



Scenario generation in stochastic programming using principal component analysis based on moment-matching approach

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Abstract

In optimization models based on stochastic programming, we often face the problem of representing expectations in proper form known as scenario generation. With advances in computational power, a number of methods starting from simple Monte-Carlo to dedicated approaches such as method of moment-matching and scenario reduction are being used for multistage scenario generation. Recently, various variations of moment-matching approach have been proposed with the aim to reduce computational time for better outputs. In this paper, we describe a methodology to speed up moment-matching based multistage scenario generation by using principal component analysis. Our proposal is to pre-process the data using dimensionality reduction approaches instead of using returns as variables for moment-matching problem directly. We also propose a hybrid multistage extension of heuristic based moment-matching algorithm and compare it with other variants of moment-matching algorithm. Computational results using non-normal and correlated returns show that the proposed approach provides better approximation of returns distribution in lesser time.

Keywords Scenario generation · Moment-matching · Principal component analysis · Stochastic programming

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1 Introduction

Stochastic programming is a common optimization technique used to solve decision problems involving uncertainty. Representing the underlying random process is the major hurdle in any application of multistage stochastic programming. To assess the risk for the financial decision making process, simulation models are widely used. These models are generally solved by taking expectation over a set of scenarios. The scenario trees are generated by using appropriate scenario generation methods such that they provide discrete approximations of assumed continuous distribution of parameters. In case of multistage stochastic programming, the main characteristics are the time and the randomness of the future events. The scenario trees are commonly used [3, 20]. See [18, 24] for a detailed overview and literature on scenario methods for portfolio optimization and risk management.

The three basic approaches for capturing the joint distribution and approximating the underlying stochastic process or the joint distribution for scenario generation process are:

- *The moment-matching approach* This approach takes into account the interdependencies between the random variables and captures the joint distribution of the scenarios via moments including the cross-moments. It matches the mathematical definition of the moments to given values and solves the set of so formed non-convex equations. Initially introduced by Høyland and Wallace [16], this approach was extended in a more refined way to reduce the computational complexity of the resulting optimization problem by Date et al. [6], Høyland et al. [15]. Høyland and Wallace [16] proposed a method based on nonlinear programming problem to generate a limited number of discrete outcomes with specified statistical properties. Consiglio et al. [2] formulated a moment-matching model to generate multi-factor scenario trees for stochastic optimization satisfying no-arbitrage restrictions with a minimal number of scenarios. Further, Høyland et al. [15] proposed a moment-matching method with the idea of constructing approximated distribution of returns similar to the original distribution in terms of first few moments. Mehrotra and Papp [19] proposed an optimization problem by formulating the problem as a semi-infinite linear programming to generate moment-matching scenarios. Their method is capable of generating scenarios matching any prescribed set of moments of the underlying instead of matching moments upto a fixed order. Geyer et al. [8] pointed that in order to get meaningful scenarios, the arbitrage opportunities must be ruled out. They also compared two popular scenario generation methods: moment-matching and scenario reduction [9] (by approximately minimizing a metric given by Heitsch and Romisch [11]) in the context of financial optimization. Rubasheuski et al. [21] proposed a faster method for scenario generation using a combination of moment-matching and scenario reduction method. Consiglio et al. [5] also formulated a global optimization model to generate moment-matching, arbitrage-free trees for an arbi-

trary number of risk factors. The dimensionality reduction based approach can be extended to the decomposed moment-matching algorithm as well, but the data needs to be scaled properly.

- *The copula approach* This approach splits the task of modeling the joint distribution for scenario generation into two. First the marginals are obtained and second the multivariate joint distribution is captured. This method takes into account the asymmetry, leptokurticity, heteroskedasticity and fat tails present in the financial data. For more details see Cherubini et al. [4], Goel et al. [10].
- *The distance minimization approach* With the help of a few points, this approach aims to approximate the true distribution (continuous or discrete) such that the Kantorovich distance between the original and approximated stochastic optimization model is minimized [13].

We focus on the first approach in this article, on multistage and multiple variable scenarios generation in the context of financial optimization.

Principal component analysis (PCA) is a commonly used method in data analysis for identification of key factors in multidimensional data. It was introduced by Pearson and Hotelling [14] with a purpose to reduce the number of variables while still retaining the pertinent information describing the major variance in a sample. This is achieved by linearly transforming the original variables to a new set of uncorrelated variables in such a way that the first principal component has the largest possible variance. Also, each succeeding component in turn has the highest variance possible under the constraint that it is uncorrelated with the preceding components. Topaloglou et al. [23] applied principal component analysis followed by an empirical sampling procedure for scenario generation. Other recent articles on PCA includes Abdi and Williams [1], Hess and Hess [12]. For a detailed study on PCA, reader can refer to Jolliffe [17].

In this work, we propose multistage extensions of heuristic based moment-matching algorithm coupled with PCA. Principal components have an identity correlation matrix by construction, the problem reduces to the problem of matching moments. In order to test the stability conditions of models, we use a stochastic programming based portfolio optimization model proposed by Sakar and Koksalan [22].

The paper is organized as follows: Sect. 2 briefly explains the original and the decomposed multistage moment-matching. Section 3 discusses the heuristic based moment-matching scenario generation, proposed multistage extension and its comparison with the original decomposed approach. Section 4 presents motivation for PCA approach and its application with multistage extension. Also, this section presents the results of numerical experiments to compare the performance of the proposed approaches with results obtained from [9] and [21]. Section 5 concludes our findings.

2 The moment-matching method for scenario generation

General principle in applying statistical methods is to determine various statistical properties (e.g., mean, variance or higher order moments) of given data. Values of these statistical properties are then used to determine the best theoretical distribution

for the data. The idea behind the moment-matching approach is to match the statistical properties of the generated scenarios with those of the observed data process.

2.1 Original moment-matching algorithm

Let S be the set of all specified statistical properties (data) and ρ_i be the specified value (observed value) of statistical property i in S . Let T be the total number of stages where each stage denotes the state of underlying at a point in time, x be the scenario vector where $x_{n,t,k}$ denotes the value of underlying returns for product $n \in 1, 2, \dots$ in outcome $k = 1, 2, \dots, \prod_{h=1}^t \Theta_h$ on stage $t \in T$. ρ be the probability vector where $\rho_{t,k}$ expresses the probability of the outcome $k = 1, 2, \dots, \prod_{h=1}^t \Theta_h$ in stage $t = 1, 2, \dots, T$. $f^i(x, \rho)$ be the i th moment, w_i be its weight and Θ_t be the number of branches in stage t . The non-linear optimization problem proposed by Høyland and Wallace [16] is given as follows:

$$\begin{aligned} & \min_{x, \rho} \sum_{i \in S} w_i (f^i(x, \rho) - \tau_i)^2 \\ \text{s.t.} \quad & \sum_{k=(j-1)\Theta_t+1}^{j\Theta_t} \rho_{t,k} = 1 \quad \forall t = 2, 3, \dots, T; \quad j = 1, 2, \dots, \prod_{h=1}^{t-1} \Theta_h \\ & \rho_{1,1} = 1 \\ & \rho_{t,k} > 0 \quad \forall t \in T, \quad k \in 1, 2, \dots, \prod_{h=1}^t \Theta_h. \end{aligned}$$

In general, this optimization problem is not convex and convergences to a solution which is not guaranteed. When the moments are derived from actual data, e.g., the historical stock prices for practical application, this optimization problem has a locally optimal solution in general.

2.2 Multistage decomposed moment-matching

Rubasheuski et al. [21] recently proposed a more efficient algorithm to solve multistage optimization problem. They proposed to decompose the above non-linear programming problem into sub-problems such that the matching problem can be solved for each stage separately. Let $x_{n,t,k}$ be the value of variable x for product $n \in 1, 2, \dots$ in outcome $k = 1, 2, \dots, \prod_{h=1}^t \Theta_h$ on stage $t \in T$. Let μ_n be the grand mean demand for product $n \in N$ and $\alpha_n \in [0, 1]$ be the mean reversion factor for product $n \in 1, 2, \dots$. Steps of decomposed algorithm are explained as follows:

Step 1: Set $t = 1$ and $\tau_i = \mu_n$ for each $x_{n,t,1}$ for every n .

Step 2: Set $t = t + 1$. For each parent $x_{n,t-1,k}$, compute $\tau_i = \alpha_n x_{n,t-1,k} + (1 - \alpha_n) \mu_n$ for its children.

Step 3: Solve the non-linear optimization problem with respect to t th stage components only.

Step 4: If $t \leq T$, repeat for $t = t + 1$.

They matched first three moments and correlation matrix for different configurations (N, T, b) where N denotes the number of underlying products being considered for portfolio optimization, T denotes the number of stages in the scenario tree and b is the branching factor, indicating the constant number of child nodes generated from each node.

3 A heuristic for moment-matching scenario generation

In both the moment-matching based algorithms discussed in previous section, the number of variables in non-linear optimization problem is proportional to the size of generated scenario set. Due to this, a large amount of time is consumed in solving each non-linear optimization problem. In order to overcome this limitation, Høyland et al. [15] proposed an iterative process for scenario generation using cubic transform. This process requires a fixed number of variables in the non-linear optimization problem, thus reduces the calculation time.

3.1 Single stage algorithm

This algorithm generates n discrete random variables and transforms them in such a way that the first four moments approximately match the given values. By construction, the correlation matrix of random variables at this stage is close to an identity matrix. Then, it uses another transformation to get correlation matrix close to the given matrix. These two transformations are discussed in detail in the following subsections.

3.1.1 Cubic transform

Fleishman [7] discussed this transformation as a method to convert a standard normal random variable, i.e., $\tilde{X}_i \sim N(0, 1)$ to a non-normal random variable $\tilde{Y}_i$ with the given first four moments as follows:

$$\tilde{Y}_i = a + b\tilde{X}_i + c\tilde{X}_i^2 + d\tilde{X}_i^3.$$

The parameters a , b , c and d are approximated by solving a system of non-linear equations. First four moments of $\tilde{Y}_i$ are written as functions of the first 12 moments of $\tilde{X}_i$ and the decision variables a , b , c and d . The non-linear optimization problem is to minimize the distance between those moments and their target values. The results obtained with this transformation are the approximate solution. Even if the solution does not exist, it gives the closest approximation.

3.1.2 Cholesky decomposition

If $\tilde{X}_i$, $i = 1, 2, \dots, n$ are mutually independent standard normal, i.e., $N(0, 1)$ random variables, the random vector $\tilde{Y}$ defined by $\tilde{Y} = L\tilde{X}$ gives an n -dimensional random vector with the correlation matrix $R = LL^T$ such that diagonal entries are 1. Further, if $\tilde{X}$ is a non-normal random variable with mean 0 and standard deviation 1, the third and the fourth order moments of $\tilde{Y} = L\tilde{X}$ are given by:

$$E(\tilde{Y}_i^3) = \sum_{j=1}^i L_{ij}^3 E[\tilde{X}_j^3],$$

$$E(\tilde{Y}_i^4) - 3 = \sum_{j=1}^i L_{ij}^4 (E[\tilde{X}_j^4] - 3)$$

where L_{ij} are the elements of the lower triangular matrix L .

3.1.3 Iterative approach

In order to use this algorithm on non-independent variables, Høyland et al. [15] recommended an iterative approach. Steps of this iterative approach are given as follows:

Step 1: Let target vector be $\tilde{Z}$ with target moments *tarmom* and target correlation matrix R .

Step 2: Calculate moments *mom* of $\tilde{Y}$ such that:

$$\begin{aligned}\tilde{Z} &= \alpha \tilde{Y} + \beta \\ mom_1 &= 0, \quad mom_2 = 1 \\ \alpha &= tarmom_2^{1/2}, \quad \beta = tarmom_1 \\ mom_3 &= \frac{tarmom_3}{\alpha^3}, \quad mom_4 = \frac{tarmom_4}{\alpha^4}.\end{aligned}$$

Step 3: Calculate L such that $R = LL^T$ using Cholesky decomposition.

Step 4: Calculate the moments *trsfmom* of $\tilde{X}_i$ such that $\tilde{Y} = L\tilde{X}$ where $\tilde{X}_i$ are uncorrelated univariate random variables.

$$E[\tilde{X}_i^3] = \frac{1}{L_{ii}^3} \left(E[\tilde{Y}_i^3] - \sum_{j=1}^{i-1} L_{ij}^3 E[\tilde{X}_j^3] \right).$$

$$E[\tilde{X}_i^4] - 3 = \frac{1}{L_{ii}^4} \left(E[\tilde{Y}_i^4] - \sum_{j=1}^{i-1} L_{ij}^4 (E[\tilde{X}_j^4] - 3) \right).$$

- Step 5: Generate X using random number generator with $\mu = 0$ and $\sigma = 1$.
 Step 6: Transform these values using cubic transform to get moments close to *trsf-mom* keeping them independent using Algorithm 1.
 Step 7: Transform variables such that they have the target correlation with moments preserved using Algorithm 2.
 Step 8: Calculate $\tilde{Z}$ with the target moments

$$\tilde{Z} = \alpha \tilde{Y} + \beta.$$

Algorithm 1 Moment-matching algorithm: Part 1

```

 $p = 1$  and  $\tilde{X}_1 = \tilde{X}$ 
while  $RMSE(R_p; I) > \varepsilon$  do
  do Cholesky decomposition:  $R_p = L_p L_p^T$ 
  do backward transform  $X_p^* = L_p^{-1} \tilde{X}_p$ 
  do cubic transform of  $X_p^*$  with target moments of  $\tilde{X}$ 
  compute correlation matrix  $R_{p+1}$ 
   $p = p + 1$ 
end while
 $\tilde{X} = \tilde{X}_p$  with  $RMSE(R_p; I) \leq \varepsilon$ 
  
```

However, it is possible to specify a combination of values for moments with no possible solution. Therefore, this algorithm may not converge in some cases. The chances of convergence are more if the number of scenarios generated is higher. Also if a fixed number of iterations are used in steps 6 and 7, the final output is a close approximation with respect to the required moments.

Algorithm 2 Moment-matching algorithm: Part 2

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 $\tilde{Y}_1 = L \tilde{X}^*$ 
 $p = 1$  and  $R_1$  is correlation matrix of  $\tilde{Y}_1$ 
while  $RMSE(R_p; R) > \varepsilon$  do
  do Cholesky decomposition:  $R_p = L_p L_p^T$ 
  do backward transform  $Y_p^* = L_p^{-1} \tilde{Y}_p$ 
  do forward transform  $Y^{**}_p = L Y_p^*$ 
  do cubic transform of  $Y^{**}_p$  with target moments of  $\tilde{Y}$ 
  compute correlation matrix  $R_{p+1}$ 
   $p = p + 1$ 
end while
 $\tilde{Y} = \tilde{Y}_p$  with  $RMSE(R_p; R) \leq \varepsilon$ 
  
```

3.2 Multistage decomposed extension

The multistage algorithm discussed in Sect. 2 uses a non-linear optimization on all the variables, therefore, the chances of getting a good solution decreases as the number of assets increases. Hence, instead of solving the non-linear optimization problem at each stage, we propose to use heuristic approach for matching moments at

each stage. Steps of the algorithm are similar to the decomposed approach proposed by Rubasheuski et al. [21]:

- Step 1: Set $t = 1$ and $tarmom_1(n, t) = \mu$. Set $t = t + 1$.
 Step 2: Compute $tarmom_1(n, t) = \alpha_n \cdot x_{n,t-1} + (1 - \alpha_n) \cdot tarmom_1(n, t - 1)$.
 Step 3: Generate scenarios using algorithm in Sect. 3.1.3 for t th stage components.
 Step 4: If $t \leq T$, repeat for $t = t + 1$.

3.3 Numerical experiments

We have implemented both these algorithms using GAMS with IPOPT non-linear solver for complete non-linear optimization problem as well as for the cubic transform optimization problem in heuristic approach. We have used stock prices of N stocks from Indian stock market for different configurations (N, T, b) . Here, the error term represents the objective function given in Sect. 2.1. Both these algorithms are compared in Table 1 using 4 configurations.

We observe that the original decomposed version gives a good output when the number of variables is small. As variable size increases, either the algorithm does not converge or it converges to a trivial solution with all the points having the same values. Further, we observe that the computation time increases as the number of variables increases. A comparison is shown in Table 1. We observe from the comparison that heuristic based approach provides better approximation in each case for same configurations. As it starts with the random numbers and transforms them to give the desired moments, it provides an output in every case. After testing this algorithm on different data sets, we conclude that for smaller number of variables, even one iteration of both the transformations works well.

4 Dimensionality reduction based approach

4.1 Principal components

Let $X = (X_1, X_2, \dots, X_n)$ be n random variables with covariance matrix Q . Principal components are uncorrelated vectors that can best represent the correlation and the covariance of the original data set. They are given by the eigenvectors of the

Table 1 Comparison between original decomposed approach and heuristic based decomposed approach

Configuration (N, T, b)	Original algorithm error term	Original algorithm time (s)	Heuristic algorithm error term	Heuristic algorithm time (s)
(3,1,20) Base	$10^{-9}, 0.012$	1.421	$10^{-18}, 10^{-4}$	2.556
(3,1,20)	$10^{-9}, 0.001$	1.862	$10^{-10}, 10^{-4}$	2.324
(2,1,6)	$10^{-10}, 0.021$	1.791	$10^{-8}, 10^{-4}$	1.103
(3,1,10)	$10^{-9}, 0.01$	1.723	$10^{-8}, 10^{-4}$	1.924

covariance matrix Q and are ranked according to the corresponding eigenvalues. More precisely, if λ_i , $i = 1, 2, \dots, n$ are the eigenvalues of the matrix Q such that $\lambda_1 > \dots > \lambda_n$ and u_i , $i = 1, 2, \dots, n$, are orthonormal eigenvectors corresponding to these eigenvalues, then the principal components are given by

$$u_i^T x; \quad i = 1, 2, \dots, n.$$

Principal components are uncorrelated and have the eigenvalue λ_i corresponding to the eigenvector u_i . Eigenvector corresponding to the highest eigenvalue accounts for the maximum variability in the data.

4.2 Modified algorithm

In the algorithm discussed in the previous section, the first step was to convert the random variables such that their correlation matrix R becomes an identity matrix and the moments were close to the target moments. In the second step, variables were transformed in such a way that the new correlation matrix was the target correlation matrix but preserving the moments obtained in the last step. In this modified version, we propose the use of principal components calculated using principal component analysis in place of the original random variables. Scenario generation task is now performed on these principal components considering their properties. Scenarios generated are then converted back to the original data form using back projection on the principal components.

According to the construction of the principal components, their correlation matrix is an identity matrix. Although using these components reduce the computation time in second step, it increases the computation time by twice the time required to compute the principal components. In our analysis, we observe that the modified algorithm is computationally more efficient. Further, if the historical data is used to estimate the moments in the moment-matching scenario generation algorithm, then this algorithm can be used on lesser number of the principal components which were sorted by the eigenvalues. Scenarios can be constructed from these generated values of principal components and the constant value of the other components. Given the correlation property of the principal components, this approach reduces the computation in the moment-matching problem at each level. Steps followed by the algorithm are given in Algorithm 3. In further sections, we discuss some experimental results to compare the heuristics based original algorithm with the proposed modified algorithm.

Algorithm 3 Modified algorithm

Take historical data of n entities
 Calculate n_a principal components of data and conversion matrix
 Calculate target moments and generate X using random number generator
 $p = 1$ and $\tilde{X}_1 = \tilde{X}$
while $RMSE(R_p; I) > \varepsilon$ **do**
 do Cholesky decomposition: $R_p = L_p L_p^T$
 do backward transform $X_p^* = L^{-1} X_p$
 do cubic transform of X_p^* with target moments of $\tilde{X}$
 compute correlation matrix R_{p+1}
 $p = p + 1$
end while
 $\tilde{X} = \tilde{X}_p$ with $RMSE(R_p; I) \leq \varepsilon$
 Convert these principal component scenarios to actual scenarios using the conversion factors

4.3 Numerical experiments

We compare simple moment-matching approach with dimensionality reduction based moment-matching approach using data sets obtained from Indian stock market data. We selected 10 stocks randomly from NSE indices for the single stage algorithm and 3 stocks for the multistage algorithm. Results for this analysis are given in Table 2, where the error term represents value of objective function as given in Sect. 2.1 and time represents the reference time taken to compute the scenarios. Comparison of results for single stage shows that the modified algorithm takes almost half time to generate the scenarios and matches the target moments more accurately. For the multistage case, the time taken to generate scenarios using components is 40% lesser compared to the original algorithm even for 3 stocks.

5 Conclusion and future work

We propose a new approach for generating scenario trees for financial optimization models based on the principal component analysis and the moment-matching method. This new procedure is expected to reduce the time required for scenario

Table 2 Heuristic based moment-matching algorithm results on returns versus principal component of returns

Configuration (N, T, b)	Using returns error term	Using returns time (s)	Using components error term	Using components time (s)
(3,1,20)	$10^{-7}, 0.097$	2.123	$10^{-11}, 0.001$	1.060
(10,1,100)	$10^{-6}, 0.758$	2.038	$10^{-9}, 0.007$	1.428
(10,1,200)	$10^{-5}, 1.667$	2.327	$10^{-9}, 0.093$	1.528
(3,4,10)	–	183.92	–	112.03

generation and improve the quality of scenarios in terms of less error in moment-matching problem. We also propose a modification for the decomposed moment-matching method and compare it with the original method. To show the applicability of the proposed approach, we have covered the numerical analysis on small set of stock returns giving small 1–4 stage trees. The computational experiments show that the dimensionality reduction based method takes 50% less time than the original method and gives better output, i.e., the scenarios with the moments close to the target moments.

In future, we plan to investigate the performance of the proposed method on larger data sets and comparison with the other models. In future, we plan to verify the results for the proposed algorithm mathematically as well as empirically on different data sets and larger tree sizes. Also, we plan to test this modification on other variants of moment-matching algorithm.

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