Probabilistic Methods for Model Validation, Verification and Refinement

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Background

- **Postdoctoral Research Fellow (June 2014 - current)**
  - Department of Electrical and Computer Engineering
    Texas A&M University
- **Ph.D (Aug. 2008 - May 2014)**
  - Department of Aerospace Engineering
    Texas A&M University
  - Dissertation: *Probabilistic Methods for Model Validation*
- **Bachelors and Masters (June 2003 - June 2008)**
  - Department of Aerospace Engineering
    Indian Institute of Technology Kharagpur, India
  - Thesis: *Development of An Autonomous Reconfigurable UAV*

Model validation problem: introduction

- Given
  - Time varying measurements
    - vector (trajectory)
    - set
    - concentration / density
  - Candiate model
    - flow
    - map
  - Input
    - open loop command
    - stochastic disturbance
    - initial condition
- Question
  - How well does the model replicate the measurements?

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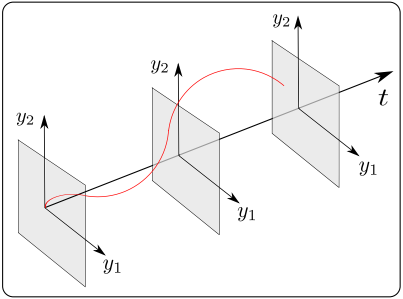

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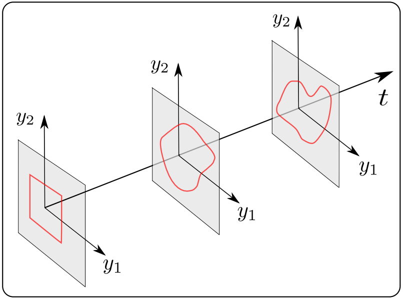

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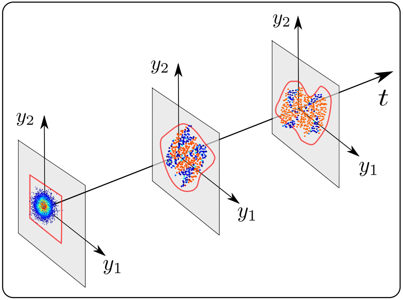

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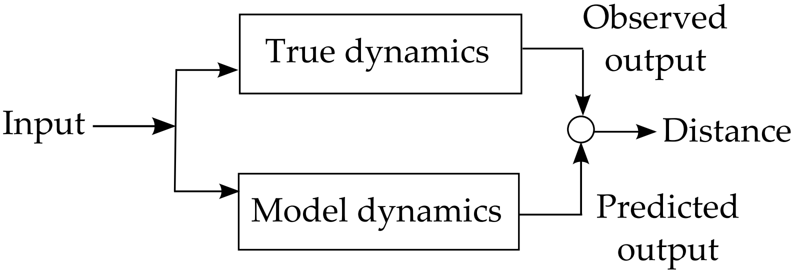
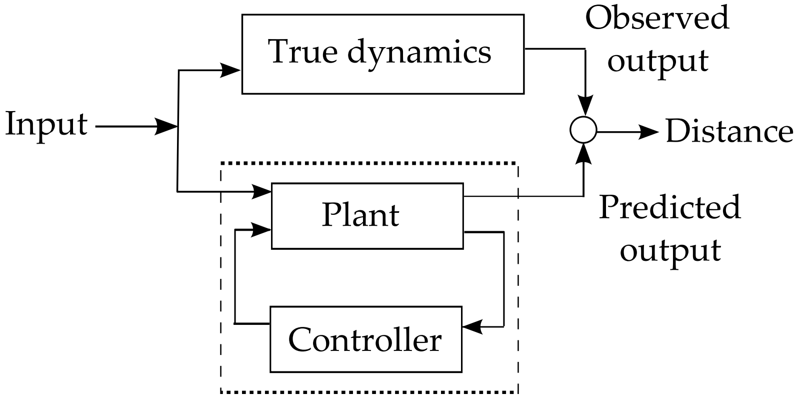
Generic validation problem: is the physics correct?



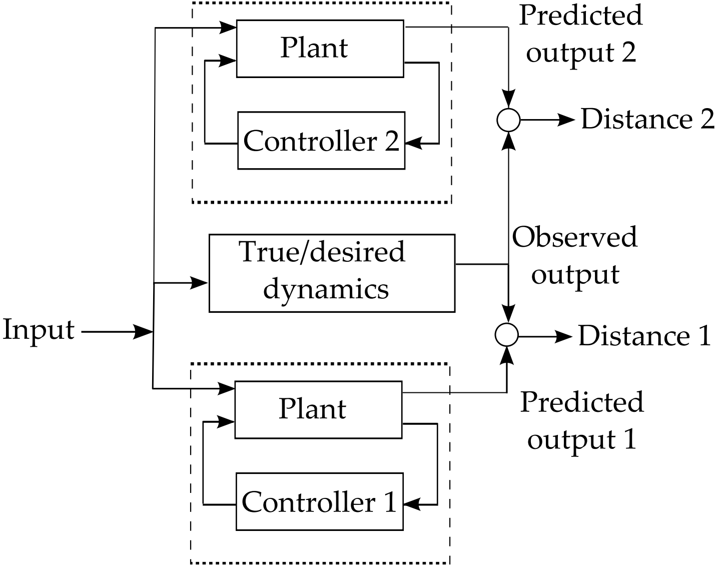
- Applications: predictive modeling
  - Systems biology
  - Atmospheric modeling in planetary entry-descent-landing (EDL)

Generic verification problem: is the implementation correct?

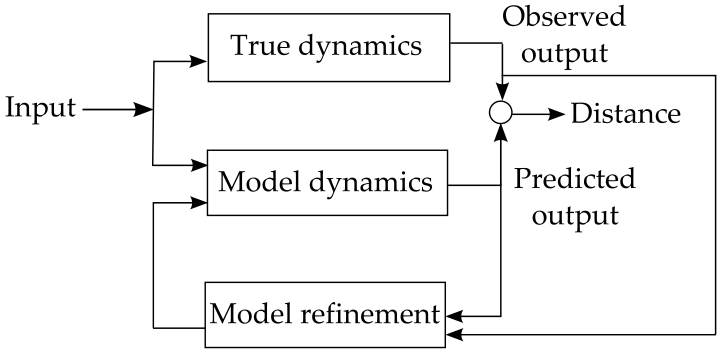


- Applications: performance assessment
  - Flight control software certification
  - Fault detection

Generic verification problem: which implementation is better?



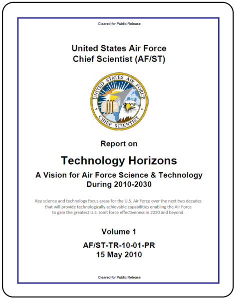
Generic refinement problem: how to improve the model?



- Applications
  - Data driven modeling
  - Density control
  - Fault reconfiguration

Model validation problem: motivation

- U.S. Air Force 2010 Report on Technology Horizons
  - "It is possible to develop systems having high levels of autonomy, but it is the lack of suitable V&V methods that prevents all but relatively low levels of autonomy from being certified for use."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United States Air Force
Chief Scientist (AF/ST)

Report on

Technology Horizons

A Vision for Air Force Science & Technology
During 2010-2030

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Volume 1

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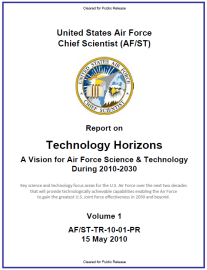
- F/A-18 Hornet Falling Leaf Mode
  - 47 out-of-control flights during 1983-2000
  - Controller revised in 2001
  - Linear analysis found insufficient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Model validation: state-of-the-art

- Linear model validation
  - Robust control framework
    - Smith & Doyle, 1992
    - Poolla *et. al.*, 1994
    - Smith & Dullerud, 1996
    - Chen & Wang, 1996
    - Steele & Vinnicombe, 2001
    - Gevers *et. al.*, 2003
  - Statistical setting
    - Lee & Poolla, 1996
    - Ljung & Guo, 1997

- Noninear model validation
  - Barrier certificate
    - Prajna, 2006
  - Polynomial chaos
    - Ghanem *et. al.*, 2008

"For the general case of nonparametric (uncertainty) models, the situation is significantly more complicated."

– *[Lee and Poolla, 1996]*

- Most existing methods focus on invalidation/falsification
- Overly conservative?
- Binary oracle vs. "degree" of (in)validation

Our approach: intuitive idea

- Our proposal:
  - Compare shapes of the output PDFs at $\{t_j\}_{j=1}^{\tau}$
- Why PDFs instead of
  - trajectories?
  - sets?
  - moments?
- Why shapes?

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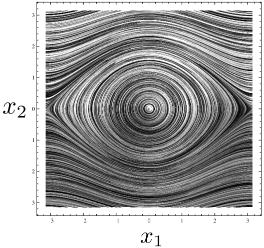
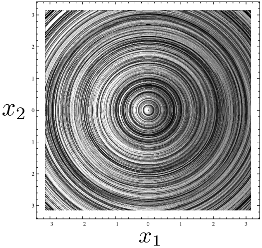


$$\dot{x}_1 = -x_2, \quad \dot{x}_2 = \sin x_1,$$



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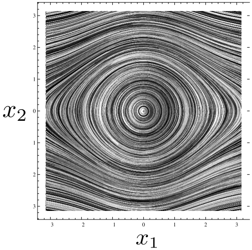
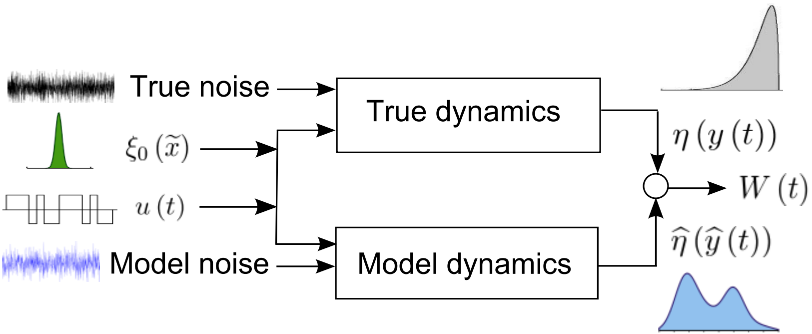


$$\dot{x}_1 = -x_2, \quad \dot{x}_2 = x_1 - \frac{x_1^3}{3!} + \frac{x_1^5}{5!},$$

Outline

- Introduction
- State-of-the-art
- Intuitive idea
- Problem formulation
- Uncertainty propagation
- Distributional comparison
- Examples
- Systems-theoretic results for probabilistic V&V
- Probabilistic model refinement
- Conclusions

Problem formulation



Proposed framework: Valid if $W(t_j) \leqslant \gamma_j, \forall j = 1, 2, \ldots, \tau$

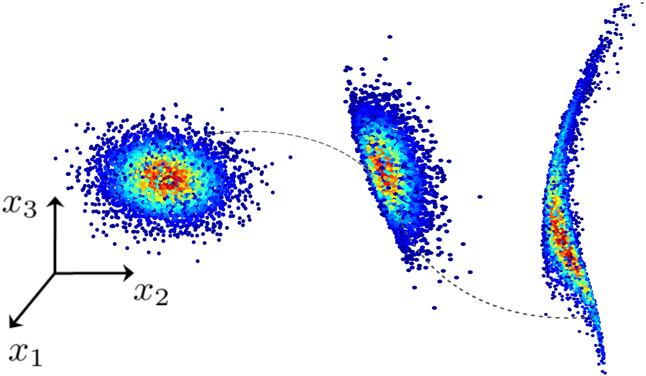
Step 1. Uncertainty propagation

Step 2. Distributional comparison

Uncertainty propagation: deterministic model

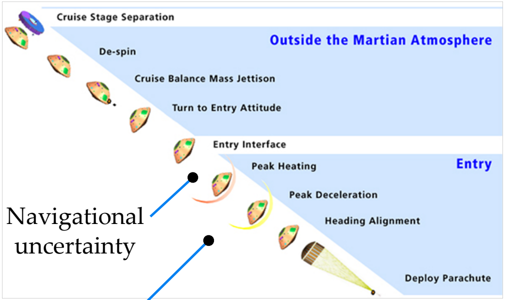
- Model
  - State equation: $\dot{\widehat{x}} = \widehat{f}\left(\widehat{x}, \widehat{p}\right), \widehat{x}\left(t\right) \in \widehat{\mathcal{X}} \subseteq \mathbb{R}^{\widehat{n}_s}, \widehat{p} \in \widehat{\mathcal{P}} \subseteq \mathbb{R}^{\widehat{n}_p}$
  - Extended state space form:
    $$\dot{\widehat{\widehat{x}}} = \widehat{\widehat{f}}\left(\widehat{\widehat{x}}\right), \widehat{\widehat{x}} \in \widehat{\mathcal{X}} \times \widehat{\mathcal{P}} \subseteq \mathbb{R}^{\widehat{n}_s + \widehat{n}_p}, \widehat{\widehat{f}} = \begin{Bmatrix} \widehat{f}_{\widehat{n}_s \times 1} \\ \mathbf{0}_{\widehat{n}_p \times 1} \end{Bmatrix}$$
  - Output equation: $\widehat{y} = \widehat{h}\left(\widehat{\widehat{x}}\right), \widehat{h} : \widehat{\mathcal{X}} \times \widehat{\mathcal{P}} \mapsto \widehat{\mathcal{Y}} \subseteq \mathbb{R}^{n_o}$
- PDF evolution
  - State PDF via Liouville equation: $\dfrac{\partial \widehat{\xi}}{\partial t} = -\displaystyle\sum_{i=1}^{\widehat{n}_s} \dfrac{\partial}{\partial \widehat{x}_i}\left(\widehat{\xi} \widehat{f}_i\right)$
  - MOC for Liouville equation: $\dfrac{d\widehat{\xi}}{dt} = -\widehat{\xi}\, \nabla . \widehat{f}$, initial PDF ξ_0
  - Output PDF: $\widehat{\eta}\left(\widehat{y}, t\right) = \displaystyle\sum_{j=1}^{\nu} \dfrac{\widehat{\xi}\left(\widehat{\widehat{x}}_j^{\star}, t\right)}{\left|\det\left(\mathcal{J}_{\widehat{h}}\left(\widehat{\widehat{x}}_j^{\star}, t\right)\right)\right|}$

Uncertainty propagation: deterministic model



MC simulation	Liouville MOC
Offline post-processing	Online
Histogram approximation	Exact arithmetic
Grid based	Meshless
$\widehat{n}_s$ ODEs per sample	$\widehat{n}_s + 1$ ODEs per sample

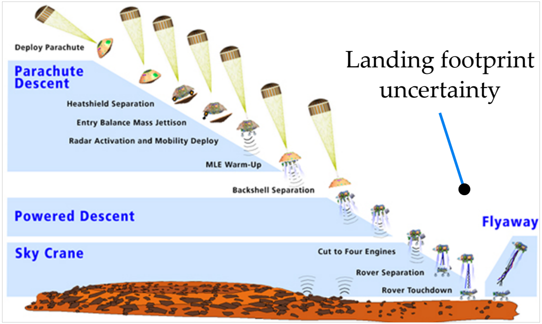
Case study: Mars EDL uncertainty analysis



Navigational uncertainty

Heating uncertainty

Chute deployment uncertainty



Landing footprint uncertainty

Image credit: NASA JPL

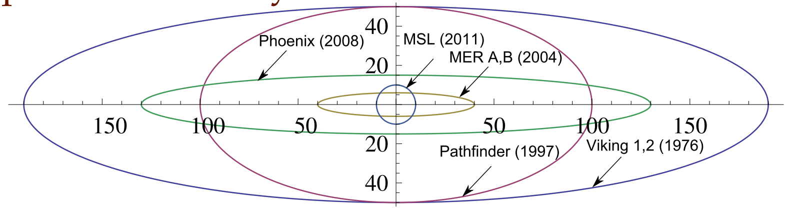
Case study: Mars EDL uncertainty analysis

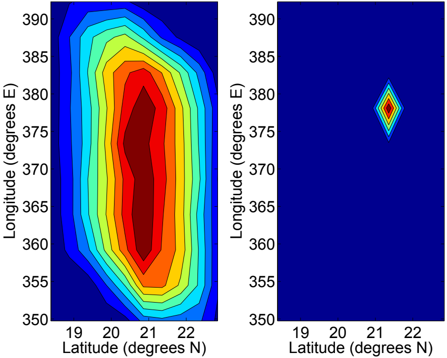
6-state Vinh's equation with 3 parameters: $\rho_0, B_c, \dfrac{C_L}{C_D}$

Atmospheric model: $\rho = \rho_0 \exp\left(\dfrac{h_2 - hR_0}{h_1}\right)$

$$
\begin{aligned}
\dot{h} &= V \sin\gamma \\
\dot{\zeta} &= \frac{V\cos\gamma\sin\chi}{(1+h)} \\
\dot{\lambda} &= \frac{V\cos\gamma\cos\chi}{(1+h)\cos\zeta} \\
\dot{V} &= -\frac{\rho R_0}{2B_c}V^2 - \frac{gR_0}{v_c^2}\sin\gamma + \frac{R_0^2\Omega^2}{v_c^2}(1+h)\cos\zeta\,(\sin\gamma\cos\zeta - \cos\gamma\sin\zeta\sin\chi) \\
\dot{\gamma} &= \frac{\rho R_0}{2B_c}\frac{C_L}{C_D}V\cos\sigma + \frac{gR_0}{v_c^2}\cos\gamma\left(\frac{V}{1+h} - \frac{1}{V}\right) \\
\dot{\chi} &= \frac{\rho R_0}{2B_c}\frac{C_L}{C_D}\frac{V\sin\sigma}{\cos\gamma} - \frac{V\cos\gamma}{(1+h)}\tan\zeta\cos\chi + \frac{2R_0\Omega}{v_c}(\tan\gamma\cos\zeta\sin\chi - \sin\zeta) - \\
&\quad \frac{R_0^2\Omega^2}{v_c^2}\frac{(1+h)}{V\cos\gamma}\sin\zeta\cos\zeta\cos\chi
\end{aligned}
$$

Case study: Mars EDL uncertainty analysis – landing footprint uncertainty

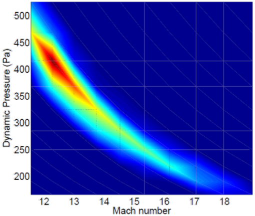


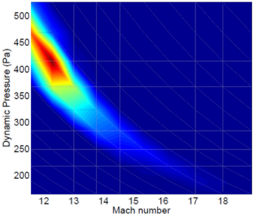


Case study: Mars EDL uncertainty analysis

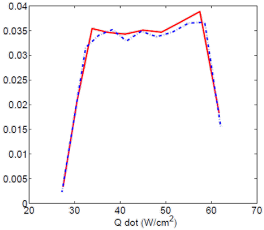
MC | Liouville MOC

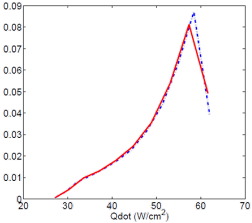
Chute deployment uncertainty





Heating rate uncertainty





Uncertainty propagation: stochastic model

- Model
  - State equation: $d\widehat{\widehat{x}}(t) = \widehat{\widehat{\widetilde{f}}}\left(\widehat{\widehat{x}}(t)\right)\, dt + \widehat{g}\left(\widehat{\widehat{x}}(t)\right)\, d\mathcal{W}$,
  - Output equation: $\widehat{y}(t) = \widehat{h}\left(\widehat{\widehat{x}}(t)\right)$,
- PDF evolution
  - State PDF via Fokker-Planck equation:
    $$\frac{\partial\widehat{\xi}}{\partial t} = -\sum_{i=1}^{\widehat{n}_s}\frac{\partial}{\partial\widehat{x}_i}\left(\widehat{\xi}\widehat{\widetilde{f}}_i\right) + \sum_{i=1}^{\widehat{n}_s}\sum_{j=1}^{\widehat{n}_s}\frac{\partial^2}{\partial\widehat{x}_i\partial\widehat{x}_j}\left(\left(\widehat{g}Q\widehat{g}^\top\right)_{ij}\widehat{\xi}\right),$$
  - Main idea: design a dynamics whose Liouville MOC approximates the Fokker-Planck soltuion
  - Proposed KL + MOC formulation:
    $$\dot{\widehat{x}}_N^{(j)} = \widehat{f}^{(j)}\left(\widehat{x}_N, t\right) + \sum_{k=1}^{n_{\text{noise}}} g^{(j,k)}\left(\widehat{x}_N, t\right)\text{KL}_N^{(k)},$$

Uncertainty propagation: stochastic model

- Theorem
  - Asymptotic consistency: $x_N(t) \xrightarrow[\text{m.s.}]{N\to\infty} x(t)$, $\forall\, t > 0$.
  - Rate-of-convergence: $\lesssim \exp(-N)$ for OU, GBM.

Uncertainty propagation: stochastic model

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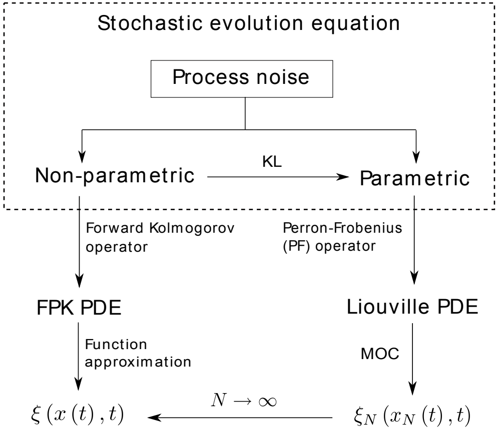
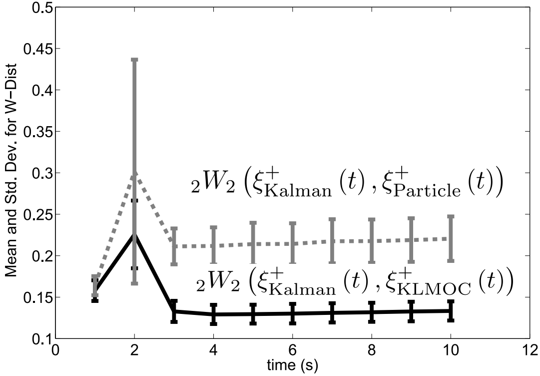


Numerical results: Kalman filter

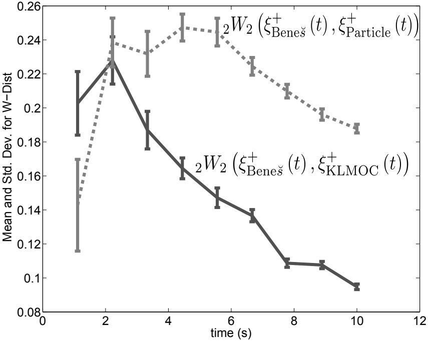
- Process model: $\dot{x}(t) = -0.05 I_2\, x(t) + \begin{bmatrix} 1 & 1 \end{bmatrix}^\top \eta(t)$
- Measurement model: $y_k = \begin{bmatrix} 1 & 1 \end{bmatrix} x_k + v_k, \qquad k \in \mathbb{N}$
- $\eta(t), v_k$ are independent GWN with $Q = 1/8$, $R = 1/4$
- Initial PDF $\varphi_0 = \mathcal{N}\left(\begin{bmatrix} 1 & 1 \end{bmatrix}^\top, \mathrm{diag}(1,1) \right)$
- From ξ_0, we draw 100 sample sets, each with 500 samples



Numerical results: Beneš filter

- Process model: $dx(t) = \dfrac{\kappa e^{x} - e^{-x}}{\kappa e^{x} + e^{-x}}\, dt + d\mathcal{W}(t)$
- Measurement model: $dy(t) = x(t)\, dt + d\mathcal{V}(t)$
- Noise variances: $Q = 1$, $R = 10$; deterministic x_0
- Normalized posterior:

$$\xi^{+}\left(x(t), t|\mathcal{Y}_t\right) = \sqrt{\frac{\coth(t)}{2\pi}} \left(\frac{\kappa e^{x} + e^{-x}}{\kappa e^{I_t(y)} + e^{-I_t(y)}}\right) \exp\left(-\tfrac{1}{2}\Gamma(t)\right)$$



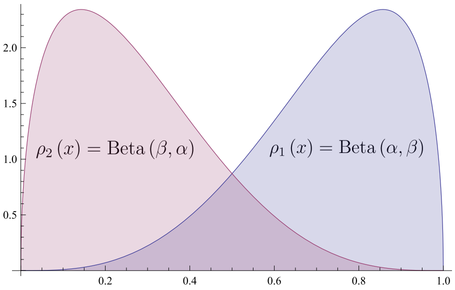
Distributional comparison: axiomatic approach

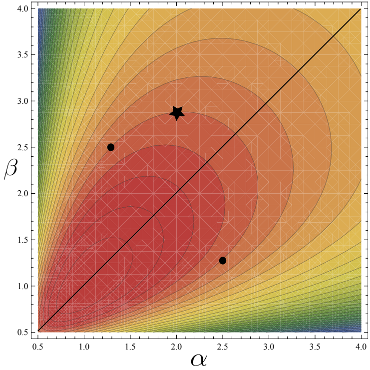
- Candidates for validation distance
  - Kullback-Leibler divergence $D_{KL}(\rho_1||\rho_2) := \int_{\mathbb{R}^d} \rho_1(x) \log\left(\frac{\rho_1(x)}{\rho_2(x)}\right) dx$
  - Symmetric KL divergence
    $D_{KL}^{\text{symm}}(\rho_1||\rho_2) := \frac{1}{2}\left(D_{KL}(\rho_1||\rho_2) + D_{KL}(\rho_2||\rho_1)\right)$
  - Wasserstein distance
    ${}_pW_q(\mu_1, \mu_2) := \left[\inf_{\mu \in \mathcal{M}_2(\mu_1,\mu_2)} \int_\Omega \| \underline{x} - \underline{y} \|_p^q \, d\mu\left(\underline{x}, \underline{y}\right)\right]^{1/q}$

What we want	D_{KL}	D_{KL}^{symm}	W
$\geqslant 0$	✓	✓	✓
Symmetry	×	✓	✓
Triangle inequality	×	×	✓
$\text{supp}(\eta) \neq \text{supp}(\widehat{\eta})$	×	×	✓
$\dim(\text{supp}(\eta)) \neq \dim(\text{supp}(\widehat{\eta}))$	×	×	✓
$\#\text{sample}(\eta) \neq \#\text{sample}(\widehat{\eta})$	×	×	✓
Convexity	✓	✓	✓
Finite range	$[0, \infty)$	$[0, \infty)$	$[0, \text{diam}(\Omega)]$

Distributional comparison: axiomatic approach

- Counterexample 1: randomness $\neq$ shape
  $W(\rho_1, \rho_2) \neq 0$, for $\alpha \neq \beta$ (e.g. $\alpha = 4$, $\beta = \frac{3}{2}$ below)



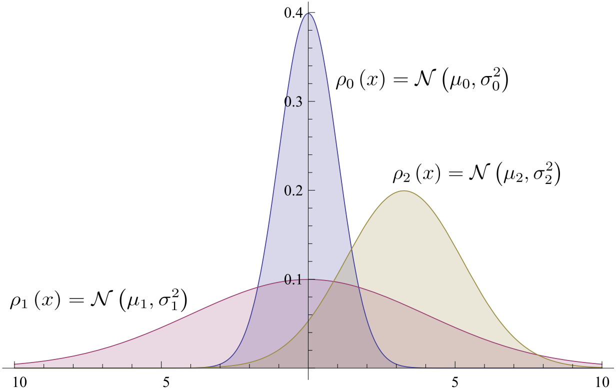


$$H(\rho_1) = H(\rho_2) = \log B(\alpha, \beta) - (\alpha - 1)(\Psi(\alpha) - \Psi(\alpha + \beta)) - (\beta - 1)(\Psi(\beta) - \Psi(\alpha + \beta))$$

Distributional comparison: axiomatic approach

- Counterexample 2: $D_{KL} \neq$ shape

$(\mu_0, \sigma_0) = (0, 1)\,;\ (\mu_1, \sigma_1) = (0, 4)\,;\ (\mu_2, \sigma_2) = \left(\sqrt{12 - 2\log 2}, 2\right)$



$$D_{KL}(\rho_1, \rho_0) = D_{KL}(\rho_2, \rho_0), \text{ but } W(\rho_1, \rho_0) \neq W(\rho_2, \rho_0)$$

Distributional comparison: W for model validation

Wasserstein distance in validation context

- $_pW_q(\eta,\widehat{\eta}) = \left(\inf_{\varrho\in\mathcal{M}_2(\eta,\widehat{\eta})} \int_{\mathcal{Y}\times\widehat{\mathcal{Y}}} \| y-\widehat{y} \|_p^q \; \varrho(y,\widehat{y})\, dy d\widehat{y}\right)^{1/q}$
- Minimum effort required to convert one shape to another
- We choose $p=q=2$, and denote $_2W_2$ as W

When can we write W in closed-form:

- Single output case: $W^2(\eta,\widehat{\eta}) = \int_0^1 \left(F^{-1}(u) - G^{-1}(u)\right)^2 du$
- Multivariate Normal case (comparing Linear Gaussian systems): $W\left((A,C);\left(\widehat{A},\widehat{C}\right)\right) = W(\eta,\widehat{\eta}) = W\left(\mathcal{N}(\mu_1,\Sigma_1), \mathcal{N}(\mu_2,\Sigma_2)\right) = \sqrt{\| \mu_1-\mu_2 \|_2^2 + \operatorname{tr}(\Sigma_1) + \operatorname{tr}(\Sigma_2) - 2\operatorname{tr}\left(\left(\sqrt{\Sigma_1}\Sigma_2\sqrt{\Sigma_1}\right)^{1/2}\right)}$

Distributional comparison: computing W

- At each time $\{t_j\}_{j=1}^{\tau}$, we have two sets of colored scattered data
- Construct complete, weighted, directed bipartite graph $K_{m,n}(U \cup V, E)$ with $\#(U) = m$ and $\#(V) = n$
- Assign edge weight $c_{ij} := \| u_i - v_j \|_{\ell_2}^2$, $u_i \in U$, $v_j \in V$
- minimize $\displaystyle\sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}\,\varphi_{ij}$ subject to

$$\sum_{j=1}^{n} \varphi_{ij} = \alpha_i, \qquad \forall\, u_i \in U, \qquad \text{(C1)}$$

$$\sum_{i=1}^{m} \varphi_{ij} = \beta_j, \qquad \forall\, v_j \in V, \qquad \text{(C2)}$$

$$\varphi_{ij} \geqslant 0, \qquad \forall\, (u_i, v_j) \in U \times V. \qquad \text{(C3)}$$

- Necessary feasibility condition: $\displaystyle\sum_{i=1}^{m} \alpha_i = \sum_{j=1}^{n} \beta_j$

Distributional comparison: computing W

Sample complexity

- Rate-of-convergence of empirical Wasserstein estimate

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

Runtime complexity

- An LP with mn unknowns and $(m+n+mn)$ constraints
- For $m = n$, runtime is $\mathcal{O}\left(n_o n^{2.5} \log n\right)$

Storage complexity

- For $m = n$, constraint is a binary matrix of size $2n \times n^2$
- Each row has n ones. Total # of ones = $2n^2$
- At a given snapshot, sparse storage complexity is $2n\left(3n + n_o + 1\right) = \mathcal{O}\left(n^2\right)$
- Non-sparse storage complexity is $2n\left(n^2 + n_o + 1\right) = \mathcal{O}\left(n^3\right)$

Distributional comparison: computing W

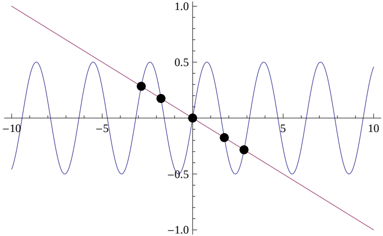
In standard LP form

$$\underset{x \geqslant 0}{\text{minimize}} \quad \tilde{c}^\top x,$$
$$\text{subject to} \quad Ax = b,$$

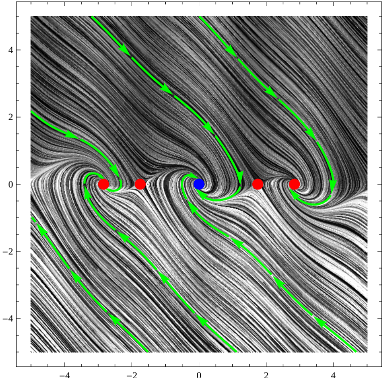
with $\tilde{c}_{mn \times 1} = \text{vec}(c)$, $x_{mn \times 1} = \text{vec}(\varphi)$, $b_{(m+n) \times 1} = [\alpha_{m \times 1}; \beta_{n \times 1}]^\top$, Let $e_n = \Big[\underbrace{1, 1, \ldots, 1}_{n \text{ times}}\Big]^\top$. Then fast construction of $A_{(m+n) \times mn} = \begin{bmatrix} e_n^\top \otimes I_m \\ I_n \otimes e_m^\top \end{bmatrix}$.

Solver used: Large scale sparse LP solver MOSEK®

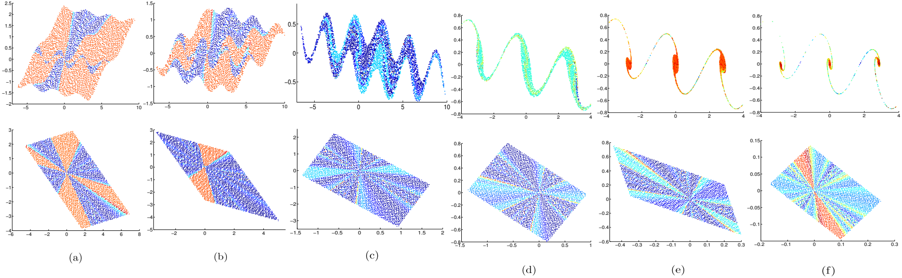
Example 1: model validation

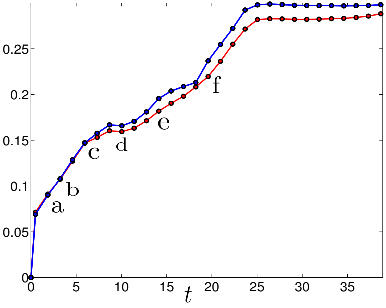


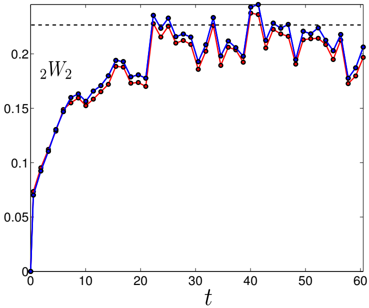
- Truth: $\ddot{x} = -ax - b\sin 2x - c\dot{x}$, $a = 0.1, b = 0.5, c = 1$.
- Five equilibria
- Model: Linearization about origin
- $\xi_0 = \mathcal{U}\left([-4,6] \times [-4,6]\right)$
- Let $y_1 = x$, $y_2 = \dot{x}$
- We plot time history of $W\left(\eta_k, \widehat{\eta}_k\right)$



Example 1 (contd.): W vs. t



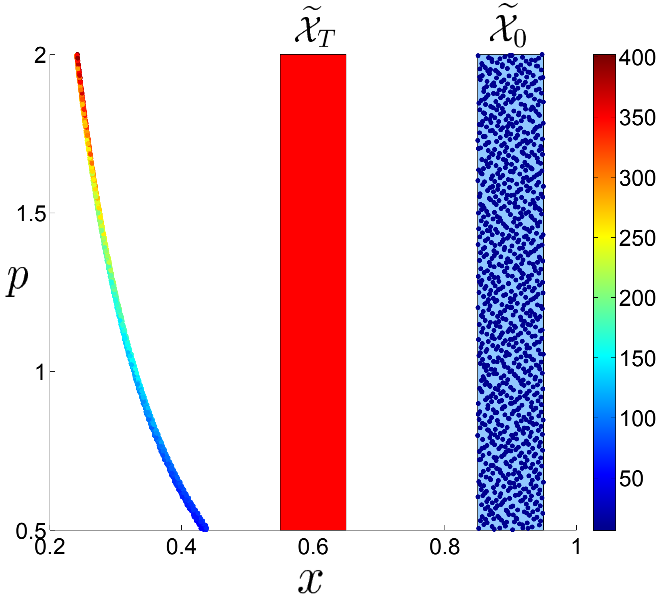




Example 2: model falsification

- Model: $\dot{x} = -px^3$,
- Parameter: $p \in \mathcal{P} = [0.5, 2]$,
- Measurement data: $\mathcal{X}_0 = [0.85, 0.95]$ at $t = 0$, and $\mathcal{X}_T = [0.55, 0.65]$ at $t = T = 4$,
- Prajna's Barrier certificate (from SOS optimization):
  $B(x,t) = B_1(x) + tB_2(x)$,
  $B_1(x) = 8.35x + 10.40x^2 - 21.50x^3 + 9.86x^4$,
  $B_2(x) = -1.78 + 6.58x - 4.12x^2 - 1.19x^3 + 1.54x^4$.
- Our approach: Show that the final measure $\xi_T(x_T, p, T) \sim \mathcal{U}(x_T, p) = \dfrac{1}{\text{vol}\left(\widetilde{\mathcal{X}}_T\right)}$ is not reachable from the initial measure $\xi_0(x_0, p) \sim \mathcal{U}(x_0, p) = \dfrac{1}{\text{vol}\left(\widetilde{\mathcal{X}}_0\right)}$ in $T = 4$.

Example 2: model falsification (contd.)



Example 3: F-16 controller robustness verification

Constant altitude longitudinal flight: $x = (\theta, V, \alpha, q)^{\top}$, $u = (T, \delta_e)^{\top}$

$$\begin{aligned}
\dot{\theta} &= q, \\
\dot{V} &= \frac{1}{m}\cos\alpha\left[T - mg\sin\theta + \bar{q}S\left(C_X + \frac{\bar{c}}{2V}C_{X_q}q\right)\right] + \frac{1}{m}\sin\alpha\left[mg\cos\theta + \bar{q}S\left(C_Z + \frac{\bar{c}}{2V}C_{Z_q}q\right)\right], \\
\dot{\alpha} &= q - \frac{\sin\alpha}{mV}\left[T - mg\sin\theta + \bar{q}S\left(C_X + \frac{\bar{c}}{2V}C_{X_q}q\right)\right] + \frac{\cos\alpha}{mV}\left[mg\cos\theta + \bar{q}S\left(C_Z + \frac{\bar{c}}{2V}C_{Z_q}q\right)\right], \\
\dot{q} &= \frac{\bar{q}S\bar{c}}{J_{yy}}\left[C_m + \frac{\bar{c}}{2V}C_{m_q}q + \frac{\left(x_{\text{cg}}^{\text{ref}} - x_{\text{cg}}\right)}{\bar{c}}\left(C_Z + \frac{\bar{c}}{2V}C_{Z_q}q\right)\right].
\end{aligned}$$

Stochastic initial condition: $x_0 = \underbrace{x_{\text{trim}}}_{\text{from SNOPT}} + x_{\text{pert}}$.

Admissible perturbation:

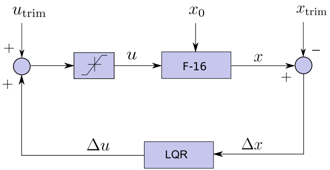
$x_{\text{pert}} \sim \mathcal{U}\left([-35^\circ, 35^\circ] \times [-50\text{ ft/s}, 50\text{ ft/s}] \times [-10^\circ, 45^\circ] \times [-60^\circ/\text{s}, 60^\circ/\text{s}]\right)$

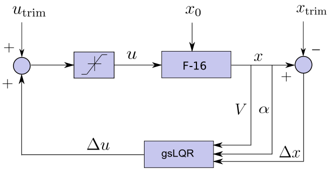
Control objective: $\min_u \mathcal{J} = \int_0^\infty \left(x^\top Q x + u^\top R u\right) dt$,

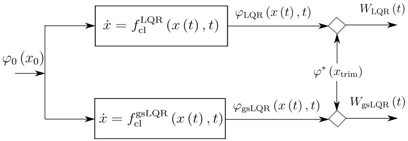
$Q = \text{diag}\left(100, 0.25, 100, 10^{-4}\right), R = \text{diag}\left(10^{-6}, 625\right)$.

Control saturation: $1000\text{ lb} \leqslant T \leqslant 28{,}000\text{ lb}, \quad -25^\circ \leqslant \delta_e \leqslant +25^\circ$.

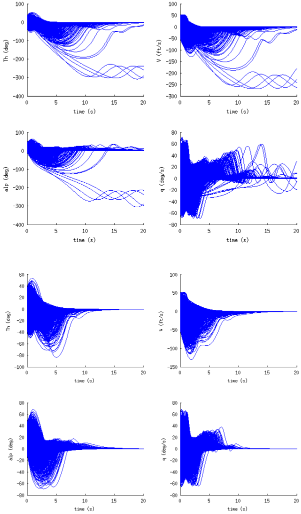
Case Study: F-16 controller robustness verification



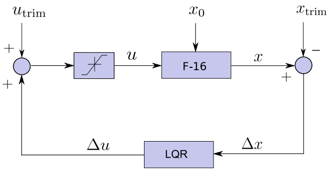


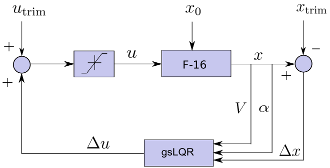


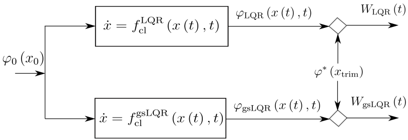
LQR vs. gsLQR Results: (MC)



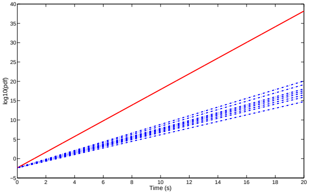
Case Study: F-16 controller robustness verification

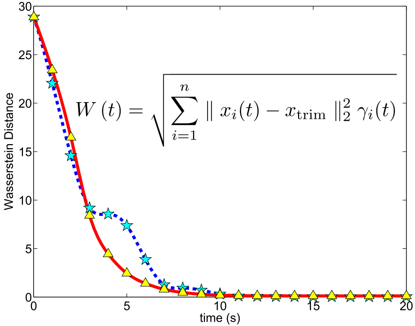






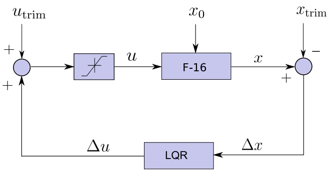
LQR vs. gsLQR Results: (MOC)

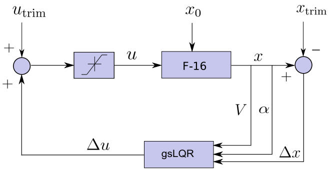


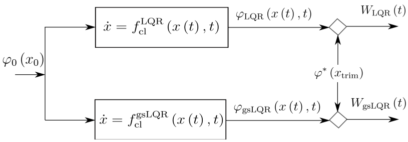


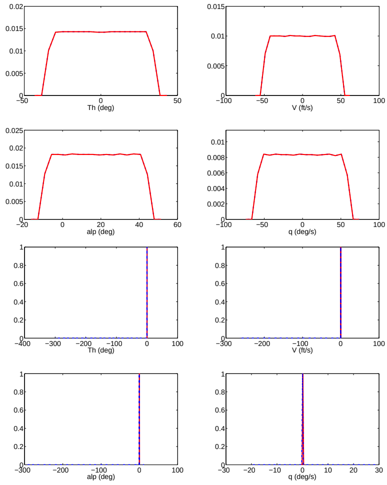
Case Study: F-16 controller robustness verification

Error marginals at $t = 0.01$ and 20 s

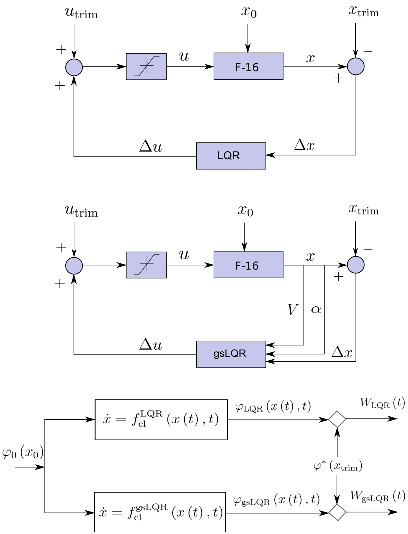




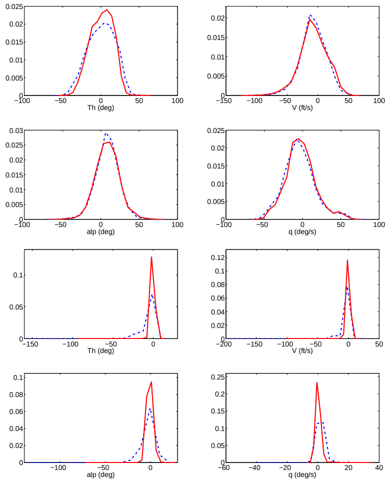




Case Study: F-16 controller robustness verification



Error marginals at $t = 1$ and 5 s



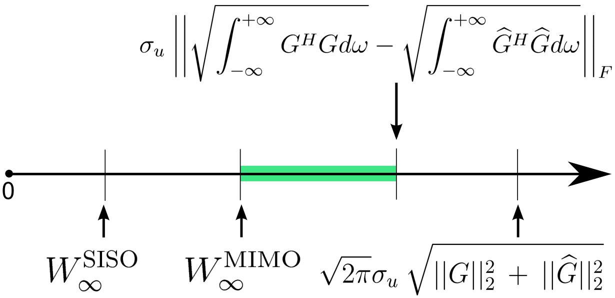
Input-Output Model Validation for LTI Systems

Theorem

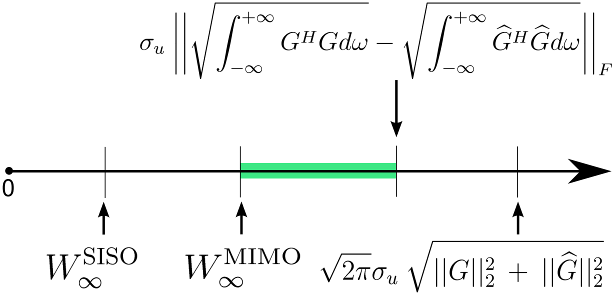
1. **SISO and MISO:** $W_\infty\left(G,\widehat{G}\right) = \sqrt{2\pi}\sigma_u \left| \, ||G(j\omega)||_2 - ||\widehat{G}(j\omega)||_2 \, \right|,$

2. **MIMO:** $$W_\infty\left(G,\widehat{G}\right) = \sqrt{2\pi}\sigma_u \left(||G(j\omega)||_2^2 + ||\widehat{G}(j\omega)||_2^2 - 2\,\mathrm{tr}\left[\left(\frac{1}{2\pi}\int_{-\infty}^{+\infty} G^H(j\omega)\,G(j\omega)\,d\omega\right)^{1/2}\left(\frac{1}{2\pi}\int_{-\infty}^{+\infty} \widehat{G}^H(j\omega)\,\widehat{G}(j\omega)\,d\omega\right)\left(\frac{1}{2\pi}\int_{-\infty}^{+\infty} G^H(j\omega)\,G(j\omega)\,d\omega\right)^{1/2}\right]^{1/2}\right)^{1/2}$$

Bounds for MIMO W_∞

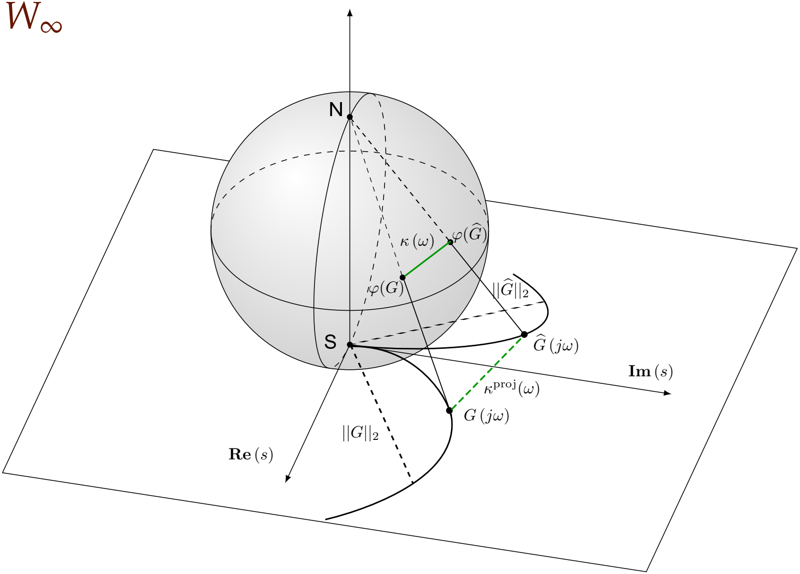


Bounds for MIMO W_∞

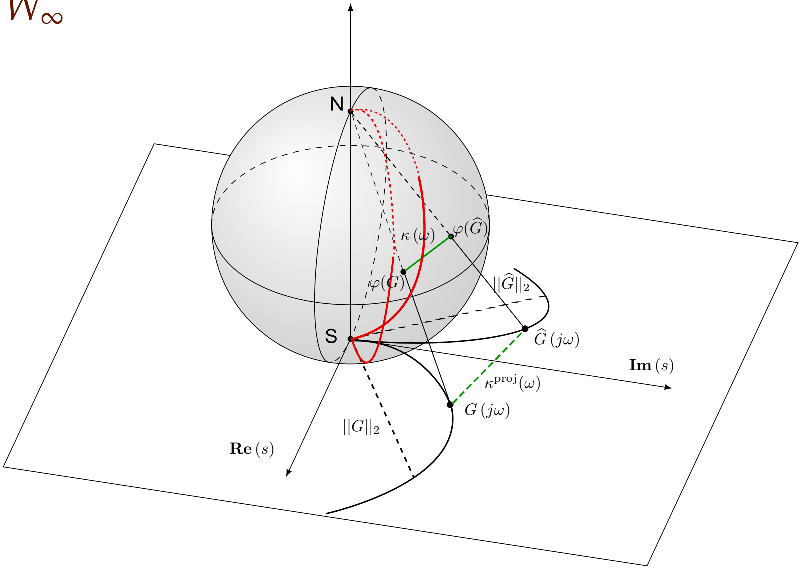


Observation: the **"green gap"** $\to 0$, if $\left[\Sigma_\infty, \widehat{\Sigma}_\infty\right] \to 0$.

Geometric Meaning & Intrinsic Normalization of SISO W_∞



Geometric Meaning & Intrinsic Normalization of SISO W_∞

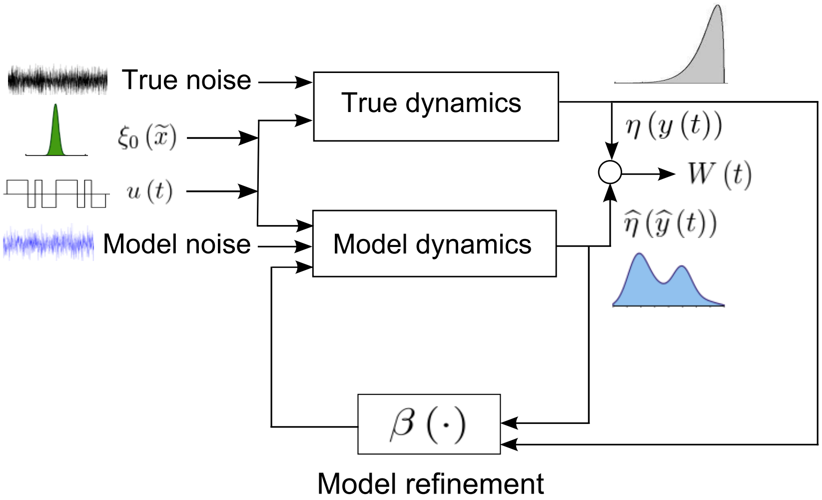


Comparing W_∞ and $\delta_\nu := \sup_\omega \kappa(\omega)$

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

- **Normalized comparison on Riemann sphere:**
  $\overline{W}_{\mathcal{S}}\left(G, \widehat{G}\right) = \frac{2}{\pi}\left|\ \arctan||G||_2 - \arctan||\widehat{G}||_2\right|$, we find $\delta_\nu \geqslant \overline{W}_{\mathcal{S}}$ under some technical conditions.

Probabilistic model refinement



Probabilistic model refinement: formulation

- Startegy: Only refine the output model (why?)
- For example, consider proposed model $\dot{\widehat{x}} = \widehat{f}\left(\widehat{x}\right), \widehat{y} = \widehat{h}\left(\widehat{x}\right)$
- Call $\widehat{y}_j^- \triangleq \widehat{y}\left(t_j\right)$. We know η_j and $\widehat{\eta}_j$.
- We seek $\beta_j : \mathbb{R}^{n_o} \mapsto \mathbb{R}^{n_o}$, so that $\widehat{y}_j^+ = \beta_j\left(\widehat{y}_j^-\right)$ satisying $\widehat{y}_j^+ \sim \eta_j$ and $\widehat{y}_j^- \sim \widehat{\eta}_j$
- Then the refined model is: $\dot{\widehat{x}} = \widehat{f}\left(\widehat{x}\right), \widehat{y}_j^+ = \beta_j \circ \widehat{h}\left(\widehat{x}\right)$
- Seek optimal push-forward:
  $\inf\limits_{\beta(\cdot)} \underbrace{\int_{\widehat{\mathcal{Y}}} \| \beta_j\left(\widehat{y}_j^-\right) - \widehat{y}_j^- \|^2_{\ell_2(\mathbb{R}^{n_o})} \; \widehat{\eta}_j d\widehat{y}_j^-}_{J_2(\beta)}$, subject to $\eta_j = \beta_j \sharp \widehat{\eta}_j$.

Probabilistic model refinement: some background

- (Brenier, 1991): optimal $\beta^{\star}(\cdot)$ exists and is unique. Further, $\beta^{\star}(\cdot) = \nabla\psi$. Here $\psi : \mathbb{R}^{n_o} \mapsto \mathbb{R}$, and is convex.

- (Benamou & Brenier, 2001): Consider the space-time variational formulation

  $$T \inf_{(\varphi,v)} \underbrace{\int_{\mathbb{R}^{n_o}} \int_0^T \varphi(\widehat{y},s) \parallel v(\widehat{y},s) \parallel^2_{\ell_2(\mathbb{R}^{n_o})} \, d\widehat{y} ds}_{J_3(\varphi,v)}$$ subject to

  $$\frac{\partial\varphi}{\partial s} + \nabla\cdot(\varphi v) = 0,\ \varphi(\cdot,0) = \widehat{\eta},\ \varphi(\cdot,T) = \eta.$$ Then $J_3^{\star} = W^2$ and $v^{\star}$ is gradient flow.

- $$W^2 = \underbrace{\inf_{\varrho \in \mathcal{P}_2(\rho,\widehat{\rho})} J_1(\varrho)}_{\text{infinite dimensional LP}} = \underbrace{\inf_{\beta : c(\beta)=0} J_2(\beta)}_{\text{Nonlinear nonconvex optimization}} = \underbrace{T \inf_{(\varphi,v)} J_3(\varphi,v)}_{\text{Nonsmooth convex optimization}}$$

Linear Gaussian model refinement

- Theorem: Consider discrete-time deterministic LTI pairs: (A, C), $\left(\widehat{A}, \widehat{C}\right)$, sarting with $\xi_0 = \mathcal{N}\left(\mu_0, \Sigma_0\right)$. Then refined model is: $\widehat{x}_{j+1} = \widehat{A}\widehat{x}_j$, $\widehat{y}_j^+ = \Theta_j \widehat{C}\widehat{x}_j + \theta_j$.

  $\Theta_j = \Sigma_j^{1/2}\left(\Sigma_j^{1/2}\widehat{\Sigma}_j\Sigma_j^{1/2}\right)^{-1/2}\Sigma_j^{1/2}$, and $\theta_j = \mu_j - \widehat{\mu}_j$.

  The s^{th} synthetic time PDF at j^{th} physical time is: $\mathcal{N}\left(\mu_{\widehat{y}\to y}\left(s\right), \Sigma_{\widehat{y}\to y}\left(s\right)\right)$, where

$$\mu_{\widehat{y}\to y}\left(s\right) = \left[\left(1-s\right)\,\widehat{C}\widehat{A}^j + s\,CA^j\right]\mu_0,$$

$$\Sigma_{\widehat{y}\to y}\left(s\right) = \left[\left(1-s\right)\,I + s\,\Theta\left(j\right)\right]\left(\left(\widehat{C}\widehat{A}^j\right)\Sigma_0\left(\widehat{C}\widehat{A}^j\right)^\top\right)\left[\left(1-s\right)\,I + s\,\Theta\left(j\right)\right].$$

Linear Gaussian model refinement

- Theorem: Consider discrete-time deterministic LTI pairs: (A, C), $\left(\widehat{A}, \widehat{C}\right)$, sarting with $\xi_0 = \mathcal{N}\left(\mu_0, \Sigma_0\right)$. Then refined model is: $\widehat{x}_{j+1} = \widehat{A}\widehat{x}_j$, $\widehat{y}_j^+ = \Theta_j \widehat{C}\widehat{x}_j + \theta_j$.
  $\Theta_j = \Sigma_j^{1/2}\left(\Sigma_j^{1/2}\widehat{\Sigma}_j\Sigma_j^{1/2}\right)^{-1/2}\Sigma_j^{1/2}$, and $\theta_j = \mu_j - \widehat{\mu}_j$.
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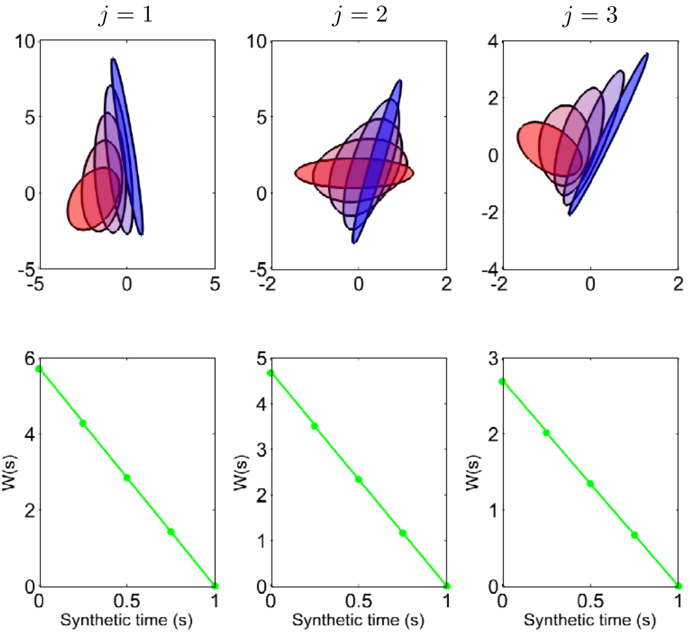
$$\mu_{\widehat{y}\to y}(s) = \left[(1-s)\ \widehat{C}\widehat{A}^j + s\, CA^j\right]\mu_0,$$

$$\Sigma_{\widehat{y}\to y}(s) = \left[(1-s)\ I + s\,\Theta(j)\right]\left(\left(\widehat{C}\widehat{A}^j\right)\Sigma_0\left(\widehat{C}\widehat{A}^j\right)^\top\right)\left[(1-s)\ I + s\,\Theta(j)\right].$$

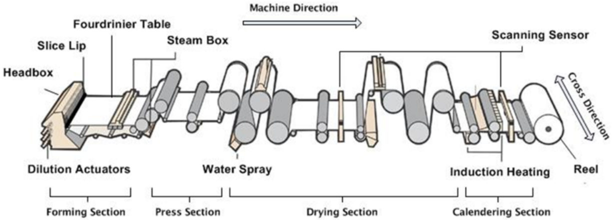
- Example: $A = \begin{bmatrix} 0.4 & -0.1 \\ 2 & 0.6 \end{bmatrix}$, $\widehat{A} = \begin{bmatrix} 0.2 & -0.7 \\ -0.7 & 0.1 \end{bmatrix}$, $C = \begin{bmatrix} -1 & 0.03 \\ -0.2 & 0.8 \end{bmatrix}$, $\widehat{C} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. $\mu_0 = \{1, 3\}^\top, \Sigma_0 = \begin{bmatrix} 10 & 6 \\ 6 & 7 \end{bmatrix}$

Linear Gaussian model refinement: example



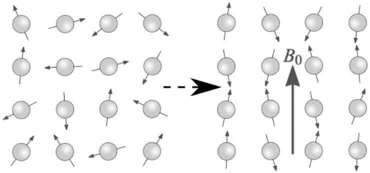
Application: finite horizon density tracking

- Process industry applications

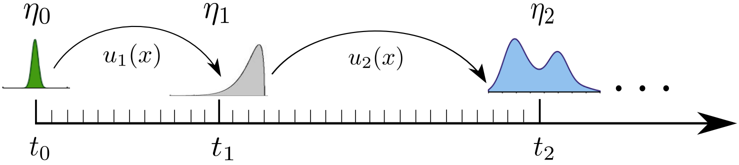


Source: Chu *et.al.* (2011), "Model Predictive Control and Optimization for Papermaking Process", doi: 10.5772/18535.

- NMR spectroscopy and MRI applications



Application: linear Gaussian tracking

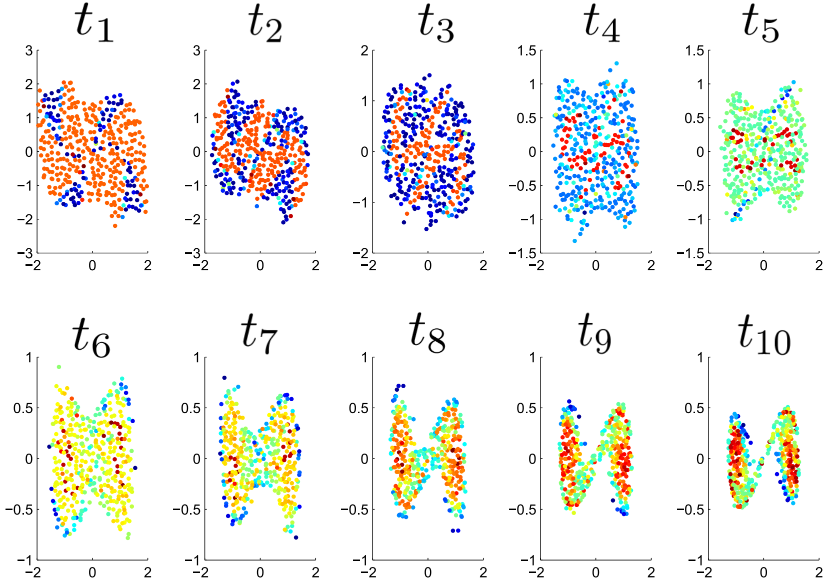


- Theorem: Consider tracking Gaussians $\eta_j = \mathcal{N}\left(\mu_j, \Sigma_j\right)$, under LTI structure $x_{j+1} = Ax_j + Bu_j$. The state feedback $u_j^{\star} \triangleq u^{\star}\left(x_j\right)$ guaranteeing optimal transport
  1. exists iff $\left(\Theta_j - A\right), \theta_j \in \ker\left(I - BB^{\dagger}\right)$
  2. if exists, then must be affine form $u_j^{\star} = K_j x_j + \kappa_j$, where $K_j = B^{\dagger}\left(\Theta_j - A\right) - \left(I - BB^{\dagger}\right) R$, and $\kappa_j = B^{\dagger}\theta_j - \left(I - BB^{\dagger}\right) r$
  3. is unique, if B is full rank.

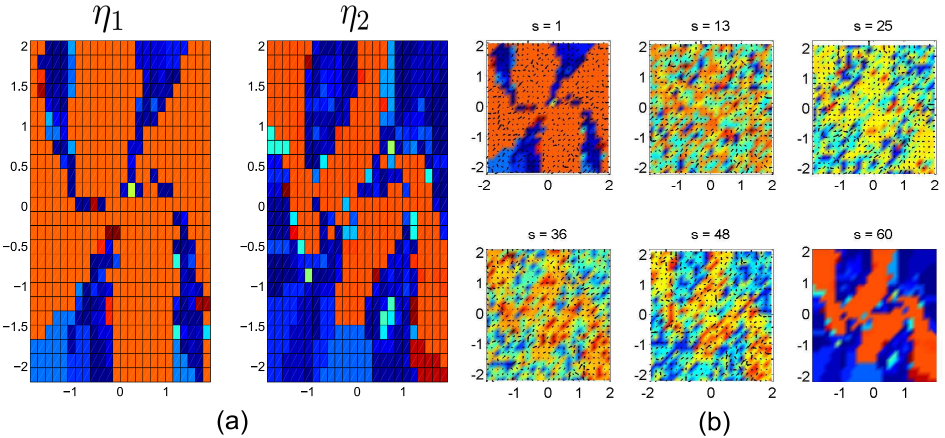
Application: data-driven modeling

- Duffing vector field (unknown to modeler) to generate data: $\dot{x}_1 = x_2, \quad \dot{x}_2 = -\alpha x_1^3 - \beta x_1 - \delta x_2$, $y = \{x_1, x_2\}^\top$, $\alpha = 1$, $\beta = -1$, $\delta = 0.5$
- Lioville MOC with 500 samples from $\xi_0 = \mathcal{U}\left([-2, 2]^2\right)$
- 10 snapshot data $\{t_j, \eta_j\}_{j=1}^{10}$
- Subdivided each of the 10 intervals $[t_j, t_{j+1})$, $j = 0, \ldots, 9$ into 60 sub-intervals.
- Want to compute optimal transport vector field $v_{j \to j+1}$ for each of those intervals

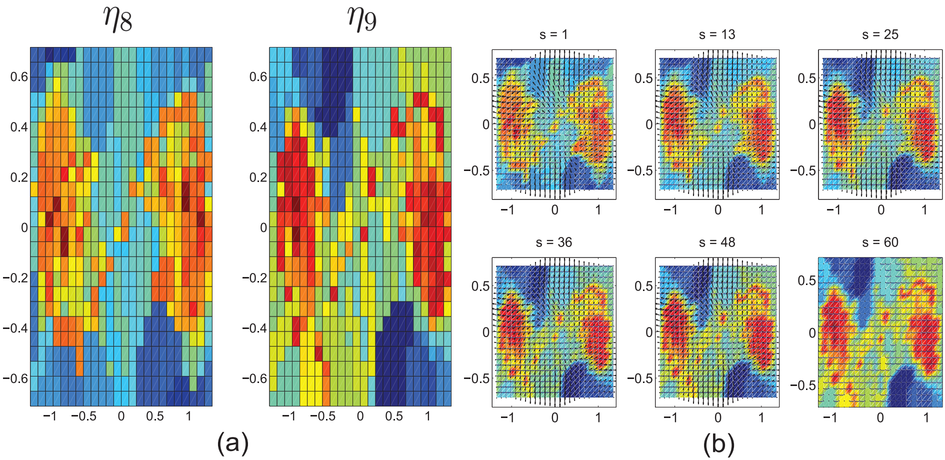
Application: data-driven modeling



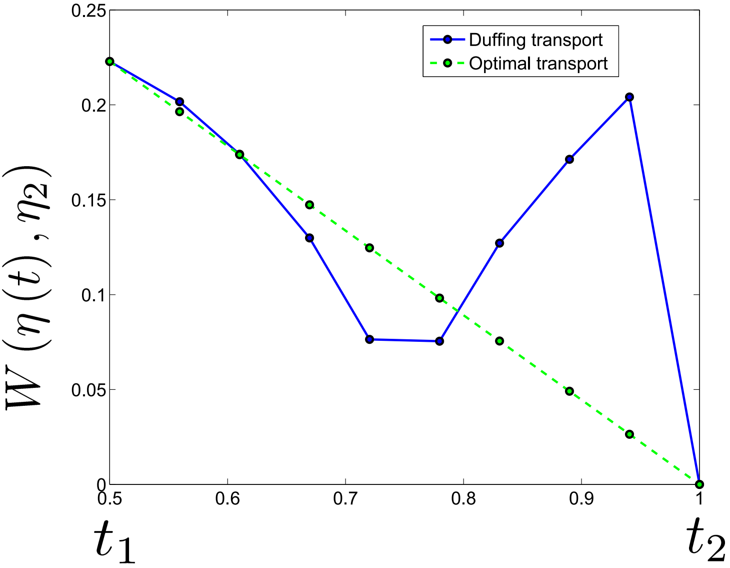
Application: data-driven modeling of $v_{1\to2}$



Application: data-driven modeling of $v_{8\to 9}$



Application: Duffing transport vs. optimal transport for $[t_1, t_2)$



Conclusions

- Unifying framework for probabilistic V&V
- Transport-theoretic Wasserstein distance as (in)validation measure
- Probabilistic framework for model refinement
- Possible extensions:
  (i) compositionality in probabilistic V&V
  (ii) optimal transport based model reduction
  (iii) application to ensemble tracking, e.g. MRI and NMR

Conclusions

- Unifying framework for probabilistic V&V
- Transport-theoretic Wasserstein distance as (in)validation measure
- Probabilistic framework for model refinement
- Possible extensions:
  (i) compositionality in probabilistic V&V
  (ii) optimal transport based model reduction
  (iii) application to ensemble tracking, e.g. MRI and NMR

Thank You

Backup Slides

Some details on noise KL expansion

- KL expansion of $\eta(\omega, t) \in L_2(\Omega, \mathscr{F}, \mathbb{P})$, is:
$\eta(\omega, t) \overset{\text{m.s.}}{=} \sum_{i=1}^{\infty} \sqrt{\Lambda_i} \zeta_i(\omega) e_i(t)$
- Covariance function $C(t_1, t_2) \triangleq$
$\text{cov}(\eta(\omega, t_1) - \mathbb{E}[\eta(\omega, t_1)], \eta(\omega, t_2) - \mathbb{E}[\eta(\omega, t_2)])$,
$t_1, t_2 \in [0, T]$
- Fredholm integral eqn. of second kind:
$\int_0^T C(t_1, t_2) e_i(t_2) dt_2 = \Lambda_i e_i(t_1)$

Noise $\mathcal{W}(\omega, t)$ in SDE	$C(t_1, t_2)$ **for** $\mathcal{W}(\omega, t)$	$\eta(\omega, t)$	**KL expansion of** $\eta(\omega, t)$**,** $0 < t \leqslant T$
Wiener process	$\sigma^2 (t_1 \wedge t_2)$	GWN	$\sqrt{\frac{2}{T}} \sum_{i=1}^{\infty} \zeta_i(\omega) \cos\left(\left(i - \frac{1}{2}\right) \frac{\pi t}{T}\right)$
Compound Poisson process	$\lambda\sigma^2 (t_1 \wedge t_2) + (\lambda\mu)^2 t_1 t_2$	PWN	$\sum_{i=1}^{\infty} \bar{\zeta}_i(\omega) \frac{\frac{2}{\beta_i} \sqrt{\Lambda_i}}{\sqrt{2T - \beta_i \sin \frac{2T}{\beta_i}}} \cos\left(\frac{t}{\beta_i}\right)$

On the KL expansion of compound Poisson process

$\overline{\zeta}_i(\omega)$ are i.i.d random variables from $\mathcal{N}(0,1)$, $\beta_i \triangleq \sqrt{\frac{\Lambda_i}{\lambda\sigma^2}}$, $\forall\, i \in \mathbb{N}$, and $\Lambda_i > 0$ solves

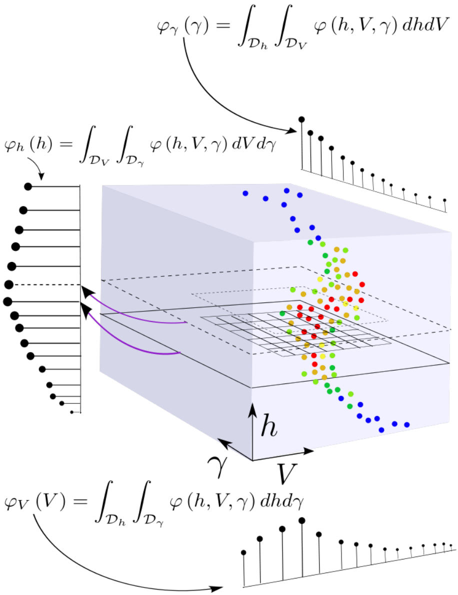
$$\tan\left(\sigma T\sqrt{\frac{\lambda}{\Lambda_i}}\right) = \left[1 + \frac{1}{\lambda T}\left(\frac{\sigma}{\mu}\right)^2\right]\left(\sigma T\sqrt{\frac{\lambda}{\Lambda_i}}\right),$$

where the parameters $\lambda, \sigma, \mu, T > 0$.

Application of KL+ MOC algorithm to nonlinear estimation

- Compute particle filter posterior: $\xi^{+}_{\text{Particle}}\left(x(t), t\right)$
- Compute posterior from our proposed method: $\xi^{+}_{\text{KLMOC}}\left(x(t), t\right)$
- Compute the "distances" of $\xi^{+}_{\text{Particle}}\left(x(t), t\right)$ and $\xi^{+}_{\text{KLMOC}}\left(x(t), t\right)$ from the true posterior $\xi^{+}_{\text{True}}\left(x(t), t\right)$
- Distance metric on the space of PDFs: Wasserstein distance W
- $W \triangleq \left(\inf\limits_{\gamma \in \mathcal{M}(\varphi, \widehat{\varphi})} \mathbb{E}\left[\| x - \widehat{x} \|_2^2\right]\right)^{\frac{1}{2}}$, $\mathcal{M}\left(\varphi, \widehat{\varphi}\right) = \{\text{All joint PDFs}\, \gamma\left(x, \widehat{x}\right) \,: x \sim \varphi, \widehat{x} \sim \widehat{\varphi}\}$.
- W = minimum amount of work needed to morph one PDF to other

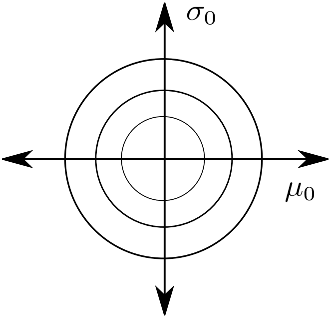
Marginal computation



Worst case initial PDF: model discrimination problem

Scalar linear systems

- Deterministic (continuous and discrete time): gap $\propto \sqrt{m_{20}}$
- Construction:



- Stochastic: depends on m_{20}, m_{10} and
  $s\left(F_0\right) := \sqrt{2}\,\mathbb{E}\left[x_0 \operatorname{erf}^{-1}\left(2F_0\left(x_0\right) - 1\right)\right]$.

Vector linear systems: Conjecture

- Deterministic: gap $\propto \sqrt{\parallel \mu_0 \parallel_2^2 + \left(\operatorname{tr}\left(P_0\right)\right)^2}$
- Can prove for Gaussian family

Worst case initial PDF: example

Uniform PDF $\not\Leftrightarrow \sup_{\rho_0} {}_2W_2(t)$