Constraint Back-Offs for Safe, Sufficient Excitation: A General Theory with Application to Experimental Optimization

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Abstract

In many experimental settings, one is tasked with obtaining information about certain relationships by applying perturbations to a set of independent variables and noting the changes in the set of dependent ones. While traditional design-of-experiments methods are often well-suited for this, the task becomes significantly more difficult in the presence of constraints, which may make it impossible for one to sufficiently excite the experimental system without incurring constraint violations. The key contribution of this paper consists in deriving back-off sizes for the constraints that are sufficient to guarantee that one can always perturb in a ball of radius \( \delta \) without leaving the constrained space, with \( \delta \) set by the user. Additionally, this result is exploited in the context of experimental optimization to propose a constrained version of G. E. P. Box’s evolutionary operation technique. The proposed algorithm is then applied to three case studies and is shown to consistently converge to the neighborhood of the optimum without violating any of the problem constraints.

Keywords: design measures for robustness, sufficient excitation, evolutionary operation, optimization under uncertainties, experiment design

1 Introduction

Systems where the relationship between some experimental response and a finite number of independent variables needs to be studied are found in most branches of science (Myers et al., 2009; Montgomery, 2012), and it is generally assumed that the response is a dependent variable and a function of the independent ones. Allowing this, one may write the experimental quantity as \( f(u) \), with \( u \in \mathbb{R}^n \) used to denote the vector of independent variables \( u = (u_1, ..., u_n) \). Having established these mathematical foundations, one is then left with the job of identifying \( f : \mathbb{R}^n \rightarrow \mathbb{R} \), either locally or globally, by conducting a series of experiments with different values of \( u \), observing the resulting \( f(u) \) values, and often performing some sort of regression. Such procedures are typically used to:

(i) construct data-driven model approximations of \( f \) for when \( f \) is difficult to model via first principles (Jones et al., 1998; Myers et al., 2009; Montgomery, 2012),

(ii) estimate the uncertain parameters of an already available model (Box, 1990; Chen & Joseph 1987; Pfaff et al., 2006; Quelhas et al., 2013).

(iii) explore how the function changes so as to find conditions where it is minimized, maximized, or achieves a certain value (Robbins & Monro, 1951; Box & Wilson, 1951; Lewis et al., 2000; Conn et al., 2009).

It is the case for many problems that the experimental space of interest is a box defined by the constraints \( u_i^L \leq u_i \leq u_i^U \), \( i = 1, ..., n_u \), where \( u^L = (u_1^L, ..., u_n^L) \) and \( u^U = (u_1^U, ..., u_n^U) \) are the lower and upper limits on the independent variables, respectively. Such problems typically correspond to simple set-ups that do not possess major safety limitations, and where testing any variable combination in the experimental space is permissible. Obtaining knowledge about \( f \) is not difficult in such conditions, and the traditional design-of-experiments techniques (Montgomery, 2012) are perfectly appropriate here.

However, there still exists a fair share of problems – many of them corresponding to continuous or batch chemical processes (Bunin, 2015) – where additional constraints enter to reduce the experimental space in a nontrivial manner. These constraints may be expressed as the \( n_g \) inequalities

\[
g_j(u) \leq 0, \ j = 1, ..., n_g.
\]
In some problems, the functions \( g_j \) may represent experimental relationships that, like \( f \), can only be made clear by experimentation. It often happens that such experimental constraints are safety or economic limitations – they could, for example, represent an upper limit on the temperature in a continuous reactor, or a lower limit on the purity of a batch-produced chemical. Despite violation of such constraints being highly undesirable, or even dangerous, there currently exists no theoretically rigorous method for guaranteeing that the perturbations carried out on the system satisfy these constraints, with virtually every method developed to date accepting constraint violation as a potential side effect, oft unavoidable, of the perturbation procedure.

The present work simplifies and generalizes results previously reported in the unpublished document of Bunin et al. (2014a) to derive positive back-off values, \( b_j \), so that, for a given \( u^* \), one has the guarantee

\[
g_j(u^*) \leq -b_j \Rightarrow g_j(u) \leq 0, \quad \forall u \in B_c, \tag{1}
\]

where \( B_c = \{ u : \| u - u^* \|_2 \leq \delta_e \} \). Verbally, this means that given a variable set \( u^* \) known to satisfy the constraints with some slack, one is able to provide a guarantee that the entire ball of radius \( \delta_e \) surrounding \( u^* \) will satisfy the constraints as well, thereby allowing the user to perturb anywhere within this ball without fear of constraint violation. Despite being local, such a result is nevertheless very useful as it allows a high degree of freedom – a ball being sufficient to allow for perturbation of any geometry. As will be shown, the value \( b_j \) will depend on the local sensitivities of \( g_j \) around \( u^* \), but can nevertheless be computed without requiring much effort from the user. Conversely, \( \delta_e \) is the sole tuning parameter set by user and represents, in some sense, the magnitude of perturbation considered as “sufficiently exciting” for identification given the particular problem.

To date, this result has already been integrated into the SCFO experimental optimization solver (Bunin et al., 2014c), where it is used to ensure accurate linear and quadratic regression. However, it is expected that the generality of the result make it applicable to many algorithms and contexts. In this paper, its usefulness is illustrated for a much simpler optimization algorithm – the evolutionary operation (EVOP) method of Box (1957; Box & Draper, 1969). As the original method searches to maximize an experimental function (Box, 1957; Box & Draper, 1969), it is made coherent with the result here by ensuring that the cube lie inside \( B_c \), with \( u^* \) then defined as the best known reference point. By forcing \( u^* \) to always satisfy (1), it thus follows that all exploration by the modified EVOP version satisfy the constraints.

The remainder of this paper is organized as follows. All of the required mathematical preliminaries are presented in Section 2. Section 3 then provides the derivation of the back-off values sufficient for (1), with a robust extension of the conditions that accounts for noise/error in the function values provided in Section 4, together with a general discussion of implementation issues. The constrained EVOP algorithm is presented in Section 5, and its effectiveness is illustrated for three case-study problems. Section 6 concludes the paper.

## 2 Mathematical Preliminaries

So as to keep the forthcoming analysis relatively simple, the following assumption on the continuity and differentiability of \( g_j \) is made.

**Assumption 1** The functions \( g_j \) are twice continuously differentiable (\( C^2 \)) on an open set containing \( B_c \).

This then allows for the definition of bounds on the sensitivities of \( g_j \).

**Definition 1** The local Lipschitz constants of \( g_j \) are defined as constants \( \kappa_{ji} \) satisfying

\[-\kappa_{ji} \leq \frac{\partial g_j}{\partial u_i}\bigg|_{u} \leq \kappa_{ji}, \quad \forall u \in B_c. \tag{2}\]

The existence of these constants follows from Assumption 1 and the boundedness of \( B_c \).

The local Lipschitz upper bound for a given function \( g_j \) follows.

**Lemma 1** Let \( u_a, u_b \in B_c \). It follows that

\[ g_j(u_b) \leq g_j(u_a) + \sum_{i=1}^{n_u} \kappa_{ji} |u_{b,i} - u_{a,i}|. \tag{3} \]

**PROOF.** See Bunin et al. (2014b). \( \Box \)

Finally, the Lipschitz bound may be exploited with \( u_a = u^* \) to generate a Lipschitz polytope around the point \( u^* \).

**Definition 2** Let \( \mathcal{L}_j \) denote the Lipschitz polytope of constraint \( g_j \) around \( u^* \), defined as the set

\[ \mathcal{L}_j = \left\{ u : g_j(u^*) + \sum_{i=1}^{n_u} \kappa_{ji} |u_i - u^*| \leq 0 \right\}. \tag{4} \]

The Lipschitz polytope has two important properties that should be apparent by inspection:

(i) \( u \in \mathcal{L}_j \cap B_c \Rightarrow g_j(u) \leq 0 \),
(ii) \( g_j(u^*) \leq 0 \Rightarrow \mathcal{L}_j \neq \emptyset \).
Fig. 1. Geometric illustration of the concept behind using back-offs to enforce the existence of an excitation ball $B_e$. The back-off is chosen large enough so that a ball of radius $\delta_e$ may be inscribed inside the Lipschitz polytope corresponding to the back-off.

Furthermore, it is clear that the size of $L_j$ grows monotonically as $g_j(u^*)$ decreases – i.e., $L_j$ admits more and more points because of the summation term being allowed to grow larger while satisfying the inequality.

It is this observation that inspires the foundations of the present work, illustrated geometrically in Figure 1. If $g_j(u^*)$ can be forced to remain sufficiently low – i.e., $L_j$ is monotonic – then one can always guarantee the existence of a non-empty Lipschitz polytope centered at $u^*$. Additionally, because the ball $B_e$ is also centered at $u^*$, it may be inscribed inside the polytope, with Property (i) above then sufficient to guarantee that all points in this ball satisfy the constraint $g_j(u) \leq 0$.

Before proceeding with the derivation of the minimum back-off sizes sufficient to guarantee the feasibility of $B_e$, let us conclude this section with the following preliminary lemma.

**Lemma 2** The equivalence

$$B_e \subseteq L_j \Leftrightarrow \text{bd}(B_e) \subseteq L_j$$

holds, with $\text{bd}(B_e)$ denoting the boundary of $B_e$.

**PROOF.** The forward implication,

$$B_e \subseteq L_j \Rightarrow \text{bd}(B_e) \subseteq L_j,$$

is trivial since $\text{bd}(B_e) \subseteq B_e$. For the other direction, note that (a) $L_j$ is a convex set and (b) any point in the interior of $B_e$ may be written as a convex combination of the boundary points of $B_e$. Because the convex combination of any two points in a convex set must also belong to that set, it follows that the interior of $B_e$ lie in $L_j$ as well. $\square$

### 3 Derivation of Sufficient Back-Offs

The key theoretical result of the paper is stated and derived in the following theorem.

**Theorem 1** Let the point $u^*$ satisfy $g_j(u^*) \leq -b_j$. Defining $\kappa_j$ as the vector $(\kappa_{j1}, ..., \kappa_{jn_u})$ and setting the back-off as

$$b_j := \delta_e \|\kappa_j\|_2$$

guarantees that $g_j(u) \leq 0$, $\forall u \in B_e$.

**PROOF.** The proof is done by showing that $\text{bd}(B_e) \subseteq L_j$ and exploiting Lemma 2. First, let us parameterize the boundary points of $B_e$ as

$$u_{bd} = u^* + \delta_e \Delta u,$$

where $\Delta u \in \mathbb{R}^{n_u}$ is a unit vector. Since the mapping between $u_{bd}$ and $\Delta u$ is bijective, one may prove that $\text{bd}(B_e) \subseteq L_j$ by showing that $u_{bd} \in L_j$ for any choice of $\Delta u$. Since the statement $u_{bd} \in L_j$ is equivalent to the inequality of (4) holding for $u_{bd}$, $u_{bd}$ is substituted into the inequality to obtain

$$g_j(u^*) + \sum_{i=1}^{n_u} \kappa_{j|i} |u_{bd,i} - u_{i}^*| \leq 0$$

$$\Leftrightarrow g_j(u^*) + \delta_e \sum_{i=1}^{n_u} \kappa_{j|i} |\Delta u_{i}| \leq 0.$$  \hspace{1cm} (5)

To prove that this inequality holds for all $\Delta u$, it is sufficient to only consider the vector $\Delta u$ that maximizes the summation term:

$$g_j(u^*) + \delta_e \max_{\|\Delta u\|_2 = 1} \sum_{i=1}^{n_u} \kappa_{j|i} |\Delta u_{i}| \leq 0.$$  \hspace{1cm} (6)

To simplify the analysis, it is first shown that the maximum is achieved on the positive orthant ($\Delta u \in \mathbb{R}_{+}^{n_u}$), with

$$\max_{\|\Delta u\|_2 = 1} \sum_{i=1}^{n_u} \kappa_{j|i} |\Delta u_{i}| = \max_{\Delta u \geq 0} \sum_{i=1}^{n_u} \kappa_{j|i} |\Delta u_{i}|.$$


To prove this, suppose by contradiction that there exists a unit vector $\Delta v \notin \mathbb{R}_+^n$ such that

$$\sum_{i=1}^{n_u} \kappa_{ji} |\Delta v_i| > \max_{\|\Delta u\|_2^2=1} \sum_{i=1}^{n_u} \kappa_{ji} |\Delta u_i|. \quad (6)$$

Clearly, the choice $\Delta u_i := |\Delta v_i|$, $i = 1, ..., n_u$ shows that there exists a unit vector $\Delta u \in \mathbb{R}_+^n$ with a value equal to the left-hand side of (6), thereby proving that (6) cannot hold for any choice of $\Delta v$. The inequality of (5) may thus be simplified to

$$g_j(u^*) + \delta_c \max_{\|\Delta u\|_2^2=1} \sum_{i=1}^{n_u} \kappa_{ji} |\Delta u_i| \leq 0 \quad (7)$$

$$\Leftrightarrow g_j(u^*) + \delta_c \max_{\|\Delta u\|_2^2=1} \kappa_j^T \Delta u \leq 0. \quad (7)$$

The maximum term may be upper bounded by relaxing the constraints to which it is subject. Let us thus consider a more restricting inequality:

$$g_j(u^*) + \delta_c \max_{\|\Delta u\|_2^2\leq 1} \kappa_j^T \Delta u \leq 0, \quad (8)$$

the satisfaction of which implies the satisfaction of (7). As the evaluation of the maximum term is now equivalent to maximizing a linear function over a unit sphere, writing out the stationary conditions for such a problem readily yields the solution

$$\frac{\kappa_j}{\|\kappa_j\|_2} = \arg \max_{\Delta u} \kappa_j^T \Delta u$$

subject to $\Delta u^T \Delta u \leq 1,$

which, when substituted into (8), yields the more tractable form

$$g_{p,j}(u^*) + \delta_c \|\kappa_j\|_2 \leq 0.$$

It is evident that this condition holds given the definition of the back-off and the assumption that $g_j(u^*) \leq -b_j$, and proves that $bd(B_c) \subseteq L_j$, which implies $B_c \subseteq L_j$ by Lemma 2. This leads to the conclusion that $B_c \cap L_j = B_c$, which by Property (i) of the Lipschitz polytope finally yields the desired result. □

4 Implementation Issues

On the surface, the result seems easy to implement as it simply states that if one wants to perturb anywhere in $B_c$ without fear of constraint violation, one only needs to ensure that $g_j(u^*) \leq -\delta_c \|\kappa_j\|_2$, $\forall j$. Conversely, if no such $u^*$ is available, $\delta_c$ may be decreased until $g_j(u^*) \leq -\delta_c \|\kappa_j\|_2$, $\forall j$ holds, which clearly must occur for $\delta_c > 0$ sufficiently small unless one of the constraints is right on its boundary. However, there remain a number of implementation aspects that merit discussion.

4.1 Setting of Lipschitz Constants

Theorem 1 provides a robust guarantee only if it is assumed that the Lipschitz constants provided satisfy (2). While one can argue that picking very large, conservative values is sufficient, this has the obvious performance drawback of increasing $b_j$, which could make satisfying $g_j(u^*) \leq -b_j$ impossible. As such, one would prefer more intelligent ways of setting these constants.

Apart from some scarce and limited results in the global optimization literature (Hansen et al., 1992; Strongin, 1973; Wood & Zhang, 1996), the problem of how to estimate these constants effectively is still very open. A number of techniques have been proposed in Section 3 of [Bunin et al., 2014a], and generally suggest mixing a priori knowledge about the functions $g_j$, which may provide good initial guesses of the constants, together with data-driven refinements, which make explicit use of the fact that for a sufficiently local or nonlinear region the Lipschitz constants differ little from the local function derivatives. Such techniques have been employed in the SCFO solver [Bunin et al., 2014d] and have often led to relatively robust performance in test problems, although constraint violations do occur sometimes [Bunin, 2013].

It is worth noting that the EVOP method proposed in Section 5 appears to handle this issue very well, using iterative local linear regression to estimate the Lipschitz constants in a manner that requires no input from the user and yet avoids constraint violation completely.

4.2 Accounting for Noise/Error

Enforcing $g_j(u^*) \leq -b_j$ relies on having accurate knowledge of $g_j(u^*)$. While it is reasonable that in most applications one will be able to either measure or estimate the values of these functions at $u^*$, for experimental functions it is generally the case that a perfect measurement or estimation will be impossible, and that access to only the corrupted values, $\tilde{g}_j(u^*)$, will be available. A typical assumption is that this corruption is additive – i.e., that
\[ g_j(u^*) = g_j(u^*) + w, \]

with \( w \) a stochastic element for which estimates of at least the mean and variance are available. In this case, it becomes possible to compute a high-probability bound \( g_j(u^*) \leq \overline{g}_j(u^*) \) using, in the most general case, Chebyshev’s inequality \cite{MoreWill11}, or something less conservative if better assumptions on the nature of the noise are available. More involved techniques for computing \( \overline{g}_j(u^*) \) are also outlined in \cite{Bunin14a}.

One may then work with the robust condition \( \overline{g}_j(u^*) \leq -b_j \) instead, since satisfaction of this condition implies the satisfaction of \( g_j(u^*) \leq -b_j \) with high probability.

### 4.3 Accomodating Numerical Constraints

So far, \( g_j \) has been treated from a very general perspective, and has been assumed only to be a \( C^2 \) function over \( B_e \). However, there are plenty of constraints for which much more knowledge is available. In particular, when the constraint \( g_j \) is a numerical function that can be evaluated by hand or by computer for any desired \( u \in B_e \), the guarantee of perturbing in \( B_e \) without incurring violation of the given constraint is fairly easy. Namely, it suffices to ensure that

\[
\max_{u \in B_e} g_j(u) \leq 0,
\]

since this trivially guarantees that all perturbations in \( B_e \) are feasible for that constraint, without requiring Lipschitz constants or robust upper bounds. For some cases, it may be that \( g_j \) is an involved nonconcave function, potentially making its maximization over a ball a numerically challenging (global optimization) task. When this occurs, one could attempt to take a concave upper bound or, if worse comes to worst, estimate its Lipschitz constants – a significantly easier task for a numerical function – and then employ the general (albeit conservative) result of Theorem 1.

A special subclass of numerical constraints that is even easier to work with is that of the bound constraints, \( u^L_i \leq u_i \leq u^U_i \), which are extremely relevant since they tend to occur in virtually any well-defined experimental investigation. By simple intuition and quick inspection, one should be able to see that employing a back-off of \( \delta_e \) is sufficient for these bounds. Not surprisingly, it is possible to arrive at this same result by Theorem 1, as the \( \kappa_j \) vector for these constraints is simply a vector of \( n_u - 1 \) zeros with unity in the \( i \)th spot, thus leading to \( \delta_e \| \kappa_j \|_2 = \delta_e \).

One could, however, choose not to back off from the bound constraints since, given their orthogonal nature, one is always guaranteed to retain a full orthant in which one can perturb. Given with the feasibility of \( B_e \), this means that one could ignore these back-offs and still retain \( 1/2^n \) of \( B_e \) for safe perturbation. For most cases, this fraction of \( B_e \) still offers enough room for the user to accomplish what they aim to (e.g., to estimate a derivative or to locally explore the function’s behavior).

### 4.4 Scaling and the Tuning of the Excitation Radius

It is evident that the results provided are not scale-invariant, and that a ball of radius \( \delta_e \) could offer very poor perturbation in directions which vary over a much greater domain than others – geometrically, this may be seen as the question of efficiency of inscribing a ball inside a Lipschitz polytope. One solution could be to generalize the notion of the ball to an ellipse, and to rederive the result for this more versatile case. However, a simple approach found to work well has been to simply scale the independent variables so that each \( u_i \) varies between 0 and 1, in which case perturbing in a ball is reasonable.

This aside, one may still have to make a nontrivial decision about what \( \delta_e \) to set. Ultimately, this choice should depend on the particular problem that the user is trying to solve, with all available a priori knowledge exploited to yield an appropriate choice. For example, if the goal is to explore as much of the experimental space as possible and to build a model that encompasses a large, perhaps even global, domain, it may be of interest to set \( \delta_e \) to be as large as possible. If the goal is to perturb just enough to estimate a derivative while avoiding significant corruption due to noise, one may want to choose \( \delta_e \) as a function of the expected signal-to-noise ratio \cite{Bunin14c}.

### 5 Feasible-Side Evolutionary Operation

An evolutionary operation (EVOP) algorithm is constructed for the feasible-side solution of experimental optimization problems having the form

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

where both \( \phi \) and \( g_j \) will, in general, represent experimental functions. As in many experimental optimization problems of this type, there is a constant trade-off between adapting the decision variables \( u \) so as to minimize \( \phi \) and perturbing them so as to learn more about the local or general nature of \( \phi \) and \( g_j \). Both tasks are necessary – one cannot optimize without perturbation, but one cannot optimize if one spends all
of the experimental resources perturbing the system for knowledge, either.

This choice of application is motivated by two main reasons. First, the derived result of Theorem 1 is innately coherent with the direct-search algorithmic nature of EVOP, which iteratively perturbs in a local region and then shifts this region so that it is centered around the best found point. It is thus quite natural to let EVOP perturb in \( B \) and then shift \( \mathbf{u}^\ast \) accordingly, which immediately provides the traditional EVOP with constraint satisfaction guarantees. The second reason has to do with the practical usefulness of the constructed scheme. Ever since its inception in 1957 (Box, 1957), EVOP has enjoyed great popularity in industry, which has largely been due to its extreme simplicity. In addition to being simple, it would later be shown to be theoretically well founded as well, a slight step-size modification allowing it to enjoy the global convergence properties of Torczon’s generalized pattern search algorithms (Torczon, 1997). However, both its industrial and theoretical success has largely been limited to simple problems with bound constraints, and while one could use the standard (i.e., penalty-function) methods (Conn et al., 2000, Ch. 14) to convert problems with \( g \) constraints into the bound-constrained form for which EVOP is readily applicable, these approaches are ultimately not robust and only offer the guarantee that the constraints are satisfied upon convergence.

From this point of view, the algorithm proposed in this section is believed to carry great potential as a stand-alone contribution that, in addition to being effective for the problems tested, is also extremely easy to apply and requires minimal input from the user.

### 5.1 Description of the Algorithm

Prior to stating the algorithm, let us first make some knowledge assumptions so as to ensure its basic functionality.

First, it is assumed that, for a given tested \( \mathbf{u} \), one measures both \( \phi \) and \( g_j \) with additive white Gaussian noise:

\[
\begin{align*}
\hat{\phi}(\mathbf{u}) &= \phi(\mathbf{u}) + \phi, \quad \phi \sim \mathcal{N}(0, \sigma^2_{\phi}) \\
\hat{g}_j(\mathbf{u}) &= g_j(\mathbf{u}) + w_j, \quad w_j \sim \mathcal{N}(0, \sigma^2_j).
\end{align*}
\]

For simplicity, it will be assumed that \( \sigma_{\phi} \) and \( \sigma = (\sigma_1, \ldots, \sigma_n) \) are known.

It will also be assumed that a sufficiently “safe” initial \( \mathbf{u}^\ast \) is available, so that the \( 2n_u \) test points generated by perturbing the individual elements \( \mathbf{u}^\ast \) by \( \pm \delta_c \):

\[
\begin{align*}
& (u_1^\ast \pm \delta_c, \ldots, u_{n_u}^\ast), \\
& (u_1^\ast, u_2^\ast \pm \delta_c, \ldots, u_{n_u}^\ast), \\
& \vdots \\
& (u_1^\ast, u_2^\ast, \ldots, u_{n_u}^\ast \pm \delta_c)
\end{align*}
\]

are, together with \( \mathbf{u}^\ast \), safe and satisfy the constraints.

The scaled variables will be denoted with (\( \tilde{\cdot} \)) and defined as

\[
\tilde{u}_i = \frac{u_i - u_{L_i}}{u_{U_i} - u_{L_i}}, \quad i = 1, \ldots, n_u.
\]

This scaling step will be implicit in the algorithm statement that follows — i.e., we will switch between the scaled and unscaled variables as needed without explicitly including the affine operation above in the algorithm steps.

#### Algorithm 1 (Feasible-Side EVOP)

1. **(Initialization)** The initial reference point \( \mathbf{u}^\ast \), the standard deviations \( \sigma_{\phi} \) and \( \sigma \), and the variable bounds \( \mathbf{u}^L \), \( \mathbf{u}^U \) are provided. The excitation radius \( 0.5 \geq \delta_c > 0 \) is set by the user.

2. **(Evaluation at Reference Point)** Apply \( \mathbf{u}^\ast \) to the experimental system to obtain \( \hat{\phi}(\mathbf{u}^\ast) \) and \( \hat{g}_j(\mathbf{u}^\ast) \). Define \( \hat{\mathbf{U}} := (\hat{\mathbf{u}}^\ast)^T \), \( \phi := \hat{\phi}(\mathbf{u}^\ast) \), \( \mathbf{G} := [\hat{g}_1(\mathbf{u}^\ast) \cdots \hat{g}_n(\mathbf{u}^\ast)] \).

3. **(Perturbation)** For \( i = 1, \ldots, n_u \):
   1. \( (\text{Perturbing by } \pm \delta_c) \) Obtain \( \hat{\mathbf{u}}_+ \) and \( \hat{\mathbf{u}}_- \) by perturbing the \( i \)th element of \( \hat{\mathbf{u}} \) by \( \delta_c \) and \( -\delta_c \), respectively.
   2. **(Upper Bound Constraint Check)** If \( u_{i,+} \leq u_i^L \), apply \( \mathbf{u}_+ \) to the experimental system to obtain \( \hat{\phi}(\mathbf{u}_+) \) and \( \hat{g}_j(\mathbf{u}_+) \) and augment \( \hat{\mathbf{U}}, \phi, \) and \( \mathbf{G} \):

\[
\hat{\mathbf{U}} := \begin{bmatrix} \hat{\mathbf{U}}^T \\ \hat{\mathbf{u}}_+^T \end{bmatrix}, \quad \phi := \begin{bmatrix} \phi \\ \hat{\phi}(\mathbf{u}_+) \end{bmatrix},
\]

\[
\mathbf{G} := \begin{bmatrix} \hat{g}_1(\mathbf{u}_+) & \cdots & \hat{g}_n(\mathbf{u}_+) \end{bmatrix}.
\]

   3. **(Lower Bound Constraint Check)** If \( u_{i,-} \geq u_i^U \), apply \( \mathbf{u}_- \) to the experimental system to obtain \( \hat{\phi}(\mathbf{u}_-) \) and \( \hat{g}_j(\mathbf{u}_-) \) and augment \( \hat{\mathbf{U}}, \phi, \) and \( \mathbf{G} \):

\[
\hat{\mathbf{U}} := \begin{bmatrix} \hat{\mathbf{U}}^T \\ \hat{\mathbf{u}}_-^T \end{bmatrix}, \quad \phi := \begin{bmatrix} \phi \\ \hat{\phi}(\mathbf{u}_-) \end{bmatrix},
\]

\[
\mathbf{G} := \begin{bmatrix} \hat{g}_1(\mathbf{u}_-) & \cdots & \hat{g}_n(\mathbf{u}_-) \end{bmatrix}.
\]
A number of remarks are in order:

- As suggested in Section 4.3, no back-offs are used for the bound constraints, ensuring instead that they are never violated during the perturbation phase.
- It is not difficult to show that the derivative estimates obtained by linear regression of the local data set are, as a result of the orthogonality and symmetry of the perturbations, identical to the finite-difference estimates

\[
\frac{\partial \hat{g}_j}{\partial u_i} u^* = \frac{\hat{g}_j(u^+) - \hat{g}_j(u^-)}{2\delta c}
\]

when \(s_i = 2\), or to either

\[
\frac{\hat{g}_j(u^+) - \hat{g}_j(u^+)}{\delta c}
\]

or

\[
\frac{\hat{g}_j(u^+) - \hat{g}_j(u^-)}{\delta c}
\]

when \(s_i = 1\). It is well known (see, e.g., Daniel & Heerema (1950)) that the standard deviation for such estimates is equal to \(\sigma_j \sqrt{2/s_i \delta c}\). In adding six times this quantity to the absolute value of the derivative estimates, we use half of that amount (“three sigma”) to account for potential errors in the estimates due to noise, and the other half to compensate for the fact that the Lipschitz constants only match the derivatives very locally, and may actually be larger for the \(B_i\) at the future cycle (i.e., the Lipschitz-constants estimation is always one cycle behind).

- The quantity of \(3\sigma_j\) is added to the constraint measurements so as to robustify the scheme, with

\[
\tilde{g}_j(u) := \hat{g}_j(u) + 3\sigma_j.
\]

Because the problem addressed is constrained and uses Lipschitz bounds to guarantee robust constraint satisfaction, it follows that the scheme may converge suboptimally if it gets too close to a constraint. This issue was first observed in Bunin et al. (2011) and dealt with rigorously in Bunin et al. (2013), and represents a main drawback of using Lipschitz constants for constraint satisfaction. So as to avoid this issue here, it has been proposed to minimize an approximation of the Lagrangian instead of simply minimizing \(\phi\). Note that when \(u^*\) is far from any constraints, the scheme simply sets \(\lambda := 0\) and the two objectives are equal. However, when \(u^*\) start to get close to activity, the scheme defines the objective as a trade-off between minimizing \(\phi\) and lowering the active constraint values, which tends to allow the algorithm to “slide off” active constraints in application. The theoretical rigor of this scheme is not entirely clear, but it may be seen to be consistent upon convergence, in that finding \(\lambda\) such that \(\nabla L(u^*, \lambda) \approx 0\) implies \(u^*\) being a constrained stationary point, provided that the gradient estimates are not too erroneous.

5.2 Application to Case-Study Examples

Three problems are chosen from the ExpOpt Test Problem Database (Bunin, 2015, Problems P2, P3, P6) so as to illustrate the performance of the algorithm.

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(d) (Set Number of Points Tested) If

\[ u^L_i \leq u^*_i \pm \delta e \leq u^U_i, \]

set \(s_i := 2\). Otherwise, set \(s_i := 1\).

(4) (Local Linear Regression) Fit a linear model,

\[ \beta_0 + \sum_{i=1}^{n_u} \beta_i u_i, \]

to the observed cost function values, with the \(\beta_1, \ldots, \beta_{n_u}\) coefficients recovered as the first \(n_u\) elements of the least-squares solution \([\tilde{U}] [1] \phi\).

Set \(\nabla \hat{\phi}(\tilde{u}^*) = (\beta_1, \ldots, \beta_{n_u})\) as the estimate of the gradient of \(\phi\) at \(\tilde{u}^*\). Repeat the same with the columns of \(\mathbf{G}\) to obtain the gradient estimates \(\nabla \hat{g}_j(\tilde{u}^*)\) for \(j = 1, \ldots, n_g\).

(5) (Lipschitz Constants) For each \(i = 1, \ldots, n_u\) and \(j = 1, \ldots, n_g\), set

\[ \kappa_{ji} := \frac{\left| \frac{\partial \hat{g}_j}{\partial u_i} \right|}{\sigma_j \sqrt{2/s_i \delta e}} + 0, \]

(6) (Nearly Active Constraints) Define the index set

\[ j_A := \{ j : \hat{g}_j(u) + 3\sigma_j \geq -\delta e ||\kappa_{ji}||_2 \text{ for some } u \text{ in } U \} \]

as the index set of nearly active constraints.

(7) (Approximation of Lagrangian) Find the coefficients \(\lambda = (\lambda_1, \ldots, \lambda_{n_u})\) that satisfy

\[ \nabla L(\tilde{u}^*, \lambda) = \nabla \hat{\phi}(\tilde{u}^*) + \sum_{j=1}^{n_g} \lambda_j \nabla \hat{g}_j(\tilde{u}^*) = 0 \]

in the least-squares subject to the constraint that \(\lambda_j = 0\), \(\forall j \notin j_A\). For any \(j\) for which the least-squares solution yields \(\lambda_j < 0\), set \(\lambda_j := 0\).

(8) (Choose New Reference) Set as \(\tilde{u}^*\) the point in \(U\) that minimizes \(\nabla L(\tilde{u}^*, \lambda)^T \tilde{u}\) while ensuring that \(\hat{g}_j(u^*) + 3\sigma_j \leq -\delta e ||\kappa_{ji}||_2\), \(\forall j\). If no such \(u^*\) exists, maintain the same reference point as before. Define \(\tilde{U} := (\tilde{u}^*)^T, \phi := \hat{\phi}(u^*), \mathbf{G} := [\hat{g}_1(u^*) \cdots \hat{g}_{n_g}(u^*)]\) and return to Step 3.

A number of remarks are in order:

- As the scaling reduces the variable space to a unit hypercube, there is no need for \(\delta e\) to be set above 0.5, as this would preclude the existence of a feasible \(B_e\).
- The perturbation scheme used here differs from that of the traditional EVOP methods, which use a \(2^{n_u}\) factorial scheme to define the test points (Box, 1957; Box & Draper, 1969), and is in this sense more similar to a coordinate search (Conn et al., 2009, Ch. 7).
- The rationale for doing this is that requiring \(2^{n_u}\) perturbations leads to better efficiency as \(n_u\) increases (linear as opposed to geometrical), requires fewer perturbations for \(n_u > 2\), and appears to be sufficient for the given tasks.
Table 1
Problem specifications for the case-study examples.

| #  | Initial \( \mathbf{u}^* \) | \( \sigma_{\phi} \) | \( \sigma \) | \( \mathbf{u}^{\ell} \) | \( \mathbf{u}^{U} \) |
|----|----------------|----------------|----------|----------------|----------------|
| P2 | (3.5, 72)     | 0.5            | \( 5 \cdot 10^{-4} \) | (3, 70)        | (6, 100)       |
| P3 | (242, 945)    | 60             | \( 10^4 \)      | (50, 600)      | (450, 1000)    |
| P6 | (14.5, 14.9)  | 0.1            | (0.03, 0.03)    | (1, 1)         | (50, 50)       |

when applied to realistic case-study scenarios. The first problem consists in varying the feed rate and temperature of a Williams-Otto plant so as to maximize its steady-state profit while honoring an upper limit on a noxious product, and is originally taken from the work of Marchetti (2013). The second, adapted from the paper of François et al. (2005), deals with minimizing the operating time of a polystyrene batch reactor while honoring a minimal molecular weight specification. Here, two “switching times” that help define the temperature profile of the batch are taken as the decision variables. Finally, the third problem comes from François & Bonvin (2013) and seeks to maximize the steady-state production of a continuous reactor by varying two feed rates subject to two experimental constraints. Two-dimensional problems have intentionally been chosen as they allow for easy visualization and interpretation of the results. The different problem specifications are provided in Table 1.

Inputting the specifications into Algorithm 1, the algorithm’s performance is tested for \( \delta_e := 0.05 \). The results are given in Figure 2 and show that the algorithm is robust with regard to exploring the decision-variable space while satisfying the constraints – absolutely no violations are observed. By contrast, suppose that one tried to apply the same algorithm to Problem P2 but without the application of the robust back-off derived in Theorem 1. This is done by substituting \(-\delta_e \| \kappa \|_2 \to 0\) in Steps 6 and 8 of Algorithm 1. The result is given in Figure 3. Again, it is seen that the use of the Lagrangian leads to the algorithm successfully converging to a neighborhood of the optimum. However, constraint violations occur repeatedly along the convergence trajectory.

The convergence properties of the algorithm are of interest – in particular, one notices that the algorithm converges to a region that is relatively suboptimal in Problem P6. This is due to the geometry of the problem, the conservatism of the back-offs, and the size of the noise in the constraint measurements. In other words, the algorithm cannot make further progress while robustly (to \( 3\sigma \)) satisfying the specified back-offs. While proving convergence to an optimum in a mathematically rigorous manner is outside the scope of this paper, for \( C^2 \) functions one should expect the algorithm to converge properly if both the noise and back-offs go to 0 asymptotically, as \( \delta_e \to 0 \) would lead to the linear regression converging to the true function gradient in the absence of noise, with the removal of noise also removing

Fig. 2. Plots of the decision variables and cost function values for Problems P2 (top), P3 (middle), and P6 (bottom). Green points in the decision-variable plots denote the true optimum, red points denote the individual experiments, and blue points denote the reference (best) point at the final tested EVOP cycle. Red regions denote the infeasible (not safe) portions of the operating space as defined by the constraints. In plotting the cost function values, the blue lines denote the true (noiseless) values, while the constant black line denotes the value at the optimum.

Fig. 3. Illustration of EVOP performance for Problem P2 when the back-off is not employed.
the conservatism introduced by using the upper bounds $g_j(u) + 3\sigma_j$. To test this hypothesis empirically, let us use a modified version of Algorithm 1 where

$$
\delta_e(k) := \delta_e / \sqrt{k}, \quad \sigma_\phi(k) := \sigma_\phi / \sqrt{k}, \quad \sigma(k) := \sigma / \sqrt{k},
$$

with $k$ starting at 1 and being incremented by 1 after each cycle of the algorithm. The results are presented in Figure 4 and largely confirm one’s expectations, with feasible-side convergence very close to the optimum achieved for all problems. Although the neighborhood of convergence appears to be geometrically far from the optimum in Problem P3, this is due to the geometry of the problem — because both the cost and constraint functions are close to linear in the region of the optimum, there is a wide range of points that achieve a low cost and are close to stationarity all along the constraint.

6 Closing Remarks

This paper has contributed to the problem of obtaining information about an experimental function in the presence of general $C^2$ constraints, and a rigorous constraint back-off has been derived that, when satisfied at some $u^*$, guarantees that the user may perturb anywhere in the ball of radius $\delta_e$ around $u^*$ without incurring constraint violations. This result is believed to constitute a useful contribution to scientific problems dealing with constrained experimental spaces, as it offers a straightforward way to guarantee safety while exploring the experimental space.

While the results simplify greatly for numerical constraints, in the case of general (and likely experimental) constraints one is forced to obtain local sensitivity bounds (Lipschitz constants) for the constraint function in order to compute the appropriate back-offs. To do this well may be challenging, but relevant methods do exist and may work quite well in certain contexts (e.g., in the EVOP algorithm proposed and tested here).

The feasible-side EVOP optimization algorithm has provided an interesting application of the derived back-off result, and has been shown to work very well with respect to feasibility and convergence for three different case studies. While more involved than the traditional EVOP procedure, the algorithm nevertheless retains its simplicity, requiring the user to only set $\delta_e$ prior to applying it to a problem. It goes without saying that numerous performance improvements are possible but are not the goal of this paper. One could, for example, use all of the measurements obtained since initialization to filter out the noise. One could attempt to choose search directions in a more intelligent manner, such as what is done in some derivative-free methods (Conn et al., 2009; Lewis et al., 2000). Clearly, one could also generalize the method to handle noise that is not white Gaussian, although the computational effort may increase due to a lack of closed-form expressions.

References

Box, G. E. P. (1957). Evolutionary operation: a method for increasing industrial productivity. *J. Royal Stat. Society. Series C (Applied Statistics)*, 6, 1–45.

Box, G. E. P. (1990). Integration of techniques in process development. *Qual. Eng.*, 3, 9–26.

Box, G. E. P., & Draper, N. R. (1969). *Evolutionary Operation: A Statistical Method for Process Improvement*. John Wiley & Sons.

Box, G. E. P., & Wilson, K. B. (1951). On the experimental attainment of optimum conditions. *J. Royal Stat. Society. Series B (Methodological)*, 13, 1–45.

Bunin, G. A. (2015). Test problem database for experimental optimization (ver. 1.2). Http://www.ccapprox.info/expopt/. Accessed March 2015.

Bunin, G. A., François, G., & Bouvin, D. (2014a). Implementation techniques for the...
SCFO experimental optimization framework. arXiv:1406.3997 [math.OC], (pp. 1–66).

Bunin, G. A., François, G., & Bonvin, D. (2014b). On linear and quadratic Lipschitz bounds for twice continuously differentiable functions. arXiv:1406.3991 [math.OC], (pp. 1–4).

Bunin, G. A., François, G., & Bonvin, D. (2014c). The SCFO Experimental Optimization Solver: Users’ Guide (version 0.91.1). Http://www.ccapprox.info/soft/.

Bunin, G. A., François, G., & Bonvin, D. (2013). Feasible-side global convergence in experimental optimization. arXiv:1406.4063 [math.OC], (pp. 1–35).

Bunin, G. A., François, G., Srinivasan, B., & Bonvin, D. (2011). Input filter design for feasibility in constraint-adaptation schemes. In 18th World Congress of the International Federation of Automatic Control (IFAC) (Milan) (pp. 5585–5590).

Chen, C., & Joseph, B. (1987). On-line optimization using a two-phase approach: An application study. Ind. Eng. Chem. Res., 26, 1924–1930.

Conn, A., Scheinberg, K., & Vicente, L. (2009). Introduction to Derivative-Free Optimization. Cambridge University Press.

Conn, A. R., Gould, N. I. M., & Toint, P. L. (2000). Trust-Region Methods. SIAM.

Daniel, C., & Heerema, N. (1950). Design of experiments for most precise slope estimation or linear extrapolation. J. Am. Statist. Assoc., 45, 546–556.

François, G., & Bonvin, D. (2013). Use of convex model approximations for real-time optimization via modifier adaptation. Ind. Eng. Chem. Res., 52, 11614–11625.

François, G., Srinivasan, B., & Bonvin, D. (2005). Use of measurements for enforcing the necessary conditions of optimality in the presence of constraints and uncertainty. J. Process Control, 15, 701–712.

Hansen, P., Jaumard, B., & Lu, S. (1992). On using estimates of Lipschitz constants in global optimization. J. Optim. Theory Appl., 75, 195–200.

Jones, D. R., Schonlau, M., & Welch, W. J. (1998). Efficient global optimization of expensive black-box functions. J. Global Optim., 13, 455–492.

Lewis, R. M., Torczon, V., & Trosset, M. W. (2000). Direct search methods: then and now. J. Comput. Appl. Math., 124, 191–207.

Marchetti, A. G. (2013). A new dual modifier-adaptation approach for iterative process optimization with inaccurate models. Comput. Chem. Eng., 59, 89–100.

Montgomery, D. C. (2012). Design and Analysis of Experiments. Wiley.

Moré, J. J., & Wild, S. M. (2011). Estimating computational noise. SIAM J. Sci. Comput., 33, 1292–1314.

Myers, R., Montgomery, D., & Anderson-Cook, C. (2009). Response Surface Methodology. John Wiley & Sons.