

Multidisciplinary Optimization under Uncertainty Using Bayesian Network

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ABSTRACT

This paper proposes a novel probabilistic approach for multidisciplinary design optimization (MDO) under uncertainty, especially for systems with feedback coupled analyses with multiple coupling variables. The proposed approach consists of four components: multidisciplinary analysis, Bayesian network, copula-based sampling, and design optimization. The Bayesian network represents the joint distribution of multiple variables through marginal distributions and conditional probabilities, and updates the distributions based on new data. In this methodology, the Bayesian network is pursued in two directions: (1) probabilistic surrogate modeling to estimate the output uncertainty given values of the design variables, and (2) probabilistic multidisciplinary analysis (MDA) to infer the distributions of the coupling and output variables that satisfy interdisciplinary compatibility conditions. A copula-based sampling technique is employed for efficient sampling from the joint and conditional distributions. The proposed MDO methodology is implemented within a framework of reliability-based design optimization. The proposed Bayesian network surrogate model and copula sampling are used for efficient reliability assessment within the optimization framework. A mathematical example and an aeroelastic aircraft wing design are used to demonstrate the proposed probabilistic MDO methodology.

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INTRODUCTION

Multidisciplinary design optimization (MDO) aims at developing optimization methodologies for systems that are modeled through simulation codes in individual disciplines that interact with each other [1,2]. Based on the direction of the information flow, the coupling between two individual disciplinary analyses can be feedforward coupling (unidirectional), or feedback coupling (bidirectional). The latter (feedback coupling) needs iterative analysis of the individual codes to convergence, thus considerably increasing the computational effort for even deterministic analysis. Computational methods such as the fixed point iteration (FPI) approach (repeated analysis until convergence of coupling variables) is commonly used. The consideration of uncertainty sources further increases the computational effort in MDA, since probabilistic assessment requires repeated runs of the deterministic analysis. The computational effort is amplified further in the case of MDO under uncertainty, which requires probabilistic MDA within each optimization iteration.

Review of the previous studies reveals that the existing methods for efficient MDA and MDO under uncertainty introduce several approximations to reduce the computational effort by trading off the accuracy. For example, in the decoupled approach to MDA adopted by Du and Chen [3] and Mahadevan and Smith [4], the probability density functions (PDF) of the coupling variables are calculated by Taylor's series-based first-order second moment approximation. In

the context of MDO under uncertainty, surrogate models have often been used for individual disciplinary analyses when the original disciplinary analysis codes are expensive [5]. Based on surrogate modeling (or metamodeling), Kokkolaras et al. [6] developed an advanced mean value method, which was extended by Liu et al. [7] by using moment-matching and considering the first two moments. Surrogate models such as Kriging models [8], neural network [9] etc. can be expensive to train, since converged analysis of the physics model is required for each training point. Also, many surrogate models become unreliable for high-dimensional problems. Thus there is a need for effective surrogate models in feedback-coupled MDA and MDO problems.

The central motivation of this paper is to investigate efficient approaches need to be developed for MDA and MDO under uncertainty. A framework is proposed for efficient MDO under uncertainty using the Bayesian network, which functions as an effective surrogate model for high dimensional problems.

The Bayesian network is a powerful tool to incorporate different sources of uncertainty and support several applications such as model calibration [10], model validation [11], and uncertainty quantification [12]. Given specific values of the input variables, we can obtain the probability distribution of the output variables (uncertainty

propagation), or given observed or desired values of the outputs, we can obtain the posterior distributions of unknown inputs (Bayesian inference). Both abilities of the BN are exploited in this paper.

The forward uncertainty propagation property of the BN is first exploited to consider a novel surrogate modeling technique for efficient optimization under uncertainty. The ability to obtain the probability distribution of the output for a given specific value of the input makes the BN a *probabilistic* surrogate model. The inversion capability of the Bayesian network is exploited in a novel manner to enforce the interdisciplinary compatibility condition in feedback-coupled MDA, by setting the difference between the values of the same coupling variable from two successive iterations to zero. This approach only requires a few iterations of the feedback coupled analysis (usually 2 to 4 iterations), thus achieving great computational savings by not performing the fully converged physics analysis.

Optimization methods under uncertainty within engineering design have generally been pursued in two directions: (1) reliability-based design optimization (RBDO) [13, 14, 15], and (2) robust design optimization (RDO) [16, 17, 18]. The MDO approach proposed in this paper is in the context of RBDO, but it can be extended to solve RDO problems as well. A BN is built as a surrogate model, both MDA and design evaluation are achieved simultaneously during each call to the BN by the optimizer, providing tremendous computational advantage.

For practical problems, the conditional distribution estimation of the quantities of interest is often accomplished by sampling techniques. However, regular sampling approaches can be quite expensive, especially when the dimension of the joint distribution. A copula-based sampling technique is explored in this research. Copulas have been used in reliability analysis and RBDO for correlated [15] and non-Gaussian [19] input random variables. An approach that combines Bayesian network and copula-sampling as a probabilistic surrogate model is proposed in [20]. In this paper, a Gaussian copula-based sampling technique is adopted. Sampling from a Gaussian copula makes use of analytical solutions and is very fast, whereas sampling from non-Gaussian copula is more complicated.

Three types of uncertainty sources need to be considered in design optimization: physical variability (aleatory uncertainty), data uncertainty and model uncertainty (epistemic uncertainty, due to the lack of knowledge). Treatment of both aleatory and epistemic uncertainty sources in feedback-coupled MDA can be found in [21]. Only a brief explanation of their treatment in the context of Bayesian network will be given in the numerical example.

The contributions of this paper are as follows:

1. A new concept of probabilistic surrogate modeling technique based on the Bayesian network and copula-based sampling is pursued which is able to consider large numbers of input variables and accurately represent the stochastic dependence among the inputs, outputs and coupling variables.
2. The BNC approach is used to formulate a Bayesian network for efficient MDO under uncertainty using the RBDO format, which simultaneously enforces interdisciplinary compatibility

and evaluates the optimization objectives and constraints, without any further evaluations of the original physics models, thus significantly reducing the computational effort in MDO.

The rest of the paper is organized as follows: Section 2 provides the mathematical formulation of MDO under uncertainty used in this paper. Section 3 develops the proposed innovation of probabilistic graphical surrogate modeling based on Bayesian Network and Copula-based sampling (BNC). Section 4 introduces the enforcement of interdisciplinary compatibility based on the proposed BNC for stochastic MDA. Section 5 introduces the BNC-MDO approach, building on the BNC surrogate model and BNC-MDA. A mathematical example and an aeroelastic wing design problem are used to illustrate proposed the methodology in Section 6. Section 7 provides concluding remarks.

MULTIDISCIPLINARY OPTIMIZATION UNDER UNCERTAINTY

Fig.1 is a diagram of a multidisciplinary system which consists of three analyses. A feedback analysis is required between analyses 1 and 2. The input variables are $X = \{X_1, X_2, X_s\}$ where X_1 and X_2 are the input vectors for each individual analysis, and X_s is shared by both analyses. Given a realization of X , the interdisciplinary analysis between analyses 1 and 2 is conducted; the coupling variables, i.e. U' and V' , will converge to particular values.

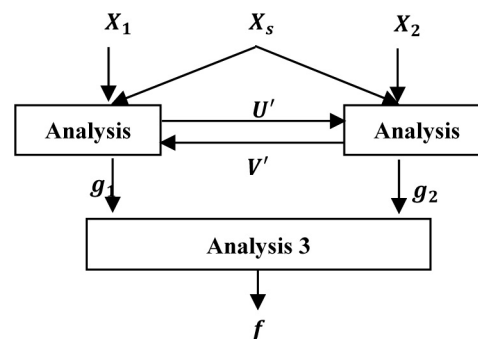


Figure 1. Multidisciplinary analysis

A simplistic implementation of this iterative analysis is fixed point iteration (FPI). After convergence, each disciplinary analysis releases a subsystem output, i.e., g_1 and g_2 , to analysis 3 to evaluate the system level output, i.e., f . For the purpose of illustration, in the optimization statement, the system output f is treated as the objective function, and the disciplinary output g_i is regarded as the constraints. A typical deterministic MDO problem statement is provided in [22] and as shown in Eq. 1.

$$\begin{aligned}
 & \min_{\mathbf{x}} f(\mathbf{x}) \\
 & s.t. \quad g_i(\mathbf{x}, \mathbf{u}(\mathbf{x}), \mathbf{v}(\mathbf{x})) \leq 0 \quad i = \{1, \dots, n_q\} \\
 & \quad h_i(\mathbf{x}, \mathbf{u}, \mathbf{v}) = 0, i = 1, 2
 \end{aligned} \tag{1}$$

where f is the performance function or objective to be minimized; $\mathbf{x}$ is the vector of design variables, $\mathbf{u}(\mathbf{x})$ and $\mathbf{v}(\mathbf{x})$ are coupling variables, and the interdisciplinary compatibility is defined by the

constraints on h_1 and h_2 . Therefore, if $\mathbf{u}$ and $\mathbf{v}$ satisfy the last two constraints of Eq. 2 simultaneously, then they are said to be compatible, and in practical engineering applications, h_i ($i = 1, 2$) are implicit functions. For example, in the two disciplinary example shown in Fig. 1, h_i can be written as:

$$\begin{aligned} U(\mathbf{x}, \mathbf{v}') - u' &= 0 \\ V(\mathbf{x}, \mathbf{u}') - v' &= 0 \end{aligned} \quad (2)$$

When uncertainty is considered in the MDO formulation above, the probabilistic formulation can be written as:

$$\begin{aligned} \min_{\mu_x} \mu_f(\mathbf{x}) \\ P(g_i(\mathbf{x}, \xi, \mathbf{u}(\mathbf{x}, \xi), \mathbf{v}(\mathbf{x}, \xi)) \geq 0) \leq \alpha_i, \quad i \\ = \{1, \dots, n_q\} \\ \text{s.t.} \\ h_j(\mathbf{x}, \xi^*, \mathbf{u}, \mathbf{v}) = 0, j = 1, 2 \end{aligned} \quad (3)$$

In Eq. 3, ξ is a vector of random variables $\xi_1, \dots, \xi_m$, that model the uncertainty in the system, whereas ξ^* is one set of realizations of the random variables ξ . α_i represents the desired reliability level for the probabilistic constraint of g_i . It can be seen from the equation that, the MDO under uncertainty requires the interdisciplinary compatibility to be satisfied for each set of realizations of the random variables ξ , which can be expensive if the uncertainty assessment is performed with feedback-coupled iterative analysis (optimization with SOFPI).

Therefore, surrogate modeling techniques are usually pursued to replace the original model with computationally less expensive models for the objective and constraints estimation. For feedback-coupled MDA, a sufficient number of training samples need to be obtained by running the fixed-point-iteration method. As the number of model inputs and outputs increase, the number of training samples needed also increases, and consequently generates a lot of computational burden. Further, when the coupling variables between individual disciplines are large in number, characterizing the dependence among input, coupling and output variables can be very complicated for most of the existing surrogate modeling techniques. To overcome these challenges, several innovations are developed in the proposed methodology, which consists of four components: (1) probabilistic graphical surrogate modeling; (2) copula-based sampling; (3) interdisciplinary compatibility enforcement in stochastic MDA; and (4) multidisciplinary design optimization under uncertainty.

PROBABILISTIC GRAPHICAL SURROGATE MODEL

A new probabilistic surrogate modeling technique is proposed based on the concept of Bayesian network. A copula-based sampling approach is introduced to further improve the sampling efficiency.

Probabilistic Surrogate Modeling with Bayesian Network

A Bayesian network is a directed acyclic graph that represents a multivariate joint probability distribution of random variables using their marginal distributions (nodes) and the conditional probabilities (arrows). In the proposed method, the Bayesian network is used as a probabilistic surrogate model that connects the input and output variables through a joint distribution. A simple model shown in Fig. 2(a) is used to illustrate the proposed approach. The model M has 2 input variables X_1 and X_2 ; and 2 output variables Y_1 and Y_2 . Assume that there is correlation between inputs X_1 and X_2 , and the outputs Y_1 and Y_2 . Based on the model in Fig. 2(a), a Bayesian network can be built as shown in Fig. 2(b). Each node represents a variable, and the edges denote the dependence relations.

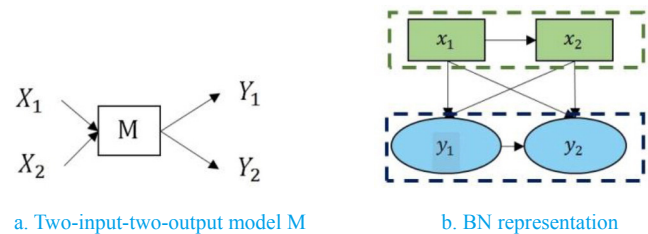


Figure 2. Bayesian network representation of a model with input and output variables

In forward uncertainty propagation, for a given realization of the input values (x_1, x_2) , the conditional joint distribution of the output variables $f(Y_1, Y_2 | X_1 = x_1, X_2 = x_2)$ is estimated. This joint distribution is often evaluated using sampling approaches, which may be time consuming especially when Bayesian network contains a large number of variables. A copula-based strategy is therefore adopted to efficiently generate conditional samples.

Probabilistic Surrogate Modeling with Bayesian Network

A copula is simply a joint CDF of marginal CDFs [23]. Consider n random variables $X_1 \dots X_n$, with continuous CDFs $F_1(x_1) \dots F_n(x_n)$. The copula function related to $X_1 \dots X_n$ is defined as Eq. 4.

$$C(u_1 \dots u_n) = P[F_1(X_1) \leq u_1, \dots, F_n(X_n) \leq u_n] \quad (4)$$

The copula C contains the dependence information between the variables, and can be used to model the joint distribution of random variables. Multiple choices for copula type are available, such as Gaussian, Clayton, Frank and Gumbel copula [24]. In practice, Gaussian copula is widely used because of the availability of analytical solutions, which makes it much easier to model high-dimensional dependence.

Gaussian Copula

A Gaussian copula represents the joint CDF of all marginal CDFs using a multivariate Gaussian distribution. To apply the Gaussian copula, the Spearman's rank correlations between all the pairs of

variables are first computed, denoted as r_{ij} . Then, Pearson's transform [25] is applied to get the conditional linear product moment correlations:

A Gaussian copula that represents the relationships in Fig. 2 can be written as:

$$c_R(\mathbf{u}) = \frac{1}{\sqrt{\det(R)}} \exp \left(-\frac{1}{2} \begin{pmatrix} \Phi^{-1}(x_1) \\ \Phi^{-1}(x_2) \\ \Phi^{-1}(y_1) \\ \Phi^{-1}(y_2) \end{pmatrix} \cdot (R^{-1} - I) \cdot \begin{pmatrix} \Phi^{-1}(x_1) \\ \Phi^{-1}(x_2) \\ \Phi^{-1}(y_1) \\ \Phi^{-1}(y_2) \end{pmatrix} \right) \quad (5)$$

where Φ^{-1} represents the inverse CDF of a standard normal random variable. $\mathbf{u}$ are independent uniform random variables from the interval [0,1]. I is an identity matrix. R is the covariance matrix of the four variables, and since the marginals of the Gaussian copula are standard normals, R is essentially the correlation coefficient matrix composed of the unconditional product moment correlations ρ_{ij} .

The multivariate Gaussian distribution in Eq. 5 can be used to rapidly generate a large number of samples of correlated normal random variables. In this case, samples of 4 variables from this joint normal distribution are generated and denoted as X'_1, X'_2, Y'_1, Y'_2 . For each sample of the variables, compute the CDF with respect to the marginal distributions of standard normal distribution, and denote the CDF values as $u_{X'_1}, u_{X'_2}, u_{Y'_1}$ and $u_{Y'_2}$. Samples of X_1, X_2, Y_1 and Y_2 are then obtained by taking the inverse CDFs of $u_{X'_1}, u_{X'_2}, u_{Y'_1}$ and $u_{Y'_2}$ with respect to their marginal distributions.

Conditional Sampling

To use this framework as a surrogate model, the conditional distributions of outputs $\mathbf{y}$ for given values of input $\mathbf{x}$ needs to be estimated. Conditionally sampling with the Gaussian copula assumption is very easy to implement since Eq. 5 can be converted to conditional Gaussian copula analytically. For example, the conditional samples of Y_1 and Y_2 need to be generated given $X_1 = x_1, X_2 = x_2$. The equivalent normals corresponding to $X_1 = x_1, X_2 = x_2$ are first calculated as $x'_1 = \Phi^{-1}(F_{X_1}(x_1)), x'_2 = \Phi^{-1}(F_{X_2}(x_2))$.

Let μ be the mean vector of X_1, X_2, Y_1 and Y_2 in the equivalent normal space $[X'_1, X'_2, Y'_1, Y'_2]$; μ is a vector of zeros with 4 entries, and R is the covariance matrix:

$$R = \begin{bmatrix} 1 & \rho_{x_1 x_2} & \rho_{x_1 y_1} & \rho_{x_1 y_2} \\ \rho_{x_1 x_2} & 1 & \rho_{x_2 y_1} & \rho_{x_2 y_2} \\ \rho_{x_1 y_1} & \rho_{x_2 y_1} & 1 & \rho_{y_1 y_2} \\ \rho_{x_1 y_2} & \rho_{x_2 y_2} & \rho_{y_1 y_2} & 1 \end{bmatrix} \quad \left. \begin{matrix} \Sigma_2 & \Sigma_1 \\ \hline \hline \end{matrix} \right\} \Sigma_2 \quad (6)$$

Then the conditional joint distribution of Y'_1 and Y'_2 given

$X'_1 = x'_1, X'_2 = x'_2$ is denoted as:

$f(Y'_1, Y'_2 | X'_1 = x'_1, X'_2 = x'_2) \sim N(\tilde{\mu}, \tilde{\Sigma})$ where the conditioned mean vector $\tilde{\mu}$ and covariance matrix $\tilde{\Sigma}$ are

$$\tilde{\mu} = \Sigma_1 \Sigma_3^{-1} * \begin{bmatrix} x'_1 \\ x'_2 \end{bmatrix} \quad (7)$$

$$\tilde{\Sigma} = \Sigma_2 - \Sigma_1 \Sigma_3^{-1} \Sigma_1^T \quad (8)$$

Samples Y'_1 and Y'_2 are jointly generated from a multivariate normal distribution, of which the mean and covariance matrix are calculated as in Eqs. 8 and 9. The CDF values of each Y'_1 and Y'_2 sample with respect to the standard normal distribution ($u_{Y'_1}, u_{Y'_2}$) are computed, and the inverse CDF is taken to obtain the conditional samples of Y_1 and Y_2 .

Note that the Gaussian copula assumption is only for connecting the CDFs of the random variables, which is less restrictive than assuming a joint Gaussian distribution for the variables themselves. The individual variables can have any arbitrary distribution. Connections between the nodes (i.e. network topology) could be based on the analyst's underlying knowledge of the dependence relations among the variables (e.g., correlation between x_1 and x_2), whereas marginal and conditional probability distributions (and unknown connections) could be learned from data (samples).

A verification approach has been proposed in [26] to test the Gaussian copula assumption. When the Gaussian copula assumption is not valid, other types of copula need to be pursued. However, most of the copulas only have analytical forms for bi-variate dependence, which is difficult to be extended for modeling high-dimensional correlations. A vine-based strategy was proposed to overcome this challenge [25, 26]. Nevertheless, when the number of variables within the BN (hence the vine structure) is large, this series of inverse copula estimations required by the vine-based strategy can be computationally intensive. In the rest of the paper, Gaussian copula is adopted in the BNC approach but verified before application.

In summary, the two essential elements for the proposed BNC method are (1) Bayesian network, which establishes the conditional relationship among variables; and (2) copula-based sampling, which rapidly generates samples and allows conditional sampling.

ENFORCING INTERDISCIPLINARY COMPATIBILITY IN BN

An efficient strategy is introduced in the section, which avoids the full convergence physics analysis and enforces interdisciplinary compatibility using the BNC approach, thus makes the training of the BN more efficient. Consider an MDA problem with two coupling variables in each direction as shown in Fig. 3(a). A single iteration is shown in Fig. 3(b).