

A Generalized Unscented Transformation for Probability Distributions

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Abstract—The unscented transform uses a weighted set of samples called sigma points to propagate the means and covariances of nonlinear transformations of random variables. However, unscented transforms developed using either the Gaussian assumption or a minimum set of sigma points typically fall short when the random variable is not Gaussian distributed and the nonlinearities are substantial. In this paper, we develop the generalized unscented transform (GenUT), which uses adaptable sigma points that can be positively constrained, and accurately approximates the mean, covariance, and skewness of an independent random vector of most probability distributions, while being able to partially approximate the kurtosis. For correlated random vectors, the GenUT can accurately approximate the mean and covariance. In addition to its superior accuracy in propagating means and covariances, the GenUT uses the same order of calculations as most unscented transforms that guarantee third-order accuracy, which makes it applicable to a wide variety of applications, including the assimilation of observations in the modeling of the coronavirus (SARS-CoV-2) causing COVID-19.

Index Terms—Unscented transform, Probability distributions, Estimation, Kalman filtering, Infectious disease, COVID-19

I. INTRODUCTION

THE Kalman filter provides the basis for most of the popular state estimation techniques used for linear and nonlinear dynamic systems. The linear Kalman filter works by propagating the means and covariance of the state of a dynamic system [1], [2]. Originally developed under the Gaussian assumption for measurement and process noise, the

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Kalman filter is the optimal estimator when this assumption is satisfied. Under non-Gaussian noise, the Kalman filter is the optimal linear estimator but its performance can sometimes deteriorate [1], [3].

For many dynamic systems in practice, linearity is a reasonable assumption. For others, system non-linearities cause methods based on linear models to perform poorly. Most nonlinear systems can behave approximately linearly over small operation ranges. The extended Kalman filter (EKF) is one of the most widely used Kalman filter for nonlinear dynamic systems. The EKF employs a linear approximation of the nonlinear system around a nominal state trajectory [1], [2]. However, for highly nonlinear systems, linear approximations can introduce errors that can lead to divergence of the state estimate.

To address the drawbacks of the EKF, several well-known state estimators such as the ensemble Kalman filter [4]–[7], the unscented Kalman filter (UKF) [8], [9], and the particle filter [1], [10] have been developed. Although the particle filter can give better performance than the UKF, this comes at the cost of a higher computational effort. In some applications, the improved performance might not be worth the additional computational costs [1].

The UKF is a nonlinear filter that uses the unscented transformation to approximate the mean and covariance of a Gaussian random variable [8], [11]. The unscented transform uses the intuition that *with a fixed number of parameters it should be easier to approximate a Gaussian distribution than it is to approximate an arbitrary nonlinear function or transformation* [8]. It produces sets of vectors called *sigma points* that capture the moments of the standard Gaussian distribution. The UKF uses the generated sigma points to obtain estimates of the states and the state estimation error covariance. The UKF has been used to generate proposal distributions which improve the performance of a particle filter [12], [13]. It has also been employed to improve the performance of the EnKF [14]. Despite the several types of sigma points that exist in the literature [15], [16], a majority of them that were not developed using the Gaussian assumption do not try to match the skewness or kurtosis of a random variable, thereby ensuring only second-order accuracy.

The need to effectively monitor, predict, and control the spread of infectious disease has led to the application of numerous state estimation techniques. The EKF [17], [18] and the particle filter [19] have been used to estimate the parameters of the measles virus transmission dynamics from real data. The ensemble adjustment Kalman filter (EAKF) has

been employed in the forecasting of influenza [20] and dengue fever [21]. Several infectious disease such as Ebola [22], HIV [23], and neonatal sepsis [24] have seen implementation of different Kalman filters. More recently, the outbreak of the novel coronavirus (SARS-CoV-2) causing COVID-19 has led to concerted efforts to properly understand its transmission and offer policy guidelines that can mitigate its spread. Recent efforts have employed the iterated EAKF to assimilate daily observations in the modeling of COVID-19 [25]. Distributions such as Poisson, negative-binomial, and binomial are typically used for modeling infectious disease from count data. Additionally, the number of patients arriving at a hospital or a testing center can be modeled by a Poisson distribution whose rate is proportional to the infected population. Although the use of standard Kalman filters in infectious disease estimation and prediction under the Poisson assumption can be justified with the fact that a Poisson distribution with a large rate can be approximated by a Gaussian distribution of the same mean and variance, the approximation breaks down when the rates are small [26].

The usage of Kalman filters to assimilate data generated by the transformation of random variables from different probability distributions has revealed a fundamental mismatch in the application of the filters – the accuracy of the filter is reduced if the Gaussian assumption is not satisfied and the nonlinearities are high. Given the mismatch between current Kalman filter assumptions and modeling frameworks that employ a wide range of transformed variables, we present a new method that uses a fixed number of sigma points to approximate an arbitrary probability distribution. The intuition is that *employing sigma points more suitable to the inherent distributions of a random vector can lead to a more accurate propagation of means and covariances*. We develop the *generalized unscented transform* (GenUT) which is able to adapt to the unique statistics of most probability distributions. We show that for any random vector of an arbitrary probability distribution, the GenUT gives accurate approximations up to its second moment (second-order accuracy). Additionally, for any independent random vector of an arbitrary probability distribution, the GenUT gives accurate approximations up to its third moment, while achieving partial accuracy in approximating the fourth moment.

In Section II, we discuss the problems that arise when the Gaussian assumption is employed in the unscented transform. In Section III, we develop the GenUT sigma points that can capture certain properties of most probability distributions, such as its mean, covariance, and skewness. In Section IV, we show that these sigma points are accurate in approximating the first three moments of an arbitrarily distributed independent random vector, thus exceeding the performance of the original unscented transform [8]. In Section V, we address positivity constraints and develop additional sigma points that ensure that such constraints are never violated while maintaining third-order accuracy. In Section VI, we evaluate the accuracy of the GenUT sigma points in propagating the mean and covariance of nonlinear transformations of arbitrarily distributed random vectors and we give several examples that demonstrate its effectiveness. We discuss the conclusions in Section VII.

II. THE GAUSSIAN ASSUMPTION PROBLEM

We analyze the performance of the unscented transform developed in [8], [11]. We only focus the UT of [8], [11] as opposed to other unscented transforms existing in the literature because, to our best knowledge, a majority were developed under the Gaussian assumption. The resulting problem even extends to unscented transforms that were developed without using the Gaussian assumption [27], where no probability distribution was considered in the development of the sigma points. We will show how linearization approximations, via Taylor series expansion of a nonlinear transformation of a random vector x evaluated about its mean \bar{x} , introduces errors in the propagation of means and covariances. We will see that errors can be introduced in the propagation of means and covariances beyond the second order when sigma points developed under the Gaussian assumption [8], [11] are used to approximate the nonlinear function $\lambda(x)$ of a non-Gaussian distributed random vector x . We note that the nonlinear transformation $y \in \mathbb{R}^n$ is given by

$$y = \lambda(x) \quad (1)$$

Given the mean \bar{x} and covariance matrix P , the sample mean and covariance of the nonlinear transformation of (1) can be calculated as follows [8].

- 1) Calculate the $2n + 1$ sigma points given by

$$\begin{aligned} \chi_0 &= \bar{x} & w_0 &= \frac{\kappa}{n + \kappa} \\ \chi_i &= \bar{x} + \left(\sqrt{(n + \kappa)P} \right)_i & w_i &= \frac{1}{2(n + \kappa)} \\ \chi_{i+n} &= \bar{x} - \left(\sqrt{(n + \kappa)P} \right)_i & w_i &= \frac{1}{2(n + \kappa)} \end{aligned} \quad (2)$$

where $\left(\sqrt{(n + \kappa)P} \right)_i$ is the i th row or column of $\sqrt{(n + \kappa)P}$, w_i is the weight associated with the i th sigma point, and κ is a free parameter. We typically set $\kappa = n - 3$ to minimize the fourth-order moment mismatch [8].

- 2) Pass the sigma points through the known nonlinear function to get the transformed sigma points

$$\mathcal{Y}_i = \lambda(\chi_i) \quad (3)$$

- 3) Evaluate the sample mean of the transformed sigma points

$$\bar{y} = \sum_{i=0}^{2n} w_i \mathcal{Y}_i \quad (4)$$

- 4) Evaluate the sample covariance of the transformed sigma points

$$P_y = \sum_{i=0}^{2n} w_i (\mathcal{Y}_i - \bar{y})(\mathcal{Y}_i - \bar{y})^T \quad (5)$$

A. Accuracy in Approximating the True Mean

Applying a Taylor series expansion of $\lambda(x)$ about its mean \bar{x} , we show in Appendix A-A that the true mean of $y = \lambda(x)$ is given as

$$\bar{y} = \lambda(\bar{x}) + \left\{ \sum_{i,j=1}^n \frac{P_{ij}}{2!} \frac{\partial^2 \lambda}{\partial x_i \partial x_j} + \sum_{i,j,k=1}^n \frac{S_{ijk}}{3!} \frac{\partial^3 \lambda}{\partial x_i \partial x_j \partial x_k} \right. \\ \left. + \sum_{i,j,k,l=1}^n \frac{K_{ijkl}}{4!} \frac{\partial^4 \lambda}{\partial x_i \partial x_j \partial x_k \partial x_l} \right\}_{x=\bar{x}} \\ + \mathbb{E} \left[\frac{D_{\bar{x}}^5 \lambda}{5!} + \frac{D_{\bar{x}}^6 \lambda}{6!} + \dots \right] \quad (6)$$

where the elements of the skewness tensor S are defined as

$$S_{ijk} = \mathbb{E}[(x - \bar{x})_i (x - \bar{x})_j (x - \bar{x})_k] \quad (7)$$

and the elements of the kurtosis tensor K are defined as

$$K_{ijkl} = \mathbb{E}[(x - \bar{x})_i (x - \bar{x})_j (x - \bar{x})_k (x - \bar{x})_l] \quad (8)$$

Using the sigma points of (2), the analytical expression for the approximated mean from [8] is given as

$$\bar{y}_u = \lambda(\bar{x}) + \frac{1}{2} \sum_{i,j=1}^n P_{ij} \left. \frac{\partial \lambda}{\partial x_i \partial x_j} \right|_{x=\bar{x}} \\ + \frac{1}{2(n+\kappa)} \sum_{i=1}^{2n} \left(\frac{D_{\sigma_i}^4 \lambda}{4!} + \frac{D_{\sigma_i}^6 \lambda}{6!} + \dots \right) \quad (9)$$

Comparing the above equation with the true mean of (6), we notice the following problems about the sigma points developed using the Gaussian assumption

- 1) The odd-powered moments in the approximation of the true mean are always zero due to their symmetry. This introduces significant approximation errors in situations where the odd-powered moments of the distribution of x are non-zero and the transformation $y = \lambda(x)$ is highly nonlinear.
- 2) The fourth-order term fails to capture a part of the true Kurtosis even when the optimal value of $\kappa = n - 3$ is selected because of the Gaussian assumption.

We note that we can arrive at the same conclusion of errors in approximating the mean beyond the second order when the reduced sigma points existing in the literature are analyzed – this is because they do not account for the skewness and kurtosis of x when it is not Gaussian distributed.

B. Accuracy in Approximating the True Covariance Matrix

The true covariance matrix, which was evaluated in Appendix A-B, is given as

$$P_y = \Lambda P \Lambda^T + \left\{ \sum_{i,j,k=1}^n \frac{S_{ijk}}{2!} \left[\frac{\partial^2 \lambda}{\partial x_i \partial x_j} \frac{\partial \lambda^T}{\partial x_k} + \frac{\partial \lambda}{\partial x_i} \frac{\partial^2 \lambda^T}{\partial x_j \partial x_k} \right] \right. \\ + \sum_{i,j,k,l=1}^n K_{ijkl} \left[\frac{1}{3!} \frac{\partial^3 \lambda}{\partial x_i \partial x_j \partial x_k} \frac{\partial \lambda^T}{\partial x_l} \right. \\ \left. + \frac{1}{3!} \frac{\partial \lambda}{\partial x_i} \frac{\partial^3 \lambda^T}{\partial x_j \partial x_k \partial x_l} + \frac{1}{4} \frac{\partial^2 \lambda}{\partial x_i \partial x_j} \frac{\partial^2 \lambda^T}{\partial x_k \partial x_l} \right] \\ \left. + \left[\sum_{i,j=1}^n \frac{P_{ij}}{2} \frac{\partial^2 \lambda}{\partial x_i \partial x_j} \right] \left[\dots \right]^T \right\}_{x=\bar{x}} + \dots \quad (10)$$

where we have used the notation $XX^T = X[\dots]^T$. The analytical expression for the approximated covariance matrix from [8] is given as

$$P_u = \Lambda P \Lambda^T + \frac{1}{2(n+\kappa)} \sum_i^{2n} \left(\frac{D_{\sigma_i} \lambda (D_{\sigma_i}^3 \lambda)^T}{3!} \right. \\ \left. + \frac{D_{\sigma_i}^3 \lambda (D_{\sigma_i} \lambda)^T}{3!} + \frac{D_{\sigma_i}^2 \lambda (D_{\sigma_i}^2 \lambda)^T}{2! \times 2!} \right) \\ + \left[\frac{1}{2} \sum_{i,j=1}^n P_{ij} \left. \frac{\partial^2 \lambda}{\partial x_i \partial x_j} \right|_{x=\bar{x}} \right] \left[\dots \right]^T + \dots \quad (11)$$

Comparing the above equation with the true covariance matrix of (10), we notice similar issues that were pointed out in approximating the mean – the approximation is only accurate up to the second order when x is not Gaussian distributed. All the odd-powered moments are zero because of the symmetric nature of the sigma points, while the fourth-powered moment is also inaccurate because of the Gaussian nature of the sigma points. As with the mean approximation, errors in the covariance matrix approximation are introduced beyond the second order when the reduced sigma points existing in the literature are used to approximate x because its skewness and kurtosis are not captured.

III. GENERALIZED UNSCENTED TRANSFORM

A third-order unscented transform uses a set of sigma points to accurately capture the first three moments of a random vector. Following [11], we define $x \in \mathbb{R}^n$ as a random vector that can follow any probability distribution.

Theorem III.1. *Given a random vector x with mean \bar{x} and covariance P , a user-specified arbitrarily distributed random vector z with zero mean and unit variance is defined as*

$$z = C^{-1}(x - \bar{x}) \quad (12)$$

where C is the matrix square root of P , $CC^T = P$.

Proof. Taking the expected value of (12) gives the mean as

$$\mathbb{E}[z] = C^{-1}\mathbb{E}[x - \bar{x}] \\ = 0 \quad (13)$$

The covariance of (12) is evaluated as

$$\mathbb{E}[zz^T] = C^{-1}\mathbb{E}[(x - \bar{x})(x - \bar{x})^T]C^{-1} \\ = C^{-1}PC^{-1} = I \quad (14)$$

where I is the identity matrix. \square

To accurately capture the higher moments of x , we use the following assumption

Assumption III.1. *Let $x \in \mathbb{R}^n$ be an independent random vector that can follow any probability distribution.*

Assumption III.2. *In addition to the availability of its mean \bar{x} and covariance P , the skewness (third central moment) $\mathcal{S}_i = \mathbb{E}[(x - \bar{x})_i^3]$ and the kurtosis (fourth central moment) $\mathcal{K}_i = \mathbb{E}[(x - \bar{x})_i^4]$ of x_i for $i = 1, \dots, n$ are also available.*

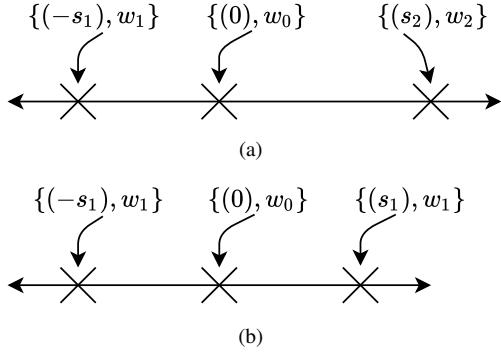


Fig. 1. (a) Samples chosen for a one-dimensional distribution for the GenUT. The locations and weights of the sigma points are determined by the moments of the probability distribution. (b) Symmetric samples chosen for a one-dimensional Gaussian distribution [11].

Using the assumption that x is an independent random vector, the third central moment can be evaluated as

$$S_{ijk} = \mathbb{E}[(x - \bar{x})_i(x - \bar{x})_j(x - \bar{x})_k] = \begin{cases} \mathcal{S}_i & \text{if } i = j = k \\ 0 & \text{otherwise} \end{cases} \quad (15)$$

while the fourth central moment can be evaluated as

$$K_{ijkl} = \mathbb{E}[(x - \bar{x})_i(x - \bar{x})_j(x - \bar{x})_k(x - \bar{x})_l] = \begin{cases} \mathcal{K}_i & \text{if } i = j = k = l \\ P_{ii}P_{jj} & \text{if } i = k \neq j = l \\ 0 & \text{otherwise} \end{cases} \quad (16)$$

where P_{ij} is the i th element in the j th column of P . We select the higher-order central moments of z in (12) to match the standardized moments of x up to at least the third order. This is done by selecting sigma point distributions that have the flexibility to either be symmetric when x is symmetrically distributed or be asymmetric when x is asymmetrically distributed. To aid in the selection of our sigma points, we define the standardized moments $\tilde{\mathcal{S}}_i$ and $\tilde{\mathcal{K}}_i$ for $i \in [1, n]$ such that

$$\tilde{\mathcal{S}}_i = \frac{\mathcal{S}_i}{\sigma_i^3} \quad (17)$$

$$\tilde{\mathcal{K}}_i = \frac{\mathcal{K}_i}{\sigma_i^4} \quad (18)$$

where $\sigma_i = \sqrt{P_{ii}}$ is the standard deviation of x_i . Let z_i be the i th element of the user-selected arbitrarily distributed random vector z , and let \bar{z}_i be the mean of z_i . The first four moments are selected as

$$\mathbb{E}[z_i] = 0 \quad (19)$$

$$\mathbb{E}[(z - \bar{z})_i^2] = 1 \quad (20)$$

$$\mathbb{E}[(z - \bar{z})_i^3] = \tilde{\mathcal{S}}_i \quad (21)$$

$$\mathbb{E}[(z - \bar{z})_i^4] = \tilde{\mathcal{K}}_i \quad (22)$$

A. One-Dimensional Distribution

We develop sigma points that match the first three moments of z in a single dimension, and then constrain those points to

try to capture the fourth moment of z . To capture the first three moments in a single dimension, three points are used: the first point lies at the origin with a weight of w_0 ; the second point lies at a distance $-s_1$ from the origin with a weight of w_1 ; the third point lies at a distance s_2 from the origin with a weight of w_2 . A comparison between our sigma points and the sigma points of [11] in one dimension is shown in Fig. 1. In our sigma points, we have two points that have their own adjustable weight and adjustable distance away from their mean while the sigmas point of [11] have two points that share the same weights and distance away from their mean. Therefore, in one-dimension, we use the following 3 sigma points

$$\begin{aligned} \chi^{(0)} &= \{0\}, w_0 \\ \chi^{(1)} &= \{-s_1\}, w_1 \\ \chi^{(2)} &= \{s_2\}, w_2 \end{aligned}$$

where w_0 , w_1 , and w_2 are the weights for the respective sigma points. Obeying the moments of z in (19)–(21) and the fact that the sum of all weights should equal 1, we write

$$w_0 + w_1 + w_2 = 1 \quad (23)$$

$$-w_1 s_1 + w_2 s_2 = 0 \quad (24)$$

$$w_1 s_1^2 + w_2 s_2^2 = 1 \quad (25)$$

$$-w_1 s_1^3 + w_2 s_2^3 = \tilde{\mathcal{S}} \quad (26)$$

From (24), we see that $w_1 = \frac{s_2}{s_1} w_2$. Rewriting (25) using (26) gives

$$w_2 s_2 (s_1 + s_2) = 1 \quad (27)$$

$$w_2 s_2 (s_2^2 - s_1^2) = \tilde{\mathcal{S}} \quad (28)$$

We designate s_1 as the free parameter while assuming that $s_1 > 0$. Using the fact that $s_2^2 - s_1^2 = (s_1 + s_2)(s_2 - s_1)$, substituting (27) into (28) gives

$$s_2 = s_1 + \tilde{\mathcal{S}} \quad (29)$$

From (23) and (27), we see that the weights are given as

$$w_2 = \frac{1}{s_2(s_1 + s_2)}, \quad w_0 = 1 - w_1 - w_2 \quad (30)$$

We note that the free parameter s_1 can be selected to match the fourth moment of z . We now attempt to satisfy the fourth moment constraint given by

$$w_1 s_1^4 + w_2 s_2^4 = \tilde{\mathcal{K}} \quad (31)$$

Eliminating w_1 using $w_1 = \frac{s_2}{s_1} w_2$ gives

$$w_2 s_2 (s_1^3 + s_2^3) = \tilde{\mathcal{K}} \quad (32)$$

Using the relationships $w_2 s_2 (s_1 + s_2) = 1$, $s_1^3 + s_2^3 = (s_1 + s_2)(s_1^2 + s_2^2 - s_1 s_2)$, and $s_2 = s_1 + \tilde{\mathcal{S}}$, the above equation reduces to

$$s_1^2 + \tilde{\mathcal{S}} s_1 + \tilde{\mathcal{S}}^2 - \tilde{\mathcal{K}} = 0$$

The solution to the above quadratic equation is

$$s_1 = \frac{1}{2} \left[-\tilde{\mathcal{S}} + \sqrt{4\tilde{\mathcal{K}} - 3\tilde{\mathcal{S}}^2} \right] \quad (33)$$

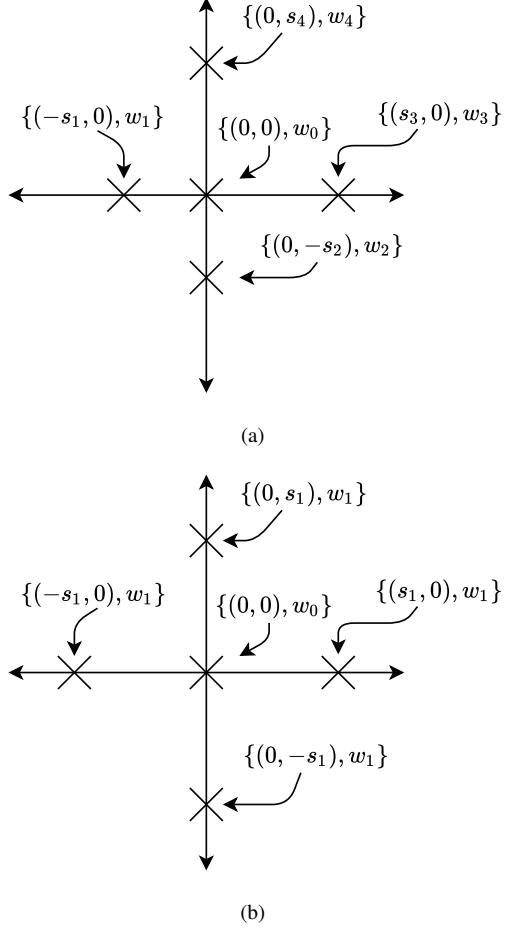


Fig. 2. (a) Samples chosen for a two-dimensional distribution for the GenUT. The locations and weights of the sigma points are determined by the moments of the probability distribution. (b) Symmetric samples chosen for a two-dimensional Gaussian distribution [11].

where s_2 is given in (29). The equations for w_1 , w_2 , and w_0 remain unchanged.

We note that the sigma points described above, which accurately capture the kurtosis when constrained, were designed for when the state has a dimension of 1. In the next section, we extend this to multiple dimensions.

B. Multi-Dimensional Distribution

We develop a set of sigma points that accurately capture the first moment, second central moment, and third central moment of an n -dimensional vector z . We then use the developed sigma points, by constraining them, to try to capture part of the kurtosis. The points whose distribution obey the moments in (19)–(21) for a two-dimensional distribution are shown in Fig. 2 where they are contrasted against the original symmetric sigma points of [11]. Our first points lie at $(0, 0)$ with a weight of w_0 . Our second points lie on the coordinate axes a distance $-s_1$ from the origin with a weight of w_1 . Our third points lie on the coordinate axes a distance $-s_2$ from the origin with a weight of w_2 . Our fourth points lie on the coordinate axes a distance s_3 from the origin with a weight of w_3 . Our fifth points lie on the coordinate axes a

distance s_4 from the origin with a weight of w_4 . In summary, in each dimension, our sigma points are characterized by two points that have their own adjustable weight and adjustable distance away from their mean while the sigma points of [11] are characterized by two points that share the same weight and distance away from their mean. Therefore, our unscented transform uses the following $2n + 1$ sigma points

$$\begin{aligned}\chi^{(0)} &= \{\mathbf{0}\}, w_0 \\ \chi^{(i)} &= \{-s_i I_i\}, w_i \quad i = 1, \dots, n \\ \chi^{(i+n)} &= \{s_{i+n} I_i\}, w_{i+n} \quad i = 1, \dots, n\end{aligned}$$

where $\mathbf{0} \in \mathbb{R}^n$ is a vector of zeros and I_i is the i th column of the $n \times n$ identity matrix. Obeying the moments of z , we write

$$w_0 + \sum_{i=1}^{2n} w_i = 1 \quad (34)$$

$$-w_i s_i + w_{i+n} s_{i+n} = 0 \quad (35)$$

$$w_i s_i^2 + w_{i+n} s_{i+n}^2 = 1 \quad (36)$$

$$-w_i s_i^3 + w_{i+n} s_{i+n}^3 = \tilde{\mathcal{S}}_i \quad (37)$$

From (35), we see that $w_i = \frac{s_{i+n}}{s_i} w_{i+n}$. Rewriting (36) and (37) by eliminating w_i gives

$$w_{i+n} s_{i+n} (s_i + s_{i+n}) = 1 \quad (38)$$

$$w_{i+n} s_{i+n} (s_i + s_{i+n})(s_{i+n} - s_i) = \tilde{\mathcal{S}}_i \quad (39)$$

Selecting $s_i > 0$ for $i \in [1, n]$ as the free parameters, we get

$$s_{i+n} = s_i + \tilde{\mathcal{S}}_i \quad (40)$$

Therefore, from (34) and (38), we see that

$$w_{i+n} = \frac{1}{s_{i+n}(s_i + s_{i+n})}, \quad w_0 = 1 - \sum_{i=1}^{2n} w_i \quad (41)$$

To match the term $\mathbb{E}[(z - \bar{z})_i^4]$, which is a part of the Kurtosis of the n -dimensional vector z , we need to satisfy

$$w_i s_i^4 + w_{i+n} s_{i+n}^4 = \tilde{\mathcal{K}}_i \quad (42)$$

Solving the above equation results in constrained values for s_i , such that

$$s_i = \frac{1}{2} \left(-\tilde{\mathcal{S}}_i + \sqrt{4\tilde{\mathcal{K}}_i - 3\tilde{\mathcal{S}}_i^2} \right) \quad \text{for } i = 1, \dots, n \quad (43)$$

It can be shown from (12) that after pre-multiplying by C , the algorithm for selecting the $2n + 1$ sigma points for any random vector x is given in Algorithm 1.

We recall from (40) that $s_i > 0$. Applying this constraint on (43), we see that

$$\begin{aligned}\frac{1}{2} \left(-\tilde{\mathcal{S}}_i + \sqrt{4\tilde{\mathcal{K}}_i - 3\tilde{\mathcal{S}}_i^2} \right) &> 0 \\ \sqrt{4\tilde{\mathcal{K}}_i - 3\tilde{\mathcal{S}}_i^2} &> \tilde{\mathcal{S}}_i \\ \tilde{\mathcal{K}}_i &> \frac{\tilde{\mathcal{S}}_i^2}{\sigma_i^2}\end{aligned} \quad (44)$$

where we have used the fact that $\tilde{\mathcal{S}}_i = \frac{s_i}{\sigma_i^3}$ (see (17)) and $\tilde{\mathcal{K}}_i = \frac{\mathcal{K}_i}{\sigma_i^4}$ (see (18)). The inequality in (44) agrees with the

fact that for probability distributions, the standardized kurtosis always exceeds the squared of the standardized skewness [28]. Therefore, we can conclude from (43) that s_i for $i \in [1, n]$ is always feasible.

There might be concerns that s_{i+n} in (40) might be negative whenever the standardized skewness $\tilde{\mathcal{S}}_i$ is negative. Substituting (43) into (40) gives

$$\begin{aligned} s_{i+n} &= \frac{1}{2} \left(-\tilde{\mathcal{S}}_i + \sqrt{4\tilde{\mathcal{K}}_i - 3\tilde{\mathcal{S}}_i^2} \right) + \tilde{\mathcal{S}}_i \\ &= \frac{1}{2} \left(\tilde{\mathcal{S}}_i + \sqrt{4\tilde{\mathcal{K}}_i - 3\tilde{\mathcal{S}}_i^2} \right) > 0 \end{aligned} \quad (45)$$

Irrespective of the sign of the standardized skewness $\tilde{\mathcal{S}}_i$, we see from the above equation that $s_{i+n} > 0$ whenever (44) is satisfied.

Algorithm 1 can be used to create sigma points that satisfy some prescribed mean, variance, skewness, and kurtosis only when (44) is satisfied. For example, let $\bar{x} = 0.1$, $P = 0.2$, and $\mathcal{S} = -0.5$. To satisfy (44), we require $\mathcal{K} > \frac{-0.5^2}{0.2} = 1.25$ so we select $\mathcal{K} = 1.3$. Using Algorithm 1, we see that $w_0 = 0.2$, $w_1 = 0.0286$, $w_2 = 0.7714$, $s_1 = 5.8055$, and $s_2 = 0.2153$. The sample mean, sample covariance, sample skewness, and sample kurtosis exactly match their true values. We show how to calculate the sample statistics in Section IV.

C. Selecting the Parameters $\tilde{\mathcal{S}}_i$ and $\tilde{\mathcal{K}}_i$

We use the moment generating function (MGF) $M(t)$ to evaluate the mean and higher-order central moments of a probability distribution. For any random variable X [29], its MGF and n -th moment are given by

$$M(t) = \mathbb{E}[e^{tX}], \quad \mathbb{E}[X^n] = \left. \frac{\partial^n M}{\partial t^n} \right|_{t=0} \quad (46)$$

We also use the gamma notation

$$\Gamma(k) = \int_0^\infty x^{k-1} e^{-x} dx \quad (47)$$

The first four moments, as well as the standardized moments $\tilde{\mathcal{S}}_i$ and $\tilde{\mathcal{K}}_i$ for some probability distributions can be found in Table I.

IV. ACCURACY OF SIGMA POINT SAMPLE STATISTICS

We demonstrate the accuracy of our sigma points in approximating any random vector $X \in \mathbb{R}^n$.

Theorem IV.1. Let $X \in \mathbb{R}^n$ be any random vector with mean \bar{X} and covariance matrix $P > 0$ and let the $2n+1$ sigma points be defined as shown in Algorithm 1, then the following statements are true:

- 1) The sample mean of $\{\chi^{(i)}, w_i\}$, $\mu_\chi = \sum_{i=0}^{2n} w_i \chi^{(i)}$, is equal to the true mean of X .
- 2) The sample covariance matrix of $\{\chi^{(i)}, w_i\}$, $\Sigma_P = \sum_{i=0}^{2n} w_i (\chi^{(i)} - \mu_\chi)(\chi^{(i)} - \mu_\chi)^T$, is equal to the true covariance of X .

1 Make available the mean \bar{x} , covariance P , skewness \mathcal{S}_i for $i \in [1, n]$, and kurtosis \mathcal{K}_i for $i \in [1, n]$

2 Calculate the standardized skewness $\tilde{\mathcal{S}}_i$ and kurtosis $\tilde{\mathcal{K}}_i$;

$$\tilde{\mathcal{S}}_i = \frac{\mathcal{S}_i}{\sigma_i^3}, \quad \tilde{\mathcal{K}}_i = \frac{\mathcal{K}_i}{\sigma_i^4}$$

where σ_i is the standard deviation of x_i .

3 Choose the free parameters $s_i > 0$ for $i \in [1, n]$;

4 Calculate the scaling parameter s_{i+n} , as well as the weights w_i , w_{i+n} , and w_0 ;

$$\begin{aligned} s_{i+n} &= s_i + \tilde{\mathcal{S}}_i, \quad w_{i+n} = \frac{1}{s_{i+n}(s_i + s_{i+n})} \\ w_i &= \frac{s_{i+n}}{s_i} w_{i+n}, \quad w_0 = 1 - \sum_{i=1}^{2n} w_i \end{aligned}$$

5 Calculate the $2n+1$ sigma points;

$$\begin{aligned} \chi^{(0)} &= \bar{x} & w_0 \\ \chi^{(i)} &= \bar{x} - s_i \left(\sqrt{P} \right)_i & w_i \quad i \in [1, n] \\ \chi^{(i+n)} &= \bar{x} + s_{i+n} \left(\sqrt{P} \right)_i & w_{i+n} \quad i \in [1, n] \end{aligned}$$

where $(\sqrt{P})_i$ is the i th column of the matrix square root of P .

Note : To partially match the Kurtosis, select

$$s_i = \frac{1}{2} \left(-\tilde{\mathcal{S}}_i + \sqrt{4\tilde{\mathcal{K}}_i - 3\tilde{\mathcal{S}}_i^2} \right)$$

Algorithm 1: Sigma Points for the Generalized Unscented Transform

Proof. We use the notation $C_i = (\sqrt{P})_i$, where $CC^T = P$. Evaluating the sample mean, we get

$$\begin{aligned} \mu_\chi &= \sum_{i=0}^{2n} w_i \chi^{(i)} \\ &= w_0 \bar{X} + \sum_{i=1}^n w_i [\bar{X} - s_i C_i] + \sum_{i=1}^n w_{i+n} [\bar{X} + s_{i+n} C_i] \\ &= \bar{X} \sum_{i=0}^{2n} w_i + \sum_{i=1}^n w_i [(w_{i+n} s_{i+n} - w_i s_i) C_i] = \bar{X} \end{aligned} \quad (48)$$

because $\sum_{i=0}^{2n} w_i = 1$ and $w_{i+n} s_{i+n} - w_i s_i = 0$. We see that the sample mean equals the actual mean. Evaluating the sample covariance matrix, we get

$$\begin{aligned} \Sigma_P &= \sum_{i=0}^{2n} w_i (\chi^{(i)} - \mu_\chi)(\chi^{(i)} - \mu_\chi)^T, \\ &= \sum_{i=1}^n [w_i s_i^2 C_i C_i^T] + \sum_{i=1}^n [w_{i+n} s_{i+n}^2 C_i C_i^T] \\ &= \sum_{i=1}^n [(w_i s_i^2 + w_{i+n} s_{i+n}^2) C_i C_i^T] = P \end{aligned} \quad (49)$$

TABLE I
PROBABILITY DISTRIBUTIONS

Random Variable	Probability density function	Mean $\mathbb{E}[x_i]$	Variance $\mathbb{E}[(x - \bar{x})_i^2]$	Skewness $\mathbb{E}[(x - \bar{x})_i^3]$	Kurtosis $\mathbb{E}[(x - \bar{x})_i^4]$	GenUT $\tilde{\mathcal{S}}_i$	GenUT $\tilde{\mathcal{K}}_i$
Gaussian $N(\mu, \sigma^2)$	$\frac{1}{\sqrt{2\pi}\sigma^2} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$, $x \in (-\infty, \infty)$	μ_i	σ_i^2	0	$3\sigma_i^4$	0	3
Exponential $E(\lambda)$	$\lambda e^{-\lambda x}, x \geq 0, \lambda > 0$	$\frac{1}{\lambda_i}$	$\frac{1}{\lambda_i^2}$	$\frac{2}{\lambda_i^3}$	$\frac{9}{\lambda_i^4}$	2	9
Gamma $G(a, b)$	$\frac{x^{a-1}}{\Gamma(a)b^a} e^{-\frac{x}{b}}$, $x \geq 0, a > 0, b > 0$	$a_i b_i$	$a_i b_i^2$	$2a_i b_i^3$	$3a_i b_i^4(a_i + 2)$	$\frac{2}{\sqrt{a_i}}$	$3 + \frac{6}{a_i}$
Weibull $W(a, b)$	$\frac{b}{a} \left(\frac{x}{a} \right)^{b-1} e^{-\left(\frac{x}{a} \right)^b}$, $x \geq 0, a > 0, b > 0$	$a \Gamma_{1b_i}$	$a^2 [\Gamma_{2b_i} - \Gamma_{1b_i}^2]$	$\frac{a_i^3 (T_{3b_i} + 2T_{1b_i}^3)}{-3\Gamma_{1b_i} \Gamma_{2b_i}}$	$\frac{a^4 (4\Gamma_{4b_i} - 3\Gamma_{1b_i}^4)}{-4\Gamma_{1b_i} \Gamma_{3b_i}}$ $+ 6\Gamma_{1b_i}^2 \Gamma_{2b_i}^2$	$(\Gamma_{4b_i} - 3\Gamma_{1b_i}^4)$ $- 4\Gamma_{1b_i} \Gamma_{3b_i}$ $+ 2\Gamma_{1b_i}^2 \Gamma_{2b_i}^2$	$\frac{(\Gamma_{3b_i} - 3\Gamma_{1b_i} \Gamma_{2b_i})}{(\Gamma_{2b_i} - \Gamma_{1b_i}^2)^2}$
$\Gamma_{kb_i} = \Gamma \left(\frac{k}{b_i} + 1 \right)$				$\frac{2a_i b_i}{6\Gamma_{1b_i}^2 \Gamma_{2b_i}}$	$\frac{\left(\Gamma_{2b_i} - \Gamma_{1b_i}^2 \right)^3}{\left(\Gamma_{2b_i} - \Gamma_{1b_i}^2 \right)^2}$		
Rayleigh $R(\sigma)$	$\frac{x}{\sigma^2} e^{-\frac{x^2}{2\sigma^2}}, x \geq 0$		$\sigma_i \sqrt{\frac{\pi}{2}}$	$\sigma_i^2 (2 - \frac{\pi}{2})$	$\sigma_i^3 (\pi - 3) \sqrt{\frac{\pi}{2}}$	$\frac{2\sqrt{\pi}(\pi - 3)}{(4 - \pi)\frac{3}{2}}$	$\frac{32 - 3\pi^2}{(\pi - 4)\frac{3}{2}}$
Beta $BE(a, b)$	$\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} x^{a-1} (1-x)^{b-1}$, $x \in (0, 1), a > 0, b > 0$	$\frac{a_i}{\zeta_0}$		$\frac{2a_i b_i (b_i - a_i)}{\zeta_0^3 \zeta_1 \zeta_2}$	$\frac{3a_i b_i (2(b_i - a_i)^2 + ab\zeta_2)}{\zeta_0^4 \zeta_1 \zeta_2 \zeta_3}$	$\frac{2(b-a)\sqrt{\zeta_1}}{\zeta_2 \sqrt{a_b}}$	$\frac{6\zeta_1 (a_i - b_i)^2 + 3a_i b_i \zeta_1 \zeta_2}{a_i b_i \zeta_2 \zeta_3}$
Binomial $B(n, p)$	$\binom{n}{k} p^k (1-p)^{n-k}$, $p \in [0, 1], k = 0, 1, 2, \dots, n$	$n_i p_i$	$n_i p_i (1 - p_i)$	$n_i p_i (1 - p_i)(1 - 2p_i)$	$\frac{n_i p_i (1 - p_i)(1 + p(1 - p_i)(3n_i - 6))}{p(1 - p_i)}$	$\frac{1 - 2n_i}{\sqrt{n_i p_i (1 - p_i)}}$	$\frac{1 - 6p_i (1 - p_i)}{n_i p_i (1 - p_i)}$
Poisson $P(\lambda)$	$\frac{\lambda^k}{k!} e^{-\lambda}, \lambda > 0$, $k = 0, 1, 2, \dots, \infty$	λ_i	λ_i	λ_i	$3\lambda_i^2 + \lambda_i$	$\lambda_i^{-\frac{1}{2}}$	$3 + \lambda_i^{-1}$
Geometric $GE(p)$	$p(1-p)^k, p \in (0, 1],$ $k = 0, 1, 2, \dots, \infty$	$\frac{(1-p_i)}{p_i}$	$\frac{(1-p_i)}{p_i^2}$	$\frac{(p_i - 1)(p_i - 2)}{p_i^3}$	$\frac{(1 - p_i)(p_i^2 - 9p_i + 9)}{p_i^4}$	$\frac{(2 - p_i)}{\sqrt{1 - p_i}}$	$\frac{p^2}{1 - p_i} + 9$
Negative Binomial $NB(r, p)$	$\binom{r+k-1}{k} p^r (1-p)^r$, $k = 0, 1, 2, \dots, \infty$	$\frac{r_i(1-p_i)}{p_i}$	$\frac{r_i(1-p_i)}{p_i^2}$	$\frac{r(p_i - 1)(p_i - 2)}{p_i^3}$	$\frac{r(1-p)(p^2 - 6p - 3pr + 3r + 6)}{p^4}$	$\frac{1 + p_i}{\sqrt{p_i} \Gamma_i}$	$\frac{(3r_i + 6)(p_i - 1) - p^2}{r_i(p_i - 1)}$

because $w_i s_i^2 + w_{i+n} s_{i+n}^2 = 1$ and $\sum_{i=1}^n C_i C_i^T = P$. We see that the sample covariance matrix equals the actual covariance matrix. \square

Theorem IV.2. Let $X \in \mathbb{R}^n$ be an independent random vector with mean \bar{X} and covariance matrix $P > 0$. Let the skewness and kurtosis for x_i be given as \mathcal{S}_i and \mathcal{K}_i respectively. Let the $2n+1$ sigma points be defined as shown in Algorithm 1. Then the following statements are true:

- 1) The sample skewness tensor of $\{\chi^{(i)}, w_i\}$, $\Sigma_{S_{jkl}} = \sum_{i=1}^{2n} w_i (\chi^{(i)} - \mu_\chi)_j (\chi^{(i)} - \mu_\chi)_k (\chi^{(i)} - \mu_\chi)_l$, is equal to the skewness tensor of X .
- 2) The sample Kurtosis tensor of $\{\chi^{(i)}, w_i\}$, $\Sigma_{K_{jklm}} = \sum_{i=1}^{2n} w_i (\chi^{(i)} - \mu_\chi)_j (\chi^{(i)} - \mu_\chi)_k (\chi^{(i)} - \mu_\chi)_l (\chi^{(i)} - \mu_\chi)_m$, only approximates a part of the Kurtosis tensor of X if $s_i = \frac{1}{2} (-\tilde{S}_i + \sqrt{4\tilde{K}_i - 3\tilde{S}_i^2})$.

Proof. The true skewness and kurtosis are given in (15) and (16) respectively. We evaluate the sample skewness tensor as

$$\begin{aligned} \Sigma_{S_{jkl}} &= \sum_{i=1}^{2n} w_i (\chi^{(i)} - \mu_\chi)_j (\chi^{(i)} - \mu_\chi)_k (\chi^{(i)} - \mu_\chi)_l \\ &= \sum_{i=1}^n (-w_i s_i^3 + w_{i+n} s_{i+n}^3) C_{ji} C_{ki} C_{li} \\ &= \sum_{i=1}^n \frac{\mathcal{S}_i}{\sigma_i^3} C_{ji} C_{ki} C_{li} \\ &= \begin{cases} \mathcal{S}_j & \text{if } i = j = k = l \\ 0 & \text{otherwise} \end{cases} \end{aligned} \quad (50)$$

because $C_{ij} = 0$ whenever $i \neq j$ and $C_{ii} = \sigma_i$. We note that C_{ij} is the i th row in the j th column of \sqrt{P} . We see that the sample skewness tensor equals the actual skewness tensor of (15). Finally, we evaluate the sample Kurtosis tensor as

$$\begin{aligned} \Sigma_{K_{jklm}} &= \sum_{i=1}^n (w_i s_i^4 + w_{i+n} s_{i+n}^4) C_{ji} C_{ki} C_{li} C_{mi} \\ &= \sum_{i=1}^n \frac{\mathcal{K}_i}{\sigma_i^4} C_{ji} C_{ki} C_{li} C_{mi} \\ &= \begin{cases} \mathcal{K}_j & \text{if } i = j = k = l = m \\ 0 & \text{otherwise} \end{cases} \end{aligned} \quad (51)$$

because $C_{ij} = 0$ whenever $i \neq j$ and $C_{ii} = \sigma_i$. We see that, for an independent random vector, the sample Kurtosis tensor only matches a part of the true Kurtosis tensor of (16). \square

Theorem IV.1 shows that our sigma points in Algorithm 1 can accurately approximate the mean and covariance of any random vector – this makes it applicable to a wide variety of applications. In the special case of an arbitrarily distributed independent random vector with known skewness and kurtosis for each element, Theorem IV.2 shows that our sigma points accurately approximates the skewness tensor. It also shows that with proper selection of the proportionality constants, the Kurtosis tensor can be partially approximated.

V. POSITIVELY CONSTRAINED SIGMA POINTS

Several probability distributions, such as Poisson and negative binomial, only permit random variables that take positive values. Although several sigma point transformations that exist in the literature can be employed [9], [11], they sometimes give sigma points that violate the positive assumption inherent to some probability distributions despite being able to capture the mean and covariance of the random variable. This might make them inapplicable in situations/models that only permit positive values. For example, in applications that assume a Poisson distribution for the states, such as count data, the states are usually positive by default and can never be negative. When our sigma point of Algorithm 1 is applied, the positive constraint on an independent random vector can be violated. We demonstrate this using the following example.

Example V.1. We generate sigma points for an independent Poisson random vector x with mean \bar{x} and covariance P such that

$$\bar{x} = \begin{bmatrix} 1.5 \\ 1 \end{bmatrix}, \quad P = \begin{bmatrix} 1.5 & 0 \\ 0 & 1 \end{bmatrix}$$

Using Algorithm 1, we see that $w_0 = 0.3333$, $w_1 = 0.2049$, $w_2 = 0.2129$, $w_3 = 0.1284$, $w_4 = 0.1204$, $s_1 = 1.3713$, $s_2 = 1.3028$, $s_3 = 2.1878$, and $s_4 = 2.3028$. The $2n+1$ sigma points in matrix form is

$$\chi = \begin{bmatrix} 1.5000 & -0.1794 & 1.5000 & 4.1794 & 1.5000 \\ 1.0000 & 1.0000 & -0.3028 & 1.0000 & 3.3028 \end{bmatrix} \quad (52)$$

The sample mean and sample covariance are

$$\mu_\chi = \begin{bmatrix} 1.5 \\ 1 \end{bmatrix}, \quad \Sigma_P = \begin{bmatrix} 1.5 & 0 \\ 0 & 1 \end{bmatrix}$$

We see from Example V.1 that despite the accuracy of the sample mean and sample covariance, two sigma points $\chi^{(1)}$ and $\chi^{(2)}$ in (52) had negative values. The negative sigma points do not satisfy the non-negativity of Poisson draws. Hence, we would like to come up with analytical expressions for sigma points that do not violate the positive constraints, while still maintaining accuracy in approximating the true mean and covariance of a random vector. To do this, we employ the following assumption about the sigma points in Algorithm 1.

Assumption V.1. The mean \bar{x} is positive, the sigma points $\chi^{(i)} = \bar{x} - s_i (\sqrt{P})_i$ can either be positive or negative for $i \in [1, n]$, and the sigma points $\chi^{(i+n)} = \bar{x} + s_{i+n} (\sqrt{P})_i$ are always positive for $i \in [1, n]$.

We analytically enforce positive constraints on the sigma points in Algorithm 1 by ensuring that the inequality $(\bar{x} - s_i (\sqrt{P})_i) \geq 0$ will not be violated – we enforce this constraint by redefining the free parameters s_i for $i \in [1, n]$. After calculating the sigma points using Algorithm 1, we select the free parameter s_i such that

$$s_i = \min \left(\bar{x} \oslash (\sqrt{P})_i \right) \quad \text{if } \min \left(\chi^{(i)} \right) < 0$$

where $(\sqrt{P})_i$ is the i th column of \sqrt{P} and the Hadamard division \oslash implies an element-wise division. Although the above

representation always guarantees that one of the elements of the sigma point $\chi^{(i)}$ attains a value of zero, some models might not permit zero values for the sigma points. To address this, we introduce a *slack parameter* $k \in (0, 1]$ which is a user selected constant. Using k , we now redefine the free parameter s_i as

$$s_i = k \left[\min \left(\bar{x} \oslash (\sqrt{P})_i \right) \right] \quad \text{if } \min \left(\chi^{(i)} \right) < 0 \quad (53)$$

where a value of $k = 1$ ensures that at least one of the elements of $\chi^{(i)}$ is zero. The sigma point gets farther away from 0 as $k \rightarrow 0$. Using a new value for s_i , we note that the equations for s_{i+n} , w_{i+n} , and w_i are unchanged.

For an arbitrarily distributed independent random vector, the positively constrained sigma points designed here are only accurate up to the third order – the extra degree of freedom in capturing a part of the kurtosis tensor is lost. The positively constrained sigma point algorithm is given in Algorithm 2. We now show a benefit of Algorithm 2 in the following example.

```

1 Implement Algorithm 1
2 for i = 1 to n do
3   if min (χ(i)) < 0 then
4     Redefine si;
      
$$s_i = k \left[ \min \left( \bar{x} \oslash (\sqrt{P})_i \right) \right]$$

      where the Hadamard division  $\oslash$  implies an
      element-wise division. The user-selected
      slack parameter  $k$  should be selected such
      that  $0 < k \leq 1$ . A value of  $k = 1$  yields a
      zero sigma point. The sigma point gets
      farther away from 0 as  $k \rightarrow 0$ .
5   end
6 end
7 Repeat steps 4 and 5 of Algorithm 1;

```

Algorithm 2: Positively Constrained Sigma Points for the General Unscented Transform

Example V.2. Using Algorithm 2 to generate positively constrained sigma points for the Poisson random vector, we select $k = 0.9$. We see that $w_0 = -0.0576$, $w_1 = 0.3003$, $w_2 = 0.3968$, $w_3 = 0.1725$, $w_4 = 0.1880$, $s_1 = 1.1023$, $s_2 = 0.9000$, $s_3 = 1.9188$, and $s_4 = 1.9000$. The $2n + 1$ positive sigma points in matrix form is

$$\chi = \begin{bmatrix} 1.5000 & 0.1500 & 1.5000 & 3.8500 & 1.5000 \\ 1.0000 & 1.0000 & 0.1000 & 1.0000 & 2.9000 \end{bmatrix} \quad (54)$$

while the corresponding sample mean and sample covariance are

$$\mu_\chi = \begin{bmatrix} 1.5 \\ 1 \end{bmatrix}, \quad \Sigma_P = \begin{bmatrix} 1.5 & 0 \\ 0 & 1 \end{bmatrix}$$

We see from Example V.2 that using Algorithm 2 ensures that the sigma points are always positive while ensuring accuracy in approximating the true mean and covariance of a random vector. A graphical representation of Examples V.1

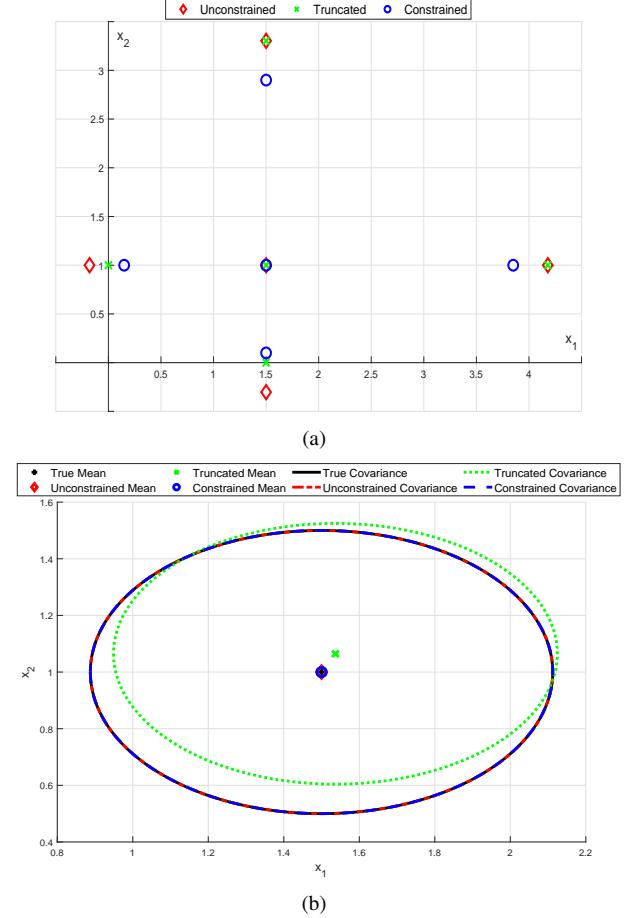


Fig. 3. (a) Locations of sigma points for the unconstrained (Algorithm 1), truncated, and constrained (Algorithm 2) sigma points. (b) Mean and covariance of the unconstrained (Algorithm 1), truncated, and constrained (Algorithm 2) sigma points.

and V.2 is shown in Figure V.2 where we plot the sigma points and the covariance. We note that the accuracy in approximating the true mean and true covariance of a random vector is also valid for any arbitrary distribution whenever the positively constrained sigma points of Algorithm 2 are used.

VI. PROPAGATION OF MEANS AND COVARIANCES OF NONLINEAR TRANSFORMATIONS

We analyze the performance of our new sigma point algorithm when they undergo nonlinear transformations. We will show how linearization approximations, via Taylor series expansion of a nonlinear transformation of a random vector x evaluated about its mean \bar{x} , introduce errors in the propagation of means and covariances. We evaluate the true mean and true covariance of an independent random vector in Appendices A-A and A-B respectively. We then evaluate the approximated mean and approximated covariance in Appendices B-A and B-B respectively. We see that errors are introduced beyond the third order when approximating a nonlinear transformation of an independent random vector. We also see that errors are introduced beyond the second order when the random vector is not independent.

We will see that errors can be introduced in the propagation of means and covariances beyond the second order when sigma points developed under the Gaussian assumption [8], [11], [30] are used to approximate the nonlinear function $\lambda(x)$ when x is an independent random vector. We note that the nonlinear transformation $y \in \mathbb{R}^n$ is given by

$$y = \lambda(x) \quad (55)$$

where $\mathbb{E}[x] = \bar{x}$. We use the GenUT of Algorithm 1, which guarantees fourth-order accuracy for random variables. Given \bar{x} , P , S_i , and \mathcal{K}_i , the sample mean and covariance of the nonlinear transformation of (55) when the GenUT is used can be calculated as follows.

- 1) Calculate the $2n + 1$ sigma points using Algorithm 1.
- 2) Evaluate the sample mean and sample covariance using (3)–(5).

For our comparison, we use the scaled unscented transform of [30], which is denoted as UT for the remainder of this paper. The sigma points of the UT is given as

$$\begin{aligned} \chi_0 &= \bar{x} & w_0 &= \frac{1}{2\alpha} \\ \chi_i &= \bar{x} + \left(\sqrt{\alpha P}\right)_i & w_i &= 1 - \frac{n}{\alpha} \\ \chi_{i+n} &= \bar{x} - \left(\sqrt{\alpha P}\right)_i & w_i &= 1 - \frac{n}{\alpha} \end{aligned} \quad (56)$$

where α defines the scaling of the sigma points. A value of $\alpha = 3$ is typically recommended to partially match the kurtosis of a random vector [30]. The sample mean and sample covariance of the UT can also be evaluated using (3)–(5).

A. Case Study 1 – Transformation of Random Variables

Defining x as a random variable that can follow any of the probability distributions given in Table I, we evaluate the mean and covariance of two nonlinear transformations: a quadratic function of the random variable $y = 3x + 2x^2$, and a trigonometric function of the random variable $y = \sin(x)$. We also use 100000 Monte Carlo draws from the different probability distributions to evaluate the sample mean and sample covariance of the nonlinear transformations. The true mean and covariance of the quadratic function can be easily evaluated using the raw moments of x up to its fourth order. The true mean and covariance of the trigonometric function can be evaluated using their characteristic functions. A comparison between the accuracy of the GenUT, UT, and 100000 Monte Carlo draws in approximating the true mean and true covariance of the nonlinear transformations for the different probability distributions is shown in Tables II–V.

For the quadratic function, we see that the GenUT gave an exact approximation of the true mean and true covariance for all the probability distributions while the UT was only accurate in approximating the true mean when the probability distribution was not Gaussian. This is because the Taylor series expansion of the mean is characterized by the existence of second-order moments of x , the Taylor series expansion of the covariance is characterized by the existence of fourth-order moments of x , and the UT is only accurate up to the second order when the distribution is not Gaussian. The GenUT

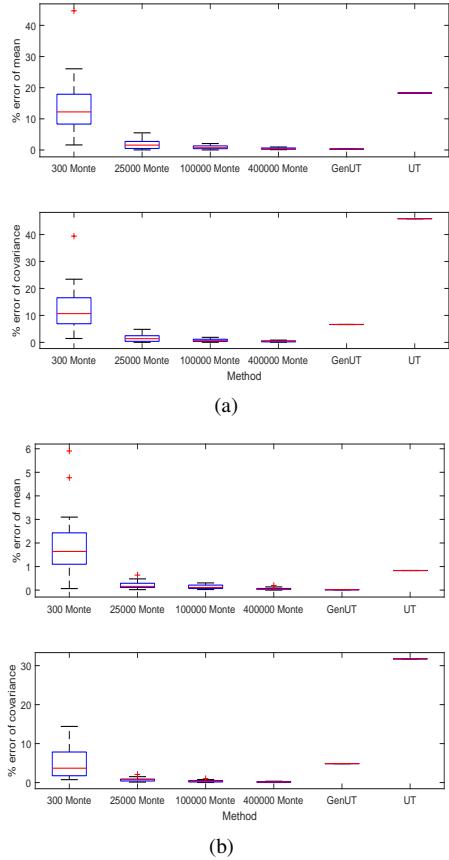


Fig. 4. (a) Moments of $y = \sin(x)$ when x is a Poisson random variable.
(b) Moments of $y = \sin(x)$ when x is a Weibull random variable.

is accurate up fourth order because it is adaptable to the unique skewness and kurtosis of most probability distributions. Although the 100000 Monte Carlo draws gave relatively good approximations, they were not as accurate as the GenUT.

For the trigonometric function, we see that the GenUT and UT were unable to give exact approximations of the true mean and true covariance in most cases because the Taylor series expansion of the nonlinear transformation is characterized by the existence of the central moments of x beyond the fourth order. The GenUT was more accurate than the UT for all the non-Gaussian probability distributions because the GenUT is accurate up to the fourth order while the UT is accurate up to the second order. The GenUT and UT gave similar accuracy when x was Gaussian distributed because fourth-order accuracy was guaranteed by both methods. The 100000 Monte Carlo draws sometimes gave better accuracy than the GenUT because of the random nature of its draws. A box plot of the accuracy of the GenUT, UT, and several Monte Carlo draws of different sizes is shown in Figure 4 for the trigonometric function. We see that a significant number of Monte Carlo draws is needed to achieve the accuracy of the GenUT when approximating the mean. A significant number of Monte Carlo draws gives better accuracy in approximating the variance.

TABLE II
PERCENTAGE ERROR IN PROPAGATING THE MEAN OF $y = 3x + 2x^2$

x	GenUT	UT	MC
$\mathcal{N}(1, 4)$	0	0	0.015
$E(2)$	0	0	0.069
$G(1, 2)$	0	0	0.452
$W(1, 2)$	0	0	0.005
$R(1)$	0	0	0.097
$BE(3, 4)$	0	0	0.063
$B(3, 0.3)$	0	0	0.457
$P(2)$	0	0	0.270
$GE(0.5)$	0	0	1.251
$NB(4, 0.67)$	0	0	0.668

TABLE III
PERCENTAGE ERROR IN PROPAGATING THE COVARIANCE OF $y = 3x + 2x^2$

x	GenUT	UT	MC
$\mathcal{N}(1, 4)$	0	0	0.029
$E(2)$	0	49.057	0.249
$G(1, 2)$	0	64	1.889
$W(1, 2)$	0	15.003	0.310
$R(1)$	0	16.815	0.381
$BE(3, 4)$	0	2.307	0.613
$B(3, 0.3)$	0	16.380	0.359
$P(2)$	0	25.946	1.061
$GE(0.5)$	0	67.662	1.036
$NB(4, 0.67)$	0	43.224	2.356

TABLE IV
PERCENTAGE ERROR IN PROPAGATING THE MEAN OF $y = \sin(x)$

x	GenUT	UT	MC
$\mathcal{N}(0.25, 0.1)$	0.001	0.001	0.012
$E(2)$	0.219	5.788	0.110
$G(0.5, 0.5)$	0.312	6.964	0.050
$W(1, 2)$	0.017	0.831	0.029
$R(1)$	0.049	0.912	0.007
$BE(3, 4)$	0	0.038	0.037
$B(3, 0.3)$	0.158	4.814	0.046
$P(0.1)$	0.275	18.305	0.531
$GE(0.7)$	2.416	32.906	0.138
$NB(0.4, 0.67)$	0.176	44.172	0.383

TABLE V
PERCENTAGE ERROR IN PROPAGATING THE COVARIANCE OF $y = \sin(x)$

x	GenUT	UT	MC
$\mathcal{N}(0.25, 0.1)$	5.026	5.026	0.444
$E(2)$	23.499	72.557	0.213
$G(0.5, 0.5)$	20.749	61.391	0.372
$W(1, 2)$	4.862	31.760	0.043
$R(1)$	12.158	50.678	0.531
$BE(3, 4)$	0.031	0.940	0.225
$B(3, 0.3)$	11.033	24.806	0.060
$P(0.1)$	6.646	45.895	0.461
$GE(0.7)$	12.074	87.637	0.070
$NB(0.4, 0.67)$	39.068	135.783	0.366

B. Case Study 2 - Infectious Disease Models

We consider an SIR (susceptible-infectious-recovered) infectious disease model given by the difference equation [31]

$$\begin{aligned} S_{k+1} &= S_k - \frac{\beta S_k I_k}{N} \\ I_{k+1} &= I_t + \frac{\beta S_k I_k}{N} - \gamma I_k \\ R_{k+1} &= R_k + \gamma I_k \end{aligned} \quad (57)$$

where β is the infection rate, γ is the recovery rate, and $N = S_k + I_k + R_k$. We examine the performance of the GenUT and the UT in approximating the true mean and covariance of (57) when its right hand side is linear in the random variables or nonlinear in the random variables. We note that by defining the state $x_k = [S_k, I_k, R_k]^T$, we can write (57) in a more compact form.

1) *Linear in random variables:* We modify (57) to be a linear combination of independent Poisson random variables such that

$$x_{k+1} = x_k + AX \quad (58)$$

where

$$A = \begin{bmatrix} -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix}, \quad X = \text{Poisson} \begin{bmatrix} \frac{\beta S_k I_k}{N} \\ \gamma I_k \end{bmatrix}$$

We note that although one of the Poisson rates is nonlinear in the variables S_k and I_k , the difference equation of (58) is comprised of linear combinations of the Poisson random vector X . Variants of this particular formulaion can be found in [25], [31]. Evaluating the mean and covariance of (58) conditioned on the state at index k , the GenUT and UT will both give the correct mean and correct covariance despite the fact that the independent random vector X is Poisson distributed. To better understand why they both give similar values, we briefly analyze the Taylor series expansion of (58) by using the results in (6) and (10). Assuming that $\lambda = x_t + AX$, we see that the following partial derivative holds true.

$$\frac{\partial^2 \lambda}{\partial X_i \partial X_j} = [0 \ 0 \ 0]^T \quad \text{for } i, j \in [1, 2]$$

We see from the above equation that all second, third, and fourth partial derivatives are zero. Therefore, only the terms $\lambda(\bar{X})$ and $\Lambda P \Lambda^T$ exist in the Taylor series expansion in (6) and (10) respectively, which are accurately approximated by the GenUT and UT.

2) *Nonlinear in random variables – model 1:* We deviate from the more common representation in (58) by assuming that the SIR dynamics is made up of Poisson draws of the states such that

$$x_{k+1} = x_k + \lambda(X) \quad (59)$$

where

$$\lambda(X) = \begin{bmatrix} -\frac{\beta X_1 X_2}{N} \\ \frac{\beta X_1 X_2}{N} - \gamma X_2 \\ \gamma X_2 \end{bmatrix}, \quad X = \text{Poisson} \begin{bmatrix} S_k \\ I_k \end{bmatrix}$$

The difference equation of (59) is comprised of nonlinear combinations of the Poisson random vector X whose rates depend on S_k and I_k . Evaluating the mean and covariance of (59) conditioned on the state at index k , the GenUT and UT will both give the same sample mean and sample covariance for (59). We however note that although the sample mean would be accurate, the sample covariance would be inaccurate because of errors in approximating the fourth-order terms in the Taylor series expansion of the covariance of (59). To better understand why they both give the correct mean and an inaccurate covariance matrix despite the fact that the independent random vector was Poisson distributed, we briefly analyze the Taylor series expansion of (59) using the results in (6) and (10). We see that the following partial derivative of $\lambda(X)$ holds true.

$$\frac{\partial^2 \lambda}{\partial X_i \partial X_j} = \begin{cases} \begin{bmatrix} -\frac{\beta}{N} & \frac{\beta}{N} & 0 \end{bmatrix}^T & \text{if } i \neq j \\ \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T & \text{otherwise} \end{cases} \quad \text{for } i, j \in [1, 2]$$

From the above equation, we see that all partial derivatives beyond the second order are zero. Therefore, from (6), we can see that the GenUT and UT give the accurate mean because they both accurately capture the second-order terms. For the covariance matrix, we analyze the third-order and fourth-order terms. Although the term $\frac{\partial^2 \lambda}{\partial X_i \partial X_j}$ has some nonzero elements if $i \neq j$, the term $S_{ijk} = 0$ whenever $i = j = k$ is violated. Therefore, in the third-order terms, the partial derivatives always equal zero when the skewness exists while the skewness always equals zero when the partial derivatives exist. This is why the GenUT and UT arrive at the same value of zero for all third-order terms even though the UT inaccurately approximates the skewness by always guaranteeing zero skewness. For the fourth-order terms, only the term $\frac{\partial^2 \lambda}{\partial X_i \partial X_j} \frac{\partial^2 \lambda^T}{\partial X_i \partial X_j} \neq 0$ whenever $i \neq j$. From (10), we can see that this term is multiplied by the kurtosis term K_{ijkl} which is defined in (16) as $K_{ijkl} = P_{ii} P_{jj}$ whenever $i = k \neq j = l$. However, we see from (51) that the GenUT gives a value of $K_{ijkl} = 0$ whenever $i = k \neq j = l$ – the same can be said about the UT. Therefore, the GenUT and UT both arrive at zero values for the fourth-order terms thereby leading to inaccurate approximations of the true covariance matrix.

3) *Nonlinear in random variables – model 2:* Using the conservation principle $S + I + R = N$, we reduce the model of (57) to

$$\begin{aligned} I_{k+1} &= I_k + \beta(N - I_k - R_k) \frac{I_k}{N} - \gamma I_k \\ R_{k+1} &= R_k + \gamma I_k \end{aligned} \quad (60)$$

We now assume that the reduced dynamics of (60) is made up of Poisson draws of the state I_k such that

$$x_{k+1} = x_k + \lambda(X) \quad (61)$$

where $x_k = \begin{bmatrix} I_k \\ R_k \end{bmatrix}$, and

$$\lambda(X) = \begin{bmatrix} \beta(N - X_1 - R_k) \frac{X_1}{N} - X_2 \\ X_2 \end{bmatrix}, \quad X = \text{Poisson} \begin{bmatrix} I_k \\ \gamma I_k \end{bmatrix}$$

Evaluating the mean and covariance of (59) conditioned on the state at index k , the GenUT will accurately approximate the mean and covariance matrix, while the UT will accurately approximate the mean but inaccurately approximate the covariance matrix. To understand the performance of the GenUT and UT, we briefly analyze the Taylor series expansion of (61) using the results in (6) and (10). We see that the following partial derivative of $\lambda(X)$ holds true.

$$\frac{\partial^2 \lambda}{\partial X_i \partial X_j} = \begin{cases} \begin{bmatrix} -\frac{2\beta}{N} & 0 \end{bmatrix}^T & \text{if } i = j = 1 \\ \begin{bmatrix} 0 & 0 \end{bmatrix}^T & \text{otherwise} \end{cases} \quad \text{for } i, j \in [1, 2]$$

From the above equation, we see that all partial derivatives beyond the second order are zero. Therefore, from (6), we can see that the GenUT and UT give the accurate mean because they both accurately capture the second-order terms. For the covariance, using (10), we see that the third-order terms are nonzero if $i = j = k = 1$ and only the GenUT is able to accurately approximate S_{ijk} , with the UT always giving a value of zero for S_{ijk} . Furthermore, from (10), we see that the only nonzero fourth-order term is $\frac{\partial^2 \lambda}{\partial X_i \partial X_j} \frac{\partial^2 \lambda^T}{\partial X_k \partial X_l}$ whenever $i = j = k = l = 1$. However, only the GenUT is able to accurately approximate K_{ijkl} if $i = j = k = l$. This is why the GenUT gives an accurate approximation of the covariance matrix.

During the implementation of a Kalman filter on the reduced dynamics of (61), using the GenUT and UT to estimate the system noise covariance matrix will give filter performances that might be indistinguishable from each other. This can happen for two reasons: (i) Whenever the infected population I is very small such that the Poisson random variable X_1 can not be well approximated by a Gaussian of the same mean and variance, the contribution of the third-order and fourth-order terms in (10) will be very small because of the presence of the $\frac{\beta}{N}$ term and the relatively small values of β that are typically used in infectious disease modeling. The resulting small difference in covariance matrix accuracy will be made negligible during the measurement update step of the Kalman filter. (ii) Whenever the infected population I is large enough such that the Poisson random variable X_1 can be well approximated by a Gaussian of the same mean and variance,

due to the presence of the $\frac{\beta}{N}$ term and small β values, the GenUT and UT will both give similar values for the third-order and fourth-order terms in (10).

VII. CONCLUSION

In this paper we have developed the generalized unscented transform (GenUT) that is capable of adapting to the unique statistics of an arbitrarily distributed random variable. We showed that due to its ability to match up to at least the skewness of any random variable, the GenUT is preferable to the unscented transforms that were either developed using the Gaussian assumption or were developed without any probability distribution in mind. In terms of ease of implementation, we demonstrated that like the unscented transform originally developed in [11] which uses $2n+1$ sigma points, the GenUT uses the same number of sigma points ($2n+1$) to achieve third-order accuracy for independent random vectors. In terms of performance, the GenUT and unscented transforms developed under the Gaussian assumption give the same performance when the random variable is Gaussian distributed. We also showed that the GenUT formulation makes it easy to enforce positive constraints on the sigma points while still guaranteeing third-order accuracy, which makes it appealing in models that permit only positive values for random variables.

When compared against many unscented transforms existing in the literature, the GenUT gives better accuracy if the nonlinearity of the transformations are significant and the random variable is not Gaussian distributed, which makes it suitable for numerous real world applications. For example, several infectious disease models use linear combinations of random variables such as Poisson or Negative Binomial [31] – a linear combination of independent Poisson random variables was used in the modeling and assimilation of daily COVID-19 infection data [25]. In such an application, for estimating the noise covariance matrix, the use of the GenUT, UT, and other unscented transforms existing in the literature that guarantee at least a second-order accuracy will yield no noticeable difference in performance. We showed in Section VI-B1 that this is because higher order terms beyond the first order in the Taylor series expansion of a linear transformation of an independent random vector are all zero – this explains why using the EKF, which uses first-order linearization, for such applications might produce similar results. We showed in Section VI-B2 that the GenUT and UT performance are indistinguishable from each other if the each random variable in the product is a monomial of degree 1. We showed in Section VI-B3 that a noticeable increase in performance of the GenUT will be observed when any of the random variable in the product is a monomial of degree 2 or more – this implies that terms beyond the third order exist in the Taylor series expansion of the transformation.

For uncertainty quantification, estimation, or prediction applications, the GenUT can typically give better accuracy when compared to other unscented transforms. This accuracy will have more significant consequences if the nonlinearities are strong.

In summary, the GenUT is a new form of adaptable sigma points that can match a prescribed mean, variance, and

skewness of most independent random vectors, while being able to partially match its kurtosis. In the case of a single random variable, the GenUT can match up to its kurtosis. For correlated random vectors, the GenUT can accurately match up to its covariance. The GenUT can be applied to any filter that uses linear or nonlinear transformations of random variables.

APPENDIX A TRUE MEAN AND COVARIANCE OF NONLINEAR TRANSFORMATIONS

We derive analytical expressions for the true mean and covariance when we take the Taylor series expansion of the nonlinear function $y = \lambda(x)$ where x is a random vector that follows an arbitrary distribution.

A. True Mean of the Nonlinear Transformation

Applying Taylor series expansion around \bar{x} , where $\tilde{x} = x - \bar{x}$, we write the true mean of y as

$$\bar{y} = \mathbb{E}[\lambda(x)] = \lambda(\bar{x}) + \mathbb{E}\left[D_{\tilde{x}}\lambda + \frac{D_{\tilde{x}}^2\lambda}{2!} + \frac{D_{\tilde{x}}^3\lambda}{3!} + \frac{D_{\tilde{x}}^4\lambda}{4!} + \dots\right] \quad (62)$$

where $D_{\tilde{x}}\lambda$ is the total differential of $\lambda(x)$ when perturbed around a nominal value \bar{x} by \tilde{x} . We note that

$$D_{\tilde{x}}^k\lambda = \left(\sum_{i=1}^n \tilde{x}_i \frac{\partial}{\partial x_i}\right)^k \lambda(x) \Big|_{x=\bar{x}} \quad (63)$$

Using (63), we can evaluate the true mean of (62) as

$$\begin{aligned} \bar{y} = & \lambda(\bar{x}) + \left\{ \sum_{i,j=1}^n \frac{P_{ij}}{2!} \frac{\partial^2\lambda}{\partial x_i \partial x_j} + \sum_{i,j,k=1}^n \frac{S_{ijk}}{3!} \frac{\partial^3\lambda}{\partial x_i \partial x_j \partial x_k} \right. \\ & \left. + \sum_{i,j,k,l=1}^n \frac{K_{ijkl}}{4!} \frac{\partial^4\lambda}{\partial x_i \partial x_j \partial x_k \partial x_l} \right\}_{x=\bar{x}} + \dots \end{aligned} \quad (64)$$

where $P_{ij} = \mathbb{E}[\tilde{x}_i \tilde{x}_j]$, while S_{ijk} , and K_{ijkl} are defined in (7) and (8) respectively.

B. True Covariance of the Nonlinear Transformation

The true covariance of y is given as

$$P_y = \mathbb{E}[(y - \bar{y})(y - \bar{y})^T] \quad (65)$$

Evaluating the expression $y - \bar{y}$, we write

$$y - \bar{y}_T = D_{\tilde{x}}\lambda + \frac{D_{\tilde{x}}^2\lambda}{2!} + \frac{D_{\tilde{x}}^3\lambda}{3!} - \mathbb{E}\left[\frac{D_{\tilde{x}}^2\lambda}{2!} + \frac{D_{\tilde{x}}^3\lambda}{3!}\right] + \dots \quad (66)$$

Substituting (66) into (65) gives

$$\begin{aligned} P_y = & \mathbb{E}\left[D_{\tilde{x}}\lambda(D_{\tilde{x}}\lambda)^T + \frac{D_{\tilde{x}}^2\lambda(D_{\tilde{x}}\lambda)^T}{2!} + \frac{D_{\tilde{x}}\lambda(D_{\tilde{x}}^2\lambda)^T}{2!}\right. \\ & \left. + \frac{D_{\tilde{x}}^3\lambda(D_{\tilde{x}}\lambda)^T}{3!} + \frac{D_{\tilde{x}}\lambda(D_{\tilde{x}}^3\lambda)^T}{3!} + \frac{D_{\tilde{x}}^2\lambda(D_{\tilde{x}}^2\lambda)^T}{2! \times 2!}\right] \\ & + \mathbb{E}\left[\frac{D_{\tilde{x}}^2\lambda}{2!}\right] \mathbb{E}\left[\frac{D_{\tilde{x}}^2\lambda}{2!}\right]^T + \dots \end{aligned} \quad (67)$$

We note that we can write the first term in the above equation as

$$\mathbb{E} [D_{\tilde{x}} \lambda (D_{\tilde{x}} \lambda)^T] = \frac{\partial \lambda}{\partial x} \Big|_{x=\bar{x}} \mathbb{E} [\tilde{x} \tilde{x}^T] \frac{\partial \lambda^T}{\partial x} \Big|_{x=\bar{x}} = \Lambda P \Lambda^T \quad (68)$$

Using (63) and (68), we can rewrite the true covariance matrix of (67) as

$$\begin{aligned} P_y = & \Lambda P \Lambda^T + \left\{ \sum_{i,j,k=1}^n \frac{S_{ijk}}{2!} \left[\frac{\partial^2 \lambda}{\partial x_i \partial x_j} \frac{\partial \lambda^T}{\partial x_k} + \frac{\partial \lambda}{\partial x_i} \frac{\partial^2 \lambda^T}{\partial x_j \partial x_k} \right] \right. \\ & + \sum_{i,j,k,l=1}^n K_{ijkl} \left[\frac{1}{3!} \frac{\partial^3 \lambda}{\partial x_i \partial x_j \partial x_k} \frac{\partial \lambda^T}{\partial x_l} \right. \\ & \left. + \frac{1}{3!} \frac{\partial \lambda}{\partial x_i} \frac{\partial^3 \lambda^T}{\partial x_j \partial x_k \partial x_l} + \frac{1}{4} \frac{\partial^2 \lambda}{\partial x_i \partial x_j} \frac{\partial^2 \lambda^T}{\partial x_k \partial x_l} \right] \\ & \left. + \left[\sum_{i,j=1}^n \frac{P_{ij}}{2} \frac{\partial^2 \lambda}{\partial x_i \partial x_j} \right] \left[\dots \right]^T \right\}_{x=\bar{x}} + \dots \end{aligned} \quad (69)$$

where we have used the notation $XX^T = X[\dots]^T$.

APPENDIX B

APPROXIMATION OF THE MEAN AND COVARIANCE USING GENERALIZED UNSCENTED TRANSFORMATION

We analytically show the accuracy in capturing the true mean and true covariance of $y = \lambda(x)$ when using our $2n+1$ sigma points of Algorithm 1. We show that our sigma point transformations are accurate up to the third order for independent random vectors. We also show that our sigma points can partially capture some of the fourth-order moments. In this section, we define the matrix square root of P as $C = \sqrt{P}$. We note that

$$\sum_{i=1}^{2n} w_i D_{\tilde{x}}^k \lambda = \sum_{i=1}^{2n} w_i \left(\sum_{j=1}^n \tilde{x}_j \frac{\partial}{\partial x_j} \right)^k \lambda(x) \Big|_{x=\bar{x}} \quad (70)$$

A. Approximation of the Mean

The approximated mean is given as

$$\begin{aligned} \bar{y}_u &= \sum_{i=0}^{2n} w_i \lambda(\chi^{(i)}) \\ &= \sum_{i=0}^{2n} w_i \left[\lambda(\bar{x}) + D_{\tilde{x}^{(i)}} \lambda + \frac{D_{\tilde{x}^{(i)}}^2 \lambda}{2!} + \frac{D_{\tilde{x}^{(i)}}^3 \lambda}{3!} + \dots \right] \\ &= \lambda(\bar{x}) + \sum_{i=1}^{2n} w_i \left[D_{\tilde{x}^{(i)}} \lambda + \frac{D_{\tilde{x}^{(i)}}^2 \lambda}{2!} + \frac{D_{\tilde{x}^{(i)}}^3 \lambda}{3!} + \dots \right] \end{aligned} \quad (71)$$

Using (70), we can evaluate the approximated mean of (71) as

$$\begin{aligned} \bar{y}_u = & \lambda(\bar{x}) + \left\{ \sum_{i,j=1}^n \frac{P_{ij}}{2} \frac{\partial \lambda}{\partial x_i \partial x_j} + \sum_{i,j,k=1}^n \frac{\Sigma_{S_{ijk}}}{3!} \frac{\partial^3 \lambda}{\partial x_i \partial x_j \partial x_k} \right. \\ & \left. + \sum_{i,j,k,l=1}^n \frac{\Sigma_{K_{ijkl}}}{4!} \frac{\partial^4 \lambda}{\partial x_i \partial x_j \partial x_k \partial x_l} \right\}_{x=\bar{x}} + \dots \end{aligned} \quad (72)$$

where $\sum_{i=1}^{2n} w_i \tilde{x}_j^{(i)} \tilde{x}_k^{(i)} = P_{jk}$, while $\Sigma_{S_{ijk}}$ and $\Sigma_{K_{ijkl}}$ are defined in (50) and (51) respectively.

We see that, for an independent random vector, the approximated mean of (72) correctly matches the true mean of (64) up to the third order, and only partial accuracy is achieved for the fourth order. This is because $\Sigma_{S_{ijk}} = S_{ijk}$ (see (15) and (50)) and $\Sigma_{K_{ijkl}}$ only partially approximates K_{ijkl} (see (16) and (51)).

B. Approximation of the Covariance

The approximated covariance can be evaluated using the expression

$$P_u = \sum_{i=1}^{2n} w_i \left[\mathcal{Y}^{(i)} - \bar{y}_u \right] \left[\mathcal{Y}^{(i)} - \bar{y}_u \right]^T \quad (73)$$

From

$$\begin{aligned} \mathcal{Y}^{(i)} - \bar{y}_u &= D_{\tilde{x}^{(i)}} \lambda + \frac{D_{\tilde{x}^{(i)}}^2 \lambda}{2!} + \frac{D_{\tilde{x}^{(i)}}^3 \lambda}{3!} \\ &\quad - \sum_{j=1}^{2n} w_j \left[\frac{D_{\tilde{x}^{(j)}}^2 \lambda}{2!} + \frac{D_{\tilde{x}^{(j)}}^3 \lambda}{3!} \right] + \dots \end{aligned} \quad (74)$$

Substituting (74) into (73) and multiplying out gives

$$\begin{aligned} P_u = & \sum_{i=1}^{2n} w_i \left[D_{\tilde{x}^{(i)}} \lambda (D_{\tilde{x}^{(i)}} \lambda)^T + \frac{D_{\tilde{x}^{(i)}}^2 \lambda (D_{\tilde{x}^{(i)}} \lambda)^T}{2!} \right. \\ & + \frac{D_{\tilde{x}^{(i)}} \lambda (D_{\tilde{x}^{(i)}}^2 \lambda)^T}{2!} + \frac{D_{\tilde{x}^{(i)}}^3 \lambda (D_{\tilde{x}^{(i)}} \lambda)^T}{3!} \\ & \left. + \frac{D_{\tilde{x}^{(i)}} \lambda (D_{\tilde{x}^{(i)}}^3 \lambda)^T}{3!} + \frac{D_{\tilde{x}^{(i)}}^2 \lambda (D_{\tilde{x}^{(i)}}^2 \lambda)^T}{2! \times 2!} \right] \\ & + \left[\sum_{j=1}^{2n} w_j \frac{D_{\tilde{x}^{(j)}}^2 \lambda}{2!} \right] \left[\dots \right]^T + \dots \end{aligned} \quad (75)$$

For the first term in (75),

$$\begin{aligned} \sum_{i=1}^{2n} w_i D_{\tilde{x}^{(i)}} \lambda (D_{\tilde{x}^{(i)}} \lambda)^T &= \sum_{j,k=1}^n \sum_{i=1}^{2n} w_i \tilde{x}_j^{(i)} \tilde{x}_k^{(i)} \frac{\partial \lambda}{\partial x_j} \frac{\partial \lambda^T}{\partial x_k} \Big|_{x=\bar{x}} \\ &= \sum_{j,k=1}^n \frac{\partial \lambda}{\partial x_j} \Big|_{x=\bar{x}} P_{jk} \frac{\partial \lambda^T}{\partial x_k} \Big|_{x=\bar{x}} \\ &= \Lambda P \Lambda^T \end{aligned} \quad (76)$$

Using (70) and (76), we can rewrite the approximated covariance matrix of (75) as

$$\begin{aligned} P_u = & \Lambda P \Lambda^T + \left\{ \sum_{i,j,k=1}^n \frac{\Sigma_{S_{ijk}}}{2!} \left[\frac{\partial^2 \lambda}{\partial x_i \partial x_j} \frac{\partial \lambda^T}{\partial x_k} + \frac{\partial \lambda}{\partial x_i} \frac{\partial^2 \lambda^T}{\partial x_j \partial x_k} \right] \right. \\ & + \sum_{i,j,k,l=1}^n \Sigma_{K_{ijkl}} \left[\frac{1}{3!} \frac{\partial^3 \lambda}{\partial x_i \partial x_j \partial x_k} \frac{\partial \lambda^T}{\partial x_l} \right. \\ & \left. + \frac{1}{3!} \frac{\partial \lambda}{\partial x_i} \frac{\partial^3 \lambda^T}{\partial x_j \partial x_k \partial x_l} + \frac{1}{4} \frac{\partial^2 \lambda}{\partial x_i \partial x_j} \frac{\partial^2 \lambda^T}{\partial x_k \partial x_l} \right] \\ & \left. + \left[\sum_{i,j=1}^n \frac{P_{ij}}{2} \frac{\partial^2 \lambda}{\partial x_i \partial x_j} \right] \left[\dots \right]^T \right\}_{x=\bar{x}} + \dots \end{aligned} \quad (77)$$

where we have also used the notation $XX^T = X[\dots]^T$. We see that, for an independent random vector, the approximated covariance matrix of (77) correctly matches the true covariance matrix of (69) up to the third order, and only partial accuracy is achieved for the fourth order.

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