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Measuring data drift with the unstable population indicator[1]

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Abstract. Measuring data drift is essential in machine learning applications where model scoring (evaluation) is done on data samples that differ from those used in training. The Kullback-Leibler divergence is a common measure of shifted probability distributions, for which discretized versions are invented to deal with binned or categorical data. We present the Unstable Population Indicator, a robust, flexible and numerically stable, discretized implementation of Jeffrey's divergence, along with an implementation in a `Python` package that can deal with continuous, discrete, ordinal and nominal data in a variety of popular data types. We show the numerical and statistical properties in controlled experiments. It is not advised to employ a common cut-off to distinguish stable from unstable populations, but rather to let that cut-off depend on the use case.

Keywords: Data drift, data shift, machine learning, kl-divergence

1. Introduction

In studies where populations are compared, it is often required to quantify the change of the population from one sample to the next. The term population is used in the broad sense here: it can be a group of people, but it can also refer to a general ensemble of elements, about which we have data that will be statistically investigated. We will refer to populations in the broad sense throughout this article, and will use the term "entities" to denote the elements making up the population (e.g. the people in a group).

[1] As RDF/nanopublications: https://w3id.org/kpxl/ios/ds/np/RAw9z6Zz148e1e6v4dyLObRaoOP97lMMPSLePvaGUMObA.
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Changes in populations can be interesting in their own right [13,22], but they can also be a necessary prerequisite for modeling a particular property of the population in question or its entities [7,15]. Common use cases are machine learning models that have been trained on a training data set that has been collected in the past (the “historical” data) while it is currently running in production, predicting properties of interest on “current” data, that may or may not still be representative of the training data [1,11]. Usually, the model will be re-trained every once in a while to accommodate the model running in an ever-changing world. It is useful to know how dissimilar your population can become from your training population in either the target variable or any one of the features employed by the predictive model.

Whether to retrain or not, or even whether to make any prediction at all can, and probably *should* be dependent on a measure of similarity between training target or model features and the properties of the data set the model faces in production. This requires a quantitative measure of data drift (also known as data shift or concept drift) between populations. This drift can, and if possible *should* be measured on both predictor and target values, as noted by [2,14]. Such a measure should be well-behaved, i.e. it should give numerical values that actually mean something, no matter how subtle or extreme the data shift is and it should be able to contrast between changes that are perhaps not important and changes that really require action from the data scientist. Note that this decision, whether or not to take action, will very much depend on the use case of the model in question, and can never depend only on the numerical value of a measure of data drift.

When comparing two populations, many measures of (dis-)similarity exist [3]. Some work exclusively for continuous data, some only for categorical data and many are commonly employed in niche branches of applications of machine learning. Some care about the reason why the data has drifted, while some do not [7]. Software implementations do exist, especially for the more “classical” examples, which are commonly included in statistical packages available for many programming languages.

In this paper we introduce a new measure to flexibly overcome some (numerical) shortcomings in existing ones. Our new data drift quantification is a small modification to a popularly used existing parameter, the Population Stability Index [PSI, 23,24]. We describe the PSI and our new implementation, the Unstable Population Indicator, in some detail, while connecting it to its underlying information theoretical foundation. We take away some numerical issues in the implementation that are arise when numerical bins, or categories of data are empty in either one of the populations and we release an implementation in `Python` that is stable, flexible and fast. Therefore, with just our UPI, users can identify data drift in target or feature variables, which can be continuous, discrete, ordinal or nominal in nature and may come in a variety of different popular data formats.

We will start with a brief outline of relative entropy-based measures of dissimilarity from information theory in Section 2, which will give the reader an understanding of how previous and our new implementation fit in the landscape of divergence measures. After that, we will introduce our new measure, the Unstable Population Indicator in Section 3. The numerical and statistical properties of the UPI are discussed in Section 4 and a short summary of a publicly released `Python` implementation is given in Section 5. We will conclude in Section 6.

2. Relative entropy based divergence between probability distributions

Quantitative comparisons of distribution functions are valuable for a great variety of reasons. They are mostly based on Information Theory, and in particular on the Shannon entropy [9], which is a measure of the “disorder” of a system based on the number of possible configuration of entities in a population that would result in the observed distribution function. For a discrete random variable X with possible values $x_i = x_1, x_2, \ldots, x_n$ (respectively, a continuous variable X), all occurring with probability $P(x_i)$ (respectively, of which the probability densities are described by a PDF $P(x)$), the Shannon entropy [16,17] is given by

$$H(X) = -\sum_{i=1}^{n} P_i(x_i) \cdot \log\bigl(P_i(x_i)\bigr) \tag{1}$$

$$H(X) = -\int_{-\infty}^{\infty} P(x) \cdot \log\bigl(P(x)\bigr)\, \mathrm{d}x \tag{2}$$

Note that summation in Eq. (1) is over all possible values of $x_i \in \mathcal{X}$, in which the space of all possible values $\mathcal{X}$ can be countable, or uncountable (like, e.g., in the binomial distribution). The units of this entropy are set by the base of the logarithm. In this paper we take the natural logarithm, which measures entropy in “nats” (base 2 would give “bits” or “shannons”, and base 10 would give “dits”, “bans” or “hartleys”). In words, this entropy describes the PDF-averaged negative log probability mass (or density) and is thus the expectation value of that probability mass or density. The normalization for the expectation values would after all be $\sum_{i=1}^{n} P_i(x_i) = 1$ and $\int_{-\infty}^{\infty} P(x)\,\mathrm{d}x = 1$, respectively.

Adding information (or: “learning something” about X) should make $P(X)$ better-determined, which lowers the entropy and increases the average probability mass/density.

2.1. Symmetrized Kullback-Leibler divergence

A change from one distribution function to another can be quantified by the *relative* entropy. The relative entropy of one distribution function P to another distribution function Q is known as the Kullback-Leibler divergence [8], which is given by

$$D_{\mathrm{KL}}\bigl(P \,||\, Q\bigr) = \int_{-\infty}^{\infty} p(x) \cdot \ln\left(\frac{p(x)}{q(x)}\right) \mathrm{d}x \tag{3}$$

where $p(x)$ and $q(x)$ are the probability densities of P and Q. KL-divergence is not a metric, as it is neither symmetric nor does it obey the triangle inequality and is the expectation of the logarithmic difference between the probabilities P and Q. The asymmetry can be understood: when shifting the mean of a Gaussian, while leaving the standard deviation the same, the average probability density does not change. The PDF does, nevertheless, requiring information to be added and the KL-divergence to be non-zero. Shifting the same Gaussian back to its original position requires the same amount of information added (not subtracted): one added information twice so the total KL-divergence is non-zero, even though we are back at the original distribution function: the KL-divergence measures how far we have diverged before returning to the original distribution function.

A symmetrized version measures the relative entropy from P to Q and adds the relative entropy from Q to P, which has become known as the Jeffrey’s divergence. For discrete probability density functions (or, rather, probability mass functions), this can be written as

$$D_{\text{Jeffrey's, discr.}} = \sum_{x \in \mathcal{X}} \bigl(P(x) - Q(x)\bigr) \cdot \ln\left(\frac{P(x)}{Q(x)}\right) \tag{4}$$

where the summation is over the same probability space $\mathcal{X}$: $P(x) = 0$ implies $Q(x) = 0$.

As this quantity is defined on a discrete probability space, it works for binned continuous variables as well as for categorical variables and it is not necessary for the space $\mathcal{X}$ to be continuous. A related quantity, the Jensen-Shannon divergence [9] has been implemented in `scipy` for discrete and finite probability vectors. This quantity is bounded between zero and one.

2.2. The population stability index

The Jeffrey's divergence, in simple implementations, is popularly known as the Population Stability Index [PSI, 23,24]. Another such measure is the Population Accuracy Index [PAI, 19], but that definition seems to gain less traction. The PSI measures the amount of change in a population, based on a single (continuous, discrete or categorical) variable and measures the change of the fraction of entities at several possible values for the value of that variable. This is completely equivalent to the Jeffrey's divergence in Eq. (4) and usually written as

$$\mathrm{PSI} = \sum_{\text{bins, } i} (f_{1,i} - f_{0,i}) \cdot \ln\left(\frac{f_{1,i}}{f_{0,i}}\right) \tag{5}$$

where $f_{0,i}$ and $f_{1,i}$ are the fraction of the entities in bin or category i in the original and new population, respectively.

In many implementations, like described in a variety of online blog posts,[2] but also e.g. in [6,23], PSI is used on both categorical as well as on discretized versions of continuous variables. Often, 10 or 20 bins are chosen without too much justification. Note how the definition of PSI does not take into account any order in the bins, nor (potentially non-uniform) distances between the bins, which makes the measure equally suitable for categorical/nominal data. Interestingly, this is rarely done. Besides, many posts and papers suggest the same, uninformed cut-off values for the PSI as a distinction between stable and shifted or drifted data sets. What counts as an important shift in your data should be strongly use case dependent and investigated on a per-feature basis. Blindly applying cut-off values found elsewhere is likely to result in less than optimal data drift detection. See Section 4.3 for more discussion on cut-off values.

2.3. The relation with chi-squared tests

For categorical data, the χ^2-test is often used to determine whether the distribution in question (the new data set) is significantly different from the original data set. It is a method from the frequentist realm of hypothesis testing where some null-hypothesis (e.g. no change) is contrasted with an alternative (e.g. a change). Significance levels need to be hand-picked (just going for $P < 0.05$ would be rather naive, given the large variation in data set sizes occurring in practice), resulting in either a significant detection of change, or not [e.g. 18]. As we will motivate below, a hard cut-off is not advised. Given the definition of the statistic, $\chi^2 = \sum(N - O)/O^2$, where the sum is over all independent categories, with N and O being the counts in the New vs Ooriginal data sets, respectively, the same numerical issues as with the original definitions of PSI exist.

[2] See, e.g., these clickable links: this medium post, this github page, this SAS paper, this post on Machine Learning+ and this CRAN R package.

3. The unstable population indicator

It will seem obvious that the evaluation of the logarithm in Eq. (5) is impossible or meaningless when either $f_{0,i} = 0$ or $f_{1,i} = 0$, which is what occurs when a bin or category is un-populated in either the original or new population, respectively, as also noted by [2]. In practice, this may happen fairly often, depending on the use case for the PSI.

3.1. Defining UPI

We therefore propose a low-impact numerical adaptation to the original formulation of the PSI, and release a more flexible implementation of it. As the Index is close to zero for stable populations and higher for unstable populations, we name our new index the *Unstable Population Indicator*: UPI.

In order to solve the numerical nuisances in the evaluation of the logarithm, we add a fraction to every bin or category, equal to one extra entity in the combination of both populations, which is saying we divide one extra entity equally over all bins, in both the original and the new population. In well-populated bins, this difference is marginal, while in (almost) empty bins or categories the difference may be larger. Adding one to a logarithm to ensure positive evaluation is an easy solution, but the effect differs strongly between almost empty and very well filled bins. The justification is that for most use cases, a population should be sufficiently large that adding one entity to the total of the populations, n_{tot}, should make little difference (i.e. $1 \ll n_{\text{tot}}$) and that by spreading out that one extra entity over all bins (i.e. a flat distribution) results in a very small change in the population distribution; one that shouldn't be picked up by doing this analysis in the first place. We will add some more numerical justification below.

Our implementation conserves the symmetry of Jeffrey's divergence, which would have been broken by only adding (fractions of) elements to either one of the populations. Often, the algorithms following this investigation have been trained on the original population, which therefore determines the existing bins or categories. This could make it attractive to only add elements to the new population, when empty bins or categories arise. For many applications, though, having a symmetric distance measure is convenient, and in our implementation we lose nothing by ensuring just that.

For the UPI, we arrive at the following expression:

$$\text{UPI} = \sum_{\text{bins},\, i} (f_{1,i} - f_{0,i}) \cdot \ln\left(\frac{f_{1,i} + 1/n_{\text{tot}}}{f_{0,i} + 1/n_{\text{tot}}}\right) \tag{6}$$

where n_{tot} is the number of entities in the original and new populations together and N_{bins} is the number of bins or categories.

For very large populations ($n \to \infty$) this reduces to the expression for the PSI, but including the extra terms in the logarithm solves the problem of empty bins or categories. It is not a problem when new categories are introduced in the new population, that did not yet exist in the original population. This definition, and our implementation of it, look at both the original and the new data at once and determine all possible values for categorical as well as numerical data in both sets and calculate population stability based on that complete set of possible values.

3.2. UPI in higher dimensions

UPI is defined for the comparison of two one-dimensional probability mass or density functions. In practice, a data set often comprises many dimensions, of which a drift in any constituent dimension can be assessed using the above definition. It can nevertheless be useful to capture drift of the full high-dimensional data set in one metric. Essentially, going to higher dimensions can be done by counting bins of unique combinations of all values in all dimensions. Typically, this is going to result in ever more sparsely filled bins. We have not implemented such a higher-dimensional version (potentially, if demand is there, this is left for future work). One trivial way to extend to higher dimensions and capture the drift of a data set in many dimensions simultaneously is to combine the separate dimensions just like it is done for, e.g. the Euclidean distance: by summing the squared distances in all constituent dimensions to arrive at the total squared distance. UPI is symmetric, positive definite and obeys the triangle inequality (as long as the same two populations are compared along all dimensions; not doing so makes the calculation meaningless) and is thus a distance metric. The total multi-dimensional UPI_{tot} is then

$$\mathrm{UPI}_{\mathrm{tot}}^2 = \sum_{\mathrm{dim}} \mathrm{UPI}_d^2 \tag{7}$$

where UPI_d is UPI as defined in Eq. (6) for every dimension separately and the sum is over all dimensions. It should be noted, though, that drift in one feature may be more important than others, which is ignored in this definition (see also Section 4.3).

4. Numerical and statistical properties of the UPI

In this section we compare UPI, PSI and their underlying theoretical divergences to measure data drift for (samples of) known distribution functions, in order to illustrate the numerical and statistical behavior of such distance measures.

4.1. Sampling from known continuous distribution functions

As a numerical experiment we will start by calculating the UPI and PSI for random samples from distribution functions, for which we also know the actual KL-divergence analytically.

As a base population to compare with, we sample 1000 values from a Gaussian distribution with a mean of zero and a standard deviation of one. We then draw a second population with either 50, 100 or 1000 samples from Gaussians that have a standard deviation of one and means (0, 0.5, 1, 1.5, 2, 2.5). We bin these using `numpy`'s `auto` setting[3] (which we supply with both populations pooled).

The Gaussian distribution may seem like the simplest possible case, with the risk of over-simplification of the general behavior of the UPI. Nevertheless, by binning the random samples, the distribution becomes discrete, and because the order of the bins, nor their position matters for the value of UPI, the distributions could as well be multi-modal or asymmetric. What is important here is that the peak(s) shift away from one another and that the peak of one distribution coincides with lower probability density (or mass) in the other.

[3] The `auto` setting determines the number of equal-width bins by taking the maximum of the Freedman Diaconis estimator (in which the binwidth $h = 2 \cdot \mathrm{IQR}/N^{1/3}$, with IQR the inter-quartile range and N the number of elements in the population), which is supposed to work well for large data sets and is robust to outliers (but can be conservative for small data sets) and the Sturges method ($n_{\mathrm{bins}} = \log_2(N) + 1$), which is the default in R, but can be conservative for large, non-gaussian populations.

Also, the KL-divergence between two Guassian PDFs can be calculated analytically, which allows comparison to the value of the UPI, and is given by

$$D_{\mathrm{KL}}\bigl(P \,||\, Q\bigr) = \ln\frac{\sigma_Q}{\sigma_P} + \frac{\sigma_P^2 + (\mu_P - \mu_Q)^2}{2\sigma_Q^2} - \frac{1}{2} \tag{8}$$

which for $\sigma_P = \sigma_Q = 1$ and $\mu_P = 0$ simply reduces to $D_{\mathrm{KL}}(P \,||\, Q) = \mu_Q^2/2$ and for the symmetrized divergence under the same conditions just to μ_Q^2. We show boxplots of UPI as a function of the offset between the distributions for 100 realizations of the set-up above in Fig. 1. The binning scheme results in very many empty bins for the second population. In fact, only 4 in 1800 simulations have a PSI value that can be calculated, all other realisations had empty bins in either population. This is in part a result of the binning scheme and we come back to this below. It is, nevertheless, an obvious sign that using the original implementation of PSI comes with severe drawbacks when used on continuous data, for which the binning scheme will need to be fine-tuned by hand. UPI gets rid of this problem and is compared to the analytical symmetrized KL-divergence with the stars in the upper panels of Fig. 1. As can be seen, the correspondence between UPI and KL-divergence is very good, especially for large sample sizes and large offsets.

For small sample sizes, as shown in the left panels of Fig. 1 the difference in UPI values gets less pronounced: the vertical difference between the small and large offsets become smaller and the values of the UPI become larger than those of the analytical KL-divergence. This shows that the smaller the sample size, the harder it is for a discretized measure like UPI to find very small drifts of a data set. There is no minimum sample size necessary, but one should keep in mind that UPI measures a difference in *distributions*, not in separate values, so a sample should at least capture the essential behavior of the distributions. Therefore, a few tens of sample seems a sensible minimum data set size to require. It is up to the user of the UPI to set their own limits, given their own use case.

To get around the problems of the binning scheme and to mimic the use of the data drift measures for discrete variables, we bin all of the data into bins with edges at $(-\infty, -1, 0, 1, \infty)$, which ensures well-filled bins at least for population 1. Population 2 is then binned into the same bins and the UPI and PSI are measured for those bins (or categories, if preferred) and displayed in the lower panels of Fig. 1. Here we also include the probability mass based KL-divergence for completeness. The grey bars show the fraction of the samples for which PSI is still undefined because of empty bins. For small samples and large offsets this can still be very common. As long as they are both well-determined, the measures largely agree. Mass-based KL-divergence is asymmetric and is therefore more often finite than PSI.

4.2. *Measuring data drift in probability mass functions*

In a second experiment we create some artificial categorical distributions and show how the values for UPI develop as a function of the difference in bin distributions. Specifically, we create a three-category data set. In the first experiment, the baseline population is a uniform categorical distribution of 3×300 entities per category. For the second population, while leaving the first category (‘A’) untouched, we gradually move all of the items from category ‘B’ to category ‘C’. In Fig. 2, left panels, we show what values UPI takes (upper panel) and what the distributions over the categories look like before, halfway and at the end of the process (lower panel). For comparison, we also plot the value for UPI for distributions of 20 objects per category, initially.

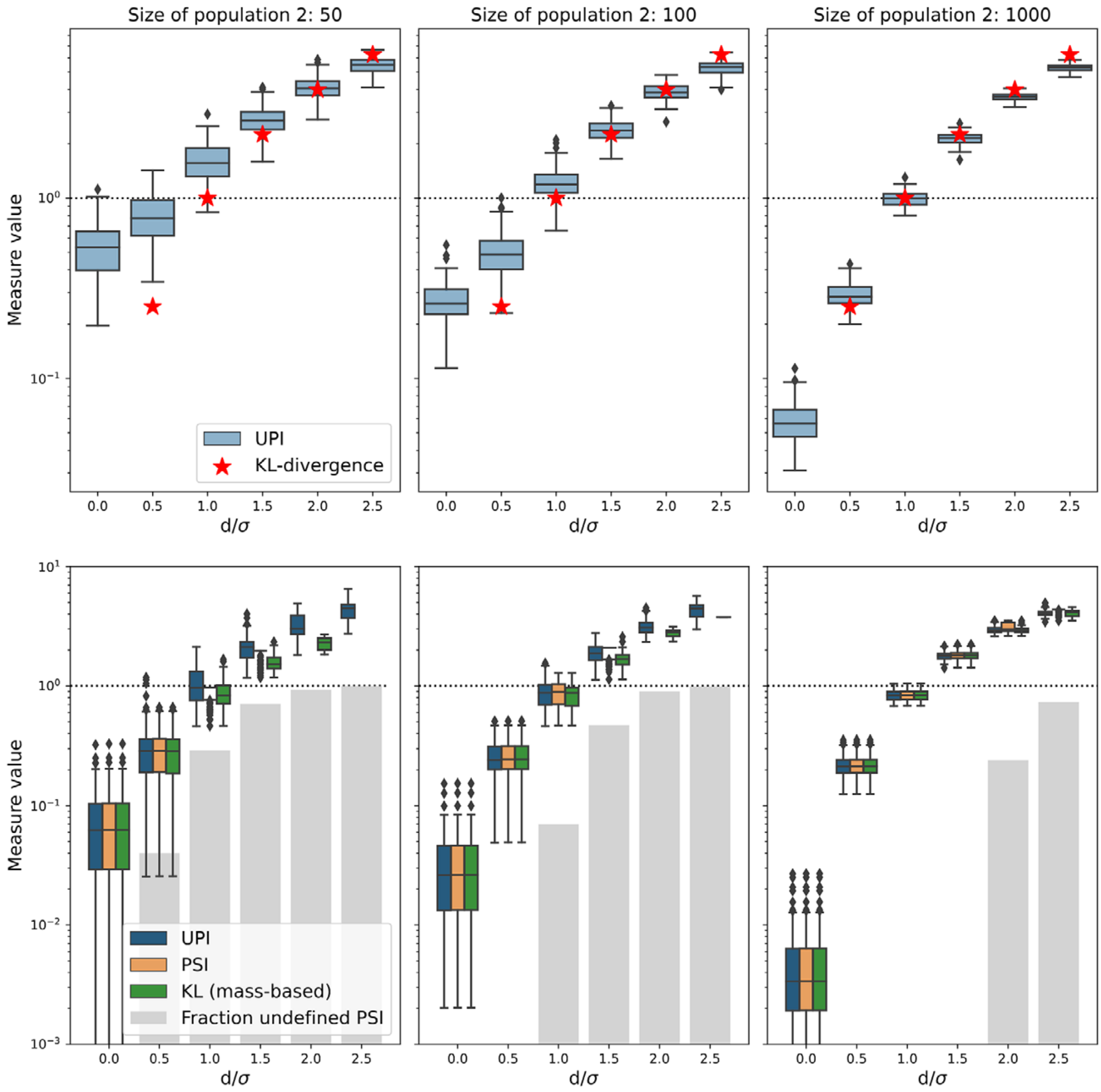

Fig. 1. The values for different measures of data shift in numerical experiments in which populations are randomly drawn from a Gaussian distribution function. One population always consist of 1000 entities, the second has 50, 100 or 1000 entities (the facet columns) from a Gaussian with the same standard deviation, but shifted by a number of standard deviations, indicated on the horizontal axis by d/σ. The vertical axis indicates the value of either of the data shift measures, as indicated by the colors. The reference line helps guide the eye and shows that a value of 1 roughly corresponds to a difference of 1 standard deviation, but the relation between the value of the shift measure and the distance between the Gaussians is non-linear. The upper panels are created with variable binning using NUMPY's AUTO setting, and the stars indicate the exact KL-divergence for two shifted Gaussians (which is 0 for $d/\sigma = 0$). The lower panels use bins with bin edges at $(-\infty, -1, 0, 1, \infty)$ to ensure the PSI has mostly finite values). The fraction of populations that have undetermined PSI values (see text for more details) is indicated with the grey bars.

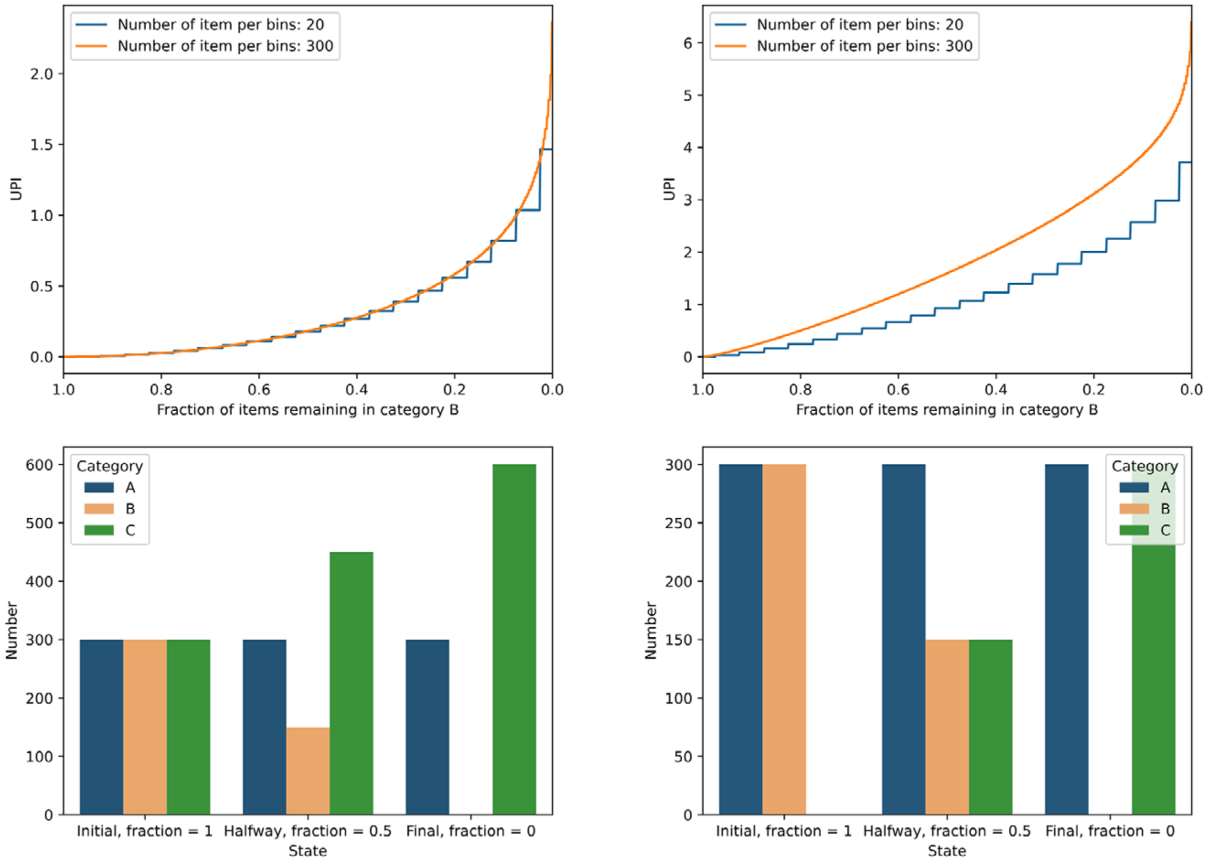

Fig. 2. Values for UPI for categorical distributions in which items from category ‘B’ are gradually moved into category ‘C’, while leaving category ‘A’ untouched. In the left panels, ‘A’, ‘B’ and ‘C’ start out uniformly while in the right panels ‘C’ starts out empty. The evolution of UPI with the remaining fraction in category ‘B’ is shown in the upper panels for 20 (step-wise line) and 300 items (smooth line) per filled category, respectively. The distribution over categories is shown in the lower panel, where the ‘original’ state of category ‘B’ is identical to the distribution of the population that is compared to.

PSI values are almost identical to UPI values, except that they are undefined for situations in which either of the categories is empty (which occurs in either ‘Original’ or ‘Final’ states).

As another example, we repeat the above experiment, except that category ‘C’ (that receives items) starts out empty, and gradually takes over the elements from category ‘B’ (which starts with the same number of elements as category ‘A’ and ends up empty, like before). Note that the total number of elements in the population is smaller in this experiment and in the right panel of Fig. 2 we show that in this case, the value of UPI is more sensitive to the total size of the populations as well. An important difference is that the values for UPI are in general much higher than in the previous exercise, which is explained by the larger relative difference in the populations displayed in the lower right panel (as compared to the lower left panel).

4.3. A cut-off value for UPI to determine significant data drift

It would be tempting to use one value as a cut-off above which populations are “different” and below which they are “the same”. This is common [14,24], but uninformed practice, also when using the conventional PSI. As is shown in Fig. 1 the values for UPI and PSI vary smoothly with increasing difference in underlying populations, for both variable bins and fixed bins. What counts as an "important" difference depends on the use case and should be evaluated whenever UPI or PSI is used in practice. Even for the same distribution function shapes, with the same difference in peak location, a cut-off value will also depend on the two (and relative) sample sizes. Furthermore, as can be seen from the extent of the bar plots in Fig. 1, there is a sizable spread in UPI values for different random realizations of the same two underlying distribution functions. In Fig. 2 we show that depending on how relative categories are filled in categorical data, rather different choices may be made as cut-off values for UPI, which again should be largely informed by the use case. If, for example, a machine learning model is evaluated on the new data set, the target variable will be more sensitive to some predictors than to others, justifying different UPI limits before re-training is warranted. Also, some target predictions are much more critical than others, demanding a more strict definition of data stability or drift, which in turn translates to different cut-off values for the UPI. Numerical experimentation will generally be the preferred way to determine what UPI values to use to ring the digital alarm bell.

5. A `Python` implementation

With this paper, we release a `Python 3` package to calculate the UPI for two distributions of data. The package also allows to calculate the original PSI and the one-directional mass-based KL-divergence. The package is called unstable_populations and can be installed from PyPI via "`pip install unstable_populations`". It allows continuous data as well as categorical (and, thus, ordinal and nominal) data. It is possible to feed the function with binned continuous data, or let the function do the binning of it, based on `numpy`'s `histogram` methods. The populations that are to be compared can be supplied as `list`, `tuple`, `dictionary`, `numpy.ndarray`, `pandas.Series` and `pandas.DataFrame`. With these features it is more flexible and more generic than previous packages to calculate (a subset of) these population stability parameters.

The documentation for the functions is included with the packages. The package comes with an extensive set of test cases, demonstrating the flexibility of the package in terms of input.

The main repository for the package, where issues can be raised (and pull requests submitted) and where a notebook can be found that shows example code using the package is located on GitHub: https://github.com/harcel/unstable_populations.

6. Conclusions

Popular methods to measure the difference between two distributions functions, either of continuous or categorical nature, are based on the concept of relative entropy. Many such measures are implemented in a variety of packages or downloadable functions, but very often come with numerical nuisances that render them less than flexible in everyday use.

We introduce the Unstable Population Indicator, and release a `Python` package that implements it for continuous and discrete data sets in a variety of popular data types alongside. The definition of UPI is very close to that of Jeffrey's Divergence, which itself a symmetrized version (and hence a metric) of the Kullback-Leibler Divergence, i.e. the relative entropy between two distribution functions. With that, the definition is well-motivated by Information Theory, and we explained how to get from the entropy of a distribution to our definition of data shift, also known as data drift.

We have shown that UPI is a smoothly increasing function of data drift, regardless of the underlying distributions being categorical or continuous in nature and that it is largely insensitive to the binning scheme of a continuous variable. This smoothly increasing behavior leads us to strongly advise against the use of a "rule-of-thumb" like cut-off value between distributions that show no significant shift, versus those that do. On a case-by-case basis, users should evaluate what values of UPI are acceptable and which indicate that further action (e.g. re-training a machine learning model) is necessary.

The released code is easy to obtain, install and use and is fully open source.

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The code and this paper use `Python 3` [20], `numpy` [4], `pandas` [10,12], `matplotlib` [5] and `seaborn` [21]. The reviewers are acknowledged for their comments that improved the clarity of the paper. The authors thank Joris Huese for valuable and inspiring discussions during the onset of this study. Dan Foreman-Mackey and Adrian Price-Whelan are acknowledged for technical help and Bluesky for taking over the role of what once was Twitter for enabling such help.

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