The Use of Lipschitz Constants in Experimental Optimization

Citation for published version:

Link:
Link to publication record in Edinburgh Research Explorer

Published In:
Journal of Process Control

General rights
Copyright for the publications made accessible via the Edinburgh Research Explorer is retained by the author(s) and/or other copyright owners and it is a condition of accessing these publications that users recognise and abide by the legal requirements associated with these rights.

Take down policy
The University of Edinburgh has made every reasonable effort to ensure that Edinburgh Research Explorer content complies with UK legislation. If you believe that the public display of this file breaches copyright please contact openaccess@ed.ac.uk providing details, and we will remove access to the work immediately and investigate your claim.
The Use of Lipschitz Constants in Experimental Optimization

Gene A. Bunin\textsuperscript{a*}, Gréory François\textsuperscript{b}

\textsuperscript{a}Tuanjie Road, Fourth North Alley 86, Urumqi, Xinjiang Uyghur Autonomous Region, People’s Republic of China 830001
\textsuperscript{b}Institute for Materials and Processes, School of Engineering, The University of Edinburgh, Edinburgh EH9 3FB, UK

Abstract

Given a certain response surface function, its Lipschitz constants may be defined as the limits on its largest derivatives (sensitivities), and as such provide important information about the function’s behavior. In this paper, it is argued that the explicit use of these constants may prove useful in the domain of experimental optimization. Most notably, it is shown that they offer a simple and robust way of rigorously guaranteeing constraint satisfaction, but may also be exploited to remove suboptimal portions of the decision-variable space, to filter out noise/error from the obtained experimental measurements, and to serve as regularizing bounds in the experimental derivative estimation problem. Because the constants are often conservative, a number of performance-improving refinements are outlined. Finally, some techniques for estimating the constants in practice are proposed.

Keywords: Lipschitz constants, upper-bounding functions, experimental optimization, process constraints, real-time optimization

1. Introduction: Experimental Optimization and Lipschitz Constants

Let the function $f_p : \mathbb{R}^n \rightarrow \mathbb{R}$ denote an experimental relationship between the decision-variable vector, $\mathbf{u} \in \mathbb{R}^n$, and an experimental output quantity, $y$:

$$y = f_p(\mathbf{u}),$$

where the qualifier “experimental” implies that evaluating the corresponding $y$ for a given $\mathbf{u}$ requires carrying out a physical experiment that cannot be performed solely with a computer – i.e., the evaluation intrinsic to $f_p$ is defined as being a physical act and not a series of numerical computations.
Such relationships appear virtually everywhere in the sciences (Montgomery, 2012), with systematic studies that attempt to discover the nature of some particular \( f_p \) dating very far back – a notable example is John Lind’s 1747 study of scurvy patients (Dunn, 1997). The most influential early work on quantitatively identifying \( f_p \) is arguably that of Ronald Fisher, with his work on the design of experiments (Fisher, 1935) containing many concepts that are still in use today.

In many cases, simply identifying an experimental relationship is not the end goal, as one is often searching to manipulate experimental conditions in such a way so as to obtain the “best” response while satisfying a number of safety or physical restrictions. In such scenarios, the following experimental optimization problem usually arises:

\[
\begin{align*}
\text{minimize} \quad & \phi_p(u) \\
\text{subject to} \quad & g_{p,j}(u) \leq 0, \quad j = 1, \ldots, n_g \\
& g_j(u) \leq 0, \quad j = 1, \ldots, n_g \\
& u^L_i \leq u_i \leq u^U_i, \quad i = 1, \ldots, n_u,
\end{align*}
\]

with \( \phi : \mathbb{R}^{n_u} \to \mathbb{R} \) denoting the cost function to be minimized, the functions \( g : \mathbb{R}^{n_u} \to \mathbb{R} \) denoting the \( n_g + n_p \) constraints, and the constants \( u^L_i, u^U_i \) denoting the lower and upper limits on the decision variables, respectively. The subscript \( p \) denotes explicitly those relationships that are experimental in nature, while its absence indicates that the function is numerical and only requires a computer or basic algebra to evaluate.

Problem (1) is a canonical form originally proposed in Bunin et al. (2014c), and is employed here as it is both convenient and general, encompassing a number of practical engineering problems (Bunin, 2016b). In fact, many of the oft-encountered design or recipe problems traditionally solved by the response-surface methodology (Myers et al., 2009) – as well as steady-state real-time optimization (Brdys & Tatjewski, 2005; Chen & Joseph, 1987; Quelhas et al., 2013), batch-process optimization (Costello et al., 2011; François et al., 2005; Georgakis, 2009), and iterative controller tuning (Bunin et al., 2013b; Hjalmarsson et al., 1998; Killingsworth & Krstić, 2006) problems – may be cast and solved in this form. Because the experimental functions \( \phi_p \) and \( g_{p,j} \) are essentially unknown, solving (1) entails running a series of experiments at \( u_0, u_1, \ldots, u_k \) with each new experiment chosen, in the general case, via some algorithmic function of the previously applied \( u \) and the corresponding function values:

\[
u_{k+1} = \Gamma \left( u_0, u_1, \ldots, u_k, \phi_p(u_0), \phi_p(u_1), \ldots, \phi_p(u_k), \\
g_{p,1}(u_0), g_{p,1}(u_1), \ldots, g_{p,1}(u_k), \\
\vdots \\
g_{p,n_p}(u_0), g_{p,n_p}(u_1), \ldots, g_{p,n_p}(u_k) \right),
\]

where \( \Gamma \) is the particular algorithm applied. Throughout this paper, the index \( k \) will be used to denote the latest experimental iteration.
The seminal paper with regard to solving experimental optimization problems is due to Box & Wilson (1951), where \( \Gamma \) essentially takes the form of a standard gradient-based descent method. Numerous other methods (\( \Gamma \)) and frameworks have also been proposed in various domains since (Bunin et al., 2014c, §2). In the present work, we explore a single facet of Problem (1) that may improve the solution procedure significantly, but which has not received much attention – that of the experimental functions’ Lipschitz constants. These constants, denoted here by \( \kappa \), will be implicitly defined by the inequalities

\[
-\kappa_i \leq \frac{\partial f_p}{\partial u_i} \mid_{u_i} \leq \kappa_i, \quad \forall u_i \in I,
\]

for the general experimental function \( f_p \), with \( I = \{ u_i : u_i^L \leq u_i \leq u_i^U, \quad i = 1, \ldots, n_u \} \) denoting the experimental space. Similar notations will be used for the optimization problem functions \( \phi_p \) and \( g_{p,j} \), with \( \kappa_{\phi,i} \) and \( \kappa_{p,ji} \) denoting their Lipschitz constants, respectively. Throughout this work, it will be assumed that these constants exist – i.e., that the experimental-function derivatives can be bounded. From a mathematical perspective, it is sufficient to assume that \( \phi_p \) and \( g_{p,j} \) are continuously differentiable for this to be the case, and our empirical experience suggests that such an assumption is not unreasonable for many, if not most, practical problems.

The mathematical meaning of these constants is thus straightforward – they are nothing but “\( I \)-global” bounds on the magnitudes of the derivatives of the functions. In more engineering-oriented language, they may be thought of as the maximal sensitivities of the experimental quantities with respect to individual changes in the decision variables, and are essentially the answers to the question: “If the variable \( u_i \) were changed by such-and-such amount, what is the greatest possible change that would be seen in such-and-such experimental quantity?”

As might be expected, there are many useful things that one can do with such knowledge. Namely, the Lipschitz constants \( \kappa \) may be used to:

- provide rigorous conditions to guarantee that a certain decision-variable set \( u \) will not violate the problem constraints (Bunin et al., 2014c; 2011; Jun et al., 2015),
- remove from consideration those parts of the experimental space where a solution of (1) cannot lie (Bunin et al., 2014a, §3.4),
- help filter out the uncertainty due to noise or error from the experimental measurements of \( \phi_p \) and \( g_{p,j} \) (Bunin et al., 2014a, §4.3),
- improve the quality of experimental derivative estimates (Bunin et al., 2013a, 2012; Serralunga et al., 2013).

Despite these potential benefits, the use of these constants in the experimental optimization setting is not standard practice and is fairly under-researched – of the work cited above, much is unpublished, while in the rest the usefulness of the constants is mentioned briefly or in passing. In the numerical optimization
context, Lipschitz constants have seen more use, but usually either as (a) conceptual stepping blocks in proving the convergence of a given algorithm (Boyd & Vandenberghe, 2008, §9) (Fletcher, 1987, §3) (Conn et al., 2000, §11) or (b) coefficients of bounding linear functions in Lipschitz global optimization (Cartis et al., 2014; Strongin, 1973) (Horst et al., 1995, §5).

It is the authors’ opinion that these constants can and should be a natural part of the design and thought process when approaching experimental optimization problems, and that they should be incorporated explicitly into the relevant algorithms whenever possible. The first half of this paper details this argument by illustrating the prominent role of the constants as constraint-satisfaction guarantors (Section 2) and their less prominent – though nevertheless useful – roles in experimental-space reduction, noise/error removal, and derivative estimation (Section 3). Multiple case studies, taken from the first author’s ExpOpt database of test problems (Bunin, 2016b), are used to demonstrate the points in realistic – albeit simulated – conditions. The second half of the paper then seeks to address the constants’ potential pitfalls – namely, the conservatism that may result in slow optimization and the fundamental issue of actually choosing and setting the constants. In particular, Section 4 presents to the reader some refinements that may partially remove the conservatism by exploiting direction, locality, and convexity properties, while Section 5 proposes several techniques for obtaining estimates of the Lipschitz constants and then refining these estimates during the optimization procedure. Some concluding remarks wrap up the paper in Section 6.

We emphasize that the contribution of the present work is intended to be tutorial and organizational in nature, and will not focus much on the proofs and derivations of the stated results, largely in the interest of space. The reader interested in the relevant mathematical details is referred to the cited references.

2. Experimental-Constraint Satisfaction Guarantees

The issue of satisfying the experimental constraints, \( g_{p,j}(u) \leq 0 \), at all of the experiments is one that is usually overlooked in the literature. In considering three large domains where the solution of (1) has been addressed – those of derivative-free, response-surface, and real-time optimization – one observes the following:

- derivative-free optimization (DFO) methods, developed mostly by the mathematical community and often dealing with numerical optimization problems, only take precautions against constraints asymptotically – i.e., they ensure, usually via penalty-function methods, that \( u_k \) satisfies the constraints as \( k \to \infty \) (Biegler et al., 2014; Liuzzi et al., 2010) (Conn et al., 2000, §14);
- response-surface optimization (RSO) methods often deal with experimental systems and are used in a wide number of fields (Myers et al., 2009), but neither do they address the problem of constraint satisfaction
during the experiments used to construct the response-surface model, nor do they rigorously attack the potential issue of the model optimum violating the constraints (Michaels & Pengilly, 1963; Umland & Smith, 1959);

- real-time optimization (RTO), as typically done in the chemical-engineering community (Chachuat et al., 2009; Darby et al., 2011), is arguably the most concerned with consistent constraint satisfaction, since \( g_{p,j}(u) > 0 \) may represent a dangerous or economically disastrous operating regime; however, while both theoretical and practical methods have been developed for promoting the satisfaction of constraints, the former are often too complex and restrictive while the latter suffer from a lack of rigorous guarantees, with both types of methods tending to find solutions that are significantly suboptimal because of conservatism (Quelhas et al., 2013).

In this section, we will address those problems where rigorous experimental-constraint satisfaction is highly desired, and as such we will examine what the Lipschitz-constant approach offers with respect to the methods already proposed in the literature. Namely, we will restrict ourselves to the RTO literature, as both DFO and RSO methods make no attempt at constraint satisfaction for all experiments. The satisfaction of the numerical constraints \( g_j(u) \leq 0 \) and \( u_i^L \leq u_i \leq u_i^U \) will not be discussed as this is relatively trivial, and one can simply do the numerical work before running the experiment to see if these restrictions are met or not.


One very simple and traditional approach (Govatsmark & Skogstad, 2005; Loeblein & Perkins, 1998; Loeblein et al., 1999) for satisfying the experimental constraints in RTO has been to add positive safety “back-offs” \( b \) to the optimization problem, with the problem constraints becoming

\[
g_{p,j}(u) + b_{p,j} \leq 0, \quad j = 1, \ldots, n_g.
\]

The constraints (3) are then used in place of \( g_{p,j}(u) \leq 0, \quad j = 1, \ldots, n_g \) in (1), and any algorithm or method that is employed to solve (1) now solves it with these tighter constraints instead. The logic is simple: by staying further away from the original constraints, one is less likely to violate them. However, rigorously setting proper back-off values is hardly trivial, as it requires accounting for a number of unknown components (Loeblein & Perkins, 1998) and ultimately introduces conservatism into the solution of (1), since one may not be able to converge to the optimum of the problem when this optimum happens to be on one of the original constraint boundaries (Quelhas et al., 2013). An ad hoc alternative is to simply set the \( b \) values by employing some heuristics or intuitive guesses, but this retains the issue of conservatism and ultimately offers no real guarantees of constraint satisfaction.
Another method involves employing stochastic-optimization tools, which require one to have *parametric models* of the experimental constraint functions (Zhang et al., 2002). The model $g_{p,j}(\mathbf{u}, \theta)$ – where $\hat{p}$ denotes the model nature of the function and $\theta$ the vector of uncertain parameters – then acts as the parametric approximation of $g_{p,j}(\mathbf{u})$. Additionally, it is assumed that one has knowledge of the uncertainty distributions of $\theta$, thus making it possible to pose chance constraints of the form

$$P(g_{\hat{p},j}(\mathbf{u}, \theta) \leq 0) \geq \alpha, \quad j = 1, ..., n_{g_p},$$

(4)

with $\alpha$ being a lower limit on the acceptable probability (e.g., 0.9 or 0.95). These constraints are then used as surrogates for $g_{p,j}(\mathbf{u}) \leq 0, \quad j = 1, ..., n_{g_p}$ in (1), and no experiment $\mathbf{u}$ failing to satisfy (4) is run, with the expectation that

$$P(g_{\hat{p},j}(\mathbf{u}, \theta) \leq 0) \geq \frac{1}{1 - \alpha} \Rightarrow g_{p,j}(\mathbf{u}) \leq 0$$

with a probability of at least $\frac{1}{1 - \alpha}$. In many ways, this second approach is similar to setting a robust back-off as discussed by Loeblein & Perkins (1998) – in fact, Loeblein & Perkins (1998) require much of the same information, such as the model and the parametric uncertainty distributions. The difference is that the back-offs are *implied* in the stochastic-optimization approach, rather than being set explicitly. Like the back-off method, this approach also suffers from conservatism, but additionally requires that a “sufficiently good” parametric model be available and that the nature of the uncertainty of the parameters be known. Numerical difficulties may arise since ensuring (4) may be very computationally intensive, especially when there are many constraints and parameters (Quelhas et al., 2013).

2.2. Lipschitz Bounds for Satisfying Experimental Constraints

With access to the experimental constraints’ Lipschitz constants, one has a brutally simple, yet rigorous, method for guaranteeing their satisfaction without employing any back-offs. The key idea lies in the recognition that the constants of (2) give rise to the following inequalities:

$$f_{\hat{p}}(\mathbf{u}_a) - \sum_{i=1}^{n_u} \kappa_i |u_{b,i} - u_{a,i}| \leq f_{\hat{p}}(\mathbf{u}_b) \leq f_{\hat{p}}(\mathbf{u}_a) + \sum_{i=1}^{n_u} \kappa_i |u_{b,i} - u_{a,i}|,$$

(5)

which are valid for any pair $\mathbf{u}_a, \mathbf{u}_b \in \mathcal{I}$ (Bunin et al., 2014b). We will refer to the two expressions on the left and right as *Lipschitz bounds*, although one can also refer to them more generally as lower- and upper-bounding functions, or even as (very local) surrogate models. Only the upper bound will be required for the constraint-satisfaction guarantees discussed in this section, but the lower bound is included now for the sake of completeness, as it will be used later.

Suppose now that, at the latest experimental iteration $k$, one has $g_{p,j}(\mathbf{u}_k) \leq 0$. It follows that one can guarantee $g_{p,j}(\mathbf{u}) \leq 0$ by guaranteeing that its upper
bound be non-positive. Substituting $f_p \rightarrow g_{p,j}$, $\kappa_i \rightarrow \kappa_{p,ji}$, $u_0 \rightarrow u_k$, and $u_0 \rightarrow u$ in the upper bound of (5) then yields

$$g_{p,j}(u_k) + \sum_{i=1}^{n_u} \kappa_{p,ji}|u_i - u_{k,i}| \leq 0 \Rightarrow g_{p,j}(u) \leq 0. \quad (6)$$

Clearly, one can recursively guarantee constraint satisfaction by starting with $u_0$ such that $g_{p,j}(u_0) \leq 0$ and then ensuring

$$g_{p,j}(u_0) + \sum_{i=1}^{n_u} \kappa_{p,ji}|u_{1,i} - u_{0,i}| \leq 0 \Rightarrow g_{p,j}(u_1) \leq 0$$

$$g_{p,j}(u_1) + \sum_{i=1}^{n_u} \kappa_{p,ji}|u_{2,i} - u_{1,i}| \leq 0 \Rightarrow g_{p,j}(u_2) \leq 0$$

$$\vdots$$

$$g_{p,j}(u_k) + \sum_{i=1}^{n_u} \kappa_{p,ji}|u_{k+1,i} - u_{k,i}| \leq 0 \Rightarrow g_{p,j}(u_{k+1}) \leq 0,$$

which is relatively straightforward and does not involve any complicated numerics.

2.3. Limitations of the Lipschitz-Bound Approach

Despite its apparent advantages, the Lipschitz-bound method has three important caveats.

The first, and likely the most minor, is that one must start at a point $u_0$ satisfying $g_{p,j}(u_0) \leq 0, \forall j = 1, ..., n_{g_p}$. Otherwise, Condition (6) becomes irrelevant for $k := 0$ as it is violated for all $u$. In principle, this first requirement should not be restricting, since one would not expect to start the operation of an experimental system at hazardous conditions – indeed, if this were the case, then it is very questionable if optimization should be the user’s top priority.

Another limitation lies, of course, in the setting of the Lipschitz constants. This is an important issue and one that is addressed in greater detail in Section 5. Here, let us remark only on the ramifications of setting $\kappa$ improperly. If the set Lipschitz constants are so small that they do not satisfy (2) for $f_p \rightarrow g_{p,j}$, then (6) is invalid and the approach loses its rigor. Setting the constants high thus seems to be the natural safeguard, but values that are too high make (6) very restrictive, implicitly reducing the distances between $u_1$ and $u_0$, $u_2$ and $u_1$, and so on. For an iterative optimization algorithm, this has the performance drawback of requiring many iterations to achieve near-optimality.

Finally, the last point is a subtle but very vital one – an algorithm that approaches a constraint faster than it approaches an optimum solution is likely to converge prematurely without ever reaching the solution. This is evident if one considers $g_{p,j}(u_k) \approx 0$ for some $j$, which in turn forces $u \approx u_k$ for (6) to hold. This issue was pointed out in the work of Bunin et al. (2011), where the Lipschitz-bound approach to guaranteeing constraint satisfaction...
was first proposed. There, the authors argued, incorrectly, that premature convergence is an issue present only for multiple-constraint systems \((n_p > 1)\), but this is not true—depending on the problem and algorithm, one can converge prematurely regardless of the number of experimental constraints. Avoiding this behavior generally requires a mechanism to ensure that one never approaches the constraints “too close, too quickly” (Bunin et al., 2014c).

2.4. Case-Study Example: Model-Based Minimization of the Batch Time of Polystyrene Production

To illustrate with what results the three different methods (explicit back-off, stochastic optimization, and Lipschitz bounding) may be applied to a practical problem, let us take the case-study example of minimizing the batch time of a polystyrene production reactor, originally reported by Gentric et al. (1999). Following the solution approach of François et al. (2005), one is interested in choosing the “switching times” of the reactor’s temperature profile so as to (a) minimize the time required to reach the desired conversion, favored by higher temperatures, and (b) meet a terminal lower limit on the molecular weight of the product, favored by lower temperatures. The original problem is a dynamic optimization problem as it seeks to find an optimal profile, but the piecewise definition of the profile via prescribed “arcs” and switching times essentially turns this into an experimental optimization problem, which can then be solved in a batch-to-batch manner by varying the switching times (and thus the profile) from batch to batch until an optimal profile is hopefully found. As formulated, the problem has an experimental cost function (the time of the batch) and a single experimental constraint (the lower limit on the molecular weight). Because the molecular weight is a product specification, it would be very wasteful to run batches that violate this constraint, as all such batches may be discarded as inadequate for failing to meet specifications. It follows that an effort to satisfy this constraint for all batches should be made.

The exact problem solved is Problem P3 from the ExpOpt database (Bunin, 2016b), which the interested reader may access to find a more detailed problem description, the steps taken to place the problem into the standard form (1), and the actual code used to simulate the case study. Only the problem as written in standard form is given here:

\[
\begin{align*}
\text{minimize} \quad & \phi_p(u) := t_b(u) \\
\text{subject to} \quad & g_{p,1}(u) := -M(u) + 2 \cdot 10^6 \leq 0 \\
& 50 \leq u_1 \leq 450 \\
& 600 \leq u_2 \leq 1000,
\end{align*}
\]

(7)

noting that \(t_b\) denotes the final batch time to be minimized (in seconds), \(M\) denotes the number average molecular weight (in grams per mole), and \(u_1\) and \(u_2\) are the two switching times that define the temperature profile (in seconds). So as to avoid unnecessary numerical complications, (7) is scaled prior to being solved, with \(t_b\) divided by 8000, the constraint divided by \(4 \cdot 10^6\), and the two
decision variables normalized to lie in the unit box defined by the coordinates 
(0, 0) and (1, 1).

In comparing the three approaches, we try and simplify as much as possible 
without comprisoing the key message. Because a parametric model is required 
for the stochastic-optimization approach, one is assumed to be available, with 
g_p,1(u, \theta_1, \theta_2) \approx g_p,1(u). The model chosen is the one provided in the ExpOpt 
database and, following what was done in the work of François et al. (2005), 
supposes parametric uncertainty in the rate constants for propagation (\theta_1) 
and transfer to monomer (\theta_2), both of which influence the dynamics of the 
polymerization and ultimately the end-batch result. When these parameters 
are at their true values of \( \theta_1^* = 5.7 \cdot 10^6 \) and \( \theta_2^* = 1.5 \cdot 10^{11} \) (liters per 
mole per second), the model is a perfect description of the true pr
ocess, and 
g_p,1(u, \theta_1^*, \theta_2^*) = g_p,1(u). By allowing a model with only parametric uncertainty, 
we avoid the complications of judging the stochastic-optimization approach in 
a scenario where it may not be appropriate – i.e., in the cases of potentially 
severe structural model mismatch.

Additionally, we will initialize all methods by first carrying out two initial 
experiments at \( u_0 = (250, 950) \) and \( u_1 = (200, 950) \), and then assuming that the 
collected data is su
fficient to identify \( \theta_1 = \theta_1^* \) and \( \theta_2 = \theta_2^* \), thereby obtaining 
a perfect model directly from the initialization. This is done so as to avoid 
the numerical complications that would arise in the stochastic-optimization 
approach, since the estimation may not always be easy and could potentially 
hurt the performance of the method. However, some uncertainty on the part of 
the user must be retained, and so these estimates are not assumed to be perfect, 
even though they are made so here. The same model is used to identify the cost 
function, with \( \phi_p(u, \theta_1^*, \theta_2^*) = \phi_p(u) \).

2.4.1. Explicit Back-off Approach

Following the two initial experiments to determine \( \theta_1^* \) and \( \theta_2^* \), a model-based 
optimization is carried out by numerically solving the problem

\[
\begin{align*}
\text{minimize} & \quad \phi_p(u, \theta_1^*, \theta_2^*) \\
\text{subject to} & \quad g_p,1(u, \theta_1^*, \theta_2^*) + b_{p,1} \leq 0 \\
& \quad 50 \leq u_1 \leq 450 \\
& \quad 600 \leq u_2 \leq 1000,
\end{align*}
\]

(8)

with \( b_{p,1} \) set as \( 4 \cdot 10^5 \) (10% of the normalizing scaling factor). This choice is not 
rigorous and represents what a typical operator might do to safeguard against 
the possibility of the model structure being incorrect. The solution of (8) is then 
applied to the reactor at the next batch and new measurements are collected. 
In this case, because the model is already perfect, future measurements will not 
refine the estimates of \( \theta_1 \) and \( \theta_2 \), and one would not wish them to. Convergence 
after a single numerical optimization is thus obtained.
2.4.2. Stochastic-Optimization Approach

Let us suppose that the obtained estimates $\theta^*_1$ and $\theta^*_2$ are uncertain with uniform distributions, and that the true parameter values are assumed to lie in the intervals $\theta_1 \in [0.9\theta^*_1, 1.1\theta^*_1]$ and $\theta_2 \in [0.7\theta^*_2, 1.3\theta^*_2]$ with a sufficiently large probability $P$. Following the initial two experiments, a model-based optimization is performed by solving the problem

$$\begin{align*}
\text{minimize} & \quad \phi_p(u, \theta^*_1, \theta^*_2) \\
\text{subject to} & \quad g_{p,1}(u, \theta_1, \theta_2) \leq 0, \quad \forall \theta_1 \in [0.9\theta^*_1, 1.1\theta^*_1], \quad \theta_2 \in [0.7\theta^*_2, 1.3\theta^*_2] \\
& \quad 50 \leq u_1 \leq 450 \\
& \quad 600 \leq u_2 \leq 1000.
\end{align*}$$ (9)

Because Problem (9) is semi-infinite in nature (Hettich & Kortanek, 1993), it presents a challenge numerically and can, in the general case, only be solved approximately. In this study, we use a simple approximation by only analyzing the constraint values at the nine edge-plus-center points:

$$\begin{align*}
(0.9\theta^*_1, 1.3\theta^*_2) & \quad (\theta^*_1, 1.3\theta^*_2) & \quad (1.1\theta^*_1, 1.3\theta^*_2) \\
(0.9\theta^*_1, \theta^*_2) & \quad (\theta^*_1, \theta^*_2) & \quad (1.1\theta^*_1, \theta^*_2) \\
(0.9\theta^*_1, 0.7\theta^*_2) & \quad (\theta^*_1, 0.7\theta^*_2) & \quad (1.1\theta^*_1, 0.7\theta^*_2).
\end{align*}$$

Here, such an approximation happens to be sufficiently robust because the point $(\theta^*_1, \theta^*_2)$ is included, and including the other points only offers additional security. As in the previous approach, future measurements will not refine future parameter estimates, and convergence is obtained after a single numerical optimization.

2.4.3. Lipschitz-Bound Approach

Once again, the two initial experiments are carried out to identify the model, after which Condition (6) is enforced in one of two ways. Both are examined here as they yield fairly different convergence behaviors.

The first, “direct” way consists in placing the condition right into the model-based optimization for the current iteration $k$, in lieu of the model constraint:

$$\begin{align*}
\text{u}_{k+1} := \arg \min_{u} & \quad \phi_p(u, \theta^*_1, \theta^*_2) \\
\text{subject to} & \quad g_{p,1}(u_k) + \sum_{i=1}^{2} \kappa_{p,1}|u_i - u_{k,i}| \leq 0 \\
& \quad 50 \leq u_1 \leq 450 \\
& \quad 600 \leq u_2 \leq 1000.
\end{align*}$$ (10)

The resulting solution is then applied to the reactor at the next batch, new measurements are taken, $k$ is updated, and the steps are repeated again.

The alternate, “indirect” method is to first solve the model-based problem with no modifications:
\[
\begin{align*}
\bar{u}_{k+1}^* &:= \arg \min_u \phi_p(u, \theta_1^*, \theta_2^*) \\
\text{subject to} & \quad g_{p,1}(u, \theta_1^*, \theta_2^*) \leq 0 \\
 & \quad 50 \leq u_1 \leq 450 \\
 & \quad 600 \leq u_2 \leq 1000,
\end{align*}
\]
and to then “filter” the step towards \(\bar{u}_{k+1}^*\):

\[
\begin{align*}
\bar{u}_{k+1}^* &:= u_k + K_k \left( \bar{u}_{k+1}^* - u_k \right).
\end{align*}
\]
In accordance with (6), setting

\[
K_k := \frac{-g_{p,1}(u_k)}{\sum_{i=1}^2 \kappa_{p,1,i} |\bar{u}_{k+1,i}^* - u_{k,i}|}
\]
is then sufficient to ensure that \(g_{p,1}(u_{k+1}) \leq 0\) (Bunin et al., 2011).

The Lipschitz constants are set as \(\kappa_{p,11} := 2\) and \(\kappa_{p,12} := 1\), as these are values that are sufficient and correct for the (scaled) problem of the case study.

2.4.4. Results and Comparisons

The results of applying the different methods are presented graphically in Figure 1. As expected, both the explicit back-off and stochastic-optimization approaches, despite having perfect parameter estimates, converge to suboptimal points due to the back-offs (explicit or implicit) shrinking the feasible space of the optimization problem. By contrast, the Lipschitz-bound approaches have no difficulty in this regard because of their adaptive nature, as they iteratively converge to a point with a cost value close to that at the optimum, and ultimately touch the constraint without ever violating it.

It is of interest to remark that the “direct” approach leads one to take steps along a single direction. This is most likely due to the rhombus shape (Bunin et al., 2012) of the safety-guaranteeing constraint region in (10) and the almost linear nature of the cost, which leads to the next iterate always being found on the bottom vertex of the rhombus, thus leading the iterates straight down until the constraint is hit. It may be worth noting that this is very similar in nature to what is obtained with the \(l_1\)-norm steepest descent algorithm (Boyd & Vandenberghe, 2008, §9). The “indirect” approach avoids this issue and converges to a point that is, for all practical purposes, as good as the true optimum, and the one found by the numerical optimization solver – MATLAB’s \texttt{patternsearch} derivative-free optimization package, which was employed here, did not find the true, exact optimum of (7).

In addition to the Lipschitz-bound approach being rigorously safe and able to approach the constraint without the need of back-offs, it is worth observing that its ease of implementation is much superior to that of the first two methods. Apart from the fact that it does not require a model and only necessitates two parameters (the two Lipschitz constants), its simplicity and usefulness becomes further apparent when one considers the following:
Figure 1: Results obtained from applying the explicit back-off, stochastic-optimization, and Lipschitz-bound methods to Problem (7). The lighter (green) area in the left-hand plot represents the region where the constraint is satisfied, while the darker (red) area represents the region where it is violated. The leftmost and darker dashed line shows the implicit back-off achieved by the stochastic-optimization method, while the lighter dashed line to the right gives the explicit back-off set by the user. The iterates for the different methods are denoted as follows: light blue squares for the explicit back-off approach, blue diamonds for the stochastic-optimization approach, yellow triangles for the direct Lipschitz-bound approach, and red circles for the indirect Lipschitz-bound approach. The true optimum is marked by the green circle.

- Constraint satisfaction in the first two approaches is ensured by the fact that a perfect model is obtained after the initial two experiments. In most real problems, model error will not be parametric only (Quelhas et al., 2013), in which case neither of the methods will be robust. The Lipschitz approach does not suffer from this as its constraint-satisfaction guarantees are not model-dependent. An exception to this statement is the case where one relies on a model for estimating the Lipschitz constants – see Section 5.2.

- The stochastic optimization approach requires the user to know the uncertainty distributions of the parameters. This assumption, besides already implying the other assumption of having parametric uncertainty only, may be very restrictive in practice, since tight distributions that do not result in overly conservative implicit back-offs may be very difficult or impossible to obtain (Li et al., 2008; Quelhas et al., 2013).

- As mentioned above, solving the semi-infinite programming problems that often arise from chance constraints may be a very difficult task numerically – the light approximation employed here was sufficient only because the true parameter values were in the set of the nine combinations considered. Although the numerical difficulties may be alleviated significantly by linearizing the probability constraints (Zhang et al., 2002), this technique
comes with a number of robustness issues.

However, it would be improper to completely dismiss either of the first two approaches for problems where the structural, non-parametric uncertainty is relatively small, and it is worth noting that the suboptimality of both methods clearly comes from their lack of adaptation — i.e., the back-offs, explicit or implicit, never go away. It is certainly conceivable that one could gradually diminish the back-off in the first scheme as a function of model fidelity. For the second scheme, one could implicitly remove the back-off by gradually tightening the uncertainty intervals around the true parameter values with each new experiment — in estimation theory lingo, this would require that the estimator of the parameters be consistent.

2.5. An Extension: Lipschitz Bounds for Safe Excitation

In experimental optimization problems there is often the need for some sort of continuous excitation for estimation purposes. This may be done to identify the parameters of a locally valid model (Conn et al., 2000; Pfaff et al., 2006), to estimate the local function derivatives (Gao & Engell, 2005; Marchetti et al., 2010), or to continuously optimize by locally exploring the decision-variable space (Box & Draper, 1969; Conn et al., 2009; Martínez, 2005). There thus arises a natural conflict between constraint satisfaction and obtaining information when one approaches a constraint, since the information-gathering perturbations then become a potential constraint-violation hazard.

The Lipschitz condition (6) allows for a simple extension that handles this case very well. Namely, if one has an experimental iterate $u_k$ that satisfies the constraint $g_{p,j}$ with a back-off of $\delta_\epsilon \|\kappa_{p,j}\|_2$, where the vector $\kappa_{p,j}$ is simply the collection of the individual Lipschitz constants ($\kappa_{p,j1}, \ldots, \kappa_{p,jn_u}$), then one has the guarantee that

$$g_{p,j}(u_k) + \delta_\epsilon \|\kappa_{p,j}\|_2 \leq 0 \Rightarrow g_{p,j}(u) \leq 0, \forall u \in B_{\epsilon} \cap \Omega, \quad (12)$$

with $B_{\epsilon} = \{ u : \|u - u_k\|_2 \leq \delta_\epsilon \}$ the ball of radius $\delta_\epsilon$ centered around $u_k$. For the proof of the above statement and further discussion, the reader is referred to the recently submitted manuscript of Bunin (2016a).

The exact manner in which one may use (12) to allow for excitation while robustly satisfying the constraints would almost certainly be method-dependent. The general principles, however, are quite simple. Because one has the guarantee that satisfying the constraint with a specified back-off allows for one to perturb safely anywhere in a $\delta_\epsilon$-ball around that point, it follows that one can choose $\delta_\epsilon$ a priori and to then only perturb around those experimental iterates that satisfy the corresponding back-off, since all such information-gathering experiments will satisfy the constraints. This is now illustrated for a specific case-study example.

2.5.1. Case Study: A Modifier-Adaptation Algorithm for Minimizing the Steady-State Production Cost of a Gold Cyanidation Leaching Process

One algorithm that depends heavily on perturbations is the modifier-adaptation method (Brdys & Tatjewski, 2005; Gao & Engell,
which solves Problem (1) by iteratively solving a corrected model-based problem:

\[
\begin{align*}
\text{minimize} & \quad \phi(p(u, \theta) + \lambda^T_{\phi,k} u \\
\text{subject to} & \quad g_{p,j}(u, \theta) + \epsilon_{j,k} + \lambda^T_{j,k}(u - u_k) \leq 0, \quad j = 1, \ldots, n_p \\
& \quad g_j(u) \leq 0, \quad j = 1, \ldots, n_g \\
& \quad u_i^L \leq u_i \leq u_i^U, \quad i = 1, \ldots, n_u,
\end{align*}
\]

with \( \epsilon \) and \( \lambda \) denoting the “modifiers” used to correct the local zero- and first-order errors of the model, respectively:

\[
\begin{align*}
\epsilon_{j,k} & := g_{p,j}(u_k) - g_{p,j}(u_k, \theta) \\
\lambda_{j,k} & := \nabla_{g_{p,j}(u_k)} - \nabla_{g_{p,j}(u_k, \theta)} \\
\lambda_{\phi,k} & := \nabla_{\phi_p(u_k)} - \nabla_{\phi_p(u_k, \theta)}.
\end{align*}
\]

The uncertain parameters of the model are not updated between iterations and are kept at some nominal, constant values, although a version of the algorithm that estimates and updates the parameters as well may certainly be used (Brdys & Tatjewski, 2005). One could also filter the updates in (14) to promote algorithm stability (Marchetti et al., 2009), but this is not done here.

The zero-order modifier values \( \epsilon_{j,k} \) may be easily obtained by physically measuring the experimental function values and numerically evaluating the model at \( u_k \). The first-order corrections, however, require experimental derivative estimates. A number of approaches may be proposed for obtaining such estimates (Bunin et al., 2013a), and the method employed here will be that of taking the difference quotients

\[
\left. \frac{\partial f_p}{\partial u_i} \right|_{u_k} \approx \frac{f_p(u_k) - f_p(u_{k,1}, \ldots, u_{k,i} - \delta_e, \ldots, u_{k,n_u})}{\delta_e},
\]

or, if \( u_{k,i} - \delta_e < u_i^L \),

\[
\left. \frac{\partial f_p}{\partial u_i} \right|_{u_k} \approx \frac{f_p(u_{k,1}, \ldots, u_{k,i} + \delta_e, \ldots, u_{k,n_u}) - f_p(u_k)}{\delta_e},
\]

where \( \delta_e \) is chosen as some non-zero value. The choice to use \( \delta_e \) as the perturbation step is, of course, not coincidental and is intended to be used in synergy with (12) to ensure that all perturbations performed for estimating the derivatives satisfy the constraints.

The outline of the employed algorithm, where one starts at the iteration \( k := 0 \) with some \( u_0 \) that satisfies the problem constraints with the additional back-offs of \( \delta_e \), is as follows:

1. Define the modifiers as in (14), with the experimental gradients obtained by carrying out an additional \( n_u \) experiments and then applying (15) or (16).
2. Solve Problem (13) and let $\bar{u}_{k+1}^*$ denote the solution.

3. Guarantee that the next experimental iterate satisfy the constraints with the back-offs accounted for by applying the filter rule (11) and defining $K_k$ as

$$K_k := \min_{j=1,\ldots,n_g} \frac{-g_{p,j}(u_k) - \delta_e \| \kappa_{p,j} \|_2}{\sum_{i=1}^{n_u} |\kappa_{p,ji}|(\bar{u}_{k+1,i}^* - u_{k,i})}$$ (17)

(Bunin et al., 2014a). In the case that this $K_k$ does not lead to all $g_j$ being satisfied, lower $K_k$ until it does. If $K_k > 1$, trim it down to $K_k := 1$.

4. Apply the new decision variables to the experimental system, obtain the new measurements, augment the value of $k$, and return to Step 1.

This algorithm is applied to Problem P11 from the ExpOpt database (Bunin, 2016b). The problem itself is adapted from the work of Jun et al. (2015) and deals with the minimization of the steady-state production cost of a gold cyanidation leaching process. Only the skeleton of the problem is provided here, with interested readers once more referred to the aforementioned references for more in-depth descriptions.

In our standard form, the problem may be written as

$$\begin{align*}
\text{minimize} & \quad \phi_p(u) := \phi_{\text{econ}}(u) \\
\text{subject to} & \quad g_{p,1}(u) := \frac{C_s(u) - C_{s,0}}{C_{s,0}} + 0.75 \leq 0 \\
& \quad 10 \leq u_1 \leq 80 \\
& \quad 5 \leq u_2 \leq 20,
\end{align*}$$ (18)

with $u$ consisting of two variables – the flow rate of the sodium cyanide (in kilograms per hour) and the concentration of the dissolved oxygen in the liquid (in milligrams per kilogram). The function $\phi_{\text{econ}}$ is the economical cost function to be minimized (in Chinese RMB per hour), while $C_s$ denotes the gold concentration in the ore (in milligrams per kilograms; $C_{s,0}$ denotes its initial value). The single experimental constraint ensures that the gold recovery is at least 75% – the solution, although not on this constraint, is nevertheless very close to it. The model used for the case study is that provided in the database and differs from the simulated “real” process by virtue of errors in the kinetic parameters. As in the previous case-study example, the decision variables are scaled down to a unit box, with the cost and constraint values divided by the scaling factors of 200 and 0.04, respectively. A $\delta_e$ value of 0.05 (for the scaled variables) is chosen, with the Lipschitz constants of the scaled problem set as $\kappa_{p,11} := 3$ and $\kappa_{p,12} := 1$. The process starts operating at the suboptimal point
of $u_0 = (52, 18)$, which satisfies the experimental constraint with a slack greater than $\delta_e \| \kappa_{p,1} \|_2$.

The results of applying the above algorithm to this problem are given in Figure 2. As expected, one sees that the main experimental iterates all satisfy the experimental constraint with the back-off, while the $\delta_e$-perturbations for derivative estimation all satisfy the original constraint. In this case, we see that the modifier-adaptation algorithm converges fairly close to the optimum fairly quickly, with full convergence to the optimum being precluded by the back-off.

3. Other Uses of the Lipschitz Constants

Guaranteeing constraint satisfaction is arguably the most important potential role of the Lipschitz constants in the experimental optimization setting. However, they have other possible uses as well, which, though of less importance, may nevertheless bring some benefits to the solution procedure and are thus worth mentioning. Namely, the Lipschitz constants and bounds may be used for:

- the “fathoming” of certain regions of the experimental space that cannot contain an optimum,
- the reduction of uncertainty due to measurement noise/error,
- the regularization of derivative estimates.

We now present these one by one.
3.1. Lipschitz-Based Fathoming

A fairly general approach to globally minimizing a black-box function in the numerical optimization community is that of Lipschitz-based branch and bound (Horst et al., 1995, §5). Because experimental relationships are black-box in nature, exactly the same concepts may be employed in the experimental optimization setting and may be employed to remove those portions of the experimental space that are proven to not contain the (global) optimum, as based on previously measured values and the Lipschitz constants.

Suppose that \( k + 1 \) experiments have already been carried out with the decision-variable sets \( u_0, u_1, \ldots, u_k \) and that the corresponding cost function measurements, \( \phi_p(u_0), \phi_p(u_1), \ldots, \phi_p(u_k) \), have been obtained. It is assumed that all of these experiments satisfy the constraints.

Let \( k^* \) denote the index – assumed, for simplicity, to be unique – of the experiment with the minimum cost value:

\[
\phi_p(u_{k^*}) \leq \phi_p(u_k), \quad \forall k = 0, \ldots, k.
\]

For any of the points \( u_0, u_1, \ldots, u_k \), one has a corresponding lower bound on the cost function value, obtained by substituting \( f_p \to \phi_p, \quad \kappa_i \to \kappa_{\phi,i}, \quad u_a \to u_{\bar{k}} \), and \( u_b \to u \) in (5):

\[
\phi_p(u) - \sum_{i=1}^{n_u} \kappa_{\phi,i} |u_i - u_{\bar{k},i}| \leq \phi_p(u), \quad \forall u \in I.
\]

So as to have a single tightest bound, one can simply take the piecewise maximum of the individual ones:

\[
\max_{k=0, \ldots, k} \left( \phi_p(u_k) - \sum_{i=1}^{n_u} \kappa_{\phi,i} |u_i - u_{\bar{k},i}| \right) \leq \phi_p(u), \quad \forall u \in I.
\]

Suppose now that we wish to test a new point \( u_{k+1} \), but compute the lower bound for this point and find that

\[
\phi_p(u_{k^*}) < \max_{k=0, \ldots, k} \left( \phi_p(u_k) - \sum_{i=1}^{n_u} \kappa_{\phi,i} |u_{k+1,i} - u_{\bar{k},i}| \right).
\]

Since this clearly implies that \( \phi_p(u_{k^*}) < \phi_p(u_{k+1}) \), there appears to be little sense in trying this experiment unless we are specifically interested in information gathering. However, it is likely that there are other decision-variable sets that could also give good information without being provably suboptimal.

We may therefore proceed to “fathom” (remove from consideration) the entire set

\[
I_{\text{sub},k} = \left\{ u : \phi_p(u_{k^*}) < \max_{k=0, \ldots, k} \left( \phi_p(u_k) - \sum_{i=1}^{n_u} \kappa_{\phi,i} |u_i - u_{\bar{k},i}| \right) \right\}.
\]
and only consider optimizing over the remaining $I \setminus I_{\text{sub},k}$.

How this information is used, and to what degree of success, would naturally be dependent on the problem and the optimization algorithm. We now consider the global optimization of a Williams-Otto reactor by a random sampling method as an illustration of the potential usefulness of this technique.

### 3.1.1. Maximization of Steady-State Profit in a Williams-Otto Reactor via Random Sampling

For this case study, let us take Problem P1 from ExpOpt (Bunin, 2016b), which deals with the maximization of a steady-state profit function for the reactor model originally proposed by Williams & Otto (1960). In our standard form, this problem appears as

$$\begin{align*}
\text{minimize} \quad & \phi_p(u) := -\phi_{\text{profit}}(u) \\
\text{subject to} \quad & 3 \leq u_1 \leq 6 \\
& 70 \leq u_2 \leq 100,
\end{align*}$$

where $\phi_{\text{profit}}$ denotes the steady-state profit function, while the two decision variables $u_1$ and $u_2$ denote the feed rate of one of the reactants (in kilograms per second) and the reactor temperature (in degrees Celsius), respectively. The problem is scaled as in the previous examples – the decision variables are affinely transformed to lie in the unit box, while the cost function is divided by a factor of 100. Values of $\kappa_{\phi,1} := 4$ and $\kappa_{\phi,2} := 6$ are used for the scaled problem. Global optimization is then performed by running a hundred experiments at random points in the reduced experimental space $I \setminus I_{\text{sub},k}$. Figure 3 presents the results, and one sees that the fathoming leads to a greater number of samples with lower cost-function values due to many suboptimal regions being removed from consideration.

The illustrative nature of this example cannot be overstated – clearly, these results are anything but surprising. Nor is the choice of a random-sampling method pragmatic for this example, since the cost function has a single optimum and could be optimized much more efficiently by any local-descent algorithm. However, regardless of what algorithm one may choose, it is important to realize that one cannot, provided a correct choice of $\kappa_\phi$, do worse by restricting the space to $I \setminus I_{\text{sub},k}$ and, depending on the problem and algorithm, may even do noticeably better.

### 3.2. Lipschitz-Based Noise/Error Reduction

Up to now, the discussion has been kept simple by assuming that the function values $f_p$ could be measured perfectly. However, in practice it is almost always the case that the measurements are corrupted by some sort of noise or error, and what one observes are actually the corrupted values, $\hat{f}_p$, with

$$\hat{f}_p(u_k) = f_p(u_k) + w_k, \quad k = 0, \ldots, k,$$

and with $w$ denoting stochastic elements. Naturally, it is still desired that something useful be said about the true function values when all that one has
Figure 3: Results for the global optimization of Problem (19) by random sampling over $I \setminus I_{\text{sub,}k}$ (top) and $I$ (bottom). The individual yellow polytope regions correspond to the regions around each sampled point that have been fathomed from consideration by applying the Lipschitz bound to that point and measurement. The union of the polytopes in the figure is equivalent to $I_{\text{sub,100}}$. 
access to are the corrupted measurements. One such piece of information comes in the form of the lower and upper bounding values

\[ f_p(u_k) \leq f_p(u_k) \leq \overline{f}_p(u_k). \]

as this allows one to derive a robust version of (5) (Bunin et al., 2014a).

The simplest way to obtain \( f_p \) and \( \overline{f}_p \) involves bounding the stochastic elements in some high-probability sense, which may be done by Monte Carlo simulation when the probability distribution functions (PDFs) of \( w \) are known, or by the use of Chebyshev’s inequality for the general case when only the means and the variances of the different \( w \) are available (Moré & Wild, 2011).

Let us assume then that, with high probability, one has

\[ w_{\bar{k}} \leq w_{\bar{k}} \leq w_{\bar{k}}, \]

with \( w \) and \( w \) denoting the lower and upper magnitudes of the corruption, respectively. By rearranging the measurement equality (20), one then obtains

the lower and upper bounding values

\[ f_p(u_{\bar{k}}) := \hat{f}_p(u_{\bar{k}}) - w_{\bar{k}} \leq f_p(u_{\bar{k}}) \leq \hat{f}_p(u_{\bar{k}}) - w_{\bar{k}} := \overline{f}_p(u_{\bar{k}}). \]

Although these bounds may be fairly rigorous and useful, they can be too conservative when the variance of the noise/error is large. By exploiting the Lipschitz bounds (5), it is possible to tighten \( f_p \) and \( \overline{f}_p \) by coupling the Lipschitz bounds with the lower/upper bounding values for the other obtained measurements. Consider the robust version of (5) for the general \( \tilde{k} \in \{0, \ldots, k\} \):

\[ f_p(u_{\tilde{k}}) - \sum_{i=1}^{n_{\tilde{k}}} \kappa_i |u_{\tilde{k},i} - u_{\tilde{k},i}| \leq f_p(u_{\tilde{k}}) \leq \overline{f}_p(u_{\tilde{k}}) + \sum_{i=1}^{n_{\tilde{k}}} \kappa_i |u_{\tilde{k},i} - u_{\tilde{k},i}|. \]

Clearly, the bounds obtained in (21) are a special case of the above (i.e., when \( \tilde{k} := \bar{k} \)). However, it should be evident that we may be able to improve the bounds by considering the tightest values over all \( \{0, \ldots, k\} \):

\[ f_p(u_k) := \max_{k=0, \ldots, k} \left( f_p(u_k) - \sum_{i=1}^{n_{\bar{k}}} \kappa_i |u_{\bar{k},i} - u_{\bar{k},i}| \right) \leq f_p(u_k), \]

\[ f_p(u_k) \leq \min_{k=0, \ldots, k} \left( \overline{f}_p(u_k) + \sum_{i=1}^{n_{\bar{k}}} \kappa_i |u_{\bar{k},i} - u_{\bar{k},i}| \right) := \overline{f}_p(u_k). \]

Note that after using (22)-(23) to assign lower/upper bounding values to the measurements at \( u_0, u_1, \ldots, u_k \), one may run through the process again, since changes in some of the values may lead to additional changes in the others. The iterative scheme may be outlined as follows:

1. Set the nominal \( f_p \) and \( \overline{f}_p \) for \( \bar{k} = 0, \ldots, k \) as given in (21).
2. Refine the bounds by applying (22)-(23) for $k = 0, ..., k$.

3. If the largest refinement obtained is negligible (e.g., < $10^{-6}$), terminate. Otherwise, return to Step 2.

A conceptual illustration of removing noise or error via this procedure is given in Figure 4, where we consider a simple one-dimensional case with white Gaussian noise of variance $\sigma^2$, and high-probability bounds of $-3\sigma$ and $3\sigma$ on the noise elements. As shown in the figure, it happens that a very poor nominal upper bounding value is obtained at $u_k$ while a very tight upper bounding value is obtained at the previous experiment of $u_{k-1}$. The tightness at the latter may then be partially “inherited” by the former because of the Lipschitz bound, thereby leading to significant refinement in the upper bounding value at $u_k$. Naturally, this method will lose its effectiveness when the decision-variable points are further apart and when the Lipschitz constants used are more conservative.

3.2.1. Case Study: Gold Cyanidation Leaching Process with Noise

Let us return to the case-study example of Section 2.5.1, where we seek to minimize the steady-state operating cost of a gold cyanidation leaching process by varying the flow rate of sodium cyanide and the concentration of dissolved oxygen, subject to a gold recovery constraint. This time, let us suppose a more realistic scenario where all of the measurements obtained, for both the cost and constraints, are corrupted by noise elements from the PDF of $\mathcal{N}(0, \sigma^2)$.
with a value of \( \sigma := 0.07 \) used here (this corruption is applied to the problem post-scaling). The nominal lower and upper magnitudes of the corruption are then chosen as \( \underline{w} := -3\sigma \) and \( \bar{w} := 3\sigma \) for all measurements at all iterations, from which the nominal lower and upper bounding values on the true function values are obtained as in (21).

Two realizations of the modifier-adaptation algorithm are compared here. Both use a corrupted modifier update, with the zero-order correction defined as

\[
\epsilon_{j,k} := \hat{\delta}_{p,j}(u_k) - g_{\hat{\delta}_{p,j}}(u_k, \theta),
\]

and the derivative estimates for the first-order terms obtained as corruptions

\[
\frac{\partial f_{\hat{\delta}}}{\partial u_i} \bigg|_{u_k} \approx \frac{\hat{f}_{p}(u_k) - \hat{f}_{p}(u_{k,\delta_{c},\ldots,u_{k,n}))}{\delta_{c}}
\]

or, if \( u_{k,i} - \delta_{c} < u_{i}^{L} \),

\[
\frac{\partial f_{\hat{\delta}}}{\partial u_i} \bigg|_{u_k} \approx \frac{\hat{f}_{p}(u_{k,\delta_{c},\ldots,u_{k,n})} - \hat{f}_{p}(u_k)}{\delta_{c}}.
\]

The filter gain setting of (17) is modified to

\[
K_k := \min_{j=1,\ldots,n_p} \left[ \frac{-\overline{\gamma}_{p,j}(u_k) - \delta_{c} \| \kappa_{p,j} \|_2}{\sum_{i=1}^{n_{\phi}} |u_{k+1,i}^\phi - u_{k,i}|} \right]
\]

to robustify the algorithms against noise (Bunin et al., 2013c).

In the first algorithm, the Lipschitz constants are not used to refine the bounding value, with the \( \overline{\gamma}_{p,j} \) value obtained from (21) used in (27). The measured, noisy values are used directly in (24)-(26). In the second algorithm, the Lipschitz-bound refinement procedure as outlined in the previous section is run through all of the measurements – the “key” iterations \( 0, \ldots, k \) and the additional perturbations around the key iterations used for derivative estimation. The resulting \( \overline{\gamma}_{p,j}(u_k) \) is then used in (27). Additionally, the measured values \( \hat{\phi} \) and \( \hat{\delta}_{p,j} \) as employed in (24)-(26) are trimmed in the case that they do not satisfy the refined bounds (e.g., \( \hat{\phi}(u_k) \rightarrow \overline{\phi}(u_k) \) if \( \hat{\phi}(u_k) > \overline{\phi}(u_k) \)). The Lipschitz constants for the cost are chosen as \( \kappa_{\phi,1} := 4 \) and \( \kappa_{\phi,2} := 2 \).

A comparison for a single noise realization is given in Figure 5, from which it is seen that applying the Lipschitz-based refinements leads to improved performance in the form of less suboptimal experiments. As would be expected, the performances of the two methods for the early iterations are almost identical – because there are fewer experiments, there are fewer data for Lipschitz-based refinement and thus almost none takes place. However, the difference becomes apparent once more data are accumulated, with tighter bounding values leading to less corruption and to better algorithm performance.

22
Without carrying out an intensive statistical study, a broader comparison of these two methods was carried out by applying them side by side for an additional nineteen noise realizations. The average differences between the cost function values obtained – the cost function values for the algorithm without Lipschitz-based refinement minus the values for the algorithm with the refinement – were recorded. The obtained average differences were

8.25, 5.74, 0.65, 3.78, 9.21, 2.90, 0.43, 3.05, 9.89, 2.96, 3.39, 5.60, 6.17, 1.18, −4.11, 0.85, −0.06, −1.12, 1.62, 1.07 (RMB/hour),

showing that the version of the algorithm that used the refinement usually did better, though to different extents.

3.3. Use of Lipschitz Constants for Regularization of Derivative Estimates

As pointed out by Bunin et al. (2013a), the Lipschitz constants act as the most brute and fundamental tool for regularizing experimental derivative estimates – i.e., for ensuring that the estimation succumbs to some sort of additional structure that makes it impossible for the estimates to explode in value when sample points are too close together and there are noise errors. Simply put, the estimates must satisfy the corresponding Lipschitz limits imposed by (2). It is therefore natural to take the Lipschitz constants and use them to bound the derivative estimates, and this may be seen as the first-order analogue of what has already been discussed in the previous subsection with regard to the function, rather than derivative, values.

Such regularization is expected to be particularly useful in those optimization schemes where the algorithm is fairly sensitive to errors in the estimated derivatives. The following case-study example illustrates one such case.

3.3.1. Case Study: Williams-Otto Reactor Optimized by an Approximate Gradient-Descent Method

We consider again the problem addressed in Section 3.1.1, this time starting at the (pre-scaled) point \( u_0 = (4.8, 77) \) and dictating future experiments by the approximate gradient-descent update

\[
 u_{k+1} := u_k - \frac{1}{k+1} \nabla \phi_p(u_k),
\]

where the gradient is obtained from the corrupted difference-quotient estimates (25), with \( \delta_\sigma \) set as 0.01 and a noise corruption of \( \sigma = 0.05 \) present. This simple algorithm was essentially first proposed by Kiefer & Wolfowitz (1952) for the case of a single decision variable, before being generalized by Blum (1954) to the multidimensional case. In the case that the provided \( u_{k+1} \) falls outside of the experimental space, those elements of \( u_{k+1} \) failing to satisfy \( u^L \) and \( u^U \) are simply trimmed to the lower or upper limits, as appropriate.

Two versions of the algorithm are compared here – one where the estimates (25) are trimmed to the Lipschitz constants when they violate them, and one
Figure 5: Solving the noisy gold cyanidation leaching problem with modifier-adaptation algorithms that do not refine the bounding values (top), and that do refine them by exploiting the Lipschitz bounds (bottom). Only the cost function values for the key iterations (excluding perturbations for derivative estimation) are shown in the right-hand plots. The values obtained by the first method are superimposed on the plot for the second, via the dashed line, to demonstrate the noticeable improvement when using the Lipschitz constants – numerically, there is an average positive difference of 8.25 Chinese RMB/hour between the top and bottom curves.
where they are not. Figure 6 presents the results for a single noise realization, from which one sees that the trimming helps significantly in reducing the suboptimality of the experiments and making the algorithm less prone to take undesirable steps.

As in the previous section, we test the repeatability of these results for an additional nineteen noise realizations, with the average differences between the cost function values obtained for the two algorithms – those without the trimming minus those with – observed as

\[ 12.97, -0.04, -1.65, -3.01, 5.06, 2.00, -1.42, 5.16, 11.44, 8.12, 10.64, 6.44, 3.62, 2.37, 10.43, 6.01, 4.49, 0.95, 8.30, 7.95 \text{ (thousand USD)}. \]

From these numbers, it is seen that trimming the estimates does indeed seem to lead to fairly consistent improvements in performance for this problem.

4. Refinements

The price to pay for the simplicity of the Lipschitz constants and the corresponding bounds of (5) is their potential conservatism. Namely, if the constants \( \kappa \) are chosen so that (2) is satisfied with a very large margin, the resulting bounds (5) will not be very tight. This can have several drawbacks:

- the constraint-satisfaction condition (6) becomes too restrictive, forcing the algorithm to take overly small steps;
- the back-off, \( \delta \| \kappa_{p,j} \|_2 \), needed for safe excitation in (12) becomes too large and difficult to satisfy;
- the techniques of Section 3 degrade and become of no use.

In this section, we will review three types of refinements that may, at the cost of additional assumptions, remove some of this conservatism. For each refinement, we will summarize the changes that result in the general bounds (5), the constraint-satisfaction condition (6), the safe-excitation condition (12), and the bounding values (22)-(23). Finally, after detailing the refinements one by one, we will provide the versions of (5), (6), (12), and (22)-(23) that incorporate all three refinements simultaneously.

4.1. Refinement with Respect to Direction

Rather than use the same value to define both the lower (\( -\kappa \)) and upper (\( \kappa \)) bounds on the derivatives, as was done in (2), a more general definition with different lower (\( \kappa_l \)) and upper (\( \kappa_u \)) limits may be employed:

\[
\kappa_l \leq \frac{\partial f_p}{\partial u_i} \mid _u \leq \kappa_u, \quad \forall u \in I.
\]
Figure 6: Solving the noisy Williams-Otto problem with gradient-descent algorithms that do (bottom) and do not (top) trim the derivative estimates in accordance with the Lipschitz constants. Only the cost function values for the key iterations (excluding perturbations for derivative estimation) are shown in the right-hand plots. The values obtained by the first method are superimposed on the plot for the second, via the dashed line, to demonstrate the noticeable improvement when using the Lipschitz constants—numerically, there is an average positive difference of 12.97 thousand USD between the top and bottom curves.
Mathematically, this leads to the \( \kappa_i |u_{b,i} - u_{a,i}| \) absolute-value term being replaced by piecewise minimums and maximums (Bunin et al., 2014b), and results in the following refinements.

### Lipschitz Bounds

\[
f_p(u_b) \geq f_p(u_a) + \sum_{i=1}^{n_u} \min \left[ \frac{\kappa_i (u_{b,i} - u_{a,i})}{\zeta_i (u_{b,i} - u_{a,i})} \right], \quad \forall u_a, u_b \in \mathcal{I},
\]

\[
f_p(u_b) \leq f_p(u_a) + \sum_{i=1}^{n_u} \max \left[ \frac{\kappa_i (u_{b,i} - u_{a,i})}{\zeta_i (u_{b,i} - u_{a,i})} \right], \quad \forall u_a, u_b \in \mathcal{I}.
\]

### Constraint-Satisfaction Condition

\[
g_{p,j}(u_k) + \sum_{i=1}^{n_u} \max \left[ \frac{\kappa_{p,ji} (u_i - u_{k,i})}{\zeta_{p,ji} (u_i - u_{k,i})} \right] \leq 0 \Rightarrow g_{p,j}(u) \leq 0.
\]

### Safe-Excitation Condition

\[
g_{p,j}(u_k) + \delta_e \| \kappa_{p,j}^* \|_2 \leq 0 \Rightarrow g_{p,j}(u) \leq 0, \quad \forall u \in \mathcal{B}_e \cap \mathcal{I},
\]

\[
\kappa_{p,ji}^* = \max \left( |\kappa_{p,ji}|, |\zeta_{p,ji}| \right).
\]

### Bounding Values

\[
f_p(u_k) := \max_{k=0,...,k} \left( \mathcal{L}_i(u_k) + \sum_{i=1}^{n_u} \min \left[ \frac{\kappa_i (u_{k,i} - u_{k,i})}{\zeta_i (u_{k,i} - u_{k,i})} \right] \right) \leq f_p(u_k),
\]

\[
f_p(u_k) \leq \min_{k=0,...,k} \left( \mathcal{T}_p(u_k) + \sum_{i=1}^{n_u} \max \left[ \frac{\kappa_i (u_{k,i} - u_{k,i})}{\zeta_i (u_{k,i} - u_{k,i})} \right] \right) := \mathcal{T}_p(u_k).\]

#### 4.2. Refinement with Respect to Locality

Because the Lipschitz bounds are only required to be valid over a local subspace of the experimental space, there is no need for the Lipschitz constants to be valid over all of \( \mathcal{I} \). Let us define \( \mathcal{T}_{u_a}^{u_b} \) as the line segment

\[
\mathcal{T}_{u_a}^{u_b} = \{ u_a + \gamma (u_b - u_a) : \gamma \in [0, 1] \},
\]

and the Lipschitz constants local to this line as

\[
-\kappa_{u_a, u_b} \leq \frac{\partial f_p}{\partial u_i} |_{u_a} \leq \kappa_{u_a, u_b}, \quad \forall u \in \mathcal{T}_{u_a}^{u_b}.
\]

Likewise, one may also define local Lipschitz constants for the constraints over the ball \( \mathcal{B}_e \):
\[-\kappa^e_{p,ji} \leq \frac{\partial g_{p,ji}}{\partial u_j} \bigg|_{\mathbf{u}} \leq \kappa^e_{p,ji}, \quad \forall \mathbf{u} \in \mathcal{B}_e.\]

The refinements of (5), (6), (12), and (22)-(23) are then derived by simply substituting in the local variants.

**Lipschitz Bounds**

\[
f_p(\mathbf{u}_b) \geq f_p(\mathbf{u}_a) - \sum_{i=1}^{n_u} \kappa^e_{u_i, u_{b,i}} |u_{b,i} - u_{a,i}|, \quad \forall \mathbf{u}_a, \mathbf{u}_b \in \mathcal{I}_{u_b},
\]

\[
f_p(\mathbf{u}_b) \leq f_p(\mathbf{u}_a) + \sum_{i=1}^{n_u} \kappa^e_{u_i, u_{b,i}} |u_{b,i} - u_{a,i}|, \quad \forall \mathbf{u}_a, \mathbf{u}_b \in \mathcal{I}_{u_b}.
\]

**Constraint-Satisfaction Condition**

\[
g_{p,j}(\mathbf{u}_k) + \sum_{i=1}^{n_u} \kappa^e_{u_i, u_{k,i}} |u_{k,i} - u_{a,i}| \leq 0 \Rightarrow g_{p,j}(\mathbf{u}) \leq 0.
\]

**Safe-Excitation Condition**

\[
g_{p,j}(\mathbf{u}_k) + \delta_e \|\kappa^e_{p,ji}\|_2 \leq 0 \Rightarrow g_{p,j}(\mathbf{u}) \leq 0, \quad \forall \mathbf{u} \in \mathcal{B}_e.
\]

**Bounding Values**

\[
\ell_p(\mathbf{u}_k) := \max_{k=0, \ldots, k} \left( \ell_p(\mathbf{u}_k) - \sum_{i=1}^{n_u} \kappa^e_{u_i, u_{k,i}} |u_{k,i} - u_{a,i}| \right) \leq f_p(\mathbf{u}_k),
\]

\[
f_p(\mathbf{u}_k) \leq \min_{k=0, \ldots, k} \left( \ell_p(\mathbf{u}_k) + \sum_{i=1}^{n_u} \kappa^e_{u_i, u_{k,i}} |u_{k,i} - u_{a,i}| \right) := f_p(\mathbf{u}_k).
\]

### 4.3. Refinement with Respect to Convexity/Concavity

Sometimes, experimental relationships are known to be either convex or concave in certain decision variables - i.e., if one were to keep all of the variables except a particular \(u_i\) constant, the experimental relationship between the function and \(u_i\) would either be convex or concave. For example, the relationship between power and current in a fuel-cell system, whose nature is almost always concave (Marchetti et al., 2011), is precisely such a case.

Letting \(\mathcal{I}^{cvx}\) and \(\mathcal{I}^{ccv}\) denote the subsets of the indices \(\{1, \ldots, n_u\}\) in which the functions are convex or concave, respectively, the following refinements to the Lipschitz bounds (5) may be made (Bunin et al., 2014a, §3.2):

\[
f_p(\mathbf{u}_b) \geq f_p(\mathbf{u}_a) + \sum_{i \in \mathcal{I}^{cvx}} \frac{\partial f_p}{\partial u_i} \bigg|_{\mathbf{u}_a} (u_{b,i} - u_{a,i}) - \sum_{i \notin \mathcal{I}^{cvx}} \kappa_i |u_{b,i} - u_{a,i}|, \quad \forall \mathbf{u}_a, \mathbf{u}_b \in \mathcal{I}.
\]
\[ f_p(u_b) \leq f_p(u_a) + \sum_{i \in F^{\text{cv}}} \left( \max \left[ \frac{\partial f_p}{\partial u_i} \bigg|_{u_a} (u_{b,i} - u_{a,i}), \frac{\partial f_p}{\partial u_i} \bigg|_{u_a} (u_{b,i} - u_{a,i}) \right] - \sum_{i \in F^{\text{cv}}} \kappa_i |u_{b,i} - u_{a,i}| \right) \]

However, it is very unlikely that the derivatives \( \frac{\partial f_p}{\partial u_i} \bigg|_{u_a} \) be known exactly in practice, and so it is better to bound the true derivatives as

\[ \kappa_i \leq \frac{\partial f_p}{\partial u_i} \bigg|_{u_a} \leq \frac{\partial f_p}{\partial u_i} \bigg|_{u_a} \leq \kappa_i \]

and to replace the \( \frac{\partial f_p}{\partial u_i} \bigg|_{u_a} (u_{b,i} - u_{a,i}) \) terms by piecewise minimums and maximums, as was done with the Lipschitz-constant terms in Section 4.1. A data-driven approach for obtaining such bounds has been proposed by Bunin et al. (2013a). In the case where no useful bounds can be found, they may be set as the Lipschitz constants (2), which then results in the Lipschitz bounds above reverting to (5) – i.e., there is no refinement.

**Lipschitz Bounds**

\[ f_p(u_b) \geq f_p(u_a) + \sum_{i \in F^{\text{cv}}} \min \left[ \frac{\partial f_p}{\partial u_i} \bigg|_{u_a} (u_{b,i} - u_{a,i}), \frac{\partial f_p}{\partial u_i} \bigg|_{u_a} (u_{b,i} - u_{a,i}) \right] \]

Constraint-Satisfaction Condition

\[ g_{p,j}(u_k) + \sum_{i \in F_{p,j}^{\text{cv}}} \max \left[ \frac{\partial g_{p,j}}{\partial u_i} \bigg|_{u_k} (u_i - u_{k,i}), \frac{\partial g_{p,j}}{\partial u_i} \bigg|_{u_k} (u_i - u_{k,i}) \right] \]

\[ + \sum_{i \in F_{p,j}^{\text{cv}}} \kappa_{p,j} |u_i - u_{k,i}| \leq 0 \Rightarrow g_{p,j}(u) \leq 0. \]

Safe-Excitation Condition

\[ g_{p,j}(u_k) + \delta_c \| (\kappa_{p,j})^* \|_2 \leq 0 \Rightarrow g_{p,j}(u) \leq 0, \forall u \in \mathcal{B}_c \cap \mathcal{I}, \]
4.4. Combined Refinement Results

Lipschitz Bounds

Bounding Values

\[ \kappa_{p,j} := \max \left( \frac{\partial g_{p,j}}{\partial u_i} |_{u_a} \right), \quad i \in I_{p,j}^{cv}, \]

\[ \kappa_{p,j} := \max \left( \frac{\partial g_{p,j}}{\partial u_i} |_{u_a} \right), \quad i \notin I_{p,j}^{cv}. \]

\[
\begin{align*}
f_p(u_k) := \max_{k=0,\ldots,k} \left( f_p(u_k) + \sum_{i \in I_{p,k}^{cv}} \min \left[ \frac{\partial f_p}{\partial u_i} \big|_{u_k} (u_{k,i} - u_{k,i}), \quad \frac{\partial f_p}{\partial u_i} \big|_{u_k} (u_{k,i} - u_{k,i}) \right] \right) \leq f_p(u_k), \\
f_p(u_k) \leq \min_{k=0,\ldots,k} \left( T_p(u_k) + \sum_{i \in I_{p,k}^{cv}} \max \left[ \frac{\partial f_p}{\partial u_i} \big|_{u_k} (u_{k,i} - u_{k,i}), \quad \frac{\partial f_p}{\partial u_i} \big|_{u_k} (u_{k,i} - u_{k,i}) \right] \right) := T_p(u_k).
\end{align*}
\]

4.4. Combined Refinement Results

The three refinements discussed just above may be combined and their potential benefits may be superposed. The derivations consist in simple algebra and need not be done out here, with most of the results fairly intuitive.

Lipschitz Bounds

\[
\begin{align*}
f_p(u_a) & \geq f_p(u_a) + \sum_{i \in I_{p,a}^{cv}} \min \left[ \frac{\partial f_p}{\partial u_i} \big|_{u_a} (u_{a,i} - u_{a,i}), \quad \frac{\partial f_p}{\partial u_i} \big|_{u_a} (u_{a,i} - u_{a,i}) \right] \quad (28) \\
& \quad + \sum_{i \notin I_{p,a}^{cv}} \min \left[ \frac{\kappa_{a,i}}{\kappa_{a,i}} (u_{a,i} - u_{a,i}), \quad \frac{\kappa_{a,i}}{\kappa_{a,i}} (u_{a,i} - u_{a,i}) \right], \quad \forall u_a, u_b \in T_{u_a}^{u_b}, \\
f_p(u_a) & \leq f_p(u_a) + \sum_{i \in I_{p,a}^{cv}} \max \left[ \frac{\partial f_p}{\partial u_i} \big|_{u_a} (u_{a,i} - u_{a,i}), \quad \frac{\partial f_p}{\partial u_i} \big|_{u_a} (u_{a,i} - u_{a,i}) \right] \quad (29) \\
& \quad + \sum_{i \notin I_{p,a}^{cv}} \max \left[ \frac{\kappa_{a,i}}{\kappa_{a,i}} (u_{a,i} - u_{a,i}), \quad \frac{\kappa_{a,i}}{\kappa_{a,i}} (u_{a,i} - u_{a,i}) \right], \quad \forall u_a, u_b \in T_{u_a}^{u_b},
\end{align*}
\]
\[
\begin{aligned}
&\sum_{i=1}^n u_i u_k \leq \frac{\partial f_p}{\partial u_i}|_{u_k} \leq \sum_{i=1}^n u_i u_k, \quad \forall u \in T_u^u. \\
\text{Constraint-Satisfaction Condition} \\
&g_{p,j}(u_k) + \sum_{i \in I_{p,j}^{cv}} \max \left[ \frac{\partial g_{p,j}}{\partial u_i}|_{u_k} (u_i - u_{k,i}), \frac{\partial f_0}{\partial u_i}|_{u_k} (u_i - u_{k,i}) \right] \\
&\quad + \sum_{i \notin I_{p,j}^{cv}} \max \left[ \frac{\partial g_{p,j}}{\partial u_i}|_{u_k} (u_i - u_{k,i}), \frac{\partial f_0}{\partial u_i}|_{u_k} (u_i - u_{k,i}) \right] \leq 0 \Rightarrow g_{p,j}(u) \leq 0. \\
\text{Safe-Excitation Condition} \\
&(k_e^{p,j})^* = \left\{ \begin{array}{ll}
\max \left( \left| \frac{\partial g_{p,j}}{\partial u_i}|_{u_k} \right|, \left| \frac{\partial f_0}{\partial u_i}|_{u_k} \right| \right), & i \in I_{p,j}^{cv}, \\
\max \left( |k_e^{p,j}|, |\kappa_e^{p,j}| \right), & i \notin I_{p,j}^{cv},
\end{array} \right. \\
&k_e^{p,j} \leq \frac{\partial g_{p,j}}{\partial u_i}|_{u_k} \leq \kappa_e^{p,j}, \quad \forall u \in B_c, \\
\text{Bounding Values} \\
f_p(u_k) := \max_{k=0, \ldots, k} \left( f_p(u_k) + \sum_{i \in I_{p,j}^{cv}} \min \left[ \frac{\partial f_0}{\partial u_i}|_{u_k} (u_{k,i} - u_{k,i}), \frac{\partial f_0}{\partial u_i}|_{u_k} (u_{k,i} - u_{k,i}) \right] \right) \leq f_p(u_k), \\
&\quad + \sum_{i \notin I_{p,j}^{cv}} \min \left[ \frac{\partial g_{p,j}}{\partial u_i}|_{u_k} (u_{k,i} - u_{k,i}), \frac{\partial g_{p,j}}{\partial u_i}|_{u_k} (u_{k,i} - u_{k,i}) \right] \\
&f_p(u_k) \leq \min_{k=0, \ldots, k} \left( f_p(u_k) + \sum_{i \in I_{p,j}^{cv}} \max \left[ \frac{\partial f_0}{\partial u_i}|_{u_k} (u_{k,i} - u_{k,i}), \frac{\partial f_0}{\partial u_i}|_{u_k} (u_{k,i} - u_{k,i}) \right] \right) : = f_p(u_k).
\end{aligned}
\]
5. The Setting and Estimation of Lipschitz Constants

Setting the Lipschitz constants in implementation so that they satisfy (2) or, more generally, (30) is usually not trivial and requires some care. As already mentioned, choosing constants that do not satisfy these inequalities potentially makes the aforementioned techniques invalid because of the possibility that the corresponding Lipschitz bounds may no longer hold. At the same time, as discussed in the beginning of Section 4, satisfying the inequalities with too much conservatism may affect performance undesirably.

It is thus the goal of this section to offer some insight into how one may set and refine the Lipschitz constants intelligently. We begin with the special and desirable case where these constants are easily known from the physical laws governing a given experimental system (Section 5.1). Unfortunately, as there exists no means to rigorously guarantee that the Lipschitz constants chosen for a general experimental function be correct, one must inevitably turn to heuristic methods in the general case, and some of these are discussed in Sections 5.2-5.3. Despite lacking the desired rigor, the methods proposed are not doomed to failure for this reason, and can certainly be applied with success, as has been demonstrated with some empirical evidence from both simulated and experimental case studies. This last point is discussed in Section 5.4.

5.1. Setting Lipschitz Constants by Exploiting Physical Laws

Virtually all experimental relationships are subject to physical laws, and for some relationships such laws are so well known and documented that they may be assumed to hold, with their existence exploited in setting the Lipschitz constants. A simple example previously employed by the authors is the exchange of heat between a heating and heated element – e.g., a jacket (heating element) surrounding a reactor (heated element). If the temperature of the heated element is an experimental function, and the temperature of the heating element is one of the decision variables under the user’s control, then much can be said about the sensitivity relating the changes in the temperatures of the two. For very many systems, it would be expected that raising the temperature of the heating element will raise the temperature of the heated element, and that, symmetrically, lowering the temperature of one will lead to a lower temperature in the other. As such, the sensitivity would always be positive, and the lower Lipschitz constant, $\kappa$, could safely be set to 0. Additionally, heat losses are likely to ensure that a change in the temperature of the heating element will lead to a smaller change in temperature in the heated one, thus allowing us to set $\overline{\kappa}$ as 1.

While this particular example is somewhat trivial, there are others that are less so. For example, in the solid oxide fuel-cell system where one manipulates the current while needing to respect a lower-limit constraint on the cell voltage (Marchetti et al., 2011), it is known that the relationship between voltage and current is always inverse proportional, thus allowing one to set the corresponding $\overline{\kappa}$ as 0. And although the physical laws could not tell us the value of $\underline{\kappa}$ in this case, one could nevertheless rely on the multitude of available experimental data
to come up with a good estimate. For the polymerization example of Section 2.4, one may know that both extended heating (increased u₁), together with shortened cooling (decreased u₂) and thus increased temperature, will generally lead to a favorization of the termination reactions and shorter polymer chains, thus resulting in a final product with a lower molecular weight. This knowledge may then be used to set the Lipschitz constants accordingly.

Identifying such relationships and their relevance to the setting of Lipschitz constants may be an important step to include in the experimental and theoretical work that normally goes into understanding a given system prior to optimization.

5.2. Model-Based Estimation

Many of the relationships that appear in experimental optimization problems will have undergone a fair amount of theoretical investigation, resulting in first-principles parametric models being available for them:

\[ f_p(\mathbf{u}) \approx f_p(\mathbf{u}, \theta), \]

where the uncertain parameters are assumed to belong to a bounded set, \( \Theta \).

If the assumption of parametric uncertainty is not too egregious, and if the uncertainty set \( \Theta \) is not too erroneously defined, then a reasonable choice of the Lipschitz constants in (30) may be obtained by minimizing and maximizing the derivatives of the model over \( I_{u_{ia}, u_{ib}} \) and \( \Theta \):

\[ \kappa_{u_{ia}, u_{ib}} := \arg \min_{\mathbf{u} \in I_{u_{ia}, u_{ib}}} \max_{\theta \in \Theta} \left| \frac{\partial f_p}{\partial \mathbf{u}_i} \right|_{\mathbf{u}, \theta}, \]  

(35)

\[ \kappa_{u_{ia}, u_{ib}} := \arg \max_{\mathbf{u} \in I_{u_{ia}, u_{ib}}} \min_{\theta \in \Theta} \left| \frac{\partial f_p}{\partial \mathbf{u}_i} \right|_{\mathbf{u}, \theta}. \]  

(36)

While solving these optimization problems may not be trivial, it is conceivable that they would be solved off-line prior to any optimization algorithm being applied, thus making the associated computational burdens of lesser concern. If an additional layer of safety is desired, one can heuristically lower and increase the estimates of (35) and (36), respectively – for example, by either doubling or halving them, as appropriate.

For the very general case where no model is available, one could still apply the above approach but in a data-driven fashion. One could, for example, construct a linear or quadratic model from several obtained measurements, choose \( \theta \) as the coefficients of the model, let their confidence intervals define \( \Theta \) (Montgomery, 2012, §10.5), and then apply (35) and (36).
5.3. Refinement of Estimates via Data-Driven Consistency Checks

The previous two sections have addressed the problem of setting Lipschitz constants when none are initially provided. Now, let us consider a technique for refining these initial estimates so that they are consistent with the obtained data. To keep things as simple as possible, we will focus on just the upper Lipschitz bound of (5) in its rudimentary form – prior to any refinements of Section 4, although these could certainly be incorporated.

Suppose now that we have obtained an estimate of a valid set of Lipschitz constants, denoted by $\hat{\kappa}_i$, and as such have the hypothetically valid bound

$$f_p(u_a) \leq f_p(u_b) + \sum_{i=1}^{n_u} \hat{\kappa}_i |u_{b,i} - u_{a,i}|, \quad \forall u_a, u_b \in I.$$  \hfill (37)

Although there exists no way to prove the validity of (37) for an experimental function $f_p$ in the general case, we can and should make sure that this bound is at least satisfied for those experimental measurements that have been collected.

Letting $k_1$ and $k_2$ denote two (different) indices, a basic consistency-check algorithm would consist of the following two steps being carried out for every combination $(k_1, k_2)$ of $k_1, k_2 \in [0, ..., k]$:

(i) Check if the inequality

$$f_p(u_{k_2}) \leq f_p(u_{k_1}) + \sum_{i=1}^{n_u} \hat{\kappa}_i |u_{k_2,i} - u_{k_1,i}|$$  \hfill (38)

is satisfied.

(ii) If (38) is satisfied, proceed to the next $(k_1, k_2)$ combination. Otherwise, increase the values of $\hat{\kappa}_i$ by a preset, strictly positive quantity and return to (i).

It is easy to show that such an algorithm will terminate with $\hat{\kappa}_i$ values that are consistent with the obtained data. There is no apparent “best way” to increase the $\hat{\kappa}_i$ values when they are not consistent, and so here one would rely on heuristics (e.g., doubling the values, although more robust schemes may be proposed (Bunin et al., 2014a, §3.5.3)).

5.4. Empirical Evidence for Lipschitz-Constant Estimation

Clearly, since Lipschitz constants are often unknown, it is difficult to test, in any sort of closed-loop manner, whether different estimation methods are actually successful at identifying proper values for these constants in practice. Instead, one may apply the methods during the solution procedure of (1) and see if the problem is solved in a satisfactory manner. When the problem comes with experimental constraints, the strongest criterion is to verify that the constraints were met during optimization – if they were not, then this is strong evidence for poor estimates, as it suggests that the constraint-satisfaction condition (6) was
not valid. The speed of decrease in the cost function value is another telling criterion – if progress is very slow, then this may be a sign of the estimates being too conservative. In other cases, the quality of the estimates may be difficult to evaluate, although strange behavior during optimization may be an indicator that the constants are not being estimated properly. To date, much of the available empirical evidence for the effectiveness of Lipschitz-constant estimation methods comes from problems that have been tackled by the SCFO solver (Bunin, 2015), as this solver incorporates almost all of the techniques discussed in this paper and relies heavily on the Lipschitz constants to operate.

Of the experimental results available, perhaps the most telling are those obtained in the experimental optimization of a laboratory solid-oxide fuel cell stack (François & Bonvin, 2014), where no theoretical model was used and the Lipschitz constants were initialized using a data-driven model and the methods of Section 5.2, before being refined by consistency checks as more data became available. Of the limited results reported, one does see that the estimation is sufficiently good from the safety perspective – the constants are conservative enough so as to keep the system from violating its two experimental constraints, and a close-to-optimal system efficiency is achieved without requiring too many iterations, the latter point suggesting that the constants are not too conservative.

Other experimental results have been obtained by applying an earlier version of the SCFO to the problem of run-to-run controller tuning, where the tuning parameters of the controllers were treated as the decision variables, with different trajectory tracking metrics defined to judge controller performance for a given setpoint profile (Bunin et al., 2013b). The solver managed to successfully autotune a model-predictive controller for a water-tank system and a fixed-order controller for a mechanical torsional plant – however, these results are less validating since no experimental constraints were present and so it was impossible to evaluate the quality of the Lipschitz-constant estimates with regard to their ability to enforce constraints. At the same time, the constants for the experimental cost function were used to help filter out the measurement variance/noise, to limit the search space, and to place bounds on the experimental derivative estimates as detailed in Section 3, and this is likely to have aided in the optimization (though there is no way to say how much, since testing the quality of the estimators was not the goal of this largely proof-of-concept study). Once again, no a priori models were used – the solver constructed a data-driven model from \( n_u + 1 \) initial experiments, and then refined the initial estimates via the consistency checks.

In simulated tests, a good quantity of results is now available for a number of case-study test problems, including six with experimental constraints, courtesy of the ExpOpt database (Bunin, 2016b). Examining the results of the SCFO solver for these problems shows that the current estimation methods employed by the solver are certainly not perfect, and one can indeed have Lipschitz-constant estimates that are not valid and that allow for constraint violations, although this varies significantly from problem to problem. For certain problems, the estimates are consistently good and violations are minimal, with the violations being of very small magnitude even when they are present.
For other problems, violations may be larger and more frequent, but it is nevertheless rare to see consistently large constraint violations, suggesting that consistency checks are eventually able to improve on poor initial estimates.

With regard to results not obtained with the SCFO solver, an application of a data-driven approach of Section 5.2 has recently been reported by Bunin (2016a). Here, a modification of G. E. P. Box’s evolutionary-operation method (Box & Draper, 1969) was proposed, with the Lipschitz bound used to ensure that the experiments carried out by the algorithm would never violate the problem constraints. After each set of \(2n_a\) axially distributed experiments, the Lipschitz constants were estimated locally as the derivatives of a linear model for the \(2n_a + 1\) axial-plus-center data points, with additional conservatism added to the estimates to account for noise and nonlinearity effects. The end result was very satisfactory – in testing the algorithm for three problems from the ExpOpt database, the estimated Lipschitz constants were always sufficiently conservative and the experimental constraints were not violated even once. While this method comes at the price of a relatively large number of experiments and slow progression to the optimum, it does present an alluring candidate for those problems that both require a simple algorithm (arguably the most attractive trait of Box’s method) and demand stringent constraint satisfaction at all experiments.

6. Concluding Remarks

It is the authors’ hope that the present document has helped convince the reader that Lipschitz constants – despite being an implicit, age-old mathematical concept – may be made explicit and thereby bring multiple benefits to the experimental optimization domain. Most importantly, the use of these constants appears to offer an extremely simple way to guarantee constraint satisfaction in problems with experimental constraints, which is something that may be exploited during both the optimization and data-collection (excitation) phases of the solution process. Because constraint satisfaction may be immensely important in experimental settings, this alone presents a very strong argument for the implementation of Lipschitz constants and bounds. However, multiple additional uses of the constants – to restrict the experimental space, to help filter out measurement error, and to bound the experimental derivative domain during derivative estimation – may be beneficial as well and serve to strengthen the argument further. There are no major implementation difficulties involved with the techniques described, and so it is the authors’ recommendation that these techniques be made a part of a “standard protocol” when approaching experimental optimization problems, even if a single such protocol may not be well-defined or agreed upon at the time of writing.

This paper has also addressed the two major concerns regarding the use of Lipschitz constants in practice – the concern that the set constants may be too conservative and the concern that the task of setting them may be difficult. Both are, of course, valid and represent potential issues. However, as has been shown in Section 4, there do exist several ways to reduce conservatism
– namely, one may refine the bounds by exploiting direction, locality, and
the potential convexity/concavity properties of the function. With regard to
estimation, Section 5 has outlined a number of methods to set and refine
the Lipschitz-constant estimates, and empirical evidence has shown that such
methods can, in fact, be sufficient for many problems.

Despite the different arguments for incorporating the Lipschitz bounds into
the experimental optimization setting as a matter of routine, the use of these
bounds is not at all standard now and is mainly limited to the context of the
SCFO solver (Bunin, 2015). Some researchers have picked up on the idea
and have used it (Jun et al., 2015; Serralunga et al., 2013), but widespread
acceptance is still very far off. It is hoped that the techniques outlined and
argued for here will help lay the foundations of a new standard practice.

Acknowledgements

The authors would like to thank Professor Dominique Bonvin of the
Laboratoire d’Automatique (École Polytechnique Fédérale de Lausanne) for his
insights and input.

References


for Process Improvement*. John Wiley & Sons.

Box, G., & Wilson, K. (1951). On the experimental attainment of optimum

University Press.

Optimizing Control*. Imperial College Press.

Guide (version 0.91.2)*. Http://www.ccapprox.info/#soft.

a general theory with application to experimental optimization.


