Convex Relaxations for Global Optimization Under Uncertainty Described by Continuous Random Variables

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Abstract

This article considers nonconvex global optimization problems subject to uncertainties described by continuous random variables. Such problems arise in chemical process design, renewable energy systems, stochastic model predictive control, etc. Here, we restrict our attention to problems with expected-value objectives and no recourse decisions. In principle, such problems can be solved globally using spatial branch-and-bound (B&B). However, B&B requires the ability to bound the optimal objective value on subintervals of the search space, and existing techniques are not generally applicable because expected-value objectives often cannot be written in closed-form. To address this, this article presents a new method for computing convex and concave relaxations of nonconvex expected-value functions, which can be used to obtain rigorous bounds for use in B&B. Furthermore, these relaxations obey a second-order pointwise convergence property, which is sufficient for finite termination of B&B under standard assumptions. Empirical results are shown for three simple examples.

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1 Introduction

This article presents a new method for automatically constructing convex underestimators and concave overestimators (i.e., convex and concave relaxations) of functions of the form $F(x) \equiv \mathbb{E}[f(x, \omega)]$, where $\mathbb{E}$ denotes the expected value over continuous random variables $\omega \in \Omega \subset \mathbb{R}^n$ and $f$ may be nonconvex in both arguments. The ability to construct convex and concave relaxations of nonconvex functions is central to algorithms for solving nonlinear optimization problems to guaranteed global optimality [1–4]. Here, we are specifically motivated by the following global optimization problem under uncertainty:

$$\min_{x \in C} \mathbb{E}[f(x, \omega)]$$  \hspace{1cm} (1)

Such problems arise broadly in chemical process design [5], structural design [6], renewable energy systems [7, 8], portfolio optimization [9], stochastic model predictive control [10, 11], discrete event systems [12], etc. Moreover, although we restrict our attention to single-stage problems in this article (i.e., problems with no recourse decisions), more flexible two-stage and multistage formulations can also be reduced to (1) through the use of parameterized decision rules, which is an increasingly popular method for obtaining tractable approximate solutions [13].

In the applications above, many uncertainties are best modeled by continuous random variables, including process yields, material properties, renewable power generation, product demands, returns on investments, etc. [6–9]. However, when $f$ is nonlinear, this very often precludes writing the function $F(x) \equiv \mathbb{E}[f(x, \omega)]$ analytically in closed form. Moreover, expressing $F(x)$ via quadrature rules quickly becomes intractable as the dimension of $\omega$ increases. In this situation, $F(x)$ must be evaluated by sampling, which fundamentally limits the applicability of guaranteed global optimization algorithms such as spatial Branch-and-Bound (B&B). Specifically, to perform an exhaustive global search, B&B requires the ability to compute guaranteed lower and upper bounds on the optimal value of $F$ on any given subinterval $X$ of its domain. Assuming for simplicity that the set $C$ in (1) is convex, these bounds are typically computed by minimizing a convex relaxation.
of $F$ over $X \cap C$ (for the lower bound) and evaluating $F$ at a feasible point in $X \cap C$ (for the upper bound). However, conventional methods for constructing convex relaxations are only applicable to functions that are known explicitly in closed form \cite{1-4}. Moreover, using only sample-based approximations of $F$, it is not even possible to bound its value at a single feasible point with finitely many computations.

At present, the most common approach for solving (1) globally is sample-average approximation (SAA), which approximates $F$ using fixed samples of the random variables chosen prior to optimization. This results in a deterministic optimization problem that can be solved globally using conventional methods \cite{1-4}. However, SAA has several critical limitations that often lead to inaccurate solutions or excessive computational cost for nonconvex problems. Most notably, it only guarantees convergence to a global solution (with probability one) as the sample size tends to infinity \cite{14}. Moreover, the number of samples required to achieve a high-quality solution in practice is unknown and can be quite large \cite{15} (also see ‘ill-conditioned’ problems in \cite{16}). Perhaps more importantly, a sufficient sample size is typically not known \textit{a priori}. Theoretical bounds are available \cite{17}, but are not generally computable and are often excessively large \cite{14}. Instead, state-of-the-art SAA methods solve multiple deterministic approximations with independent samples to compute statistical bounds on the approximation error \cite{16}. However, these are only asymptotically valid. Moreover, this typically involves solving 10–40 independent instances to global optimality, and the entire procedure must be repeated from scratch if a larger sample size is deemed necessary \cite{16}. This is clearly problematic for nonconvex problems, where solving just one instance to global optimality is already computationally demanding.

An alternative approach is the stochastic branch-and-bound algorithm \cite{18}, which applies spatial B&B to (1) using probabilistic upper and lower bounds on each node $X$ based on a finite number of samples. Relative to SAA, a strength of this approach is that the sample size can be dynamically adapted as the search proceeds. However, since the computed bounds are only statistically valid, there is a nonzero probability of fathoming optimal solutions. Thus, stochastic B&B only ensures convergence to a global solution when no fathoming is done, and even then only in
the limit of infinite branching.

In the case where \( f \) is convex, a number of deterministic (i.e., sample-free) methods are available for computing rigorous underestimators and overestimators of \( F(x) = \mathbb{E}[f(x, \omega)] \) that can be used for globally solving (1). The simplest underestimator is given by Jensen’s inequality \([19]\), which states that \( \mathbb{E}[f(x, \omega)] \geq f(x, \mathbb{E}[\omega]) \) for convex \( f \). This leads to a deterministic lower bounding problem for (1) that can be solved using standard methods \([20]\). Moreover, \( F(x) \) can be bounded above at any feasible point \( x \) using, e.g., the Edmunson-Madansky upper bound \([21]\), which uses values of \( f(x, \omega) \) at the extreme points of the uncertainty set \( \Omega \). Notably, these upper and lower bounds can be made arbitrarily tight using successively refined partitions of \( \Omega \), which allows (1) to be solved to guaranteed \( \varepsilon \)-global optimality \([20, 22]\). Moreover, refinements of the Jensen and Edmunson-Madansky bounds using higher order moments of \( \omega \) have been studied in \([23, 24]\). However, all of these methods require \( f \) to be convex or, more generally, to satisfy a convex-concave saddle property. Moreover, achieving convergence by partitioning \( \Omega \) requires the ability to efficiently compute probabilities and conditional expectations on subintervals of \( \bar{\Omega} \), which severely limits the distributions of \( \omega \) that can be handled efficiently (e.g., to multivariate uniform or Gaussian distributions with independent elements).

To address these limitations, this article presents a new method for computing deterministic convex and concave relaxations of \( F(x) = \mathbb{E}[f(x, \omega)] \) on subintervals \( X \) of its domain. This method applies to arbitrary nonconvex functions \( f \) and a very general class of multivariate probability density functions for \( \omega \). In brief, nonconvexity is addressed through a novel combination of Jensen’s inequality and existing relaxation techniques for deterministic functions, such as McCormick’s technique \([25]\). Similarly, general multivariate densities are addressed by relaxing non-convex transformations that relate \( \omega \) to random variables with simpler distributions. We show that the resulting relaxations of \( F \) can be improved by partitioning \( \bar{\Omega} \). More importantly, we establish second-order pointwise convergence of the relaxations to \( F \) as the diameter of \( X \) tends to 0, provided that the partition of \( \bar{\Omega} \) is appropriately refined.

The proposed relaxations can be used to compute both upper and lower bounds for (1) restricted
to any given $X$. In principle, this enables the global solution of (1) by spatial B&B. We leave the
details of this algorithm for future work. However, we note here some potentially significant ad-
vantages of this approach relative to existing methods. First, unlike the stochastic B&B algorithm,
our relaxations provide deterministic upper and lower bounds for (1) on any $X$, so there is zero
probability of incorrectly fathoming an optimal solution during B&B. Second, the convergence of
our relaxations as the diameter of $X$ tends to 0 implies that spatial B&B will terminate finitely with
an $\varepsilon$-global solution under standard assumptions [1, 26]. This is in contrast to both stochastic B&B
and SAA, which only converge in the limit of infinite sampling. In fact, the second-order conver-
gence rate established here is known to be critical for avoiding the so-called cluster effect in B&B,
and hence avoiding exponential run-time in practice [27]. Third, although refining the partition of
$\Omega$ is required for convergence, valid relaxations on $X$ can be obtained using any partition of $\Omega$, no
matter how coarse. Thus, the partition of $\Omega$ can be adaptively refined as the B&B search proceeds.
This is potentially a very significant advantage over SAA, which must determine an appropriate
number of samples a priori, and must solve the problem again from scratch if more samples are
deemed necessary.

The remainder of this article is organized as follows. Section 2 establishes the necessary def-
initions and notation, followed by a formal problem statement in Section 3. Next, Sections 4 and
5 present the main theoretical results establishing the validity and convergence of the proposed
relaxations, respectively. Section 6 develops an extension of the basic relaxation technique that
enables efficient computations with a wide variety of multivariate probability density functions.
Finally Section 7 concludes the article.

2 Preliminaries

Convex and concave relaxations are defined as follows.

**Definition 2.1.** Let $S \subset \mathbb{R}^n$ be convex and $h : S \to \mathbb{R}$. Functions $h^{cv}, h^{cc} : S \to \mathbb{R}$ are convex and
concave relaxations of $h$ on $S$, respectively, if $h^{cv}$ is convex on $S$, $h^{cc}$ is concave on $S$, and

$$h^{cv}(s) \leq h(s) \leq h^{cc}(s), \quad \forall s \in S.$$  

The following extension of Definition 2.1 is useful for convergence analysis. First, for any $s^L, s^U \in \mathbb{R}^n$ with $s^L \leq s^U$, let $S = [s^L, s^U]$ denote the compact $n$-dimensional interval $\{s \in \mathbb{R}^n : s^L \leq s \leq s^U\}$. Moreover, for $\overline{S} \subset \mathbb{R}^n$, let $\overline{I}S$ denote the set of all compact interval subsets $S$ of $\overline{S}$. In particular, let $\overline{I}\mathbb{R}^n$ denote the set of all compact interval subsets of $\mathbb{R}^n$. Finally, denote the width of $S$ by $w(S) = \max_i |s^U_i - s^L_i|$.

**Definition 2.2.** Let $\overline{S} \subset \mathbb{R}^n$ and $h : \overline{S} \to \mathbb{R}$. A collection of functions $h^{cv}_S, h^{cc}_S : \overline{S} \to \mathbb{R}$ indexed by $S \in \overline{I}S$ is called a scheme of relaxations for $h$ in $\overline{S}$ if, for every $S \in \overline{I}S$, $h^{cv}_S$ and $h^{cc}_S$ are convex and concave relaxations of $h$ on $S$.

**Remark 2.3.** The notion of a scheme of relaxations was first introduced in [26] with the alternative name scheme of estimators. Here, we use the term relaxations in place of estimators to avoid possible confusion with the common meaning of estimation in the stochastic setting.

The following notion of convergence for schemes of relaxations originates in [26].

**Definition 2.4.** Let $\overline{S} \subset \mathbb{R}^n$ and $h : \overline{S} \to \mathbb{R}$. A scheme of relaxations $(h^{cv}_S, h^{cc}_S)_{S \in \overline{I}S}$ for $h$ in $\overline{S}$ has pointwise convergence of order $\gamma$ if $\exists \tau \in \mathbb{R}^+$ such that

$$\sup_{s \in S} |h^{cc}_S(s) - h^{cv}_S(s)| \leq \tau w(S)\gamma, \quad \forall S \in \overline{I}S.$$  

Note that the constants $\gamma$ and $\tau$ in Definition 2.4 may depend on $\overline{S}$, but not on $S$. First-order convergence is necessary for finite termination of spatial-B&B algorithms, while second-order convergence is known to be critical for efficient B&B because it can eliminate the cluster effect, which refers to the accumulation of a large number of B&B nodes near a global solution [1, 26, 27].

Several methods are available for automatically computing schemes of relaxations for factorable functions. A function $h$ is called factorable if it is a finite recursive composition of ba-
sic operations including \{+, −, ×, ÷\} and standard univariate functions such as \(x^n\), \(e^x\), \(\sin x\), etc. Roughly, factorable functions include every function that can be written explicitly in computer code. Schemes of relaxations for factorable functions can be computed by the \(\alpha\)BB method, McCormick’s relaxation technique, the addition of variables and constraints, and several advanced techniques. Moreover, both \(\alpha\)BB and McCormick relaxations are known to exhibit second-order pointwise convergence. However, for functions \(h\) that are not known in closed form, and hence are not factorable, none of the aforementioned techniques apply. Some recent extensions of \(\alpha\)BB and McCormick relaxations do address certain types of implicitly defined functions, such as the parametric solutions of fixed-point equations, ordinary differential equations, and differential-algebraic equations. However, no techniques are currently available for relaxing the expected-value function of interest here.

3 Problem Statement

Let \(\omega \in \mathbb{R}^{n_\omega}\) be a vector of continuous random variables (RVs) distributed according to a probability density function (PDF) \(p : \mathbb{R}^{n_\omega} \rightarrow \mathbb{R}\). We assume throughout that \(p\) is zero outside of a compact interval \(\Omega \subset \mathbb{R}^{n_\omega}\). Let \(X \subset \mathbb{R}^{n_x}\) be compact, let \(f : X \times \Omega \rightarrow \mathbb{R}\) be a potentially nonconvex function, and assume that the expected value \(E[f(x, \omega)] \equiv \int_\Omega f(x, \omega)p(\omega)d\omega\) exists for all \(x \in X\). Moreover, define \(F : X \rightarrow \mathbb{R}\) by \(F(x) \equiv E[f(x, \omega)], \forall x \in X\).

The objective of this article is to present a new scheme of relaxations for \(F\) in \(X\) with second-order pointwise convergence. In particular, this scheme addresses the general case where \(F\) cannot be expressed explicitly as a factorable function of \(x\), and standard relaxation techniques cannot be applied. In such cases, \(F\) is most often approximated via sampling and, in general, \(F(x)\) cannot even be evaluated exactly with finitely many computations. Critically, our new scheme consists of relaxations that provide bounds on \(F\) itself, rather than a finite approximation of \(F\), but are nonetheless finitely computable. Therefore, these relaxations can be used within a spatial-B&B framework to solve \((1)\) to \(\varepsilon\)-global optimality without approximation errors.

A central assumption in the remainder of the article is that the integrand \(f\) is a factorable
function, or that a scheme of relaxations is available by some other means.

**Assumption 3.1.** A scheme of relaxations for $f$ in $X \times \Omega$, denoted by $(f_{cv}^{X \times \Omega}, f_{cc}^{X \times \Omega})_{X \times \Omega \in \Xi \times \Omega}$, is available. $f_{cv}^{X \times \Omega}$ and $f_{cc}^{X \times \Omega}$ denote convex and concave relaxations of $f$ jointly on $X \times \Omega$.

**Remark 3.2.** We will sometimes make use of relaxations of $f$ with respect to either $x$ or $\omega$ independently, with the other treated as a constant. We denote these naturally by $f_{cv}^{X}(x, \omega)$ and $f_{cc}^{\Omega}(x, \omega)$. Within the scheme of Assumption 3.1, these relaxations are equivalent to the more cumbersome notations $f_{cv}^{X}(x, \omega) \equiv f_{cv}^{X\{\omega, \omega\}}(x, \omega)$ and $f_{cc}^{\Omega}(x, \omega) \equiv f_{cc}^{[x, x] \times \Omega}(x, \omega)$.  

### 4 Relaxing Expected-Value Functions

This section presents a general approach for constructing finitely computable convex and concave relaxations of the expected value function $F(x) = E[f(x, \omega)]$. Let $(f_{cv}^{X \times \Omega}, f_{cc}^{X \times \Omega})$ be a scheme of relaxations for $f$ on $X \times \Omega$ as per Assumption 3.1 and choose any $X \in \mathbb{I}^{X}$. To begin, note that a direct application of integral monotonicity gives ([39], p.101)

$$E[f_{cv}^{X}(x, \omega)] \leq E[f(x, \omega)] \leq E[f_{cc}^{X}(x, \omega)], \quad \forall x \in X,$$

which suggests defining relaxations of $F$ by $F_{cv}(x) \equiv E[f_{cv}^{X}(x, \omega)]$ and $F_{cc}(x) \equiv E[f_{cc}^{X}(x, \omega)]$. However, although these functions are indeed convex and concave on $X$, respectively, they are not finitely computable because they need to be evaluated by sampling in general. To overcome this limitation, we apply Jensen’s inequality, which is stated as follows.

**Lemma 4.1.** Let $\Omega \subset \overline{\Omega}$ be convex and let $g: \Omega \rightarrow \mathbb{R}$. If $g$ is convex and $E[g(\omega)]$ exists, then $E[g(\omega)] \geq g(E[\omega])$. If $g$ is concave, then $E[g(\omega)] \leq g(E[\omega])$.

**Proof.** See Proposition 1.1 in [19].

Although Jensen’s inequality is widely used to relax stochastic programs, it has so far only been applied in the case where $f(x, \cdot)$ is convex on $\overline{\Omega}$ for all $x \in X$, which we do not assume
here. Instead, we propose to combine existing convex relaxation techniques such as McCormick relaxations with Jensen’s inequality. To do this, it is necessary to relax \( f \) jointly on \( X \times \Omega \). Then, integral monotonicity and Jensen’s inequality imply that

\[
\mathbb{E}[f(x, \omega)] \geq \mathbb{E}[f_{cv}^{X \times \Omega}(x, \omega)] \geq f_{cv}^{X \times \Omega}(x, \mathbb{E}[\omega]), \tag{3}
\]

\[
\mathbb{E}[f(x, \omega)] \leq \mathbb{E}[f_{cc}^{X \times \Omega}(x, \omega)] \leq f_{cc}^{X \times \Omega}(x, \mathbb{E}[\omega]). \tag{4}
\]

for all \( x \in X \). Note that the integrals \( \mathbb{E}[f_{cv}^{X \times \Omega}(x, \omega)] \) and \( \mathbb{E}[f_{cc}^{X \times \Omega}(x, \omega)] \) exist because the convexity and concavity of the integrands implies that they are continuous on the interior of \( X \times \Omega \), and the boundary of \( X \times \Omega \) has measure zero because \( X \times \Omega \) is an interval. The inequalities (3)–(4) suggest defining relaxations for \( F \) by

\[
F_{cv}^{X \times \mathcal{P}}(x) \equiv f_{cv}^{X \times \Omega}(x, \mathbb{E}[\omega]),
\]

\[
F_{cc}^{X \times \mathcal{P}}(x) \equiv f_{cc}^{X \times \Omega}(x, \mathbb{E}[\omega]).
\]

These relaxations are clearly convex and concave on \( X \), respectively, and are finitely computable provided that \( \mathbb{E}[\omega] \) is known. However, a remaining difficulty is that the under/over-estimation caused by the use of Jensen’s inequality does not converge to zero as \( w(X) \to 0 \), which is required for finite termination of spatial-B&B. We address this problem by considering relaxations constructed on interval partitions of \( \Omega \).

**Definition 4.2.** A collection \( \mathcal{P} = \{ \Omega_i \}_{i=1}^n \) of compact intervals \( \Omega_i \in \overline{\Omega} \) is called an interval partition of \( \overline{\Omega} \) if \( \overline{\Omega} = \bigcup_{i=1}^n \Omega_i \) and \( \text{int}(\Omega_i) \cap \text{int}(\Omega_j) = \emptyset \) for all distinct \( i \) and \( j \).

**Definition 4.3.** For any measurable \( \Omega \subset \overline{\Omega} \), let \( \mathbb{P}(\Omega) \) denote the probability of the event \( \omega \in \Omega \), and let \( \mathbb{E}[\cdot|\Omega] \) denote the conditional expected-value conditioned on the event \( \omega \in \Omega \).

The following theorem extends the relaxations defined above to partitions of \( \overline{\Omega} \).

**Theorem 4.4.** Let \( \mathcal{P} = \{ \Omega_i \}_{i=1}^n \) be an interval partition of \( \overline{\Omega} \). For every \( X \in \mathcal{I} \) and every \( x \in X \), define

\[
F_{cv}^{X \times \mathcal{P}}(x) \equiv \sum_{i=1}^n \mathbb{P}(\Omega_i) f_{cv}^{X \times \Omega_i}(x, \mathbb{E}[\omega|\Omega_i]),
\]

\[
F_{cc}^{X \times \mathcal{P}}(x) \equiv \sum_{i=1}^n \mathbb{P}(\Omega_i) f_{cc}^{X \times \Omega_i}(x, \mathbb{E}[\omega|\Omega_i]).
\]
$F_{X \times \mathcal{P}}^{cv}$ and $F_{X \times \mathcal{P}}^{cc}$ are convex and concave relaxations of $F$ on $X$, respectively.

**Proof.** By the law of total expectation (Proposition 5.1 in [40]),

$$F(x) = \mathbb{E}[f(x, \omega)] = \sum_{i=1}^{n} P(\Omega_i) \mathbb{E}[f(x, \omega)|\Omega_i],$$  \hspace{1cm} (7)

for all $x \in X$. Thus, for any $X \in \mathbb{X}$ and any $x \in X$, integral monotonicity and Jensen’s inequality give,

$$F(x) \geq \sum_{i=1}^{n} P(\Omega_i) \mathbb{E}[f_{X \times \Omega_i}^{cv}(x, \omega)|\Omega_i],$$ \hspace{1cm} (8)

$$\geq \sum_{i=1}^{n} P(\Omega_i) f_{X \times \Omega_i}^{cv}(x, \mathbb{E}[\omega|\Omega_i]),$$ \hspace{1cm} (9)

$$= F_{X \times \mathcal{P}}^{cv}(x).$$ \hspace{1cm} (10)

Moreover, $F_{X \times \mathcal{P}}^{cv}$ is convex on $X$ because it is a sum of convex functions. Thus, $F_{X \times \mathcal{P}}^{cv}$ is a convex relaxation of $F$ on $X$, and the proof for $F_{X \times \mathcal{P}}^{cc}$ is analogous.

The relaxations (5)–(6) are finitely computable provided that the probabilities $P(\Omega_i)$ and conditional expectations $\mathbb{E}[\omega|\Omega_i]$ are computable for any subinterval $\Omega_i \subset \overline{\Omega}$. This is trivial when $\omega$ is uniformly distributed, but requires difficult multidimensional integrations even for Gaussian random variables. We develop a general approach for avoiding such integrals for a broad class of RVs called *factorable RVs* in §6. Given these probabilities and expected values, the required relaxations of the integrand $f$ can be computed using any standard technique. In the following example we apply McCormick relaxations [3, 25]. In this case, we call the relaxations (5)–(6) *Jensen-McCormick (JMC) relaxations*.

**Example 1.** Let $X \equiv [-1,1] \times [-1,1]$, let $\omega = (\omega_1, \omega_2)$ be uniformly distributed in $\Omega \equiv [0,1] \times [0,2]$, and define $F : X \to \mathbb{R}$ by $F(x) \equiv \mathbb{E}[f(x, \omega)]$ with

$$f(x, \omega) \equiv \frac{x_1 x_2 \ln(3 + x_1 \omega_1 \omega_2) - (x_1^2 - 1)(x_2^2 - 1) \omega_2^2}{2 + \omega_1 x_1}.$$
The nonlinearity of \( f \) makes it difficult if not impossible to evaluate \( F \) analytically. Nonetheless, a rigorous convex relaxation for \( F \) can be constructed using Theorem 4.4. Figure 1 shows the relaxation \( F_{cv}^{\mathcal{X} \times \mathcal{P}}(x) \) computed using three different partitions \( \mathcal{P} \) of \( \Omega \) with 1, 16, and 64 uniform subintervals each. The required relaxations \( f_{cv}^{\mathcal{X} \times \Omega_i} \) were automatically constructed on each \( \mathcal{X} \times \Omega_i \) by McCormick’s relaxation technique [3, 25]. Figure 1 also shows simulated \( f(x, \omega) \) values and a sample-average approximation of \( F \) using 100 samples. Clearly, the Jensen-McCormick relaxations are convex and underestimate the expected value \( F(x) \). Interestingly, however, they do not underestimate \( f(x, \omega) \) for every \( \omega \in \Omega \). Figure 1 also shows that \( F_{cv}^{\mathcal{X} \times \mathcal{P}}(x) \) gets significantly tighter as the partition of \( \Omega \) is refined from 1 subinterval to 16, while the additional improvement from 16 to 64 is small. This shows that sharp results are obtained with few subintervals in this case. Note that \( F_{cv}^{\mathcal{X} \times \mathcal{P}}(x) \) will not converge to \( F(x) \) under further \( \Omega \) partitioning unless \( \mathcal{X} \) is also partitioned, as in spatial B&B.

Spatial B&B algorithms compute a lower bound on the optimal objective value in a given subinterval \( \mathcal{X} \) by minimizing a convex relaxation of the objective function, while an upper bound is most often obtained by simply evaluating the objective at a feasible point. Theorem 4.4 provides a suitable convex relaxation for the lower bounding problem. However, in the presence of continuous RVs, computing a valid upper bound becomes nontrivial because, in general, \( F \) cannot be evaluated finitely. One possible solution is to evaluate the concave relaxation \( F_{cc}^{\mathcal{X} \times \mathcal{P}} \) instead. However, this is unnecessarily conservative. Instead, rigorous upper (and lower) bounds can be computed at feasible points, without sampling error, by the following simple corollary of Theorem 4.4.

**Corollary 4.5.** Let \( \mathcal{P} = \{\Omega_i\}_{i=1}^n \) be an interval partition of \( \Omega \). For any \( x \in \mathcal{X} \), the following bounds hold:

\[
F(x) \geq \sum_{i=1}^n \mathbb{P}(\Omega_i) f_{cc}^{\mathcal{X} \times \Omega_i}(x, \mathbb{E}[\omega|\Omega_i]), \quad (11)
\]

\[
F(x) \leq \sum_{i=1}^n \mathbb{P}(\Omega_i) f_{cc}^{\mathcal{X} \times \Omega_i}(x, \mathbb{E}[\omega|\Omega_i]). \quad (12)
\]

**Proof.** The result follows by simply applying Theorem 4.4 with the degenerate interval \( \mathcal{X} = [x, x] \).
Figure 1: Jensen-McCormick convex relaxations of $F$ in Example 1 (shaded surfaces) with partitions of $\Omega$ into 1 (top), 16 (middle), and 64 (bottom) uniform subintervals, along with simulated values of $f(x, \omega)$ at sampled $\omega$ values (◦) and a sample-average approximation of $F$ with 100 samples (black mesh).
Clearly, the need to exhaustively partition $\Omega$ in Theorem 4.4 and Corollary ?? is potentially prohibitive for problems with high-dimensional uncertainty spaces. However, it is essential for obtaining deterministic bounds on $F$, rather than bounds that are only statistically valid. Moreover, Theorem 4.4 and Corollary 4.5 provide valid bounds on $F$ for any choice of partition $\mathcal{P}$, no matter how coarse, and this has significant implications in the context of spatial B&B. Specifically, since valid bounds are obtained with any $\mathcal{P}$, it is possible to fathom a given node $X$ with certainty using only a coarse partition of $\Omega$. In other words, if $X$ is proven to be infeasible or suboptimal based on such a coarse description of uncertainty, then this decision cannot be overturned at any later stage based on a more detailed representation (i.e., a finer partition). This is distinctly different from the case with sample-based bounds, where bounds based on few samples can always be invalidated by additional samples in the future. Thus, when using the bounds and relaxations of Theorem 4.4 and Corollary 4.5 in B&B, it is possible to refine the partition of $\Omega$ adaptively as the search proceeds. It is therefore conceivable that, in some cases, much of the search space could be ruled out using only coarse partitions at low cost, while fine partitions are required only in the vicinity of global solutions. We leave the development and testing of such an adaptive B&B scheme for future work. However, as a step in this direction, we now turn to the study of the convergence behavior of $F_{cv}^X\times\mathcal{P}$ and $F_{cc}^X\times\mathcal{P}$ as both $X$ and the elements of $\mathcal{P}$ are refined towards degeneracy.

5 Convergence

Consider any $X \in \mathbb{X}$ and any interval partition $\mathcal{P} = \{\Omega_i\}_{i=1}^n$ of $\Omega$, and let the relaxations $F_{cv}^{X,\mathcal{P}}$ and $F_{cc}^{X,\mathcal{P}}$ be defined as in Theorem 4.4. This section considers the convergence of these relaxations to $F(x) = \mathbb{E}[f(x, \omega)]$ as the width of $X$ and the elements $\Omega_i$ of $\mathcal{P}$ tend towards zero. We require the following assumption on the scheme of relaxations used for $f$.

Assumption 5.1. The scheme of relaxations $(f_{cv}^X, f_{cc}^X)$ from Assumption 3.7 has second-order...
pointwise convergence in $\mathbb{I}X \times \mathbb{I}\Omega$; i.e., $\exists \tau \in \mathbb{R}_+$ such that

$$\sup_{(x,\omega) \in X \times \Omega} |f^\text{cc}_{X \times \Omega}(x,\omega) - f^\text{cv}_{X \times \Omega}(x,\omega)| \leq \tau w(X \times \Omega)^2,$$

for all $(X \times \Omega) \in \mathbb{I}X \times \mathbb{I}\Omega$.

Both McCormick and $\alpha$BB relaxations are known to satisfy Assumption 5.1 [26]. We now show that this implies a convergence bound for $F^\text{cv}_{X \times \mathcal{P}}$ and $F^\text{cc}_{X \times \mathcal{P}}$ in terms of $w(X)^2$ and the ‘average’ square-width of partition elements $\Omega_i \in \mathcal{P}$.

**Lemma 5.2.** If Assumption 5.1 holds with $\tau \in \mathbb{R}_+$, then, for any $X \in \mathbb{I}X$ and any interval partition $\mathcal{P} = \{\Omega_i\}_{i=1}^n$ of $\Omega$, we have

$$\sup_{x \in X} |F^\text{cc}_{X \times \mathcal{P}}(x) - F^\text{cv}_{X \times \mathcal{P}}(x)| \leq \tau \left[ w(X)^2 + \sum_{i=1}^n \mathbb{P}(\Omega_i) w(\Omega_i)^2 \right].$$

**Proof.** Choose any $X \in \mathbb{I}X$ and any $x \in X$. Moreover, choose any interval partition $\mathcal{P} = \{\Omega_i\}_{i=1}^n$ of $\Omega$ and define the shorthand $\hat{\Omega}_i \equiv \mathbb{E}[\omega|\Omega_i]$. From (5)–(6), we have

$$\sup_{x \in X} |F^\text{cc}_{X \times \mathcal{P}}(x) - F^\text{cv}_{X \times \mathcal{P}}(x)| \leq \tau \left[ w(X)^2 + \sum_{i=1}^n \mathbb{P}(\Omega_i) w(\Omega_i)^2 \right].$$

In order to use the relaxations $F^\text{cv}_{X \times \mathcal{P}}$ and $F^\text{cc}_{X \times \mathcal{P}}$ in a spatial B&B algorithm, it is impor-
tant that the relaxation error \( \sup_{x \in X} |F_{cc,X}^{cv}(x) - F_{cv,X}^{cv}(x)| \) converges to zero as \( w(X) \to 0 \). However, Lemma 5.2 suggests that this will not occur if \( \mathcal{P} \) remains constant, since the term \( \sum_{i=1}^{n} P(\Omega_i)w(\Omega_i)^2 \) will not converge to zero. However, convergence as \( w(X) \to 0 \) can be achieved if \( \mathcal{P} \) is refined appropriately as \( X \) diminishes. We formalize this next.

**Definition 5.3.** For every \( X \in I \), let \( \Phi(X) = \{ \Omega_i \}_{i=1}^{n} \) denote an interval partition of \( \overline{\Omega} \) satisfying the condition

\[
\sum_{i=1}^{n} P(\Omega_i)w(\Omega_i)^2 \leq Kw(X)^2,
\]

(19)

for some constant \( K \in \mathbb{R}_+ \) that is independent of \( X \). Moreover, let \( (\mathcal{F}_X^{cv}, \mathcal{F}_X^{cc})_{X \in I} \) be a scheme of relaxations for \( F \) defined for all \( X \in I \) by

\[
\mathcal{F}_X^{cv}(x) \equiv F_{X \times \Phi(X)}^{cv}(x), \quad \forall x \in X,
\]

(20)

\[
\mathcal{F}_X^{cc}(x) \equiv F_{X \times \Phi(X)}^{cc}(x), \quad \forall x \in X,
\]

(21)

where \( F_{X \times \Phi(X)}^{cv} \) and \( F_{X \times \Phi(X)}^{cc} \) are defined as in (5)–(6).

**Theorem 5.4.** The scheme of relaxations \( (\mathcal{F}_X^{cv}, \mathcal{F}_X^{cc})_{X \in I} \) for \( F \) has second-order pointwise convergence; i.e., there exists \( \hat{\tau} \in \mathbb{R}_+ \) such that

\[
\sup_{x \in X} |\mathcal{F}_X^{cc}(x) - \mathcal{F}_X^{cv}(x)| \leq \hat{\tau}w(X)^2, \quad \forall X \in I.
\]

**Proof.** Let \( \tau \in \mathbb{R}_+ \) satisfy Assumption 5.1 and choose any \( X \in I \). By Definition 5.3 and Lemma 5.2

\[
\sup_{x \in X} |\mathcal{F}_X^{cc}(x) - \mathcal{F}_X^{cv}(x)| = \sup_{x \in X} |F_{X \times \Phi(X)}^{cc}(x) - F_{X \times \Phi(X)}^{cv}(x)|
\]

\[
\leq \tau \left[ w(X)^2 + \sum_{i=1}^{n} P(\Omega_i)w(\Omega_i)^2 \right],
\]

15
where $\Phi(X) = \{\Omega_i\}_{i=1}^n$. Applying (19),

$$\sup_{x \in X} |F_{cc}^X(x) - F_{cv}^X(x)| \leq \tau (1 + K) w(X)^2, \quad (22)$$

which proves the result with $\hat{\tau} = \tau (1 + K)$.

The partitioning condition (19) is easily satisfied in practice. For example, choosing any $K \in \mathbb{R}_+$, it is satisfied by simply partitioning $\Omega$ uniformly until each element satisfies $w(\Omega_i)^2 \leq Kw(X)^2$. The following example demonstrates the convergence result of Theorem 5.4 using this simple scheme. Although this scheme is likely to generate much larger partitions than are necessary for convergence, we leave the issue of efficient adaptive partitioning schemes for future work.

**Example 2.** Let $X \equiv [24, 26]$, let $\omega$ be uniformly distributed in $\Omega \equiv [10, 13]$, and define $F : X \to \mathbb{R}$ by $F(x) \equiv \mathbb{E}[f(x, \omega)]$ with

$$f(x, \omega) \equiv \frac{(\omega - 10)^2 \ln(x) + (x - 5)^2}{\omega}.$$

Consider the sequence of intervals $X_\varepsilon \equiv [25 - \varepsilon, 25 + \varepsilon] \subset X$ with $\varepsilon \to 0$, so that $w(X_\varepsilon) \to 0$. For every $X_\varepsilon$, let $\Phi(X_\varepsilon) = \{\Omega_i\}_{i=1}^n$ be generated by uniformly partitioning $\Omega$ until $w(\Omega_i) \leq 10w(X_\varepsilon) = 20\varepsilon$, which verifies (19) with $K = 100$. Moreover, define the relaxations $F_{cv}^X$ and $F_{cc}^X$ of $F$ on $X_\varepsilon$ as in Definition 5.3, where McCormick’s relaxations are used to compute $(f_{cv}^X, f_{cc}^X)$ satisfying Assumptions 3.1 and 5.1. Figure 2 shows the pointwise relaxation error $|F_{cc}^X(x) - F_{cv}^X(x)|$ versus $\varepsilon$ for the point $x = 25$. The observed slope of 2 on log-log axes indicates that the convergence is indeed second-order.

6 Non-Uniform Random Variables

The relaxation theory presented in the previous sections puts two significant restrictions on the random variables (RVs) $\omega$. First, $\omega$ must be compactly supported in the interval $\Omega \in \mathbb{R}^{n_\omega}$. Therefore,
if we wish to use, e.g., normal random variables, we must use a truncated density function. However, this is not a major limitation since the truncated distribution can be made arbitrarily close to the original by choosing $\Omega$ large. Second, computing the relaxations $F_{cv}^X$ and $F_{cc}^X$ for a given partition $\mathcal{P}$ of $\Omega$ requires the ability to compute the probability $P(\Omega)$ and conditional expectation $E[\omega | \Omega]$ for any given subinterval $\Omega$ of $\Omega$. While this is trivial for uniform RVs, it may involve very cumbersome multidimensional integrals for other types of RVs. In this section, we address this issue in two steps. First, in §6.1, we compile a library of so-called primitive RVs for which the required probabilities and expectations are easily computed by well-known formulas. Second, in §6.2, we extend our relaxation theory to problems with factorable RVs, which are those RVs that can be transformed into primitive RVs by a factorable function. We then provide some general strategies for finding such transformations.
6.1 Primitive RVs

Recall from §3 that $\omega$ is a vector of random variables with PDF $p : \mathbb{R}^{n_\omega} \to \mathbb{R}$ compactly supported in the interval $\Omega \in \mathbb{R}^{n_\omega}$. We will call $\omega$ a primitive random vector if, for any $\Omega \in \mathbb{I} \Omega$, the quantities $P(\Omega)$ and $E[\omega|\Omega]$ can be computed efficiently through simple formulas. Clearly, uniformly distributed RVs are primitive. Moreover, if the elements of $\omega = (\omega_1, \ldots, \omega_{n_\omega})$ are independent, then several other distributions for each $\omega_i$ result in a primitive $\omega$. To see this, let $\Omega = \overline{W_1} \times \cdots \times \overline{W_{n_\omega}}$ and let $\Omega = W_1 \times \cdots \times W_{n_\omega} \in \mathbb{I} \Omega$. With this notation, independence implies that

\begin{align*}
P(\Omega) &= \Pi_{i=1}^{n_\omega} P(W_i), \quad (23) \\
E[\omega|\Omega] &= (E[\omega_1|W_1], \ldots, E[\omega_{n_\omega}|W_{n_\omega}]). \quad (24)
\end{align*}

Thus, $\omega$ is primitive if formulas are known for the one-dimensional probabilities $P(W_i)$ and expectations $E[\omega_i|W_i]$. Such formulas are well known for many common distributions. However, recall that distributions with non-interval supports must be truncated to $\overline{W_i}$ here. The following lemma provides a means to translate formulas for $P(W_i)$ and $E[\omega_i|W_i]$ for an arbitrary one-dimensional distribution to corresponding formulas for the same distribution truncated on $\overline{W_i}$.

**Lemma 6.1.** Let $\eta$ be a random variable with probability density function (PDF) $p_\eta : \mathbb{R} \to \mathbb{R}$, and let $P_\eta$ and $E_\eta$ denote the probability and expected value with respect to $p_\eta$, respectively. Moreover, choose any $\overline{W} \in \mathbb{I} \mathbb{R}$ and let $\omega$ be a random variable with the truncated PDF $p : \mathbb{R} \to \mathbb{R}$ defined by

\[
p(\omega) \equiv p_\eta(\omega|\overline{W}) = \begin{cases} 
p_\eta(\omega)/P_\eta(\overline{W}) & \text{if } \omega \in \overline{W} \\
0 & \text{otherwise}
\end{cases}.
\]

Let $P$ and $E$ denote the probability and expected value with respect to $p$. For any $W \in \mathbb{I} \overline{W}$, the
following relations hold:

\[ P(W) = \frac{P_\eta(W)}{P_\eta(W)} , \]
\[ E[\omega|W] = E_\eta[\omega|W] , \]

**Proof.** For any \( W \in \mathbb{W} \),

\[ P(W) = \int_W p(\omega) d\omega = \int_W \frac{p_\eta(\omega)}{P_\eta(W)} d\omega = \frac{P_\eta(W)}{P_\eta(W)} , \]

which proves (25). Similarly,

\[ E[\omega|W] = \frac{1}{P(W)} \int_W \omega p(\omega) d\omega , \]
\[ = \frac{1}{P(W)} \int_W \omega \frac{p_\eta(\omega)}{P_\eta(W)} d\omega . \]

Applying (25),

\[ E[\omega|W] = \frac{1}{P_\eta(W)} \int_W \omega p_\eta(\omega) d\omega = E_\eta[\omega|W] . \]

Table 1 lists formulas for the cumulative probability distributions (CDFs) \( P \) and conditional expectations \( E[\omega|W] \) for several common one-dimensional distributions. When necessary, distributions are truncated to an interval \( \mathbb{W} = [\omega_L, \omega_U] \). The listed CDFs can be used to compute \( P(W) \) via \( P(W) = P(\omega_U) - P(\omega_L) \). The formulas in Table 1 follow directly from Lemma 6.1 and standard formulas for probabilities and conditional expectations in [41, 42].

### 6.2 Factorable RVs

We now extend our relaxation method to a flexible class of non-primitive RVs. For the following definition, recall the definition of a *factorable function* discussed at the end of §2.
Table 1: Primitive one-dimensional distributions on $W = [\bar{\omega}^L, \bar{\omega}^U]$ with formulas for the CDFs $P(\omega)$ and the conditional expectations $\mathbb{E}(\omega | W)$ with $\omega \in W = [\omega^L, \omega^U] \in \bar{W}$. Normal and Gamma distributions are truncated to $\bar{W}$ \cite{42}. Formulas for the Beta distribution are for $W = [0,1]$, but arbitrary $W$ can be achieved by linear transformation of the RV (see \S 6.2).

| Distribution          | Notation | $P(\omega)$ | $\mathbb{E}(\omega | W)$ |
|-----------------------|----------|-------------|--------------------------|
| Uniform $\mathcal{U}(\underline{\omega}^L, \underline{\omega}^U)$ | $\omega - \underline{\omega}^L$ | $\frac{\omega^L + \omega^U}{2}$ |
| Truncated Normal $\mathcal{N}(\mu, \sigma^2, \bar{\omega}^L, \bar{\omega}^U)$ | $\frac{\phi(\xi) - \phi(\bar{\omega}^L)}{\bar{\omega}^L - \bar{\omega}^U}$ | $\frac{\mu}{2}$ |
| Truncated Gamma $\Gamma(\alpha, \beta, \bar{\omega}^L, \bar{\omega}^U)$ | $\Gamma(a, \infty) = \int_{-\infty}^a t^\alpha e^{-t} dt$ | $\Gamma(\alpha, \beta, \omega^L) - \Gamma(\alpha, \beta, \omega^U)$ | $\beta(\Gamma(\alpha + 1, \omega^L) - \Gamma(\alpha + 1, \omega^U))$ |
| Beta $(W = [0,1])$ $\mathcal{B}(\alpha, \beta)$ | $\Gamma(a, b) = \int_0^a t^{a-1}(1-t)^{b-1} dt$ | $\frac{\beta(a, \omega^U) - \beta(a, \omega^L)}{\beta(a, 1)}$ | $\frac{\beta(1 + \alpha, \omega^L) - \beta(1 + \alpha, \omega^U)}{\beta(1 + \alpha, 1)}$ |

**Definition 6.2.** The random vector $\omega$ is called factorable if there exists an open set $\Gamma_0 \subset \mathbb{R}^n_\omega$, an interval $\Gamma \in \Gamma_0$, and a function $\psi : \Gamma_0 \rightarrow \mathbb{R}^n_\omega$ such that (i) $\psi$ is continuously differentiable on $\Gamma_0$ and $\det(\frac{\partial \psi}{\partial \gamma}(\gamma)) \neq 0$, $\forall \gamma \in \Gamma_0$; (ii) $\psi$ is one-to-one on $\Gamma_0$, and hence invertible on the image set $\psi(\Gamma_0)$; (iii) $\omega$ has zero probability density outside of $\psi(\Gamma)$; (iv) $\gamma = \psi^{-1}(\omega)$ is a primitive RV; and (v) $\psi$ can be expressed as a factorable function on $\Gamma$.

**Remark 6.3.** A standard result in probability theory (\S 6.7 in \cite{42}) shows that, under the conditions of Definition 6.2, $\gamma = \psi^{-1}(\omega)$ obeys the PDF $p_\gamma : \mathbb{R}^n_\omega \rightarrow \mathbb{R}$ defined by

$$p_\gamma(\gamma) = \begin{cases} p(\psi(\gamma)) \left| \det \left( \frac{\partial \psi}{\partial \gamma}(\gamma) \right) \right| & \text{if } \gamma \in \bar{\Gamma} \\ 0 & \text{otherwise.} \end{cases}$$

where $p$ is the PDF of $\omega$. Thus, the fourth condition of Definition 6.2 is equivalent to the statement that $p_\gamma$ is the PDF of a primitive RV.

The following theorem shows that the expected value $F(x) = \mathbb{E}[f(x, \omega)]$ of a factorable function $f$ with respect to a factorable RV $\omega$ can be reformulated as an equivalent expected value over a primitive RV $\gamma$, and the reformulated integrand is again a factorable function.
Theorem 6.4. Assume that $\omega$ is factorable and let $\psi$, $\Gamma$, $\gamma$, and $p_\gamma$ be defined as in Definition 6.2 and Remark 6.3. Moreover, denote the expected value with respect to $p_\gamma$ by $E_\gamma$. If $\hat{f} : \mathbb{X} \times \Gamma \rightarrow \mathbb{R}$ is defined by $\hat{f}(x, \gamma) = f(x, \psi(\gamma))$, then $\hat{f}$ is a factorable function and

$$
E[f(x, \omega)] = E_\gamma[\hat{f}(x, \gamma)].
$$

Proof. By condition (v) of Definition 6.2, $\hat{f}$ is a composition of factorable functions, and is therefore factorable [3]. Now, by condition (iii) of Definition 6.2, $p(\omega) = 0$ for all $\omega \notin \psi(\Gamma)$. Therefore,

$$
E[f(x, \omega)] = \int_{\psi(\Gamma)} f(x, \omega) p(\omega) d\omega.
$$

Conditions (i) and (ii) imply that $\psi$ is a diffeomorphism from $\Gamma_0$ to $\psi(\Gamma_0)$. Since the boundary of $\Gamma_0$ has measure zero, it follows that the boundary of $\psi(\Gamma)$ has measure zero (Lemma 18.1 in [43]) and can be excluded from the integral above. Moreover, $\psi$ is a valid change-of-variables from $\omega$ in the open set $\text{int}(\psi(\Gamma))$ to $\gamma$ in the open set $\psi^{-1}(\text{int}(\psi(\Gamma)))$ (p.147 in [43]). Furthermore, the latter set is equivalent to $\text{int}(\Gamma)$ by Theorem 18.2 in [43]. Then, applying the Change of Variables Theorem 17.2 in [43] and noting that the boundary of $\Gamma$ has measure zero,

$$
E[f(x, \omega)] = \int_{\Gamma} f(x, \psi(\gamma)) p(\psi(\gamma)) \left|\det \left( \frac{\partial \psi}{\partial \gamma}(\gamma) \right) \right| d\gamma.
$$

Then, using (31),

$$
E[f(x, \omega)] = \int_{\Gamma} f(x, \psi(\gamma)) p_\gamma(\gamma) d\gamma = E_\gamma[\hat{f}(x, \gamma)].
$$

When $\omega$ is factorable, Theorem 6.4 implies that valid relaxations for $F(x) = E[f(x, \omega)]$ can be obtained by relaxing the equivalent representation $F(x) = E_\gamma[\hat{f}(x, \gamma)]$. Relaxations of the latter expression can be readily computed as described in [4], since $\hat{f}$ is factorable and $\gamma$ is a primitive RV.
Specifically, letting $\mathcal{P} = \{\Gamma_i\}_{i=1}^n$ denote an interval partition of $\Gamma$, valid relaxations are given by

$$
F_{X \times \mathcal{P}}^{cv}(x) \equiv \sum_{i=1}^n \mathbb{P}_\gamma(\Gamma_i) \hat{f}_{X \times \Gamma_i}(x, \mathbb{E}_\gamma[\gamma|\Gamma_i]),
$$

(33)

$$
F_{X \times \mathcal{P}}^{cc}(x) \equiv \sum_{i=1}^n \mathbb{P}_\gamma(\Gamma_i) \hat{f}_{X \times \Gamma_i}(x, \mathbb{E}_\gamma[\gamma|\Gamma_i]).
$$

(34)

Thus, relaxations can be computed without explicitly computing $\mathbb{P}(\Omega)$ and $\mathbb{E}[(\omega|\Omega)]$ for non-primitive distributions.

In the following subsections, we discuss several methods for computing the factorable transformation $\psi$ required by Definition 6.2. We first consider one-dimensional transformations that can be used to handle RVs $\omega$ with more general distributions than in Table 1 but still restricted to having independent elements. Subsequently, we show how RVs with independent elements can be transformed into RVs with any desired covariance matrix.

### 6.3 The Inverse Transform Method

Let $P : \mathbb{R} \to [0, 1]$ be the cumulative distribution function (CDF) for $\omega$. It is well known that the RV defined by $\gamma = P(\omega)$ is uniformly distributed on $[0, 1]$ [44]. Thus, $\gamma$ is a primitive RV, and $\omega = P^{-1}(\gamma)$ is a factorable RV as per Definition 6.2 under the following assumptions.

**Assumption 6.5.** Let $\omega$ be compactly supported in the interval $\mathbb{W} \in \mathbb{R}$. Assume that $P$ is continuously differentiable on $\mathbb{W}$ and satisfies $\frac{dP}{d\omega}(\omega) = p(\omega) > 0$ for all $\omega \in \mathbb{W}$. Moreover, assume that $P^{-1}$ is a factorable function.

Under Assumption 6.5, it is always possible to define an open set $W_0$ containing $\mathbb{W}$ and a continuously differentiable function $\psi^{-1} : W_0 \to \mathbb{R}$ that agrees with $P$ on $\mathbb{W}$ and satisfies $\frac{d\psi^{-1}}{d\omega}(\omega) > 0$ for all $\omega \in W_0$. This last condition ensures that $\psi^{-1}$ has an inverse $\psi$ defined on $\Gamma_0 \equiv \psi^{-1}(W_0)$, which contains the interval $\Gamma \equiv \psi^{-1}(\mathbb{W}) = P(\mathbb{W}) = [0, 1]$. By Theorem 8.2 in [43], $\Gamma_0$ is open and $\psi$ is continuously differentiable on $\Gamma_0$. Moreover, an application of the chain rule to the identity
\[
\psi^{-1}(\psi(\gamma)) = \gamma \text{ gives }
\]
\[
\frac{d\psi}{d\gamma}(\gamma) = \left(\frac{d\psi^{-1}}{d\omega}(\psi(\gamma))\right)^{-1} > 0, \quad \gamma \in \Gamma_0.
\] (35)

Thus, conditions (i) and (ii) of Definition 6.2 are satisfied. Condition (iii) states that \( \psi(\Gamma) = P^{-1}([0, 1]) \) contains the support of \( \omega \), which holds by definition of \( P \). Condition (iv) holds because, by Remark 6.3 and (35),

\[
p_\gamma(\gamma) = p(\psi(\gamma)) \left(\frac{d\psi^{-1}}{d\omega}(\psi(\gamma))\right)^{-1}
\] (36)
\[
= p(\psi(\gamma)) \left(\frac{dP}{d\omega}(\psi(\gamma))\right)^{-1},
\] (37)
\[
= p(\psi(\gamma)) [p(\psi(\gamma))]^{-1},
\] (38)
\[
= 1,
\] (39)

for all \( \gamma \in \Gamma \), and \( p_\gamma(\gamma) = 0 \) otherwise. Thus, \( \gamma \) is uniform. Finally, condition (v) of Definition 6.2 holds by the assumption that \( P^{-1} \) is factorable. Thus, \( \omega \) is a factorable RV under the transformation \( \omega = P^{-1}(\gamma) \).

For example, let \( \omega \sim W(\alpha, \beta, \omega^L, \omega^U) \) be a truncated Weibull RV with coefficients \( \alpha \) and \( \beta \). The standard (untruncated) Weibull CDF and inverse CDF are given by

\[
P_\eta(\eta) = 1 - e^{-(\eta/\alpha)^\beta},
\] (40)
\[
P_\eta^{-1}(\gamma) = \alpha \left(\sqrt{-\ln(1 - \gamma)}\right).
\] (41)

The CDF of the truncated distribution is given by

\[
P(\omega) = \frac{P_\eta(\omega) - P_\eta(\omega^L)}{P_\eta(\omega^U) - P_\eta(\omega^L)}, \quad \forall \omega \in \bar{W},
\] (42)
Table 2: Some common RVs $\omega$ that are factorable in the sense of Definition 6.2 with $\gamma$ uniformly distributed on $\Gamma = [0, 1]$ and factorable transformations $\psi(\gamma) = P^{-1}(\gamma)$ given by inverse CDFs. All RVs $\omega$ are truncated on the interval $\bar{W} = [\bar{\omega}^L, \bar{\omega}^U]$. $P^{-1}_\eta(\gamma)$ is the inverse CDF of the corresponding untruncated RV, so that $P^{-1}(\gamma) = P^{-1}_\eta \left[ P_\eta(\bar{\omega}^L) + (P_\eta(\bar{\omega}^U) - P_\eta(\bar{\omega}^L))\gamma \right]$.

| Distribution          | $P^{-1}_\eta(\gamma)$ | $P^{-1}(\gamma)$ |
|-----------------------|------------------------|------------------|
| Truncated Exponential | $\text{Exp}(\lambda, \bar{\omega}^L, \bar{\omega}^U)$ | $\lambda > 0$ | $-\frac{1}{\lambda} \ln(1 - \gamma)$ | $-\frac{1}{\lambda} \ln[e^{-\lambda \bar{\omega}^L} + (e^{-\lambda \bar{\omega}^U} - e^{-\lambda \bar{\omega}^L})\gamma]$ |
| Truncated Weibull     | $W(\alpha, \beta, \bar{\omega}^L, \bar{\omega}^U)$ | $\alpha, \beta > 0$ | $\alpha \sqrt{-\ln(1 - \gamma)}$ | $\alpha \sqrt{-\ln\left[e^\beta \left(\frac{\bar{\omega}^L}{\bar{\omega}^U} \right)^\beta + e^{-\beta} - e^{-(\frac{\bar{\omega}^L}{\bar{\omega}^U})^\beta}\gamma\right]}$ |
| Truncated Cauchy      | $C(\alpha, \beta, \bar{\omega}^L, \bar{\omega}^U)$ | $\beta \tan((\gamma - \frac{1}{2})\pi) + \alpha$ | $\beta \tan[\arctan(\frac{\bar{\omega}^L - \alpha}{\bar{\omega}^U})] + (\arctan(\frac{\bar{\omega}^U - \alpha}{\bar{\omega}^L}) - \arctan(\frac{\bar{\omega}^L - \alpha}{\bar{\omega}^U}))\gamma] + \alpha$ |
| Truncated Rayleigh    | $Ru(\sigma, \bar{\omega}^L, \bar{\omega}^U)$ | $\sigma > 0$ | $\sqrt{-2\sigma^2 \ln(1 - \gamma)}$ | $\sqrt{-2\sigma^2 \ln\left[\frac{\bar{\omega}^L}{\bar{\omega}^U} + \frac{(\bar{\omega}^L)^\beta}{\bar{\omega}^U} - \frac{(\bar{\omega}^L)^\beta - (\bar{\omega}^U)^\beta}{\bar{\omega}^U}\gamma\right]}$ |
| Truncated Pareto      | $Pa(m, \alpha, \bar{\omega}^L, \bar{\omega}^U)$ | $m, \alpha > 0$ | $m(1 - \gamma)^{-\frac{1}{\alpha}}$ | $m\left(\frac{m}{\bar{\omega}^L}\right)^\alpha + (\frac{m}{\bar{\omega}^L})^\alpha - (\frac{m}{\bar{\omega}^L})^\alpha\gamma^{-\frac{1}{\alpha}}$ |

and hence

$$P^{-1}(\gamma) = P^{-1}_\eta \left[ P_\eta(\bar{\omega}^L) + (P_\eta(\bar{\omega}^U) - P_\eta(\bar{\omega}^L))\gamma \right], \quad (43)$$

$$= \alpha \sqrt{-\ln\left[\frac{\bar{\omega}^L}{\bar{\omega}^U} + \frac{(\bar{\omega}^L)^\beta}{\bar{\omega}^U} - \frac{(\bar{\omega}^L)^\beta - (\bar{\omega}^U)^\beta}{\bar{\omega}^U}\gamma\right]}.$$

This gives the desired factorable transformation $\omega = \psi(\gamma) = P^{-1}(\gamma)$. Similar transformations for several common distributions are collected in Table 2.

### 6.4 Other Transformations

For many common RVs, explicit transformations from simpler RVs have been developed for the purpose of generating samples computationally. One example is the Box-Muller transformation, which transforms the two-dimensional uniform RV $\gamma$ on $(0, 1] \times [0, 1]$ into two independent standard normal RVs $\omega$ via

$$\omega_1 = \sqrt{-2 \ln \gamma_1 \cos(2\pi \gamma_2)}, \quad (44)$$

$$\omega_2 = \sqrt{-2 \ln \gamma_1 \sin(2\pi \gamma_2)}.$$
According to [45], the Box-Muller transform can also be used to generate independent bivariate normal RVs truncated on a disc of radius $r$; i.e., with $\Omega \equiv \{ \omega \in \mathbb{R}^2 : \omega_1^2 + \omega_2^2 \leq r^2 \}$. This is accomplished by simply setting $\gamma_1 = \exp(-r^2/2)$, $\Gamma = [\gamma_1, 1] \times [0, 1]$, and defining $\gamma$ on $\Gamma$ by (44), which is clearly factorable.

Many other factorable transformations can be readily devised. Naturally, we can replace log-normal RVs by the log of normal RVs, $\chi^2$ RVs by summations of squared standard normal RVs, etc.

### 6.5 Dependent RVs

Using the techniques outlined in the previous subsections, factorable random vectors can be generated with elements obeying a wide variety of common distributions, but all elements must be independent. Let $\hat{\omega}$ denote such a random vector, so that $\text{Cov}(\hat{\omega}) = \mathbf{I}$. In this subsection, we show that another factorable (in fact linear) transformation can be used to generate a random vector $\omega$ from $\hat{\omega}$ with any desired mean $d$ and positive definite (PD) covariance matrix $C$. For any such $C$, positive definiteness implies that there exists a unique PD matrix $C^{1/2}$ such that $(C^{1/2})^2 = C$. Thus, defining $\omega = d + C^{1/2}(\hat{\omega} - \mathbb{E}[\hat{\omega}])$, we readily obtain $\mathbb{E}[\omega] = d$ and

$$\text{Cov}(\omega) = \mathbb{E}[(\omega - \mathbb{E}[\omega])(\omega - \mathbb{E}[\omega])^T],$$  \hspace{1cm} (45)

$$= \mathbb{E}[C^{1/2}(\hat{\omega} - \mathbb{E}[\hat{\omega}])^T(\hat{\omega} - \mathbb{E}[\hat{\omega}])^T(C^{1/2})^T],$$  \hspace{1cm} (46)

$$= C^{1/2}\text{Cov}(\hat{\omega})C^{1/2},$$  \hspace{1cm} (47)

$$= C,$$  \hspace{1cm} (48)

as desired. Note that this linear transformation can be applied directly to any of the primitive RVs listed in Table 1 (e.g., to obtain a multivariate normal distribution with mean $d$ and covariance $C$) or to more general factorable RVs constructed via the methods in the previous subsections.

**Example 3.** To demonstrate the use of non-primitive factorable RVs, we consider relaxing the objective function of the following stochastic optimization problem modified from [46], which
considers the optimal design of two consecutive continuous stirred-tank reactors of volumes $x_1$ and $x_2$ carrying out the reactions $A \rightleftharpoons B \rightleftharpoons C$:

$$\min_x -\mathbb{E} \left[ \frac{k_{f,2} x_2 (1 + k_{r,1} x_1) + k_{f,1} x_1 (1 + k_{f,2} x_2)}{(1 + k_{f,1} x_1)(1 + k_{f,2} x_2)(1 + k_{r,1} x_1)(1 + k_{r,2} x_2)} \right]$$

s.t. $x_1^{0.5} + x_2^{0.5} \leq 4$

$0 \leq x_1, x_2 \leq 16$

$k_{r,1} = 0.99 k_{f,1}$

$k_{r,2} = 0.90 k_{f,2}$

$$\begin{bmatrix} k_{f,1} \\ k_{f,2} \end{bmatrix} = \begin{bmatrix} 0.097 \\ 0.039 \end{bmatrix} + \begin{bmatrix} 0.0072 & 0.0004 \\ 0.0008 & 0.0036 \end{bmatrix} \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix}$$

$\gamma_1 \sim \mathcal{N}(\mu_1, \sigma_1^2, \gamma_1^U, \gamma_1^L)$

$\gamma_2 \sim \mathcal{N}(\mu_2, \sigma_2^2, \gamma_2^U, \gamma_2^L)$

The objective is to maximize the expected value of the concentration of product B in the exit stream of the second reactor. We assume that the forward reaction rates $(k_{f,1}, k_{f,2})$ follow a bivariate normal distribution with

$$\mathbf{d} = \mathbb{E} \left( \begin{bmatrix} k_{f,1} \\ k_{f,2} \end{bmatrix} \right) = \begin{bmatrix} 0.097 \\ 0.039 \end{bmatrix},$$

$$\mathbf{C}^{1/2} = \sqrt{\text{Cov} \left( \begin{bmatrix} k_{f,1} \\ k_{f,2} \end{bmatrix} \right)} = \begin{bmatrix} 0.0072 & 0.0004 \\ 0.0008 & 0.0036 \end{bmatrix}.$$

To avoid computing probabilities and conditional expected values of this distribution over subintervals, we introduce a primitive random vector $\gamma$ consisting of two independent random variables $(\gamma_1, \gamma_2)$ satisfying standard normal distributions ($\mu_1 = \mu_2 = 0$ and $\sigma_1 = \sigma_2 = 1$) truncated at plus
and minus five standard deviations, giving the truncation bounds

\[
[\gamma^L_1, \gamma^U_1] = [\gamma^L_2, \gamma^U_2] = [-5, 5].
\] (51)

After truncation, \( \text{Var}(\gamma_1) = \text{Var}(\gamma_2) = 0.9999 \approx 1 \). We then transform \((\gamma_1, \gamma_2)\) into a bivariate normal RV \((k_{f,1}, k_{f,2})\) with the desired mean and covariance as discussed in §6.5. With these definitions, Figure 3 shows convex relaxations for the objective function on \( X \equiv [2.5, 4] \times [2.5, 4] \) computed as in (33) with partitions \( \mathcal{P} = \{\Gamma_i\}_{i=1}^{n_0} \) of \( \bar{\Gamma} \) consisting of 1, 16, and 64 elements. The required relaxations of \( \hat{f}(x, \gamma) = f(x, d + C^{1/2} \gamma) \) on each \( X \times \Gamma_i \) were computed using McCormick relaxations [3]. Figure 3 shows that the relaxation computed with a partition consisting of only one element is fairly weak, but improves significantly with 16 elements. On the other hand, the additional improvement achieved with 64 elements is minor.

Figure 4 shows the pointwise convergence of the computed relaxations on a sequence of intervals \( X_\varepsilon \equiv [5 - \varepsilon, 5 + \varepsilon] \times [6 - \varepsilon, 6 + \varepsilon] \) as \( \varepsilon \to 0 \). Specifically, Figure 4 shows the convergence of the scheme of relaxations \((\mathcal{T}^{cv}_X, \mathcal{T}^{cc}_X)\) defined analogously to (20)–(21) by imposing an \( X \)-dependent uniform partitioning rule to \( \Gamma \) such that

\[
\sum_{i=1}^{n} \mathbb{P}(\Gamma_i) w(\Gamma_i)^2 \leq Kw(X)^2.
\] (52)

Again, the observed slope of 2 on log-log axes verifies the theoretical second-order pointwise convergence ensured by Theorem 5.4.

7 Conclusions

In this article, we developed a new method for computing convex and concave relaxations of non-convex expected-value functions over continuous random variables (RVs). These relaxations can provide rigorous lower and upper bounds for use in spatial branch-and-bound (B&B) algorithms, thereby enabling the global solution of nonconvex optimization problems subject to continuous
Figure 3: Jensen-McCormick convex relaxations of the objective function $F$ in Example 3 (shaded surfaces) with partitions of $\Gamma$ into 1 (top), 16 (middle), and 64 (bottom) uniform subintervals, along with simulated values of $f(x, \omega)$ at sampled $\omega$ values (◦) and a sample average approximation of $F$ with 100 samples (black mesh).
uncertainties (e.g., process yields, renewable renewable resources, product demands, etc.). Importantly, these relaxations are not sample-based. Instead, they make use of an exhaustive partition of the uncertainty set. As a consequence, they can be evaluated finitely, even when the original expected-value cannot be. Empirical results with simple uniform partitions showed that tight relaxations can be obtained with fairly coarse partitions. Moreover, when the uncertainty partition is refined appropriately, we established second-order pointwise convergence of the relaxations to the true expected value as the relaxation domain tends to a singleton. Such convergence is critical for ensuring finite termination of spatial B&B and avoiding the cluster effect. Finally, using the notion factorable RVs, we extended our relaxation technique to a wide variety of multivariate probability distributions in a manner that avoids the need to compute any difficult multidimensional integrals.

In a forthcoming paper, we plan to develop a complete spatial B&B algorithm for nonconvex op-
timization problems with continuous uncertainties by combining the relaxations developed here with efficient, adaptive uncertainty partitioning strategies.

References

[1] Horst, R., Tuy, H.: Global Optimization: Deterministic Approaches, third edn. Springer, New York (1996)

[2] Tawarmalani, M., Sahinidis, N.V.: Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming. Kluwer Academic Publishers (2002)

[3] McCormick, G.: Computability of global solutions to factorable nonconvex programs: Part I - convex underestimating problems. Mathematical Programming 10, 147–175 (1976)

[4] Adjiman, C.S., Dallwig, S., Floudas, C.A., Neumaier, A.: A global optimization method, αBB, for general twice-differentiable constrained NLPs - I. Theoretical advances. Computers & Chemical Engineering 22(9), 1137–1158 (1998)

[5] Ahmadian Behrooz, H.: Robust design and control of extractive distillation processes under feed disturbances. Industrial & Engineering Chemistry Research 56(15), 4446–4462 (2017)

[6] Liem, R.P., Martins, J.R., Kenway, G.K.: Expected drag minimization for aerodynamic design optimization based on aircraft operational data. Aerospace Science and Technology 63, 344–362 (2017)

[7] Hakizimana, A., Scott, J.: Differentiability conditions for stochastic hybrid systems arising in the optimal design of microgrids. J. Optim. Theor. Appl. 173(2), 658–682 (2017)

[8] Papadopoulos, A.I., Giannakoudis, G., Voutetakis, S.: Efficient design under uncertainty of renewable power generation systems using partitioning and regression in the course of optimization. Ind. Eng. Chem. Res. 51(39), 12,862–12,876 (2012)

[9] Pang, L.P., Chen, S., Wang, J.H.: Risk management in portfolio applications of non-convex stochastic programming. Applied Mathematics and Computation 258, 565–575 (2015)

[10] Farina, M., Giulioni, L., Magni, L., Scattolini, R.: An approach to output-feedback MPC of stochastic linear discrete-time systems. Automatica 55, 140–149 (2015)

[11] Mesbah, A.: Stochastic model predictive control: An overview and perspectives for future research. IEEE Control Systems 36(6), 30–44 (2016)
[12] E., Y.M., Norkin, V.I.: On nonsmooth and discontinuous problems of stochastic systems optimization. European Journal of Operational Research 101(2), 230–244 (1997)

[13] Georghiou, A., Wiesemann, W., Kuhn, D.: Generalized decision rule approximations for stochastic programming via liftings. Mathematical Programming 152(1), 301–338 (2015)

[14] Shapiro, A.: Stochastic programming approach to optimization under uncertainty. Mathematical Programming 112(1), 183–220 (2008)

[15] Verweij, B., Ahmed, S., Kleywegt, A.J., Nemhauser, G., Shapiro, A.: The sample average approximation method applied to stochastic routing problems: A computational study. Computational Optimization and Applications 24(2), 289–333 (2003)

[16] Linderoth, J., Shapiro, A., Wright, S.: The empirical behavior of sampling methods for stochastic programming. Annals of Operations Research 142(1), 215–241 (2006)

[17] Shapiro, A.: On complexity of multistage stochastic programs. Operations Research Letters 34(1), 1–8 (2006)

[18] Norkin, V.I., Pflug, G.C., Ruszczyński, A.: A branch and bound method for stochastic global optimization. Mathematical Programming 83(1), 425–450 (1998)

[19] Perlman, M.D.: Jensen’s inequality for a convex vector-valued function on an infinite-dimensional space. Journal of Multivariate Analysis 4(1), 52–65 (1974)

[20] Birge, J.R., Wets, R.J.B.: Designing approximation schemes for stochastic optimization problems, in particular for stochastic programs with recourse, pp. 54–102. Springer Berlin Heidelberg, Berlin, Heidelberg (1986)

[21] Madansky, A.: Bounds on the expectation of a convex function of a multivariate random variable. Annals of Mathematical Statistics 30(3), 743–746 (1959)

[22] Frauendorfer, K., Kuhn, D., Schurle, M.: Barycentric Bounds in Stochastic Programming: Theory and Application, International Series in Operations Research & Management Science, vol. 150, pp. 67–96. Springer, New York (2011)

[23] Dokov, S.P., Morton, D.P.: Higher-Order Upper Bounds on the Expectation of a Convex Function. Humboldt-Universitat zu Berlin, Mathematisch-Naturwissenschaftliche Fakultat II, Institut fur Mathematik (2002)

[24] Edirisinghe, N.C.P.: New second-order bounds on the expectation of saddle functions with applications to stochastic linear programming. Operations Research 44(6), 909–922 (1996)
[25] Scott, J., Stuber, M., Barton, P.: Generalized McCormick relaxations. Journal of Global Optimization 51, 569–606 (2011)

[26] Bompadre, A., Mitsos, A.: Convergence rate of McCormick relaxations. J. Glob. Optim. 52(1), 1–28 (2012)

[27] Kannan, R., Barton, P.I.: The cluster problem in constrained global optimization. J. Glob. Optim. (2017)

[28] Skjäl, A., Westerlund, T., Misener, R., Floudas, C.A.: A generalization of the classical αBB convex underestimation via diagonal and nondiagonal quadratic terms. Journal of Optimization Theory and Applications 154(2), 462–490 (2012)

[29] Meyer, C.A., Floudas, C.A.: Convex envelopes for edge-concave functions. Mathematical Programming 103(2), 207–224 (2005)

[30] Gounaris, C.E., Floudas, C.A.: Tight convex underestimators for C(2)-continuous problems: II. multivariate functions. Journal of Global Optimization 42(1), 69–89 (2008)

[31] Bao, X., Khajavirad, A., Sahinidis, N., Tawarmalani, M.: Global optimization of nonconvex problems with multilinear intermediates. Mathematical Programming Computation 7(1), 1–37 (2015)

[32] Tsoukalas, A., Mitsos, A.: Multivariate McCormick relaxations. J. Glob. Optim. 59(2), 633–662 (2014)

[33] Khan, K.A., Watson, H.A.J., Barton, P.I.: Differentiable McCormick relaxations. J. Glob. Optim. 67(4), 687–729 (2017)

[34] Wechsung, A., Scott, J., Watson, H., Barton, P.: Reverse propagation of McCormick relaxations. J. Glob. Optim. 63(1), 1–36 (2015)

[35] Stuber, M., Scott, J., Barton, P.: Convex and concave relaxations of implicit functions. Optimization Methods and Software 30(3), 424–460 (2015)

[36] Esposito, W.R., Floudas, C.A.: Deterministic global optimization in nonlinear optimal control problems. J. Glob. Optim. 17, 97–126 (2000)

[37] Scott, J., Barton, P.: Improved relaxations for the parametric solutions of ODEs using differential inequalities. J. Glob. Optim. 57(1), 143–176 (2013)

[38] Scott, J., Barton, P.: Convex and concave relaxations for the parametric solutions of semi-explicit index-one DAEs. Journal of Optimization Theory and Applications 156(3), 617–649 (2013)
[39] Karr, A.: Probability. Springer-Verlag (1993)

[40] Ross, S.: A First Course in Probability. Prentice Hall (2002)

[41] Johnson, N.L., Kotz, S., Balakrishnan, N.: Continuous Univariate Distributions, vol. 1. Wiley-Interscience (1994)

[42] Okasha, M.K., Alqanoo, I.M.: Inference on the doubly truncated gamma distribution for lifetime data. Int. J. Math. Stat. Invent 2, 1–17 (2014)

[43] Munkres, J.R.: Analysis on Manifolds. Westview Press, Cambridge, MA (1991)

[44] Ripley, B.D.: Stochastic Simulation. John Wiley & Sons (2006)

[45] Martino, L., Luengo, D., Miguez, J.: Efficient sampling from truncated bivariate Gaussians via Box-Muller transformation. Electronics Letters 48(24), 1533–1534 (2012)

[46] Ryoo, H.S., Sahinidis, N.V.: Global optimization of nonconvex NLPs and MINLPs with applications in process design. Computers & Chemical Engineering 19(5), 551–566 (1995)