Inverse Problem for Dynamic Computer Simulators via Multiple Scalar-valued Contour Estimation

Joseph Resch
University of California, Los Angeles, USA

Pritam Ranjan
OM&QT, Indian Institute of Management Indore, MP, India

Abhyuday Mandal
University of Georgia, Athens, USA

Abstract

The inverse problem refers to finding a set of inputs that generates a pre-specified simulator output. A dynamic computer simulator produces a time-series response, \( y_t(x) \) over time points \( t = 1, 2, \ldots, T \), for every given input parameter \( x \). The motivating application uses a rainfall-runoff measurement model (called Matlab-Simulink model) to predict the rate of runoff and sediment yield in a watershed, using several inputs on the soil, weather (e.g., precipitation, temperature, and humidity), elevation, and land characteristics. The input parameters \( x \)'s are typically unknown and our aim is to identify the ones that correspond to the target response, which is to be used further for calibrating the computer model and make more accurate predictions of water level.

The proposed approach starts with discretizing the target response series on \( T_k \) (<< \( L \)) time points, and then iteratively solve \( T_k \) scalar-valued inverse problems with respect to the discretized targets. We investigate a sequential approach of contour estimation via expected improvement criterion developed by Ranjan et al. (2008, DOI: 10.1198/004017008000000541). We also propose to use spline smoothing of the target response series to identify \( k \) as the optimal number of knots, and the discretization time points as the actual location of the knots. The performance of the proposed methods are compared for several test-function based computer simulators and the real-life Matlab-Simulink model.

Keywords: History matching, Gaussian process model, Expected improvement criterion, Spline smoothing, Matlab-Simulink model.

1 Introduction

Physical experiments are frequently expensive and impractical to perform. The growth in computing power during modern times offers an alternative to carrying out such experiments in the real world. Due to the cost of resources that comes with each iteration of a physical experiment, less expensive computer simulators are used to represent phenomena such as the dynamic traffic patterns of a metropolitan intersection, the hydrological behaviors of an ecosystem, the spread behaviors of a wildfire, and the formation patterns of galaxies. The application of computer simulation span a variety of sectors such as industrial experiments, ecology, medicine, engineering, nuclear research, manufacturing, climatology, and astronomy.
Whereas scalar-valued simulators represent experimental environments where time is not a factor, dynamic simulators account for the change in response over time. In this paper, we focus on the inverse problem, otherwise referred to as a calibration problem, of dynamic simulator models. The objective of the problem is to calibrate the input parameters to produce output closely resembles the target in context for all time points that the experiment uses. Actual computer experiments tend to be complex and have a high dimensional input space, therefore simply attempting to solve the inverse problem is infeasible. Thus, less computationally expensive surrogates such as the Gaussian Process model — fitted using training data of $n$ observations $(x_1, y_1), \ldots, (x_n, y_n)$ to emulate computer models — are a useful tool in algorithms to approach the calibration problem.

In order for the surrogate to accurately produce an output that represents the simulator output for a given input, we carefully choose the training data set. This is typically done by selecting an initial training set of a space-filling design, augmented by some other approaches. Ranjan et al. (2016) and Zhang et al. (2018) proposed to choose the follow-up training points for the surrogate model in a sequential design for solving the calibration problem. More recently, Bhattacharjee et al. (2019) used history matching approach where they augmented the training set in batches using a model improvement criterion that extracted points from a large space-filling design.

To optimize the inverse solution at all time points for a dynamic simulator model, Vernon et al. (2010) proposed to discretize the time-series response on a set of time points and then take common solution for the scalar-valued inverse problems at the discretized time points, as a part of the history matching algorithm. Bhattacharjee et al. (2019) adopted the same concept to discretize time points called discretization-point-set (DPS), to augment the training set for fitting a surrogate model in their modified history matching approach. Although it is suggested for the discretization-point-set is to be selected such that the time points would capture features of the target response, no methods were given to explicitly choose the time points.

In this paper, we propose to solve the calibration problem for dynamic computer simulators by taking the intersection of solutions for scalar-valued inverse problems at a discretization-point-set of size. To systematically select the discretization-point-set, we set the time points to be the optimal knots for fitting cubic splines to the target time-series response in a forward selection method. We approach each scalar-value inverse solution by augmenting the training sets used to fit Gaussian Process model surrogates. Jones et al. (1998) proposed the expected improvement (EI) criterion for a sequential strategy, which was then modified by Ranjan et al. (2012) for estimating a pre-specified contour. Expected improvement for contour estimation is the augmenting criterion chosen for the sequential design here. Four applications of the proposed approach are discussed in this paper. To illustrate the advantage of the proposed method, a comparison to the modified history matching approach was also performance.

The remaining sections are outlined as follows. Sections 2 reviews the concepts integral to the proposed method and review the competing modified history matching approach proposed by Bhattacharjee et al. (2019). Section 3 provides the elements of the proposed multiple scalar contour estimation method along with a thorough implementation of each step of the proposed method. In Section 4, the proposed method is implemented onto three examples and the results are compared. Section 5 applies the proposed method to the real rainfall-runoff simulation, Matlab-Simulink model. Section 6 concludes with the findings of this paper.
2 Review of Existing Methodology

In this section, the existing methods that set precedence for this paper are reviewed. We examine the use of the Gaussian Process model as a surrogate to deterministic simulators and the use of the expected improvement criterion as a part of sequential design. The preexisting modified history matching approach and the use of a discretization-point-set is designed to approximate the best solution for the inverse problem for dynamic computer simulators.

2.1 Gaussian Process Models

Deterministic computer model simulators are complex and computationally expensive to evaluate, but a surrogate fitted to emulate the model becomes much more practical. A useful surrogate for this purpose is the Gaussian Process (GP) model (Sacks et al., 1989; Jones et al., 1998). Fitting a set of inputs and outputs, a stationary GP model, called ordinary Kriging, will follow the form of:

\[ y(x_i) = \mu + Z(x_i), \quad i = 1, \ldots, n, \]  

where \( \mu \) is the mean and \( Z(x_i) \) is a Gaussian Process with \( E(Z(x_i)) = 0 \) and a covariance structure of \( \text{Cov}(Z(x_i), Z(x_j)) = \sigma^2 R(\theta; x_i, x_j) \). There are several popular choices of \( R \). The power-exponential correlation structure will have the \((i, j)\)th term \( R_{ij}(\theta) \) as:

\[ R(Z(x_i), Z(x_j)) = \prod_{k=1}^{d} \exp \left( -\theta_k | x_{ik} - x_{jk} |^{p_k} \right) \quad \text{for all } i, j, \]  

where \( p_k \) are smoothness parameters and \( \theta_k \) measure correlations lengths. In this paper, we assume Gaussian correlation which corresponds to \( p_k = 2 \). The best linear unbiased predictor for the response at any unsampled point \( x^* \) is given by:

\[ \hat{y}(x^*) = \hat{\mu} + r(x^*)^T R^{-1} (y - 1_n \hat{\mu}), \]  

where \( r(x^*) = [\text{corr}(z(x^*), z(x_1)), \ldots, \text{corr}(z(x^*), z(x_n))] \) with the mean squared error of

\[ s^2(x^*) = \hat{\sigma}^2 \left( 1 - r(x^*)^T R^{-1} r(x^*) \right). \]  

The flexibility of its correlation structure makes the GP model a popular surrogate for complex computer models. Throughout this paper, the \( R \) package \texttt{GPfit} (MacDonald et al., 2015) is used to fit GP models.

2.2 Sequential Design

The process of sequential design, discussed in Ranjan et al. (2016) and Zhang et al. (2018), uses available budget in a sequential manner to augment a training set, that is used to fit surrogates such as the GP model. With each iteration and augmentation of the training set, the surrogate needs to increasingly resemble the simulator for the purpose of inverse solution extraction.
In computer experiments, space-filling designs are popular choices for the initial design. Suppose we have \(d\) input variables, a space-filling design such as a maximum projection Latin hypercube design (Joseph et al., 2015), is used to create a training input set of initial size \(n_0\) from the scaled input space \([0,1]^d\). The corresponding response set is generated by evaluating the simulator at each input of the training set. A surrogate model is then fitted to the simulator responses and the training set inputs. After which, a sequential design criterion such as expected improvement (EI) is evaluated using the GP model over the entire input space to find the input, \(x_{\text{new}}\), that leads to the greatest expected improvement. Practically, we evaluate EI over a dense, randomly generated spacing-filling test set \(\chi_i\) of large size \(M\) in \([0,1]^d\). The \(x_{\text{new}}\) is added to the training set and evaluated in the simulator. The new training set is refitted to a new GP surrogate to selected the following \(x_{\text{new}}\). This process is repeated until the total budget of \(N\) points is exhausted, resulting in a training set of size \(N\) and a final GP surrogate fitted using that training set.

### 2.3 Expected Improvement Criterion for Contour Estimation

Jones et al., (1998) proposed a sequential design criterion, expected improvement (EI), to determine points to be added to the training set sequentially. For the purpose of estimating the response that will lead us the closest to the true target contour, Ranjan et al., (2008) developed the expected improvement criterion for contour estimation. With the latter fitting our purposes, the improvement function becomes:

\[
I(x^*) = \epsilon^2(x^*) - \min\{\{y(x^*) - a\}^2, \epsilon^2(x^*)\}. \tag{5}
\]

Hence, the expected value of the improvement function is:

\[
E[I(x^*)] = \left[\epsilon^2(x^*) - \{\hat{y}(x^*) - a\}^2\right]\left\{\Phi(u_2) - \Phi(u_1)\right\} + \epsilon^2(x^*)\left\{\Phi(u_2) - \Phi(u_1)\right\} + 2\left\{\hat{y}(x^*) - a\right\}s(x^*)\left\{\phi(u_2) - \phi(u_1)\right\}, \tag{6}
\]

where \(\epsilon(x^*) = \alpha s(x^*)\) for a positive constant \(\alpha\) (e.g., \(\alpha = 0.67\), corresponding to 50% confidence under approximate normality), \(u_1 = [a - \hat{y}(x^*) - \epsilon(x^*)]/s(x^*)\), and \(u_2 = [a - \hat{y}(x^*) + \epsilon(x^*)]/s(x^*)\). Here \(\Phi\) and \(\phi\) are the cumulative distribution function and probability density function of the standard normal distribution for input \(x^*\). The term \(a\) is the target response contour and \(\hat{y}(x^*)\) denotes the simulator output for input \(x^*\) derived from the GP model.

The components of expected improvement allow us to explore the input space enough to not be stuck at a local optimal while exploiting the areas of interest for more information. This allows for a healthy balance in deciding the follow-up point.

### 2.4 Modified History Matching Approach for the Inverse Problem

For a time-series function, the continuous time variable has to be discretized into \(L\) distinct time-points. Let \(g(x) = \{g(x,t_i), i = 1, \ldots, L\}\) denote the time-series valued simulator response with the input scaled such as \(x \in [0,1]^d\). The aim of the inverse problem (or calibration problem) is to find \(x\) such that
$g(x)$ resembles the target response $g_0 = \{g_0(t_i), i = 1, \ldots, L\}$. The history matching approach was first proposed by Vernon et al. (2010) and was modified by Bhattacharjee et al. (2019) to solve the inverse problem for dynamic simulators. The modified history matching approach adopted a nontraditional sequential design and used the space-filling design Maximin Latin Hypercube (Johnson et al., 1990) as the initial design for fitting a GP surrogate.

Although data are observed at $L$ distinct time-points, in history matching approach, a handful of time-points are selected. This set of time-points is known as a discretization-point-set (DPS) and has size $T_k$ such that $T_k << L$. It is important for the DPS $(t^*_1, t^*_2, \ldots, t^*_k)$ to be representative of the computer simulator, since we would use only the DPS to improve the surrogate to match the computer model. Thus, the history matching algorithm finds $g$ in such a way that $g(x, t^*_j) = g_0(t^*_j)$ for all $j = 1, \ldots, T_k$.

The modified history matching uses a multi-stage design to augment a training set using the Gaussian Process model surrogate generated at each stage to evaluate the implausibility criteria, which is defined as

$$I_j(x) = \frac{|\hat{g}(x, t^*_j) - g_0(t^*_j)|}{s_{t_j}(x)},$$

where $\hat{g}(x, t^*_j)$ is the predicted response derived from the GP surrogate and $s_{t_j}(x)$ is the associated uncertainty value. Design points are deemed implausible if $I_{max}(x) > c$, where $c$ is a pre-determined cutoff and

$$I_{max}(x) = \max[I(1)(x), I(2)(x), \ldots, I(T_k)(x)].$$

The training set is augmented, in batches of multiple new training points, with inputs from a randomly generated test set $\chi_i$ that satisfy the threshold $c$ for the implausibility function such that each augmentation of the training set can be defined as $\{x \in \chi_i : I_{max}(x) \leq c\}$. This pre-determined cutoff $c$ is selected in an ad-hoc manner, subjectively.

Following each batch augmentation of the training set, an updated GP surrogate is fitted using the augmented training set to determine the following batch of design points that satisfy the implausibility criteria. This process is halted once no additional points are added to the training set in an iteration. At the end of the procedure, the best approximate inverse solution is extracted from the training set or from the final GP surrogate.

3 Proposed Methodology: Multiple Scalar-valued Sequential Design via Contour Estimation

Departing from the existing methods to tackle the calibration problem of dynamic computer simulators, we proposed to solve multiple scalar-valued inverse problems at discrete time points under a set budget constraint. Similar to the modified history matching method, a discretization-point-set is used to capture the characteristics of the target time-series response on $k$ ($<< L$) time points. Following the discretization, we iteratively solve $k$ scalar-valued inverse problems with respect to the discretized targets. To solve each of the $k$ scalar-valued inverse problems, we use sequential design and the improvement criteria for contour estimation to derive $k$ sets of respective inverse solutions. The intersection of these sets of in-
verse solution is taken and used as the optimal solution for the calibration problem of dynamic computer simulator. The proposed method follows the general outline below:

**Selection of Discretization-Point-Set**

In our proposed method, we aim to improve upon history matching’s arbitrary choice of the discretization-point-set (DPS). The DPS is a set of time-stamps from the space of time - where the size of DPS is much smaller than the number of points in the discretized space of time - that allows for the features of the target response contour to be captured. The history matching discussed in Section 2.4 chooses DPS is rather subjectively and is not based on a systematic algorithm. Here we introduce an algorithmic approach for choosing the DPS.

We propose to use the optimal knots for cubic basis splines fitted to the target time-series response as the DPS. For implementation, the R package “splines” is called upon for this purpose while the command for B-spline “bs()” is used in the linear model environment. The idea is that if we find the inverse solution at these knots (time points), then the inverse solutions at time points between the knots would also be covered by solving these inverse problems.

We propose to generate the optimal knots iteratively in a forward selection method, in the sense that the previously chosen knots are held constant while new knots are selected one at a time. The size of the set is determined by viewing the mean squared errors of spline fits for optimal set of knots for each $k$ number of knots. The plot of the relationship between mean squared error and number of knots tends to show an elbow shape. Thus, the number of knots is optimized at the elbow. To set a constraint for the size of the DPS and to observe an elbow shape when plotting mean squared errors of the fits against the number of knots used in spline fitting, a thumb rule of $1 \leq k \leq 10$ is suggested.

**Extraction of the Inverse Solution**

The intersection of the $k$ solution at the time points of the discretization-point-set (DPS) is approximated as the inverse solution. To implement this, GP model surrogate fitted at DPS following the final iteration is used to extract $x_{opt}$.

We accept the solution sets at each of the $k$ DPS time point such that solution set $S_i = \{ x^* : \hat{g}(x^*, t_i) = g_0(t_i) \pm \epsilon \}$, for $i = 1, \ldots, k$ and $\epsilon$ is subjectively small enough to limit the size of the inverse solution set. Taking the intersection of the $k$ solution sets ($S_1 \cap S_2 \cap \ldots \cap S_k$), our $x_{opt}$ is selected by minimizing the Euclidean distance or $L_2$ norm such that

$$x_{opt} = \arg\min \| g(x) - g_0 \| .$$

(8)

Alternatively, $x_{opt}$ could be extracted directly from the training set by minimizing the Euclidean distance. While the alternative extraction method requires less computation, it produces a less desirable inverse solution in most cases. It is recommended to implement both extraction methods to produce the most optimal solution.
Illustration:

We illustrate details of the proposed method by applying it to a test function. The simulator Easom function (Michalewicz, 1996) is defined as,

$$g(x, t_i) = \cos(x_1) \cos(x_2) \exp \left\{ - (x_1 - \pi t_i)^2 - (x_2 - \pi)^2 \right\},$$

(9)

where \(t_i\) are \(L\) equidistant time points in \([0, 1]\) for \(i = 1, \ldots, L = 200\). The input space is scaled to \((x_1, x_2) \in [0, 1]^2\). The true target response \((g_0)\) of simulator corresponds to the input set \(x_0 = (0.8, 0.2)\). Here the objective is to solve the inverse problem by calibrating the parameters \(x_1\) and \(x_2\) such that \(g(x_1, x_2) \approx g_0\).

We begin by choosing the discretization-point-set from the 200 time points that the simulator lies on. To use the forward selection method, the first point of the DPS is optimized by comparing the mean square errors of the cubic splines fit onto the target response using each of the possible 200 time points as the sole knot. We find that the optimal first knot at time point 145. Keeping that knot at time point 145 fixed, we repeat the process and find the second knot at point at 37. The process continues using forward selection to optimize ten knots, we produce the ordered set \(\{145, 37, 132, 47, 120, 55, 113, 63, 104, 174\}\).

We can see the goodness-of-fit using the first one through ten knots in this list to fit cubic splines onto the target response in Figure 1.

Figure 1: (Left) The positions of the ordered optimal knots for fitting cubic splines are labeled and shown as the dotted lines.

Figure 2: (Right) Taking mean squared errors of the fits corresponding to the number of knots used for spline fitting, we identify the elbow by the red line and optimize the number of knots, therefore the size of the DPS, to be three.

In Figure 2, we see an elbow shape in the relationship between number of knots and mean square error. Choosing the cutoff for the optimal number of knots at the elbow, which would be optimized at the point where the second derivative of the relationship initially reaches a positive value, would allow for a good fit while maintaining the efficiency of the knots used. In this case, the elbow cutoff for the number of knots is 3. Taking the first 3 values of the previously mentioned ordered set, we have the discretization-point-set of \(DPS = \{145, 37, 132\}\).
Figure 3: The training set is shown by points while the solution sets are shown by lines. The black points indicate the initial $n_0$ training points while the colors red, green, and blue correspond to the follow-up training points and solution sets at the ordered DPS.

For the inverse problem, we use a budget of $n_0 = 15$ for the initial training set and a total budget of $N = 50$. The remaining budget of $N - n_0 = 35$ is divided approximately evenly among the three points of DPS. When implementing the expected improvement criterion for contour estimation to allow for both global and local exploration of space when choosing the follow-up points sequentially, we default $\alpha = 0.67$ to correspond to 50% confidence under approximate normality. In the same step, the resolution of the space-filling set $\chi_i$ for the sequential design is set to $M = 5000$ to explore the space of the GP surrogates. Lastly, to limit the size of the intersection of the solution sets, we have set $\epsilon = 1 \times 10^{-5}$.

As the training set is augmented and the GP model surrogate improves, the follow-up training points become increasingly precise relative to the solution set. In Figure 4, we see the intersection of solutions sets to be approximately $x_0$, after the final iteration of the sequential design. We extract the intersectional inverse solution $x_{opt} = (0.8188406, 0.2028986)$. Figure 4 demonstrates that the response for $x_{opt}$ has close resemblance to the target response.

4 Simulation studies

In this section, we use two different test simulators to compare the proposed multiple scalar contour estimation method with the modified history matching algorithm. The multiple scalar contour estimation method is implemented and compared at two levels, using the original budget and the budget matching that of the modified history matching method, since the budget is not predetermined in the latter method.

To demonstrate the comparison between the proposed method and modified history matching method, we use the following four popular goodness of fit measures:
Figure 4: To illustrate the result of the procedure, the target response is shown by the solid black line and the response for $x_{opt}$ is shown by the dotted red line.

- Root mean squared error

$$RMSE = \left( \frac{1}{L} \sum_{i=1}^{L} |g(\hat{x}_{opt}, t_i) - g_0(t_i)|^2 \right)^{1/2}.$$ 

- Coefficient of determination $R^2$ of the simple linear regression model fitted to the inverse solution and its corresponding response, i.e., $R^2$ of the SLR model:

$$g_0(t_i) = g(\hat{x}_{opt}, t_i) + \epsilon_i, i = 1, 2, \ldots, L,$$

with the assumption of i.i.d. errors $\epsilon_i$.

- Nash–Sutcliffe Efficiency (Nash and Sutcliffe, 1970)

$$NSE = 1 - \frac{\sum_{i=1}^{L} [g(\hat{x}_{opt}, t_i) - g_0(t_i)]^2}{\sum_{i=1}^{L} [g_0(t_i) - \bar{g}_0]^2}$$

- Normalized discrepancy

$$normD_{g_0(t_i)} = \frac{\|g_0(t_i) - g(\hat{x}^*)\|_2^2}{\|g_0(t_i) - g_0(t_i)1_L\|_2^2}$$

where $\bar{g}_0(t_i) = \sum_{i=1}^{L} g_0(t_i)/L$ and $1_L$ is an L-dimension vector of ones.

The goal is for the time series solution corresponding to $x_{opt}$ to maximize $R^2$ and NSE while minimizing RMSE and normD. The goodness of fit comparisons for modified history matching methods and the two budget levels of multiple scalar contour estimation are shown at the end of each example.
4.1 Example 1: Easom Function (Michalewicz, 1996) Continued

We begin by revisiting the example discussed in Section 3 to compare the inverse solutions that we arrived at. The modified history matching approach used a budget size of $N = 230$; thus, a budget of the matching size was used for the proposed method as well along with the original budget size of $N = 50$.

Table 1: Goodness-of-fit comparisons of the proposed multiple scalar valued contour estimation using $N = 66$ and $N = 93$, and the modified history matching method.

| Methods                      | Total Budget | RMSE       | $R^2$     | NSE      | normD    |
|------------------------------|--------------|------------|-----------|----------|----------|
| modified history matching    | $N = 230$   | $2.46 \times 10^{-7}$ | 0.999    | 0.999    | $3.157 \times 10^{-6}$ |
| multiple scalar contour estimation | $N = 50$  | $3.10 \times 10^{-7}$ | 0.999    | 0.999    | $4.993 \times 10^{-6}$ |
| multiple scalar contour estimation | $N = 230$ | $1.48 \times 10^{-7}$ | 0.999    | 0.998    | $1.137 \times 10^{-5}$ |

Table 2: Plots for goodness-of-fit comparison between modified history matching (gray), multiple scalar-valued contour estimation with $N = 50$ (brown), and multiple scalar-valued contour estimation with $N = 230$ (blue).

From Table 1 and Table 2, we see that the proposed multiple scalar contour estimation method using a budget size of $N = 230$ is clearly the most favored approach. Compared to the modified history matching approach, this method shows an improvement margin of $(2.46 \times 10^{-7} - 1.48 \times 10^{-7}) / 1.48 \times 10^{-7} \times 100\% \approx 66\%$ per RMSE, and $(3.157 \times 10^{-5} - 1.137 \times 10^{-5}) / 1.137 \times 10^{-5} \times 100\% \approx 178\%$ per normalized discrepancy.

4.2 Example 2: Harari and Steinberg, 2014

In another example of adapting the multiple scalar contour estimation approach to solve the inverse problem, we use a more complex test function (Harari and Steinberg, 2014) with the input space $x = (x_1, x_2, x_3)^T \in [0,1]^3$. The simulator model is shown as:

$$y_t(x) = \exp(3x_1t + t) \cos(6x_2t + 2t - 8x_3 - 6)$$

where time $t \in [0,1]$ is on a 200-point equidistant grid. The target time-series response for the calibration problem corresponds to $x_0 = (0.522, 0.950, 0.427)^T$.

Using the method of forward selected spline knots, the DPS was selected at $\{118, 26, 95\}$. An initial training set of size $n_0 = 18$ generated used a MaxPro Latin Hypercube and total budget of $N = 66$ are used. The budget used in implementing the modified history matching method is $N = 93$, thus the
proposed method with the matching budget and $n_0$ held constant was used as well. In Figure 5, we see the placement of DPS and the time series responses for the inverse solutions derived from the methods.

Figure 5: The target time series simulator response is shown by the black contour, with the DPS of size $k = 3$ being displayed by the dotted vertical lines. The time series responses corresponding to the modified history matching method, multiple scalar contour estimation method using $N = 66$, and multiple scalar contour estimation method using $N = 93$ are displayed by the red, blue, and green line respectively.

Table 3: Goodness-of-fit comparisons of the proposed multiple scalar valued contour estimation using $N = 66$ and $N = 93$, and the modified history matching method.

| Methods                     | Total Budget | RMSE  | $R^2$   | NSE   | normD   |
|-----------------------------|--------------|-------|---------|-------|---------|
| modified history matching   | $N = 93$     | 0.209 | 0.997   | 0.996 | 0.00317 |
| multiple scalar contour estimation | $N = 66$     | 0.246 | 0.996   | 0.995 | 0.00440 |
| multiple scalar contour estimation | $N = 93$     | 0.134 | 0.999   | 0.998 | 0.00132 |

In Table 3 and the graphics in Table 4, we see that while the proposed multiple scalar-valued contour estimation method at the default budget of $N = 66$ performs slightly worse than the modified history matching method, the proposed method outperforms the modified history matching method in all four of the goodness of fit measurements when its budget matches that of the modified history matching method at $N = 93$. In particular, we see the proposed method using $N = 93$ outperform the modified history matching method by a significant margin of $(0.209 - 0.134)/0.134 \times 100% \approx 56\%$ according to RMSE, and an even greater margin of $(0.00317 - 0.00132)/0.00132 \times 100% \approx 140\%$ according to normal discrepancy.

4.3 Example 3: Bliznyuk et al., 2008

In another application of the contour estimation based history matching method for solving the inverse problem, we use a complex simulator model (Bliznyuk et al., 2008) with the input space such that $x = (x_1, x_2, x_3, x_4, x_5)^T \in [7, 13] \times [0.02, 0.12] \times [0.01, 3] \times [30.01, 30.304] \times [0, 3]$. The computer simulator
Table 4: Plots for goodness-of-fit comparison between modified history matching (gray), multiple scalar-valued contour estimation with \( N = 66 \) (brown), and multiple scalar-valued contour estimation with \( N = 93 \) (blue).

Function is seen as:

\[
y_t(x) = \frac{x_1}{\sqrt{x_2 t}} \exp\left(\frac{-x_3^2}{4x_2 t}\right) + \frac{x_1}{\sqrt{x_2 (t - x_4)}} \exp\left(-\frac{(x_5 - x_3)^2}{4x_2 (t - x_4)}\right) I(x_4 < t)
\]  

where time is defined by 200 equidistant points such that \( t \in [35.3, 95] \). The true target time-series response corresponds to \( x_0 = (9.640, 0.059, 1.445, 30.277, 2.520)^T \). For the purposes of the history matching procedure, the input space is scaled such that \( x \in [0, 1]^5 \).

By optimizing the cubic spline knots onto the target response, the DPS of size \( k = 3 \) is chosen at \( \{30, 7, 61, 14\} \). A training set of size \( n_0 = 30 \) and total budget of \( N = 120 \) are used. The proposed method is implemented using \( N = 269 \) as well to match the size of budget that the modified history matching method requires for the calibration problem of the simulator model. In Figure 6 below, we see the target response, the DPS, and the results for the three procedures performed.

![Figure 6](image)

Figure 6: The target time series simulator response is shown by the black contour, with the DPS of size \( k = 4 \) being displayed by the dotted vertical lines. The time series responses corresponding to the modified history matching method, multiple scalar contour estimation method using \( N = 120 \), and multiple scalar contour estimation method using \( N = 269 \) are displayed by the red, blue, and green line respectively.
Table 5: Goodness-of-fit comparisons of the proposed multiple scalar valued contour estimation using $N = 120$ and $N = 269$, and the modified history matching method.

| Methods                              | Total Budget | RMSE  | $R^2$ | NSE     | normD   |
|--------------------------------------|--------------|-------|-------|---------|---------|
| modified history matching            | $N = 269$   | 0.129 | 0.999 | 0.984   | 0.0152  |
| multiple scalar contour estimation   | $N = 120$   | 0.0221| 0.999 | 0.999   | 0.000447|
| multiple scalar contour estimation   | $N = 269$   | 0.0194| 0.999 | 0.999   | 0.000346|

Table 6: Plots for goodness-of-fit comparison between modified history matching with $N = 269$ (gray), multiple scalar-valued contour estimation with $N = 120$ (brown), and multiple scalar-valued contour estimation with $N = 269$ (blue).

In Table 5 and the visualizations in Table 6, we see the goodness of fit measures corresponding to the three inverse solutions that were optimized by the methods implemented. We can see that the proposed multiple scalar contour estimation method at both budget levels significantly outperform the modified history matching approach by massive margins.

5 Real Application: Rainfall-Runoff Example

The motivating application for the modified history model was its using on hydrological models. The Matlab-Simulink simulator introduced by Duncan et al. (2013) and studied the rainfall-runoff relationship for the windrow composting pad. The compartmental model for estimating the amount of rainfall-runoff from the composting pad. The following four input parameters are identified to have the most significant influence on the output: depth of surface, depth of sub-surface and two coefficients of the saturated hydraulic conductivity ($K_{sat1}$ and $K_{sat2}$). See Duncan et al. (2013) for further details on the Matlab-Simulink Model.

For the inverse problem, the target response used is the rainfall-runoff data ($g_0$) observed from the Bioconversion center at the University of Georgia, Athens, USA (Bhattacharjee et al. 2019). In Figure 7, we observe the target response and some random outputs from the Matlab-Simulink model.

Using the method of forward selected cubic spline knots for DPS selection, we choose the time points at $DPS = \{4557, 3359, 4702, 4085\}$ for the multiple scalar contour estimation method. We use the initial training set with size $n_0 = 40$ generated using a Latin hypercube design and a total budget of $N = 120$. The modified history matching method exhausted a total budget of $N = 461$ (Bhattacharjee et al.), thus the budget size of $N = 461$ was made available for the proposed method as well. Figure 8 shows the positioning of DPS as well as time-series responses for the three inverse solutions with respect to the observed runoff data.
Figure 7: Observed data \((g_0)\) with random simulator outputs.

Figure 8: The target time series simulator response is shown by the black contour, with the DPS of size \(k = 4\) being displayed by the dotted vertical lines. The time series responses corresponding to the modified history matching method, multiple scalar contour estimation method using \(N = 120\), and multiple scalar contour estimation method using \(N = 461\) are displayed by the red, blue, and green line respectively.

We can see that the proposed multiple scalar contour estimation method using \(N = 120\) and \(N = 461\) slightly outperform the modified history matching approach from Table 7 and the plots in Table 8. The multiple scalar contour estimation approach using \(N = 120\) outperformed the modified history matching approach by small margins of \((55.580 - 54.215)/54.215 \times 100\% \approx 2.5\%\) per RMSE, and \((0.0841 - 0.0801)/0.0801 \times 100\% \approx 5\%\) per normal discrepancy. When the proposed method matches the budget size used by modified history matching method at \(N = 461\), the margin of improvement increases to \((55.580 - 53.585)/53.585 \times 100\% \approx 3.7\%\) per RMSE, and \((0.0841 - 0.0782)/0.0782 \times 100\% \approx 7.5\%\) per normal discrepancy.
Table 7: Goodness-of-fit comparisons of the proposed multiple scalar valued contour estimation using $N = 120$ and $N = 461$, and the modified history matching method.

| Methods                                | Total Budget | RMSE  | $R^2$ | NSE  | normD |
|----------------------------------------|--------------|-------|-------|------|-------|
| modified history matching               | $N = 461$   | 55.580| 0.926 | 0.916| 0.0841|
| multiple scalar contour estimation      | $N = 120$   | 54.215| 0.934 | 0.920| 0.0801|
| multiple scalar contour estimation      | $N = 461$   | 53.585| 0.934 | 0.922| 0.0782|

Table 8: Plots for goodness-of-fit comparison between modified history matching with $N = 461$ (gray), multiple scalar-valued contour estimation with $N = 120$ (brown), and multiple scalar-valued contour estimation with $N = 461$ (blue).

6 Concluding Remarks

In this paper, we established the proposed multiple scalar contour estimation approach to be competitive in solving the calibration problem for dynamic computer simulators. The expected improvement for contour estimation sequential criterion was successfully applied to the problem. Furthermore, our study offered a systematic approach in selecting the discretization-point-set, which is a concept in history matching adopted by the proposed approach.

The proposed approach outperformed the competing modified history matching approach in all four examples seen when using the equivalent budget. In Example 3 and the real rainfall-runoff application of Matlab-Simulink model, the proposed approach performed better than modified history matching using less budgets. In fact, a budget of $269 - 120 = 149$ in Example 3 and a budget of $461 - 120 = 341$ were saved using the proposed approach. The better performance in terms of the goodness of fit measures and the efficiency is budget usage point to multiple scalar contour estimation being favorable to the modified history matching approach.

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