

# Adaptive Global Solutions to Single-Input Optimal Control Problems via Gaussian Processes<sup>\*</sup>

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**Abstract:** Optimal control problems are found in state and parameter estimation, experimental design, and model-based control for complex dynamical systems. Parsimonious input parameterization is an approach for obtaining solutions to these problems, which comprises two tasks: the first corresponds to the generation of arc sequences and the second consists in the computation of optimal values of a small number of decision variables for each sequence. This paper proposes an adaptive method for global solutions to single-input optimal control problems that accounts for the mismatch between the true system and its model by using Gaussian processes to represent the mismatch in the cost and constraints for an arc sequence. This adaptive approach converges to the global solution for the true system and ensures constraint satisfaction with a prespecified probability. The proposed approach is illustrated by a simulation example of a reaction system.

*Keywords:* optimal control, global optimization, model uncertainty, Gaussian processes

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## 1. INTRODUCTION

Optimal control problems (OCPs) are extensively applied for optimal design, analysis, and operation of various complex dynamical systems. Efficient methods for OCPs are useful for several tasks in engineering applications, such as optimization-based state and parameter estimation, experimental design, and model-based control. The decision variables in OCPs represent time-varying functions over a time interval such that a cost is optimized subject to constraints. OCPs can be complex to solve since they involve infinitely many decision variables, and there can exist both terminal constraints at the end of the time interval and path constraints along the trajectory (Bryson and Ho, 1975).

Direct methods are a popular approach for OCPs wherein the time-varying functions represented by decision variables are discretized to approximate the original infinite-dimensional problem as a finite-dimensional one (Teo et al., 1991; Biegler et al., 2002). However, a general challenge in OCPs is that one cannot obtain a model that represents exactly the true system where the solution to the OCP will be implemented. This may result in suboptimal, or even infeasible, performance when the optimal solution for the model is applied to the true system (Yip and Marlin, 2003). The main approaches to prevent these effects of model mismatch are robust, stochastic, and adaptive optimization (Chachuat et al., 2009). Robust optimization provides performance guarantees, but can result in conservative solutions (Mönnigmann and Marquardt, 2003). Stochastic op-

timization is less conservative, but can be computationally costly due to the representation of probability (Mesbah, 2016). Adaptive optimization uses measurements to enforce optimality of the true system, but requires repetition (Krstić and Wang, 2000). Moreover, all these approaches are impaired by a large number of decision variables.

The number of decision variables in OCPs can be reduced via a parsimonious input parameterization (Rodrigues and Bonvin, 2020). In this approach, (i) all the arcs that can occur in the solution to an OCP are identified, (ii) a finite set of plausible arc sequences is generated, and (iii) each sequence is described by a small number of decision variables. Then, for a given arc sequence, the optimal values of these decision variables can be computed via numerical optimization, which only requires numerical integration of the dynamic equations of the states and adjoint variables for each value of the decision variables. Another main advantage, shown by Rodrigues and Mesbah (2022) and applied to Bayesian optimal experiment design by Rodrigues et al. (2022), is that the small number of decision variables enables efficient computation of globally optimal values of the decision variables for each arc sequence.

An approach based on parsimonious input parameterization can enforce convergence to the global optimum for the model, but not for the true system; thus, it must be extended to deal with model mismatch. The small number of decision variables enabled by the parsimonious input parameterization is useful for addressing model mismatch, as explained next. To this end, alternate parameter estimation and optimization is a typical adaptive approach, but may fail to converge to the optimum of the true system (Forbes et al., 1994). On the other hand, modifier

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adaptation is an adaptive approach that satisfies the optimality conditions of the true system upon convergence by using measurements to update modifiers that are added to the cost and constraints (Marchetti et al., 2009). This approach benefits from a small number of decision variables since it requires explicit estimation of the gradients of the cost and constraints of the true system with respect to the decision variables, which is sensitive to measurement noise (Bunin et al., 2013). However, modifier adaptation either provides no guarantees of global and feasible-side convergence, or provides them at the price of relatively slow convergence (Marchetti et al., 2017). This motivates a representation of the mismatch between the true system and the model by updating distributions rather than modifiers for the cost and constraints. In particular, Gaussian processes can be used to represent this mismatch since they deal effectively with measurement noise and can provide probabilistic bounds (Ferreira et al., 2018; Rasmussen and Williams, 2006). After each update, the modified model can be used again for optimization. The smaller number of decision variables provided by the parsimonious input parameterization facilitates the whole procedure. In fact, an approach based on parsimonious input parameterization and modifier adaptation has already been applied to data-driven adaptive optimal control of cold atmospheric plasmas by Rodrigues et al. (2023). However, the parsimonious input parameterization combined with Gaussian processes to deal with model mismatch has not been presented yet.

This paper aims to extend the parsimonious input parameterization approach for adaptive global solutions to OCPs for nonlinear dynamical systems subject to model mismatch, with particular emphasis on the case of single-input OCPs. The main contribution of this paper is an adaptive method for determining the optimal solution to the OCP in the presence of model mismatch via Gaussian processes. By using the proposed iterative approach to update the Gaussian processes, it is shown that the true system is expected to converge to its global optimum without constraint violation. Finally, the proposed approach is illustrated via a simulation example.

## 2. PROBLEM STATEMENT

Consider the general class of OCPs formulated as

$$\min_{\mathbf{u}(\cdot), t_f} \mathcal{J}(\mathbf{u}(\cdot), t_f) = \phi(\mathbf{x}(t_1), \dots, \mathbf{x}(t_T), t_f), \quad (1a)$$

$$\text{s.t. } \mathcal{T}(\mathbf{u}(\cdot), t_f) = \boldsymbol{\psi}(\mathbf{x}(t_1), \dots, \mathbf{x}(t_T), t_f) \leq \mathbf{0}_{n_\psi}, \quad (1b)$$

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t)), \quad \mathbf{x}(t_0) = \mathbf{x}_0, \quad (1c)$$

$$\underline{\mathbf{u}} \leq \mathbf{u}(t) \leq \bar{\mathbf{u}}, \quad \mathbf{h}(\mathbf{x}(t)) \leq \mathbf{0}_{n_h}, \quad (1d)$$

where  $t_0$  is the initial time,  $t_1 < \dots < t_T$  are  $T$  times,  $t_f = t_T \in [t_0, t_{max}]$  is the finite final time with upper bound  $t_{max}$ ;  $\mathbf{u}(t)$  is the  $n_u$ -dimensional vector of piecewise-continuous inputs for all  $t \in [t_0, t_f)$  with  $n_u$ -dimensional vectors of lower and upper bounds  $\underline{\mathbf{u}}$  and  $\bar{\mathbf{u}}$ ;  $\mathbf{x}(t)$  is the  $n_x$ -dimensional vector of piecewise-continuously differentiable states for all  $t \in [t_0, t_f]$ ;  $\mathbf{f}(\mathbf{x}, \mathbf{u})$  is an  $n_x$ -dimensional vector function, smooth for all  $(\mathbf{x}, \mathbf{u}) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_u}$ ;  $\mathbf{h}(\mathbf{x})$  is an  $n_h$ -dimensional vector function, smooth for all  $\mathbf{x} \in \mathbb{R}^{n_x}$ ;  $\phi(\mathbf{X}, t)$ ,  $\boldsymbol{\psi}(\mathbf{X}, t)$  are a scalar function and an  $n_\psi$ -dimensional vector function, respectively, smooth for all  $(\mathbf{X}, t) \in \mathbb{R}^{T n_x} \times [t_0, t_{max}]$ . We assume that  $\mathbf{h}^{(1)}(\mathbf{x}, \mathbf{u}) := \frac{\partial \mathbf{h}}{\partial \mathbf{x}}(\mathbf{x})\mathbf{f}(\mathbf{x}, \mathbf{u})$  depends explicitly on  $\mathbf{u}$ .

The inputs that represent the solution to Problem (1) are composed of several arcs. For each input  $u_j$ , each arc can be of type 1) bang-bang, which is determined by  $u_j = \underline{u}_j$  or  $u_j = \bar{u}_j$ , 2) active-state constraint, which is determined by  $h_k^{(1)}(\mathbf{x}, \mathbf{u}) = 0$  for some  $k = 1, \dots, n_h$ , or 3) singular, which is determined by the dynamics given by  $\mathbf{f}(\mathbf{x}(t), \mathbf{u}(t))$  (Srinivasan et al., 2003; Rodrigues and Bonvin, 2020). Hence, arc sequences can be formed from a finite number of arc types. If only arc sequences with a number of arcs no larger than some upper bound  $\bar{n}_a$  and without consecutive arcs of the same type are considered plausible, then the number of plausible sequences is also finite. Suppose that the bang-bang arcs are denoted as 1L or 1U, depending on whether they are determined by  $u_j = \underline{u}_j$  or  $u_j = \bar{u}_j$ , and note that sequences with fewer than  $\bar{n}_a$  arcs are particular cases of the sequences with  $\bar{n}_a$  arcs where some arcs vanish. In many cases, one can reasonably assume that the solution includes a relatively small number of arcs with  $\bar{n}_a$  between 3 and 5 since chattering solutions with arcs of infinitesimal duration are not practically interesting even if these solutions are globally optimal from a mathematical point of view (Srinivasan et al., 2003; Rodrigues and Bonvin, 2019).

Parsimonious input parameterization effectively describes the optimal inputs using only a few decision variables, in contrast to an infinite number of variables in the original OCP (Rodrigues and Bonvin, 2019, 2020). For a given plausible arc sequence with  $n_s + 1$  bang-bang and singular arcs, the inputs are defined by the following decision variables: the switching times  $\bar{t}_1, \dots, \bar{t}_{n_s}$  to arcs of types 1 and 3, the final time  $\bar{t}_{n_s+1} = t_f$ , and the initial conditions of the singular arcs (Xu and Antsaklis, 2004). The entry points in arcs of type 2 are given by the  $n_\eta$ -dimensional vector  $\boldsymbol{\eta} = (\eta_1, \dots, \eta_{n_\eta})$ , but the switching to these arcs cannot occur at arbitrary times since it depends on the states  $\mathbf{x}$ .

The goal of this paper is to extend the parsimonious input parameterization approach for solving OCPs formulated as (1) to global optimality in the presence of mismatch between the true system and the model. Although the proposed approach can be generalized to OCPs with multiple inputs  $\mathbf{u}(t)$ , the number of inputs affects the number of arc sequences. For this reason, we consider OCPs with  $n_u = 1$ , that is, a single input  $u(t)$ , without loss of generality, not only for the sake of clarity, but also because the approach is most efficient in this case. The proposed approach for adaptive global optimality relies on a model of the system to determine: (i) the globally optimal switching between arcs for a given plausible arc sequence; and (ii) the sequence that provides the globally optimal solution. Question (i) is addressed by computing the globally optimal values of the decision variables for the given arc sequence. For this, the cost and constraints of the OCP for each arc sequence are represented in terms of new decision variables, as shown in Section 3. Once question (i) is addressed for each sequence, question (ii) is trivially answered via parallel computing. Lastly, for the sequence chosen to address question (ii), an adaptive method is used to answer question (i) for the true system rather than for the model, as shown in Section 4.

## 3. REFORMULATION OF THE OCP VIA PARSIMONIOUS INPUT PARAMETERIZATION

For a given arc sequence, we describe the input in the  $i$ th time interval  $[\bar{t}_{i-1}, \bar{t}_i)$ , for  $i = 1, \dots, n_s + 1$ , by defining  $n_{z,i}$  new states and initial conditions for this interval as  $\mathbf{z}_i(t)$

and  $\mathbf{z}_{i,0}$ . One can then combine all the states into vectors with a dimension  $n_z := n_x + n_{z,1} + \dots + n_{z,n_s+1}$

$$\mathbf{z}(t) := \left[ \mathbf{x}(t)^\top \begin{bmatrix} \mathbf{z}_1(t) \\ \vdots \\ \mathbf{z}_{n_s+1}(t) \end{bmatrix}^\top \right]^\top, \quad (2)$$

with corresponding initial conditions  $\mathbf{z}_0$ .

The arc type determines the dimension and meaning of the elements of  $\mathbf{z}_i(t)$ ,  $\mathbf{z}_{i,0}$  and their effect on the input  $u(t)$  given by the control law  $u(t) = \tilde{c}(\mathbf{z}(t))$  and on the dynamics of  $\mathbf{z}_i(t)$  given by  $\dot{\mathbf{z}}_i(t) = \mathbf{q}_i(\mathbf{x}(t), \mathbf{z}_i(t))$ . For bang-bang arcs,  $\mathbf{z}_i(t)$ ,  $\mathbf{z}_{i,0}$  are of dimension 0 and  $\tilde{c}(\mathbf{z}(t)) = \underline{u}$  or  $\tilde{c}(\mathbf{z}(t)) = \bar{u}$ . For active-state constraint arcs,  $\mathbf{z}_i(t)$ ,  $\mathbf{z}_{i,0}$  are not needed and  $\tilde{c}(\mathbf{z}(t))$  is such that  $h_k^{(1)}(\mathbf{x}(t), \tilde{c}(\mathbf{z}(t))) = 0$  for some  $k = 1, \dots, n_h$ . For singular arcs, assuming that the input is approximated by a linear function, then  $\mathbf{z}_i(t) = \begin{bmatrix} \tilde{u}_i(t) \\ \tilde{p}_i(t) \end{bmatrix}$ ,  $\mathbf{z}_{i,0} = \begin{bmatrix} u_i^0 \\ p_i \end{bmatrix}$  are of dimension 2, where  $u_i^0$  and  $p_i$  are the initial value and derivative of the input and  $\tilde{u}_i(t)$  is its value at time  $t$ , which implies that  $\tilde{c}(\mathbf{z}(t)) = \tilde{u}_i(t)$  and  $\mathbf{q}_i(\mathbf{x}(t), \mathbf{z}_i(t)) = \begin{bmatrix} \tilde{p}_i(t) \\ 0 \end{bmatrix}$ . The set  $\{i : i\text{th arc of } u(\cdot) \text{ is of type 3}\}$  is denoted as  $\mathcal{S}$ , which implies that  $n_{z,1} + \dots + n_{z,n_s+1} = 2|\mathcal{S}|$ .

Then, upon eliminating input dependencies and rewriting Problem (1) in terms of the extended states  $\mathbf{z}$ , one obtains

$$\tilde{\chi}(\mathbf{z}(t_1), \dots, \mathbf{z}(t_T), t_f) := \begin{bmatrix} \tilde{\phi}(\mathbf{z}(t_1), \dots, \mathbf{z}(t_T), t_f) \\ \tilde{\psi}(\mathbf{z}(t_1), \dots, \mathbf{z}(t_T), t_f) \end{bmatrix}, \quad (3)$$

with  $\tilde{\phi}(\mathbf{z}(t_1), \dots, \mathbf{z}(t_T), t_f) := \phi(\mathbf{x}(t_1), \dots, \mathbf{x}(t_T), t_f)$  and  $\tilde{\psi}(\mathbf{z}(t_1), \dots, \mathbf{z}(t_T), t_f)$  defined similarly, and the dynamics

$$\tilde{\mathbf{f}}(\mathbf{z}(t)) := \left[ \mathbf{f}(\mathbf{x}(t), \tilde{c}(\mathbf{z}(t)))^\top \begin{bmatrix} \mathbf{q}_1(\mathbf{x}(t), \mathbf{z}_1(t)) \\ \vdots \\ \mathbf{q}_{n_s+1}(\mathbf{x}(t), \mathbf{z}_{n_s+1}(t)) \end{bmatrix}^\top \right]^\top. \quad (4)$$

Since the input parameters for the given arc sequence are  $\boldsymbol{\tau} := (\bar{t}_1, \dots, \bar{t}_{n_s}, t_f, \mathbf{z}_{1,0}, \dots, \mathbf{z}_{n_s+1,0})$ , Problem (1) can be reformulated in terms of these new decision variables as

$$\min_{\boldsymbol{\tau}} \hat{\phi}(\boldsymbol{\tau}) := \tilde{\phi}(\mathbf{z}(t_1), \dots, \mathbf{z}(t_T), t_f), \quad (5a)$$

$$\text{s.t. } \hat{\psi}(\boldsymbol{\tau}) := \tilde{\psi}(\mathbf{z}(t_1), \dots, \mathbf{z}(t_T), t_f) \leq \mathbf{0}_{n_\psi}, \quad (5b)$$

$$\bar{t}_{i-1} \leq \bar{t}_i, \quad i = 1, \dots, n_s + 1, \quad (5c)$$

$$\underline{u} \leq u_s^0 \leq \bar{u}, \quad (5d)$$

$$\underline{u} \leq u_s^0 + p_s(\bar{t}_s - \bar{t}_{s-1}) \leq \bar{u}, \quad s \in \mathcal{S}, \quad (5d)$$

$$\dot{\mathbf{z}}(t) = \tilde{\mathbf{f}}(\mathbf{z}(t)), \quad \mathbf{z}(t_0) = \mathbf{z}_0, \quad (5e)$$

which is convenient for numerical optimization since there are only  $N := n_s + 1 + n_{z,1} + \dots + n_{z,n_s+1}$  decision variables.

For each entry point  $\hat{\eta}_j(\boldsymbol{\tau}) := \eta_j$ , there exists  $k = 1, \dots, n_h$  such that  $\tilde{h}_k(\mathbf{z}(t)) \leq 0$  becomes active at  $t = \hat{\eta}_j(\boldsymbol{\tau})$ .

#### 4. ADAPTIVE APPROACH FOR A REFORMULATED OCP USING GAUSSIAN PROCESS REGRESSION

##### 4.1 Gaussian processes to adapt cost and constraints

The main goal of this paper is to develop an adaptive OCP approach that converges to the global optimum of the true system despite the mismatch between the true system and its model. Hence, we (i) estimate the mismatch between the cost and constraint functions for the true system and the ones for the model and (ii) use this estimation for

an adaptive algorithm to solve the OCP (5) to global optimality for the true system, as shown in Algorithm 1.

Each cost and constraint function is expressed for the true system and the model as

$$\hat{\chi}^p(\boldsymbol{\tau}) := \tilde{\chi}(\mathbf{z}^p(t_1), \dots, \mathbf{z}^p(t_T), t_f), \quad (6)$$

$$\hat{\chi}^m(\boldsymbol{\tau}) := \tilde{\chi}(\mathbf{z}^m(t_1), \dots, \mathbf{z}^m(t_T), t_f), \quad (7)$$

where  $\mathbf{z}^p(t)$  and  $\mathbf{z}^m(t)$  are the states  $\mathbf{z}(t)$  that correspond to  $\boldsymbol{\tau}$  in the true system and the model, respectively. Suppose that, at each iteration  $k$  of Algorithm 1, data for  $\hat{\chi}^p(\boldsymbol{\tau})$  are available in the neighborhood of a set of points  $\boldsymbol{\tau}_1, \dots, \boldsymbol{\tau}_k$  evaluated by the algorithm. More precisely, this occurs not only for the nominal points  $\boldsymbol{\tau}_i^0 = \boldsymbol{\tau}_i$ , for  $i = 1, \dots, k$ , but also for the auxiliary points  $\boldsymbol{\tau}_i^j$ , for  $i = 1, \dots, k$  and  $j = 1, \dots, N$ , where  $\boldsymbol{\tau}_1$  is the global model optimum for the OCP (5). An efficient method for solving single-input OCPs reformulated as (5) has been presented by Rodrigues and Mesbah (2022). Hence, the goal is to describe the mismatch between the functions  $\hat{\chi}^p(\boldsymbol{\tau})$  and  $\hat{\chi}^m(\boldsymbol{\tau})$  from measurements of  $\hat{\chi}^p(\boldsymbol{\tau}_i^j)$  and knowledge of  $\hat{\chi}^m(\boldsymbol{\tau}_i^j)$ , for  $i = 1, \dots, k$  and  $j = 0, \dots, N$ . For this, we use Gaussian process regression since it provides a statistical description of the mismatch in the cost and constraint functions in terms of probability distributions (Rasmussen and Williams, 2006).

Suppose that the unknown function

$$g^{x^*}(\boldsymbol{\tau}) = \hat{\chi}^p(\boldsymbol{\tau}) - \hat{\chi}^m(\boldsymbol{\tau}), \quad (8)$$

is sampled at  $\boldsymbol{\tau} = \boldsymbol{\tau}_i^j$ , for  $i = 1, \dots, k$  and  $j = 0, \dots, N$ , as

$$y_j^x(i) = g^{x^*}(\boldsymbol{\tau}_i^j) + e_j^x(i), \quad i = 1, \dots, k, \quad j = 0, \dots, N, \quad (9)$$

where  $y_j^x(i)$  is the measurement of  $g^{x^*}(\boldsymbol{\tau}_i^j)$  with noise  $e_j^x(i)$ . Based on the data  $y_j^x(i)$ , the mismatch model

$$y_j^x(i) = g_k^x(\boldsymbol{\tau}_i^j) + e_j^x(i), \quad i = 1, \dots, k, \quad j = 0, \dots, N, \quad (10)$$

and a prior distribution of the function  $g_k^x(\boldsymbol{\tau})$  that represents the mismatch between  $\hat{\chi}^p(\boldsymbol{\tau})$  and  $\hat{\chi}^m(\boldsymbol{\tau})$  in the domain  $\mathcal{D}$ , we aim to estimate the probability density function (pdf) for the posterior distribution of  $g_k^x(\boldsymbol{\tau})$ . To this end, upon defining  $\mathbf{g}_k^x(i) := [g_k^x(\boldsymbol{\tau}_i^0) \dots g_k^x(\boldsymbol{\tau}_i^N)]^\top$ ,  $\mathbf{y}^x(i) := [y_0^x(i) \dots y_N^x(i)]^\top$ ,  $\mathbf{e}^x(i) := [e_0^x(i) \dots e_N^x(i)]^\top$ ,

$$\mathbf{y}^x(i) = \mathbf{g}_k^x(i) + \mathbf{e}^x(i), \quad i = 1, \dots, k, \quad (11)$$

and, upon defining  $\mathbf{g}_k^x := [\mathbf{g}_k^x(1)^\top \dots \mathbf{g}_k^x(k)^\top]^\top$ ,  $\mathbf{y}_k^x := [\mathbf{y}^x(1)^\top \dots \mathbf{y}^x(k)^\top]^\top$ ,  $\mathbf{e}_k^x := [\mathbf{e}^x(1)^\top \dots \mathbf{e}^x(k)^\top]^\top$ ,

$$\mathbf{y}_k^x = \mathbf{g}_k^x + \mathbf{e}_k^x. \quad (12)$$

Assuming that the noise realizations in  $\mathbf{e}_k^x$  for the points  $\mathbf{T}_k = (\mathbf{t}_k^1, \dots, \mathbf{t}_k^{k(N+1)}) := (\boldsymbol{\tau}_1^0, \dots, \boldsymbol{\tau}_1^N, \dots, \boldsymbol{\tau}_k^0, \dots, \boldsymbol{\tau}_k^N)$  are independent and identically distributed (i.i.d.) and drawn from a zero-mean normal distribution with variance  $\sigma_\chi^2$ , the likelihood function is

$$p(\mathbf{y}_k^x | \mathbf{g}_k^x) = f(\mathbf{y}_k^x | \mathbf{g}_k^x, \sigma_\chi^2 \mathbf{I}_{k(N+1)}), \quad (13)$$

where  $f(\mathbf{x} | \bar{\mathbf{x}}, \boldsymbol{\Sigma}_x)$  is the pdf of a multivariate normal distribution with mean  $\bar{\mathbf{x}}$  and covariance  $\boldsymbol{\Sigma}_x$ .

Also, assume that the prior distribution of  $g_k^x(\boldsymbol{\tau})$  is given by a zero-mean squared exponential kernel, thus it follows a normal distribution with pdf

$$p(g_k^x | \boldsymbol{\eta}) = f(g_k^x | 0, K_k^x(\boldsymbol{\eta})), \quad (14)$$

with covariance  $K_k^x(\boldsymbol{\tau}, \boldsymbol{\tau}') = c \exp\left(-\frac{\|\boldsymbol{\tau} - \boldsymbol{\tau}'\|^2}{2\lambda^2}\right)$ , which depends on some hyperparameters  $\boldsymbol{\eta} = (c, \lambda)$ , where  $c \geq 0$ ,  $\lambda \geq 0$  represent the noise level and the length scale.

Hence, the posterior distribution of  $g_k^X(\boldsymbol{\tau})$  also follows a normal distribution with pdf

$$p(g_k^X | \mathbf{y}_k^X) = f(g_k^X | \bar{g}_k^X, \Sigma_{g,k}^X), \quad (15)$$

where

$$\bar{g}_k^X(\boldsymbol{\tau}) = \mathbf{k}_k^X(\boldsymbol{\tau})^T \left( \Sigma_{\mathbf{y},k}^X \right)^{-1} \mathbf{y}_k^X, \quad (16)$$

$$\Sigma_{g,k}^X(\boldsymbol{\tau}, \boldsymbol{\tau}') = K_k^X(\boldsymbol{\tau}, \boldsymbol{\tau}' | \hat{\boldsymbol{\eta}}_k^X) - \mathbf{k}_k^X(\boldsymbol{\tau})^T \left( \Sigma_{\mathbf{y},k}^X \right)^{-1} \mathbf{k}_k^X(\boldsymbol{\tau}'), \quad (17)$$

with

$$(\mathbf{k}_k^X(\boldsymbol{\tau}))_i = K_k^X(\mathbf{t}_k^i, \boldsymbol{\tau} | \hat{\boldsymbol{\eta}}_k^X), \quad (18)$$

$$\left( \Sigma_{\mathbf{y},k}^X \right)_{i,j} = \sigma_\chi^2 (\mathbf{I}_{k(N+1)})_{i,j} + K_k^X(\mathbf{t}_k^i, \mathbf{t}_k^j | \hat{\boldsymbol{\eta}}_k^X), \quad (19)$$

and the hyperparameters  $\hat{\boldsymbol{\eta}}_k^X$  computed as in Appendix A.

This allows us to obtain probabilistic bounds for the function  $g^{X*}(\boldsymbol{\tau})$  since  $\bar{g}_k^X(\boldsymbol{\tau}) + r_k \sigma_{g,k}^X(\boldsymbol{\tau})$ , with  $\sigma_{g,k}^X(\boldsymbol{\tau}) := \sqrt{\Sigma_{g,k}^X(\boldsymbol{\tau}, \boldsymbol{\tau})}$ , is an upper bound for  $g_k^X(\boldsymbol{\tau})$  with a probability that depends on  $r_k$ . To this end, we assume that the unknown function  $g^{X*}(\boldsymbol{\tau})$  is sampled from the prior distribution of  $g_k^X(\boldsymbol{\tau})$ , which is a standard assumption in Gaussian process optimization (Srinivas et al., 2012). More precisely, there is a probability  $\Phi(r_k)$  that  $g_k^X(\boldsymbol{\tau}) \leq \bar{g}_k^X(\boldsymbol{\tau}) + r_k \sigma_{g,k}^X(\boldsymbol{\tau})$ , where  $\Phi$  is the cumulative distribution function of the standard normal distribution. For example, the probability that  $g_k^X(\boldsymbol{\tau}) \leq \bar{g}_k^X(\boldsymbol{\tau}) + 2\sigma_{g,k}^X(\boldsymbol{\tau})$  is more than 97.5%. Since  $g_k^X(\boldsymbol{\tau})$  is an estimate of the mismatch  $\hat{\chi}^p(\boldsymbol{\tau}) - \hat{\chi}^m(\boldsymbol{\tau})$ ,  $\hat{\chi}_k^m(\boldsymbol{\tau}) := \hat{\chi}^m(\boldsymbol{\tau}) + \bar{g}_k^X(\boldsymbol{\tau}) + r_k \sigma_{g,k}^X(\boldsymbol{\tau})$  represents an upper bound for  $\hat{\chi}^p(\boldsymbol{\tau})$  with a probability  $\Phi(r_k)$ .

#### 4.2 Adaptive OCP approach

This idea can be used to obtain upper bounds for the cost and constraint functions  $\hat{\phi}^p(\boldsymbol{\tau})$  and  $\hat{\psi}_j^p(\boldsymbol{\tau})$  of the OCP (5) for the true system. Hence, based on the data available in the neighborhood of the set of points  $\boldsymbol{\tau}_1, \dots, \boldsymbol{\tau}_k$  at each iteration  $k$  of Algorithm 1, the following OCP is solved:

$$\boldsymbol{\tau}_{k+1} := \arg \min_{\boldsymbol{\tau}} \hat{\phi}^m(\boldsymbol{\tau}) + \bar{g}_k^{\phi}(\boldsymbol{\tau}) + r_k \sigma_{g,k}^{\phi}(\boldsymbol{\tau}), \quad (20a)$$

$$\text{s.t. } \hat{\psi}_j^m(\boldsymbol{\tau}) + \bar{g}_k^{\psi_j}(\boldsymbol{\tau}) + r_k \sigma_{g,k}^{\psi_j}(\boldsymbol{\tau}) \leq 0, \quad (20b)$$

$$j = 1, \dots, n_\psi, \quad (20b)$$

$$\bar{t}_{i-1} \leq \bar{t}_i, \quad i = 1, \dots, n_s + 1, \quad (20c)$$

$$\underline{u} \leq u_s^0 \leq \bar{u}, \quad (20d)$$

$$\underline{u} \leq u_s^0 + p_s (\bar{t}_s - \bar{t}_{s-1}) \leq \bar{u}, \quad s \in \mathcal{S}, \quad (20d)$$

$$\dot{\mathbf{z}}^m(t) = \tilde{\mathbf{f}}(\mathbf{z}^m(t)), \quad \mathbf{z}^m(t_0) = \mathbf{z}_0. \quad (20e)$$

The following theorem shows that, under some assumptions about the quality of the model used for the OCPs (5) and (20), the true system converges to its global optimum with a prespecified probability of constraint satisfaction.

*Theorem 1.* Suppose that the OCP (20) is solved at each iteration  $k$  of Algorithm 1. Assuming that the optimal arc sequence is the same for the model and the true system,  $g^{X*}(\boldsymbol{\tau})$  is sampled from the prior distribution of  $g_k^X(\boldsymbol{\tau})$ , and the points  $\boldsymbol{\tau}_1, \dots, \boldsymbol{\tau}_k$  are in the basin of attraction of a global optimum of the OCP (5) for the true system, then:

- (1) Each constraint  $\hat{\psi}_j^p(\boldsymbol{\tau}_{k+1}) \leq 0$ , for  $j = 1, \dots, n_\psi$ , is satisfied with a prespecified probability  $\Phi(r_k)$ .
- (2) The algorithm converges to a single point  $\boldsymbol{\tau}_\infty$  that is a global optimum of the OCP (5) for the true system.

**Algorithm 1:** Adaptive algorithm to solve the OCP (5) to global optimality for the true system in the presence of mismatch between the true system and its model.

- 1 Compute  $\boldsymbol{\tau}_1$ , the global solution to the OCP (5) for the model, and set the iteration  $k \leftarrow 1$ .
- 2 For each cost and constraint function, sample the mismatch  $g^{X*}(\boldsymbol{\tau})$  at the nominal point  $\boldsymbol{\tau} = \boldsymbol{\tau}_k^0 = \boldsymbol{\tau}_k$  and at the auxiliary points  $\boldsymbol{\tau} = \boldsymbol{\tau}_k^j$ , for  $j = 1, \dots, N$ , by measuring  $y_j^X(k)$ , for  $j = 0, \dots, N$ .
- 3 Use  $\mathbf{y}_k^X = [y_0^X(1) \cdots y_N^X(1) \cdots y_0^X(k) \cdots y_N^X(k)]^T$  and  $\mathbf{T}_k = (\mathbf{t}_k^1, \dots, \mathbf{t}_k^{(N+1)}) = (\boldsymbol{\tau}_1^0, \dots, \boldsymbol{\tau}_1^N, \dots, \boldsymbol{\tau}_k^0, \dots, \boldsymbol{\tau}_k^N)$  to compute the hyperparameters  $\hat{\boldsymbol{\eta}}_k^X$  according to Appendix A and to update the mean  $\bar{g}_k^X(\boldsymbol{\tau})$  and standard deviation  $\sigma_{g,k}^X(\boldsymbol{\tau}) := \sqrt{\Sigma_{g,k}^X(\boldsymbol{\tau}, \boldsymbol{\tau})}$  of each Gaussian process  $g_k^X(\boldsymbol{\tau})$  according to (16) and (17).
- 4 Compute  $\boldsymbol{\tau}_{k+1}$ , the solution to OCP (20).
- 5 Set the iteration  $k \leftarrow k + 1$  and return to Step 2.

**Proof.** Since the OCP (20) ensures that  $\hat{\psi}_j^m(\boldsymbol{\tau}_{k+1}) + \bar{g}_k^{\psi_j}(\boldsymbol{\tau}_{k+1}) + r_k \sigma_{g,k}^{\psi_j}(\boldsymbol{\tau}_{k+1}) \leq 0$ , for  $j = 1, \dots, n_\psi$ , and  $\hat{\psi}_j^m(\boldsymbol{\tau}) + \bar{g}_k^{\psi_j}(\boldsymbol{\tau}) + r_k \sigma_{g,k}^{\psi_j}(\boldsymbol{\tau})$  represents an upper bound for  $\hat{\psi}_j^p(\boldsymbol{\tau})$  with a probability  $\Phi(r_k)$  given that  $g^{X*}(\boldsymbol{\tau})$  is sampled from the prior distribution of  $g_k^X(\boldsymbol{\tau})$ , condition (1) holds.

To prove condition (2), we first prove that, if Algorithm 1 converges to a single point  $\boldsymbol{\tau}_\infty$ , then  $\boldsymbol{\tau}_\infty$  is a global optimum of the OCP (5) for the true system. Then, assume that Algorithm 1 converges to a single point  $\boldsymbol{\tau}_\infty$ . This implies that the algorithm evaluates the cost and constraint functions  $\hat{\chi}^p$  an arbitrarily large number of times, not only for  $\boldsymbol{\tau}_\infty$ , but also for the auxiliary points  $\boldsymbol{\tau}_\infty^j$ , for  $j = 1, \dots, N$ . From the properties of Gaussian processes, this implies that  $\bar{g}_\infty^X(\boldsymbol{\tau}_\infty) = g^{X*}(\boldsymbol{\tau}_\infty)$ ,  $\frac{\partial \bar{g}_\infty^X}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}_\infty) = \frac{\partial g^{X*}}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}_\infty)$ ,  $\sigma_{g,\infty}^X(\boldsymbol{\tau}_\infty) = 0$ ,  $\frac{\partial \sigma_{g,\infty}^X}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}_\infty) = 0$ , which in turn implies that  $\hat{\chi}_\infty^m(\boldsymbol{\tau}_\infty) = \hat{\chi}^p(\boldsymbol{\tau}_\infty)$ ,  $\frac{\partial \hat{\chi}_\infty^m}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}_\infty) = \frac{\partial \hat{\chi}^p}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}_\infty)$ , and  $\boldsymbol{\tau}_\infty$  is a KKT point of the OCP (20) for  $k \rightarrow \infty$  if and only if  $\boldsymbol{\tau}_\infty$  is a KKT point of the OCP (5) for the true system. However, since  $\boldsymbol{\tau}_\infty$  is the solution to the OCP (20) for  $k \rightarrow \infty$ ,  $\boldsymbol{\tau}_\infty$  is also a KKT point of the OCP (5) for the true system. Then, since the only KKT point of the OCP (5) for the true system that is in the basin of attraction of a global optimum of that OCP is the global optimum itself,  $\boldsymbol{\tau}_\infty$  is a global optimum of the OCP (5) for the true system.

Now we prove that Algorithm 1 converges to a single point  $\boldsymbol{\tau}_\infty$  by contradiction. Assume that Algorithm 1 converges to a periodic sequence of  $s$  points  $\boldsymbol{\tau}_{k+i}$ , for  $i = 1, \dots, s$ , for  $k \rightarrow \infty$ . As shown, for  $k \rightarrow \infty$ ,  $\hat{\chi}_\infty^m(\boldsymbol{\tau}_{k+i}) = \hat{\chi}^p(\boldsymbol{\tau}_{k+i})$ ,  $\frac{\partial \hat{\chi}_\infty^m}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}_{k+i}) = \frac{\partial \hat{\chi}^p}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}_{k+i})$ , and  $\boldsymbol{\tau}_{k+i}$  is a KKT point of the OCP (20) if and only if  $\boldsymbol{\tau}_{k+i}$  is a KKT point of the OCP (5) for the true system. However, since  $\boldsymbol{\tau}_{k+i}$  is a solution to the OCP (20) for  $k \rightarrow \infty$ ,  $\boldsymbol{\tau}_{k+i}$  is also a KKT point of the OCP (5) for the true system. Then, since only one KKT point of the OCP (5) for the true system is in the basin of attraction of a global optimum of that OCP, Algorithm 1 converges to a single point  $\boldsymbol{\tau}_\infty$ , which proves condition (2).

*Remark 1.* The assumption that the points  $\boldsymbol{\tau}_1, \dots, \boldsymbol{\tau}_k$  are in the basin of attraction of a global optimum of the OCP (5) for the true system required by Theorem 1 may not be easy to check. However, Theorem 1 provides sufficient conditions

for the model to ensure convergence of the true system to its global optimum: (i) the optimal arc sequence must be the same for the model and the true system; and (ii) the initial model specified by the cost and constraint functions  $\hat{\chi}^m(\boldsymbol{\tau})$  and the modified models specified by the functions  $\hat{\chi}_k^m(\boldsymbol{\tau})$  must be such that the global model optimum  $\boldsymbol{\tau}_1$  and the subsequent points  $\boldsymbol{\tau}_{k+1}$  are in the basin of attraction of a global optimum of the OCP (5) for the true system.

*Remark 2.* Although the addition of  $r_k \sigma_{g,k}^\phi(\boldsymbol{\tau})$  to the cost of the OCP (20) is not required for Theorem 1, this penalty term is useful to limit the exploration of points  $\boldsymbol{\tau}$  with a large uncertainty. This enables the implementation of an approach similar to a trust-region method, which has been shown to be beneficial for stochastic derivative-free optimization (Larson and Billups, 2016). However, instead of dedicated rules to update the trust region, the proposed adaptive algorithm uses the distribution of  $g_k^\phi(\boldsymbol{\tau})$  to implement an analogue of trust region. More precisely, it penalizes points  $\boldsymbol{\tau}$  depending on their distance to the sampled points  $\mathbf{T}_k$  and the length-scale hyperparameter  $\hat{\lambda}_k^\phi$ . In addition, with this penalty term, if the global model optimum  $\boldsymbol{\tau}_1$  is in the basin of attraction of a global optimum of the OCP (5) for the true system, the subsequent points  $\boldsymbol{\tau}_{k+1}$  are also more likely to be in that basin of attraction.

Another important advantage of the proposed adaptive algorithm is that it avoids the explicit estimation of the gradients of the cost and constraint functions of the true system with respect to the decision variables that is required by modifier adaptation. Nevertheless, the proposed approach still provides a way to account for the mismatch between the true system and the model. Moreover, as in the case of other methods to deal with model mismatch such as modifier adaptation, the proposed approach benefits from a small number of decision variables since the representation via Gaussian processes would be less accurate and more computationally involved for a high-dimensional domain.

## 5. NUMERICAL ILLUSTRATION

The simulation example corresponds to a problem of production maximization in an acetoacetylation reaction system with the species A, B, C, D, E (Rodrigues and Bonvin, 2020). This OCP is formulated mathematically with the states  $\mathbf{x}(t) := [\mathbf{x}_r(t)^T \ x_{in}(t)]^T$  as:

$$\max_{u_{in}(\cdot), t_f} \mathcal{J}(u_{in}(\cdot), t_f) = n_C(t_f), \quad (21a)$$

$$\text{s.t. } \mathcal{T}(u_{in}(\cdot), t_f) = \begin{bmatrix} n_B(t_f) - c_{B,max} V(t_f) \\ n_D(t_f) - c_{D,max} V(t_f) \\ t_f - t_{f,max} \end{bmatrix} \leq \mathbf{0}_3, \quad (21b)$$

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), u_{in}(t)) = \begin{bmatrix} \mathbf{r}_v(t) \\ \frac{u_{in}(t)}{1000} \end{bmatrix}, \quad \mathbf{x}(t_0) = \mathbf{0}_{R+1}, \quad (21c)$$

$$[u_{in}(t) - \bar{u}_{in} \ \underline{u}_{in} - u_{in}(t)]^T \leq \mathbf{0}_2, \quad (21d)$$

where  $\underline{u}_{in} = 0$ ,  $\bar{u}_{in} = 2 \text{ mL min}^{-1}$ ,  $t_{f,max} = 250 \text{ min}$ ,  $c_{B,max} = 0.025 \text{ mol L}^{-1}$ ,  $c_{D,max} = 0.15 \text{ mol L}^{-1}$ , the  $R = 3$  reaction rates are given by  $r_{v,1}(t) = k_1 \frac{n_A(t)n_B(t)}{V(t)}$ ,  $r_{v,2}(t) = k_2 \frac{n_B^2(t)}{V(t)}$ ,  $r_{v,3}(t) = k_3 n_B(t)$ , with rate constants  $k_1 = 0.053 \text{ L mol}^{-1} \text{ min}^{-1}$ ,  $k_2 = 0.128 \text{ L mol}^{-1} \text{ min}^{-1}$ ,  $k_3 = 0.028 \text{ min}^{-1}$ , the volume is given by  $V(t) = V_0 + x_{in}(t)$ , with  $V_0 = 1 \text{ L}$ , and the numbers of moles are

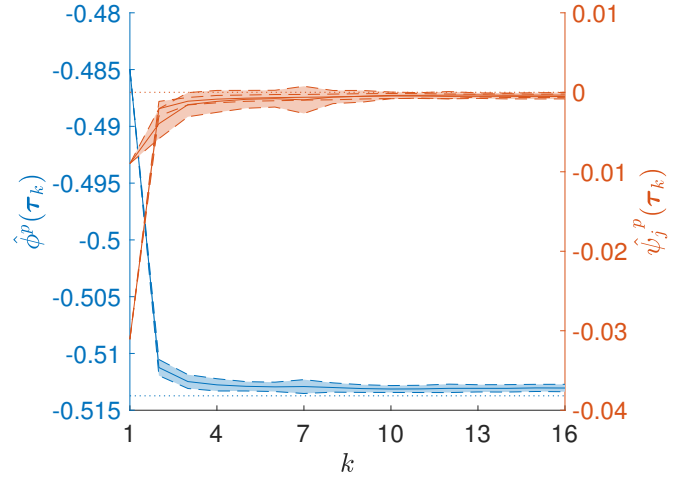


Fig. 1. Evolution of the cost (in blue) and constraints (in red) for the true system as a function of the iteration number  $k$  of the adaptive algorithm. Solid lines: mean over 50 realizations of measurement noise; dashed lines with shading in between: mean  $\pm$  standard deviation; dotted lines: optimal values.

given by  $\mathbf{n}(t) = \mathbf{N}^T \mathbf{x}_r(t) + \mathbf{c}_{in} x_{in}(t) + \mathbf{n}_0$ , with  $\mathbf{n}_1 = [-1 \ -1 \ 1 \ 0 \ 0]^T$ ,  $\mathbf{n}_2 = [0 \ -2 \ 0 \ 1 \ 0]^T$ ,  $\mathbf{n}_3 = [0 \ -1 \ 0 \ 0 \ 1]^T$ ,  $\mathbf{N} = [\mathbf{n}_1 \ \mathbf{n}_2 \ \mathbf{n}_3]^T$ ,  $\mathbf{c}_{in} = [0 \ 5 \ 0 \ 0 \ 0]^T \text{ mol L}^{-1}$ ,  $\mathbf{n}_0 = [0.72 \ 0.05 \ 0.08 \ 0.01 \ 0]^T \text{ mol}$ .

We illustrate the proposed adaptive approach to compute the global solution to the OCP for the true system. We assume that the knowledge of the true system dynamics is inaccurate, in the sense that the true values of the rate constants are  $k_1^p = 0.053 \text{ L mol}^{-1} \text{ min}^{-1}$ ,  $k_2^p = 0.128 \text{ L mol}^{-1} \text{ min}^{-1}$ , and  $k_3^p = 0.028 \text{ min}^{-1}$ , but their values in the model are  $k_1^m = 0.05 \text{ L mol}^{-1} \text{ min}^{-1}$ ,  $k_2^m = 0.12 \text{ L mol}^{-1} \text{ min}^{-1}$ , and  $k_3^m = 0.02 \text{ min}^{-1}$ .

Firstly, the global solution to the OCP is computed using the available model. This procedure yields the same optimal arc sequence as in Rodrigues and Mesbah (2022), that is, 1U-3-1L. However, in this case, the optimal values of the decision variables are  $\bar{t}_1^* = 5.56 \text{ min}$ ,  $\bar{t}_2^* = 225.45 \text{ min}$ ,  $t_f^* = 250 \text{ min}$ ,  $u_2^* = 1.129 \text{ mL min}^{-1}$ ,  $p_2^* = -1.16 \times 10^{-3} \text{ mL min}^{-2}$ . This corresponds to a worse cost  $n_C^*(t_f^*) = 0.48497 \text{ mol}$  and inactive and feasible constraints with  $n_B^*(t_f^*) - c_{B,max} V^*(t_f^*) = -0.00897 \text{ mol}$ ,  $n_D^*(t_f^*) - c_{D,max} V^*(t_f^*) = -0.03107 \text{ mol}$  for the true system, while the optimal cost for the true system would be  $n_C^*(t_f^*) = 0.51373 \text{ mol}$  and the constraints would be active. These values of the decision variables become the first point  $\boldsymbol{\tau}_1$  evaluated by Algorithm 1, from which the algorithm should converge to the true solution. To this end, the algorithm uses measurements of the cost and of the constraints corrupted by noise with variances  $\sigma_\phi^2 = 0.005^2 \text{ mol}^2$  and  $\sigma_{\psi_1}^2 = \sigma_{\psi_2}^2 = 0.001^2 \text{ mol}^2$ . At each iteration  $k$ , besides the nominal point  $\boldsymbol{\tau}_k$ ,  $N = 5$  auxiliary points  $\boldsymbol{\tau}_k^j$  are evaluated. The step away from each nominal point to obtain an auxiliary point corresponds to  $+10 \text{ min}$  for  $\bar{t}_1, \bar{t}_2, t_f$ ,  $+1 \text{ mL min}^{-1}$  for  $u_2^0$ , and  $+1 \times 10^{-3} \text{ mL min}^{-2}$  for  $p_2$ .

Fig. 1 shows the evolution of the cost and constraints for the true system over 50 realizations of measurement noise

using  $r_k = 2$ . The probability of satisfying each constraint  $\hat{\psi}_j^p(\tau_{k+1}) \leq 0$  is estimated from the frequency of satisfaction of the constraint if  $\hat{\psi}_j^p(\tau_k) \leq 0$ . This estimate equals 0.9717 and 0.9834 for  $j = 1, 2$ , while the theoretical value is  $\Phi(r_k) = 0.9772$ . The cost for the true system already approaches its optimal value for  $k = 2$ , while the constraints become nearly active. From  $k = 10$ , the cost and constraints for the true system become almost equal to their optimal values. The constraint violation remains under 0.0007 mol for all the realizations, which is comparable to the standard deviation of the measurement noise. This illustrative example shows that, despite the existence of measurement noise and the presence of parametric mismatch between the true system and its model, the adaptive algorithm enforces convergence of the true system to the global solution to the OCP with almost no constraint violation.

## 6. CONCLUSIONS

This paper presented an approach for obtaining adaptive global solutions to OCPs in the presence of mismatch between the true system and its model by using Gaussian processes to represent the mismatch in the cost and constraints for a given arc sequence. The proposed approach enables efficient solutions to OCPs for general nonlinear dynamical systems. The method for adaptive global solutions to OCPs has been detailed for the case of a single input. In future work, it would be useful to extend this method so as to provide such solutions in the case of multiple inputs and stochastic input disturbances.

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## Appendix A. ESTIMATION OF HYPERPARAMETERS FOR GAUSSIAN PROCESSES

The evidence  $p(\mathbf{y}_k^x | \boldsymbol{\eta}) := \int_{\mathcal{D}} p(\mathbf{y}_k^x | g_k^x) p(g_k^x | \boldsymbol{\eta}) d\boldsymbol{\tau}$  is the known function of the hyperparameters  $\boldsymbol{\eta}$  given by

$$p(\mathbf{y}_k^x | \boldsymbol{\eta}) = f(\mathbf{y}_k^x | \mathbf{0}_{k(N+1)}, \boldsymbol{\Sigma}_{\mathbf{y},k}^x(\boldsymbol{\eta})), \quad (\text{A.1})$$

where

$$\left( \boldsymbol{\Sigma}_{\mathbf{y},k}^x(\boldsymbol{\eta}) \right)_{i,j} = \sigma_x^2 (\mathbf{I}_{k(N+1)})_{i,j} + K_k^x(\mathbf{t}_k^i, \mathbf{t}_k^j | \boldsymbol{\eta}). \quad (\text{A.2})$$

To estimate the hyperparameters  $\boldsymbol{\eta}$  from  $\mathbf{y}_k^x$ , one can maximize  $p(\mathbf{y}_k^x | \boldsymbol{\eta})$  by solving the optimization problem

$$\begin{aligned} \hat{\boldsymbol{\eta}}_k^x &= \arg \min_{\boldsymbol{\eta}} - \frac{2}{k(N+1)} \log p(\mathbf{y}_k^x | \boldsymbol{\eta}) - \log(2\pi) \\ &= \arg \min_{\boldsymbol{\eta}} \frac{1}{k(N+1)} \|\mathbf{y}_k^x\|_{\boldsymbol{\Sigma}_{\mathbf{y},k}^x(\boldsymbol{\eta})^{-1}}^2 + \frac{\log \det(\boldsymbol{\Sigma}_{\mathbf{y},k}^x(\boldsymbol{\eta}))}{k(N+1)}, \end{aligned} \quad (\text{A.3})$$

which is nonconvex but involves only few hyperparameters.