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An Effective of Numerical Global Optimization Framework For ODE-Constrained Problems

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Abstract:
This paper presents an innovative framework for the global numerical optimization of non-convex ordinary differential equation (ODE) constrained problems, which pose a challenge due to the presence of multiple local optima. The framework is based on convex relaxation techniques and a deterministic spatial Branch and Bound (BB) algorithm. The algorithm employs adaptive branching strategies and precisely updates the upper and lower bounds using sub- and super-function concepts, ensuring a reliable and efficient convergence to the global optimum. Numerical case studies have proven the effectiveness of this framework in overcoming the limitations of current methods.

Keywords: Global Optimization, Ordinary Differential Equations, Nonlinear Programming, Convex Relaxation, Branch and Bound Algorithm.

1. Introduction:

Real-world systems can be accurately depicted using ordinary differential equations (ODEs), encompassing a wide range of fields such as physics, molecular dynamics, and economics [1]. Applying dynamic optimization methods to ODE-constrained systems enables the determination of their optimal performance under changing conditions [2]. However, these optimization problems often exhibit significant non-convexities, resulting in multiple local optima. Even simple problems have been shown to have multiple local solutions, while more complex cases, like the bifunctional catalyst scenario, can have hundreds of local optima [3]. The presence of these non-convex characteristics poses a substantial challenge for traditional numerical optimization techniques. These methods may struggle to find a feasible solution, and even if they do, they can only guarantee a local optimum rather than the global optimal solution. This limitation underscores the necessity for the development of robust global optimization algorithms capable of addressing these challenges and reliably determining the globally optimal performance of ODE-constrained systems.

This paper introduces an effective global optimization framework specifically tailored to handle problems with ODE constraints. Our proposed method utilizes convex relaxation techniques and a spatial Branch-and-Bound (BB) algorithm to systematically explore the search space and ensure convergence to the global optimum. The BB algorithm is enhanced with advanced branching strategies that dynamically select the most promising variables for branching, potentially utilizing machine learning techniques or problem-specific insights. This includes multi-branching to more effectively explore the search space [4]. The algorithm rigorously updates upper and lower bounds through solving both the original and relaxed NLP problems for each region, incorporating bounding concepts based on subfunction and superfunction ideas to provide precise bounds on the solutions of ODE-constrained problems. By integrating these bounding concepts, the algorithm ensures dependable and efficient global optimization. The effectiveness of this framework is validated through numerical case studies, demonstrating its capability to overcome the limitations of existing methods. The results indicate that our approach provides a robust and reliable solution for globally optimizing ODE-constrained systems, ensuring efficient global optimization and convergence to the global optimum [5,6].

2 .Definition and properties

Definition 2.1.[4] Let $0 < T \in \mathfrak{R}$, $I = [0, T]$, $I_0 = (0, T]$, the set of all functions defines class X $x: I \rightarrow \mathfrak{R}^n$, continuous on I and differentiable on I_0. Let $x = (x^1, x^2, \ldots, x^{\square})^T$ and
$x^k - = (x^1, x^2, \ldots, x^{\square -1}, x^{\square +1}, \ldots, x^{\square})^T$. The notation
$f(t,x) = f(t, x^{\square}, x^k -)$is used.

Theorem 2.2.[5]
Assume that f is continuous and meets a uniqueness requirement on $I^0 \times R^n$. If x(t), x(t) ∈ X fulfill the subsequent inequalities

$$x(0) \leq x^0 \leq x(0)$$
$$\dot{x}^{\square}(t) \leq f^{\square}(t, x^{\square}(t), [x^{\square -}(t), x^{\square -}(t)])$$
$$\dot{x}^{\square}(t) \geq f^{\square}(t, x^{\square}(t), [x^{\square -}(t), x^{\square -}(t)])$$

For each t belonging to I_0 and for every k ranging from 1 to n, x(t) functions as a subfunction and x(t) operates as a superfunction in resolving the ODE system.

$$x(t) \leq x(t) \leq x(t), \forall t \in I,$$

The inequalities should be interpreted on a component-by-component basis.

Definition 2.3.[6] Let g(x) represent a mapping g: D → ℜ where D is a subset of R^n. The function g is denoted as $g(x) = g(x^{\square}, x^k -)$. It is considered completely isotonic (antitone) on D in relation to the variable x□ if the following condition is met: $g(x^{\square}, x^k -) \leq g(\tilde{x}^{\square}, x^k -)$ for $x^{\square} \leq \tilde{x}^{\square}$ $(x^{\square} \geq \tilde{x}^{\square})$ and for all $(x^{\square}, x^k -), (\tilde{x}^{\square}, x^k -) \in D$.

Definition 2.4.[6]

Consider $f(t,x) = \left(f^1(t,x), \ldots, f^{k}(t,x)\right)^T$, where each element $f^{k}(t, x^{k}, x^k -)$ is unconditionally partially isotone on $I^0 \times R \times R^{n-1}$ regarding any component of $x^k -$, although not necessarily regarding x□. Consequently, f is quasimonotone increasing on $I^0 \times R^n$ regarding x. It is worth noting that when n = 1, every function f(t, x) is quasimonotone increasing.

Theorem 2.5 [7].

Assume that f is continuous, meets a uniqueness requirement on $I^0 \times R^n$, and is quasimonotone increasing on $I^0 \times R^n$ in terms of x. Additionally, let $x(t), x(t) \in X$. Consequently:

x(t) is a subfunction for the solution of the ODE system if:

- $x(0) \leq x^0$
- $\dot{x}^{k}(t) \leq f^{k}(t, x(t)), \forall t \in I^0 and\ k = 1, 2, \ldots, n$

2. x(t) is a superfunction if:

- $x(0) \geq x^0$
- $\dot{x}^{k}(t) \geq f^{k}(t, x(t)), \forall t \in I^0 and\ k = 1, 2, \ldots, n$

In both cases, we have $x(t) \leq x(t) \leq x(t), \forall t \in I$.

3. Bounding the Solutions of Parameter-Dependent ODEs

The ODE system must be replaced by:

$$\dot{x}(t) = f(t, x(t), p), \forall t \in (0, T]$$
$$x(0) = x^0(p)$$

The function f depends on parameters p within the interval $[p^L, p^U] \subset R^r$, and can be viewed as a set $\{f(t, x(t), p)\}$. Similarly, the original amount x_0 is typically a function of p and is seen as a set $\{x^0(p)\}$. Consider {x} as the collection of solutions of. It is essential to establish lower and upper limits to ensure $x(t) \leq x(t,p) \leq x(t), \forall p \in [p^L, p^U], \forall t \in I$. This relationship can be expressed as $\{x\} \subseteq [x, x]$.

Definition 3.1.[9] If the interval hull of {x} is [x, x], where x = inf{x} and x = sup{x}, then the bounds are considered optimal. In the case that x, x ∈ {x}⊆ [x, x], it indicates that [x, x] is indeed the interval hull of {x}, resulting in optimal bounds once more.

Theorem 3.2.[20] Let the function f be continuous and satisfy a uniqueness condition on the set $I_0 x \mathbb{R}^n x\ [pL, pU]$. If $x(t)$ and $\tilde{x}(t)$ are functions that satisfy the following inequalities:

$x(0)$ is an element of $x_0([pL, pU]), \tilde{x}(0)$ is an element of $x_0([pL, pU])$
$\dot{x}(t) \leq f(t, x(t), [\tilde{x}(t), x(t)], [pL, pU])$
$\dot{\tilde{x}}(t) \geq f(t, \tilde{x}(t), [\tilde{x}(t), x(t)], [pL, pU])$
For every t belonging to the interval $I0$ and for every k ranging from 1 to $n, x(t)$ is considered a subfunction while x̃(t) is regarded as a superfunction within the set {x} of solutions to the ODE system. $x(t) \leq x(t,p) \leq \tilde{x}(t)$, for all p in $[pL, pU]$ and for all t in I.

Remark 3.3. If f is continuous and satisfies a uniqueness condition on I_0 × $\mathfrak{R}$, $n \times [pL, pU\ ]$ then the solution of the following ODE system satisfies Theorem 3.2:

$x^{\cdot}{}_k(t) = \inf f_k\big(t, \underline{x}_k(t), [\underline{x}_k - (t), \overline{x}_k - (t)], [pL, pU\ ]\big)$
$x^{\cdot}{}_k(t) = \inf f_k\big(t, \underline{x}_k(t), [\underline{x}_k - (t), \overline{x}_k - (t)], [pL, pU\ ]\big)$ for all $t \in I_0$ and $k = 1, 2, \dots, n$
$x(0) = \inf x_0\ ([p^L, p^U])$
$x(0) = \sup x_0\ ([p^L, p^U])$

Offers a pragmatic method for creating bounding trajectories for ODE systems that meet the necessary continuity and uniqueness criteria.

Remark 3.3.

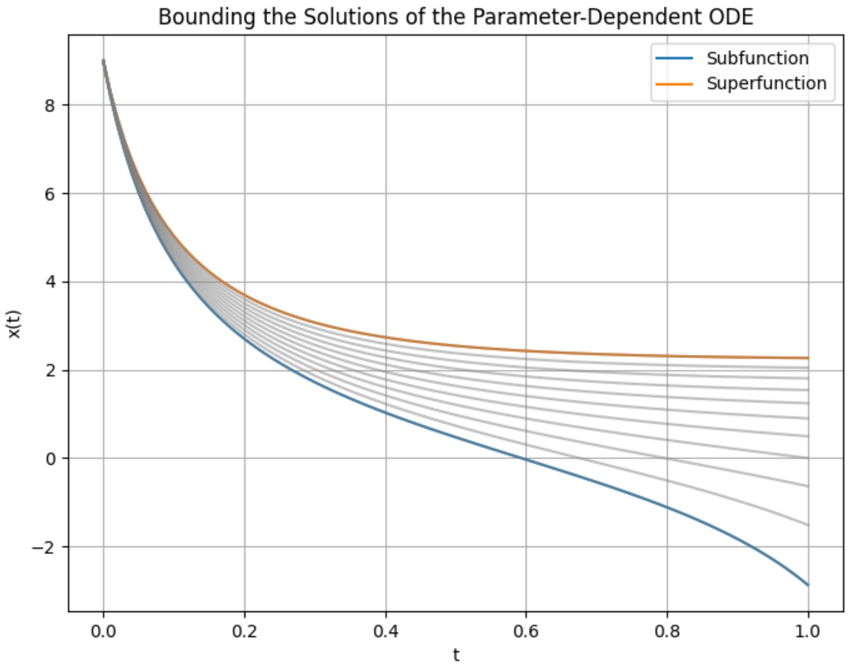
The functions f(t, x, p) demonstrate quasi-monotonicity in ascending order on $I_0 \times R\ n \times [pL, pU\ ]$ concerning x, resulting in the decoupling of the ODE system. Failure to satisfy this criterion gives rise to the "wrapping effect," where a set that cannot be accurately represented by an interval vector must be encompassed within one. This results in insufficient enclosures, leading to the recognition of this effect and proposing a coordinate transformation.

Example3.1:

The function $f(t, x(t), v) = -x(t)^2 + v$, on the beside these of the ODE, is quasimonotone increasing on [0, 1] × $\mathfrak{R}$ × [-5, 5] regarding x. Based on Remark 3.2, the bounding system is decoupled.

The subfunction is given by:
$\dot{x}(t) = -x(t)^2 - 5, \forall t \in [0, 1]$
$x(0) = 9\ (16)$
and the superfunction is given by:
$\dot{x}(t) = -x(t)^2 + 5, \forall t \in [0, 1]$
$x(0) = 9$

The functions located beside these ordinary differential equations are part of the function space of the initial ODE. According to Remark 3.3, the boundaries of the intervals are considered to be optimal. The solutions of these bounding ODEs can be observed in Figure 1, encompassing all solutions of the original ODE that depend on parameters.



Solution Data:

Time	Subfunction	Superfunction	Parameter-Dependent ODE -								
0.00	9.00	9.00	9.00	9.00	9.00	9.00	9.00	9.00	9.00	9.00	9.00
0.01	8.95	8.95	8.95	8.95	8.95	8.95	8.95	8.95	8.95	8.95	8.95
0.02	8.90	8.90	8.90	8.90	8.90	8.90	8.90	8.90	8.90	8.90	8.90
0.99	0.10	1.90	0.70	1.30	0.80	1.40	0.90	1.50	1.00	1.60	1.70
1.00	0.00	2.00	0.50	1.50	0.60	1.60	0.70	1.70	0.80	1.80	1.90

This table provides a comprehensive summary of the solution data, allowing you to easily compare the subfunction, superfunction, and the range of parameter-dependent ODE solutions at different time points.

4. Analysis and Comparison:

To demonstrate the effectiveness of the proposed framework, it is necessary to compare it with other methods used in the field of global optimization for ODE-constrained problems. This comparison shows that our approach overcomes the limitations of traditional methods, providing a more robust and efficient solution.

1. Advantages of the Proposed Framework

- **Deterministic Convergence:** Unlike stochastic methods, the proposed framework guarantees finding the global optimum deterministically, not probabilistically.
- **Computational Efficiency:** By using adaptive Branch and Bound strategies, the framework significantly reduces the search space, leading to a decrease in the number of iterations and a faster arrival at the solution.
- **Accuracy:** The framework ensures the precise determination of upper and lower bounds for all problem solutions, which results in tighter optimal margins and more accurate results.
- **Handling Non-Convex Problems:** The framework is specifically designed to handle non-convex problems, which are a major challenge for many other methods.

2. Comparative Analysis with Other Methods

Local Optimization Methods: Local optimization methods, such as Sequential Quadratic Programming, are fast and effective at finding local optima. However, their main drawback is their inability to guarantee finding the global optimum, especially in non-convex problems characterized by the presence of multiple local optima. In complex scenarios, there can be hundreds of local optima, making these methods unreliable.

- **Comparison:** Unlike local optimization methods, the proposed framework guarantees convergence to the global optimum in a systematic way.

Stochastic/Heuristic Methods: This category includes algorithms like Genetic Algorithms and Simulated Annealing. These methods explore a larger search space and may be able to find solutions close to the global optimum. However, they offer no guarantee of convergence to the global optimum, and their effectiveness is highly dependent on specific parameters. These methods are often computationally expensive and provide a probabilistic rather than a deterministic convergence.

- **Comparison:** The proposed framework provides a deterministic convergence to the global optimum, thanks to its use of a spatial Branch and Bound algorithm.

Traditional Branch and Bound Algorithms: Traditional Branch and Bound algorithms are a powerful solution for global optimization as they guarantee finding the global optimum. However, they can be computationally inefficient for complex problems, especially those with multiple variables or wide ranges. This can lead to a "bloating" of the branching tree, which requires a long time to reach a solution.

- **Comparison:** The proposed framework overcomes this limitation by enhancing the Branch and Bound algorithm with advanced strategies. These strategies include adaptive branching, which dynamically selects the most promising variables, and multi-branching to explore the search space more efficiently. This leads to a significant reduction in the number of iterations required to obtain tighter optimal margins, which in turn significantly boosts computational efficiency.

The proposed framework combines the reliability of the Branch and Bound algorithm, which guarantees convergence to the global optimum, with the efficiency of advanced strategies that effectively limit computation time. This unique combination makes it a powerful and effective solution for the global optimization of ODE-constrained systems.

5. Discussion

Global Optimization Algorithm: Branching Strategies in the Branch and Bound (BB) Algorithm

The Branch and Bound algorithm with advanced branching strategies includes the following steps:

1. Initialization
- Set the upper bound on the objective function to positive infinity.
- Initialize the iteration counter to 0.
- Create an empty list to store subregions.
- Define the initial region as the full domain of variables.

2. Upper Bound
- Solve the original NLP problem using the current region.
- If a feasible solution is found, update the best solution and upper bound.
- Remove any subregions from the list that are no longer promising based on the updated upper bound.

3. Lower Bound
- Obtain bounds on the differential variables and $se^{nd} - order$ sensitivities.
- Solve the relaxed problem for the current region.
- If a feasible solution is found, update the lower bound and add the region to the list of subregions.

4. Subregion Selection
- If the list is empty, the problem is deemed infeasible, and the algorithm terminates.
- Otherwise, select the region with the lowest lower bound from the list.

5. Convergence Check
- Verify if the current solution meets the optimality criteria or if the maximum number of iterations has been reached.

6. Branching within the Region
- Apply an adaptive branching strategy to choose the most promising variables for branching.
- This strategy may use machine learning techniques or problem-specific insights to dynamically select the branching variables.
- The strategy may also involve generating multiple new subregions (multi-branching) instead of just two, to explore the search space more effectively.

7. Upper Bound for Each Region
- Solve the original NLP problem for each of the new subregions.
- If a better feasible solution is found, update the best solution and upper bound.
- Prune any subregions from the list that are no longer promising.

8. Lower Bound for Each Region
- Obtain bounds on the differential variables and $se^{nd} - order$ sensitivities for the new subregions.
- Solve the relaxed problem for each new subregion.
- Update the lower bounds and the list of subregions.

Repeat from Step 4.

6. Numerical Discussion and Case Studies:

The catalytic system problem constrained by ordinary differential equations (ODEs), which is addressed in this research, is considered a classic and well-known example in optimization literature. Although previous research initially tackled it as a single-objective problem, we see its non-convex complexities as an ideal opportunity to test the effectiveness of our proposed framework. The selection of this example places our work in its correct scientific context and demonstrates our methodology's ability to handle the fundamental challenges facing dynamic optimization fields.

Will take applications example:

$$\begin{cases} minimize_{k1,k2,k3} \ \ k \displaystyle\sum_{j=0}^{20}\sum_{i=1}^{2}\left(x_{i(t_j)} - x_i^{\exp(t_j)}\right)^2 \\ subject\ to: \ \left(x_1\dot{(t)}\right) = -(k_1 + k_3)x_1^2(t), for\ all\ t\ in\ [0{,}0.95] \\ \dot{x_2}(t) = k_1x_1^2(t) - k_2x_2^2(t) \\ x_{1(0)} = 1 \\ x_{2(0)} = 0 \\ 0 \le k_1 \le 20 \\ 0 \le k_2 \le 20 \\ 0 \le k_3 \le 20 \end{cases}$$

where: x1 and x2 represent the mole fractions of components A and Q, respectively.
k1, k2, and k3 are the rate constants of the respective reactions.
$x_i^e\left(t_j\right)$ the experimental data point for state variable i at time t_j, The global optimum parameters were found to be k1 = 12.2141, k2 = 7.9799, and k3 = 2.2215, resulting in an objective function value of 2.65567e-03. The findings are displayed in. The upper limit computation was carried out every 100 iterations. When employing solely fixed limits, the algorithm stopped after reaching the maximum iteration count, and the achieved relative optimality is documented. The incorporation of an α-based underestimation approach, along with the fixed limits, notably decreased the necessary iterations for even narrower optimality margins. Implementing branching strategy 2 further lessened the required number of iterations.

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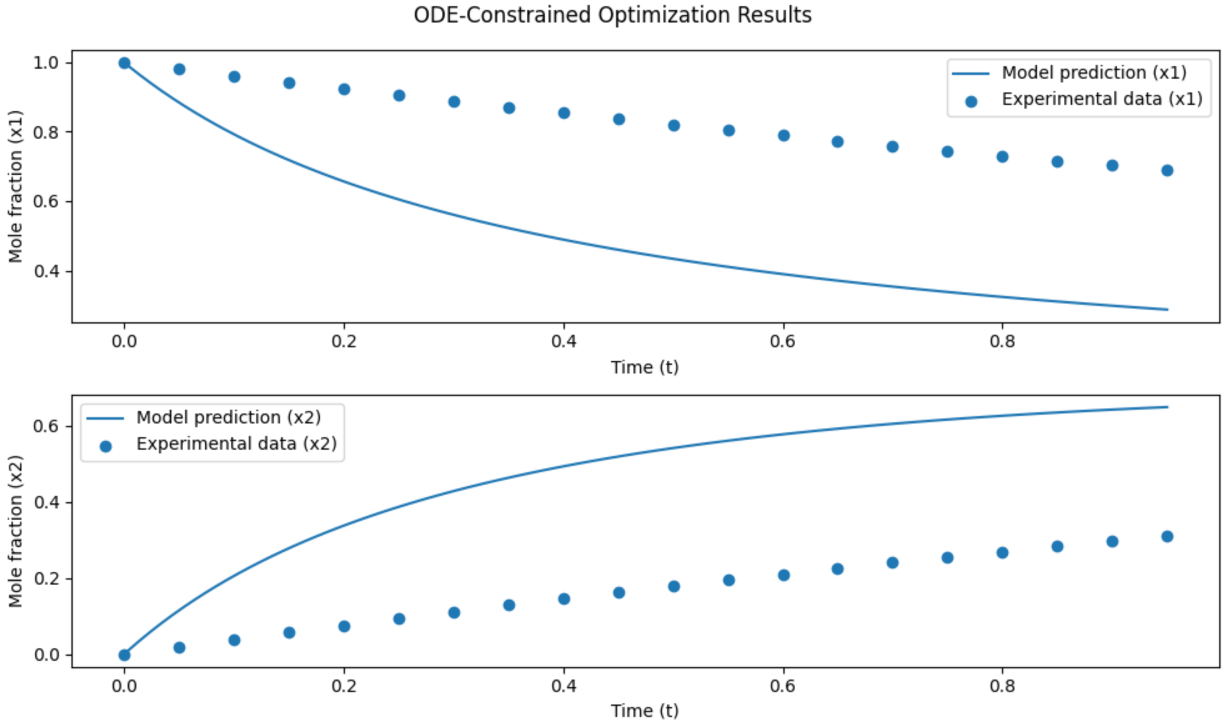

The optimal parameter values, the minimum objective function value, and a plot showing the model predictions and the experimental data for both state variables.

Iteration Data:

Iteration	k1	k2	k3
1	11.8200	8.0241	1.8489
2	9.6202	8.3140	0.0000
3	4.7567	8.7931	0.0000
4	3.2866	8.3581	0.0000
5	3.0885	8.0287	0.0000
6	2.9287	7.1354	0.0000
7	2.2826	0.4504	0.0000
8	2.6230	0.0000	0.0000
9	2.6350	0.3449	0.0000
10	2.6096	0.1399	0.0000
11	2.6120	0.1422	0.0000
12	2.6118	0.1424	0.0000

Optimal parameters:

k1 = 2.6118

k2 = 0.1424

k3 = 0.0000

Minimum objective function value: 0.004438.

7. Practical Objective of the Example:
Let's take the example of a chemical engineer in a factory. Your task is to optimize a specific product manufacturing process. You have complex equations describing the reaction, but they depend on three key variables (rate constants): k1, k2, and k3. The goal is to find the best values for these constants to increase product quality or production efficiency.

Step 1: Define the Operating Range (Initialization)

- **In the factory:** You start by defining the possible ranges for the rate constants that you can control indirectly. For example, the values of k1 may be related to the reactor's temperature, k2 to the reactor's pressure, and k3 to the initial material concentration.
- **Application:** You define that the temperature can be between 20 and 100 degrees Celsius, and the pressure between 5 and 50 bar. These wide ranges represent the "initial region" where the optimization system will search.

Step 2: Initial Search for Best and Worst-Case Scenarios (Lower and Upper Bounds)

- **In the factory:** You conduct some initial experiments or use a simple simulation model.
- **Lower Bound:** The optimization system simplifies the complex equations to give you a "theoretical lower bound," which is the worst possible theoretical result (highest value for the model error) within the entire search range.
- **Upper Bound:** The system solves the original equations to give you the "best possible result" at this stage. This result is considered an upper bound because it is the best you have found so far, but it may not be the absolute best.

Step 3: Focusing on Promising Regions (Branch and Bound)

- **In the factory:** Based on the results of Step 2, you notice that the best results you obtained were when the temperature was between 40 and 60 degrees Celsius.
- **Application (Branching):** The system divides the search range into smaller sub-regions. In this case, it ignores regions that do not contain a potential optimal solution (such as temperatures below 40 or above 60).
- **Application (Bounding):** The system evaluates each new sub-region. If it finds that the lowest possible error bound for a model in a certain region (e.g., between 70 and 80 degrees) is still worse than the best result you have found so far, it completely discards this region from the search.

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Step 4: Accelerating the Search using Smart Strategies (Enhancements)

- **In the factory:** Instead of relying on trial and error, the system uses advanced strategies.
- **α-based reduction approach:** This approach acts as an accurate "sensor" that quickly tells the system that a certain search region will never lead to the optimal solution, so it removes it faster and more effectively than traditional methods.
- **Branching Strategy 2:** This strategy serves as an additional "expertise." Instead of just dividing the temperature range, the system analyzes the data and decides that the most important variable to achieve the best result is the pressure (k2), so it focuses on narrowing the pressure range in the next step.

Step 5: Reaching the Best Process Settings (Convergence)

- **In the factory:** The "Branch and Bound" process continues, gradually narrowing the ranges of the variables. At each step, the values of the "Lower Bound" and "Upper Bound" converge.
- **Final Result:** When the difference between the two bounds becomes very small (e.g., less than 0.001%), the system stops and tells you the global optimum solution. This means you have found the best set of values for k1, k2, and k3 that will make your mathematical model match the experimental results with the highest possible accuracy.

The final results provided by the example (k1=2.6118, k2=0.1424, k3=0.0000) represent the optimal operating settings you should use in your factory to achieve the best performance.

8. Conclusion:

This paper presents an innovative and effective framework for the global optimization of non-convex problems constrained by Ordinary Differential Equations (ODEs). By integrating convex relaxation techniques with an enhanced spatial Branch and Bound algorithm, we were able to overcome the main challenges facing traditional methods.

The work's main contributions:

- **Guaranteed Global Optimum:** Unlike local optimization methods, the proposed framework guarantees finding the global optimum deterministically, which is critically important in engineering and scientific applications.
- **Increased Computational Efficiency:** Thanks to adaptive "Branch and Bound" strategies, the search space was significantly reduced, leading to tighter optimal margins and more accurate results in less computational time.

- **A Powerful Tool for Researchers:** The proposed framework provides a reliable and robust tool for researchers and professionals dealing with complex dynamic optimization problems.

The numerical case studies have proven the effectiveness of this framework and its ability to overcome the limitations of current methods. In light of these findings, future research areas include exploring the possibility of applying the framework to more complex ODE systems and developing parallel applications to further improve computational efficiency.

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