Piecewise Kriging Metamodeling

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Abstract**—**Approximation models are used to replace simulators to reduce computation time for engineering system design. These approximation models are called metamodels or surrogate models. For design spaces with wide and complex variation, partitioning the whole design space into multi subregions (pieces), then constructing a metamodel for each piece reduces complexity of variation and enhances accuracy of the resulting piecewise metamodel. In this paper a piecewise-Kriging metamodel methodology is proposed, whereby partitioning of the design variables space is based on using data displays called ordinal plots. These plots are constructed from the same validation samples that are used to test the accuracy of an initial and other intermediate global-Kriging metamodels, thus requiring no additional simulation runs. Comparisons with global-Kriging metamodels having equivalent accuracy show that the piecewise-Kriging metamodels are generated at lower computational costs in terms of the simulation runs used.

Keywords**—**Kriging, Metamodeling, Metamodel validation, Piecewise metamodels, Simulation, Space partitioning.

I. INTRODUCTION

SIMULATORS are used in engineering system design to predict the response of multidimensional systems. These simulators are used to perform the analysis and to predict system response to satisfy certain specifications for the design problem. In the design of multivariable systems each simulation run requires excessive computational times; in some cases up to a few hours or even longer based on the variation and complexity of the design problem.

Approximation models (called metamodels or surrogate models) are used to replace simulators to overcome such drawbacks. A metamodel is constructed using a set of sample data to build an approximate model of the function (simulator) which is used to evaluate responses at the sample data points. The metamodel may then be used as a surrogate for the original function; this enables design processes to be carried out more easily, faster, and cheaper.

There are a wide variety of metamodeling techniques such as Kriging (KG) [1-4], Response Surface Models (RSM) [3,4], Radial Basis Functions (RBF) [2,4], Multivariate Adaptive Regression Splines (MARS) [1], Piecewise (PW) metamodels [5-7], and Artificial Neural Networks (ANN) [3,8]. Which metamodel type to use is dependent on its ability to model the functionality of the response in an accurate and efficient manner.

For problems with complex variation over the whole design space a global metamodel may be accurate in regions and not accurate for others. Thus, piecewise metamodeling can be used to divide the whole design space to subregions (pieces), and construct the most suitable metamodel for each piece. This enhances the accuracy of the metamodel over the entire design space. The main challenge in partitioning the design space is related to the number and location of the pieces in the design variables space.

Piecewise RSMs are constructed in [6] using data displays called acceptance score distribution (ASD) plots to delineate the design variables space into appropriate subregions. In [5], ordinal plots are used in partitioning the space to construct piecewise RSMs. In this paper a piecewise-Kriging metamodeling methodology is introduced based on ordinal plots [5,9] as the data displays to guide space-partitioning. Ordinal plots are constructed based on whatever validation samples that are used to test the accuracy of global-Kriging metamodels; no extra simulation runs are required. An extensive discussion about validation samples and their sizes is presented in [6].

The proposed methodology is tested on two problems and the resulting piecewise metamodels are validated based on multiple statistical validation criteria. More problems are presented in [10]. Comparisons between global-Kriging and piecewise-Kriging metamodels show that more accurate metamodels can be achieved using piecewise metamodels. The computational cost of building the piecewise-Kriging metamodel is reduced by comparison to a global-Kriging metamodel with equivalent accuracy, provided that the space is partitioned correctly, as will be demonstrated.

This paper is organized as follows. In section 2, we start by illustrating metamodeling concepts in engineering system design, including experimental design and Kriging metamodeling concepts. Ordinal plots and their use in space partitioning are also presented in section 2. In section 3 the proposed methodology is outlined and applied to an analytic problem to demonstrate the validity of the proposed method, an electronic circuit design problem is also given in section 3. Finally, the paper is concluded in section 4.

II. METAMODELING IN ENGINEERING SYSTEM DESIGN

The goal for engineering system design is to determine design variables to meet certain specifications. For example in electronic circuits design variables include component values such as transistor widths, resistors, capacitors, etc. These component values represent the design variables for the circuit which influence design specifications like the gain and the bandwidth of an amplifier.

Engineers often rely on models to facilitate system design. The most widely used modeling technique in engineering system design is via simulators. Many simulation runs are needed to optimize the system to meet the required design specification. However, a simulation run can take several hours depending on the problem complexity; so metamodels are used to replace simulators in engineering system design to increase the computation efficiency.

Metamodels are constructed using data samples based on design variables locations and the corresponding system responses given by the simulator. Experimental design methods are used to sample the design variables space. Sampling methods include classical techniques used for RSM such as central composite designs [11] and minimum bias designs [12]. More recent techniques that are primarily used for computer experiments include space-filling designs [13] such as the Latin hypercube sampling (LHS) methods [3].

III. KRIGING METAMODELS

After selecting an appropriate experimental design, the next step is to choose an approximation model type (such as KG, RSM, RBF, MARS, etc., as mentioned earlier).

Kriging metamodels are used extensively to build metamodels in engineering system design. The basic idea in Kriging metamodeling is that the predictions are weighted averages of the simulated responses, where the weights depend on the distances between the design variables points location to be predicted and the locations already observed in the experimental design. The weights are chosen so as to minimize the prediction variance and should provide a best linear unbiased estimator of the response.

The Kriging metamodel $\hat{y}$ postulates a combination of a polynomial model and departures from it for k-design variables $x = x_1, x_2, \ldots, x_k$ as given in Equation (1):

$$\hat{y}(x) = \sum_{j=1}^{k} \beta_j f_j(x) + Z(x), \tag{1}$$

where β_j are the coefficients of linear regression functions $f_j(x)$ · $Z(x)$ is assumed to be a realization of a stochastic process with zero mean and a spatial correlation function given by:

$$Cov\left[Z(x^i), Z(x^j)\right] = \sigma^2 R\left[r(x^i, x^j)\right] \tag{2}$$

where

σ^2 is the process variance.

R is the correlation Matrix.

$r(x^i, x^j)$ is the correlation function between x^i and x^j. In our work a constant linear regression function is used. Also, we utilize the Gaussian correlation function of the form given in Equation (3).

$$r(x^i, x^j) = \exp\left[-\sum_{n=1}^{k} \theta_n \left|x_n^i - x_n^j\right|^2\right] \tag{3}$$

where

θ_n are the unknown correlation parameters used to fit the model. x_n^i and x_n^j are the nth component of sample points x^i and x^j for k variables.

Kriging method is extremely flexible in capturing nonlinear behavior because the correlation functions can be tuned by the sample data. See [1] for recent discussion of Kriging metamodeling and [13] for more details about correlation functions that can be used.

IV. ORDINAL PLOTS

In this paper ordinal plots [5,9] play an important role to divide the design space into several pieces for piecewise metamodels. Ordinal plots are data displays that can be used to show the relationship between the response y_i and the metamodel $\hat{y}_i$ for all sample points over the entire design space . In ordinal plots, the ratio $\frac{\hat{y}_i}{y_i}$ for data points $i = 1, 2, \ldots, N$ are plotted (points with simulation results y_i equal to zero are simply removed from the validation sample. This should have no effect on the plots credentials; see [5,9]). Two lines that represent acceptable prediction accuracy limits as ratios are also plotted. Thus, an ordinal plot shows graphically regions in the design space of acceptable accuracy for the metamodel relative to the response.

In general, if the design space is k-dimensional, then k ordinal plots are generated. Data is ordered along each of the k dimensions in turn and the corresponding ordinal plot for the current dimension is generated. Therefore, to generate an ordinal plot for the first dimension x_1, the N data points are first ordered in ascending order of x_1. The resulting ($x_{1,i}$, $\hat{y}_i/y_i$) points are then plotted for $i = 1, 2, \ldots, N$. This procedure is repeated for each of the k dimensions in turn, thus generating k ordinal plots. Points in ordinal plots with y-coordinates closer to 1 indicate a better match between the metamodel and the simulation response. See [5,9] for more details on ordinal plots construction and uses.

V. Metamodel Validation

Validation is a critical step in metamodeling which determines the accuracy of the metamodel to ascertain if the estimated metamodel adequately fits the simulation data. The purpose of metamodel validation is thus to investigate whether the metamodel adequately approximates the simulator.

In this paper statistical validation is used to determine the accuracy of the constructed metamodels, whereby multiple measures are used. These validation statistics are presented in this section. In the following discussion metamodel results are denoted by $\hat{y}_i$ in a test sample with N points, and compared to evaluations of the original response y_i for all N points in a k-dimensional space.

The validation statistics used in this work are the Root-Mean-Square Error (RMSE), the coefficient of determination (R^2), and the adjusted$-R^2$ ($\bar{R}^2$). These are defined in Equations (4) - (7):

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(\hat{y}_i - y_i)^2}{N}} \tag{4}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{N}\left(\hat{y}_i - y_i\right)^2}{\sum_{i=1}^{N}\left(\hat{y}_i - \bar{y}\right)^2} \tag{5}$$

where; $$\bar{y} = \frac{1}{N}\sum_{i=1}^{N} y_i \tag{6}$$

$$\bar{R}^2 = 1 - (1 - R^2)\frac{N-1}{N-k-1} \tag{7}$$

These error measures are useful in determining the accuracy of a given metamodel, but they all require additional simulation evaluations using the simulator if a validation sample is used. As stated earlier, the methodology presented in this paper makes further use of the available validation samples by generating ordinal plots using these samples.

VI. Picewise Kriging Metamodeling

It is difficult to construct a metamodel to predict the desired output accurately over the entire design space for complex variations over wide design spaces,. In this paper, the procedure presented in Figure 1 uses ordinal plots to divide the whole design space into several pieces. This reduces the complexity of response variation per piece and produces more accurate piecewise metamodels, as will be demonstrated.

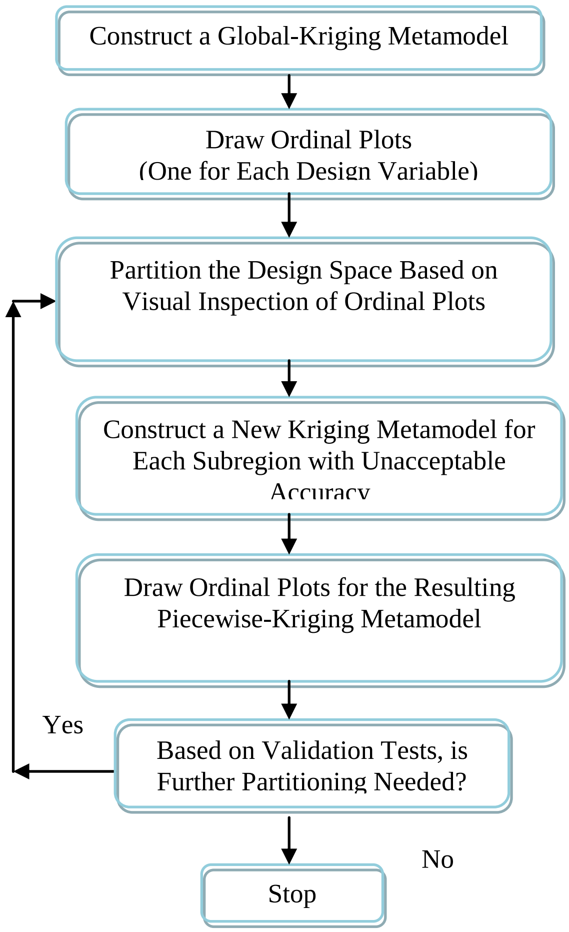

Figure 1: Piecewise-Kriging Metamodeling Methodology

The proposed methodology is illustrated using a one-dimensional analytic problem, then applied to a two-dimensional problem using an active-load inverting amplifier circuit.

VII. A One-Dimensional Analytic Problem

The proposed methodology is demonstrated by a one-dimensional analytic example in this subsection. The function is given in Equation (8).

$$f(x) = \sum_{i=1}^{9} a_i (x - 900)^{(i-1)} \tag{8}$$

Where; $x \in [905, 995]$

and,

$a_1 = -659.23$, $a_2 = 190.22$, $a_3 = -17.802$, $a_4 = 0.82691$, $a_5 = -0.021885$, $a_6 = 0.0003463$, $a_7 = -3.2446 \times 10^{-6}$, $a_8 = 1.6606 \times 10^{-8}$, $a_9 = -3.5757 \times 10^{-11}$.

Matlab commands [15] and DACE toolbox [16] are used to construct the Kriging metamodels. Initially, a Latin Hypercube Sample (LHS) is used for model construction; we call this the model sample. After constructing a metamodel another set of points is generated and called the validation sample. This sample is used to assess the accuracy of the metamodel for response prediction over the entire design space. For a *k*-variables design space the model sample size is chosen between 5 *k* and 10 *k* depending on the size of error as displayed by ordinal plots (in [17], a sample size of $10k$ is recommended) . The size of validation samples is arbitrarily chosen to be $20k$ (The size of the validation sample in ordinal plots has minimal effects as demonstrated in [5]). For this problem we have one design variable, we use 10-points for model construction and 20-points for validation.

After constructing and validating the global metamodel, an ordinal plot is used to display the variation of metamodel accuracy over the entire design space (see Figure 2).

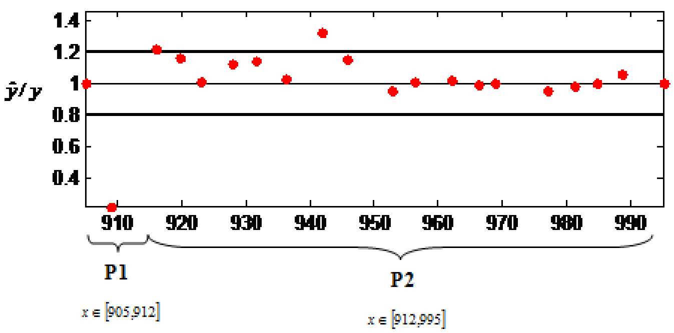

Figure 2: Ordinal Plot for Global-Kriging metamodel and space partitioning.

Visual inspection of the figure reveals that accuracy is acceptable over some regions (with dots inside the two lines at ($\hat{y}/y = 1 \pm 0.2$)), while other regions have unacceptable performance (with dots outside the two lines). Various partitioning schemes are possible; an example is shown in Figure 2, where the space is divided into two pieces P1 and P2 as shown. A new Kriging metamodel is constructed for each piece using 5- points for P1 metamodel and 10 points for P2 metamodel. These sizes are chosen depending on the complexity of error variation and/or the range of the design variable over each piece. Then the overall new piecewise metamodel is validated over the same validation sample that is used to validate the global metamodel. A comparison between both metamodels is given in Table 1. Beta and Theta coefficients of the Kriging metamodels are listed in Table 2.

Table 1: Validation Statistics for Piecewise- and Global-Kriging (KG) Metamodels.

Metamodel Method	$RMSE$	R^2	$\bar{R}^2$
Global-KG	16.39	0.8307	0.8213
Piecewise-KG	2.394	0.9952	0.9946

Table 2: Beta and Theta coefficients for Piecewise- and Global-Kriging (KG) Metamodels.

	β_0	θ
Global KG	0.023785037	20.0000000
$P1$ **Metamod**el	-2.3688601	0.12599210
$P2$ **Metamodel**	0.49517744	2.50000000

From Table 1, it is clear that the piecewise-Kriging metamodel is more accurate than the global-Kriging metamodel with lower values of $RMSE$ and higher values of R^2 and $\bar{R}^2$.

Note that 15 points are used to construct the piecewise-Kriging metamodel. In order to demonstrate the ability of the proposed piecewise methodology in producing more accurate metamodels by comparison to a methodology whereby the accuracy of the initial metamodel is improved at the global level, a global-Kriging metamodel is constructed using 15 points. A comparison with the piecewise-Kriging metamodel is presented in Tables 3-4.

Table 3: Validation Statistics for Piecewise- and Global-Kriging (KG) Metamodels Using N = 15.

Metamodel Method	$RMSE$	R^2	$\bar{R}^2$
Global-KG	12.85	0.8959	0.8901
Piecewise-KG	2.394	0.9952	0.9947

Table 4: Beta and Theta coefficients for Piecewise- and Global-Kriging (KG) Metamodels.

	β_0	θ
Global-KG Using N=15	-0.060406472	10.68179281
$P1$ **Metamodel** Using N = 5	-2.3688601	0.12599210
$P2$ **Metamodel** Using N = 10	0.49517744	2.50000000

VIII. An Electronic Circuit Design Problem

The two-dimensional design problem considered in this section is the active-load inverting amplifier circuit shown in Figure 3:

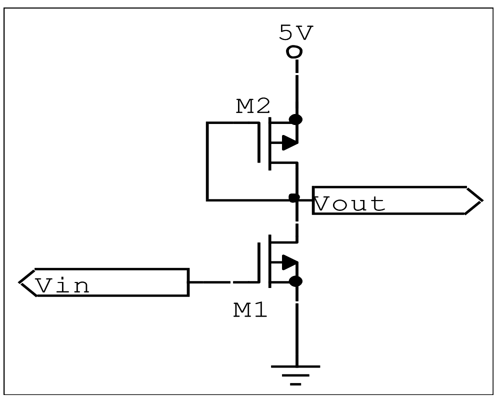

Figure 3: Active-Load Inverting Amplifier Circuit Diagram.

The Hspice simulator [18] is used to obtain the small-signal gain defined by:

$$gain = \frac{V_{out}}{V_{in}} \tag{9}$$

Where Vout and Vin are the output and input signal strengths, respectively. The small-signal gain is a function of W_1 and W_2, the widths of transistors M1 and M2, respectively (see Figure 3). We choose to sweep W_1 and W_2 over the range from 2µm to 200µm. Hspice simulator is used to obtain the small-signal values for model and validation samples then a global-Kriging metamodel is constructed using 20- points and validated using 40- points. These points are generated using the LHS sampling method. Using ordinal plots for both design variables in Figure 4 and Figure 5, one possible scheme is to divide the design space into three pieces as shown in Figure 6:

1. P1 for $W_1 \epsilon [2µm, 55µm]$.
2. P2 for $W_1 \epsilon [55uµ, 123µm]$.
3. P3 for $W_1 \epsilon [123µm, 200µm]$.

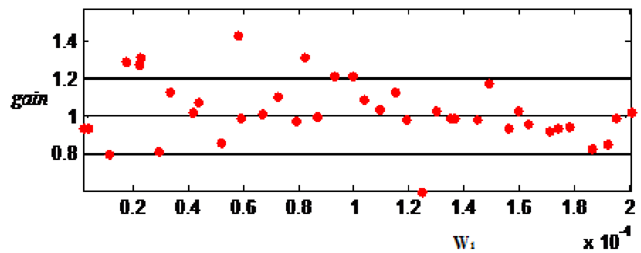

Figure 4: Ordinal Plot Over W_1 for $gain$ Global-Kriging Metamodel.

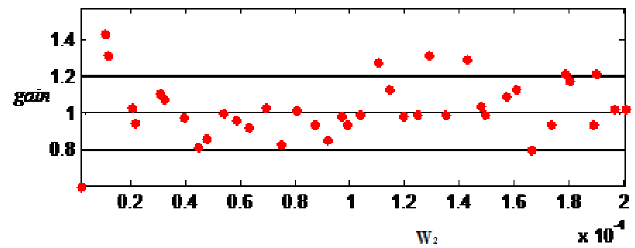

Figure 5: Ordinal Plot Over W_2 for $gain$ Global-Kriging Metamodel.

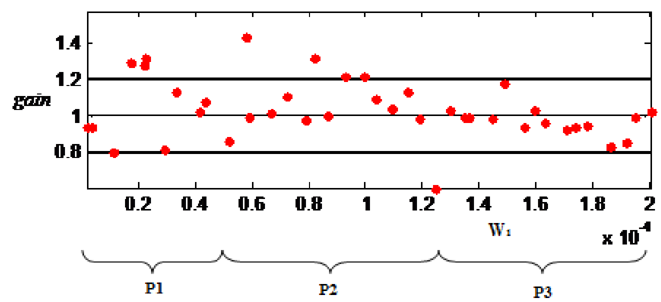

Figure 6: Ordinal Plot for Piecewise Partitioning along W_1 .

A new Kriging metamodel is constructed for P1 and another for P2 because the ratio between $\hat{y}$ and y is far from the acceptable limits (see Figure 6). For P3 the ratio between $\hat{y}$ and y is within the acceptable limits; so we keep the global-Kriging metamodel for P3. A model sample size N = 20 is used to construct a new Kriging metamodel each for P1 and P2. After constructing the piecewise-Kriging metamodel, ordinal plots over the design variables in Figures 7-8 show the need for yet another partitioning to enhance the accuracy of constructed metamodel. The design space is divided into two pieces P1 and P2 as shown in Figure 9, and a new Kriging metamodel is constructed for P1 using 20-points. The gain metamodel for the first piecewise-Kriging metamodel is kept for P2.

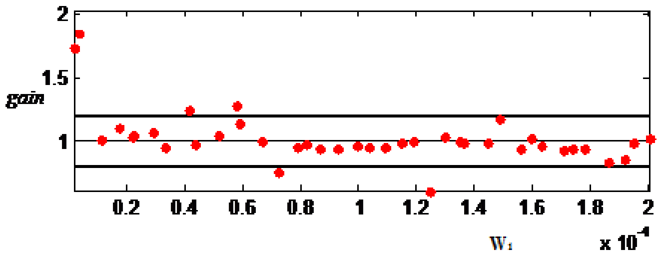

Figure 7: Ordinal Plot over W_1 for *gain* Piecewise-Kriging Metamodel.

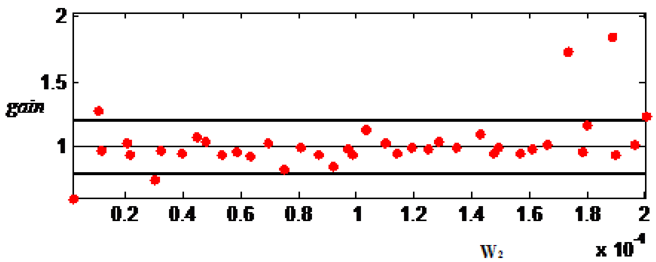

Figure 8: Ordinal Plot over W_2 for *gain* Piecewise-Kriging Metamodel.

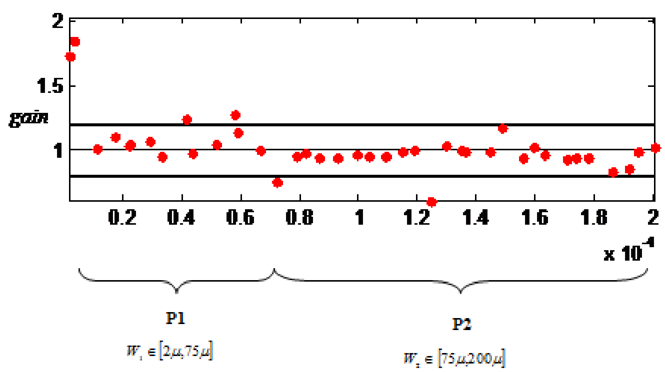

Figure 9: Ordinal Plot for Piecewise Partitioning along W_1

A comparison between the global-Kriging, the first piecewise-Kriging and the second piecewise-Kriging metamodels is listed in Table 5; the coefficients for each metamodel are listed in Table 6.

Table 5: Validation Statistics for Piecewise- and Global-Kriging (KG) Metamodels.

Metamodel Method	$RMSE$	R^2	$\bar{R}^2$
Global-KG	0.6807	0.8062	0.7957
First PW Metamodel	0.6338	0.8319	0.8229
Second PW Metamodel	0.3365	0.9527	0.9501

Table 6: Summary of Beta and Theta coefficients for Piecewise- and Global-Kriging (KG) Metamodels.

	β_0	θ_1	θ_2
Global-KG	-0.093293685	0.15625000	2.5000
1st **PW-Kriging** $P1$ **Metamodel**	0. 16096581	0.15625000	2.5000
1st **PW-Kriging** $P2$ **Metamodel**	0.15835763	0.10000000	14.142
2nd **PW-Kriging** $P1$ **Metamodel**	-0.053361968	0.15625000	2.5000

This example demonstrates that repeated partitioning for the design space using the proposed piecewise-Kriging methodology produces more accurate metamodels.

IX. CONCLUSION

This paper introduced a methodology that has a multidisciplinary application in engineering system design problems, specially for problems with complex response variations over wide design spaces. In the proposed methodology, partitioning the design space into several pieces enhances the accuracy of constructed piecewise-Kriging metamodel by reducing the complexity of variation over the entire design space. Ordinal plots are important tools in guiding space partitioning procedure to locate the subregions requiring remodeling. The resulting piecewise metamodel is accurate on a piece-by-piece basis, not just on average as in global metamodels.

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