

*The Institute for Integrating Statistics in Decision Sciences*

*Technical Report TR-2016-8*

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Endogenous Uncertainty**

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# Augmented Nested Sampling for Stochastic Programs with Recourse and Endogenous Uncertainty

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Monday 27<sup>th</sup> November, 2017

## Abstract

We propose a novel simulation-based approach for solving two-stage stochastic programs with recourse and endogenous (decision dependent) uncertainty. An augmented probability model with stochastic decision variables and nested sampling solves the stochastic optimization problem by simultaneously simulating the decision variables and parameters. The optimal decision is obtained via the mode of the augmented probability model. We illustrate our methodology on a newsvendor problem with stock-dependent uncertain demand both in single and multi-item (news-stand) cases. We provide performance comparisons with Markov chain Monte Carlo and traditional Monte Carlo simulation-based optimization schemes. Finally, we conclude with directions for future research.

**Keywords:** stochastic programming; augmented probability simulation; nested sampling; endogenous uncertainty; decision analysis.

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# 1 Introduction

We propose a novel augmented probability simulation approach combined with nested sampling to solve two-stage stochastic programs with recourse. Our focus is on endogenous (decision dependent) uncertainty where decision making allows for uncertainty whose probability distribution depends on past decisions. A variety of real world problems possess endogenous uncertainty, and the main challenge is the computational complexity. The scenario trees (a.k.a uncertainty nodes) are not finalized before decision making and optimal decisions need to be computed over all potential tree scenarios. This leads to computational challenges, for which decomposition methods, traditional Monte Carlo (MC) and Markov chain Monte Carlo (MCMC) based approaches can easily become inefficient. Our approach is based on augmented nested sampling and we illustrate our methodology on newsvendor and news-stand problems where the seller is faced with uncertain demand which depends on the initial inventory decision.

Our methodology builds on the augmented probability simulation (APS) framework of Bielza et al. (1999) and Müller et al. (2004). We allow the decision variable to be stochastic and we explore in the augmented space of both the decision and random variables using nested sampling. APS using MCMC methods is considered in Ekin et al. (2014) who solve two-stage stochastic programs with exogenous uncertainty. We develop a nested sampling based APS approach which effectively solves stochastic programs with decision dependent uncertainty. Nested sampling was originally introduced by Skilling (2006) for approximating expectations and normalisation constants that arise in Bayesian analysis. Our adoption of nested sampling in APS represents a contribution to the decision analysis literature. Proposed method is an efficient alternative to solve two-stage stochastic programs with decision dependent uncertainty.

There is an extensive literature on decision dependent utility maximization; see for example, Dantzig (1955), Lindley (1985), and Rubinstein (2009). Lee et al. (2012) provide a discussion of newsvendor-type problems with decision dependent uncertainty. Following the early work of Jonsbraten et al. (1998), a number of applications arise in operational planning of offshore gas development (Goel and Grossmann (2004)), aggregate workforce

planning (Fragnière et al. (2010)), reliability (Kirschenmann et al. (2014)), project portfolio management (Solak et al. (2010), Colvin and Maravelias (2010)) and scheduling (Morton and Popova (2004)). Goel and Grossmann (2006) illustrate ways that decisions can influence uncertainty or stochastic evolution. First, previous decisions may affect the probability distribution by making one outcome more likely than other. The random variable itself or parameters of its probability density can be modeled as a function of the previous decisions; see, Ahmed (2000). For instance, Peeta et al. (2010) develop a two-stage pre-disaster investment decision model for a highway network, where the discrete survival probabilities are altered by first stage investment decisions. Secondly, the decision maker could act to get more accurate information and the number of scenarios within the probability distributions may decrease with the partial resolution of uncertainty. In this manuscript, we consider the first type of decision dependent uncertainty.

The rest of the paper proceeds as follows. Section 2 provides an overview of two stage stochastic programs with recourse focusing on decision dependent uncertainty and introduces our augmented probability simulation methodology. Section 3 presents our nested sampling algorithm for simulating from the augmented distribution. Section 4 illustrates our methodology on a newsvendor problem with endogenous random demand. Section 5 presents numerical results and provides computational insights. Finally, we conclude with a discussion of future research and a brief appendix that presents the derivation of an equality.

## **2 Stochastic Programming via Augmented Probability Simulation**

### **2.1 Decision Dependent Stochastic Programs with Recourse**

Multi-stage stochastic programming with recourse allows for corrective decisions given observed realizations of variables at each stage; see, Birge and Louveaux (2011) for an extensive review. A stage corresponds to a node in a decision tree where we can optimally choose a set of decision variables. We focus on the two-stage problems with decision de-

pendent uncertainty where the probability distribution of the random variable depends on the first stage decision. The first stage decision, denoted by  $x$ , is optimized against observations of the stochastic outcome variable, denoted by  $\xi$ . Uncertainty about  $\xi$  given  $x$  is represented by a known decision dependent probability distribution  $p(\xi|x)$ . The objective of the decision maker is to choose a first stage decision that is feasible for all scenarios of the uncertainty so that the expected objective function associated with both stages is optimized. The objective function of the second stage, (a.k.a recourse function),  $Q(x, \xi)$  depends on both the first stage decision and the uncertain variable. In addition, the second stage constraints can be uncertain. After  $\xi$  is revealed, the second stage recourse decision, denoted by  $y(x, \xi)$ , is determined by solving the second stage problem for the specific combination of first stage decision and the outcome value  $(x, \xi)$ . The general two-stage problem with recourse is shown below.

$$\begin{aligned}
& \max_x \quad mx - E[Q(x, \xi)] \\
& \text{subject to} \quad Ax \leq b, x \geq 0 \\
& \text{where } Q(x, \xi) = \min_y \quad q(\xi)y \\
& \text{subject to} \quad Tx + Wy \geq h(\xi), y \geq 0.
\end{aligned} \tag{2.1}$$

Here the vectors and matrices  $m$ ,  $A$ ,  $b$ ,  $T$ , and  $W$ , are deterministic arrays with appropriate dimensions whereas  $q$  and  $h$  are vectors which are functions of the uncertainty  $\xi$  conditional on  $x$ .

A variety of approaches are available to solve stochastic programs with exogenous uncertainty, where  $x$  and  $\xi$  are independent. For instance, variants of Bender's algorithm (Benders (1962)), also widely known as L-shaped algorithm (van Slyke and Wets (1969)), have been successfully utilized to solve a range of applications (Birge and Louveaux (2011), Shapiro et al. (2009) and many references therein). This plane-cutting method has the advantage of scalability through its representation of the recourse function using a scalar variable and cuts. The scalar variable serves as an outer approximation to the expected recourse function, while the cuts represent the second-stage constraints in terms

of first-stage decision variables. These methods work very well for discrete distributions, but may be inefficient for large scenario sets or continuous distributions. Therefore, algorithms including decomposition based methods in which sampling is incorporated within the optimization algorithm such as stochastic decomposition (Higle and Sen (1996)) and importance sampling based L-shaped methods (Infanger (1993)) are proposed. Variants of Monte Carlo simulation (see Homem-de Mello and Bayraksan (2014) for a survey), gradient based stochastic approximation algorithms (Rubinstein and Shapiro (1993)) and stochastic quasi-gradient algorithms (Ermoliev (1988)) are among other solution approaches. Most of these solution approaches are efficient for stochastic programs with exogenous uncertainty, but not practical for models with endogenous uncertainty. This can be explained by the challenge of solving for the path dependent objective functions. For instance, stochastic decomposition is based on developing lower bound approximations for the expected value function that are easier to optimize. However, endogenous problems bring the challenge of scenario trees that are dependent on each decision alternative. Therefore, evaluation of the objective function and solution of the problem need to be done for all potential scenario trees that are dependent on considered decision alternatives. Hence, this limits applicability to small sets of variables with typically discrete randomness (Vayanos et al. (2011)). Therefore, to the best of our knowledge, there are not any attempts in literature to use L-shaped based decomposition methods for solving stochastic programs with endogenous uncertainty.

Current approaches to solving the class of problems with decision dependent uncertainty mostly require the inclusion of all scenarios. Such approaches include branch and bound schemes, and relaxation-based heuristic approaches such as disjunctive programming. Solak et al. (2010) is amenable to scenario based decomposition and uses Sample Average Approximation (SAA) which is a MC based optimization method. This is a modified utilization of SAA in which samples are drawn for a finite number of feasible decision points, and then the estimates of the expectation function are optimized. SAA first approximates  $E_{\xi}[Q(x, \xi)]$  by the MC average,  $\hat{E}_{\xi}[Q(x, \xi)]$ , which is computed using

$G$  independent MC samples from  $p(\xi|x)$ , namely

$$\hat{E}_{\xi}[Q(x, \xi)] = \frac{1}{G} \sum_{g=1}^G Q(x, \xi^{(g)}).$$

SAA then optimizes  $(mx - \hat{E}_{\xi}[Q(x, \xi)])$  over  $x$ . One key caveat is that MC errors associated with approximating  $\hat{E}_{\xi}[Q(x, \xi)]$  can overwhelm the calculation of the optimal decision,  $x^*$ . As an alternative, Lee et al. (2012) has proposed an iterative decision process which uses the empirical distribution of the data as the input distribution. However, the optimal decision search is still within the joint space of decision and random variables. Since sampling and optimization are done in an iterative fashion, this may result with an inefficient allocation of optimization effort. Using MC to approximate and then to optimise can lead to large errors. APS can be more efficient, since it performs the expectation and optimization simultaneously. For instance, Aktekin and Ekin (2016) utilize the APS approach of Ekin et al. (2014) to solve for their call center staffing model with random arrival, service and abandonment rates. In their application, the probabilities of abandonment and delay are functions of both decision variables and random parameters, hence indirect decision dependency exists. Ekin (2017) uses Markov chain Monte Carlo based APS to solve an integrated maintenance and production model. Next, we introduce the APS formulation in detail.

## 2.2 APS Formulation

Consider the two-stage program (2.1) with decision dependent uncertainty where the distribution of  $\xi$  depends on  $x$  via  $p(\xi|x)$ . We assume the second stage decisions can be computed by solving the resulting deterministic optimization problem, therefore are available. In the newsvendor case, the optimal recourse action,  $y^*(x, \xi)$ , is available in closed form which in turn provides the inner objective  $Q(x, \xi) = q(\xi)y^*(x, \xi)$ . Finding the optimal first stage solution  $x$ , then reduces to maximizing expected value of

$$u(x, \xi) = mx - q(\xi)y^*(x, \xi) \tag{2.2}$$

while satisfying the first stage constraints  $\{Ax \leq b, x \geq 0\}$ .

APS is based on the idea that maximization of the expected value of  $u(x, \xi)$  can be achieved by simulation from an augmented probability distribution  $\pi(x, \xi)$  of the decision variable  $x$  and uncertainty shock  $\xi$ . The distribution of  $x$ ,  $p(x)$  is generally assumed to be uniform in the decision space of search. We construct an auxiliary distribution,  $\pi(x, \xi)$ , as follows

$$\pi(x, \xi) \propto u(x, \xi)p(\xi|x)p(x) \quad (2.3)$$

with corresponding marginal distribution given by

$$\pi(x) \propto \int u(x, \xi)p(\xi|x)d\xi.$$

The optimal first stage decision  $x^*$  corresponds to the mode of the distribution  $\pi(x)$ . Notice that we assume that  $u(x, \xi) = (mx - q(\xi))y^*(x, \xi)$  is a non-negative function, so that  $\pi(x, \xi)$  is a valid probability distribution.

Our proposed algorithm will draw samples of the decision variable,  $x$ , from the regions of the decision space with high objective function values. The draws of  $\xi$  are tilted away from the conditional density  $p(\xi|x)$  toward  $u(x, \xi)p(\xi|x)$ . The algorithm then concentrates on the “smart” values of  $\xi$  where the importance function is the objective function that tightens around the optimal decision,  $x^*$ . Overall, sampling in a utility-tilted way helps to draw the random parameter  $\xi$ , more frequently from where it has higher utility in a maximization problem. This reduces the Monte Carlo error since no optimization effort is wasted in parts of the parameter space with low objective function values. This results with reduced sample variance that leads to performance improvement (Ekin et al. (2014)).

When the expected utility surface is flat, the APS can be improved by replacing the expected utility surface by a power transformation that uses a more peaked surface without changing the solution of the problem (Müller (1999)). This property is similar to simulated annealing; see Kirkpatrick et al. (1983) and van Laarhoven and Aarts (1987). Simulated annealing algorithms assume availability of  $u(x, \xi)$  for direct evaluation which is not re-

quired by the APS approach. Müller et al. (2004) present the convergence results of a similarly constructed simulation of an inhomogeneous Markov chain.

Following Müller (1999), we define the augmented probability model using  $J$  copies of  $\xi$  denoted by  $\xi_J = (\xi_1, \dots, \xi_J)$ . This leads to the distribution

$$\pi_J(x, \xi_J) \propto \prod_{j=1}^J (mx - q(\xi_j)y_j^*) p(\xi_j|x) p(x) \mathbb{I}(Ax \leq b, x \geq 0), \quad (2.4)$$

where again  $(mx - q(\xi_j)y_j^*) \geq 0$  for all  $j$ . For each pair of  $x$  and  $\xi_j$ ,  $y_j^* = y_j^*(x, \xi_j)$  are available or computed by solving the resulting deterministic optimization problem.

Since  $\xi_j$ 's are conditionally independent, the marginal distribution of  $x$  is given by

$$\pi_J(x) \propto \left[ E_{\xi} (mx - q(\xi)y^*(x, \xi)) \mathbb{I}(Ax \leq b, x \geq 0) \right]^J$$

with the normalisation constant

$$\left[ E_{\xi} (mx - q(\xi)y^*(x, \xi)) \right]^J = \left[ \int (mx - q(\xi)y^*(x, \xi)) \mathbb{I}(Ax \leq b, x \geq 0) p(\xi|x) d\xi \right]^J.$$

For sufficiently large  $J$ , simulations from a probability density proportional to the  $J^{\text{th}}$  power of the original target function cluster tightly around the mode. As pointed out by Müller (1999), substituting the average instead of the product of the objective functions would have implied a marginal distribution of  $\pi(x)$ , not the desired power  $\pi^J(x)$ ; therefore is not used.

The key feature is that the marginal distribution's mode is the optimal decision,  $x^*$ . When we deal with discrete alternatives or low dimensional continuous alternatives, it is straightforward to determine the mode. In the case of high dimensional continuous alternatives, Bielza et al. (1999) propose the use of a hierarchical cluster tree of the simulation output. This evaluation can also help the decision maker to conduct sensitivity analysis at no extra cost.

### 3 Nested Augmented Probability Sampling

Augmented probability sampling differs from other simulation based algorithms such as SAA, by not using simulation to evaluate expected utilities for each decision alternative. APS is based on sampling from the artificial augmented distributions. But, the marginal distribution  $\pi_J(x)$  is not analytically available. Hence, one alternative is to use MCMC methods to sample from  $\pi_J(x, \xi_J)$  to find the mode of  $\pi_J(x)$  (Ekin et al. (2014)). However, application of MCMC in the cases of decision dependent randomness and multi-dimensionality can result in computational inefficiencies. The decision dependence in the probability density  $p(\zeta|x)$  can lead to MCMC sampling from the augmented distribution to be inefficient due to slow convergence. In addition, high dimensionality of the variables and potential multi-modality of the distributions may create problems in the implementation of the MCMC (Feroz and Hobson (2008)). In cases with many local optima separated by low-probability barriers, the Markov chain can become stuck in a local optimum and fail to generate samples from the correct distribution with practical run-times (Polson and Scott (2015)). MCMC also requires careful tuning of the proposal distribution to sample efficiently. Thus, in our development below we introduce nested sampling and propose a new nested sampling based simulation method for APS.

#### 3.1 Nested Sampling

Nested sampling is initially proposed by Skilling (2006) as a numerical approximation method for integrals that arise in Bayesian inference. It is an iterative integration procedure that shrinks the prior volume towards higher likelihood values. The replacement points are drawn uniformly from the prior distribution above an ever-increasing likelihood threshold. The integrand to be considered is one-dimensional, and the task becomes finding a one dimensional sum along the states ordered by the likelihood over unit prior mass. Nested sampling ignores dimensionality, offloading such complications to the task of sampling within the likelihood constraint. Skilling (2006) shows nested sampling cannot detect dimensionality and shape of the likelihood. Therefore, it can be especially beneficial for multi-modal and challenging likelihood function shapes. It differs from an-

nealing methods in which it is based on sampling using a hard constraint on likelihood, whereas annealing methods are based on soft constraints. This method has been successfully applied to astronomical data analyses; see for instance Mukherjee et al. (2006) and Feroz and Hobson (2008) among others. In this paper, we utilize nested sampling to solve stochastic programs with recourse and decision dependent uncertainty.

Suppose we need to sample from

$$\pi(x) = U(x)p(x)/E(U(x))$$

where  $E(U(x)) = \int U(x)p(x)dx$  and  $E(U(x)) < \infty$

with  $U(x) \geq 0$  and  $p(x)$  is a density that is easy to sample from. We define the random variable  $Y \equiv U(x)$  where  $x \sim p(x)$ . Then we can define the standard stationary-excess operation (Cox (1962)) which transforms  $Y$  to  $Z(Y)$  with density

$$q_Z(z) = \frac{\mathbb{P}(Y > z)}{\mathbb{E}(Y)} = \frac{\mathbb{P}(U(x) > z)}{\mathbb{E}(U(x))}$$

The expectation,  $\mathbb{E}(Y)$ , satisfies the identity  $\mathbb{E}(Y) = \int_0^\infty \mathbb{P}(Y > z) dz$  so that  $q_Z$  forms a proper density.

The key representation is to express the density  $\pi(x)$  as a one-dimensional mixture of constrained prior densities  $p(x|U(x) > z)$  as follows

$$\begin{aligned} \pi(x) &= \int_0^\infty \frac{\mathbb{P}(Y > z)}{\mathbb{E}(Y)} p(x|U(x) > z) dz \\ &= \int_0^\infty p(x|U(x) > z) q_Z(z) dz \end{aligned} \tag{3.1}$$

The derivation of Equation (3.1) is provided in Appendix.

If we can sample from the conditional prior densities  $p(x|U(x) > z)$  for a carefully chosen schedule of utility ordinates  $z_1, \dots, z_R$  we can then use a stochastic Riemann approximation for  $\pi(x)$ , namely

$$\pi^R(x) = \sum_{i=1}^R w_i p(x|U(x) > z_i)$$

where each weight,  $w_i$ , is equal to  $\mathbb{P}(Y > z_i) / \sum_{j=1}^R \mathbb{P}(Y > z_j)$ . A practical choice of computing  $z_i$  is to pick  $q_i = 0.9$  and solve  $\mathbb{P}(Y > z_i) = q_i$ . We can find the cutoffs in a sequential stochastic manner by sampling from  $p(x|U(x) > z_i)$  and finding the  $q$ -th quantile of this conditional distribution which corresponds to  $z_{i+1}$ . This can be repeated  $R$  times. The existing sequence of points  $x_1, x_2, \dots, x_R$  provides an estimate of posterior (marginal) distribution given they are appropriately weighted.

The convergence of the approximation error between the expectation function and its estimate is shown to be in mean square of number of iterations (Skilling (2009)). Evans (2007) shows that nested sampling estimates converge in probability. Furthermore, Chopin and Robert (2010) study the formal properties of nested sampling and show that the approximation error vanishes at the standard Monte Carlo rate, and it is asymptotically Gaussian.

### 3.2 Nested Augmented Sampling

To illustrate nested sampling idea, we show how to simulate from the joint distribution  $\pi(x, \xi)$  with  $J = 1$ : namely,

$$\pi(x, \xi) = \frac{u(x, \xi) p(x, \xi)}{Z} \mathbb{I}(Ax \leq b, x \geq 0)$$

where the normalisation constant  $Z$  is given by  $Z = \int u(x, \xi) p(x, \xi) d\xi dx$  (See also Pincus (1968) and Pincus (1970)).

For the sake of parsimony we suppress the conditioning  $\mathbb{I}(Ax \leq b, x \geq 0)$  for the augmented distributions, keeping in mind that all draws should be feasible and satisfy first stage constraints.

First, we represent  $\pi(x, \xi)$  as a one-dimensional mixture over the auxiliary variable  $U$  (Saumard et al. (2014)). By the so-called wedding cake representation, we have

$$u(x, \xi) = \int_0^\infty \mathbb{I}(u(x, \xi) > U) dU.$$

Then, we write

$$\pi(x, \xi) = \frac{1}{Z} \int_0^\infty \mathbb{I}(u(x, \xi) > U) p(x, \xi) dU.$$

The conditional distribution

$$p(x, \xi | u(x, \xi) > U) = \frac{\mathbb{I}(u(x, \xi) > U) p(x, \xi)}{Z(U)}$$

where normalisation constant

$$Z(U) = \int \mathbb{I}(u(x, \xi) > U) p(x, \xi) d\xi dx$$

is a tail probability, and satisfies  $\int_0^\infty Z(U) dU = Z$ . Therefore, we have

$$\pi(x, \xi) = \int_0^\infty p(x, \xi | u(x, \xi) > U) \frac{Z(U)}{Z} dU,$$

The augmented distribution of interest,  $\pi(x, \xi)$  then becomes a mixture of the joint conditional distributions  $p(x, \xi | u(x, \xi) > U)$  with weights  $Z(U)/Z$ . Our key idea is based on the relative efficiency gain by simulating from this distribution in the case of decision dependent uncertainty.

We are interested in sampling from the family of distributions  $p(x, \xi | u(x, \xi) > U)$  for a given utility level,  $U$ . This can be done by setting  $p(x)$  as uniform with pre-specified parameters, on the constraint set  $\mathbb{I}\{Ax \leq b, x \geq 0\}$ . The utility (objective) function,  $u(x, \xi)$  is  $mx - q(\xi)y^*(x, \xi)$  whereas the utility level,  $U$  is set as the current minimum utility value,  $U_{min}$ . For the augmented joint distribution with  $J$  copies,

$$\pi_J(x, \xi_J) \propto \prod_{j=1}^J u(x, \xi_j) p(\xi_j | x) p(x),$$

we want to explore the conditional sampling region of  $p_J(x, \xi_J | u_J(x, \xi_J) > U_{min})$  where  $u_J(x, \xi_J) = \prod_{j=1}^J u(x, \xi_j)$ . The samples from this joint distribution of  $(x, \xi_J)$  can be retrieved by sampling from the Uniform prior distribution of  $x$ , and then drawing samples from the decision dependent distribution. As recommended by Robert and Casella (2010), we

accept the draw if it satisfies the constraint, reject it otherwise.

In order to improve efficiency, single runs of nested sampling can be combined by ad hoc averaging to improve the accuracy. As pointed out by Skilling (2009), a more efficient alternative is to merge the utility values into a single ordered sequence. Therefore, we start with a given number of,  $S$ , live points in which the decision and random variables are drawn from the joint distribution. It records  $U_{min}$ , the lowest of the current utility values across  $S$  live points. Then for each iteration, it selects one of the remaining live points, excluding the one with the minimum, at random and explores the decision space in order to update the minimum utility level,  $U_{min}$ . Collection of  $S$  points allows to obtain a sequence  $S$  times more closely spaced and  $S^2$  times more accurate (Skilling (2006)). The algorithm is run for  $G$  iterations until the minimum utility level and the set of live points stabilize. Since we are interested in the mode of these marginal draws, the final sequence,  $x_1, x_2, \dots, x_G$ , that maximizes the utility function will be sufficient for our purposes.

The basic algorithm can be described as follows:

1. Set  $g = 0$ . Simulate draws for  $S$  live points  $(x, \xi_j)_{(s)}$  from the joint prior distribution  $p(x, \xi_j)$  and evaluate utility levels  $u_J((x, \xi_j)_{(s)}) = \prod_{j=1}^J u((x, \xi_j)_{(s)})$  for  $1 \leq s \leq S$ .
2. Set  $g = g + 1$ . Find the live point with minimum utility;  $s_{(g)}^* = \operatorname{argmin}_s [u_J((x, \xi_j)_{(s)})]$ .
3. Set  $U_{min}^{(g)} = u_J((x, \xi_j)_{(s_{(g)}^*)})$  and  $(x, \xi_j)_{min}^{(g)} = (x, \xi_j)_{(s_{(g)}^*)}$ .
4. Replace the live point,  $s_{(g)}^*$  that provides the minimum draw, by sampling from the constrained distribution  $p_J(x, \xi_j | u_J(x, \xi_j) > U_{min}^{(g)})$  so that new utility is larger than the current minimum,  $U_{min}^{(g)}$ .
5. Repeat steps 2-4 for  $G$  iterations or until a stopping criterion is satisfied.  $\square$

The idea of nested sampling is simply based on sorting points of parameters by their utility values, that are later summed to approximate the uni-dimensional integral. As a by-product, this also provides the augmented distribution samples of interest.

Nested algorithm is efficient in which the shrinkage is expected to be at a geometrical rate by a factor of  $\exp(-1/S)$  per step. In most cases maximum likelihood is not known, so

convergence is only guaranteed asymptotically. The main efficiency concern is the challenge of exploring and efficiently sampling from the hard likelihood constrained domain. Although the evaluation is done on a one-dimensional integrand, the theoretical performance of exact nested sampling algorithm depends linearly on dimension. Particularly, it is shown that the required number of iterations for a fixed error and asymptotic variance grows linearly with the dimensionality (Chopin and Robert (2010)). This is still more efficient compared to the exponential impact of dimensionality within Monte Carlo based algorithms.

The main challenge of nested sampling is the ability to draw samples from the constrained distribution  $p_J(x, \xi_J | u_J(x, \xi_J) > U_{min})$  which has the restriction that the utilities associated with the samples need to be greater than a certain threshold. Use of a basic accept-reject algorithm can be argued to be inefficient, but can work well for models without many tight constraints. This scheme can especially become inefficient as the constraint gets closer to the highest values of likelihood. There are a number of proposed alternatives in the literature. Skilling (2006) proposes MCMC with the truncated distribution as the invariant distribution. Since the starting value is distributed from the invariant distribution, finite number of iterations produce an outcome that is distributed from the marginal distribution. Chopin and Robert (2010) discuss the potential use of random walk Metropolis-Hastings with a diminishing variance factor as a potential solution to draw from the constrained distribution even in the likelihood space of concentrated values. They also introduce the nested importance sampling and discuss the use of approximations via mixtures and formal reversible jump based algorithms. Mukherjee et al. (2006) consider the case where simulations are generated within an ellipsoid, and accepted if they fit the likelihood constraint. Their idea is based on expanding the area of live points with a certain factor, then use a uniform accept-reject step to explore the point that provides a higher likelihood in that area which also conforms with the likelihood constraint.

For this paper, we use a basic accept-reject algorithm with  $N$  steps to sample from the constrained distribution. Our approach is summarized below:

1. Pick one of the  $S - 1$  live points, excluding the one that provides the minimum

utility, at random, as your initial point.

2. Simulate a candidate draw from the joint distribution,  $p_J(x, \xi_J)$ .
3. Accept the candidate draw if it results with an increased minimum utility.
4. Repeat Steps 1-3 for  $N$  iterations.

A key advantage of nested sampling is that it applies directly to the power density  $\pi_J$  without any changes in the algorithm. This is in contrast to simulated annealing that tries to directly sample from power marginal (see Skilling (2006), section 4 for a discussion of the relative efficiency gains). Nested sampling samples more sparsely from the probability distribution in regions with low likelihood and more densely where likelihood is high; resulting in greater efficiency. It also does not require knowing the value of the maximum likelihood.

Practical termination of the algorithm can be achieved simply after a number of steps in which the utility would not increase by more than a small user-defined tolerance (Skilling (2009)). While implementing the algorithm, we check for practical convergence after every so many iterations. When the utility does not increase more than our threshold, we calculate the mode of  $x$  as the estimate of the optimal solution. In case we are not able to sample from the constrained distribution in  $N$  steps in an iteration, strategies may include increasing the value of  $S$  or  $N$ . The asymptotic variance of the sampling estimates are shown to grow linearly with the dimensionality,  $d$ ; which means computational cost is  $O(d^3/\eta^2)$ , where  $\eta$  is a selected error bound. It should be noted that increased dimensionality may make sampling from the constrained distribution domain harder, especially in the areas with high values of the utility function, see the discussion by Chopin and Robert (2010).

### 3.3 Assessment of Solution Quality

Assessment of the solution quality is a fundamental issue for any simulation-based optimization algorithm. If the optimal solution and objective function values are analytically available via integration, the quality of the solution can be evaluated by comparing the

candidate solution and the optimal solution. Statistical estimates, that are computed using the same sample,  $\xi_k$  drawn from  $p(\xi)$ , can be used when the objective function is not analytically available, see for instance Higle and Sen (1996), Shapiro and Homem-de Mello (1998) for such methods. Bayraksan and Morton (2009) provide a review of statistical properties of the optimality gaps for different approaches. However, the use of these approaches are not trivial for problems with endogenous uncertainty, because the stability of the decision dependent probability distribution,  $p(\xi|x)$ , becomes a concern. There is not much literature regarding the assessment of solution quality in large scale problems. The two-step iterative technique of Solak et al. (2010) is among the limited work, and therefore a similar approach is utilized in this paper. First, using a large Monte Carlo simulation based crude search, we generate a select set of random variables for a set of feasible decision variables and compute the objective function values. A number of decisions that optimize the objective function are retrieved as the set of the candidate optimal decisions,  $x_c^*$ . Then, for each candidate,  $x_c^*$ , a large number of draws of random variables is obtained by sampling from  $p(\xi|x_c^*)$ . By using these draws, we go through a second step to solve the problem and estimate the optimal decision,  $x^*$ . We use  $x^*$  as the "true" optimal solution of the problem, and compute the optimal value of objective function,  $mx^* - E_{\xi}[Q(x^*, \xi)]$  accordingly. For assessing the performance of a particular approach, we use the estimated optimality gap which is a function of the absolute discrepancy (i.e. error) between the optimal value of the objective function at the "true" solution  $x^*$  and the value of the objective function at the solution  $x_A^*$  obtained using approach  $A$ . In our case we define the estimated optimality gap via the mean absolute percentage error (MAPE).

This procedure is summarized below.

1. For replication  $k : 1, \dots, K$ :
  - (a) Obtain  $L$  feasible first stage decision variables,  $X^k = \{x_1^k, \dots, x_L^k\}$ .
  - (b) For  $l : 1, \dots, L$ 
    - i. Draw  $N'$  samples,  $(\xi_{l,1}^k, \dots, \xi_{l,N'}^k)$ , of  $\xi_l^k$ , from  $p(\xi|x_l^k)$ .
    - ii. Solve the second stage problem for each  $(x_l^k, \xi_{l,n'}^k)$  pair to retrieve the optimal second stage decisions  $y_l^k$ .

- iii. Compute the objective function  $E_{\xi_l^k}[u(x_l^k, \xi_l^k)] = \frac{\sum_{n'=1}^{n'=N'} u(x_l^k, \xi_{l,n'}^k)}{N'}$
- (c) Compute the candidate optimal decision as  $x_c^{k*} = \operatorname{argmax}_{x_l^k} \{E_{\xi_l^k}[u(x_l^k, \xi_l^k)]\}$ .
- (d) Draw  $N''$  ( $N'' \gg N'$ ) samples,  $\{\xi_1^k, \dots, \xi_{N''}^k\}$ , of  $\xi^k$  from  $p(\xi|x_c^{k*})$ .
- (e) Compute  $E_{\xi^k}[u(x_c^{k*}, \xi^k)] = \frac{\sum_{n''=1}^{n''=N''} u(x_c^{k*}, \xi_{n''}^k)}{N''}$ .
2. Find  $x_c^{k*}$  that maximizes  $E_{\xi^k}[u(x_c^{k*}, \xi^k)]$  as the "true" optimal decision  $x^*$  and estimate the "true" optimal value of the objective function,  $U(x^*) = E_{\xi}[u(x^*, \xi)]$ .
3. For approach  $A$  with estimated objective function value,  $U_A(x_A^*)$ , compute the estimated optimality gap based on absolute percentage error:  $|\frac{U(x^*) - U_A(x_A^*)}{U(x^*)}|$ .

## 4 Newsvendor Problem with Endogenous Uncertainty

In order to illustrate our algorithm by solving a classical decision problem, we formulate the newsvendor problem as a stochastic program with recourse. The two-stage stochastic programming setup of the newsvendor has been considered by several authors including Dai et al. (2000) and Homem-de Mello and Bayraksan (2014). In this decision problem, the newsvendor needs to determine the initial inventory level (the number) of newspapers to be purchased,  $x$ , in the first stage without knowing the demand. We assume that  $\xi$  represents uncertainty within the non-negative demand function,  $d(\xi)$ . Unit purchase price, unit sales price and unit resale (salvage) price are deterministic parameters denoted by  $c$ ,  $s$  and  $r$ , respectively. It is assumed  $s \geq c \geq r$ . We let  $y_1$  and  $y_2$  denote the second stage decisions on quantities of newspapers sold and salvaged in the second stage, respectively. The newsvendor's problem is to determine  $x$  so that the overall expected profit is maximized. The problem can be formulated as

$$\max_x -cx + E_{\xi}[Q(x, \xi)] \text{ such that } x \geq 0,$$

where the recourse function,  $Q(x, \xi)$  is obtained from the linear program

$$Q(x, \xi) = \max_{y_1, y_2} sy_1 + ry_2$$

subject to  $y_1 \leq d(\xi)$  ,  $y_1 + y_2 \leq x$  ,  $y_1 \geq 0, y_2 \geq 0$ .

Given the resolution of uncertainty via the outcome of  $d(\xi)$ , we then can have an optimal recourse action given by the solution

$$y_1^*(x, \xi) = \min(d(\xi), x) \text{ and } y_2^*(x, \xi) = \max(x - d(\xi), 0).$$

Most of the literature on newsvendor problem are focused on the decision model with exogenous demand (Petruzzi and Dada (1999)). On the other hand, the modeling approaches of the impact of price, stock level and marketing effort on demand are reviewed by Qin et al. (2011). Dana Jr and Petruzzi (2001) consider the dependence of demand on both price and inventory level. We focus on so called stock-dependent or inventory-level dependent demand and treat the sales price as deterministic and exogenous from demand. Urban (2005) provide a review of such inventory control models that consider endogeneity within two distinct types; the demand rate being a deterministic function of the initial inventory level or the instantaneous inventory level. Balakrishnan et al. (2004) generalize the newsvendor problem by incorporating the stochastic and initial stock level dependent demand for a shelf space allocation problem. In order to model the demand, they use a power function,  $\lambda(x) = \alpha x^\beta$  in that  $\alpha$  is a scaling parameter and  $\beta$  denotes the inventory elasticity of the demand. Demand is shown to have a non-decreasing behavior with a diminishing rate with respect to the initial inventory level. In a related work, Ernst and Powell (1995) specify a model in which the firm's service level affects the distribution, particularly mean and standard deviation, of demand.

In our development, the demand,  $d(\xi)$  is assumed to be dependent on the initial inventory level  $x$  via  $p(\xi|x)$ . We assume that  $p(\xi|x)$  follows truncated Normal distribution over non-negative values with mean  $\alpha x^\beta$  and standard deviation  $\sigma_d$ .

## 4.1 Multi-item Newsvendor Problem

The standard newsvendor formulation considers only one product and no resource constraints. However, many practical applications include more than one product as well as

resource constraints. In the multi-item setting, the newsvendor needs to decide on the order quantities for different types of newspapers under a fixed budget. The multiple-product single-period inventory model is also referred to as the news-stand model (Lau and Lau (1996)).

Even in the case of exogenous uncertainty, the solution of this problem can be computationally more challenging due to increased dimensionality of both decision and random variables. Abdel-Malek et al. (2004) develop Lagrangian-based methods to find the optimal solution for uniformly distributed exogenous demand, and discusses near-optimal solutions for demand following a number of other continuous distributions. Abdel-Malek and Montanari (2005) and Zhang et al. (2009) point out that the existing literature generally allow potentially negative demand, and proposes a modified Lagrangian-based method and a binary method with a focus on the solution space. Other notable extensions include the consideration of preseason production (Chung et al. (2008)), consideration of outsourcing and salvaging (Zhang and Du (2010)) and the separable programming based approximation method of Niederhoff (2007). For an extensive review, we refer the reader to Turken et al. (2012).

Our application involves a similar setting with the model of Zhang and Du (2010). They consider a multi-product newsvendor system with a fixed production capacity for multiple products, with the objective of fulfilling independently uncertain demands while allowing outsourcing with zero lead time. The option of outsourcing makes the production decisions more challenging in such multi-product settings. The decision maker needs to make a budget allocation so that the total expected production and outsourcing costs are minimized while expected profit is maximized and demand is satisfied. Differently than their model, we allow decision dependent uncertain demand.

We denote the order quantity by  $x_m$  and the random demand by  $\xi_m$  for the  $m^{th}$  item. Letting  $B$  be the total budget,  $\mathbf{x} = (x_1, x_2, \dots, x_M)$ , and  $\boldsymbol{\xi} = (\xi_1, \xi_2, \dots, \xi_M)$ , then the  $M$ -item newsvendor problem can be formulated as a two-stage stochastic program with recourse as

$$\max_{\mathbf{x}} \sum_{m=1}^M -c_m x_m + E_{\boldsymbol{\xi}}[Q(\mathbf{x}, \boldsymbol{\xi})]$$

$$\text{subject to } \sum_{m=1}^M c_m x_m \leq B, x_m \geq 0, m = 1, 2, \dots, M.$$

where the recourse function,  $Q(\mathbf{x}, \boldsymbol{\xi})$  is obtained from the linear program

$$Q(\mathbf{x}, \boldsymbol{\xi}) = \max_{\mathbf{y}_1, \mathbf{y}_2} \sum_{m=1}^{m=M} s y_{1,m} + r y_{2,m}$$

$$\text{subject to } y_{1,m} \leq d(\xi_m), y_{1,m} + y_{2,m} \leq x_m, y_{1,m} \geq 0, y_{2,m} \geq 0, m = 1, 2, \dots, M.$$

Given the resolution of uncertainty via the outcome of  $d(\xi_m)$ , we then can have the optimal recourse actions given by

$$y_{1,m}^*(x_m, \xi_m) = \min(d(\xi_m), x_m) \text{ and } y_{2,m}^*(x_m, \xi_m) = \max(x_m - d(\xi_m), 0), m = 1, 2, \dots, M.$$

## 4.2 APS Formulation of the Multi-item Newsvendor Problem

We assume that the conditional distribution  $p(\boldsymbol{\xi}|\mathbf{x})$  is a truncated multivariate normal distribution with components defined over  $(0, \infty)$ . The mean vector of the conditional distribution is given by  $\boldsymbol{\mu}_M = (\alpha x_1^\beta, \dots, \alpha x_M^\beta)$ . Its variance-covariance matrix,  $\boldsymbol{\Sigma}_M$ , consists of covariance components,  $\sigma_{mn}^2$  for each  $(m, n)$  pair, with  $\sigma_{mm}^2$  denoting the variance of the  $m^{\text{th}}$  component.

Assuming  $J$  independent draws of the  $M$  dimensional random demand vector  $\boldsymbol{\xi}$ , we can write down the augmented distribution,  $\pi_J(\mathbf{x}, \boldsymbol{\xi}^J)$  as

$$\pi_J(\mathbf{x}, \boldsymbol{\xi}^J) \propto \prod_{j=1}^J \left[ \sum_{m=1}^M (-c_m x_m + s y_{1j,m}^* + r y_{2j,m}^*) \right] p(\xi_{j,m} | x_m) p(x_m) \mathbb{I} \left( \sum_{m=1}^M c_m x_m \leq B \right)$$

where  $\boldsymbol{\xi}^J = (\boldsymbol{\xi}_1^J, \boldsymbol{\xi}_2^J, \dots, \boldsymbol{\xi}_M^J)$ . As before the second stage optimal solution is given by  $y_{1j,m}^* = \min(d(\xi_{j,m}), x_m)$  and  $y_{2j,m}^* = \max(x_m - d(\xi_{j,m}), 0)$ .

We note that the joint distribution of the decision variables is subject to the budget constraint. The distribution  $p(\mathbf{x})$  of the decision variable  $\mathbf{x}$  can be specified as a uniform in the multidimensional space subject to the budget constraint. The single-item formulation can be obtained from the above by setting  $M = 1$ .

## 5 Numerical Illustration

In this section we illustrate application of the nested augmented probability sampling to solve single and multi-item newsvendor problems. In doing so, we provide comparisons with MCMC based APS and SAA approaches.

### 5.1 Single Item Problem

We first consider the single item newsvendor problem and assume that the parameters are specified as  $c = 1$ ,  $s = 2$ ,  $r = 0.8$ . Also, for the probability distribution of demand we set  $\alpha = 5$ ,  $\beta = 0.5$ , and the standard deviation as  $\sigma_d = 10$ . Since there is no analytically available solution to the problem, we use an estimate of the optimal solution,  $x^*$  by employing a similar approach to Solak et al. (2010).

In order to estimate  $x^*$  and  $-mx^* + E[Q(x^*, \xi)]$ , we utilize  $K = 100$  replications. For each replication, we obtain  $L = 10,000$  feasible decision alternatives in the decision space of  $(0, 0.1, \dots, 1000)$  and we obtain  $N' = 1,000$  realizations of the random variable for each of these decision alternatives. Then, we record the decision that maximizes the objective function as the candidate optimal decision of that replication. For each candidate optimal decision,  $N'' = 100,000$  realizations of the decision dependent random variables  $\xi$  are drawn and the optimal objective function estimate is computed. Among these, we designate the candidate with the best objective function value, as the optimal decision,  $x^*$  and its respective objective function value as the optimal objective function.

Figure 1 presents the objective function values for the decision space  $(0, 0.1, \dots, 1000)$ . The objective function is relatively flat for values of  $x$  between 150 and 300 where the objective function values are the highest. The box-plot of the 100 best candidate optimal decisions is presented in the left panel of Figure 2. We compute 225.8 as the optimal decision for our analysis. The box-plot of the objective function values for these candidate decisions is presented in the right panel of Figure 2 with an optimal value of 44.951.

The practical implementation of the nested augmented sampling algorithm requires the choice of the number of iterations,  $G$ , the number of random variable draws,  $J$ , and the number of accept-reject steps in each iteration,  $N$ . We have set the total number of

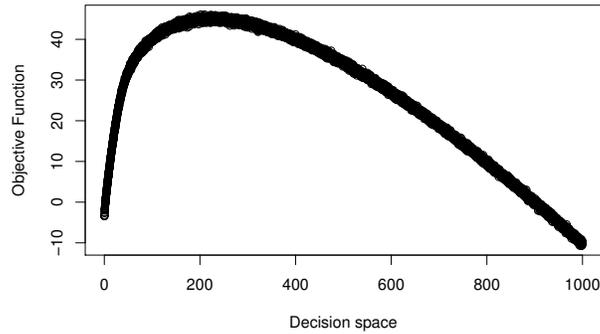


Figure 1: Objective function over the decision space (0, 1000)

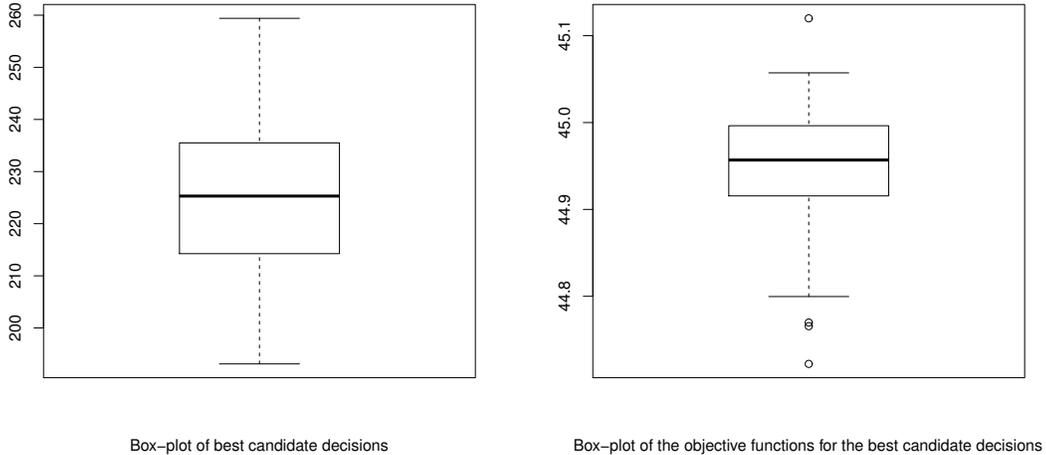


Figure 2: Box-plots of the candidate optimal decisions and candidate optimal objective function values

live points,  $S$  as 20. First, we examine the effect of  $J$  for fixed values of  $G = 500$  and  $N = 20$ . The decision variable,  $x$  is assumed to have a uniform distribution over  $(150, 300)$ . After repeated runs, the box-plots of the optimal decisions and optimal objective function values with  $J$  values of 10, 25 and 100 are shown in Figures 3 and 4 respectively.

When  $J = 10$ , the mean value of the optimal decision is 222.693 whereas the mean objective function value is 44.76. The runs where  $J = 25$  result in a mean of 224.094 for the optimal  $x$  and a mean of 44.86 for the optimal objective function value. For  $J = 100$ , the

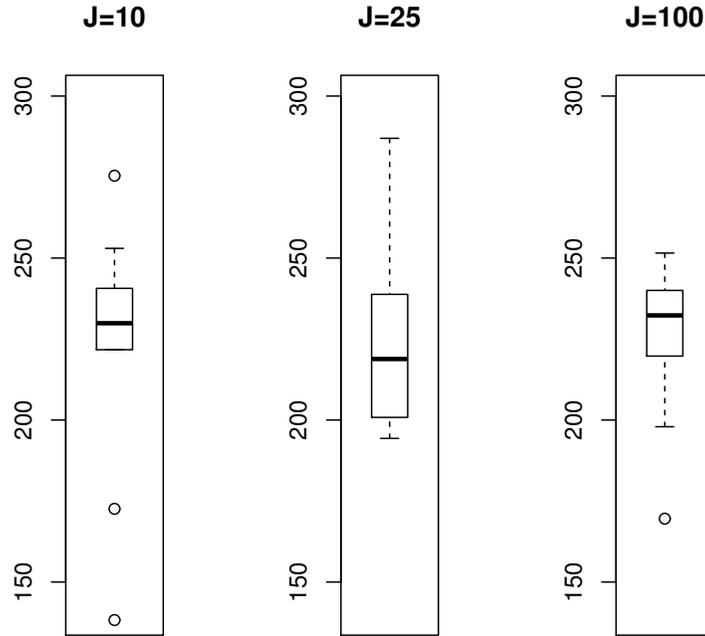


Figure 3: Box-plots of the optimal decisions with  $J$  values of 10, 25 and 100

mean of optimal  $x$  is 224.984. As  $J$  increases, the optimal decision and objective function values converge around  $x^*$  with the standard deviation values of the optimal objective function values are decreasing.

In our example, after  $G = 250$  iterations convergence has been achieved for the decision variable  $x$ . In general, the choice of  $G$  depends on the modality and flatness of the objective function and the nature of constraints. In case of slow convergence, an implementation trick would be to use a higher value of  $N$  to improve the convergence rate. We illustrate the convergence of the decision variable,  $x$  in Figure 5, by providing trace plots of 4 randomly selected live points.

Next, we compare the nested augmented sampling with MCMC based APS and SAA using a total simulation sample size of 150,000. Nested sampling is conducted with parameters  $J = 50$ ,  $N = 10$ , and  $G = 300$ . For MCMC based APS, we set  $J = 100$ ,  $G = 1,500$  and use three Markov chains to assess convergence. The Brooks-Gelman-Rubin (BGR) are

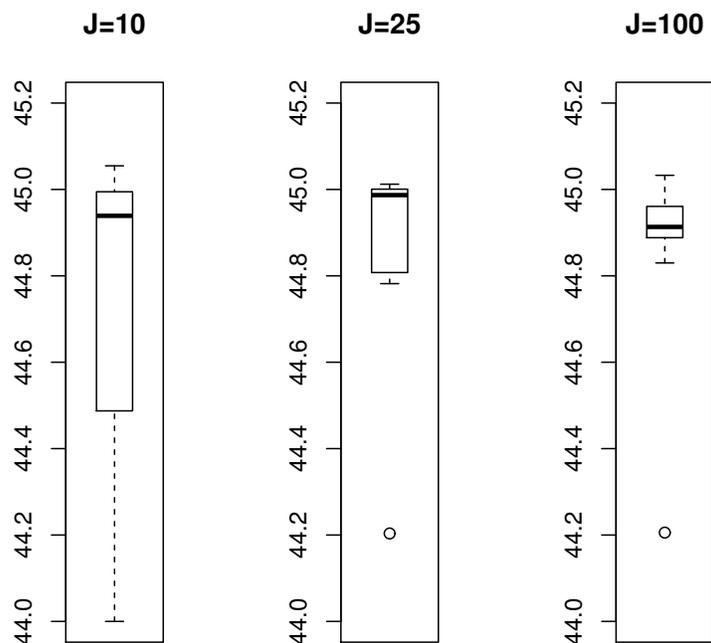


Figure 4: Box-plots of the optimal objective function values with  $J$  values of 10, 25 and 100

used as convergence diagnostics; see Gill (2014). In SAA we explore the decision space between 150 and 300 with increments of 0.1. A sample with size 100 is generated for each replication to compute the candidates for the objective function and the optimal decision.

Figure 6 provides the box-plots of the optimal decisions for each approach. The mean optimal decision is denoted with (\*) for all these approaches in Figure 6. The value of the actual optimal decision  $x^*$  is shown by the dashed horizontal line in each plot. It can be seen that augmented sampling based approaches outperform SAA approach. Based on standard deviation, it can also be seen that that nested sampling approach outperforms both the MCMC based APS and SAA.

Lastly, we have computed objective function values for these candidate optimal decisions by generating the same number of (100,000) decision dependent random variables. Using the optimal objective function value estimates, we compute the estimated optimal-

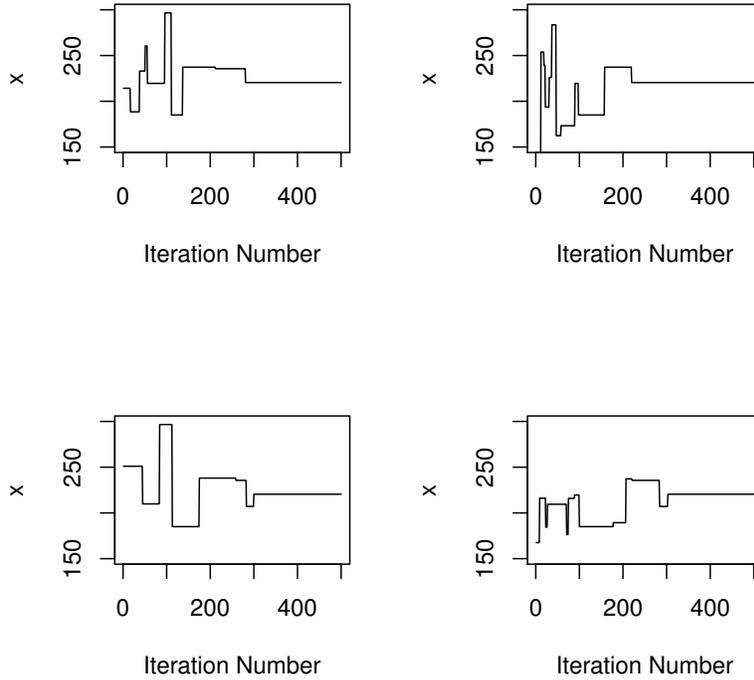


Figure 5: Trace plots of the decision variable for randomly selected live points for the nested augmented sampling formulation

ity gaps in the form of mean absolute percentage error (MAPE) as discussed in Section 3, see Figure 7. The mean optimality gaps are 0.126%, 0.206%, and 0.219% for augmented nested sampling, MCMC based APS and SAA, respectively. Augmented nested sampling also results with smaller standard deviation. This can be explained by the poor convergence of MCMC and inefficient structure of SAA. However; it should be noted that the median value of SAA is very comparable to augmented simulation approaches.

## 5.2 Multi-item Problem with Correlated Demand

Next, we solve for the multi-item newsvendor problem. In case of independent demand parameters within an incapacitated setting, the problem can be decomposed into  $M$  single item problems and its solution becomes relatively straightforward. Therefore, we consider the more challenging case of multi-items with correlated demands. Solving for

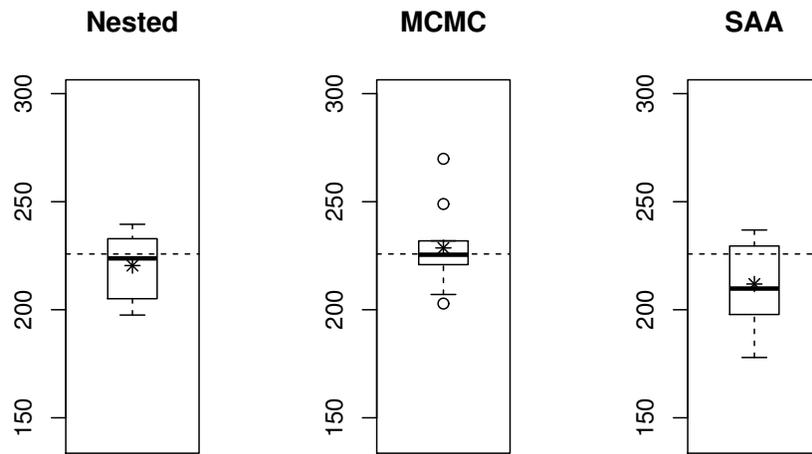


Figure 6: Box-plots of the optimal decisions for the same total sample size using augmented nested sampling, MCMC based APS and SAA

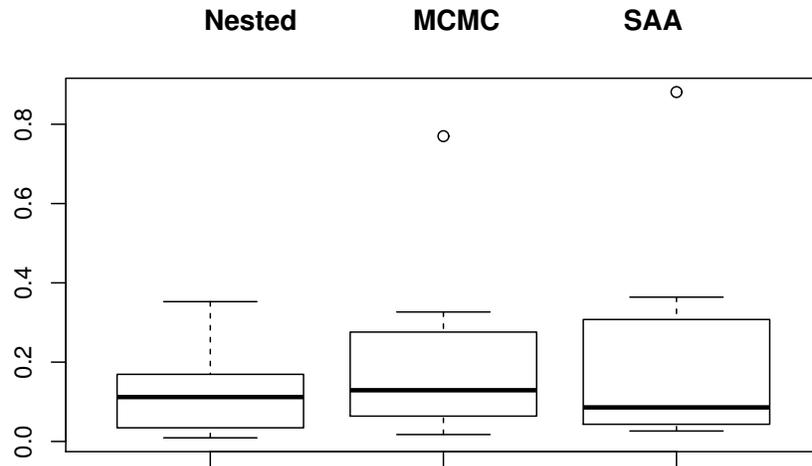


Figure 7: Estimated Optimality Gaps for the same total sample size using nested augmented sampling, MCMC based APS and SAA

the newsvendor problem with  $M = 3$  items, we set  $c = 10$ ,  $s = 12$  and  $r = 1$  for all three

items. The variance-covariance matrix of the multivariate truncated normal distribution for the demand vector is given in Table 1.

Item	1	2	3
1	1600	400	-100
2	400	576	-200
3	-100	-200	1024

Table 1: Variance covariance matrix of uncertain demand

The respective correlations are  $\rho_{1,2} = 0.417$ ,  $\rho_{1,3} = -0.078$ , and  $\rho_{2,3} = -0.260$  for the three items. The parameters of the mean for each demand distribution are specified as  $\alpha = 10$  and  $\beta = 0.5$ . It is important to note that in the decision dependent demand case, in addition to the budget constraint, the correlation structure of the item demands affect the optimal solution. Even in the case of a non-binding budget constraint, the presence of correlation among the item demands implies an optimal solution different than the one obtained by solving  $M$  single item problems. Because of this, for ease of illustration, we set the resource capacity as 1,000, which results with a non-binding resource constraint and an incapacitated newsvendor problem.

The nested augmented sampling approach is run for  $G = 250$  iterations,  $N = 5$  accept-reject steps and  $J = 100$  draws of the random variable in each iteration, resulting with a total of 125,000 samples. A uniform distribution over  $(60, 110)$  is assumed for each item. Following Solak et al. (2010), we used a similar approach as in the case of a single item and obtained the optimal objective function value as 211.179.

The estimated optimality gaps for each method via MAPE are illustrated in Figure 8. We used 1,250,000 samples for MCMC ( $G = 12,500$  and  $J = 100$ ) and SAA (10 draws for each  $50^3 = 125,000$  decision point). Whereas we already have attained convergence for nested sampling after 125,000 samples. The mean MAPE values are 3.59%, 4.54%, and 13.37% for nested augmented sampling, MCMC based APS and SAA respectively. Even with 10 times less samples, nested augmented sampling outperforms the other approaches. Even when one uses 100 draws for each decision point in SAA, the mean MAPE only improves to 7.49%, which is still outperformed by APS based approaches.

For computations, R software (Team (2014)) was utilized on a 2.8 GHz and 16 GB

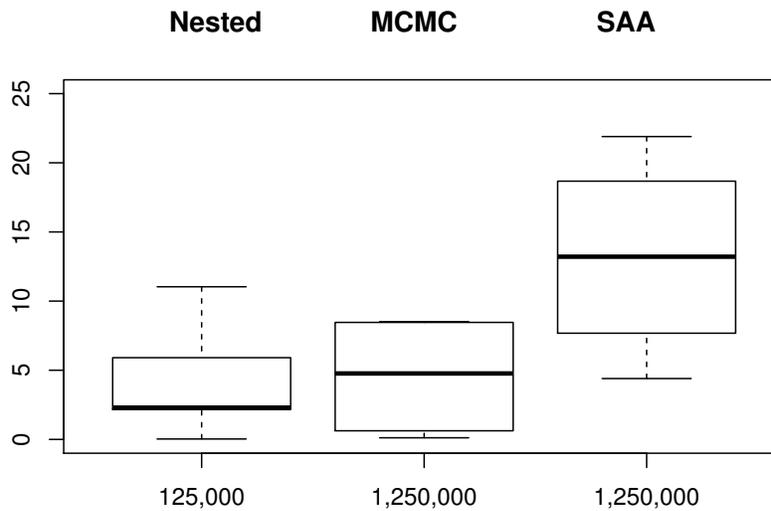


Figure 8: Estimated Optimality Gaps for the correlated demand case using nested augmented sampling, MCMC based APS and SAA

RAM MacBook. For the 1-dimensional case; a replication of drawing 150,000 samples have taken 2.034, 12.308 and 40.362 seconds for nested, SAA and MCMC algorithms, respectively. The results of these runs are visualized in Figure 6 and 7. Whereas, the runs for the multi-dimensional case have taken 395.483, 1845.839 and 4211.966 seconds for nested, SAA and MCMC algorithms, respectively. It should be noted that nested algorithm used 10 times less samples for optimality gap comparison. For the sake of a fair comparison and to retrieve equal number of samples, if SAA is run for 1 draw at each time (which would not make sense for algorithmic purposes), that would take 201.844 seconds albeit with a far worse performance. The run times have room for improvement with better array storage management. For all approaches, it should also be noted that the use of a truncated distribution in the model makes the runs considerably slower compared to the model with a non-truncated distribution.

Overall, our numerical illustrations suggest that nested augmented sampling provides an alternative approach to the solution of two stage stochastic programs with decision dependent uncertainty. The performance of the nested augmented sampling is found to be

superior and more efficient when compared to MCMC based APS and SAA. The conclusion seems to be applicable in higher dimensions as well, especially in the case of dependent random variables. Nested sampling is efficient in that its convergence is linearly affected by dimensionality. As a potential disadvantage, APS requires the estimation of mode as the optimal decision, which can be cumbersome in the multi dimensional cases. In this paper, we have computed the mode either by simply counting the draws or by using the mean as an estimate when  $J$  value is high enough (i.e.  $J > 50$ ).

## 6 Concluding Remarks

Solution of stochastic programs with decision dependent uncertainty poses challenging computational issues because the joint augmented space of decision and random variables needs to be explored. We propose a novel augmented nested sampling approach by recasting the stochastic optimization problem as a simulation problem with stochastic decision variables. We solve the stochastic program by simultaneously performing simulation and optimization, and obtain the mode of the of the stochastic decision variable as the optimal solution. Nested sampling is used to sample from the augmented space of both the random and the decision variables. We illustrate our methodology solving single and multi item two-stage newsvendor problems with continuous stock-dependent random demand. Our findings suggest that, when compared with SAA and MCMC methods, the proposed methodology provides an efficient way of simulation with reasonable estimated optimality gaps. The proposed approach can be effective in problems with objective functions and/or gradients that are difficult to compute or estimate. To the best of our knowledge, this is the first paper that proposes nested sampling within a solution approach for stochastic programs.

The biggest implementation challenge for the proposed approach is sampling from the resulting non-standard distributions in case of constrained domains. Choice of the parameters,  $G$ ,  $N$ ,  $J$  and  $S$ , of the nested sampling, is mostly problem dependent. The choice of  $S$  depends on the multi-modality of the decision. For uni-mode decisions, an  $S$  value as low as 2 can be sufficient. In cases where it is costly to draw from the constrained

prior distribution, it may be wiser to use a smaller value of  $N$  and larger value of  $S$ . Skilling (2006) provides a discussion on the choice of these parameters.

Another potential challenge is computation of the mode for multi-dimensional problems. The result of Pincus (1968), that allows us to use the ergodic mean for high values of  $J$  to estimate the optimal first stage decision  $x^*$ , can be helpful in high dimensional decision spaces where the joint mode is difficult to obtain.

Nonlinear forms for decision function  $d(\xi)$  can be easily accommodated in the proposed methodology. Another potential extension to the augmented nested simulation approach would be inclusion of the second stage decisions,  $y(x, \xi)$ , in the algorithm when it is expensive/difficult to compute  $y(x, \xi)$ . As presented in Ekin et al. (2014), this can be done by constructing an augmented joint distribution as  $\pi(x, \xi, y)$  which requires sampling from the conditional distribution  $\pi(y|x, \xi)$  using the result of Pincus (1968).

Lastly, the extension to the multi-stage setting can be considered. In the case of multi-stage newsvendor problem, at the first stage the decision maker needs to plan for several periods with endogenous uncertain demand in each period. This is especially relevant in cases where the lead time (time between the order and delivery) is long. Computationally, a  $T$  stage problem can be solved by using a nested scheme and replacing expected values with their approximations. However, it should be noted that the dimensionality grows exponentially, and it becomes more challenging to find a solution for the decision dependent problem. Generally, backward induction is utilized for the solution of these problems. However large number of scenarios need to be considered, and evaluation of potentially intractable expected utility integrals are required. For instance, Müller et al. (2007) propose the use of forward simulation and reduction of the space through a low-dimensional summary statistic for such an unconstrained decision problem. For the constrained sequential problems, this warrants further analysis and further theoretical results may be required. We are currently investigating the feasibility of nested augmented simulation for such multi-stage decision dependent problems.

## 7 Appendix

Derivation of Equation (3.1):

The key representation of the marginal distribution in nested sampling is given by

$$\begin{aligned}\pi(x) &= \int_0^\infty \frac{\mathbb{P}(Y > z)}{\mathbb{E}(Y)} p(x|U(x) > z) dz \\ &= \int_0^\infty p(x|U(x) > z) q_Z(z) dz\end{aligned}$$

There are two ways of deriving this equality: <sup>1</sup>

First, by definition from the conditional distribution:

$$p(x|U(x) > z) = \frac{p(x)\mathbb{I}(U(x) > z)}{\mathbb{P}(U(x) > z)}$$

Hence,

$$\begin{aligned}\pi(x) &= \int_0^\infty \frac{\mathbb{P}(Y > z)}{\mathbb{E}(Y)} \frac{p(x)\mathbb{I}(U(x) > z)}{\mathbb{P}(U(x) > z)} dz \\ &= \int_0^\infty \frac{\mathbb{I}(U(x) > z)}{\mathbb{E}(Y)} p(x) dz \\ &= \frac{U(x)p(x)}{\mathbb{E}(Y)} := \pi(x) \quad \square\end{aligned}$$

Alternatively, given the joint density  $p(x, y)$ , one can write

$$p(x|U(x) > z) = p(x|Y > z) = \frac{\int_z^\infty p(x, y) dy}{\mathbb{P}(Y > z)}$$

---

<sup>1</sup>We thank the anonymous reviewer for pointing this out.

Thus,

$$\begin{aligned}
\pi(x) &= \int_0^\infty \frac{\mathbb{P}(Y > z)}{\mathbb{E}(Y)} \cdot \frac{\int_z^\infty p(x, y) dy}{\mathbb{P}(Y > z)} \\
&= \frac{1}{\mathbb{E}(Y)} \int_0^\infty \int_z^\infty p(x, y) dy dz \\
&= \frac{1}{\mathbb{E}(Y)} \int_0^\infty \int_0^y p(x, y) dz dy \text{ (interchange of integrals)} \\
&= \frac{1}{\mathbb{E}(Y)} \int_0^\infty yp(x, y) dy \\
&= \frac{p(x)}{\mathbb{E}(Y)} \int_0^\infty yp(y|x) dy \\
&= \frac{p(x)}{\mathbb{E}(Y)} \mathbb{E}(Y|x) \\
&= \frac{U(x)p(x)}{\mathbb{E}(Y)} \text{ (} Y = U(x) \text{ is measurable w.r.t. } x) \\
&= \pi(x) := \pi(x) \square
\end{aligned}$$

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