



# Objective functions for information-theoretical monitoring network design: what is optimal?

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**Abstract.** This paper concerns the problem of optimal monitoring network layout using information-theoretical methods. Numerous different objectives based on information measures have been proposed in recent literature, often focusing simultaneously on maximum information and minimum dependence between the chosen locations for data collection. We discuss these objective functions and conclude that a single objective optimization of joint entropy suffices to maximize the collection of information for a given number of sensors. Minimum dependence is a secondary objective that automatically follows from the first, but has no intrinsic justification. In fact, for two networks of equal joint entropy, one with a higher amount of redundant information should be preferred for reasons of robustness against failure. In attaining the maximum joint entropy objective, we investigate exhaustive optimization, a more computationally tractable greedy approach that adds one station at a time, and we introduce the “greedy drop” approach, where the full set of sensors is reduced one at a time. We show that only exhaustive optimization will give the true optimum. The arguments are illustrated by a comparative case study.

## 1 Introduction

The objective of a hydrological monitoring network depends on its purpose, which can usually be framed as supporting decisions. The decisions can be relating to management of water systems, as for example considered by Alfonso et al. (2010a) or flood warning and evacuation decisions in uncontrolled systems. However, also purely scientific research can be formulated as involving decisions to accept or reject certain hypotheses, focus research on certain aspects, or collect more data (Raso et al., 2018). In fact, choosing monitoring locations is also a decision, whose objective can be formulated as choosing monitoring locations to optimally support subsequent decisions.

The decision problem of choosing an optimal monitoring network layout needs an explicit objective function to be optimized. While this objective could be stated in terms of a utility function (Neumann and Morgenstern, 1953), this requires knowledge of the decision problem(s) at hand and preferences of the decision maker. As a special case of utility, it is possible to state the objective of a monitoring network in terms of information (Bernardo, 1979). This can be done using the framework of information theory, originally outlined by Shannon (1948), who introduced information entropy  $H(X)$  as a measure of uncertainty or missing information in the probability distribution of random variable  $X$ , as well as many related measures.

Although ultimately the objective will be a more general utility, the focus of this paper is on information-theoretical methods for monitoring network design. Because information and utility (value of information) are linked through a complex relation-



ship, this does not necessarily optimize decisions for all decision makers. Since we do not consider a specific decision problem, the focus in the present paper is on methods for maximization of information retrieved from a sensor network.

## 1.1 Background

Over the last decade, a large number of papers on information theory based design of monitoring networks have been published. These studies apply information theoretical measures on multiple of time series from a set of sensors, to identify optimal subsets. Jointly, these papers (Alfonso et al., 2010a, b; Li et al., 2012; Ridolfi et al., 2011; Samuel et al., 2013; Stosic et al., 2017; Keum and Coulibaly, 2017; Banik et al., 2017; Wang et al., 2018; Huang et al., 2020; Khorshidi et al., 2020) have proposed a wide variety of different optimization objectives. Some have suggested that either a multi-objective approach or a single objective derived from multiple objectives is necessary to find an optimal monitoring network. These methods then were often compared to other existing methods in case studies, used to demonstrate that one objective should be preferred over the other.

In this paper, the rationale behind posing these information theoretical objectives is discussed in detail. While measures from information theory provides a strong foundation for mathematically and conceptually rigorous quantification of information content, it is important to pay attention to the exact meaning of the measures used. This paper is intended to shed some light on these meanings in the context of monitoring network optimization and provides new discussion motivated in part by recently published literature.

## 1.2 Motivation

We present three main arguments in this paper. Firstly, we argue that objective functions for optimizing monitoring networks can, in principle, not be justified by case studies. Evaluating performance of a chosen monitoring network would require a performance indicator which in itself is an objective function. Case studies could be helpful in assessing whether one objective function (the optimization objective) could be used as an approximation of another, underlying, objective function (the performance indicator). However, from case studies we cannot draw any normative conclusions as to what objective function should be preferred. In other words: the objective function is intended to assess the quality of the monitoring network, as opposed to a practice where the resulting monitoring networks are used to assess the quality of the objective function.

Secondly, we argue that the joint entropy of all signals together is in principle sufficient to characterize information content and can therefore serve as single optimization objective. Notions of minimizing dependence between monitored signals through incorporation of other information metrics in the objective function are not desirable.

Thirdly, multi-objective approaches that use some quantification of dependency or redundancy as a secondary objective, next to joint entropy, could only be justified if redundancy is interpreted as beneficial for creating a robust network, and therefore an objective to be maximized. Minimization of redundancy would mean that each sensor becomes more essential, and therefore the network as a whole more vulnerable to failures in delivering information.



### 1.2.1 Scope

In monitoring network design, other objectives, not relating to information measures have been used. Examples are cost, geographical spread, and squared error based metrics. Also some approaches use models describing spatial variability with certain assumptions, e.g. kriging (Bayat et al., 2019). In the case of network expansion to new locations, models are always needed to describe what could be measured in those locations. This could vary from simple linear models to full hydrodynamic transport models, such as for example done in (Aydin et al., 2019).

In this paper, our main focus is discussing the formulation of information-theoretical objective functions and previous literature on that topic. Therefore, we restrict our scope to those information-theory based objective functions, based on spatially distributed observed data on one single variable. Keeping this limited scope allows us to discuss the interpretation of these objective functions, which formalize what we actually want from a network. Furthermore, we investigate whether the desired optimum in the objective function can be found by greedy approaches, or whether exhaustive search is needed to prevent a loss of optimality.

Only after it is agreed on what is wanted from a network and this is captured as an optimization problem, other issues such as the solution or approximation of the solution to the problem become relevant. The numerical approach to this solution and calculation of information measures involved, warrants another, independent discussion, which is outside our current scope and presented in a future paper.

Our discussion is numerically demonstrated by using data from the case study for Brazos River in Texas, as presented in Li et al. (2012), to allow for comparisons. However, as we will argue, the case study can only serve as illustration, and not for normative arguments for use of a particular objective function. Such an argument would be circular, as the performance metric will be one of the objective functions.

### 1.2.2 Manuscript organization

The manuscript is organized as follows. In the following methodology section, we introduce the methods used to investigate and illustrate the role of objective functions. In section 3, we discuss the case study on the streamflow monitoring network of Brazos River. Section 4 introduces the results for the various methods, and then discusses the need for multiple objectives, the interpretation of trade-offs, and the feasibility of greedy algorithms reaching the optimum. The article concludes with summarizing the key messages and raising important questions about the calculation of the metrics, to be addressed in future research.

## 2 Methodology

In this paper, since we are discussing the appropriate choice of objective function, there is no experimental setup that could be used to provide evidence for one objective version versus the other. This is because to define a "best" or "optimal" golden standard network to aspire to, we need an objective function. Rather, we must make use of normative theoretical reasoning, and



shining light on the interpretation of the objectives used. The practical case studies in this paper therefore serve as illustration, but not as evidence for the conclusions advocated in this paper, which are arrived at through interpretation and argumentation in the discussion section. This methodology section introduces the elementary information measures used in this paper and previous literature we compare with. After, we discuss visualization of these information measures, and finally, we discuss the proposed and previously used objective functions for monitoring network design, which are composed of these elementary information measures.

## 2.1 Information theory terms

The concept of entropy was introduced in thermodynamics as a measure of thermal disorder or randomness of a system. Shannon (1948) developed information theory (IT) based on entropy the concept that explains system's uncertainty reduction as a function of added information. To understand how, consider set of  $N$  events for which possible outcomes are categorized into  $m$  classes, uncertainty is a measure of our knowledge about which outcome will occur. Once an event is observed, and which of the  $m$  classes it belongs to is identified, our uncertainty about the outcome decreases to 0. Therefore, information can be characterized as decrease an observer's uncertainty about the outcome (Krstanovic and Singh, 1992; Mogheir et al., 2006; Samuel et al., 2013; Foroozand and Weijs, 2017; Foroozand et al., 2018). For monitoring networks, the information each sensor provides through its observations (outcomes) is therefore linked to the uncertainty of those outcomes before measurement. These are quantified through the probability distributions of the data.

In monitoring network design, IT has been applied in the literature to evaluate data collection networks that serve a variety of purposes, including rainfall measurement, water quality monitoring, and streamflow monitoring. These evaluations are then used to optimize placement of sensors. The purpose of the network often governs which of information theory's expressions are considered. In the monitoring network optimization literature, four expressions from IT are often used in monitoring network design: (1) entropy ( $H$ ), to estimate the expected information content of observations of random variables; (2) Mutual information, often called transinformation ( $T$ ), to measure redundant information or dependency between two variables; (3) total correlation ( $C$ ), a multivariate analogue to mutual information, to measure the total nonlinear dependency among multiple random variables. Objective functions are often composed from these basic expressions. Details of each expression are presented below.

The Shannon entropy  $H(X)$  is a nonparametric measure, directly on the discrete probabilities, with no prior assumptions on data distribution. It is also referred to as discrete marginal entropy, to distinguish it both from continuous entropy and from conditional entropy. Discrete marginal entropy, defined as the average information content of observations of a random variable  $X$ , is given by:

$$H(X) = - \sum_{x \in X} p(x) \log_2 p(x) \quad (1)$$

where  $p(x)$  ( $0 \leq p(x) \leq 1$ ) is the probability of occurrence of outcome  $x$  of random variable  $X$ . Equation 1 gives the entropy in the units of "bits" since it uses a logarithm of base 2. The choice of logarithm's base for entropy calculation is determined by the desired unit — other information units are "nats" and "Hartley" for the natural and base 10 logarithms, respectively. For



monitoring network design, logarithm of base 2 is common in the literature since it can be interpreted as the needed number of answers to a series of binary questions.

Joint entropy measures the number of questions needed to determine the outcome of a multivariate system. For a bivariate case  $(X_1, X_2)$ , if two random variables are independent, then joint entropy,  $H(X_1, X_2)$ , (Eq.2) is equal to the sum of marginal entropies  $H(X_1) + H(X_2)$ . Conditional entropy (Eq.3), which explains the amount of information one variable delivers that other variable can not explain, can have a range (Eq.4) between zero when both variables are completely dependent and marginal entropy  $H(X_1)$  when they are independent. Mutual information, in this field often referred to as transinformation (Eq.5), explains the level of dependency and shared information between two variables by considering their joint distribution. The metrics are defined as follows,

$$130 \quad H(X_1, X_2) = - \sum_{x_1 \in X_1} \sum_{x_2 \in X_2} p(x_1, x_2) \log_2 p(x_1, x_2) \quad (2)$$

$$H(X_1|X_2) = - \sum_{x_1 \in X_1} \sum_{x_2 \in X_2} p(x_1, x_2) \log_2 \frac{p(x_1, x_2)}{p(x_2)} \quad (3)$$

$$0 \leq H(X_1|X_2) \leq H(X_1) \quad (4)$$

135

$$T(X_1; X_2) = - \sum_{x_1 \in X_1} \sum_{x_2 \in X_2} p(x_1, x_2) \log_2 \frac{p(x_1, x_2)}{p(x_1) * p(x_2)} \quad (5)$$

, where  $p(x_1)$  and  $p(x_2)$  constitute the marginal probability distribution of random variable  $X_1$  and  $X_2$ , respectively; and  $p(x_1, x_2)$  form their joint probability distribution. The assessment of the dependencies beyond three variables can be estimated by the concept of Total Correlation (Eq.6) (proposed by McGill (1954) and named by Watanabe (1960)). Total Correlation (C) gives the amount of information shared between all variables by taking into account their nonlinear dependencies. C can only be non-negative since sum of all marginal entropies cannot be smaller than their multivariate joint entropy (Eq.7), though in the special case of independent variables, C would become zero.

$$140 \quad C(X_1, X_2, \dots, X_n) = \left[ \sum_{i=1}^n H(X_i) \right] - H(X_1, X_2, \dots, X_n) \quad (6)$$

$$145 \quad H(X_1, X_2, \dots, X_n) = - \sum_{x_1 \in X_1} \sum_{x_2 \in X_2} \dots \sum_{x_n \in X_n} p(x_1, x_2, \dots, x_n) \log_2 p(x_1, x_2, \dots, x_n) \quad (7)$$

## 2.2 Understanding and visualizing the measures

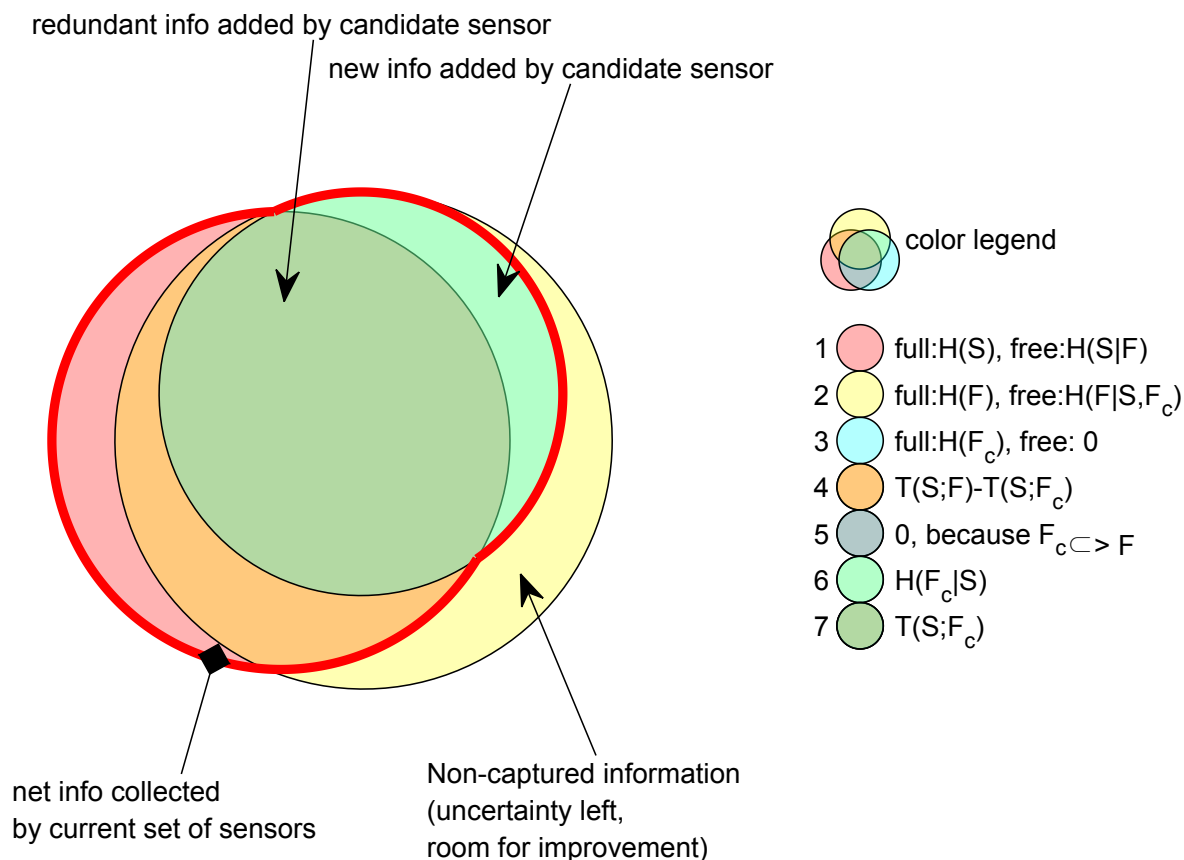
In this paper, we argue that due to the additive properties of information measures, the proposed objectives functions in the literature are unnecessarily complicated, and a single-objective optimization of the joint entropy of all selected sensors will lead



150 to a maximally informative sensor network. The additive relations between some of the information measures discussed in this paper are illustrated in Figure 1. Various types of information interactions for three variables are conceptually understandable using Venn diagram (Figure 2.a). Although Venn diagram can be used to illustrate information of more than three variables when they are grouped in three sets (Figure 1), it can't be used to illustrate pairwise information interactions beyond three variables. A chord diagram, on the other hand, can be useful to better understand pairwise information interaction beyond three variables. Figure 2 provides simple template to interpret and compare Venn and chord diagrams.

155 There are two important caveats with these visualizations. In the general Venn diagram of 3-variate interactions, the "interaction information", represented by the area where 3 circles overlap, can become negative. Hence, the Venn Diagram ceases to be an adequate visualization. For similar reasons, in the chord diagram, the sector size of outer arc lengths should not be interpreted as a total information transferred (Bennett et al., 2019). Information that can contribute to this length combination of unique, redundant and synergistic components (Goodwell and Kumar, 2017; Weijs et al., 2018). Their information entangle-  
160 ment is an active area of research in 3 or more dimensions. In this paper, the total size of the outer arc lengths is set to represent the sum of pairwise information interactions (used in Alfonso et al. (2010a)) and conditional entropy of each variable. This size may be larger than the total entropy of the variable and does not have any natural or fundamental interpretation.

In this paper, we use Venn diagrams to illustrate information relations between 3 groups of variables. Group one is the set of all sensors that are currently selected as being part of the monitoring network, which we denote as  $S$ . Group two is the set of  
165 all sensors that are currently not selected, denoted as  $F$ , and group 3 is the single candidate sensor that is currently considered for addition to the network,  $F_C$ ; see appendix B for an overview of notation. Since group 3 is a subset of group 2, one Venn circle is contained in the other, and there are only 5 distinct areas vs 7 in a general 3-set Venn diagram. In this particular case, there is no issue arising from negative interaction information.

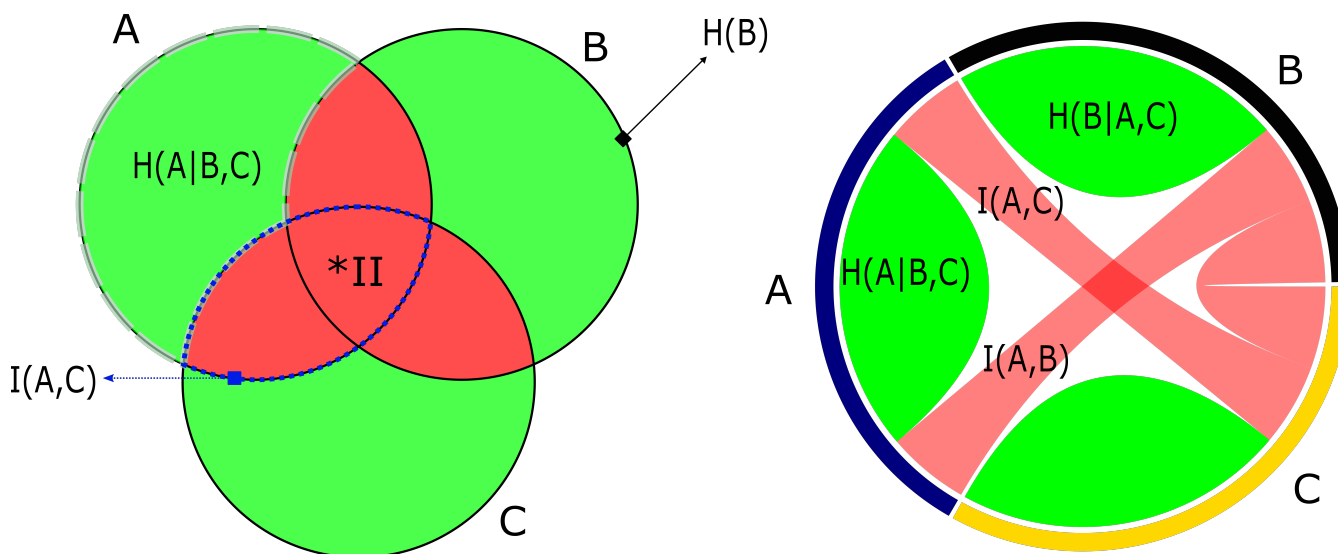


**Figure 1.** Venn diagram illustrating the relations between the relevant information measures. In the legend, the joint and marginal information-theoretical quantities (joint) entropy  $H(X)$ , conditional entropy  $H(X|Y)$ , and transinformation  $T(X;Y)$  for the sets of already selected sensors  $S$ , not yet selected sensors  $F$  and the current candidate sensor  $F_c$  are represented by the surfaces in the Venn diagram. For the 3 basic circle colors (first three circles in the legend), "free" gives the quantity represented by the non-covered part and "full" gives the quantity represented by the entire circle surface. The joint entropy that is proposed to be maximized in this paper is the area enclosed in the thick red line.



a) Sample venn diagram

b) Sample chord diagram



**Figure 2.** Template illustrations of information interactions with (a) Venn diagram, (b) chord diagram. The green and red areas in both diagrams show a graphical representation of conditional entropy and mutual information respectively. The solid line circles in Venn diagram depict single-variable entropy. \*II is information interaction between three variables. The sector size in the outer circle in chord diagram is composed of arcs whose relative lengths correspond to the sum of pairwise information interactions and conditional entropy of each variable, and are best not interpreted.

### 2.3 Multi-objective optimization

170 Information theory-based multi-objective optimization methods for monitoring networks have gained significant attention in  
 the literature. Maximizing network information content, through either the sum of marginal entropy or joint entropy, is the com-  
 mon theme among existing methods. However, there is no consensus on how to minimize redundant information. Table 1 given  
 an overview of the large number of objectives and combinations of objectives used in the last decade. On the one hand, water  
 monitoring in polders (WMP) method (Alfonso et al., 2010a) and joint permutation entropy (JPE) method (Stosic et al., 2017)  
 175 used normalized transinformation to minimize redundant information. While, on the other hand, multi-objective optimization  
 problem (MOOP) method (Alfonso et al., 2010b), Combined regionalization and dual entropy-multi-objective optimization  
 (CRDEMO) method (Samuel et al., 2013), multivariable hydrometric networks (MHN) method (Keum and Coulibaly, 2017)  
 and greedy rank based optimization (GR 5 and 6) method (Banik et al., 2017) adopted total correlation to achieve minimum  
 redundancy. Interestingly, both C and T were used as competing objectives in maximum information minimum redundancy  
 180 (MIMR) method proposed by Li et al. (2012). They argued that transinformation between selected stations in the optimal set  
 and non-selected stations should be maximized to account for the information transfer ability of a network. Meanwhile, re-  
 cently proposed methods in the literature attempted to improve monitoring network design by introducing yet other additional



objectives (Huang et al., 2020; Wang et al., 2018; Banik et al., 2017; Keum and Coulibaly, 2017). These additional objective are further discussed in the appendix.

## 185 2.4 Single-objective optimization

In this paper, we argue for the Maximum Joint Entropy (maxJE) objective for maximizing the total information collected by a monitoring network. This is equivalent to the GR3 objective proposed by Banik et al. (2017), as part of six other objectives proposed in the same paper, which did provide arguments or preference for its use. In this paper, we provide theoretical argument for using single-objective optimization of joint entropy (maxJE) instead of multi-objective optimization. The philosophy of the maxJE objective function is rooted in using multivariate joint entropy defined by Shannon's information theory (1948) for network evaluation. In the discussion, we argue that a single-objective optimization of the joint entropy of all selected sensors will lead to a maximally informative sensor network. Also, it should be noted that the maxJE objective function indirectly minimizes redundant information through its network selection process, which aims for finding a new station that produces maximum joint entropy when is combined with already selected stations in each iteration. This approach ranks stations based on growing joint information which is achievable when a new station  $F_C$  can provide maximum conditional entropy  $H(S|F_C)$  on top of an already selected set ( $S$ ) of stations (see Figure 1 for visual illustration). For case of addition of a single new station to an already existing set, it is therefore mathematically equivalent to maximizing conditional entropy of the new station by selecting it from the pool of non-selected stations  $F$ .

## 2.5 Objective functions used in comparison for this study

200 For the purpose of illustrating the main arguments of this study, we compare maxJE objective function (Eq.8) with three multi-objective optimization methods: MIMR (Eq.9), WMP (Eq.10) and minT (Eq.11). These methods were chosen since they are highly cited methods in this field, and more importantly, recent new approaches in the literature have mostly been built on one of these methods with additional objectives (see Table 1 for more details of examples).

$$\text{Objective function (maxJE):} = \text{maximize } H(\langle X_{S_1}, X_{S_2}, \dots, X_{S_k} \rangle, X_{F_C}) \quad (8)$$

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$$\text{Objective function (MIMR):} = \begin{cases} \text{maximize } H(\langle X_{S_1}, X_{S_2}, \dots, X_{S_k} \rangle, X_{F_C}) \\ \text{maximize } \sum_{i=1}^m T(\langle X_{S_1}, X_{S_2}, \dots, X_{S_k} \rangle, X_{F_i}) \\ \text{minimize } C(\langle X_{S_1}, X_{S_2}, \dots, X_{S_k} \rangle, X_{F_C}) \end{cases} \quad (9)$$

$$\text{Objective function (WMP):} = \begin{cases} \text{maximize } H(F_C) \\ \text{subject to } \sum_{i \in S} \frac{T(S_i; F_C)}{H(S_i)} < SBM \end{cases} \quad (10)$$

$$\text{Objective function (minT):} = \begin{cases} \text{maximize first } H(F_C) \\ \text{minimize } T(\langle X_{S_1}, X_{S_2}, \dots, X_{S_k} \rangle, X_{F_C}) \end{cases} \quad (11)$$



Where  $\langle X_{S_1}, X_{S_2}, \dots, X_{S_k} \rangle$  denotes selected stations in the previous iterations, and  $X_{F_C}$  denotes current candidate station. *SMB* stands for constraint where only stations are considered that are below the median score of all potential stations on that objective.  $m$  is equal to the number of non-selected station in each iteration ( $m + k = n$  total number of stations). It can be seen that a large number of different combinations of information-theoretical metrics are used as objectives.

## 215 2.6 Exhaustive search vs greedy add and drop

Apart from the objective function, the optimization of monitoring networks is also characterized by constraints. These constraints can either be implemented for numerical reasons or to reflect the problem. In existing literature, one constraint that has often implicitly been imposed is that the selection of stations is greedy, meaning that one station is added to the set of selected stations each time while trying to optimize the objective function, without reconsidering the already selected stations  
220 in the set. A practical reason for this is numerical efficiency; an exhaustive search of all subsets of  $k$  stations out of  $n$  possible stations will need to consider a large number of combinations due to combinatorial explosion. Also in practice, when gradually expanding a network, it may be undesirable to relocate existing stations each time a new station is added.

In this paper, for the maximization of joint entropy that we advocate, we will consider and compare 3 constraints that reflect strategies of placement, with the purpose of investigating whether these influence the results. Firstly, the “greedy add”  
225 strategy is the commonly applied constraint that each time the network expands, the most favorable additional station is chosen, while leaving the already chosen network intact. The optimal network for  $k$  stations is found by expanding one station at a time. Secondly, “greedy drop” is the reverse strategy, not previously discussed in literature, where the starting point is the full network with all  $n$  stations, and the optimal network for  $k$  stations is found by reducing the full network one step at a time, each step dropping the least informative station. Since all of the discussed monitoring design strategies use recorded data and  
230 hence discuss networks whose stations are already established, network reduction is perhaps a more realistic scenario. Thirdly, “exhaustive search” is the strategy where the optimal network of  $k$  stations is found by considering all subsets of  $k$  stations out of  $n$ . This is far more computationally expensive, and may not be feasible in larger networks for computational reasons, or not possible in actual placement strategy for logistical reasons. It can therefore be seen as a golden standard. Because all options are considered, this is guaranteed to find the optimal combination, given the objective function. Previous research,  
235 such as Fahle et al. (2015) and Wang et al. (2018) already discussed sub-optimality of greedy-add. Whether greedy-drop or a combination of the two greedy strategies yields the the fully optimal solutions will be investigated in this paper.

## 3 Study area and data description

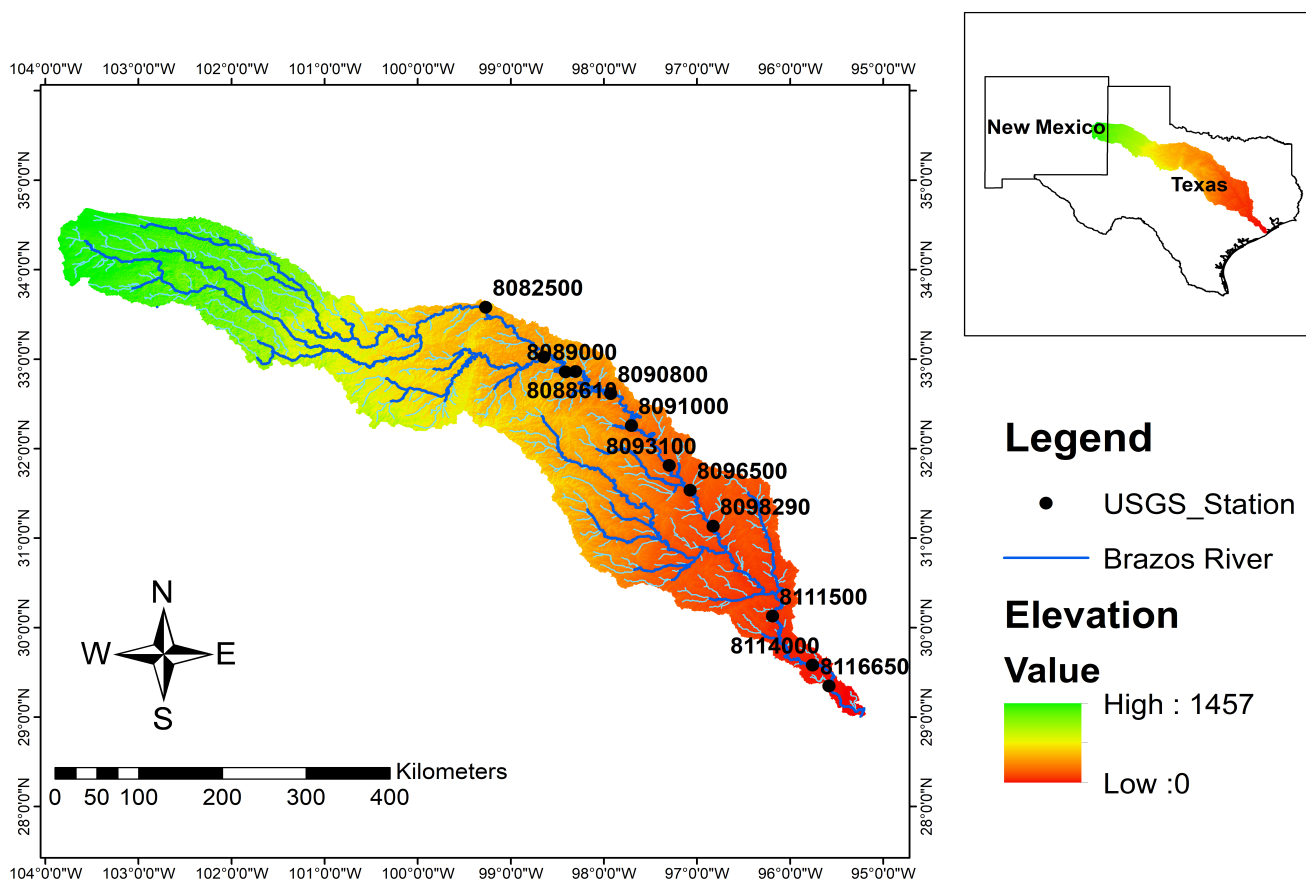
In previous studies, the focus of the research has been on finding an optimal network for the subject case study without sufficiently addressing the theoretical justification of applying a new methodology. For this reason and the primary goal of this  
240 paper, which is highlighting the unnecessary use of multiple objective functions in monitoring network design, we decided to apply our methodology in Brazos River streamflow network (Figure 3) since this network was subject of study for the MIMR method. To isolate the effect of temporal variability of data and quantization method on methodology comparison, we used the



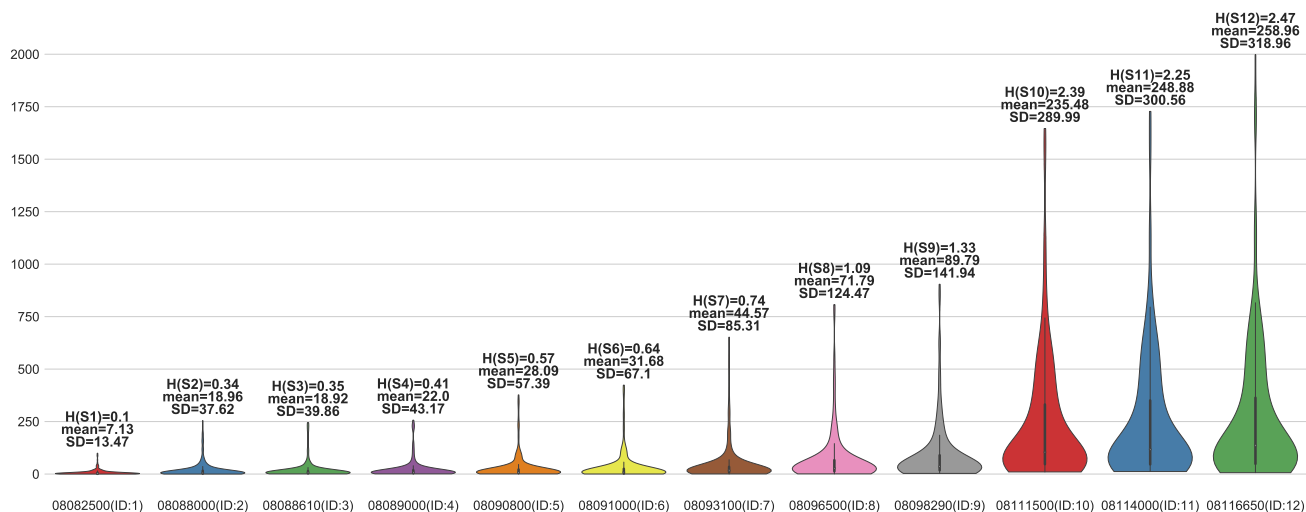
same data period and floor function quantization (Eq.12) proposed by Li et al. (2012). In that paper, 12 USGS stream gauges on the Brazos River were selected for the period of 1990-2009 with monthly temporal resolution; some statistics of the data are presented in Figure 4. For the discretization of the time series, they used a binning approach where they empirically optimized parameter  $a$  to satisfy three goals: (1) to guarantee all 12 stations have distinguishable marginal entropy, (2) to keep spatial and temporal variability of stations' time series, bin-width should be fine enough to capture the distribution of the values in the time series while being coarse enough so that enough data points are available per bin to have a representative histogram, and (3) to prevent rank fluctuation to due to the bin-width assumption, sensitivity analysis must be conducted. They carried out the sensitivity analysis and proposed  $a = 150 \text{ m}^3/\text{s}$  for this case study, the resulting marginal entropy for each station is illustrated in Figure 4.

$$x_q = a \left\lfloor \frac{2x + a}{2a} \right\rfloor \quad (12)$$

Where  $a$  is histogram bin-width for all intervals except the first one which its bin-width is equal to  $\frac{a}{2}$ .  $x$  is station's streamflow value, and  $x_q$  is its corresponding quantized value; and  $\lfloor \cdot \rfloor$  is the conventional mathematical floor function.



**Figure 3.** Brazos streamflow network and USGS stream gauges locations.



**Figure 4.** Brazos River streamflow ( $m^3/s$ ) statistics and resulting entropy values (bits).

## 255 4 Results and Discussion

### 4.1 Comparison of the objectives for Brazos River case

To assess and illustrate the workings of the different objectives in retrieving information from the water system, we compared three existing methods with a direct maximization of the joint entropy of selected sensors,  $H(S, F_c)$ , indicated with maxJE in the results, such as tables 2 and 3. The joint entropy results in table 2 indicate that maxJE is able to find a combination of 8  
 260 stations that contains joint information of all 12 stations ranked by other existing methods. We demonstrate that other methods with a separate minimum redundancy objective lead to the selection of stations with lower new information content (Figure 5). This leads to slower reduction of the remaining uncertainty that could be resolved with the full network, given by the yellow area in Figure 5. Also, Figure 6 provides auxiliary information about the evolution of pairwise information interaction between already selected stations  $\langle X_1, X_2, \dots, X_{i-1} \rangle$  in the previous iterations and new proposed station  $X_i$ . Figure 6 illustrates the  
 265 contrast between the choice of the proposed stations in the first six iterations by different methods.



**Table 2.** Resulting maximum joint entropy for different number of gauges found with different methods for Brazos River case study (JE used exhaustive optimization)

Method	Multivariate dimensions											
	1	2	3	4	5	6	7	8	9	10	11	12
MIMR	2.47	2.84	2.87	3.21	3.23	3.23	3.23	3.32	3.33	3.52	3.93	4.1
WMP1/2	2.47	3.07	3.21	3.36	3.38	3.38	3.38	3.38	3.38	3.52	3.82	4.1
minT	2.47	2.53	2.69	2.72	2.76	2.89	3.06	3.08	3.33	3.52	3.93	4.1
maxJE	2.47	3.07	3.5	3.7	3.88	4.02	4.09	4.1	4.1	4.1	4.1	4.1

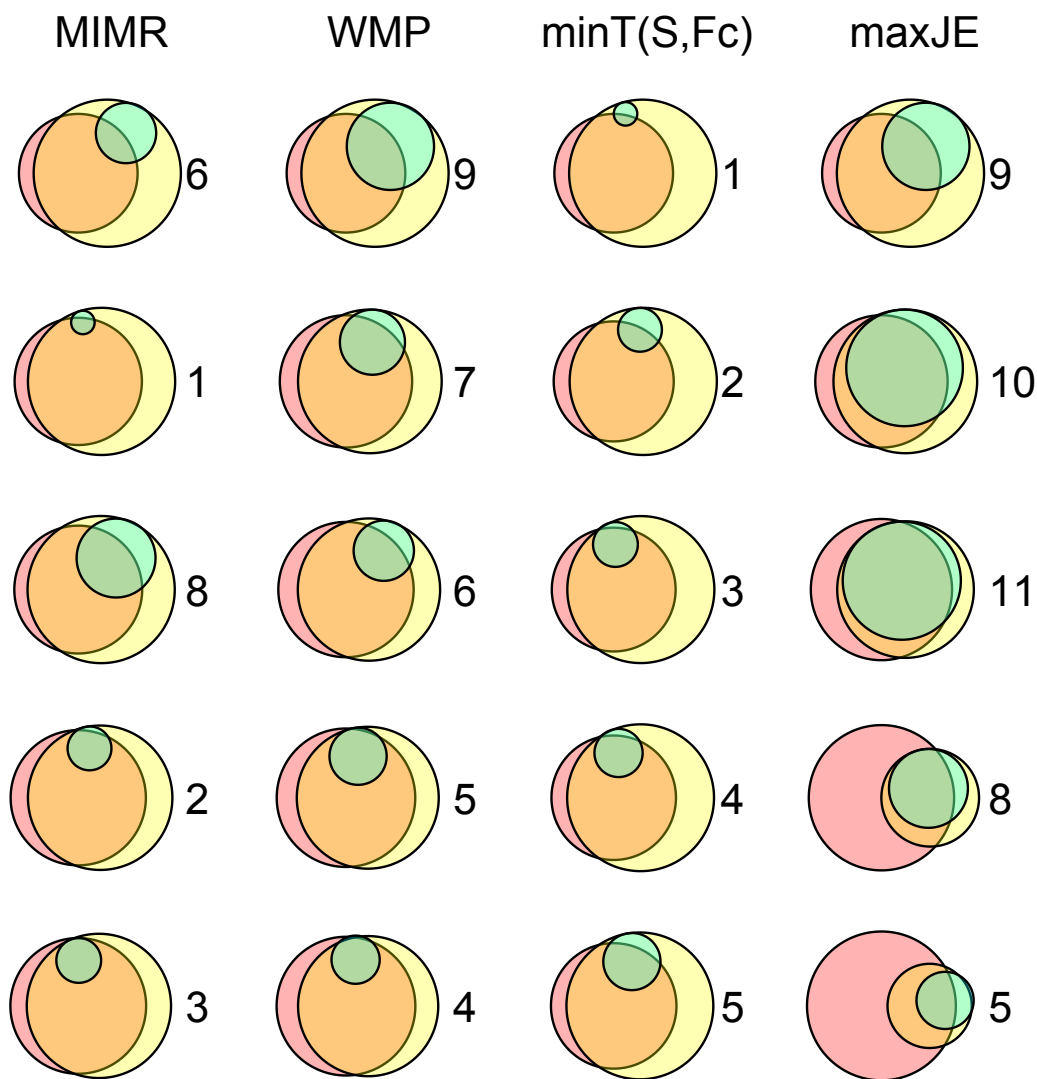
**Table 3.** Optimal gauge orders found with different methods for Brazos River case study.

Method	Station ranking in multivariate dimensions											
	1	2	3	4	5	6	7	8	9	10	11	12
MIMR	12	6	1	8	2	3	4	7	5	9	10	11
WMP1/2	12	9	7	6	5	4	3	2	1	8	11	10
minT	12	1	2	3	4	5	7	6	8	9	10	11
maxJE	12	9	10	11	8	5	7	2*	1*	3*	4*	6*

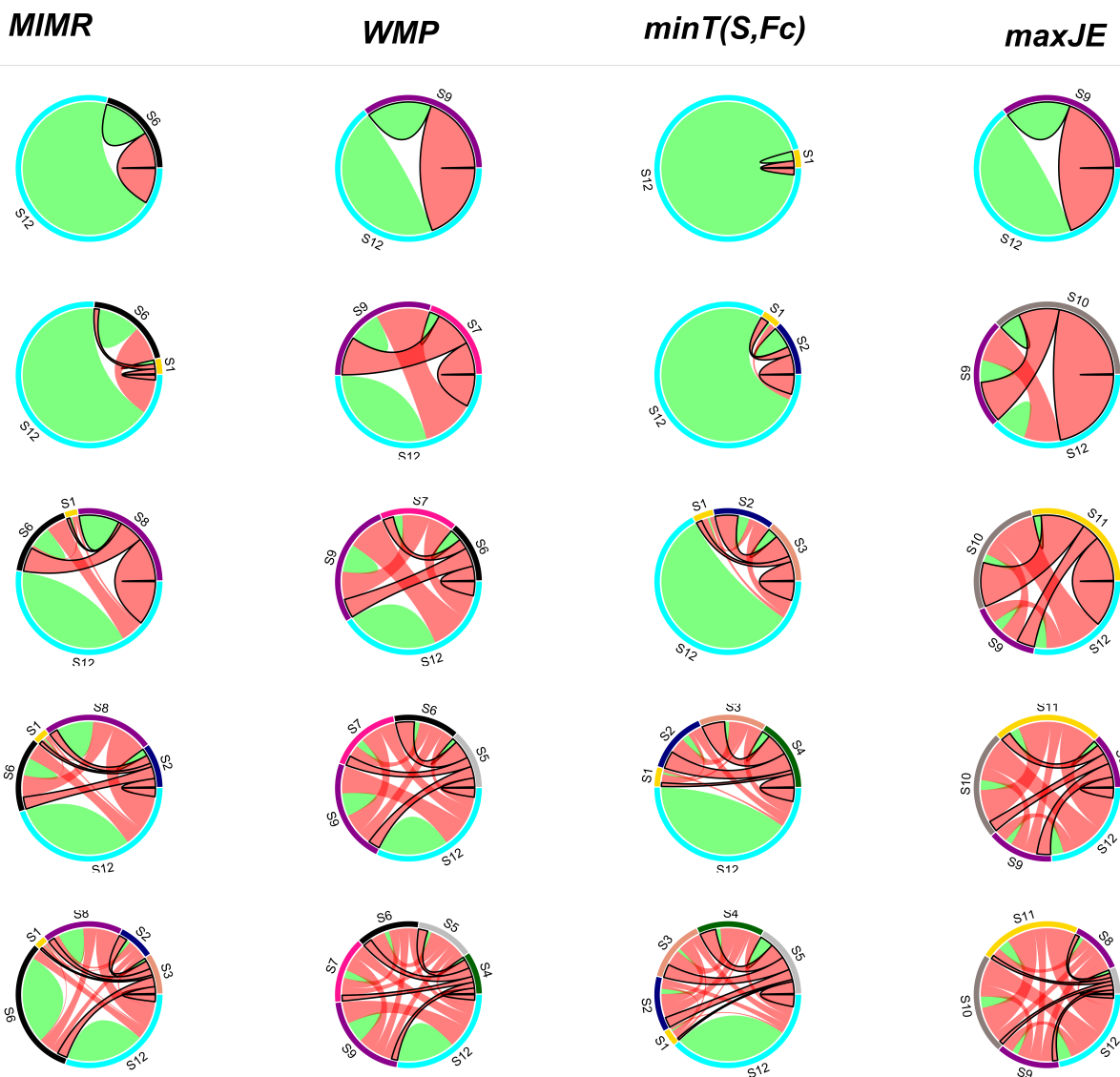
Note that for the last 5 stations, indicated with \*, multiple optimal orders are possible.

## 4.2 Is minimization of dependence needed?

The existing approaches considered above have in common that they all involve some form of dependence criterion to be minimized. Mishra and Coulibaly (2009) stated that "The fundamental basis in designing monitoring networks based the entropy approach is that, the stations should have as little transinformation as possible, meaning that the stations must be independent of each other". For example, the total correlation gives a measure of total redundant information within the selected set. This is information that is duplicated and therefore does not contribute to the total information content of the sensors, which is given by the joint entropy. Focusing fully on minimizing dependence, such as done in the minT objective optimization, makes the optimization insensitive to the amount of non-duplicated information added. This results in many low entropy sensors being selected. It is important to note that the joint entropy already accounts for duplicated information and only quantifies the non-redundant information. This is exactly the reason why it is smaller than the sum of individual entropies. In terms of joint entropy, two completely dependent monitors are not considered to be more informative than one of them. This means that the negative effect that dependency has on information content is already accounted for by maximizing joint entropy only.



**Figure 5.** Approximately proportional Venn diagrams showing the evolution of information measures when progressively (going downwards on the rows) selecting stations (selected station for each step indicated by the numbers) using four different methods (in the different columns). The interpretation of the color-coded areas representing the information measures is the same as in figure 1. All methods select station 12 as the initial station (entropy given by pink circle on row 1). As can be seen from the diagram on the bottom right, the method maximizing joint entropy leaves almost no information unmeasured (yellow part) with just 6 stations, while the other methods still miss capturing this information.



**Figure 6.** Evolution of pairwise information interaction between already selected stations in the previous iterations and new proposed station. Green and red links represent proportional conditional entropy and mutual information, respectively. Links with black border emphasizes on the information interaction of new proposed station in each iteration.

The question is then whether there is another reason, apart from information maximization, why the total correlation should be minimized. In three of the early papers (Alfonso et al., 2010a, b; Li et al., 2012) introducing the approaches that employed or evaluated total correlation, no such reason was given. Also in later citing research, no such arguments have been found. Traditional reasons for minimizing redundancy are reducing the burden of data storage and transmission, but these are not very relevant in monitoring network design, since those costs are often negligible compared to the costs of the sensor installation

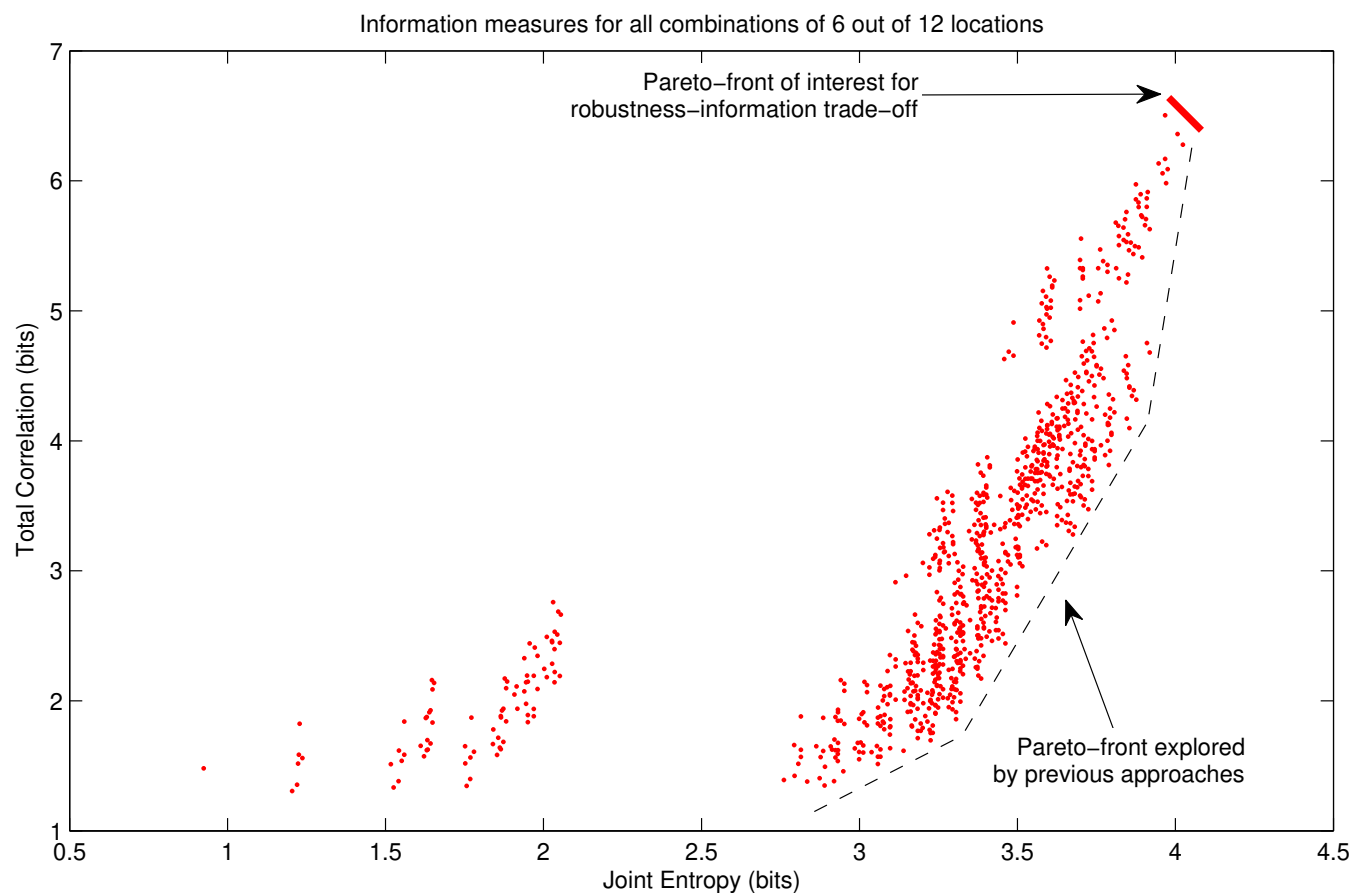


and maintenance (see (Barrenetxea et al., 2008; Nadeau et al., 2009; Simoni et al., 2011)). Moreover, information theory tells us that, if needed, redundant information can be removed before transmission and storage by employing data compression. The counter-side of minimal redundancy is less reliability, a far more relevant criterion for monitoring network design. Given that sensors often fail or give erroneous values, one could argue that redundancy (total correlation) should actually be maximized, given a maximum value of joint entropy. We might even want to gain more robustness at the cost of losing some information. One could for example imagine placing a new sensor directly next to another to gain confidence in the values and increase reliability, instead of using it to collect more informative data in other locations.

The Pareto front that would be interesting to explore in this context is the trade-off between maximum total correlation (robustness) vs. joint entropy (expected information gained from the network), indicated by the red line in Figure 7. Different points on this Pareto front reflect different levels of trust in the sensors' reliability. Less trust requires more robustness and leads to a network design yielding more redundant information. Previous approaches, such as the MOOP approach proposed by Alfonso et al. (2010b), explore the Pareto front given by the black dashed line, where minimum total correlation is conflicting with maximizing joint entropy. As argued in this section, this trade-off is not a fundamental trade-off in information-theoretical terms, but results from the fact that usually there is some redundant information as a by-product of new information, so highly informative stations also carry more redundant information. This redundant information does not reduce the utility of the new information, so does not need to be included as a minimization objective in the optimization.

Summarizing, the maximization of joint entropy while minimizing redundancy is akin to maximizing effectiveness while maximizing a form of efficiency = bits of unique info / bits collected. However bits collected do not have any significant associated cost. If installing and maintaining a monitoring location has a fixed cost, then efficiency should be expressed as unique information gathered per sensor installed, which could be found by maximizing joint entropy (effectiveness) for a given number of stations.





**Figure 7.** The resulting total correlation and joint entropy for all 924 possible combinations of 6 out of 12 sensor locations. In some past approaches, a pareto front in the lower right corner is given importance. In the paper, we argue that this trade off is irrelevant, and information can be maximized with the horizontal direction only. If a trade-off with reliability is considered, the pareto front of interest is in the top-right corner.

### 4.3 Greedy algorithms vs. exhaustive optimization of maximum joint entropy

305 For the objective function of maximum joint entropy, we investigated three different search strategies to obtain the optimal network for different numbers of sensors. The greedy-add optimization works by adding one location at a time, maximizing joint entropy, but constrained by having the already selected locations in the new set. The greedy-drop strategy has the same constraint, but works backward, starting from the maximum number of sensors and each time dropping the one sensor that retains most joint entropy in the reduced set.

310 The exhaustive optimization tests all possible new combinations, not restricted to those containing the set that was already selected. Since the joint entropy of a set of locations does not depend on the order in which they are added, the number of possible combinations is  $\binom{n}{k}$  (i.e.  $n$  choose  $k$ ), where  $n$  is the number of potential stations in the pool and  $k$  is the number of



selected stations. The computational burden is therefore greatest when about half of the stations are selected. For a number of potential sensors under 20, this is still quite tractable (4 minutes on normal PC, implemented -by a hydrologist- in MATLAB),  
315 but for larger numbers, the computation time increases very rapidly. We could make an optimistic estimate, only considering the scaling from combinatorial explosion of station sets, but not considering the dimensionality of the information measures. For 40 stations, this estimate would yield a calculation time of more than 5 years, unless a more efficient algorithm can be found.

Greedy approaches might be candidates for such algorithms. Most of the previous approaches listed in Table 1 can be  
320 categorized as greedy optimizations. For the proposed joint entropy objective, we tested the optimality of greedy approaches against the benchmark of exhaustive optimization of all possible station combinations. For the Brazos River case study, both the “add” and “drop” greedy selection strategies resulted in the global optimum sets, i.e. the same gauge order and resulting joint entropy as was found by the exhaustive optimization. These results can be read from last row of tables 2 and 3. Therefore, for this case, the greedy approaches did not result in any loss of optimality. For the last few sensors, multiple different optimal  
325 sets could be identified, which are detailed in Table 6.

In a further test, using artificially generated data, we experimentally falsified the hypothesis that this result is general. For this test. we generated a correlated random gaussian dataset for 12 monitors, based on the covariance matrix of the data from the case study. We increased the number of generated observations to 860 timesteps, to get more reliable multidimensional probability distribution. Tables 4 show the resulting orders for twelve monitors for the three different approaches. Note how for  
330 the exhaustive optimization in this example, in some instances 2 previously selected gauges are dropped in favor of selecting 3 new stations. The resulting joint entropies for the selected sets are shown in Table 5

Further research should point out 1) whether faster algorithms can be formulated that yield guaranteed optimal solutions, and 2) in which cases the greedy algorithm provides a close approximation. It is also possible to formulate greedy methods with the ability of replacing a limited number of monitors instead of just adding monitors. This leads to a significantly reduced  
335 computational burden compared to exhaustive optimization, while reaching the optimum more often than when adding monitors one at a time. In Table 4, it can be seen that allowing a maximum number of two relocated monitors would already reach the optimal configurations for this case. It would be interesting to further investigate what properties in the data drive the sub-optimality of greedy algorithms. Synergistic interactions (Goodwell and Kumar, 2017) are a possible explanation, although our generate data example shows that even when moving from 1 to 2 selected stations, a replacement occurs. Since there are  
340 only pairs of variables involved, synergy is not needed in the explanation of this behaviour. Rather, the pair with maximum joint entropy does not include the station with maximum entropy, which is perhaps to highly correlated with other high entropy variables.



**Table 4.** Resulting monitor orders for random uniform dataset, using 12 monitors with 860 data points

Method	Station ranking in multivariate dimensions											
	1	2	3	4	5	6	7	8	9	10	11	12
Exhaustive	3	1&12 -3*	6	5&7&11 -6* & -12*	2&6 -5*	9&12 -11*	3	10	5	8	4	11
Greedy Add	3	11	1	7	6	9	2	10	5	8	12	4
Greedy Drop	1	12	6	7	2	9	3	10	5	8	4	11

\* means a previously selected station is removed from optima set.

**Table 5.** Resulting joint entropy for random uniform dataset, using 12 monitors with 860 data points

Method	Multivariate dimensions											
	1	2	3	4	5	6	7	8	9	10	11	12
Exhaustive	1.538	3.0025	4.2251	5.0581	5.7322	6.1717	6.515	6.6947	6.8318	6.933	7.0237	7.0834
Greedy add	1.538	2.898	4.1635	5.0431	5.6811	6.111	6.4858	6.6462	6.7892	6.899	6.9956	7.0834
Greedy drop	1.5298	3.0025	4.2251	5.0407	5.7239	6.1717	6.515	6.6947	6.8318	6.933	7.0237	7.0834

## 5 Conclusions

Information theory provides a valid framework for monitoring network design, especially when no single users with explicit decision problems can be identified. Within this framework, maximizing the joint entropy is the only objective needed to maximize retrieved information, assuming that this joint entropy can be properly quantified. A large part of the literature on monitoring network design has put much focus on minimizing various pairwise or joint redundancy measures, while this should actually be a secondary objective, that is already considered in the first: maximizing the obtained information. Since this total information is directly given by joint entropy of all selected locations, this measure can be directly optimized.

The optimal solution for maximizing joint entropy can be found by exhaustively testing all possible combinations of monitors that are feasible given the current network. The number of possible combinations of monitors, however, becomes prohibitively large for more than some 25 possible locations, especially when around half of the stations are selected. Practical constraints on sensor placement may reduce the computational burden somewhat by limiting the combinatorial explosion. One of these constraints could be that the sensors should be placed one by one, each time optimizing the joint entropy. This so-called greedy optimization approach adds the constraint that the chosen set for  $n + 1$  stations contains the chosen set for  $n$  stations. This approach can for example be useful in Alpine terrain, where relocating a sensor requires significant effort (Simoni et al., 2011).



In this work we introduced the “greedy drop” approach that starts from the full set and deselects stations one by one. We have demonstrated that the two types of greedy approaches do not always lead to the unconstrained true optimal solution. Synergistic interactions between variable may play a role, although this is not the only possible explanation. In our case study the suboptimality of greedy algorithms was not visible, but we demonstrated its existence with artificially generated data. Differences between exhaustive and greedy approaches were small, especially when using a combination of the greedy add and greedy drop strategy, It remains to be demonstrated in further research how serious this loss of optimality is in practical situations.

### 5.1 Further work

In this paper, we focused on the theoretical arguments for choosing the right objective functions to optimize, and compared a maximization of joint entropy to other methods, while using the same data set and quantization scheme. Another important question that needs to be addressed in future research is how to numerically calculate this objective function, or other objective functions used in other approaches. What many of these objective functions have in common, is that they rely on multi-variate probability distributions. For example, in our case study, the joint entropy is calculated from a 12-dimensional probability distribution. These probability distributions are hard to reliably estimate from limited data.

Numerically, this presents a problem for the calculation of multivariate information measures. Estimating multivariate discrete joint distributions exclusively from data requires quantities of data that exponentially grow with the number of variables, i.e. potential locations. When these data-requirements are not met and joint distributions are still estimated directly based on frequencies, independent data will be falsely qualified as dependent and joint information content severely underestimated. This can also lead to apparent earlier saturation of joint entropy, at a relatively low number of stations. For the case study presented here, we do not recommend interpreting this saturation as reaching the number of needed stations, since it could be a numerical artifact. This problem applies to all methods. Before numerics can be discussed, clarity is needed on the interpretation and choice of the objective function. In other words, before thinking about how to optimize, we should be clear on what to optimize. We hope that this paper helped illuminate this.

*Code and data availability.* Data and code availability

The code and data that were used to generate the results in this manuscript are available from <https://github.com/hydroinfotheory> and the USGS <https://waterdata.usgs.gov/nwis>.

*Author contributions.* SW conceptualized study, HF and SW jointly performed analysis and wrote manuscript. SW supervised HF

*Competing interests.* The authors declare no competing interests



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## Appendix A: Additional objectives used in recent literature

Recent literature has expanded the information theoretical objectives with additional objectives. For instance: (1) Wang et al. (2018) proposed dynamic network evaluation framework (DNEF) method that follows MIMR method for network configuration in different time windows and optimal network ranking is determined by maximum Ranking disorder index (RDI) (Eq.A2), which is normalized version of apportionment entropy (AE). RDI was proposed by Fahle et al. (2015) and named by Wang et al. (2018) to analyze the uncertainty of the rank assigned to a monitoring station under different time windows; (2) Huang et al. (2020) proposed information content, spatiotemporality, and accuracy (ISA) method, which extends MIMR method by adding two objectives: maximizing spatiotemporality information (SI), and maximizing accuracy (A). The SI (Eq.A4) objective is introduced to incorporate spatiotemporality of satellite data into network design, and A (Eq.A5) objective is proposed to Maximize the interpolation accuracy of the network by minimizing the regional kriging variance; (3) Banik et al. (2017) proposed six combinations (GR 1-6) of four objectives: detection time (D) (Eq.A6), reliability (R) (Eq.A7), H (Eq.7) and C (Eq.6) for locating sensors in sewer systems; and (4) Keum and Coulibaly (2017) proposed to maximize conditional entropy as a third objective in dual entropy-multi-objective optimization to integrate multiple networks (in their case: rain gauge and streamflow networks). Although maximizing conditional entropy can indirectly be achieved in other used-objective (joint entropy), this new objective gives more preference to maximizing unique information that one network can provide when another network can't deliver. These multi-objective optimization problems are solved by either finding an optimal solution in a Pareto front (Alfonso et al., 2010b; Samuel et al., 2013; Keum and Coulibaly, 2017) or by merging multiple objectives with weight factors into a single objective function (Li et al., 2012; Banik et al., 2017; Stosic et al., 2017).

$$405 \quad AE = - \sum_{i=1}^n \frac{r_i}{M} \log_2 \frac{r_i}{M} \quad (A1)$$

$$RDI = nAE = \frac{AE}{\log_2 n} \quad (A2)$$

Where  $n$  is the number of possible ranks that a station can have (i.e.,  $n$  is equal to the total number of stations).  $\frac{r_i}{M}$  ratio is an occurrence probability of the outcome, where  $M$  is the number of ranks under different time windows, and  $r_i$  is the number of a certain  $i^{\text{th}}$  rank. Therefore, AE takes on its maximum value when the ranking probability of a station has equally probable outcome while minimum AE happens when the station's rank is constant. RDI ranges from 0 to 1, and higher RDI values indicate ranking sensitivity of a station to temporal variability of the data.

$$SI_z(X) = - \sum_{i=1}^l p(\sigma_z) \log_2 p(\sigma_z) \quad (A3)$$



$$415 \quad SI_{network}(X, \gamma_{F_i}) = \frac{1}{n+1} \left[ \sum_{j=1}^n SI_z(X_{S_j}) + SI_z(\gamma_{F_i}) \right] \quad (A4)$$

$$A_{network}(X, \gamma_{F_i}) = -\frac{1}{l} \sum_{i=1}^l \sum_{j=1}^k Var_{ij} \quad (A5)$$

Where  $SI_z(X)$  is the local spatiotemporal information of the grid  $X$  in local window  $z$  in the time series; and  $p(\sigma_z)$  is probability distribution of the standard deviation  $\sigma_z$  in time series  $l$ .  $SI_{network}(X, \gamma_{F_i})$  is spatiotemporal of the network, which  
 420 is calculated by the average of spatiotemporal information of already selected sites  $SI_z(X_{S_j})$  and a potential site  $SI_z(\gamma_{F_i})$ .  
 $A_{network}(X, \gamma_{F_i})$  is network accuracy, and  $Var$  is kriging variance over time series  $l$  and number of grids  $k$  in the study area.

$$D(\gamma) = \frac{1}{S} \sum_{s=1}^S D_{sp}(\gamma) \quad (A6)$$

$$R(\gamma) = \frac{1}{S} \sum_{s=1}^S \delta_s \quad (A7)$$

425 Where  $S$  is the total number of scenarios considered, and  $D_{sp}(\gamma)$  is the average of the shortest time among the detection times for monitoring stations, and  $\delta_s$  is binary choice of 1 or 0 for whether the contamination is detected or not.



## Appendix B: Notation and definitions

$S$	Set of indices of selected monitoring locations
$F$	Set of indices of potential monitoring locations not yet selected
$F_C$	The index of the monitoring station currently under consideration for addition
$X_S, X_F, X_{F_C}$	The (sets of) time series (variables) measured at the monitor(s) in the respective sets
$p(x_1)$	The marginal probability distribution of random variable $X_1$
$p(x_1, x_2)$	The joint probability distribution of variable $X_1$ and $X_2$
$H(X_{F_C})$	The entropy of the marginal distribution of time series $X_{F_C}$
$H(X_F)$	The joint entropy of the marginal multivariate distribution of variables in $F$
$H(X_F X_S)$	The conditional joint entropy of variables in $F$ , given knowledge of variables in $S$
$T(X_F; X_S)$	Mutual information or transinformation between set of variables in $F$ and set of variables in $S$
$C(X_1, X_2, \dots, X_n)$	Total Correlation, the amount of information shared between all variables
$SMB$	Stands for constraint where only stations are considered that are below the median score of all potential stations
$a$	Histogram bin-width
$x$	Station's streamflow value
$x_q$	Quantized value after discretization
AE	Apportionment entropy
RDI	Ranking disorder index
$SI_z(X)$	Local spatiotemporal information of the grid $X$ in local window $z$ in the time series
$p(\sigma_z)$	Probability distribution of the standard deviation $\sigma_z$ in time series
$A_{network}$	Network accuracy
$Var$	Kriging variance
$D$	Detection time
$D_{sp}(\gamma)$	The average of the shortest time among the detection times for monitoring station
$R$	Reliability
$\delta_s$	Binary choice of 1 or 0 for whether the contamination is detected or not



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**Table 1.** Various information-theoretical objectives used by methods proposed in recent literature.

Method	Reference	Objective Function												
		$H(F_C)$	SBM	$H(S, F_C)$	$C(S)$	$T(F_C; S)$	$C(F_C; S)$	$PE(F_C; S)$	$H(Q P)$	Others				
<b>WMP1</b>	Alfonso et al. (2010a)	max	$W_1$											
<b>WMP2</b>	Alfonso et al. (2010a)	max	$W_2$											
<b>WMP3</b>	Alfonso et al. (2010a)	max	$W_3$											
<b>MOOP</b>	Alfonso et al. (2010b)		max			min								
<b>minT</b>	Ridolfi et al. (2011)	$\max 1^{st}$				min								
<b>MIMR</b>	Li et al. (2012)		$\lambda_1$	$-(1 - \lambda_1)$		$\lambda_1$								
<b>CRDEMO</b>	Samuel et al. (2013)		max			min								
<b>JPE</b>	Stosic et al. (2017)		max			min		max						
<b>MHN</b>	Keum and Coulbaly (2017)		max			min		max						
<b>GR1</b>	Banik et al. (2017)												min D	
<b>GR2</b>	Banik et al. (2017)												max R	
<b>GR3</b>	Banik et al. (2017)													
<b>GR4</b>	Banik et al. (2017)												min D & max R	
<b>GR5</b>	Banik et al. (2017)		max						min					
<b>GR6</b>	Banik et al. (2017)		max						min					
<b>DNEF</b>	Wang et al. (2018)		$\lambda_1$	$-(1 - \lambda_1)$		$\lambda_1$							max RDI	
<b>ISA</b>	Huang et al. (2020)		$\lambda_1$	$-(1 - \lambda_1)$		$\lambda_1$							max SI & max A	
<b>maxJE</b>	this paper		max											

$$\text{WMP objectives: } W_1 = \sum_{i \in S} T(S_i; F_C), W_2 = \sum_{i \in S} \frac{T(S_i; F_C)}{H(S_i)}, W_3 = \sum_{i \in S} \frac{T(S_i; F_C)}{H(F_C)}$$

The table shows whether an objective is maximized (max) or minimized (min) or forms part of a weighted objective function that is maximized with weights  $\lambda$ . SBM stands for constraint where only stations are considered that are below the median score of all potential stations on that objective. D is detection time, and R is reliability. RDI stands for ranking disorder index. SI is spatiotemporal information, and A is accuracy. WMP=Water Monitoring in Polders; MOOP = Multi Objective Optimization Problem; minT = Minimum Transinformation; MIMR = Maximum Information Minimum Redundancy; CRDEMO = Combined Regionalization and Dual Entropy-Multi-objective Optimization; JPE = Joint Permutation Entropy; MHN = Multivariable Hydrometric Networks; GR = Greedy Rank; DNEF = Dynamic Network Evaluation Framework; ISA = information content, spatiotemporal and accuracy ; and maxJE = Maximum Joint Entropy.



**Table 6.** All optimal combinations of sensors for the joint entropy objective. For number of sensors above 7, multiple optimal combinations can be found due to saturation of joint entropy

Number of selected stations with multiple optimal combinations	Station ID											
	1	2	3	4	5	6	7	8	9	10	11	12
1	□	□	□	□	□	□	□	□	□	□	□	■
2	□	□	□	□	□	□	□	□	■	□	□	■
3	□	□	□	□	□	□	□	□	■	■	□	■
4	□	□	□	□	□	□	□	□	■	■	■	■
5	□	□	□	□	□	□	□	■	■	■	■	■
6	□	□	□	□	■	□	□	■	■	■	■	■
7	□	□	□	□	■	□	■	■	■	■	■	■
8	□	■	□	□	■	□	■	■	■	■	■	■
8	□	□	■	□	■	□	■	■	■	■	■	■
9	■	■	□	□	■	□	■	■	■	■	■	■
9	■	□	■	□	■	□	■	■	■	■	■	■
9	□	■	■	□	■	□	■	■	■	■	■	■
9	□	■	□	■	■	□	■	■	■	■	■	■
9	□	■	□	□	■	■	■	■	■	■	■	■
9	□	□	■	■	■	□	■	■	■	■	■	■
9	□	□	■	□	■	■	■	■	■	■	■	■
10	■	■	■	□	■	□	■	■	■	■	■	■
10	■	■	□	■	■	□	■	■	■	■	■	■
10	■	■	□	□	■	■	■	■	■	■	■	■
10	■	□	■	■	■	□	■	■	■	■	■	■
10	■	□	■	□	■	■	■	■	■	■	■	■
10	□	■	■	■	■	□	■	■	■	■	■	■
10	□	■	■	□	■	■	■	■	■	■	■	■
10	□	■	□	■	■	■	■	■	■	■	■	■
10	□	□	■	■	■	■	■	■	■	■	■	■
11	■	■	■	■	■	□	■	■	■	■	■	■
11	■	■	■	□	■	■	■	■	■	■	■	■
11	■	■	□	■	■	■	■	■	■	■	■	■
11	■	□	■	■	■	■	■	■	■	■	■	■
11	□	■	■	■	■	■	■	■	■	■	■	■
12	■	■	■	■	■	■	■	■	■	■	■	■