Supplementary Material for the Manuscript "Probabilistic Model Validation for Uncertain Nonlinear Systems"

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PROOF FOR THEOREM 1

Statement 1: ${}_2W_2\left(f_b\left(x;\alpha,\beta\right), f_b\left(x;\beta,\alpha\right)\right) = \sqrt{\dfrac{\alpha\left(\alpha+1\right)+\beta\left(\beta+1\right)}{\left(\alpha+\beta\right)\left(\alpha+\beta+1\right)} - 2\left(\dfrac{\beta}{\alpha+\beta} - \mathcal{J}\right)}$,

$$\mathcal{J} := \frac{1}{\beta+1}\int_0^1 \left(I_t^{-1}\left(\alpha,\beta\right)\right)^{1-\alpha}\left(1-I_t^{-1}\left(\alpha,\beta\right)\right)^{1-\beta}\left(I_t^{-1}\left(\beta,\alpha\right)\right)^{\beta+1}\ {}_2F_1\left(\beta+1,1-\alpha;\beta+2;\right.$$
$$\left.I_t^{-1}\left(\beta,\alpha\right)\right)\,dt.$$

Proof: From eqn.(13) in the manuscript, we have

$${}_2W_2^2\left(f_b\left(x;\alpha,\beta\right), f_b\left(x;\beta,\alpha\right)\right) = \int_0^1 \left(I_t^{-1}\left(\alpha,\beta\right) - I_t^{-1}\left(\beta,\alpha\right)\right)^2\,dt$$
$$= \int_0^1 \left(I_t^{-1}\left(\alpha,\beta\right)\right)^2\,dt + \int_0^1 \left(I_t^{-1}\left(\beta,\alpha\right)\right)^2\,dt - 2\int_0^1 I_t^{-1}\left(\alpha,\beta\right) I_t^{-1}\left(\beta,\alpha\right)\,dt, \tag{1}$$

where $I_t^{-1}\left(\alpha,\beta\right)$ is the inverse of the beta CDF $I_x\left(\alpha,\beta\right) := \dfrac{B\left(x;\alpha,\beta\right)}{B\left(\alpha,\beta\right)}$, the regularized (incomplete) beta function. Here $B\left(x;\alpha,\beta\right) := \displaystyle\int_0^x z^{\alpha-1}\left(1-z\right)^{\beta-1}\,dz$ is the incomplete beta function. The following identities, stated without proof, will be useful for the evaluation of (1).

Property 1:

$$\int I_t^{-1}\left(a,b\right)\,dt = \frac{1}{\left(a+1\right)B\left(a,b\right)}\left(I_t^{-1}\left(a,b\right)\right)^{a+1}\ {}_2F_1\left(a+1,1-b;a+2;I_t^{-1}\left(a,b\right)\right) + \text{ constant.}$$

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Property 2:

$$\int \left(I_t^{-1}(a,b)\right)^2 \, dt = \frac{1}{(a+1)\,B(a,b)} \left(I_t^{-1}(a,b)\right)^{a+1} \left({}_2F_1\left(a+1, 1-b; a+2; I_t^{-1}(a,b)\right) - {}_2F_1\left(a+1, -b; a+2; I_t^{-1}(a,b)\right)\right) + \text{constant.}$$

Property 3: $I_0^{-1}(a,b) = 0$, and $I_1^{-1}(a,b) = 1$.

Property 4: (Gauss Theorem) ${}_2F_1(A, B; C; 1) = \dfrac{\Gamma(C)\,\Gamma(C-A-B)}{\Gamma(C-A)\,\Gamma(C-B)}$.

Property 5: $\dfrac{d}{dt} I_t^{-1}(a,b) = B(a,b)\left(I_t^{-1}(a,b)\right)^{1-a}\left(1 - I_t^{-1}(a,b)\right)^{1-b}$.

Using Properties 2 and 3, we get

$$\int_0^1 \left(I_t^{-1}(\alpha,\beta)\right)^2 \, dt = \frac{1}{(\alpha+1)\,B(\alpha,\beta)} \left[{}_2F_1(\alpha+1, 1-\beta; \alpha+2; 1) - {}_2F_1(\alpha+1, -\beta; \alpha+2; 1)\right]. \tag{2}$$

Recalling that $\Gamma(k+1) = k\Gamma(k)$, Property 4 results

$$ {}_2F_1(\alpha+1, 1-\beta; \alpha+2; 1) = \frac{\Gamma(\alpha+2)\,\Gamma(\beta)}{\Gamma(\alpha+\beta+1)}, \tag{3}$$

$$ {}_2F_1(\alpha+1, -\beta; \alpha+2; 1) = \frac{\Gamma(\alpha+2)\ \beta\Gamma(\beta)}{(\alpha+\beta+1)\,\Gamma(\alpha+\beta+1)}. \tag{4}$$

Substituting the above expressions in (2), we obtain

$$\int_0^1 \left(I_t^{-1}(\alpha,\beta)\right)^2 \, dt = \frac{\alpha(\alpha+1)}{(\alpha+\beta)(\alpha+\beta+1)}, \tag{5}$$

and similarly

$$\int_0^1 \left(I_t^{-1}(\beta,\alpha)\right)^2 \, dt = \frac{\beta(\beta+1)}{(\alpha+\beta)(\alpha+\beta+1)}. \tag{6}$$

Thus (1) simplifies to

$$ {}_2W_2^2\left(f_b(x;\alpha,\beta), f_b(x;\beta,\alpha)\right) = \frac{\alpha(\alpha+1) + \beta(\beta+1)}{(\alpha+\beta)(\alpha+\beta+1)} - 2\int_0^1 I_t^{-1}(\alpha,\beta)\, I_t^{-1}(\beta,\alpha)\, dt. \tag{7}$$

To evaluate the remaining integral in (7), we employ integration-by-parts with $f(t) := I_t^{-1}(\alpha,\beta)$ as the first function and $g(t) := I_t^{-1}(\beta,\alpha)$ as the second. Now, we know that

$$\int_0^1 f(t)\,g(t)\, dt = \underbrace{\left[f(t)\int g(t)\,dt\right]\Bigg|_{t=0}^{t=1}}_{\mathcal{I}} - \underbrace{\int_0^1 \left(f'(t)\int g(t)\, dt\right) dt}_{\mathcal{J}}. \tag{8}$$

From Properties 1 and 3, we get

$$\begin{aligned}
\mathcal{I} &= \left[\frac{1}{(\beta+1)\,B(\alpha,\beta)} I_t^{-1}(\alpha,\beta)\left(I_t^{-1}(\beta,\alpha)\right)^{b+1}\ {}_2F_1(b+1,1-a;b+2;1)\right]\Bigg|_{t=0}^{t=1} \\
&= \frac{1}{(\beta+1)\,B(\alpha,\beta)}\ {}_2F_1(b+1,1-a;b+2;1) \\
&= \frac{\beta}{\alpha+\beta}. \qquad (9)
\end{aligned}$$

Further, Properties (1) and (5) yield

$$\begin{aligned}
\mathcal{J} &= \frac{1}{\beta+1}\int_0^1 \left(I_t^{-1}(\alpha,\beta)\right)^{1-\alpha}\left(1-I_t^{-1}(\alpha,\beta)\right)^{1-\beta}\left(I_t^{-1}(\beta,\alpha)\right)^{\beta+1}\ {}_2F_1(\beta+1,1-\alpha;\beta+2; \\
&\quad I_t^{-1}(\beta,\alpha))\ dt. \qquad (10)
\end{aligned}$$

Combining (7), (8), (9) and (10), the result follows. ■

Proof for Theorem 2

Statement 2: ${}_2W_2\left(f_r(x;\beta), f_w(x;c,\alpha)\right) = \sqrt{\left(\frac{2\alpha^2}{c}\right)\Gamma\left(\frac{2}{c}\right) + 2\beta^2 - 2\sqrt{2}\alpha\beta\left(\frac{1}{c}+\frac{1}{2}\right)\Gamma\left(\frac{1}{c}+\frac{1}{2}\right)}.$

Proof: The inverse of the Rayleigh and Weibull CDFs are given by

$$F_r^{-1}(t) = \begin{cases} 0, & t=0, \\ \beta\sqrt{-\log(1-t)^2}, & 0<t<1, \\ \infty, & t=1. \end{cases} \qquad (11)$$

$$F_w^{-1}(t) = \begin{cases} 0, & t=0, \\ \alpha\sqrt[c]{-\log(1-t)}, & 0<t<1, \\ \infty, & t=1. \end{cases} \qquad (12)$$

From eqn.(13) in the manuscript, we have

$$
\begin{aligned}
{}_2W_2^2\left(f_r\left(x;\beta\right), f_w\left(x;c,\alpha\right)\right) &= \lim_{\epsilon\to0+}\int_0^{1-\epsilon}\left(F_r^{-1}\left(t\right)-F_w^{-1}\left(t\right)\right)^2\,dt \\
&= \lim_{\epsilon\to0+}\int_0^{\sqrt{\log(1/\epsilon)}}\left(\sqrt{2}\beta z-\alpha z^{2/c}\right)^2 2ze^{-z^2}\,dz \quad (\text{set } z^2=-\log\left(1-t\right)) \\
&= \lim_{\epsilon\to0+}\int_0^{\sqrt{\log(1/\epsilon)}}\left(2\beta^2z^2\right)\left(2ze^{-z^2}\right)\,dz\;-\;2\sqrt{2}\alpha\beta\lim_{\epsilon\to0+}\int_0^{\sqrt{\log(1/\epsilon)}}z^{2/c+1} \\
&\quad \left(2ze^{-z^2}\right)\,dz\;+\;\alpha^2\lim_{\epsilon\to0+}\int_0^{\sqrt{\log(1/\epsilon)}}z^{4/c}\left(2ze^{-z^2}\right)\,dz \quad (\text{expanding}) \\
&= 2\beta^2\lim_{\epsilon\to0+}\int_0^{\log(1/\epsilon)}ne^{-n}\,dn\;-\;2\sqrt{2}\alpha\beta\lim_{\epsilon\to0+}\int_0^{\log(1/\epsilon)}n^{1/c+1/2}e^{-n}\,dn \\
&+\;\alpha^2\lim_{\epsilon\to0+}\int_0^{\log(1/\epsilon)}n^{2/c}e^{-n}\,dn \quad (\text{another change of variable } n=z^2) \\
&= 2\beta^2\,\Gamma\left(2\right)\;-\;2\sqrt{2}\alpha\beta\,\Gamma\left(\frac{1}{c}+\frac{1}{2}+1\right)\;+\;\alpha^2\,\Gamma\left(\frac{2}{c}+1\right) \\
&= \left(\frac{2\alpha^2}{c}\right)\Gamma\left(\frac{2}{c}\right)\;+\;2\beta^2\;-\;2\sqrt{2}\alpha\beta\left(\frac{1}{c}+\frac{1}{2}\right)\Gamma\left(\frac{1}{c}+\frac{1}{2}\right),
\end{aligned}
$$

since $\Gamma\left(k+1\right)=k\,\Gamma\left(k\right)$. Taking square root to both sides, the result follows. ■

PROOF FOR COROLLARY 1

Statement 3: If $f_r\left(x;\beta\right)$ and $f_w\left(x;c,\alpha\right)$ are isentropic, then the Wasserstein distance between them is non-zero except for $c=2$.

Proof: As the isentropic condition requires $\beta=\left(\frac{\sqrt{2}\,\alpha}{c}\right)\exp\left(\gamma\left(\frac{1}{2}-\frac{1}{c}\right)\right)$, we can substitute for β in the expression derived in Theorem 2, to get the Wasserstein distance between an isentropic Rayleigh-Weibull pair as

$$
{}_2W_2\left(c,\alpha\right)=\alpha\left[\frac{4\exp\left(\gamma\left(1-\frac{2}{c}\right)\right)}{c^2}-\frac{4\exp\left(\gamma\left(\frac{1}{2}-\frac{1}{c}\right)\right)\Gamma\left(\frac{3}{2}+\frac{1}{c}\right)}{c}+\Gamma\left(1+\frac{2}{c}\right)\right]^{1/2}. \quad (13)
$$

Since $\alpha>0$, ${}_2W_2\left(c,\alpha\right)$ can vanish only when

$$
\Omega\left(c\right):=\frac{4\exp\left(\gamma\left(1-\frac{2}{c}\right)\right)}{c^2}-\frac{4\exp\left(\gamma\left(\frac{1}{2}-\frac{1}{c}\right)\right)\Gamma\left(\frac{3}{2}+\frac{1}{c}\right)}{c}+\Gamma\left(1+\frac{2}{c}\right)=0. \quad (14)
$$

This transcendental equation has five roots $c_1 \approx -1.7762, c_2 \approx -1.0136, c_3 \approx -0.5903, c_4 \approx -0.4132, c_5 = 2$, as shown in Fig. 1. Since $c > 0$, only $c_5 = 2$ is an admissible root. This can be verified by checking the sign of

$$\begin{aligned}\frac{d}{dc}\Omega(c) &= \frac{1}{c^4}[8(\gamma - c)\exp\left(\gamma\left(1-\frac{2}{c}\right)\right) - 2c^2\Gamma\left(1+\frac{2}{c}\right)\Psi\left(1+\frac{2}{c}\right) \\ &- 4c\exp\left(\gamma\left(\frac{1}{2}-\frac{1}{c}\right)\right)\Gamma\left(\frac{3}{2}+\frac{1}{c}\right)\left(\gamma - c - \Psi\left(\frac{3}{2}+\frac{1}{c}\right)\right)],\end{aligned} \tag{15}$$

which is negative for $0 < c < 2$ and positive for $c > 2$ (Fig. 2). Hence $\Omega(c)$ is a decreasing function for $c \in (0, 2)$ and increasing function for $c \in (2, \infty)$. Thus (13) is non-zero except for $c = 2$. ■

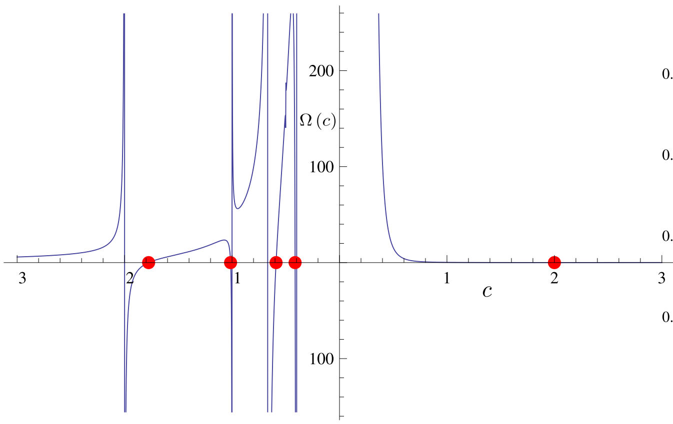

Fig. 1. The plot of $\Omega(c)$ (*blue*) and the roots (*red*) of the transcendental equation (14).

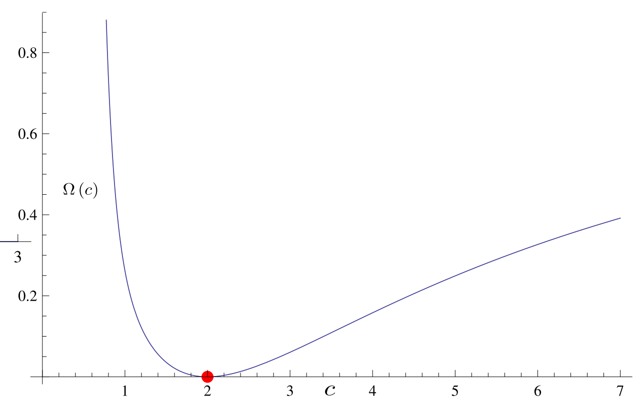

Fig. 2. For $c > 0$, $c = 2$ is also the unique inflection point for $\Omega(c)$. Hence it's the only nonnegative root for (14).

Proof for Lemma 3

Statement 4: If X, Y, Z are non-negative independent random variables such that $X \leqslant Y + Z$, then for $\epsilon > 0$, we have

$$\mathbb{P}(X > \epsilon) \leqslant \mathbb{P}(Y + Z > \epsilon) \leqslant \mathbb{P}\left(Y > \frac{\epsilon}{2}\right) + \mathbb{P}\left(Z > \frac{\epsilon}{2}\right). \tag{16}$$

Proof: (i) Proof of $\mathbb{P}(X > \epsilon) \leqslant \mathbb{P}(Y + Z > \epsilon)$: Let $A_1 := \{\omega : X(\omega) > \epsilon\}$ and $A_2 := \{\omega : Y(\omega) + Z(\omega) > \epsilon\}$. If we denote $B_1^\epsilon := \{\omega : X(\omega) \leqslant \epsilon\}$ and $B_2^\epsilon := \{\omega : Y(\omega) + Z(\omega) \leqslant \epsilon\}$, then

$$\begin{aligned} X(\omega) &\leqslant Y(\omega)+Z(\omega)<\epsilon \quad \forall\, \omega \in \Omega \\ \Rightarrow B_2^\epsilon &\subseteq B_1^\epsilon \\ \Rightarrow \mathbb{P}(B_2^\epsilon) &\leqslant \mathbb{P}(B_1^\epsilon) \qquad \text{(from monotonicity of probability measure)} \\ \Rightarrow 1-\mathbb{P}(B_2^\epsilon) &\geqslant 1-\mathbb{P}(B_1^\epsilon) \\ \Rightarrow \mathbb{P}(A_2) &\geqslant \mathbb{P}(A_1). \qquad \text{(Proved)} \end{aligned} \tag{17}$$

(ii) Proof of $\mathbb{P}(Y+Z>\epsilon) \leqslant \mathbb{P}\left(Y>\frac{\epsilon}{2}\right)+\mathbb{P}\left(Z>\frac{\epsilon}{2}\right)$: Let $A := \{\omega : Y(\omega)+Z(\omega)>\epsilon\}$, $B := \{\omega : Y(\omega) \leqslant \epsilon/2\}$, and $C := \{\omega : Z(\omega) \leqslant \epsilon/2\}$. Next, we write

$$\mathbb{P}(A) = \mathbb{P}\left((A \cap B^c \cap C^c) \cup B^c \cup C^c\right). \tag{18}$$

Taking $\mathcal{E}_1 := A \cap B^c \cap C^c$, $\mathcal{E}_2 := B^c$, $\mathcal{E}_3 := C^c$, and noting that $\mathbb{P}(\mathcal{E}_1) = \mathbb{P}(\mathcal{E}_1 \cap \mathcal{E}_2) = \mathbb{P}(\mathcal{E}_3 \cap \mathcal{E}_1) = \mathbb{P}(\mathcal{E}_1 \cap \mathcal{E}_2 \cap \mathcal{E}_3)$, from Boole-Bonferroni inequality (Appendix C, [1]), (18) yields

$$\mathbb{P}(A) = \mathbb{P}(\mathcal{E}_1 \cup \mathcal{E}_2 \cup \mathcal{E}_3) = \mathbb{P}(\mathcal{E}_2)+\mathbb{P}(\mathcal{E}_3)-\mathbb{P}(\mathcal{E}_2 \cap \mathcal{E}_3) \leqslant \mathbb{P}(\mathcal{E}_2)+\mathbb{P}(\mathcal{E}_3). \qquad \text{(Proved)} \tag{19}$$

■

PROOF FOR THEOREM 4

Statement 5: (**Rate-of-convergence of empirical Wasserstein estimate**)

$$\mathbb{P}\left(\left|\, {}_2W_2(\eta_m, \widehat{\eta}_n) \,-\, {}_2W_2(\eta, \widehat{\eta}) \right| > \epsilon\right) \leqslant K_1 \exp\left(-\frac{m\epsilon^2}{32C_1}\right) + K_2 \exp\left(-\frac{n\epsilon^2}{32C_2}\right). \tag{20}$$

Proof: Combining eqn.(20) in the manuscript with the Lemma above, we have

$$\mathbb{P}\left(\left|\, {}_2W_2(\eta_m, \widehat{\eta}_n) \,-\, {}_2W_2(\eta, \widehat{\eta}) \right| > \epsilon\right) \leqslant \mathbb{P}\left({}_2W_2(\eta_m, \eta) > \frac{\epsilon}{2}\right) \,+\, \mathbb{P}\left({}_2W_2(\widehat{\eta}_n, \widehat{\eta}) > \frac{\epsilon}{2}\right), \tag{21}$$

where each term in the RHS of (21) can be separately upper-bounded using eqn.(22) in the manuscript with $\theta \mapsto \frac{\epsilon}{2}$, i.e.

$$\mathbb{P}\left({}_2W_2(\eta_m, \eta) > \frac{\epsilon}{2}\right) \leqslant K_1 \exp\left(-\frac{m\epsilon^2}{32C_1}\right), \; \mathbb{P}\left({}_2W_2(\widehat{\eta}_n, \widehat{\eta}) > \frac{\epsilon}{2}\right) \leqslant K_2 \exp\left(-\frac{n\epsilon^2}{32C_2}\right). \tag{22}$$

Hence the result. ■

PROBABILISTICALLY WORST-CASE MODEL VALIDATION

In the manuscript, we described probabilistically robust model validation. Following [2]–[4], one can also define a probabilistic notion of the worst-case model validation performance as $\gamma_k^{\mathrm{wc}} := \sup\limits_{\Delta} {}_2W_2\left(\eta_k\left(y\right), \widehat{\eta}_k\left(y\right)\right)$, and its empirical estimate $\widehat{\gamma}_k^N := \max\limits_{i=1,\ldots,N} {}_2W_2\left(\eta_k^{(i)}\left(y\right), \widehat{\eta}_k^{(i)}\left(y\right)\right)$. The sample complexity for probabilistically worst-case model validation is given by the lemma below.

Lemma 1: (**Worst-case bound**) (p. 128, [5]) For any $\epsilon, \delta \in (0,1)$, if $N \geqslant N_{wc} := \dfrac{\log \frac{1}{\delta}}{\log \frac{1}{1-\epsilon}}$, then

$$\mathbb{P}\left(\mathbb{P}\left({}_2W_2\left(\eta_k\left(y\right), \widehat{\eta}_k\left(y\right)\right) \leqslant \widehat{\gamma}_k^N\right) \geqslant 1-\epsilon\right) > 1-\delta.$$

Notice that in general, there is no guarantee that the empirical estimate $\widehat{\gamma}_k^N$ is close to the true worst-case performance γ_k^{wc}. Also, the performance bound is obtained *a posteriori* while the robust validation framework accounted for *a priori* tolerance levels. For these reasons, the worst-case validation framework is not as useful as the robust validation. The corresponding *probabilistically worst-case validation certificate* (PWVC) $\widehat{\Gamma}_k^N$ can be constructed by normalizing $\widehat{\gamma}_k^N$, as described in the following algorithm. In summary, the algorithm, with high probability $(1-\epsilon)$, only ensures that the output PDFs are at most $\widehat{\gamma}_k^N$ far. The preceding statement can be made with probability at least $1-\delta$.

SNAPSHOTS OF TRUE AND MODEL PREDICTED OUTPUT PDFS FOR CONTINUOUS-TIME DETERMINISTIC SYSTEM (SECTION VI.A)

See Fig. 3 and 4 below.

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[2] P. Khargonekar, and A. Tikku, "Randomized Algorithms for Robust Control Analysis and Synthesis Have Polynomial Complexity". *IEEE Conference on Decision and Control*, Kobe, Japan, Dec. 11–13, 1996.

[3] R. Tempo, E.-W. Bai, and F. Dabbene, "Probabilistic Robustness Analysis: Explicit Bounds for the Minimum Number of Samples". *Systems & Control Letters*, Vol. 30, pp. 237–242, 1997.

Algorithm 1 Construct PWVC

Require: $\epsilon, \delta \in (0,1)$, T, ν, law of Δ, experimental data $\{\eta_k(y)\}_{k=1}^{T}$, model

$N \leftarrow N_{\text{wc}}(\epsilon, \delta)$ ▷ Determine sample size of initial densities using lemma 1

Draw N random functions $\xi_0^{(1)}(\widetilde{x}), \xi_0^{(2)}(\widetilde{x}), \ldots, \xi_0^{(N)}(\widetilde{x})$ according to the law of Δ ▷ Use MCMC

for $k = 1$ to T **do** ▷ Index for time step

  for $i = 1$ to N **do** ▷ Index for initial density

    for $j = 1$ to ν **do** ▷ Index for samples in the extended state space, drawn from $\xi_0^{(i)}(\widetilde{x})$

      Propagate states using dynamics

      Propagate measurements

    end for

    Propagate state PDF ▷ Use eqns.(3), (7), (9) or (11) in the manuscript

    Compute instantaneous output PDF ▷ Algebraic transformation

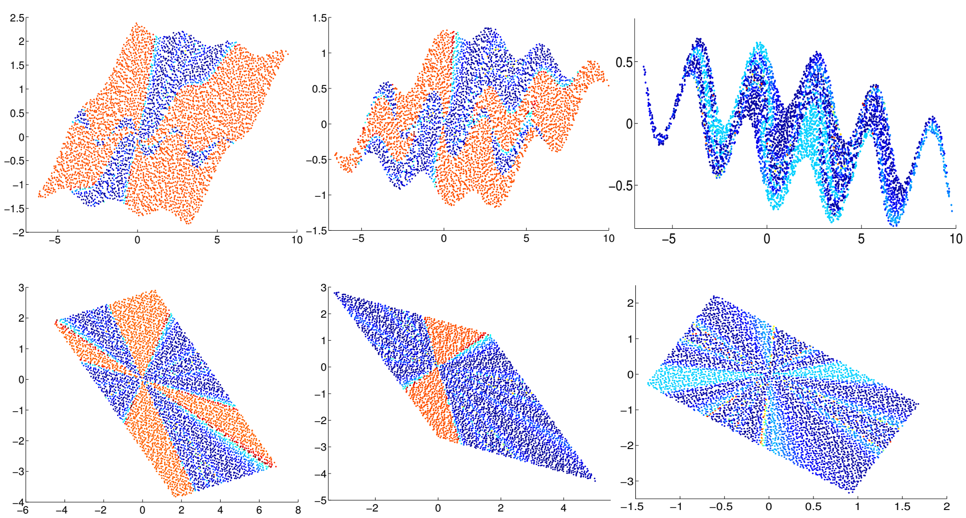
    Compute ${}_2W_2\left(\eta_k^{(i)}(y), \widehat{\eta}_k^{(i)}(y)\right)$ ▷ Distributional comparison by solving LP

    $\widehat{\gamma}_k^N \leftarrow \max\limits_{i=1,\ldots,N} {}_2W_2\left(\eta_k^{(i)}(y), \widehat{\eta}_k^{(i)}(y)\right)$ ▷ Empirically estimate worst-case performance

  end for

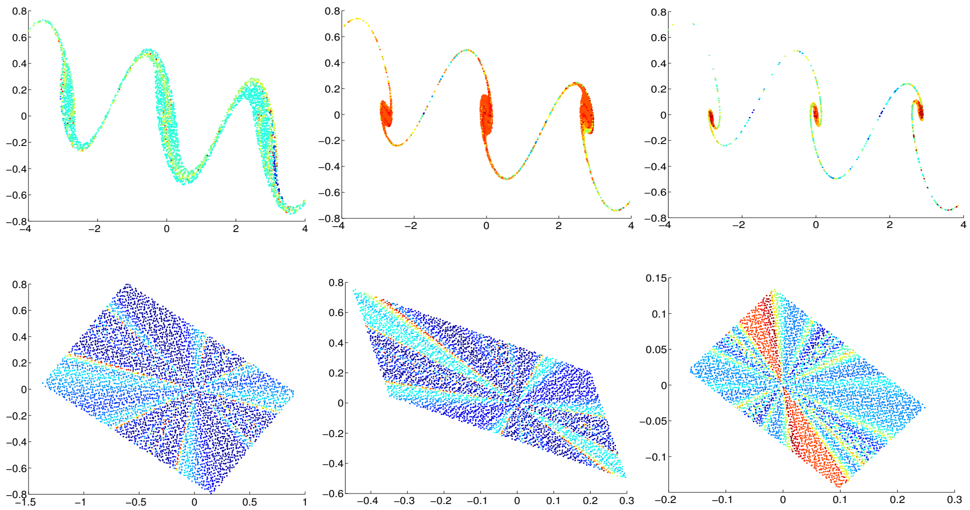
  $\widehat{\Gamma}_k^N \leftarrow \dfrac{\widehat{\gamma}_k^N}{\text{diam}(\mathcal{D}_k)}$ ▷ Construct PWVC vector of length $T \times 1$

end for



(a) (b) (c)

Fig. 3. Comparative color-coded scatter-plots of the joint PDFs for true and model dynamics over their respective output spaces. The color value stands for the magnitude of joint PDF (red = high probability and blue = low probability). The snapshots are for $t = (a)4.5, (b)6.5, (c)10.5$. The top row corresponds to the true nonlinear dynamics and the bottom row corresponds to linearized model dynamics. For the true nonlinear system, stable and unstable manifolds are visible in the transient PDFs.



(d) (e) (f)

Fig. 4. Comparative color-coded scatter-plots of the joint PDFs for true and model dynamics over their respective output spaces, at $t = (d)16.5, (e)22.5$ and (f)30.5. The convention is same as Fig.3. The true stationary density becomes dirac delta at the fixed points of the nonlinear dynamics. The model stationary density exponentially converges toward dirac delta at the origin. All computations are done by solving MOC based Liouville equation described in [6].

[4] X. Chen, and K. Zhou, "Order Statistics and Probabilistic Robust Control". *Systems & Control Letters*, Vol. 35, pp. 175–182, 1998.

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