufficient. The potential of entropy measures to provide these in hydrology has not been adequately explored. Further, flow duration (FD) curves provide a useful visual diagnostic of catchment response, but attempts to quantify the fit of modelled versus observed FD curves to date have relied on using time series measures of fit. We note that Shannon entropy of flow is strongly related to the FD relationship, so suggest it provides a more appropriate quantitative measure of fit. This paper presents initial results from a study calibrating two rainfall-runoff models to 4 years of hourly data from the Mahurangi catchment, NZ. Kling-Gupta efficiency (KGE), Nash-Sutcliffe efficiency (NSE) and two entropy measures were considered. When assessed using a range of model diagnostics, KGE was overall the single best measure, outperforming NSE at all times. Entropy outperformed KGE over particular hydrograph sections, and we show performance may improve further with careful choice of discretisation. We demonstrate entropy's strong relationship to FD and interrogate the performance of entropy measures in the presence of timing and bias errors. As entropy is insensitive to timing errors but very sensitive to most other errors (in sharp contrast to, e.g., the NSE measure) it potentially provides a useful diagnostic of the types of error present in combination with other OFs.

***Keywords**:* Shannon entropy; Model diagnostics; Model uncertainty; Rainfall-runoff modelling.

1. INTRODUCTION

Traditional "measures of fit" are commonly used in hydrological modelling to provide an objective assessment of the "closeness" between simulated and observed hydrological observations (e.g. streamflow). Different measures emphasise different systematic and/or dynamic behaviours within the hydrological system; hence a robust assessment of model performance using single measures is difficult [Krause et al., 2005; Schaefli and Gupta, 2007]. Recent papers have highlighted the importance of moving from model calibration to diagnostic model evaluation, which aims to: 1) determine the information contained in the data and in the model, 2) examine the extent to which a model can be reconciled with observations, and 3) point towards the aspects of the model (or data limitations) that need improvement [Gupta et al., 2008].

Information theoretic entropy-based measures provide a promising avenue to allow us to better identify where information is present and/or conflicting [Singh, 2000]. If placed within a hydrologically relevant context, these measures may assist in the generation of more robust modelling frameworks allowing us to better diagnose model/data/hypotheses inconsistencies [Jackson et al., 2010]. Therefore, the main objective of the current study is to investigate the potential of entropy-based measures as objective functions and as model diagnostics in hydrological modelling. Entropy-based statistics are introduced in Section 2, where we also highlight barriers to robust implementation in hydrological contexts. Section 4 describes the two rainfall-runoff model structures and the identification method followed using observed records from the Mahurangi River catchment, New Zealand. Section 5 presents initial results consisting of statistical analysis based on observed data and modelling results which use entropy as an objective function. The paper concludes with a brief discussion on possible ways forward.

2. USE OF ENTROPY AS A MODEL DIAGNOSTIC

According to Schreiber [2000], information is equivalent to the removal of uncertainty; hence uncertainty and informational entropy are in some senses identical. In recent years, entropy-based statistics have been applied to several hydrological problems [e.g. Maruyama et al., 2005; Hejaki et al., 2008; Ruddell and Kumar, 2009]; however their potential to be used as objective functions (OFs), or better as model diagnostics, is largely unexplored (exceptions are the papers of Amorocho and Espildora [1973] and Chapman [1986]). This paper is not concerned with repeating what is already discussed in previous reviews (see Singh [2000], Jackson et al. [2010]), but rather on presenting preliminary results and insights on the potential use of entropy as an objective function and model diagnostic test.

2.1 Shannon entropy

Entropy is variably described; examples include "a measure of the amount of chaos" or "of the lack of information about the system" [Koutsoyiannis, 2005]. The Shannon entropy [Shannon, 1948] of a discrete random variable *X* with *N* possible outcomes is given by:

$$H_X = -\sum_{i=1}^{N} p(x_i) \cdot \log_{base} p(x_i) \tag{1}$$

where $p(x_i)$ is the probability of occurrence of outcome x_i and *base* is the base of the logarithm used (entropy has a unit of binary digits, bits, when *base*=2). Shannon [1948] defined entropy as the average number of bits (assuming *base*=2) needed to optimally encode independent draws of *X* following a probability distribution $p(x_i)$. A low value of entropy indicates a high degree of structure and a low uncertainty. It can be easily shown that with complete information entropy equals 0, otherwise it is greater than 0. If no information is available then entropy will reach its maximum equal to $log_{base}(N)$. When using entropy as an OF or diagnostic, we suggest normalizing Equation 1 by dividing through by $log_{base}(N)$. This normalised entropy remains 0 with complete information / maximum order and takes a maximum value of 1 with no structure/maximum disorder. Note also that, if applied to flow data, this probabilistic measure is closely related to the FD curve; Shannon entropy becomes a quantification of the information (and hence shape) of the histogram or discretised distribution of flow, i.e. flow duration.

Although a continuous analog to the Shannon entropy is available, we rarely possess the analytical form of our variable *X*'s probability distribution so generally work with the discrete form given in Equation 1. Unless *X* is ordinal, a number of discrete bins must be specified, with accompanying ranges. In this case, estimation of the probability density and its associated entropy is influenced by the resolution of this data, the number of bins, and the locations of divisions between these bins. The introduction of arbitrary partitions could result in "edge effects". According to Ruddell and Kumar [2009], with too few/many partitions, "edge effects" become severe and entropy estimates are positively biased, resulting in underestimated mutual information and transfer entropy.

Different approaches can be used to discretise the data set to probability "bins". These include function fitting [Knuth, 2005], kernel estimation [Nichols, 2006], and binning with fixed mass or fixed interval partitions [Ruddell and Kumar, 2009]. Fixed interval partitions are usually applied since the approach is simple and computationally efficient [Ruddell and Kumar, 2009]. These fixed interval partitions are used in this preliminary study.

2.2 Limitations of Shannon entropy when used as an OF

Although Shannon entropy is a quantification of the amount of information within a dataset, its static probabilistic nature cannot capture the temporal variability of information. It therefore shows no sensitivity in time. In addition, this probability-based measure does not depend on the range of the data, so mass balance error could be introduced. The following example illustrates the lack of sensitivity of entropy in time and mass balance. Three streamflow hydrographs (Q_t, $Q_t/2$, and Q_{t+DT}) are generated and presented in Figure 1. $Q_t/2$ is the streamflow data of Q_t divided by 2 at each time step, while Q_{t+DT} is the Q_t data lagged by DT hours. Entropy considers the probability that a value (or range of values) occurs within the data series, and does not take into account their location within the time series. Therefore, the three hydrographs in Figure 1 have identical Shannon entropy.

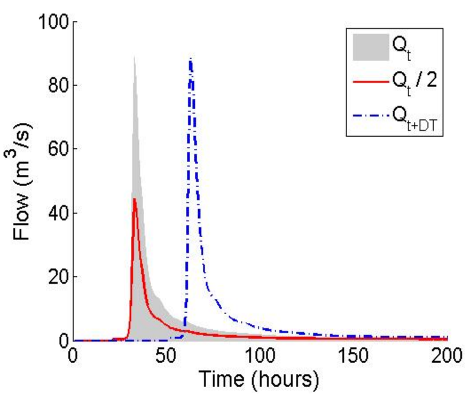

Figure 1. Example of flow times series with identical entropy. The grey band depicts the streamflow hydrograph, the blue dashed line depicts the hydrograph delayed by DT hours, and the red solid line depicts the hydrograph divided by 2.

The lack of sensitivity of entropy to mass balance was demonstrated above. However, mass conservation between observed and simulated streamflow is important in many hydrological applications. Therefore, time series analysis based on the Shannon entropy may need to introduce methodologies that can (explicitly or implicitly) account for mass balance. In this preliminary study we aimed to create a performance measure sensitive to mass balance by linearly fixing the bins between the maximum observed or modelled data range (maximum (simulated, observed) - minimum (simulated, observed)). To distinguish the binning methods from this point forward, we call *scaled*, H^S, the Shannon entropy using fixed bins for both simulated and observed data (this attempts to conserve mass), and *unscaled*, H^U, the Shannon entropy using different bin ranges for simulated and observed data based on their individual specific maximum range (this measure ignores mass conservation).

3. CATCHMENT DESCRIPTION

The analysis is based on observed data from the experimental Mahurangi River (Figure 2) in northern New Zealand, which drains 46.6 km^2 of steep hills and gently rolling lowlands. A network of 28 flowgauges and 13 raingauges has been installed, collecting records at 15 minutes intervals as part of the MARVEX project [Woods, 2004]. The catchment experiences a warm humid climate (frosts are rare and snow and ice are unknown), with mean annual rainfall and evaporation of 1,600, and 1,310 mm respectively. The catchment elevation ranges from sea level to 300 m. Most of the soils in the catchment are clay loams, no more than a metre deep, while much of the lowland area is used for grazing. Plantation forestry occupies most of the hills in the south, and a mixture of native forest, scrub and grazing occurs on the hills in the north. Further details are given in Woods [2004].

Historical hourly rainfall, streamflow and potential evapotranspiration data were provided by the National Institute of Water and Atmospheric Research, New Zealand, for the period

1998-2001. The arithmetic average of the 13 raingauge records was used as the mean areal precipitation; this was homogeneously distributed over the catchment. Only the flowgauge at the outlet of the catchment was considered in the present study.

4. RAINFALL-RUNOFF MODELLING

4.1 Model description

Two rainfall-runoff model structures within the Rainfall-Runoff Modelling Toolkit [Wagener et al., 2004] were used to describe the hydrological behaviour of the catchment. The first model is the Probability Distributed Moisture (PDM) model [Moore, 2007]. This allows for a varying distribution of storage capacity over the catchment (Figure 3), described by a Pareto distribution according to Eq. 2.

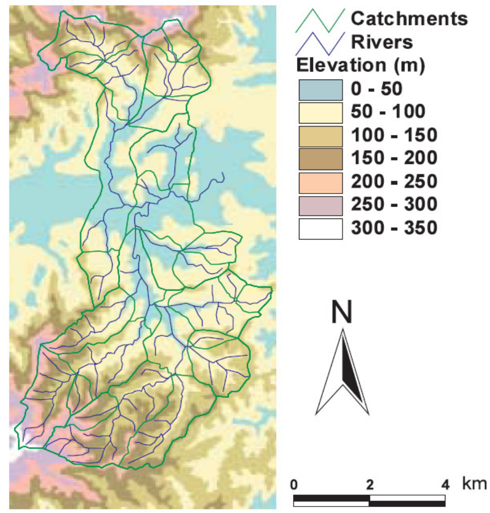

Figure 2. The Mahurangi River catchment.

$$F(C) = 1 - (1 - C / C\max)^{b} \qquad (2)$$

C is the storage capacity in the catchment, *Cmax* is the maximum capacity at any point in the catchment, and the parameter *b* (-) controls the spatial variability of storage capacity over the catchment. Within each time step, the soil moisture storage is depleted by evaporation as a linear function of the potential rate and the volume in storage, and augmented by rainfall. Effective rainfall is then equal to the soil moisture excess.

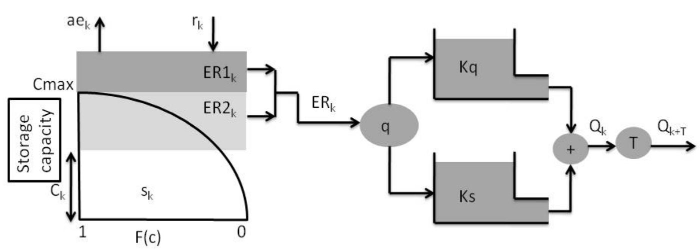

Figure 3. Structure of the Probability Distributed Moisture model.

The second model is a simple bucket model which could be described by setting parameter *b* in the PDM equal to 0. Both models were combined with a routing component consisting of two linear reservoirs in parallel, representing the quick and slow response of the system. This model component has three parameters: a residence time for each reservoir, *Kq* and *Ks* (hours) and *q,* the proportion of total effective rainfall going to the fast response reservoir. Streamflow is finally delayed by a parameter *T* (hours) to adjust time to peak response.

4.2 Model identification method

A Monte Carlo uniform random search procedure was used to explore the feasible parameter space and to investigate parameter identifiability (30,000 samples). The first year (1998) was used as a warm-up period, the next two years for calibration (1999-2000) and the final one year for independent evaluation (2001). Both models were calibrated using streamflow data at the catchment outlet using four objective functions (OFs): the Nash-

Sutcliffe Efficiency, NSE (Eq. 3) [Nash and Sutcliffe, 1970], the recently proposed Kling and Gupta Efficiency, KGE (Eq. 4) [Gupta et al., 2009], the absolute difference in unscaled entropy between simulated and observed series, US-Ent (Eq. 5), and our new entropy OF; the maximum of the scaled and unscaled Shannon entropy difference, SUS-Ent (Eq. 6).

$$NSE = 1 - \frac{\sum_{i=1}^{n}(Qobs_i - Qsim_i)^2}{\sum_{i=1}^{n}(Qobs_i - Q\overline{obs})^2} \quad (3)$$

$$KGE = 1 - \sqrt{(cc-1)^2 + (\alpha - 1)^2 + (\beta - 1)^2} \quad (4)$$

$$US - Ent = abs(H_{sim}^{U} - H_{obs}^{U}) \quad (5)$$

$$SUS - Ent = \max[abs(H_{sim}^{U} - H_{obs}^{U}), abs(H_{sim}^{S} - H_{obs}^{S})] \quad (6)$$

Qsim is the calculated flow using the parameter set θ, *Qobs* is the observed flow, n is the length of the time series, *cc* is the linear correlation coefficient between *Qobs* and *Qsim*, α is a measure of variability in the data values (equal to the standard deviation of *Qsim* over the standard deviation of *Qobs)*, and β is equal to the mean of *Qsim* over the mean of *Qobs*. See Gupta et al. [2009] for further details of the KGE and its components. As explained earlier, US-Ent is sensitive to the shape of the time series, but not scale (given the example in Section 2.2). SUS-Ent has been introduced as a trade-off between shape (and hence information) and scale conservation, in a first attempt to address the possible mass balance issue highlighted in Section 2.2. The simulated runoff using the two entropy measures is insensitive to timing errors and hence is completely insensitive to the final routing delay parameter. To overcome this, after the US-Ent and SUS-Ent calibrations were performed, this routing parameter T was individually adjusted through manual calibration. This decoupling of time sensitive versus time insensitive parameters can be seen as both an advantage (reducing problem dimension) and a potential disadvantage (it may cause issues in more complicated models where time sensitive and time insensitive parameters are strongly inter-dependent; we leave this question for future work).

5. RESULTS

Table 1 summarises model performance over both the calibration and validation period, considering NSE, KGE, US-Ent and SUS-Ent. Overall, there was no significant difference in performance of the bucket versus the PDM model when considering NSE and KGE; however, the PDM can represent the information in the data distribution (as described by the entropy OFs) better than the bucket model. As expected, information in the flow is well conserved when entropy is used as an objective function. The optimum parameter set based on SUS-Ent derives only slightly lower NSE and KGE values, highlighting the potential of this information-based OF to represent the hydrograph properties. However, also as expected, NSE and KGE performance is further reduced when US-Ent is used, probably because this OF maximises information ignoring the effect of data scale.

Table 1. Model performance (calibration and validation) using the optimum parameter set (presented horizontally) for each OF. [ ] is used for the validation period.

	Bucket model				PDM model			
	NSE	KGE	US-Ent	SUS-Ent	NSE	KGE	US-Ent	SUS-Ent
NSE	0.83 [0.81]	0.79 [0.82]	0.024 [0.036]	0.070 [0.066]	0.84 [0.79]	0.68 [0.74]	0.087 [0.079]	0.087 [0.079]
KGE	0.80 [0.77]	0.89 [0.83]	0.077 [0.114]	0.077 [0.129]	0.84 [0.78]	0.89 [0.84]	0.026 [0.008]	0.029 [0.052]
US-Ent	0.79 [0.81]	0.79 [0.85]	0.001 [0.071]	0.056 [0.071]	0.73 [0.77]	0.64 [0.78]	0.001 [0.037]	0.024 [0.037]
SUS-Ent	0.81 [0.77]	0.81 [0.80]	0.005 [0.018]	0.014 [0.039]	0.81 [0.76]	0.70 [0.76]	0.003 [0.047]	0.003 [0.047]

A graphical illustration of the bucket model behaviour is presented in Figure 4 (the PDM model showed similar behaviour, so results are not presented to avoid repetition). Overall, the four OFs simulate flow which fits well the observed data. High flow values seem to be underestimated by the NSE and better represented by the KGE and the entropy-based measures; however, fitting using US-Ent is poor during the recession. This appears to be mostly due to the low optimised *Kq* value (2.4 hours); parameter identifiability plots suggested US-Ent was not capable of identifying this parameter as robustly as the other three measures could. This is almost certainly because of its insensitivity to range and mass.

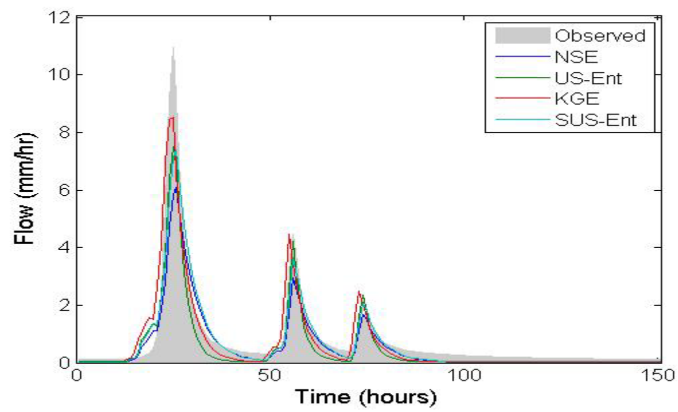

Figure 4. Time series fits depicting simulated and observed runoff in the Mahurangi catchment using different OFs with the bucket model.

Models are further evaluated using the flow duration (FD) curve as a diagnostic measure (Figure 5). Results from the SUS-Ent calibration provide a very close representation of the FD curve, which supports our insight that entropy's probabilistic derivation is closely related to FD. Low flow is not fitted well by this measure, but we believe this is an artefact of the simplistic linear binning technique we used in this preliminary study versus the logarithmic scales we are examining in Figure 5. (Further work will explore logarithmic and other binning techniques). Visual analysis suggests that the KGE fits high and low flows well; however the fitting of medium flows is poor. NSE seems able to capture the medium flows better; however high and low flow values are not accurately represented.

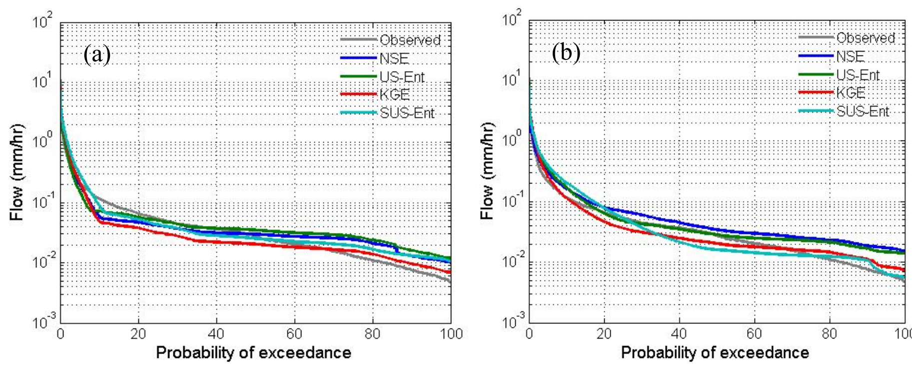

Figure 5. Flow duration curves in the Mahurangi catchment using different OFs and rainfall-runoff models: (a) bucket, and (b) PDM.

Simulated runoff time series are further analysed in a diagnostic manner. Table 2 examines performance of each of the four OF model calibrations to seven static and dynamic components of the observed flow data. These include errors in time lag, FD curve (normalised error), mass balance, peak and mean runoff respectively, correlation between modelled and observed values, and the variability measure described in Gupta et al. [2009] (standard deviation of simulated flow divided by standard deviation of observed flow-optimal at 1). The values of each of these errors or deviations are written within each cell for both calibration and validation period, while the sensitivity of the OFs to the seven individual components is qualitatively presented with colour: light grey showing low sensitivity, dark grey representing high sensitivity.

Table 2. Evaluation using the 4 OFs. [ ] denotes performance within the validation period.

	Time lag (hours)	Shape-FDC (-)	Variability (-)	Mass balance (%)	Peak flow (mm)	Mean flow ($x10^{-1}$ mm)	Correlation (-)
Bucket model							
NSE	1 [1]	0.43 [0.27]	0.82 [0.87]	-4.2 [-7.8]	4.89 [5.38]	0.03 [0.08]	0.91 [0.90]
KGE	0 [0]	0.30 [0.36]	1.07 [1.15]	0.32 [1.35]	2.45 [2.29]	0.01 [0.01]	0.91 [0.90]
US-Ent	10 [10]	0.53 [0.28]	0.84 [0.92]	-1.2 [-6.1]	3.49 [2.95]	0.01 [0.01]	0.89 [0.90]
SUS-Ent	3 [3]	0.35 [0.23]	1.03 [1.07]	15.8 [13.7]	3.58 [3.89]	0.13 [0.13]	0.90 [0.89]
PDM model							
NSE	1 [1]	0.50 [0.29]	0.81 [0.81]	18.8 [16.3]	4.41 [5.04]	0.15 [0.16]	0.92 [0.89]
KGE	0 [0]	0.21 [0.24]	1.02 [1.08]	8.2 [8.3]	3.29 [3.95]	0.07 [0.08]	0.92 [0.90]
US-Ent	9 [9]	0.36 [0.23]	1.03 [1.03]	27.3 [21.4]	1.78 [0.61]	0.22 [0.21]	0.88 [0.88]
SUS-Ent	10 [10]	0.25 [0.30]	1.02 [0.99]	26.4 [21.7]	2.85 [4.16]	0.21 [0.21]	0.91 [0.88]

Sensitivity range
Very High
High
Moderate
Low
Very Low

As explained earlier, NSE and KGE, in contrast to US-Ent and SUS-Ent, are sensitive to time to peak. However, SUS-Ent introduces less error than the NSE in the FD curve, further supporting our theoretical observation that Shannon entropy is strongly related to FD. KGE also fits the FD curve well (0.30 and 0.21 normalised error using the bucket and PDM model respectively). Both entropy-based measures are sensitive to the variability and peak flows (1.03 and 3.58 mm difference respectively using the bucket model, and 1.02 and 2.85 mm respectively using the PDM model). SUS-Ent failed to conserve the mass balance (15.8 and 26.4 % error using the bucket and PDM model respectively). This indicates that although the current scaling approach is able to represent the data range, it is unable to conserve the mass. It is important to note that the linear correlation is equally well represented for all four OFs. NSE introduced the highest errors in variability and peak runoff, probably due to its over-emphasis on obtaining high linear correlation, as explained in Gupta et al. [2009]. In contrast, the models optimised with KGE represented variability, mean flow and linear correlation well.

6. CONCLUSIONS

The potential of information entropy measures as objective functions and the use of entropy with other measures as a diagnostic in rainfall-runoff modelling was demonstrated in the present study. Two rainfall-runoff models, a simple bucket model and the PDM model, were calibrated using four objective functions (NSE, KGE, and our unscaled and scaled versions of Shannon entropy). Output was evaluated in terms of both static and dynamic properties of the streamflow data (i.e. FD curve, variability, mass balance, time to peak, peak runoff, mean and correlation). As expected, results are consistent with the many previous studies showing that not all the static and dynamic properties of the flow series can be adequately captured by a single objective function. NSE is able to capture the time to peak and linear correlation with observed flow. However, it underestimates the variability and mean of flows, and produces (at least from the four objective functions tested) the largest error in peak runoff. The new KGE measure proposed recently by Gupta et al. [2009] seems able to overcome some limitations of NSE. Variability and mean flows are well matched, while keeping the linear correlation between modelled and observed high. The mass balance and peak runoff error is also decreased. These conclusions are consistent for both rainfall-runoff models on this one catchment; however studies on further catchments and with further model structures are required to generalise the conclusions.

Results support our theoretical observations that Shannon entropy is strongly related to the FD relationship, and we suggest that this is likely to provide a more robust measure of FD curve fit than those in current use. Entropy is insensitive to timing errors. This makes it dangerous as a stand-alone measure, but potentially provides a useful diagnostic whereby (in combination with other measures) timing errors could be decoupled from other errors. It can be scaled to capture the range of data as we demonstrated; our preliminary approach is not sufficiently sensitive to mass errors. Further work will address more appropriate scaling methods. As entropy provides an OF measure with very different sensitivities and insensitivities to those currently in use, it also has obvious potential in combination with other measures in a more traditional multi-objective calibration framework.

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