Efficient estimation of divergence-based sensitivity indices with Gaussian process surrogates

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Abstract

We consider the estimation of sensitivity indices based on divergence measures such as Kullback-Leibler divergence. For sensitivity analysis of complex models, these divergence-based indices can be estimated by Monte-Carlo sampling (MCS) in combination with kernel density estimation (KDE). In a direct approach, the complex model must be evaluated at every input point generated by MCS, resulting in samples in the input-output space that can be used for density estimation. However, if the computational cost of the complex model strongly limits the number of model evaluations, this direct method gives large errors. A recent method uses polynomial dimensional decomposition (PDD), which assumes the input variables are independent. To avoid the assumption of independent inputs, we propose to use Gaussian process (GP) surrogates to increase the number of samples in the combined input-output space. By enlarging this sample set, the KDE becomes more accurate, leading to improved estimates. We investigate two estimators: one in which only the GP mean is used, and one which also accounts for the GP prediction variance. We assess the performance of both estimators, demonstrating they outperform the PDD-based method. We find the estimator based on the GP mean of the Gaussian process performs best.

Keywords: sensitivity analysis, divergence-based, Gaussian processes.

1. Introduction

Sensitivity analysis is an essential part of uncertainty quantification and a very active research field \cite{1,2,3}. Several types of sensitivity indices have been formulated, such as variance-based (including Sobol’s indices \cite{4}), density-based...
derivative-based or divergence-based. Broadly speaking, divergence-based sensitivity indices quantify the difference between the joint probability distribution (or density) of model input and output on the one hand, and the product of their marginal distributions on the other hand. A variety of divergence-based indices can be brought in a common framework built on the notion of $f$-divergence, as was shown by Da Veiga. The $f$-divergence is a generalization of several well-known divergences such as the Kullback-Leibler divergence and the Hellinger distance.

In most cases, these sensitivity indices cannot be computed analytically because the distribution of the model output given the input is not known exactly. As an alternative, one can resort to Monte Carlo (MC) sampling combined with kernel density estimation: the input distribution is sampled using MC, the model is evaluated on all sampled input points, and from resulting input-output points the joint and marginal probability densities of input and output are estimated. However, when the number of available output points is low, for example because of high computational cost of the model, the estimated densities will generally be inaccurate, resulting in large errors in the estimated sensitivity indices.

In this study we propose to increase the number of output samples by using a Gaussian process (GP) surrogate. The GP is constructed on the input-output points that are obtained with the (expensive) model. The main idea is that the additional output samples improve the kernel density estimates even though they introduce a bias due to the difference between the true model and its GP approximation.

Our approach is based on both the development of divergence-based indices and the use of Gaussian processes in sensitivity analysis. Therefore, we briefly summarize some of the advancements in these areas. Auder & Iooss presented two sensitivity analysis methods based on Shannon and Kullback-Leibler entropy, respectively, building on work in and . Da Veiga introduced sensitivity indices based on the $f$-divergence. In , besides more theoretical results, three approximate methods are discussed: one using MC, one with MC combined with kernel density estimation (KDE-MC), and one in which MC, KDE and polynomial dimensional decomposition (PDD-KDE-MC) are combined (see also ). Recently, KDE also appears in estimators of mutual information measures in , where $f$-divergences are computed between the joint distribution of two random variables and the product of their marginal distributions. In , $f$-divergence measures are computed by a $k$-nearest neighbor graph.

Marrel et al. discuss Gaussian processes and the analytical expressions for Sobol indices that arise from them. To compute the indices, two approaches are considered: one in which the predictor of the GP is used and one in which the full GP is used. The latter approach is found to be superior in convergence and robustness. Furthermore, the modeling error of the GP is integrated through confidence intervals; it is reported that the bias due to the use of the GP is negligible. In a related study, Svenson et al. estimate Sobol indices with GPs, using specific compactly supported kernel functions. Furthermore,
combining GPs with derivative-based indices has been investigated by [6] and [20]. In [21], predictions from a GP are used to rank the input variables based on their predictive relevance. Two methods for this are presented in [21], one based on Kullback-Leibler divergence and one based on the variance of the posterior mean.

Despite the developments sketched above, approaches that combine GP surrogate modeling and divergence-based sensitivity analysis have not been explored yet. The methodology proposed in this paper combines these two elements for the first time. We discuss two variants of this method, one in which only the GP mean is used, and one which also accounts for the GP prediction variance.

We note that for the approach proposed here it is not needed to assume that the inputs are mutually independent, nor does dependency of inputs make it more complicated. We present test cases with independent inputs as well as cases with dependent inputs. For the former, we compare with results obtained with PDD-KDE-MC [14, 15]. PDD-KDE-MC follows a similar philosophy of using surrogates to enlarge the set of points used for density estimation, although the type of surrogate differs. However, the PDD is connected to the ANOVA representation of a multivariate function, which becomes difficult in the case of a dependent input distribution.

Section 2 describes the sensitivity indices central to this paper, as well as the complications of estimating them. Our proposed method and the two estimators that arise from it are discussed in section 2.3. Section 3 applies these estimators to three test cases. Section 4 concludes.

2. Divergence-based sensitivity indices and their estimation

2.1. Sensitivity indices from the $f$-divergence

We consider the situation where a model takes a vector of inputs $(X^1, ..., X^d)$ and returns a (scalar) output $Y$. The input vector $X$ is random, and as a result the output $Y$ is a random variable as well. Da Veiga [8] proposed to perform global sensitivity analysis with dependence measures, especially $f$-divergences (see also [14]). In this way, the impact of the $k$th input variable $X^k$ on the output $Y$ is given by

$$S_{X^k} = \mathbb{E} [d(Y, Y|X^k)],$$

where $d(\cdot, \cdot)$ denotes a dissimilarity measure. The unnormalized first-order Sobol indices can also be written in this framework, namely with

$$d(Y, Y|X^k) = \left( \mathbb{E}(Y) - \mathbb{E}(Y|X^k) \right)^2.$$

We will use the Csiszár $f$-divergence [3], which is given by

$$d_f(Y, Y|X^k) = \int_{\mathbb{R}} f \left( \frac{p_Y(y)}{p_Y|X^k(y)} \right) p_Y|X^k(y) dy,$$
with \( f(\cdot) \) a convex function with \( f(1) = 0 \), and \( p(\cdot) \) denotes a probability distribution function. Some well-known choices for \( f \) are \( f(t) = -\log(t) \) (Kullback-Leibler divergence) and \( f(t) = (\sqrt{t} - 1)^2 \) (Hellinger distance). Combining (1) and (2) with basic probability theory gives us

\[
S^f_{X^k} = \int \int_{\mathbb{R}^2} f \left( \frac{p_Y(y)p_{X^k}(x)}{p_{X^k,Y}(x,y)} \right) p_{X^k,Y}(x,y) dy dx. \tag{3}
\]

These sensitivity indices are equal to zero for \( X^k \) and \( Y \) independent and positive otherwise. Furthermore, they are invariant with respect to smooth and uniquely invertible transformation of \( X^k \) and \( Y \) \cite{22}, in contrast to Sobol indices which are only invariant with respect to linear transformations. Moreover, it is easy to generalize (3) to multidimensional \( X^{k,l} \).

2.2. Difficulties for estimation

The main problem for computing \( S^f_{X^k} \) is that the probability densities in (3) are not known. In order to estimate \( S^f_{X^k} \) it is necessary to estimate \( p_Y(\cdot) \) and \( p_{X^k,Y}(\cdot,\cdot) \), and, depending on the type of input, \( p_{X^k}(\cdot) \) as well. In \cite{8} it is indicated that if samples \((X_L,Y_L)\) are available, only the ratio \( r(x,y) = \frac{p_Y(y)p_{X^k}(x)}{p_{X^k,Y}(x,y)} \) needs to be estimated.

The estimates of the densities can be obtained with kernel-density estimation (also in \cite{8,14}). To do so, one chooses a suitable kernel and a suitable value for the kernel bandwidth \( h \). When the density of the input \( X \) is known, this information can be used to determine \( h \), otherwise, guidelines are available \cite{23}.

Clearly, the estimate of the density \( p_Y \) will not be perfect, leading to an error in the estimation of \( S^f_{X^k} \). This is strongly related to the number of samples \((X_L,Y_L)\) available for density estimation. If high computational cost of the model limits this number, the estimation of \( S^f_{X^k} \) can be improved by using a surrogate of the model to generate more samples. An existing method for this is polynomial dimensional decomposition (PDD) \cite{24}. It is based on the assumption of mutually independent input variables, which can be unrealistic in practical cases. Furthermore, the surrogate modeled by PDD is a polynomial, thereby limiting the output function space. Another point of interest is the large number of parameters which needs to be fit for PDD.

As an alternative, we propose to use Gaussian processes \cite{25} as a surrogate model to obtain the larger sample \((X_+,Y_+)= (X_L \cup X_{L+}, Y_L \cup Y_{L+})\), in which \( Y_{L+} \) indicates the surrogate model output for the extra input samples \( X_{L+} \). For each data point in \( X_{L+} \), this \( Y_{L+} \) is a normal distribution in itself, and for each point in \( X_L \) it is a degenerated normal distribution (i.e., it has zero variance).

An additional advantage may be the availability of confidence intervals for \( S^f_{X^k} \) at almost no extra computational cost. Unfortunately, these confidence intervals do not include the bias from approximating the output by a Gaussian process.

2.3. Estimation using GPs

We assume the input samples \( X_L := \{x_i\}_{i=1}^L \) are already available, otherwise one can use Monte Carlo sampling (or Latin Hypercube sampling in the case
of independent uniform data) to select samples from the data \( X \). Then, the corresponding output \( Y_L := \{ y_l \}_{l=1}^L \) can be obtained as \( Y_L = G(X_L) \) with \( G \) the output, which is either a function or a computational model. Then, one needs to fit a Gaussian process \( \tilde{G}_{(X_L,Y_L)}(x) = N(\mu(x), \Sigma(x)) \) to \( (X_L,Y_L) \), thereby choosing an appropriate kernel. This Gaussian process is now used to obtain output \( Y_{L+} = \tilde{G}_{(X_L,Y_L)}(X_{L+}) \) for other input samples \( X_{L+} \). This leads to the augmented data set \( X := X_L \cup X_{L+} \) of size \( N = L + L+ \) with (partial) surrogate output \( Y_{L+} = Y_L \cup Y_{L+} \). Note that \( Y_{L+} \) does not consist of single values, but rather of a multivariate normal distribution. We now explain how to compute the KDE on \( (X+,Y+) \) and how it is used to approximate (3).

For a one-dimensional input \( X \), the estimators for the kernel density are given by \[14\]

\[
\hat{f}_X(x) = \frac{1}{Jh_X} \sum_{j=1}^J K_X \left( \frac{x - x_j}{h_X} \right)
\]

\[
\hat{f}_Y(y) = \frac{1}{Jh_Y} \sum_{j=1}^J K_Y \left( \frac{y - y_j}{h_Y} \right)
\]

\[
\hat{f}_{X,Y}(x,y) = \frac{1}{Jh_X h_Y} \sum_{j=1}^J K_X \left( \frac{x - x_j}{h_X} \right) K_Y \left( \frac{y - y_j}{h_Y} \right),
\]

with \( (x_j, y_j) \) the \( j \)th sample of the input data \( (X,Y) \) and \( J \) the size of the data. Note the input data \( X \) have to represent the distribution of \( X \). An extension to a higher-dimensional \( X \) is easy to obtain. For our purposes, we either have \( J = L \) and \( (X,Y) = (X_L,Y_L) \), or we have \( J = N \) and \( (X,Y) = (X_+,Y_+) \). We choose the Gaussian kernel and \( h_X = h_Y = h \) according to Scott’s rule \[23\], where we include a scaling factor if necessary. Then, the estimator for \( S_{X_k}^f \) as given by \[14\] is obtained.

\[
\overline{f}^{(j)}_{X_k} := \frac{1}{J} \sum_{j=1}^J f \left( \frac{\hat{f}_X(x_j) \hat{f}_Y(y_j)}{\hat{f}_{X,Y}(x_j, y_j)} \right).
\]

In the previous paragraph, we ignored the fact \( Y_{L+} \) is a multivariate normal distribution instead of a single value when \( J = N \). Therefore, there are two options to obtain values for \( Y_{L+} \). The first option is to use the prediction mean \( \mu(x) \) and get the resulting output samples

\[
Y_{L+} = \mu(X_{L+})
\]

to be used in (4). The other is to sample from this normal distribution \( n_s \) times. In that case, one gets the \( n_s \) output sets

\[
Y_{L+}^{(s)} \sim N(\mu(X_{L+}), \Sigma(X_{L+})),
\]

in which \( \sim \) denotes “sampled from the distribution”, and thereby \( n_s \) estimates of \( \overline{f}^{(X_k)}_{X_k,f} \). Note that this also implies the kernel density estimates have to be computed \( n_s \) times.
3. Results

We test the estimators in several ways. The first test case is with regard to random input/output data and is described in Section 3.1. In this case, the estimates should be near zero. The second test case is based on the Ishigami function and is performed for both independent and dependent input data, of which the results can be found in Section 3.2. The last test case is higher-dimensional and considers the Piston function (Section 3.3). The PDD-KDE-MC method [14] is included for comparison, where bivariate decomposition ($S = 2$) is used with polynomial order $m = 4$ is used for both random data and the Ishigami function and univariate decomposition ($S = 1$) for the Piston function (also with $m = 4$). This is due to the large amount of parameters involved. In these tests, we only use the Kullback-Leibler divergence, while other $f$-divergences can be used as well. All experiments have been performed $nr = 10^2$ times with $ns = 10^2$ samples in the case of the second estimator. The error bars in the upcoming figures indicate the empirical 95% confidence interval. The results are summarized in Section 3.4.

3.1. Random data

First, we check the behavior for random output, in which case the sensitivity indices should be zero. Both the input and output data are one-dimensional, uniformly distributed on $[0,1]$ and have size $N = 10^3$, while $L$ is varied from $L = 10$ to $L = 200$ based on [26]. The results are in Figure 1. On the right, we show the sensitivity index as computed on the complete data (green diamond). As expected, their mean is around zero and the spread of the results is small. The estimates based on $L$ samples (blue circle) are also around zero, although their spread is larger. The results for PDD-KDE-MC (red pentagon) show an even larger spread. Note that due to the numerical implementation, the sensitivity indices can become negative. For the estimates based on the Gaussian process (orange square), the situation is a little different because the Gaussian process fits a function through the data, the sensitivity index will most likely not
be equal to zero. Due to the bad fit, we chose to only include the results from (5).

Two cases appear, which have the same effect. The length scale and the process variance are either both small or both large. As a result, the predictions of the Gaussian process mean will be close to 0.

5, while the \( \mathbf{L} \) samples have values uniformly in \([0, 1]\). However, in practice one will consider a \( \mathbf{S}_X \) with such a small value as non-influential.

3.2. Ishigami function

We now continue to a non-trivial synthetic test case, of which the test function is from Ishigami & Homma [27]. This output function is defined by

\[
G(x, y, z | a, b) = (a + bz^4) \sin(x) + a \sin^2(y)
\]

on the domain \([-\pi, \pi]^3\) (dimension \(d = 3\)). We will use the well-known choice \(a = 7, b = 0.1\) in accordance with [28].

Two types of input data are constructed for this test case. One is uniformly distributed and consists of \(N = 10^3\) samples on the domain of the output function. The other is the empirical copula of a multivariate normal distribution on the same domain, which is given by

\[
Z = \mathcal{N} \left( \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.8 & 0.5 \\ 0.8 & 1 & 0.8 \\ 0.5 & 0.8 & 1 \end{bmatrix} \right),
\]

such that

\[
X = -\pi + 2\pi \cdot F(Z),
\]

with \(F\) the cumulative distribution function of the marginal distributions (which is distributed as \(N(0, 1)\)).

For these datasets, it is possible to compute the KDE on the full data for comparison. Furthermore, we can tune the length scale \(h\) because we know the input density. It turned out a scaling factor of \(\pi\) is beneficial, such that \(h = \pi \cdot N^{-1/(d+4)}\) for the complete dataset, and \(h = \pi \cdot L^{-1/(d+4)}\) for the KDE based on \(L\) samples, in which Scott’s rule [23] is used.

In the numerical experiments, we first compute a Latin Hypercube Sample (LHS) of size \(L = \{30, 50, 100, 200\}\) and combine it with KDE. For this data, we computed [4]. Then, we fit a Gaussian process with Gaussian kernel to these samples, where the length scales have been estimated by maximum likelihood estimation. Now, we can proceed with KDE on \((X, Y)\), in which we include both the choices \(Y_{L^+} = \mu(X_{L^+})\) (Equation 5) and \(Y_{L^+} = N(\mu(X_{L^+}), \Sigma(X_{L^+}))\) (Equation 6). In the first case, we obtain one estimate for \(\mathcal{H}_{X^k,f}^{(L+L^+)}\) for each repetition of the experiment and thereby one value of \(|\mathcal{H}_{X^k,f}^{(L+L^+)} - \mathcal{H}_{X^k,f}^{(N)}| \approx |\hat{S}_{X^k} - S_{X^k}|\) which is used as measure of convergence. In the second case, we take the number of samples \(ns = 10^2\). For each sample \(Y_{L^+}^{(s)}\) as a prediction of the output, we compute [4]. This leads to \(ns\) estimates of \(\mathcal{H}_{X^k,f}^{(L+L^+)}\) and the
convergence measure \( \left| \overline{H}^{(L+L+)}_{X_k,f} - \overline{H}^{(N)}_{X_k,f} \right| \). Its mean is used to determine the convergence of the estimates in Figure 4, while the standard deviation of this convergence measure is used in Figure 5. The PDD-KDE-MC method is used for comparison.

The average value and the empirical 95\% confidence interval of the sensitivity indices are shown in Figure 2.

We will first show the results for the independent data, followed by the results for the dependent data. We start with determining the goodness-of-fit of the Gaussian process by performing \( k \)-fold cross-validation (CV) with \( k = 10 \) and compute the coefficient of determination

\[
R^2 = 1 - \frac{SS_{res}}{SS_{tot}} = 1 - \frac{\frac{1}{L} \sum_l (\hat{Y}_l - Y_l)^2}{\frac{1}{L} \sum_l (Y_l - \bar{Y})^2},
\]

where \( \hat{Y}_l \) are the CV predictions for \( Y_l \) and \( \bar{Y} = \frac{1}{L} \sum_l Y_l \). In Figure 3, we show \( SS_{res} \) and we see its values are near zero for higher values of \( L \). For \( L = 30 \) and \( L = 50 \), this fraction can become larger than 1. In this case, the fit is worse than a constant function. Note that here, the Gaussian process is not fit well, while this is the case for the higher values of \( L \).

Figure 4 shows the convergence of the estimates, where “sample” indicates the KDE is based on only \( L \) samples, “GP-mean” is based on (5) and “GP-pred” is based on (6). “PDD” denotes the PDD-KDE-MC method. From left to right, variables 1 to 3 are shown. This will also be the case for all similar figures in this section. We see the differences are small for low values of \( L \), while for higher values of \( L \), the estimates based on Gaussian processes are remarkably better. Also, the mean of the sampled estimates matches the estimated mean function within sampling error, as expected. Figure 5 shows the average and the empirical 95\% confidence interval (determined from the \( nr \) repetitions) of the estimated standard deviation of the convergence measure for the sampled estimates (based on the \( ns \) samples of \( \hat{S} \)). The standard deviation decreases very fast for an increasing number of samples \( L \). Although this standard deviation
underestimates the standard deviation of the estimates for $\mathcal{H}_{X_k, f}^{(L+L+)}$ itself by approximately a factor 3, this is not enough for the 95% confidence interval for $\mathcal{H}_{X_k, f}^{(L+L+)}$ to cover zero. This is due to the bias caused by the use of the surrogate model rather than the exact output function. For the sake of completeness, note that in practice, it is not possible to compute the exact value and thereby to find out whether the confidence interval covers the real value.

The results for dependent data are shown in Figures 6, 7 and 8. Note that LHS is not an appropriate sampling method because the data is dependent, therefore, Monte Carlo sampling is used instead. Furthermore, PDD-KDE-MC is here not suitable because the input distribution is dependent. The results are
similar to previous experiments, although the cross-validation results imply the Gaussian process for this data has been fit better.

![Figure 6](image6.png)  
**Figure 6:** Cross-validation results showing the quality of the Gaussian process, dependent input data.

![Figure 7](image7.png)  
**Figure 7:** Convergence of the estimates for Kullback-Leibler divergence, dependent input data.

![Figure 8](image8.png)  
**Figure 8:** Behavior of the standard deviation of the error in the estimates based on predicted output samples for Kullback-Leibler divergence, dependent input data.

### 3.3. Piston function

We also tested a higher-dimensional test case with independent uniformly distributed input variables. In this case, the output function is defined by the
Table 1: Input variables for the piston function.

| Symbol and range | Explanation                               |
|------------------|------------------------------------------|
| \( M \in [30, 60] \) | piston weight (kg)                       |
| \( S \in [0.005, 0.020] \) | piston surface area (m\(^2\))           |
| \( V \in [0.002, 0.010] \) | initial gas volume (m\(^3\))             |
| \( k \in [1000, 5000] \) | spring coefficient (N/m)                 |
| \( P \in [90000, 110000] \) | atmospheric pressure (N/m\(^2\))        |
| \( T_a \in [290, 296] \) | ambient temperature (K)                  |
| \( T_0 \in [340, 360] \) | filling gas temperature (K)              |

Piston function from [29]. The output here is the cycle time of a piston, as given by

\[
C(x) = 2\pi \sqrt{\frac{M}{k + S^2 \frac{PV}{T_a} + \frac{V}{S}}} \\
V = \frac{S}{2k} \left( \sqrt{A^2 + 4k \frac{PV}{T_0} T_a - A} \right) \\
A = PS + 19.62M - \frac{kV}{S} \\
x = (M, S, V, k, P, T_a, T_0),
\]

of which the input ranges are given in Table 1. For numerical reasons, the data of size \( N = 10^3 \) is generated and processed on the unit hypercube: it is only transformed to the input ranges to obtain the output values. The sensitivity indices are given in Figure 9. The cross-validation results are in Figure 10.

![Figure 9](image-url) Computed values for the sensitivity indices per variable.

These last results show the Gaussian process has been fit well for all values of \( L \) and therefore we can continue with the remaining results. The results for the convergence are in Figure 11 and the results for the mean prediction standard
Figure 10: Cross-validation results showing the quality of the Gaussian process, Piston function.

deviation are in Figure 12. From left to right, top to bottom, variables 1 to 7 are shown. First of all, one sees the PDD-KDE-MC results are as accurate as the results based on only the L samples, while the results based on Gaussian processes are more accurate. Also, one can see the estimates based on the second method (Equation 6) are less accurate than the ones based on the first method (Equation 5), while they were nearly equally accurate for the earlier test cases. Furthermore, one now finds the prediction standard deviation is of the same order as the bias from using the Gaussian process. The first observation may be explained by the second: the sampling error is simply larger because of the (relatively) larger standard deviation. In this case, a constructed confidence interval for the sensitivity indices may actually cover the real value.

3.4. Recommendation

The two proposed methods perform significantly better than the PDD-KDE-MC method in the case of a low number of available input-output samples.
Figure 12: Behavior of the standard deviation of the error in the estimates based on predicted output samples for Kullback-Leibler divergence, Piston function.

Although the PDD-KDE-MC method can be performed much faster (order of seconds) than the Gaussian process based method (order of 10 minutes for $d = 3$, $L = 200$), this advantage disappears when one incorporates the resulting accuracy.

In practice, one cannot compute the bias caused by the Gaussian process and therefore, we propose to use the first estimator ($Y_{L^*} = \mu (X_{L^*})$). This is also supported by the fact the second estimator needs $ns$ computations of the kernel density estimates, while the first estimator only needs one, and by the extra sampling error involved in the second estimator.

4. Conclusion

We proposed to use Gaussian processes in order to improve the estimates of divergence-based sensitivity indices. This is advantageous in cases where the number of available input-output samples is small, for example if the computational cost of each model evaluation needed to compute the output is high. Two estimators were investigated, in which one used the prediction mean of the Gaussian process and the other used the complete multivariate normal distribution given by the Gaussian process, from which multiple samples were obtained. Both estimators performed well and much better than the reference method based on polynomial dimensional decomposition. However, we have shown that the bias from the using the Gaussian process instead of the exact output function can be larger than the width of the estimated confidence intervals and thereby can provide false confidence in the results. Therefore, and due to the extra computational cost of the second estimator, we advise to use the prediction mean of a well-fitted Gaussian process to improve the estimates of divergence-based sensitivity indices.
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