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Reach-Set Estimation for DAE Systems under Uncertainty and Disturbances Using Trajectory Sensitivity and Logarithmic Norm

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Abstract: Trajectory sensitivity analysis is useful for analyzing the dynamic behaviour of differential-algebraic equation (DAE) systems under uncertain initial conditions and/or parameters. However, the approximate trajectories obtained using trajectory sensitivities are not accompanied by explicit error bounds. In this paper, we provide an efficient method to obtain a numerical error bound for the first-order trajectory approximation. This approach uses second-order trajectory sensitivities. A theoretical result quantifying the excursion of trajectories induced by uncertain initial conditions and external disturbances is derived based on the logarithmic norm, and is extended to DAE systems. Although this result itself provides a guaranteed over-approximation of the reach-set of nonlinear DAE systems, by combining this result with the efficient bound obtained from trajectory sensitivities, we are able to provide a much less conservative reach-set estimate for systems under uncertain initial conditions and/or parameters, and external disturbances.

Keywords: Nonlinear systems, Reachability, Trajectory sensitivity, Bounded disturbances, Error estimation, Electric power systems.

1. INTRODUCTION

The concept of reach-set refers to the union of all possible states that can be visited by system trajectories originating from a set of uncertain initial conditions, under the influence of admissible parameter uncertainties and external disturbances. Given the reach-set, safety specifications can be checked by verifying there is no intersection of the reach-set and any unsafe region. This is important for safety-critical applications such as power systems (Kundu et al., 2019). However, in general it is hard to compute the exact reach-set for a nonlinear system.

Much research has been devoted to computing over-approximations of the reach-set. A Taylor flowpipe model is used in Chen et al. (2012) to over-approximate the reach-set of hybrid systems for a set of initial conditions. Other approaches to reach-set computation include abstraction-based methods (Henzinger et al., 1998), level-set methods (Mitchell et al., 2005), and differential inequalities (Scott and Barton, 2013). Reachability analysis of nonlinear differential-algebraic systems is studied in Althoff and Krogh (2013) using a conservative linearization method, where zonotopes are used to represent the reach-set. A common issue across all these methods is conservativeness, which is partially because of the accumulation of error over time, i.e., the wrapping effect. Computational burden is another issue when considering high-dimensional applications.

This paper explores reach-set approximation in the context of trajectory sensitivity analysis. Trajectory sensitivities can be used to approximate perturbed trajectories associated with uncertain initial conditions and/or parameter sets, thus avoiding repeated simulations (Hiskens and Pai, 2000; Geng and Hiskens, 2019, 2018). It is shown in Xue et al. (2017) that with sign-stable sensitivity matrices, only a small subset of the boundary of the initial set is required to be evaluated. However, sign-stability is a strong requirement. Meyer et al. (2018) provide an extension that only requires bounded sensitivity. However, the bound itself needs to be estimated through sampling and falsification. In Donzé and Maler (2007), sensitivity analysis has been used for verification through simulation of continuous and hybrid systems. However, there is no guarantee that the computed approximation is an enclosure of the true reach-set, since there is no explicit theoretical guarantee for the accuracy of such approximations. The same applies for Choi et al. (2017), where a semidefinite program is solved to search for the outermost trajectories.

In this paper, we analytically quantify the error inherent in trajectory approximation using the second-order trajectory sensitivity (Geng and Hiskens, 2019). We exploit results on multivariate Taylor's theorem and higher-order remainders to give a theoretical error bound for the first-order trajectory approximation. Sampled-data approaches (Meyer et al., 2018) can be used to estimate the bound. To ease computational effort, we also provide practical solutions for computing an error bound estimate. With an explicit numerical error bound available, we can provide a sufficiently accurate estimation of the reach-set by locating worst-case vertices of the uncertainty set (Hiskens and Alseddiqui, 2006).

The effect of external disturbances on differential-algebraic equation (DAE) systems is also investigated in this paper. We first extend to DAE systems a Lipschitz-based result from nonlinear systems theory that quantifies the effects of initial conditions and bounded external disturbances. Then we improve the result by exploiting properties of the logarithmic norm. The logarithmic norm, or matrix measure, is a useful tool for quantifying bounds on the divergence of adjacent trajectories, hence is useful for providing error bounds on linear approximation of nonlinear systems (Dahlquist, 1958), and for analyzing contractive systems (Sontag, 2010). In Maidens and Arcak (2014), the logarithmic norm has been used to compute over-approximation of the reach-set for switched nonlinear systems with uncertain initial conditions. In this paper, we also quantify the effects of external disturbances on system dynamics.

The contributions of this paper are as follows. Firstly, we provide an explicit theoretical error bound for trajectory sensitivity analysis, using second-order trajectory sensitivities. This theoretical bound is then estimated using efficient trajectory-based approach. Secondly, a theoretical result on quantifying the effects of external disturbances on nonlinear DAE systems is derived, using the mathematical tool of logarithmic norm. Thirdly, we provide an efficient approach to compute an accurate estimation of the reach-set of nonlinear DAE systems, under uncertain initial conditions and/or parameters, and external disturbances. This is achieved by combining the results on error bound for trajectory sensitivity analysis and the results on bounding the effects of external disturbances.

This paper is organized as follows: Section 2 presents system model and provides an overview of trajectory sensitivity analysis and logarithmic norm. The error bounds for trajectory approximation are derived in Section 3. Section 4 establishes theoretical results on quantifying the propagation of external disturbances. Reach-set computation with Minkowski sum formulation is described in Section 5. Simulation results are given in Section 6 and conclusions are drawn in Section 7.

2. PRELIMINARIES

In this paper, we adopt a DAE model to describe the dynamic behavior of the system,

$$\dot{x}(t) = f(x(t), y(t)) + w(t), \tag{1a}$$
$$0 = g(x(t), y(t)), \tag{1b}$$

where $x(t) \in \mathcal{D}_x \subset \mathbb{R}^n$ are the dynamic states at time t, $y(t) \in \mathcal{D}_y \subset \mathbb{R}^m$ are the algebraic states at time t, $f : \mathcal{D}_x \times \mathcal{D}_y \to \mathbb{R}^n$ is the vector field, and $g : \mathcal{D}_x \times \mathcal{D}_y \to \mathbb{R}^m$ describes the algebraic manifold. Nonlinear functions f and g are assumed to be Lipschitz in their arguments and of class $\mathcal{C}^2$. A bounded time-varying unknown external disturbance $w(t)$ is added to the differential equation. This disturbance term will not be considered until Section 4. Several technical assumptions are required for subsequent analysis:

Assumption 1. The solution of (1) exists for initial conditions and disturbances of interest, and is unique.

Assumption 2. The Jacobian $\partial g/\partial y$ is nonsingular along system trajectories.

For given initial conditions $x(t_0) = x_0$, $y(t_0) = y_0$, where $g(x_0, y_0) = 0$, the corresponding system trajectory (or flow) can be expressed as,

$$x(t) = \phi(x_0, t), \tag{2a}$$
$$y(t) = \psi(x_0, t). \tag{2b}$$

Uncertainty in initial conditions x_0 will be considered, with y_0 implicitly dependent upon x_0. To take into account uncertain parameters λ, the dynamic states x can be augmented with λ and trivial differential equations $\dot{\lambda} = 0$ added. This way, uncertain parameters are incorporated into the expanded initial conditions x_0.

2.1 Trajectory Sensitivity and Trajectory Approximation

Trajectory sensitivities describe the change in the system flow resulting from a change in initial conditions x_0. Forming the Taylor series expansion of the flow (2) with respect to x_0 along the nominal trajectory yields,

$$\phi_i(x_0 + \Delta x_0, t) = \phi_i(x_0, t) + \frac{\partial \phi_i(x_0, t)}{\partial x_0}\Delta x_0 + \frac{1}{2}\Delta x_0^\intercal \frac{\partial^2 \phi_i(x_0, t)}{\partial x_0^2}\Delta x_0 + \varepsilon_2^{\phi_i}(x_0, \Delta x_0, t), \tag{3a}$$

$$\psi_j(x_0 + \Delta x_0, t) = \psi_j(x_0, t) + \frac{\partial \psi_j(x_0, t)}{\partial x_0}\Delta x_0 + \frac{1}{2}\Delta x_0^\intercal \frac{\partial^2 \psi_j(x_0, t)}{\partial x_0^2}\Delta x_0 + \varepsilon_2^{\psi_j}(x_0, \Delta x_0, t), \tag{3b}$$

$$\forall i = 1, ...n, \ \forall j = 1, ...m,$$

where the terms $\frac{\partial \phi_i(x_0,t)}{\partial x_0} \in \mathbb{R}^{1\times n}$ and $\frac{\partial \psi_j(x_0,t)}{\partial x_0} \in \mathbb{R}^{1\times n}$ are first-order trajectory sensitivities and $\frac{\partial^2 \phi_i(x_0,t)}{\partial x_0^2} \in \mathbb{R}^{n\times n}$ and $\frac{\partial^2 \psi_j(x_0,t)}{\partial x_0^2} \in \mathbb{R}^{n\times n}$ are second-order trajectory sensitivities. The terms $\varepsilon_2^{\phi_i}(x_0, \Delta x_0, t)$ and $\varepsilon_2^{\psi_j}(x_0, \Delta x_0, t)$ capture the higher-order terms beyond the second.

The DAE variational equations describing first- and second-order trajectory sensitivities are given in Hiskens and Pai (2000) and Geng and Hiskens (2019), respectively. Due to the space limit, we only summarize the DAE model for the first-order trajectory sensitivity. Taking the derivatives of (1) with respect to x_0 yields,

$$\dot{x}_{x_0} = f_x(t)x_{x_0} + f_y(t)y_{x_0}, \tag{4a}$$
$$0 = g_x(t)x_{x_0} + g_y(t)y_{x_0}, \tag{4b}$$

where x_{x_0} and y_{x_0} denote the first-order trajectory sensitivities. We use f_x, f_y, g_x, g_y to denote $\partial f/\partial x$, $\partial f/\partial y$, $\partial g/\partial x$, $\partial g/\partial y$ respectively, which are time-varying matrices evaluated along the nominal trajectory. Initial conditions are given by $x_{x_0}(t_0) = I$, the identity matrix, and $y_{x_0}(t_0) = -(g_y(t_0))^{-1}g_x(t_0)$.

From (3), we have the first-order approximation,

$$\hat{\phi}(x_0 + \Delta x_0, t) = \phi(x_0, t) + \frac{\partial \phi(x_0, t)}{\partial x_0}\Delta x_0, \tag{5a}$$

$$\hat{\psi}(x_0 + \Delta x_0, t) = \psi(x_0, t) + \frac{\partial \psi(x_0, t)}{\partial x_0}\Delta x_0. \tag{5b}$$

Since higher-order terms are neglected, there are discrepancies between the approximated trajectory (5) and the true perturbed trajectory (3). Define the error in the first-order approximation by,

$$\varepsilon_1^{\phi}(x_0, \Delta x_0, t) \triangleq \phi(x_0 + \Delta x_0, t) - \hat{\phi}(x_0 + \Delta x_0, t), \tag{6a}$$
$$\varepsilon_1^{\psi}(x_0, \Delta x_0, t) \triangleq \psi(x_0 + \Delta x_0, t) - \hat{\psi}(x_0 + \Delta x_0, t). \tag{6b}$$

From classic perturbation theory (Khalil, 2002), we know that the first-order approximation errors are of order $\mathcal{O}(\|\Delta x_0\|^2)$. That is, there exists positive constants k^{ϕ}, k^{ψ} and c, such that $\|\varepsilon_1^{\phi}(x_0, \Delta x_0, t)\| \leq k^{\phi} \ \|\Delta x_0\|^2$ and $\|\varepsilon_1^{\psi}(x_0, \Delta x_0, t)\| \leq k^{\psi} \ \|\Delta x_0\|^2$, for all $\|\Delta x_0\| < c$. However, the magnitudes of k^{ϕ} and k^{ψ} are not known. Therefore, the big-$\mathcal{O}$ notation cannot be translated into a useful numerical error bound. This problem is investigated further in Section 3.

2.2 Logarithmic Norm

For any vector norm $\|\cdot\|$ on $\mathbb{R}^n$, and its induced matrix norm $\|\cdot\|$ on $\mathbb{R}^{n\times n}$, the logarithmic norm of a matrix

$A \in \mathbb{R}^{n\times n}$ is a real-valued functional $\mu : \mathbb{R}^{n\times n} \to \mathbb{R}$, defined by (Dahlquist, 1958),

$$\mu(A) = \lim_{s\to 0^+} \frac{\|I + sA\| - 1}{s}. \quad (7)$$

Explicit expressions exist for common vector norms such as the l_1, l_2 and l_∞-norms (Afanasiev et al., 2013). The logarithmic norm has a number of important properties (Maidens and Arcak, 2014),

(1) For any eigenvalue $\lambda_i(A)$ of A, we know, $-\|A\| \le -\mu(-A) \le \Re(\lambda_i(A)) \le \mu(A) \le \|A\|$.
(2) $\mu(cA) = c\mu(A), \forall c \ge 0$.
(3) $\mu(A + B) \le \mu(A) + \mu(B)$.

Fundamental results that connect the logarithmic norm to dynamical systems are summarized in Söderlind (2006) for linear systems and Sontag (2010) for nonlinear systems.

3. ERROR BOUND FOR TRAJECTORY APPROXIMATION

We are interested in deriving an explicit numerical bound for the error in the first-order trajectory approximation. Such an error bound provides theoretical guarantees for the accuracy of trajectory approximations and justifies their application to safety-critical scenarios such as dynamic security assessment (Kerin et al., 2014). In this section, we exploit multivariate Taylor's theorem and Lagrange's remainder, and derive an error bound for trajectory approximation by formulating an optimization problem. To ease the computational effort of solving the global optimization, we then propose an efficient approach to practically estimating the error bound.

3.1 Multivariate Taylor's Theorem and Remainder

Multi-index notation (Folland, 2005) is adopted to simplify the presentation of the following results.

Theorem 3. (Lee, 2012) Suppose $f : \mathbb{R}^n \to \mathbb{R}$ is of class $\mathcal{C}^{\kappa+1}$ on an open convex set $\mathcal{S}$. If $\boldsymbol{a} \in \mathcal{S}$ and $\boldsymbol{a} + \boldsymbol{h} \in \mathcal{S}$ then,

$$f(\boldsymbol{a} + \boldsymbol{h}) = \sum_{|\alpha|\le\kappa} \partial^\alpha f(\boldsymbol{a}) \frac{\boldsymbol{h}^\alpha}{\alpha!} + R_\kappa(\boldsymbol{a}, \boldsymbol{h}), \quad (8)$$

where the remainder is given in Lagrange's form by,

$$R_\kappa(\boldsymbol{a}, \boldsymbol{h}) = \sum_{|\alpha|=\kappa+1} \partial^\alpha f(\boldsymbol{a}+c\boldsymbol{h}) \frac{\boldsymbol{h}^\alpha}{\alpha!}, \text{ for some } c \in (0, 1). \quad (9)$$

Based on (9), an estimate for the remainder term is given by the following corollary.

Corollary 4. If f is of class $\mathcal{C}^{\kappa+1}$ on $\mathcal{S}$ and $|\partial^\alpha f(\boldsymbol{x})| \le M$ for $\boldsymbol{x} \in \mathcal{S}$ and $|\alpha| = \kappa + 1$, then

$$|R_\kappa(\boldsymbol{a}, \boldsymbol{h})| \le \frac{M}{(\kappa + 1)!} \|\boldsymbol{h}\|_1^{\kappa+1}, \quad (10)$$

where $\|\boldsymbol{h}\|_1 = |h_1| + |h_2| + ... + |h_n|$.

3.2 Error Bound by Second-Order Trajectory Sensitivity

Assigning time t to be any fixed time instant τ in (3), we obtain a regular Taylor expansion of $\phi_i(\tilde{x}_0, \tau)$ and $\psi_j(\tilde{x}_0, \tau)$, where $x_0 - \Delta x_0 \le \tilde{x}_0 \le x_0 + \Delta x_0$ with the vector inequality interpreted element-wise. Truncating all higher-order terms and applying Taylor's Inequality (10) gives remainders of the first-order approximations bounded as,

$$|R_1^{\phi_i}(x_0, \Delta x_0, \tau)| \le \frac{M^{\phi_i}(x_0, \Delta x_0, \tau)}{2} \|\Delta x_0\|_1^2, \quad (11a)$$

$$|R_1^{\psi_j}(x_0, \Delta x_0, \tau)| \le \frac{M^{\psi_j}(x_0, \Delta x_0, \tau)}{2} \|\Delta x_0\|_1^2, \quad (11b)$$

$\forall i = 1, \dots, n$ and $\forall j = 1, \dots, m$, where,

$$M^{\phi_i}(x_0, \Delta x_0, \tau) \ge \max_{\substack{x_0-\Delta x_0\le\tilde{x}_0\le x_0+\Delta x_0 \\ 1\le k\le l\le n}} \left| \left\{ \frac{\partial^2 \phi_i(\tilde{x}_0, \tau)}{\partial x_0^2} \right\}_{k,l} \right| \quad (12a)$$

$$M^{\psi_j}(x_0, \Delta x_0, \tau) \ge \max_{\substack{x_0-\Delta x_0\le\tilde{x}_0\le x_0+\Delta x_0 \\ 1\le k\le l\le n}} \left| \left\{ \frac{\partial^2 \psi_j(\tilde{x}_0, \tau)}{\partial x_0^2} \right\}_{k,l} \right| \quad (12b)$$

where the scalars k, l are indices for the entries of the symmetric second-order trajectory sensitivity matrices $\frac{\partial^2 \phi_i(\tilde{x}_0,\tau)}{\partial x_0^2}$, $\frac{\partial^2 \psi_j(\tilde{x}_0,\tau)}{\partial x_0^2}$ whose expressions are given in Geng and Hiskens (2019).

Allowing τ to vary is equivalent to replacing τ with t in (11) and (12). Also, larger Δx_0 implies larger $M^{\phi_i}(x_0, \Delta x_0, t)$ and $M^{\psi_j}(x_0, \Delta x_0, t)$, since the maximum is taken over a larger set.

3.3 Optimization Problem for the Error Bound

The question of finding a numerical error bound for the first-order trajectory approximation (relative to the true perturbed trajectory), or equivalently of quantifying the higher-order remainder of the first-order approximation, reduces to finding the entry-wise maximum absolute value for second-order trajectory sensitivities (at each time instant) corresponding to all possible trajectories originating from the initial condition set $\mathcal{X}_0 := \{\tilde{x}_0 \in \mathbb{R}^n | x_0 - \Delta x_0 \le \tilde{x}_0 \le x_0 + \Delta x_0\}$. This problem can be written explicitly as the following optimization,

$$(\mathcal{P}1) \quad M^{\phi_i}(t) = \max_{\substack{\tilde{x}_0\in\mathcal{X}_0 \\ 1\le k\le l\le n}} \left| \left\{ \frac{\partial^2 \phi_i(\tilde{x}_0, t)}{\partial x_0^2} \right\}_{k,l} \right|$$

$$M^{\psi_j}(t) = \max_{\substack{\tilde{x}_0\in\mathcal{X}_0 \\ 1\le k\le l\le n}} \left| \left\{ \frac{\partial^2 \psi_j(\tilde{x}_0, t)}{\partial x_0^2} \right\}_{k,l} \right|$$

$$\forall i = 1, \dots, n, \ \forall j = 1, \dots, m.$$

Although this establishes a theoretical form for the error bound, the global optimal solution to $(\mathcal{P}1)$ is hard to obtain. Firstly, the second-order trajectory sensitivity information is obtained by numerically integrating a DAE model, as given in Geng and Hiskens (2019). Hence, no analytical form of the function is available. Secondly, at each time instant t, for each of the n dynamic states and each of the m algebraic states, we need to solve $n(n + 1)/2$ global optimization problems. Such computational difficulty is to be expected, since in general it is hard to quantify the error resulting from a linear approximation of its nonlinear counterpart. Existing methods in Yu et al. (2013) and the recent development of Li et al. (2019) for formally solving this problem involve enforcing global conditions on a Lipschitz constant of the vector field or on the logarithmic norm of the Jacobian matrix, and finding the global maximum of a non-convex optimization problem. The resulting error bounds from such methods also tend to be overly conservative.

To solve the non-convex problem $(\mathcal{P}1)$, we can use sampling-falsification methods such as described in Meyer et al. (2018). Firstly, we can select a few samples in the space of initial conditions, and evaluate their second-order trajectory sensitivities, resulting in an initial estimate for the bound. Secondly, the previously estimated bounds are iteratively enlarged by searching for other initial conditions to falsify the prior bounds. However, numerical test cases show that computing only the nominal trajectory together with the trajectories for the extreme vertices (which can be viewed as the coarsest grid for the uncertain set $\mathcal{X}_0$) suffices to provide an accurate estimate for the error bound. In practice, if k out of n states have uncertain initial conditions, we can simply evaluate 2^k+1 trajectories (2^k vertex cases and one nominal case) and find the maximum second-order trajectory sensitivities at each time instant. This serves as an efficiently estimated error bound for the first-order trajectory approximation. Following this idea, the optimization program $(\mathcal{P}1)$ is reduced to the tractable problem,

$$(\mathcal{P}2) \quad \hat{M}^{\phi_i}(t) = \max_{\substack{\tilde{x}_0 \in (\mathrm{Vert}(\mathcal{X}_0) \cup x_0) \\ 1 \le k \le l \le n}} \left| \left\{ \frac{\partial^2 \phi_i(\tilde{x}_0, t)}{\partial x_0^2} \right\}_{k,l} \right|$$

$$\hat{M}^{\psi_j}(t) = \max_{\substack{\tilde{x}_0 \in (\mathrm{Vert}(\mathcal{X}_0) \cup x_0) \\ 1 \le k \le l \le n}} \left| \left\{ \frac{\partial^2 \psi_j(\tilde{x}_0, t)}{\partial x_0^2} \right\}_{k,l} \right|$$
$$\forall i = 1, ...n, \ \forall j = 1, ...m,$$

where the notation $\mathrm{Vert}(\mathcal{X}_0)$ denotes the operation of extracting the finite set of vertices of the polytope $\mathcal{X}_0$.

4. QUANTIFY EXTERNAL DISTURBANCES

We wish to quantify the flow excursion caused by a bounded time-varying disturbance, relative to the noise-free nominal trajectory. A well-known result for ordinary differential equation (ODE) systems is based on knowledge of the Lipschitz constant of the vector field, see for example, Theorem 3.4 in Khalil (2002). We first generalize this result to DAE systems and then establish an improved result based on the logarithmic norm.

Referring to (1), by the Implicit Function Theorem (IFT) and Assumption 2, there exists (locally) a unique function φ such that $y = \varphi(x)$. Furthermore, we make the following assumption.

Assumption 5. There exists a function $\varphi : \mathcal{D}_x \to \mathcal{D}_y$, where $\mathcal{D}_x \subset \mathbb{R}^n$ and $\mathcal{D}_y \subset \mathbb{R}^m$, such that $g(x, \varphi(x)) = 0$, and φ is Lipschitz with constant L_φ.

The existence of such a "global" implicit function holds under various conditions (Krantz and Parks, 2012; Rheinboldt, 1969), for example, if $\mathcal{D}_x$ is simply connected together with some technical conditions as discussed in Theorem 4.2 of Rheinboldt (1969). Inserting this implicit function into (1a) yields $\dot{x} = f(x, y) = f(x, \varphi(x)) \triangleq h(x)$.

We derive the following Corollary for DAE systems.

Corollary 6. Let $f(x, y)$ be Lipschitz in x and y on $\mathcal{D}_x \times \mathcal{D}_y$ with Lipschitz constants L_x and L_y, where $\mathcal{D}_x \times \mathcal{D}_y \subset \mathbb{R}^n \times \mathbb{R}^m$ is an open connected set. Let $(x(t), y^x(t))$ be the solution of $\dot{x} = f(x, y),\ 0 = g(x, y),\ x(t_0) = x_0$, and $(z(t), y^z(t))$ be the solution of $\dot{z} = f(z, y) + w(t),\ 0 = g(z, y),\ z(t_0) = z_0$, such that $(x(t),\ y^x(t)) \in \mathcal{D}_x \times \mathcal{D}_y$, $(z(t),\ y^z(t)) \in \mathcal{D}_x \times \mathcal{D}_y$ for all $t \in [t_0, t_1]$. Suppose that $\|w(t)\| \le \mathrm{w}$, $\forall t \in [t_0, t_1]$ for some $\mathrm{w} > 0$. Based on Assumption 5, we further assume that $y^x = \varphi(x)$, and $y^z = \varphi(z)$. Let $L_h = L_x + L_y L_\varphi$, where L_φ is the Lipschitz constant of the implicit function φ. Then, $\|x(t) - z(t)\| \le \|x_0 - z_0\| \exp[L_h(t - t_0)] + \frac{\mathrm{w}}{L_h}\big(\exp[L_h(t - t_0)] - 1\big)$ and $\|y^x(t) - y^z(t)\| \le L_\varphi \|x_0 - z_0\| \exp[L_h(t - t_0)] + L_\varphi \frac{\mathrm{w}}{L_h}\big(\exp[L_h(t - t_0)] - 1\big)$.

Proof. Using the implicit function φ in the differential equations gives $\dot{x} = f(x, y) = f(x, \varphi(x)) \triangleq h(x)$, $\dot{z} = f(z, y) + w(t) = f(z, \varphi(z)) + w(t) \triangleq h(z) + w(t)$. Since the implicit function φ and the vector field $f(\cdot, \cdot)$ are Lipschitz, the composite function h is also Lipschitz. For any two points $x_1,\ x_2 \in \mathcal{D}_x$,

$$\begin{aligned}
&\frac{h(x_1) - h(x_2)}{x_1 - x_2} = \frac{f(x_1, \varphi(x_1)) - f(x_2, \varphi(x_2))}{x_1 - x_2} \\
&= \frac{\big(f(x_1, \varphi(x_1)) - f(x_2, \varphi(x_1))\big) + \big(f(x_2, \varphi(x_1)) - f(x_2, \varphi(x_2))\big)}{x_1 - x_2} \\
&\le L_x + \frac{f(x_2, \varphi(x_1)) - f(x_2, \varphi(x_2))}{\varphi(x_1) - \varphi(x_2)} \cdot \frac{\varphi(x_1) - \varphi(x_2)}{x_1 - x_2} \\
&\le L_x + L_y L_\varphi.
\end{aligned} \tag{13}$$

Therefore, the Lipschitz constant L_h for the composite function h is upper bounded by $L_x + L_y L_\varphi$. Apply Theorem 3.4 in Khalil (2002) and the results follow. Furthermore, we have $\|y^x(t) - y^z(t)\| = \|\varphi(x(t)) - \varphi(z(t))\| \le L_\varphi \|x(t) - z(t)\|$. □

Next, we improve Theorem 3.4 in Khalil (2002) and Corollary 6 by deriving a tighter bound, using the logarithmic norm instead of Lipschitz constants. Property 1 in Section 2.2 indicates that the logarithmic norm of the Jacobian matrix is guaranteed to be upper-bounded by the Lipschitz constant of the vector field. Consequently, we obtain the following improved result.

Theorem 7. Let the Jacobian matrix f_x satisfy $\mu(f_x(x)) \le c$, $\forall x \in \mathcal{D}$, where $\mathcal{D} \subset \mathbb{R}^n$ is an open convex set. Let $x(t)$ be the solution of $\dot{x} = f(x),\ x(t_0) = x_0$, and $z(t)$ be the solution of $\dot{z} = f(z) + w(t),\ z(t_0) = z_0$, such that $x(t),\ z(t) \in \mathcal{D}$ for all $t \in [t_0, t_1]$. Suppose that $\|w(t)\| \le \mathrm{w}$, $\forall t \in [t_0, t_1]$ for some $\mathrm{w} > 0$. Then, $\|x(t) - z(t)\| \le \|x_0 - z_0\| \exp[c(t - t_0)] + \frac{\mathrm{w}}{c}\big(\exp[c(t - t_0)] - 1\big)$.

Proof. Based on the fundamental theorem of calculus,

$$\begin{aligned}
\dot{x} - \dot{z} &= f(x) - f(z) - w(t) \\
&= \int_0^1 f_x(z + s(x - z))(x - z)ds - w(t) \\
&= \int_0^1 f_x(z + s(x - z))ds \cdot (x - z) - w(t).
\end{aligned} \tag{14}$$

Let $x - z = e$ so that $\dot{e} = \int_0^1 f_x(z + se)ds \cdot e - w(t)$. By convexity of $\mathcal{D}$ and $s \in [0, 1]$, we have $(z + s(x - z)) \in \mathcal{D}, \forall t \in [t_0, t_1]$. Since $\mu(f_x(x)) \le c$, $\forall x \in \mathcal{D}$, apply Proposition 1 of Li et al. (2019) and the subadditivity property of the logarithmic norm to give $D_t^+ \|e\| \le c\|e\| + \|w\| \le c\|e\| + \mathrm{w}$. The notation D_t^+ is the upper right-hand Dini derivative with respect to time t. Based on Duhamel's formula and comparison lemma, we obtain,

$$\begin{aligned}
\|e(t)\| &\le \|e(t_0)\| \exp[c(t - t_0)] + \int_{t_0}^t \exp[c(t - \tau)] \cdot \mathrm{w} d\tau \\
&= \|e(t_0)\| \exp[c(t - t_0)] + \frac{\mathrm{w}}{c}\big(\exp[c(t - t_0)] - 1\big),
\end{aligned} \tag{15}$$

where $e(t_0) = x_0 - z_0$. □

Theorem 7 can be generalized to DAE systems.

Corollary 8. Let the Jacobian matrix $\frac{\partial h}{\partial x}(x, y) = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial x}$ satisfy $\mu(\frac{\partial h}{\partial x}(x, y)) \le c_h$, $\forall (x, y) \in \mathcal{D}_x \times \mathcal{D}_y$, where $\mathcal{D}_x \times \mathcal{D}_y \subset \mathbb{R}^n \times \mathbb{R}^m$ is an open convex set. Let $(x(t), y^x(t))$ be the solution of $\dot{x} = f(x, y),\ 0 = g(x, y),\ x(t_0) = x_0$, and $(z(t), y^z(t))$ be the solution of $\dot{z} = f(z, y) + w(t),\ 0 = g(z, y),\ z(t_0) = z_0$, such that $(x(t),\ y^x(t)) \in \mathcal{D}_x \times \mathcal{D}_y$,

$(z(t),\ y^z(y)) \in \mathcal{D}_x \times \mathcal{D}_y$ for all $t \in [t_0, t_1]$. Suppose that $\|w(t)\| \leq \mathrm{w}$, $\forall(t) \in [t_0, t_1]$ for some $\mathrm{w} > 0$. Based on Assumption 5, we further assume that $y^x = \varphi(x)$, and $y^z = \varphi(z)$. Let $L_h = L_x + L_y L_\varphi$, where L_φ is the Lipschitz constant of the implicit function φ. Then, $\|x(t) - z(t)\| \leq \|x_0 - z_0\| \exp[c_h(t - t_0)] + \frac{\mathrm{w}}{c_h}\big(\exp[c_h(t - t_0)] - 1\big)$ and $\|y^x(t) - y^z(t)\| \leq L_\varphi \|x_0 - z_0\| \exp[c_h(t - t_0)] + L_\varphi \frac{\mathrm{w}}{c_h}\big(\exp[c_h(t - t_0)] - 1\big)$.

Proof. Use similar techniques as in the proof for Corollary 6 and Theorem 7. □

Note that in using these results, we require the global information L_x, L_y, L_φ (Corollary 6), c (Theorem 7), and c_h(Corollary 8). Furthermore, the terms L_φ and c_h require special treatment because they involve the implicit function φ. Differentiating the algebraic equation (1b) with respect to x yields $\frac{\partial g}{\partial x} + \frac{\partial g}{\partial y}\frac{\partial y}{\partial x} = 0$, which gives,

$$\frac{\partial y}{\partial x} = -\Big(\frac{\partial g}{\partial y}\Big)^{-1}\frac{\partial g}{\partial x}. \tag{16}$$

For implementation, these terms can be computed off-line and stored for later use. However, global optimizations need to be solved. For example, computing c_h requires solving the non-convex problem,

$$(\mathcal{P}3) \quad c_h = \max_{(x,y)\in\mathcal{D}_x\times\mathcal{D}_y} \ \mu\Big(\frac{\partial h}{\partial x}(x, y)\Big).$$

We can either resort to global optimization solvers or estimate the value by sample-based methods.

5. REACH-SET COMPUTATION

Designing tractable algorithms for computing reach-sets for nonlinear systems is a challenging problem. In this section, we use results from Sections 3 and 4 to propose an efficient method for computing a sufficiently accurate reach-set estimate for nonlinear DAE systems with uncertain initial conditions and external disturbances.

5.1 Reach-Set With Uncertain Initial Conditions

The orthotope $\mathcal{X}_0 = \{\tilde{x}_0 \in \mathbb{R}^n | x_0 - \Delta x_0 \leq \tilde{x}_0 \leq x_0 + \Delta x_0\}$ of all possible initial conditions can be equivalently characterized as $\mathcal{X}_0 := x_0 \oplus \mathcal{B}$, where x_0 is the nominal initial point and $\mathcal{B} := \{\Delta\tilde{x}_0 \in R^n : -\Delta x_0 \leq \Delta\tilde{x}_0 \leq \Delta x_0\}$. In Hiskens and Alseddiqui (2006), it is shown that trajectory sensitivities can be used to approximate the reach-set efficiently, by locating worst-case vertices of the uncertainty set. Under the affine transformations (5), the orthotope $\mathcal{B}$ is shifted and distorted to form time-dependent parallelotopes:

$$\mathcal{P}^\phi(t) = \phi(x_0, t) + \frac{\partial\phi(x_0, t)}{\partial x_0}\mathcal{B}, \tag{17a}$$

$$\mathcal{P}^\psi(t) = \psi(x_0, t) + \frac{\partial\psi(x_0, t)}{\partial x_0}\mathcal{B}. \tag{17b}$$

Since the orthotope $\mathcal{B}$ is convex, the affine transformation (5) maintains its convexity. Moreover, the vertices of $\mathcal{B}$ are mapped to the vertices of $\mathcal{P}^\phi(t)$ and $\mathcal{P}^\psi(t)$, which define the approximated boundaries of the reach-set. However, there is no guarantee that such approximated boundaries will cover the true reach-set since the first-order trajectory approximations possess error. By taking advantage of the established error bounds, we can compute an over-approximation of the reach-set. In practice, the error bound is estimated from the simplified problem ($\mathcal{P}2$), which increases the confidence of covering the true reach-set.

It follows that we only need to bound approximation error for the extreme vertex cases of $\mathcal{P}^\phi(t)$, $\mathcal{P}^\psi(t)$. Define the time-dependent error bound tubes as,

$$\mathcal{E}^\phi(t) \triangleq \{\tilde{e}(t) \in \mathbb{R}^n \big| |\tilde{e}_i(t)| \leq \frac{M^{\phi_i}(t)}{2}\|\Delta x_0\|_1^2\}, \tag{18a}$$

$$\mathcal{E}^\psi(t) \triangleq \{\tilde{e}(t) \in \mathbb{R}^m \big| |\tilde{e}_j(t)| \leq \frac{M^{\psi_j}(t)}{2}\|\Delta x_0\|_1^2\}, \tag{18b}$$
$$\forall i = 1, \ldots, n,\ \forall j = 1, \ldots, m,$$

where Δx_0 denotes the maximum deviations from the nominal initial point x_0, i.e. the vertices of $\mathcal{X}_0$. Theoretically, the terms M^{ϕ_i} and M^{ψ_i} are computed from ($\mathcal{P}1$). In practice, we instead use the $\hat{M}^{\phi_i}$ and $\hat{M}^{\psi_i}$ from ($\mathcal{P}2$).

Consider uncertain initial conditions $\tilde{x}_0$ within the set $\mathcal{X}_0$, and define the reach-set of all perturbed trajectories $x(t) = \phi(\tilde{x}_0, t)$, $y(t) = \psi(\tilde{x}_0, t)$ originating from $\mathcal{X}_0$ to be,

$$\begin{bmatrix}\mathcal{X}(t)\\ \mathcal{Y}^x(t)\end{bmatrix} = \begin{bmatrix}\phi(\mathcal{X}_0, t)\\ \psi(\mathcal{X}_0, t)\end{bmatrix}$$
$$\triangleq \left\{\begin{matrix} x(t) \in \mathbb{R}^n \\ y(t) \in \mathbb{R}^m \end{matrix} \,\middle|\, \begin{matrix} \dot{x}(t) = f(x(t), y(t)) \\ 0 = g(x(t), y(t)),\ x(t_0) \in \mathcal{X}_0 \end{matrix}\right\}. \tag{19}$$

Based on the previous reasoning, we have the following over-approximation of the reach-set $\mathcal{X}(t)$, $\mathcal{Y}^x(t)$,

$$\mathcal{X}(t) \subset \mathcal{P}^\phi(t) \oplus \mathcal{E}^\phi(t), \tag{20a}$$

$$\mathcal{Y}^x(t) \subset \mathcal{P}^\psi(t) \oplus \mathcal{E}^\psi(t), \tag{20b}$$

where $\oplus$ denotes Minkowski sum. Since $\mathcal{P}^\phi(t)$, $\mathcal{P}^\psi(t)$, $\mathcal{E}^\phi(t)$, and $\mathcal{E}^\psi(t)$ are polytopes represented by vertices, their Minkowski sum can be converted to taking combinations of vertices and computing their convex hull, which is relatively tractable.

5.2 Reach-Set With External Disturbances

By using results from Section 4, we are also able to quantify the effects of external disturbances. By Corollary 8, we know that for every initial point $x_0 \in \mathcal{X}_0$, the trajectory $(x(t), y^x(t))$, $x(t_0) = x_0$ and $(z(t), y^z(t))$, $z(t_0) = x_0$ have the relationship,

$$\|x(t) - z(t)\| \leq \frac{\mathrm{w}}{c_h}\big(\exp[c_h(t - t_0)] - 1\big), \tag{21a}$$

$$\|y^x(t) - y^z(t)\| \leq L_\varphi\frac{\mathrm{w}}{c_h}\big(\exp[c_h(t - t_0)] - 1\big), \tag{21b}$$

which implies the trajectories $z(t)$, $y^z(t)$ must lie within the tubes of time-varying radius $\frac{\mathrm{w}}{c_h}\big(\exp[c_h(t - t_0)] - 1\big)$, $L_\varphi\frac{\mathrm{w}}{c_h}\big(\exp[c_h(t - t_0)] - 1\big)$ around the disturbance-free trajectories $x(t)$, $y^x(t)$, respectively. Define the tubes as:

$$\mathcal{T}^\phi(t) \triangleq \Big\{\tilde{\xi}(t) \in \mathbb{R}^n \Big| \big\|\tilde{\xi}(t)\big\| \leq \frac{\mathrm{w}}{c_h}\big(\exp[c_h(t - t_0)] - 1\big)\Big\}, \tag{22a}$$

$$\mathcal{T}^\psi(t) \triangleq \Big\{\tilde{\xi}(t) \in \mathbb{R}^m \Big| \big\|\tilde{\xi}(t)\big\| \leq L_\varphi\frac{\mathrm{w}}{c_h}\big(\exp[c_h(t - t_0)] - 1\big)\Big\}, \tag{22b}$$

where the vector norm is the same as the one used for defining the logarithmic norm.

Next consider all initial points in the set $\mathcal{X}_0$. In (19) we've defined the reach-set of all disturbance-free trajectories originating from $\mathcal{X}_0$ to be $\mathcal{X}(t)$, $\mathcal{Y}^x(t)$. Similarly, define $\mathcal{Z}(t)$, $\mathcal{Y}^z(t)$ to be the reach-set for system with disturbances,

$$\begin{bmatrix}\mathcal{Z}(t)\\ \mathcal{Y}^z(t)\end{bmatrix} \triangleq \left\{\begin{matrix} z(t) \in \mathbb{R}^n \\ y(t) \in \mathbb{R}^m \end{matrix} \middle| \begin{matrix} \dot{z}(t) = f(z(t), y(t)) + w(t) \\ 0 = g(z(t), y(t)),\ z(t_0) \in \mathcal{X}_0 \end{matrix}\right\}. \tag{23}$$

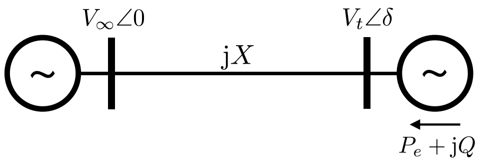

Fig. 1. Single machine infinite bus power system.

From (21), we know that the set of noisy trajectories $\mathcal{Z}(t)$, $\mathcal{Y}^z(t)$ is over-bounded by the Minkowski sum,

$$\mathcal{Z}(t) \subset \mathcal{X}(t) \oplus \mathcal{T}^\phi(t), \tag{24a}$$
$$\mathcal{Y}^z(t) \subset \mathcal{Y}^x(t) \oplus \mathcal{T}^\psi(t). \tag{24b}$$

Together with (20), we obtain the final expression for an estimated over-approximation of the reach-set,

$$\mathcal{Z}(t) \subset \mathcal{P}^\phi(t) \oplus \mathcal{E}^\phi(t) \oplus \mathcal{T}^\phi(t), \tag{25a}$$
$$\mathcal{Y}^z(t) \subset \mathcal{P}^\psi(t) \oplus \mathcal{E}^\psi(t) \oplus \mathcal{T}^\psi(t), \tag{25b}$$

where $\mathcal{P}^\phi(t)$, $\mathcal{P}^\psi(t)$ are defined in (17), $\mathcal{E}^\phi(t)$, $\mathcal{E}^\psi(t)$ are defined in (18), and $\mathcal{T}^\phi(t)$, $\mathcal{T}^\psi(t)$ are defined in (22).

6. SIMULATION RESULTS

We demonstrate the proposed reach-set computation approach through a single machine infinite bus (SMIB) power system, as shown in Fig. 1. The DAE model for the SMIB system is given by:

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{cases} x_2 \\ \dfrac{1}{M}\left(P_m - \dfrac{V_\infty V_t}{X}\sin(x_1) - Dx_2\right) + w(t) \end{cases} \tag{26a}$$

$$0 = \left(\frac{V_\infty V_t}{X}\sin(x_1)\right)^2 + \left(\frac{V_t^2}{X} - y\right)^2 - \frac{V_\infty^2 V_t^2}{X^2}. \tag{26b}$$

The dynamic states are $x = [x_1, x_2]^\intercal = [\delta, \omega]^\intercal$, where δ is the rotor angle and ω is the angular velocity. The algebraic state is $y = Q$, the reactive power generation. V_∞ is the constant voltage magnitude of the infinite bus, V_t is the voltage magnitude of the generator bus, M is the inertia constant, P_m is the mechanical power, X is the line reactance, and D is the damping. An unknown external disturbance term $w(t)$ is added to the second differential equation. It is modeled as a uniformly distributed random variable, with a bound of $\|w(t)\| \leq$ w $= 0.005$. The vector norm is defined as $\|\cdot\| = \sqrt{(\cdot)^\intercal P(\cdot)}$, where P solves the Lyapunov equation $A^\intercal P + PA + Q = 0$, where $Q = I$, and A is the Jacobian matrix evaluated at the stable equilibrium. With this vector norm, the logarithmic norm is defined accordingly as, $\mu(J) = \lambda_{max}\left(\frac{(P^{1/2}JP^{-1/2}) + (P^{1/2}JP^{-1/2})^\intercal}{2}\right)$, where λ_{max} represents the largest eigenvalue.

The system parameters are set to $V_\infty = 1$ pu, $V_t = 1$ pu, $M = 7.3784$ pu, $P_m = 3.1831$ pu, $X = 1/6$ pu, and $D = 1$ pu. For the nominal case, initial conditions are $x_0 = [0.55, 0.15]^\intercal$, giving $y_0 = 0.8849$. The implicit trapezoidal method was adopted to numerically integrate the DAE models describing the dynamics of states, the first- and second-order sensitivities. When including the stochastic disturbance, the trapezoidal integration method was modified as described in Hansen and Penland (2006) to approximate the integration of the stochastic differential equation. We assume that the initial condition for rotor angle δ is uncertain and lies within the range $[0.5, 0.6]$. The logarithmic norm is estimated off-line as $\mu(J(x,y)) \leq c_h = -0.0104$, over the operating range.

Figure 2 shows the reach-set when there are only initial condition uncertainties but no external disturbance. The red solid lines indicate the reach-set estimated using the trajectory sensitivity method. The blue dash-dot lines give the theoretical bound derived using the logarithmic norm. The green dashed lines are eleven true trajectories with their initial conditions uniformly distributed over the initial condition set. It can be observed that all trajectories are contained within the estimated and theoretical bounds. Moreover, the reach-set estimation given by the trajectory sensitivity method is much tighter than the theoretical bound, while still encompassing all the true trajectories.

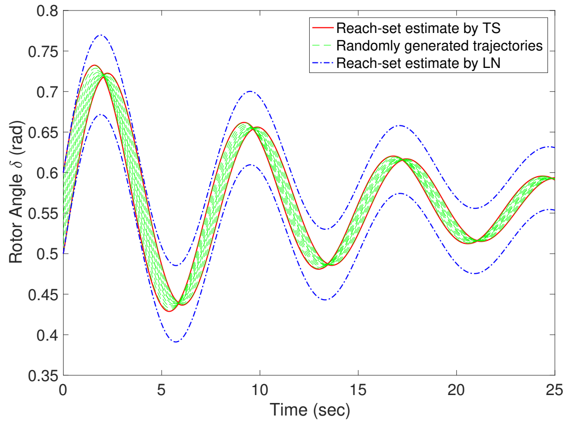

Fig. 2. Reach-set estimates based on the trajectory sensitivity and logarithmic norm methods for uncertain initial conditions.

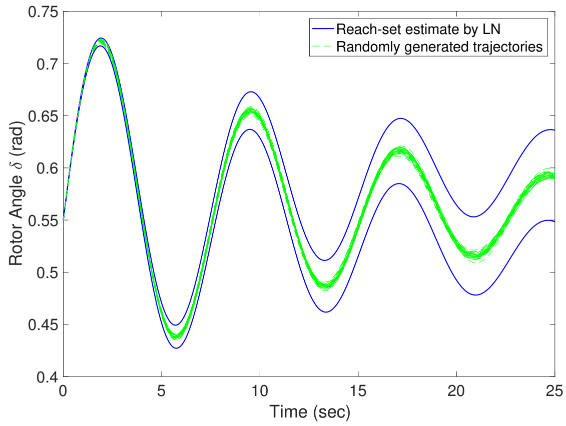

Fig. 3. Reach-set estimate based on the logarithmic norm method under external disturbances.

Figure 3 presents the case when there are only external disturbances but no initial condition uncertainty. The bound provided by the logarithmic norm is shown by blue lines. The green dashed lines are 30 randomly generated trajectories.

Finally, we consider the case when there are both uncertain initial conditions and external disturbances. The reach-set estimated by the trajectory sensitivity plus logarithmic norm (TS+LN) method and by the logarithmic norm only are presented in Fig. 4. The red solid lines refer to the bound given by the TS+LN method and the blue dash-dot lines refer to the bound given by the logarithmic norm. The green dashed lines are 55 randomly generated true trajectories emanating from the initial condition set and subjected to external disturbances. It can be observed that the reach-set estimation given by the TS+LN method is able to cover all realizations without being overly conservative, especially when the simulation horizon was quite short. The theoretical bound provided by the logarithmic

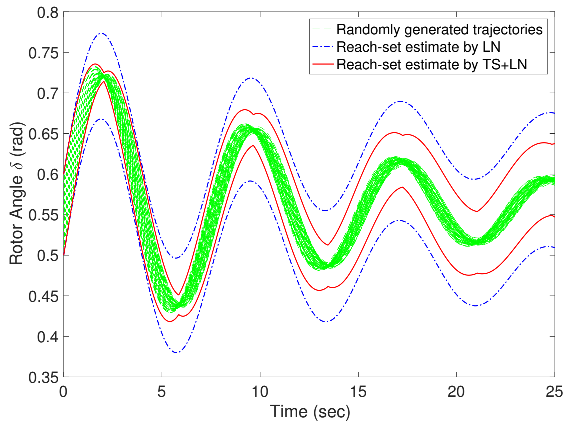

Fig. 4. Reach-set estimates based on the TS+LN and logarithmic norm methods for uncertain initial conditions and external disturbances.

norm is guaranteed to enclose all the realizations but is more conservative.

7. CONCLUSION

The paper has proposed an efficient approach to constructing a sufficiently accurate estimation of the reach-set of nonlinear DAE systems, under uncertain initial conditions and/or parameters, and external disturbances. This approach is based on establishing an error bound for the trajectory sensitivity method, as well as characterizing the effects of external disturbances using the logarithmic norm. Although the bound derived from the logarithmic norm is guaranteed to enclose the true reach-set, the trajectory sensitivity method provides a much less conservative reach-set estimation. For future work, we plan to extend the method to hybrid systems where continuous dynamics and discrete events interact.

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