12th IFAC International Symposium on
Advanced Control of Chemical Processes
July 14-17, 2024. Toronto, Canada

# Applying Sampling-Based Convex Relaxations to Dynamic Process Models ⋆

**Ho-Ching Chui** * **Kamil A. Khan** *

* *McMaster University, Hamilton, ON, Canada (e-mail: kamilkhan@mcmaster.ca).*

**Abstract:** Convex relaxations are a crucial tool in methods for global optimization, but are challenging to construct for dynamic processes. In this article, we investigate combining two recent approaches for convex relaxation generation in new nontrivial ways, to aid global optimization of dynamic chemical process models. Specifically, we combine recent approaches for automatically generating convex relaxations for solutions of parametric ordinary differential equations with a recent sampling-based approach for tractably generating lower bounds of a convex relaxation.

*Keywords:* Reachability analysis; Convex relaxations; Dynamics and control.

## 1. INTRODUCTION

Dynamic global optimization problems arise in applications such as safety verification, where we seek to verify that safety constraints are met for all realizations of uncertain parameters in a chemical process model. Typical deterministic branch-and-bound-based approaches for global minimization proceed by generating upper and lower bounds on the globally optimal value, and then refining these bounds. In this case, upper bounds are typically furnished by local minimization, while lower bounds are furnished by first generating a *convex relaxation* of the original problem, and then minimizing this relaxation (Tawarmalani and Sahinidis, 2002). Methods for global optimization thus benefit from having access to correct convex relaxations that are cheap to construct and evaluate, while staying close enough to the original system to provide useful bounding information.

However, dynamic global optimization remains difficult. While global optimization of a nonlinear program is already NP-hard, dynamic global optimization has the added complication that the system states are not available in closed-form, but may only be accessed by simulating a process model. Recent advances in convex relaxation generation (Scott and Barton, 2013; Song and Khan, 2022) apply to solutions of ordinary differential equations (ODEs), and ultimately construct useful convex relaxations that are themselves solutions of auxiliary ODEs. Hence, generating lower bounds for global optimization using these relaxation approaches nominally requires solving many of these auxiliary ODEs during the progress of a local minimization method. Outside the context of global optimization, convex relaxations for ODEs are also useful in reachability analysis.

Recent work by Song et al. (2021) shows that useful lower bounds may be generated for a convex function of $n$ variables by sampling the function $(2n+1)$ times, and arranging the results in a new tractable finite-difference formula. We expect that this approach could be deployed in dynamic global optimization, to reduce the number of ODE solves required for each lower bound computation. This article investigates how this deployment would proceed in practice, since there are nontrivial decisions to be made when combining the approaches of Song et al. (2021) and Scott and Barton (2013).

## 2. PROBLEM FORMULATION

Throughout this document, inequalities involving vectors are to be understood to apply to each component simultaneously. Let $P \subset \mathbb{R}^{n_p}$ be an interval of the form $P = \{\mathbf{p} \in \mathbb{R}^{n_p} : \mathbf{p}^{\mathrm{L}} \leq \mathbf{p} \leq \mathbf{p}^{\mathrm{U}}\}$. We consider the dynamic optimization problem:

$$\min_{\mathbf{p}\in P} J(\mathbf{p}), \tag{1}$$

where the objective function $J$ is defined in terms of a known cost function $g : \mathbb{R}^{n_p} \times \mathbb{R}^{n_x} \to \mathbb{R}$:

$$J(\mathbf{p}) := g(\mathbf{p}, \mathbf{x}(t_f, \mathbf{p})),$$

where $\mathbf{x}$ denotes the solution on $I : [0, t_f] \to \mathbb{R}^{n_x}$ of the following parametric system of ordinary differential equations:

$$\dot{\mathbf{x}}(t,\mathbf{p}) = \mathbf{f}(t,\mathbf{p},\mathbf{x}(t,\mathbf{p})), \qquad \mathbf{x}(0,\mathbf{p}) = \mathbf{x}_0(\mathbf{p}). \tag{2}$$

We suppose that the functions $g$, $\mathbf{f} : \mathbb{R} \times \mathbb{R}^{n_p} \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_x}$, and $\mathbf{x}_0 : \mathbb{R}^{n_p} \to \mathbb{R}^{n_x}$ are available in closed-form, as continuously-differentiable finite compositions of the smooth operations available on a scientific calculator. This type of assumption is standard in interval analysis (Moore et al., 2009), automatic differentiation (Griewank and Walther, 2008), and global optimization (Tawarmalani and Sahinidis, 2002). The objective function $J$ is thus continuously differentiable as well, but is not assumed to be convex.

We suppose that we seek to solve the problem (1) to global optimality by a branch-and-bound-based approach.

⋆ This work was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) under Grant RGPIN-2017-05944.

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Thus, as a critical subproblem in this approach, we seek to evaluate a useful lower bound $J^{\mathrm{L}}$ for which

$$J^{\mathrm{L}} \leq J(\mathbf{p})$$

for each $\mathbf{p} \in P$. If this can be accomplished for each choice of interval subdomain $P$, then branch and bound can proceed.

Since a convex function may be minimized with a local nonlinear programming (NLP) solver, one way to construct $J^{\mathrm{L}}$ is by minimizing a *convex relaxation* of $J$ on $P$; that is, a convex function $J^{\mathrm{cv}}$ for which

$$J^{\mathrm{cv}}(\mathbf{p}) \leq J(\mathbf{p})$$

for each $\mathbf{p} \in P$. Hence, we also seek useful new convex relaxations $J^{\mathrm{cv}}$ of $J$.

Nontrivial constraints may also be added to the optimization problem (1), and are compatible with the approaches considered here, but we neglect these for simplicity.

## 3. BACKGROUND

This article essentially combines two recent numerical methods concerning convex relaxations for process models. These methods are summarized here for convenience.

### 3.1 Convex Relaxations of Parametric ODE Solutions

Scott and Barton (2013) proposed an approach for generating convex and concave relaxations of each state variable $x_i$ of the ODE (2) with respect to $\mathbf{p}$; we briefly summarize it here.

This method requires access to *state bounds* of $\mathbf{x}$; namely functions $\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}} : I \to \mathbb{R}^{n_x}$ for which

$$\mathbf{x}^{\mathrm{L}}(t) \leq \mathbf{x}(t, \mathbf{p}) \leq \mathbf{x}^{\mathrm{U}}(t)$$

for each $t \in I$ and $\mathbf{p} \in P$. It also requires convex and concave relaxations $\mathbf{x}_0^{\mathrm{cv}}, \mathbf{x}_0^{\mathrm{cc}} : P \to \mathbb{R}^{n_x}$ of the initial-value function $\mathbf{x}_0$. Then, Scott and Barton construct the auxiliary coupled ODE:

$$\begin{aligned}
\dot{\mathbf{x}}^{\mathrm{cv}}(t, \mathbf{p}) &= \mathbf{f}^{\mathrm{SB,cv}}(t, \mathbf{p}, \mathbf{x}^{\mathrm{cv}}(t, \mathbf{p}), \mathbf{x}^{\mathrm{cc}}(t, \mathbf{p}); \mathbf{x}^{\mathrm{L}}(t), \mathbf{x}^{\mathrm{U}}(t)), \\
\dot{\mathbf{x}}^{\mathrm{cc}}(t, \mathbf{p}) &= \mathbf{f}^{\mathrm{SB,cc}}(t, \mathbf{p}, \mathbf{x}^{\mathrm{cv}}(t, \mathbf{p}), \mathbf{x}^{\mathrm{cc}}(t, \mathbf{p}); \mathbf{x}^{\mathrm{L}}(t), \mathbf{x}^{\mathrm{U}}(t)), \\
\mathbf{x}^{\mathrm{cv}}(0, \mathbf{p}) &= \mathbf{x}_0^{\mathrm{cv}}(\mathbf{p}), \qquad \mathbf{x}^{\mathrm{cc}}(0, \mathbf{p}) = \mathbf{x}_0^{\mathrm{cc}}(\mathbf{p}),
\end{aligned}$$

where $\mathbf{f}^{\mathrm{SB,cv}}$ and $\mathbf{f}^{\mathrm{SB,cc}}$ are automatically constructed as flattened *generalized McCormick relaxations* (Scott et al., 2011) of $\mathbf{f}$. This coupled ODE has a unique solution $(\mathbf{x}^{\mathrm{cv}}, \mathbf{x}^{\mathrm{cc}})$, for which, at each fixed $t \in I$, $\mathbf{x}^{\mathrm{cv}}(t, \cdot)$ is a convex relaxation of $\mathbf{x}(t, \cdot)$ on $P$, and $\mathbf{x}^{\mathrm{cv}}(t, \cdot)$ is an analogous concave relaxation. Scott and Barton refer to such functions $\mathbf{x}^{\mathrm{cv}}$ and $\mathbf{x}^{\mathrm{cc}}$ as *state relaxations* of $\mathbf{x}$.

A more recent approach by Song and Khan (2022) generates alternative state relaxations by instead constructing the functions $\mathbf{f}^{\mathrm{SB,cv}}$ and $\mathbf{f}^{\mathrm{SB,cc}}$ above as optimal-value functions involving convex/concave relaxations of the original ODE right-hand side function $\mathbf{f}$.

In either of these approaches, evaluating a state relaxation at one value of $\mathbf{p}$ requires solving an ODE system with twice as many state variables as (2). With state relaxations available, a convex relaxation $J^{\mathrm{cv}}$ of $J$ in (1) may be constructed as a McCormick composition:

$$\begin{aligned}
J^{\mathrm{cv}}(\mathbf{p}) := g^{\mathrm{GM,cv}}(&(\mathbf{p}, \mathbf{p}, \mathbf{p}^{\mathrm{L}}, \mathbf{p}^{\mathrm{U}}), \\
&(\mathbf{x}^{\mathrm{cv}}(t_f, \mathbf{p}), \mathbf{x}^{\mathrm{cc}}(t_f, \mathbf{p}), \mathbf{x}^{\mathrm{L}}(t_f), \mathbf{x}^{\mathrm{U}}(t_f))),
\end{aligned} \tag{3}$$

where $g^{\mathrm{GM,cv}}$ is a generalized McCormick relaxation of the cost function $g$. Hence, each evaluation of $J^{\mathrm{cv}}$ requires a separate evaluation of the state relaxations at time $t_f$.

### 3.2 Sampling-Based Convex Relaxations

In global optimization, obtaining a lower bound from a nonlinear convex relaxation traditionally involves either minimizing that relaxation with a local NLP solver, or evaluating a subgradient of this relaxation and minimizing the corresponding "subtangent". Theoretical convergence results by Khan (2018) show that the latter approach is viable and effective whenever subgradients are available and the original problem is sufficiently smooth.

On the other hand, Song et al. (2021) proceeded without access to subgradient information, and showed that, given a convex function $h^{\mathrm{cv}}$ on an interval $P := [\mathbf{p}^{\mathrm{L}}, \mathbf{p}^{\mathrm{U}}] \subset \mathbb{R}^{n_p}$, an affine underestimator $h^{\mathrm{aff}}$ of $h^{\mathrm{cv}}$ may be tractably generated by sampling $h^{\mathrm{cv}}$ $(2n_p + 1)$ times, and then tractably assembling the sampled information as follows. For notational simplicity, suppose that $P$ has nonempty interior, so that $\mathbf{p}^{\mathrm{L}} < \mathbf{p}^{\mathrm{U}}$.

The sampling approach of Song et al. (2021) may be summarized as follows. For each $i \in \{1, \ldots, n_p\}$, let $\mathbf{e}^{(i)}$ denote the $i^{\mathrm{th}}$ unit coordinate vector in $\mathbb{R}^{n_p}$, and choose some $\alpha_i \in (0, 1]$. Define:

- the midpoint $\mathbf{p}^{(0)} := \frac{1}{2}(\mathbf{p}^{\mathrm{L}} + \mathbf{p}^{\mathrm{U}})$ of $P$,
- perturbations $\mathbf{p}^{(\pm i)} := \mathbf{p}^{(0)} \pm \frac{\alpha_i}{2}(p_i^{\mathrm{U}} - p_i^{\mathrm{L}})\, \mathbf{e}^{(i)}$, for each $i \in \{1, \ldots, n_p\}$,
- associated sampled function values $y_0 := h^{\mathrm{cv}}(\mathbf{p}^{(0)})$ and $y_{\pm i} := h^{\mathrm{cv}}(\mathbf{p}^{(\pm i)})$, for each $i$,
- a vector $\mathbf{b} \in \mathbb{R}^{n_p}$ for which, for each $i$,
$$b_i := \frac{y_{+i} - y_{-i}}{\alpha_i(p_i^{\mathrm{U}} - p_i^{\mathrm{L}})},$$
- and a scalar:
$$c := y_0 - \frac{1}{2} \sum_{i=1}^{n_p} \left( \frac{y_{+i} + y_{-i} - 2y_0}{\alpha_i} \right).$$

Then, for each $\mathbf{p} \in P$,

$$h^{\mathrm{cv}}(\mathbf{p}) \geq c + \mathbf{b}^{\mathrm{T}}(\mathbf{p} - \mathbf{p}^{(0)}) =: h^{\mathrm{aff}}(\mathbf{p}).$$

If a constant lower bound of $h^{\mathrm{cv}}$ is desired, then the affine underestimator $h^{\mathrm{aff}}$ is trivially minimized on $P$, and Song et al. (2021) obtain a closed-form expression for the lower bound thus obtained. With

$$h^{\mathrm{L}} := y_0 - \sum_{i=1}^{n_p} \left( \frac{\max(y_{+i}, y_{-i}) - y_0}{\alpha_i} \right),$$

we have $h^{\mathrm{cv}}(\mathbf{p}) \geq h^{\mathrm{L}}$ for each $\mathbf{p} \in P$.

In the case where $h^{\mathrm{cv}}$ is itself a convex relaxation of some function $h$, then Song et al. (2021) showed that $h^{\mathrm{aff}}$ preserves certain tightness properties of the original relaxation $h^{\mathrm{cv}}$.

If a function $f$ is concave, then the mapping $\mathbf{x} \mapsto -f(\mathbf{x})$ is convex. Hence, the above approaches may also be used to obtain affine overestimators or constant upper bounds of concave functions on box domains.

## 4. SYNTHESIZING RECENT APPROACHES

A lower bound on the optimal value of the NLP (1) may be computed as the optimal value of the convex NLP:

$$\min_{\mathbf{p}\in P} J^{\mathrm{cv}}(\mathbf{p}), \tag{4}$$

with $J^{\mathrm{cv}}$ given by (3).

During this bound evaluation process, our sampling-based affine relaxations may in principle be combined with the Scott-Barton ODE relaxations in several ways; we develop some of these here. Dynamic systems were not directly considered by Song et al. (2021).

Firstly, by evaluating the Scott-Barton ODE relaxations $(2n_p+1)$ times, we may automatically construct sampling-based affine underestimators $\mathbf{x}^{\mathrm{aff,cv}}$ of $\mathbf{x}^{\mathrm{cv}}(t_f,\mathbf{p})$ with respect to $\mathbf{p}$ on $P$, simultaneously with affine overestimators $\mathbf{x}^{\mathrm{aff,cc}}$ of $\mathbf{x}^{\mathrm{cc}}(t_f,\mathbf{p})$ with respect to $\mathbf{p}$. This approach has the advantage that it only requires these $(2n_p+1)$ ODE solves, whereas applying an NLP solver to minimize $J^{\mathrm{cv}}$ given by (3) would require many more ODE solves. Once these $(2n_p+1)$ ODE solves are complete, then with the sampled information, the $\mathbf{x}^{\mathrm{cv}}$ and $\mathbf{x}^{\mathrm{cc}}$ terms in (3) may be replaced with their affine counterparts $\mathbf{x}^{\mathrm{aff,cv}}(t_f,\mathbf{p})$ and $\mathbf{x}^{\mathrm{aff,cc}}(t_f,\mathbf{p})$, at which point the bounding convex NLP (4) no longer has any embedded ODEs, and is now simply a straightforward convex NLP. In particular, if the cost function $g$ were convex quadratic, then this approach would effectively replace (4) with a convex quadratic program that is efficiently solved to yield a valid lower bound on (1).

Secondly, and independently of the previous consideration, the convex relaxation $J^{\mathrm{cv}}$ may itself be sampled $(2n_p+1)$ times, to compute a lower bound of $J$ on $P$ according to the sampling-based procedure of Song et al. (2021). This circumvents the need for local optimization when evaluating a lower bound.

An analogous optimization-free lower bound could be generated by applying interval analysis to $g$, to propagate lower/upper bounds of $\mathbf{x}(t_f,\mathbf{p})$ on $\mathbf{p}\in P$ through to lower/upper bounds of $J$ on $P$. This approach, however, would lead to lower bounds that converge relatively slowly as $P$ shrinks (Wechsung et al., 2014), which are undesirable in global optimization. We nevertheless consider this approach as well in our numerical examples, for comparison.

Whenever the sampling-based methods are deployed above, they bring the downside that they are typically less tight than the original relaxations that were sampled in their construction. Essentially, they trade relaxation tightness for savings in computational cost, by either vastly reducing the number of ODE solves required, or replacing ODE-constrained NLPs with simpler convex NLPs that are efficiently solved by off-the-shelf solvers. Depending on the original problem's structure and the way in which we deploy sampling-based methods, we may even obtain convex quadratic programs (QPs) or linear programs (LPs), which are efficiently solved virtually regardless of problem size. Moreover, it is argued by Song et al. (2021) via a rigorous convergence analysis that the sampling-based relaxations are still tight enough to be useful in global optimization.

Other combinations of these approaches are possible as well, and are currently under investigation.

## 5. IMPLEMENTATION AND EXAMPLES

### *5.1 Implementation in Julia*

The approaches described in the previous section were implemented directly in the programming language Julia v1.9. In this implementation, our own package ConvexSampling.jl was used to automatically construct sampling-based affine relaxations of convex functions, McCormick.jl (Wilhelm and Stuber, 2020) was used to build generalized McCormick relaxations of composite functions, and DifferentialEquations.jl (Rackauckas and Nie, 2017) was used to solve ODEs. Interval bounds were constructed with IntervalArithmetic.jl (Sanders and Benet, 2014), and state bounds $(\mathbf{x}^{\mathrm{L}},\mathbf{x}^{\mathrm{U}})$ were constructed by implementing an approach by Harrison et al. (1977), as was previously considered by Scott and Barton (2013).

Whenever lower bounds were computed by minimizing nonlinear convex relaxations, this was accomplished using the optimization solver IPOPT (Wächter and Biegler, 2006) in JuMP (Lubin et al., 2023).

### *5.2 Example 1*

Consider intervals $P := [5,12] \subset \mathbb{R}$ and $I := [0,0.1] \subset \mathbb{R}$, and the dynamic optimization instance:

$$\begin{aligned}\min_{p\in P}\ & 0.8(x_1(0.1,p))^2 + 0.8(x_2(0.1,p)+0.1)^2 \\ & + p(x_1(0.1,p)+x_2(0.1,p)),\end{aligned}$$

where $\mathbf{x} \equiv (x_1,x_2)$ solves the following parametric ODE system:

$$\begin{aligned}\dot{x}_1 &= 0.01p(x_1+x_2),\\ \dot{x}_2 &= (p-25)x_1 - 0.25x_2,\\ x_1(0,p) &= 2.8+\tfrac{p}{3},\\ x_2(0,p) &= 3.2+\tfrac{p}{3}.\end{aligned}$$

Corresponding convex relaxations and lower bounds for the objective function of this instance are illustrated in Figure 1. The entries in these plots' legends are as follows, and reflect the various relaxation combinations explained previously:

- $J$: the objective function of the dynamic optimization instance (as in (1)), presented for comparison.
- $J^{\mathrm{cv}}$: a convex relaxation of $J$ on $P$, generated by composing Scott-Barton state relaxations of $\mathbf{x}$ with generalized McCormick relaxations of the cost function $g$ (as in (3)), presented for comparison.
- $J^{\mathrm{cv}}_{\mathrm{affine}}$: a new convex relaxation of $J$ on $P$, similar to $J^{\mathrm{cv}}$, except that the Scott-Barton state relaxations have been sampled and replaced with sampling-based relaxations.
- $J^{\mathrm{L}}$: a lower bound of $J$, constructed using interval arithmetic during one evaluation of $J^{\mathrm{cv}}$, presented for comparison.
- $J^{\mathrm{L}}_{\mathrm{min}}$: a lower bound of $J$, constructed by using the NLP solver IPOPT to minimize $J^{\mathrm{cv}}$ from (3), presented for comparison.

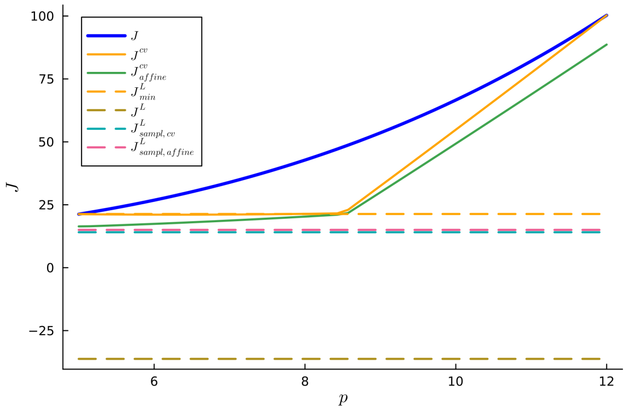


Fig. 1. Various convex relaxations and lower bounds for the dynamic optimization problem in Section 5.2. The various relaxation types are explained in the body text.

- $J^{\mathrm{L}}_{\text{sampl, cv}}$: a new lower bound on $J$, constructed by tractably sampling $J^{\mathrm{cv}}$ and constructing a sampling-based lower bound, without using an NLP solver at any point.
- $J^{\mathrm{L}}_{\text{sampl,affine}}$: a new lower bound on $J$, constructed by tractably sampling $J^{\mathrm{cv}}_{\text{affine}}$ and constructing a sampling-based lower bound, without using an NLP solver at any point.

In this case, computing $J^{\mathrm{L}}_{\min}$ via IPOPT took 20 solver iterations, each requiring ODE solves; the other methods do not require NLP solvers. The value of $J^{\mathrm{L}}$ was $-36.2$, well below the other relaxations and bounds computed. These results indicate that for this particular dynamic optimization instance, applying the sampling-based relaxations only makes the resulting relaxations of $J$ a little less tight, while significantly reducing the number of ODE solves required. Since there is only one parameter, each application of the sampling-based approach requires three samples of the underlying convex function.

### 5.3 *Example 2*

Consider intervals $P := [5, 12] \subset \mathbb{R}$ and $I := [0, 0.1] \subset \mathbb{R}$, and the dynamic optimization instance:

$$\min_{p\in P} 0.5p(-2x_1(0.1,p) - x_2(0.1,p) + (x_1(0.1,p))^2),$$

where $\mathbf{x} \equiv (x_1, x_2)$ solves the following parametric ODE system:

$$\begin{aligned}\dot{x}_1 &= 0.01p(x_1 + x_2),\\ \dot{x}_2 &= (p - 25)x_1 - 0.25x_2,\\ x_1(0,p) &= 2.8 + \tfrac{p}{3},\\ x_2(0,p) &= 3.2 + \tfrac{p}{3}.\end{aligned}$$

Observe that the embedded ODE here is retained from the previous example, but the optimization problem's cost function is different.

Corresponding convex relaxations and lower bounds for this instance are illustrated in Figure 2, with the same notation as the previous example. Here, IPOPT took 20 iterations to compute $J^{\mathrm{L}}_{\min}$.

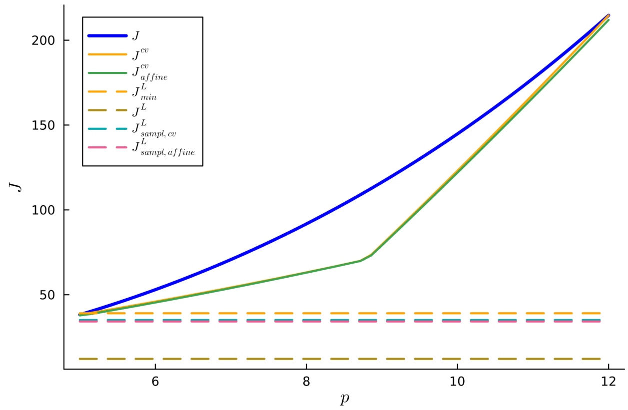


Fig. 2. Various convex relaxations and lower bounds for the dynamic optimization problem in Section 5.3. The various relaxation types are explained in the body text.

### 5.4 *Example 3*

Consider a variant of a setup previously considered by Scott et al. (2011), with intervals $P := [0.01, 0.5] \subset \mathbb{R}$ and $I := [0, 0.1] \subset \mathbb{R}$, and the dynamic optimization instance:

$$\min_{p\in P} 5x_1(0.1,p) + 0.2((x_2(0.1,p))^2 + 2.5(x_1(0.1,p))^3) + 0.3px_2(0.1,p),$$

where $\mathbf{x} \equiv (x_1, x_2)$ solves the following parametric ODE system:

$$\begin{aligned}\dot{x}_1 &= (p - \tfrac{p^3}{3})x_1x_2,\\ \dot{x}_2 &= x_1^3 - p,\\ x_1(0,p) &= 1.0,\\ x_2(0,p) &= 0.0.\end{aligned}$$

Corresponding convex relaxations and lower bounds for this instance are illustrated in Figure 3, with the same notation as the previous example. In this case, when we attempted to use IPOPT to compute $J^{\mathrm{L}}_{\min}$, the solver terminated with an error without producing a solution. As in (Song and Khan, 2022), we suspect that having ODE initial conditions independent of $\mathbf{p}$ might have contributed to this IPOPT error, since the Scott-Barton ODE relaxations depend almost negligibly on $\mathbf{p}$ for $t \approx 0$ in this case. We note that our new bounding approaches were unaffected by this issue, since they do not require solving any NLPs.

## 6. CONCLUSION AND OUTLOOK

Though the considered optimization instances are small, these numerical results illustrate the potential applicability of sampling-based affine relaxations within a procedure for generating convex relaxations of dynamic process models. These two approaches have been combined here for the first time, with the impact of significantly reducing the number of ODE solves required when computing useful lower bounds.

Future work will involve applying these approaches to larger instances, and considering other potentially effective

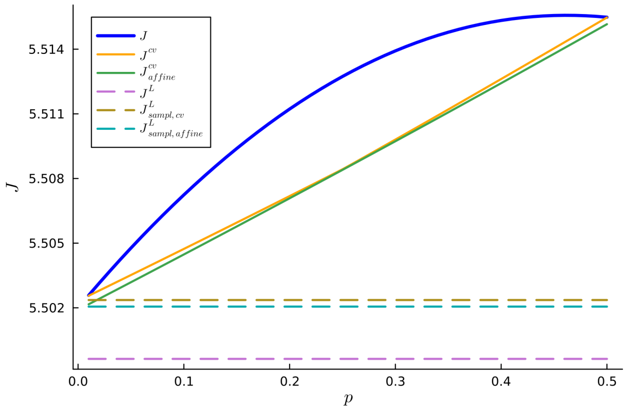


Fig. 3. Various convex relaxations and lower bounds for the dynamic optimization problem in Section 5.4. The various relaxation types are explained in the body text.

configurations of recent relaxation approaches for dynamic process models.

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