Uncertainty Quantification and Model Validation in Flight Control Applications

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Model Validation

- **Model Validation Question:** Given two systems $S_1$ and $S_2$, how close are they?
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Mathematically:

- $u(t)$
- $y_1(t)$
- $y_2(t)$

Systems are modeled using ordinary differential equations:

\[
\dot{x} = f(x, u), \quad y = g(x)
\]

Extend this to model validation with respect to experimental data.
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**Existing Methods**

\[ u(t) \rightarrow S_1 \rightarrow y_1(t) \]
\[ \quad \rightarrow S_2 \rightarrow y_2(t) \]

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### Existing Methods

![Diagram](image)

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- Model validation $\equiv$ set containment.
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- Recently sum-of-squares (SOS) based methods have been used to develop barrier certificates.
- Barrier certificates guarantee output trajectories are contained in the same set.
- Model validation $\equiv$ set containment.
- Cannot distinguish between trajectory concentrations over same support.
**New Nonlinear Model Validation Framework**

Basic Idea: Excite both systems using random signals from a given distribution $\xi(u)$. If two systems are close, their output densities $\eta(y, t)$ and $\hat{\eta}(y, t)$ will have similar shape.
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Regions of high concentration $\implies$ slow scale dynamics, invariant sets, equilibrium points.
New Nonlinear Model Validation Framework

Compute $\xi(u) \mapsto \eta(y,t)$ and $\xi(u) \mapsto \hat{\eta}(y,t)$. 

$\xi(u) \overset{\mathcal{M}}{\mapsto} \eta(y,\cdot) \overset{\mathcal{\hat{M}}}{\mapsto} \hat{\eta}(y,\cdot)$ 

$\{d(\eta, \hat{\eta}) \leq \gamma \implies \text{valid}\}$ 

- Monte-Carlo ⇔ PDF estimation using histograms.
- Polynomial Chaos to propagate moments and estimate PDF using optimization.
- Stochastic Liouville or Fokker-Planck-Kolmogorov equation.
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\[ M \hat{M} \eta (y, \cdot) \hat{\eta} (y, \cdot) \xi (u) d(\eta, \hat{\eta}) \leq \gamma \implies \text{valid} \]

Compute \( \xi(u) \leftrightarrow \eta(y, t) \) and \( \xi(u) \leftrightarrow \hat{\eta}(y, t) \).

- **Monte-Carlo** \( \leftrightarrow \) PDF estimation using histograms.
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\[ \hat{M}(y, \cdot) \rightarrow \eta(y, \cdot) \rightarrow \hat{\eta}(y, \cdot) \] \[ d(\eta, \hat{\eta}) \leq \gamma \implies \text{valid} \]

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- **Monte-Carlo** $\leftrightarrow$ PDF estimation using histograms.
- **Polynomial Chaos** to propagate moments and estimate PDF using optimization.
- **Stochastic Liouville** or Fokker-Planck-Kolmogorov equation.
What is the right metric for PDF comparison?

(a) Entropy: \( H(\rho_1) = H(\rho_2) \).

(b) \( KL(\rho_1, \rho_0) = KL(\rho_2, \rho_0) \).

Suitable definition for \( d(\eta, \hat{\eta}) \) that computes shape difference between \( \eta, \hat{\eta} \).
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**Suitable definition** for $d(\eta, \hat{\eta})$ that computes shape difference between $\eta, \hat{\eta}$.

- **Entropy** is not a shape metric.
- **Kulback Liebler Divergence** is not a shape difference metric. Requires same support.
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**Suitable definition** for \( d(\eta, \hat{\eta}) \) that computes shape difference between \( \eta, \hat{\eta} \).

- **Entropy** is not a shape metric.
- **Kulback Liebler Divergence** is not a shape difference metric. Requires same support.
- Instead use **Wasserstein distance** \( 2W_2 \). It is a shape difference metric. Has nice properties (unequal sampling, different support, etc).
Wasserstein Distance

Wasserstein distance between two densities $\rho_1(y_1)$ and $\rho_2(y_1)$ for $y_1, y_2 \in \mathbb{R}^n$ is defined as

$$2W_2 (\rho_1, \rho_2) := \left[ \inf_{\rho \in \mathcal{F}(\rho_1, \rho_2)} \int_{\mathbb{R}^n \times \mathbb{R}^n} \| y_1 - y_2 \|^2 \, d\rho (y_1, y_2) \right]^{1/2}$$

$$= \left( \inf_{\rho \in \mathcal{F}(\rho_1, \rho_2)} \mathbb{E} \left[ \| y_1 - y_2 \|^2 \right] \right)^{1/2}.$$

- $\mathcal{F}(\rho_1, \rho_2)$ is the set of all probability densities on $\mathbb{R}^n \times \mathbb{R}^n$ with first marginal as $\rho_1$ and second marginal as $\rho_2$.
- For multivariate Gaussian functions $\mathcal{N}(\mu_1, \Sigma_1)$ and $\mathcal{N}(\mu_2, \Sigma_2)$, $2W_2$ is given by,

$$2W_2 = \sqrt{\| \mu_1 - \mu_2 \|^2 + \text{tr} (\Sigma_1) + \text{tr} (\Sigma_2) - 2 \text{tr} \left( \left( \sqrt{\Sigma_1 \Sigma_2} \sqrt{\Sigma_1} \right)^{1/2} \right)}.$$
Wasserstein Distance via Linear Programming (LP)

- In general, $2W_2$ can be defined in terms of the Euclidean distance between samples of $\rho_1$ and $\rho_2$.
- Therefore, $2W_2$ can be computed by solving an LP defined over the samples of $\rho_1$ and $\rho_2$.
- LP equivalent to Monge-Kantorovich optimal transportation plan. Think of $2W_2$ as the minimum work required to convert one shape to the other.

$$2W_2(\rho_1, \rho_0) \neq 2W_2(\rho_2, \rho_0)$$
Simple Example

Consider the following nonlinear dynamical system

$$\ddot{x} = -ax - b \sin 2x - c\dot{x},$$

with $a = 0.1$, $b = 0.5$, and $c = 1$. 
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- Five fixed points of the form \((x_1^*, 0), \) where \( b \sin 2x_1^* = -ax_1^*. \)
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- Five fixed points of the form $(x^*_1, 0)$, where $b\sin 2x^*_1 = -ax^*_1$.
- Compare this with the linearized dynamics about $(0, 0)$.
- For this example, $u(t) = 0$. Both systems have same initial state distribution and $y = x$.
Consider two stable LTI systems with transfer function matrices \( G(j\omega) \) and \( \hat{G}(j\omega) \), excited by Gaussian white noise \( u(t) \sim \mathcal{N}(0, \text{diag} (\sigma_u^2)) \),

- **SISO and MISO:**

\[
2W_2^\infty(G, \hat{G}) = \sqrt{2\pi \sigma_u} \left| ||G||_2 - ||\hat{G}||_2 \right|
\]
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- **SISO and MISO:**
  \[ 2W_2^\infty(G, \hat{G}) = \sqrt{2\pi} \sigma_u \left| \|G\|_2 - \|\hat{G}\|_2 \right| \]

- **MIMO**

  \[ 2W_2^\infty(G, \hat{G}) = \sqrt{2\pi} \sigma_u \left[ \|G\|_2^2 + \|\hat{G}\|_2^2 - 2\text{tr} \left\{\mathcal{I}(G)^{1/2} \mathcal{I}(\hat{G}) \mathcal{I}(G)^{1/2}\right\} \right]^{1/2} \]

  where $\mathcal{I}(\cdot)$ is defined as

  \[ \mathcal{I}(G) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} G^H(j\omega) G(j\omega) d\omega. \]

See CDC Paper "Frequency Domain Model Validation in Wasserstein Metric", A. Halder, R. Bhattacharya, for derivations.
Bounds for MIMO $W^\infty$

$$\sigma_u \left\| \sqrt{\int_{-\infty}^{+\infty} G^H G d\omega} - \sqrt{\int_{-\infty}^{+\infty} \hat{G}^H \hat{G} d\omega} \right\|_F$$

$$W_{\infty}^{\text{SISO}} \quad W_{\infty}^{\text{MIMO}} \quad \sqrt{2\pi \sigma_u \sqrt{\|G\|_2^2 + \|\hat{G}\|_2^2}}$$
Sensitivity of $W^\infty$ in Frequency Domain

- **Sensitive to scaling:** linear relative amplification $\leadsto$ linear amplification of gap

- **Cannot discriminate between minimum and non-minimum phase systems:** e.g. $G_\pm = \frac{14s \pm \zeta}{s^2 + 5s + 6}$, $\zeta > 0$. Plot $W^\infty(G_+, G_-)$ vs. $\zeta \in (0, 40)$. 

![Diagram showing sensitivity of $W^\infty$ with examples of $G_\pm$ and corresponding plots of magnitude and phase vs. $\zeta$.]
Geometric Meaning of SISO $W^\infty$ and $\nu$-gap Metric

\[
\begin{align*}
\hat{G}(j\omega) & \quad \hat{\phi}(\hat{G}) \\
G(j\omega) & \quad \phi(G) \\
|G|_2 & \quad |\hat{G}|_2 \\
\kappa(\omega) & \quad \kappa_{\text{proj}}(\omega)
\end{align*}
\]
Geometric Meaning of SISO $W^\infty$ and $\nu$-gap Metric

\[ G(j\omega) \]
\[ \hat{G}(j\omega) \]
\[ ||G||^2 \]
\[ ||\hat{G}||^2 \]
\[ \text{Re}(s) \]
\[ \text{Im}(s) \]
\[ \kappa(\omega) \]
\[ \phi(\hat{G}) \]
\[ \phi(G) \]
\[ \kappa_{\text{proj}}(\omega) \]
Comparing SISO $W_\infty$ and $\delta_\nu := \sup_\omega \kappa(\omega)$

- **Un-normalized comparison on Complex plane:**
  $$\sup_\omega \kappa^{\text{proj}}(\omega) \geq W_\infty$$

- **Normalized comparison on Riemann sphere:**
  $$\overline{W}_S \left( G, \hat{G} \right) = \frac{2}{\pi} \left| \arctan \| G \|_2 - \arctan \| \hat{G} \|_2 \right|$$, compare $\overline{W}_S$ with $\delta_\nu$
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Questions?