

Automatic Uncertainty Propagation Based on the Unscented Transform.

Dailys Arronde Pérez, Harald Gietler and Hubert Zangl
Institute of Smart Systems Technologies, Sensors and Actuators
University of Klagenfurt
Universitätsstraße 65-67, 9020 Klagenfurt
Email: {dailys.arronde,harald.gietler,hubert.zangl}@aau.at

Abstract—Automatic uncertainty propagation reduces the effort for computation of uncertainty and is thus a useful tool in a variety of applications. Typically, such tools utilize Taylor series approximations (in particular linearization) or Monte Carlo Methods to perform the calculations. In this paper, we propose the use of the Unscented Transform for automatic uncertainty propagation. A comparison between the approaches - realized in a toolbox for the MATLAB environment and illustrated in two application examples - shows that the Unscented Transform overcomes some of the limitations of linearization and Monte Carlo methods, providing reliable estimates of the output expectation and standard deviation in nonlinear problems evaluating a reduced number of sigma points.

Index Terms—measurement uncertainty, linearization, Monte Carlo, unscented transformation, GUM, nonlinear systems

I. INTRODUCTION

Uncertainty evaluation plays a key role in accessing and comparing measurement results. With respect to metrology, the quality of measurement results has been expressed in terms of uncertainty, which quantifies the lack of knowledge or doubt about the validity of the result of a measurement usually composed of realization of random variables. In order to establish an international consensus on evaluating and expressing uncertainties, the Guide to the Expression of Uncertainty in Measurement (GUM) [1] and its subsequent supplements [2], [3], were developed.

In prior works [4]–[8], the use of software tools which provides GUM conform uncertainty estimates has been suggested. A general purpose library for measurement uncertainty evaluation, has been proposed in [5], as part of the metrology software for vector network analyzer (VNA). A stochastic calculator for Monte Carlo methods to perform non-order specific error propagation is available in [9] and a software tools for evaluation of complex-valued measurement models using both linear error propagation and MC, was addressed in [8]. On the other hand, the Unscented Transform (UT) originally proposed

in [10] have been considered for uncertainty analysis in [11], [12]. In [13] the UT is used to perform error propagation. The authors claim that it is an efficient method to estimate the first two moments of random distributions that are subject to nonlinear transformations.

A list of software tools to perform propagation of uncertainty calculations is available in [14]. However, none of them is based on the UT principle. In order to provide a more complete software solution for the evaluation of uncertainty in measurements the toolbox presented in [6], namely An Uncertainty Toolbox (AUT), is extended with the UT methodology. Initially, AUT provided an automatic evaluation of the propagated uncertainty using the GUM Tree method. In this approach, here called Linearization, the measurement model is linearized, and the standard deviation of the output is estimated by applying the law of propagation of uncertainty. As other frameworks already support, Monte Carlo (MC) based uncertainty propagation functionality is added to the toolbox. It increases the accuracy, especially when dealing with highly nonlinear systems and non-Gaussian distributions. Depending on the number of parameters and MC sample points this approach can be very accurate and handy to use. Contrary, its computational complexity can be very high. Additionally, a new method to perform uncertainty propagation using the UT is introduced and implemented in the AUT framework. UT is a suitable solution when linearization of the model provides an inadequate representation, estimating the mean and standard uncertainty through the evaluation of a small number of the so-called sigma points. The introduced method is compared to the existing methodologies using application examples. It is shown that even though Linearization is inaccurate when dealing with nonlinear problems, it allows to keep track of the dependencies between the variables. On the other hand, UT is computationally less expensive than MC, but providing similar results in terms of accuracy.

II. METHODS FOR AUTOMATIC UNCERTAINTY PROPAGATION. AN UNCERTAINTY TOOLBOX

An AUT for MATLAB was developed for the evaluation of uncertainty in advanced measurement problems. The toolbox is extended so that it provides three different approaches of uncertainty propagation: Linearization, MC method and UT based propagation. This sections briefly explains the

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commonly used Linearization and MC method for uncertainty propagation. Additionally, it deeply investigates how the UT approach can be used in that scenario, showing why it is beneficial in many applications. Some details about the implementation of the methods are also explained.

The measurement model is, in general, nonlinear and should include all quantities that significantly contribute to the measurement result uncertainty. It relates multiple output quantities to multiple input parameters through the measurement equations, that can be written as

$$\mathbf{y} = \mathbf{f}(\mathbf{x}), \quad (1)$$

where \mathbf{f} models a multivariate measurement process, \mathbf{x} denotes the vector of input quantities and \mathbf{y} , the vector of output quantities with arbitrary dimensions n and m , respectively. The input quantities are indicated as realizations of Random Variables (RVs). The standard deviation is interpreted as the combined standard uncertainty attributed to the input quantity, which should combine in a simple way all the a priori known sources of uncertainty.

AUT is implemented based on the object-oriented programming (OOP) capabilities of MATLAB, which allows to redefine operators and functions for different types of input arguments. This is known as operator overloading and is one of the features of modern OOP languages. A new uncertain data type is defined for each approach, enabling a customized implementation of methods and properties. For Linearization, MC and UT approaches are defined the data types *unc*, *unc_t* and *unc_ut*, respectively. The toolbox also considers that in a computer program, every complex mathematical expression can be executed as a sequence of basic arithmetic operations and elementary functions. This fact is exploited for performing the automatic propagation of uncertainty according to the specifications of each approach.

AUT overloads basic and advanced math operators and functions for real and complex valued quantities. It also supports algebraic operations on arrays and matrices, handling the multivariate treatment of measurement uncertainty described in [3]. It is possible to track the correlation between the variables, arising for the propagation toward the measurement model. The toolbox also includes more advanced functionalities as fast Fourier transform and linear interpolation.

A. Linearization

The Linearization approach is based on the so-called GUM Tree method, where the measurement model is linearized and the standard deviation of the output quantities is estimated by applying the law of propagation of uncertainty [15]. In order to present an universal, internally consistent and transferable approach, the original GUM [1] treats all uncertainty contributions identically, i.e. linear relations and Gaussian distributions. Considering the measurement model in (1) and the first order Taylor series approximation, the mean and uncertainties of the output quantities are estimated by applying

the multivariate linear uncertainty propagation, expressed in matrix form as

$$\begin{aligned} \mathbf{m}_y &= \mathbf{f}(\mathbf{m}_x), \\ \mathbf{C}_y &= \mathbf{J}_x \mathbf{C}_x \mathbf{J}_x^T, \end{aligned} \quad (2)$$

where \mathbf{m}_y and \mathbf{m}_x represent the mean vectors of output and input quantities, respectively. \mathbf{C}_y is the covariance matrix of the output vector \mathbf{y} , where the elements in the main diagonal are the squared standard uncertainties (or variances) associated with the output quantities $[y_1, \dots, y_m]$ and off-diagonal elements containing the information about the correlation between them. In a similar way, \mathbf{C}_x denotes the covariance matrix of the input vector \mathbf{x} and \mathbf{J}_x is the Jacobian matrix, which encodes the sensitivity coefficients of outputs with respect to each input quantity. It is worthy to highlight that for the implementation of this approach in AUT, (2) is not directly applied. Each measurement equation in (1) is split in terms of its elementary operations (+, -, *, ÷) and functions (sin, cos, exp, etc). We assume that each f can be executed as a series of P basic operations. In fact, to compute the sensitivity coefficients AUT uses the automatic differentiation (AD) mechanism, covered also in [5], [16], where the derivatives of each elementary operation and function are explicitly programmed and updated at each step of the calculation. With this principle, the sensitivity coefficients associated to the uncertain objects of data type *unc* are sequentially updated and the user does not need to concern about it while performing the calculations. With the Linearization approach, it is not only possible to track the correlation between the variables arising from common dependencies, but also to specify correlations between the input quantities. When the inputs are correlated, Karhunen-Loève Decomposition (KLD) is performed and a new set of primary uncorrelated input quantities is introduced. The idea is to keep track of the correlation information in a more efficient way, where only the dependencies with respect to primary uncorrelated inputs have to be stored. The implementation procedure is summarized in Fig. 1.

In general, each measurement quantity is represented by an *unc* object. It contains information about the sensitivities with respect to primary uncorrelated inputs, which makes it possible to propagate uncertainties on demand and to take care of correlations automatically. One of the drawbacks of this approach is that the computational complexity grows with the number of stored dependencies, which can lead to overheads in terms of memory and computation time.

B. Monte Carlo

The Monte Carlo approach describes a numerical method for estimating measurement uncertainty, addressed in detail in [2], [3]. It offers an alternative for the estimation of the output quantity and its associated standard uncertainty in cases when linearization of the model provides an inadequate representation or the probability density function (pdf) for the output quantity departs appreciably from a Gaussian distribution. MC methods have been widely adopted, in many scientific fields to numerically approximate pdfs.

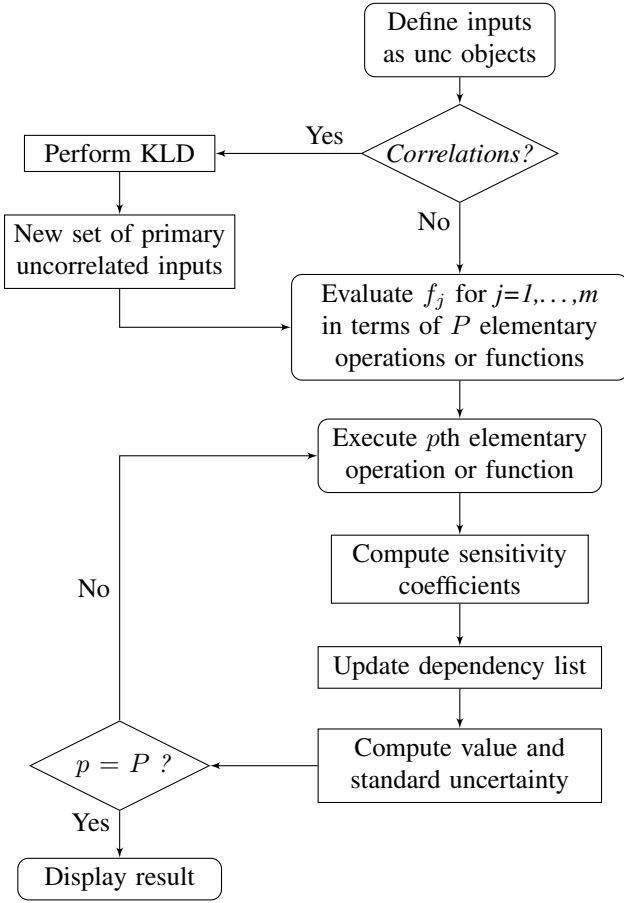


Fig. 1. Implementation of linear uncertainty propagation.

MC is based on iterative calculations. The output samples are generated by feeding realizations of the input RVs to the measurement model. This results in a single output for each input. For large numbers of samples, the Monte Carlo method provides an accurate estimate of the output probability distribution. Typically numbers in the range of $10^4 - 10^6$ are used, which makes it computationally expensive. AUT defines uncertain objects evaluated using the MC approach with data type *unc_t* and the number of required MC samples can be changed according to the accuracy requirements.

Given that the MC approach is always applicable and outperforms linear uncertainty propagation in terms of the accuracy of the results. Consequently, it can be used as a validation tool. Unlike Linearization, the MC approach can not provide sensitivity coefficients with respect to the input parameters.

C. Unscented Transform

The approach presented in this section is based on the principle of the UT. This approach was originally presented in [10], to improve the performance provided by the extended Kalman Filter in nonlinear state estimation problems. It allows for an efficient estimation of the first two moments, the propagated expectation and variance. UT is based on the

key idea that it should be easier to approximate a probability distribution than to approximate an arbitrary nonlinear function. According to this basic principle, the pdf of an n -dimensional set of inputs variables can be approximated by a set of points (referred to as sigma points). The sigma points are deterministically chosen in such a way that their statistics match the known statistics of the inputs quantities. Each sigma point is sequentially propagated through the nonlinear function, leading to a cloud of transformed sigma points. Then the statistics of the transformed variables are calculated from the function values at the sigma points. In order to obtain an estimate for the output mean and covariance of an n -dimensional function, a set of $(2n + 1)$ sigma points has to be chosen. Despite the apparent similarities between MC and UT methods, the main difference is that sigma points are chosen in a deterministic way, i.e. no random selection is applied. Consequently, a very small number of sigma points is required when comparing with the number of MC samples needed to obtain an accurate estimation. This statement is in general true, but also depends on the dimension of the set of input quantities.

In the following, the fundamental steps of the UT approach are described and some details are given about its implementation in AUT that considers the scaled UT addressed in [11], [13], [17]. This method allows any set of sigma points to be modified by a scaling parameter, in such a way that the first two moments are preserved. The scaled UT also helps to partially incorporate contributions of higher order information into the estimates and to overcome the difficulties arising from sampling non-local effects, when the radius of the sphere that bounds all the sigma points increases proportionally with the dimension of the state space.

Let us consider the n -dimensional measurement equation in (1), where the mean and variance of the input quantities are comprised in \mathbf{m}_x and \mathbf{C}_x , respectively. The first step consists of determining the coordinates of the $2n + 1$ sigma points χ_i given by

$$\begin{aligned} \chi_0 &= \mathbf{m}_x, \\ \chi_{2i-1} &= \mathbf{m}_x + \sqrt{n + \lambda} \left[\sqrt{\mathbf{C}_x} \right]_i, \\ \chi_{2i} &= \mathbf{m}_x - \sqrt{n + \lambda} \left[\sqrt{\mathbf{C}_x} \right]_i, \text{ for } i = 1, \dots, n \end{aligned} \quad (3)$$

where $[\sqrt{(\cdot)}]_i$ denotes the i th column of a matrix square root and λ is the scaling factor. Note that for uncorrelated input parameters \mathbf{C}_x is diagonal, then its squared root is obtained by taking the square root of the main diagonal elements, i.e. the matrix square root is diagonal with the standard deviation of the associated inputs as main diagonal elements. The scaling factor is defined such that $\lambda = \alpha^2(n + \kappa) - n$, with the parameters $\alpha \in (0, 1]$ and $\kappa \geq 0$ influencing how far the sigma points are away from the mean.

The second step comprises the propagation of the sigma points through the nonlinear transformation to yield a set of transformed sigma points $\mathcal{Y}_i = \mathbf{f}[\chi_i]$, for $i = 0, \dots, 2n$. The

third step lies in the estimation of the mean and covariance matrix from the weighted average and weighted product of the transformed points respectively, given by

$$\begin{aligned} \mathbf{m}_y &= \sum_{i=0}^{2n} w_i^m \mathcal{Y}_i, \\ \mathbf{C}_y &= \sum_{i=0}^{2n} w_i^c (\mathcal{Y}_i - \mathbf{m}_y)(\mathcal{Y}_i - \mathbf{m}_y)^T, \end{aligned} \quad (4)$$

with w_i denoting the weight associated with the i th sigma point and indexes m and c denoting mean and covariance respectively. The expressions for computing the weights are given by (5). For Gaussian distributed inputs the optimal value of $\beta = 2$ [17].

$$\begin{aligned} w_0^m &= \frac{\lambda}{n + \lambda}, \\ w_0^c &= w_0^m + (1 - \alpha^2 + \beta), \\ w_i^m &= w_i^c = \frac{1}{2(n + \lambda)}, \text{ for } i = 1, \dots, n. \end{aligned} \quad (5)$$

For the implementation of this approach in AUT we follow the general procedure explained in Fig. 1. Then the matricial form in (3)-(4) is not directly implemented but each input quantity and its associated sigma points are individually defined and the output quantities are sequentially computed during overloading each elementary operation and function. The computational cost of implementing the scaled UT approach is comparable to Linearization, except that UT does not require the calculation of the sensitivity coefficients. However, UT provides more accurate results in problems where nonlinearities can not be neglected.

III. APPLICATION EXAMPLES

In the following we will present two application examples in order to show how to use the toolbox and compare the results given by the different approaches addressed above.

A. Cartesian to Polar Transformation

The simple example of transforming the coordinates of a point from the Cartesian to the Polar plane is considered. We assume that the mean and standard uncertainty of the cartesian coordinates (x, y) are known a priori and the quantities are declared as uncertain objects as depicted in Fig. 2. The radial and angular coordinates (r, θ) are computed by applying the transformation equations $r = \sqrt{x^2 + y^2}$ and $\theta = \arctan(y/x)$, respectively. Their estimated values and propagated standard uncertainties are automatically displayed. The results are represented in a compact format, where the combined standard uncertainty is reported in parenthesis after the estimated value of the measurement. Two significant digits are used for reporting the standard uncertainty, which are referred to the corresponding last digits of the quoted result, following the recommendation given in [1]. Fig. 2 shows how to declare the variables using Linearization. For MC and UT

```
>> x = unc(0.4, 0.03, 'x'); ← Declaration
>> y = unc(0.3, 0.01, 'y');
>> r = sqrt(x^2 + y^2);
>> th = atan2(y, x)
th =
    0.645(40) ← Reporting
```

Fig. 2. Defining and reporting uncertain variables with Linearization approach in MATLAB. The first and second arguments in the declaration of x are the mean and standard uncertainty respectively. The third argument ' x ' is the name assigned to the variable. Uncertain variable are displayed in the format *estimate(standard uncertainty)*. For reporting the standard uncertainty two significant digits are used in terms of the least significant digits of the estimated value.

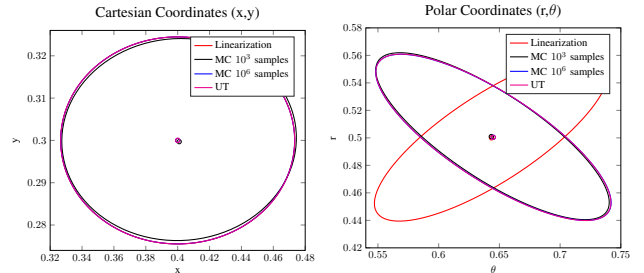


Fig. 3. Comparison of mean and covariance ellipse (3σ) in Cartesian and Polar planes.

methods, a slight modification in the syntax shall be done replacing *unc* by *unc_t* and *unc_ut*, respectively.¹

Calculations were performed using the three methods available in AUT. Figure 3 shows the results of comparing the calculated values of the moments (mean and covariance ellipse) when Linearization, MC and UT were employed. To have a better idea about the precision of each approach, MC method was executed considering 10^3 and 10^6 samples. In the Cartesian case, all the approaches lead to accurate results but MC with 10^3 samples, which is explained by the reduced number of samples. One of the drawbacks of MC is that a large number of sample points is required to obtain an accurate estimation, which is not feasible in many complex problems. In the case of the polar coordinates, Linearization leads to significant errors in calculating the covariance matrix, while UT gives a result comparable to the one obtained performing MC with 10^6 points. It is important to highlight that UT only requires the evaluation of 5 sigma points in each case, which offers a remarkable reduction in term of computational cost.

B. Forward Kinematics Model of Log Crane

The example presented in this section considers the forward kinematic model of an hydraulic forestry crane, which is being under investigation as part of a project intended for the

¹Switching between the methods can be done by including *unc = @unc_t* at the beginning of the MATLAB script for MC and *unc = @unc_ut* for UT. The toolbox is available at <https://www.aau.at/en/smart-systems-technologies/sensors-and-actuators/downloads/>

automation of log manipulation in the forestry industry. A geometric model of the crane is shown in Fig. 4. The focus of this investigation is the movement of the end-effector by means of moving hydraulic cylinders. The respective hydraulic cylinders are denoted as p_1, p_2 and p_3 . A change of cylinder length results in a change of crane constellation which ultimately moves the end-effector. In order to model the end-effector displacement, individual local coordinate frames for each arm of the crane, are introduced. The base frame of the crane is considered as global coordinate frame. A backward projection from coordinates in the end-effector local frame to the global frame is done by means of homogeneous transformation matrices [18]. The individual transformation matrices for each joint use the linear displacement from one joint to another, as well as the rotation performed in euclidean space. For the rotation the angles between the individual coordinate frames have to be known. Consequently, the nonlinear function which maps the cylinder length to the transformation angle has to be determined. Ultimately, any coordinate in the end-effector frame can be expressed in global frame as

$$\mathbf{P}_{GF} = f(\mathbf{l}, \boldsymbol{\theta}) = \left(\prod_{n=0}^3 \mathbf{T}_n(l_n, \theta_n) \right) \mathbf{P}_{EF}, \quad (6)$$

where \mathbf{P}_{GF} denotes the position \mathbf{P}_{EF} in end-effector frame expressed in global frame. The nonlinear function f is defined as multiplication of the individual homogeneous transformation matrices \mathbf{T} . Commonly, the inputs to the system, i.e. the cylinder lengths, are subject to noise. The reason are measurement noise of displacement sensors or process noise of the dynamical model of the cylinder. Consequently the inputs can be treated as RVs. The position of each piston are declared as input uncertain quantities with the toolbox, as well as the dimension of each rigid part, which are measured given by the crane model. The end-effector position is found by applying the direct kinematics equations. Fig. 5 shows the end-effector path from position A to B. The solid red lines depict a simplified model of the crane and have been plotted to have a better perception of the operational space. The standard uncertainty information of each coordinate is available for each position. The simulations were performed using Linearization, UT and MC (10^4 samples). It can be observed that the estimated mean and elliptical region of uncertainty obtained with Linearization are less accurate than the results given by MC and UT. Nevertheless, with the Linearization approach, it is possible to obtain additional information about how much the uncertainty of the inputs contribute to the combined standard uncertainty of the result. Fig. 6 a) shows all the quantities that contribute to the uncertainty of the end-effector in position A. The reported values represent the squared root of the contribution of each input quantity to the squared standard uncertainty of the output. Fig. 6 b) and c) show how to get the covariance and correlation matrices of an array of uncertain objects, respectively. The functions `get_cov_mat()` and `get_cor_mat()` are available for all the approaches.

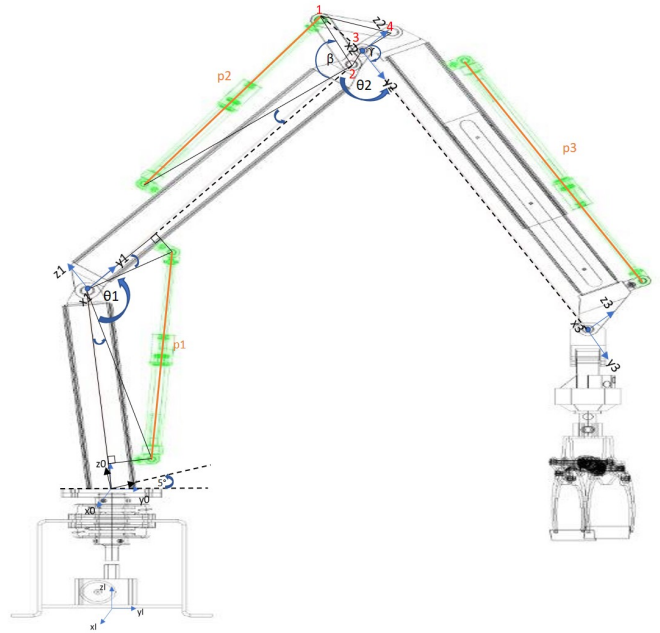


Fig. 4. The schematic of a real-world hydraulic driven forestry crane is reported.

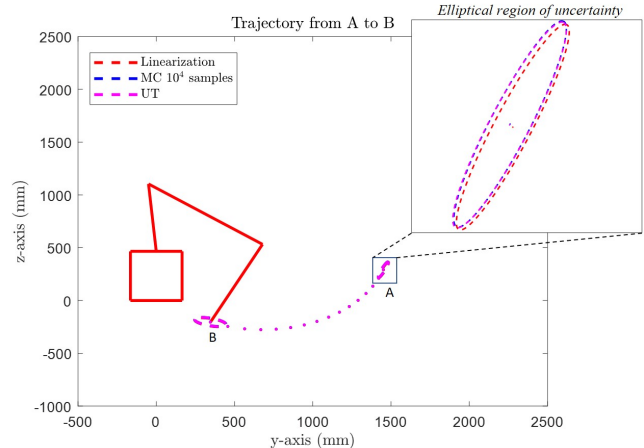


Fig. 5. End-effector path from position A to B estimated with Linearization, MC and UT approaches. The solid red lines are a representation of the simplified model of the crane, that have been plotted only to have a better perception of the work space.

Further examples and more detailed explanation about the use of the Toolbox can be found in [6], [19], [20].

IV. DISCUSSION

The previous sections showed that the three uncertainty propagation schemes come with different properties. We would like to emphasize that each approach has pros and cons, hence the choice of the method will depend on the application. Linearization is not adequate when nonlinearities can not be neglected and it requires the computation of the sensitivity coefficients. However, it provides some special functionalities, such as `disp_contribution`, which can be useful for system

```

>> disp_contribution(A)          >> Cov = get_cov_mat([Ay Az thetal theta2])

Uncertainty Contribution:      Cov =
Variable Name | Contribution                1.0e+03 *
-----
piston1 ..... | 20.7                          0.7238  1.5446  0.0329  0.0510
piston2 ..... | 10                             1.5446  3.8241  0.0607  0.1632
gamma .....   | 6.33                           0.0329  0.0607  0.0023  0
dist_p11 .....| 5.83                            0.0510  0.1632  0        0.0121
d41 .....     | 5.13
d23 .....     | 5.08
piston3 ..... | 4.77
.....         | 3
dist_p21 .....| 2.92
d12 .....     | 2.76
d34 .....     | 2.67
.....         | 2.31
dist_p12 .....| 2.06
.....         | 1.92
a)

b)
>> Corr = get_cor_mat([Ay Az thetal theta2])

Corr =
1.0000  0.9284  0.8035  0.5456
0.9284  1.0000  0.6450  0.7588
0.8035  0.6450  1.0000  0
0.5456  0.7588  0        1.0000
c)

```

Fig. 6. Analysing dependencies between uncertain quantities. a) List of main sources of uncertainty that contributes to the standard uncertainty in A. The values no identified corresponds to no named quantities. The reported values represent the squared root of the contribution of each quantity to the squared standard uncertainty of A. The method `disp_contribution()` is only available for `unc` data type. Determination of b) Covariance and c) Correlation matrices.

analysis and optimization. It gives an idea of the influence of the individual input uncertainty on the output uncertainty. Contrary, the UT approach can be effectively used for nonlinear models. The results are comparable to the gold standard, i.e. MC method with a large number of samples, where as the UT requires a small sample set. Nevertheless, in cases where the number of input parameters (n) is significantly high, MC can be less expensive than UT and Linearization, as they have the disadvantage that the required dependency lists grow with the number of input parameters. Generally, the used model needs to be analyzed in order to make a decision about the suitability of the individual methods.

V. CONCLUSIONS

In this paper we demonstrate that the unscented transform can be utilized for automatic uncertainty propagation and that in many situations it offers advantages such as higher accuracy or lower computational efforts compared to the common methods. The presented approach and realization of UT, linearization and MC in a common toolbox is very flexible, provides an intuitive way of switching between propagation methods and does not require a lot of training. We believe this is crucial for a wide utilization of automatic uncertainty propagation and consideration of uncertainty through the entire development process from the early concept and design phase all the way to the final production phase of a certain device.

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