Control Optimization for Uncertain Systems via the Koopman Operator

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Optimal Decision-Making Under Uncertainty

- The need to make decisions under uncertainty arises often in engineering and scientific applications

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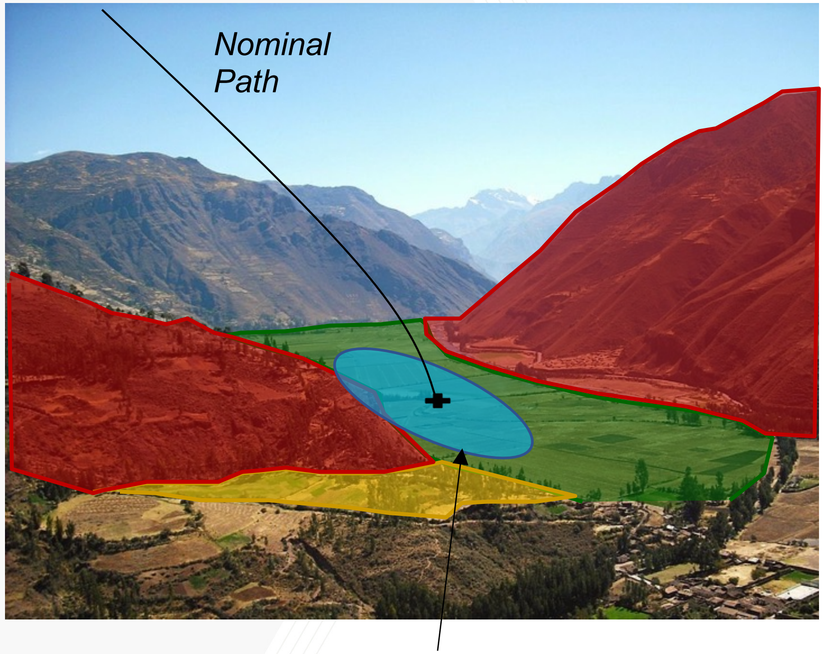
Airdrop Package Delivery Using Ballistic Parachute



Predicted Dispersion

Q: Where should the package be dropped?

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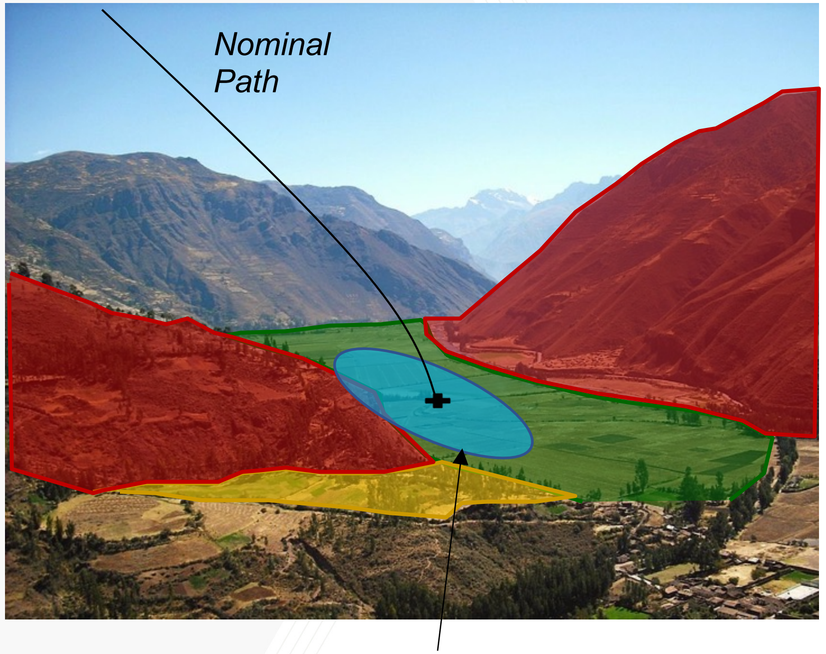

Predicted Dispersion

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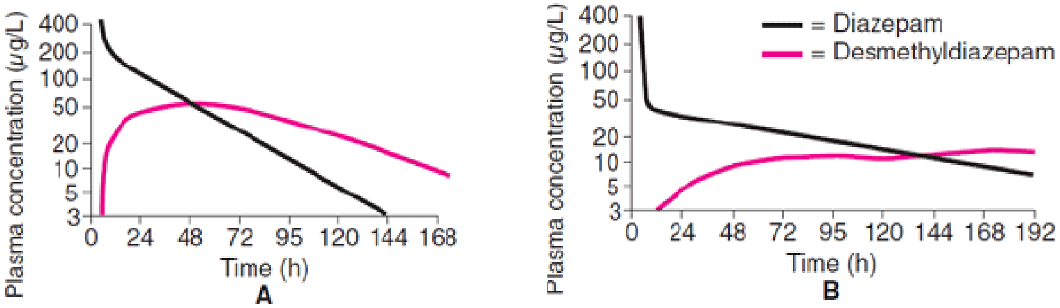
Pharmacokinetics

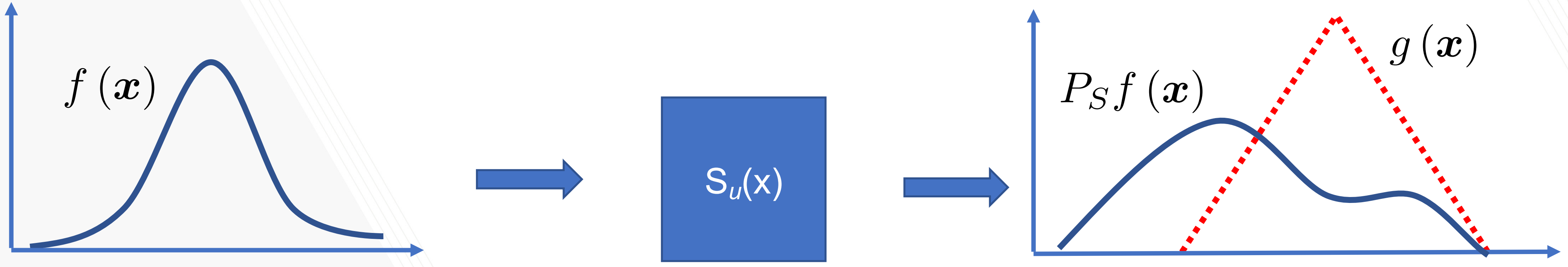
Patient A ***Patient B***



Data from Allen et al., 1980

Q: What dose should we give patients?

Optimal Decision-Making Under Uncertainty



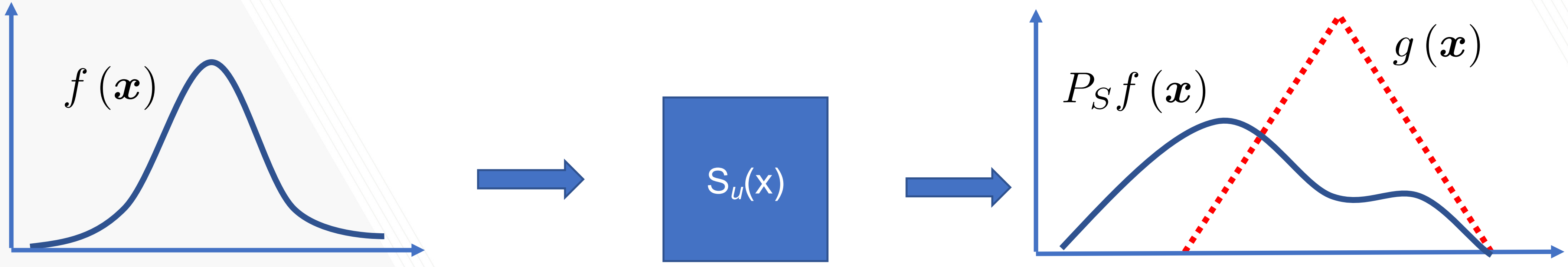
Initial density over uncertain states and parameters

State transformation under control selection u

"Pushed-forward" density and objective function

Choose u that maximizes $\mathbb{E}\left[g(X)\,|X \sim P_S f\right] = \int_{S(\Omega)} P_S f(\boldsymbol{x})\, g(\boldsymbol{x})\, d\boldsymbol{x}$

Optimal Decision-Making Under Uncertainty



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Okay…but how do we compute $P_S f(x)$ for nonlinear/non-Gaussian systems?

Forward Density Propagation for Uncertain Systems

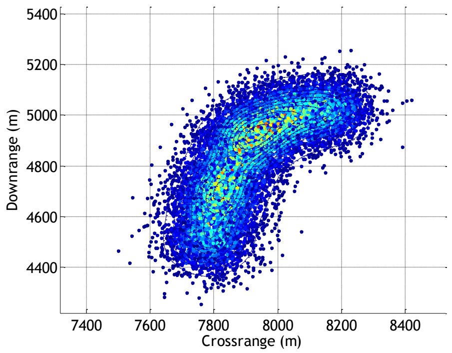
Frobenius-Perron (FP) Operator

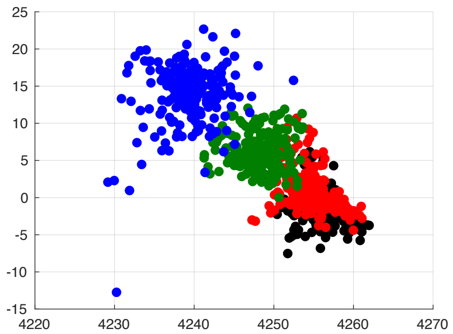
$$\int_A P_S f \, d\mu = \int_{S^{-1}(A)} f \, d\mu$$

$$S: X \to X$$

(measure preserving)

Monte Carlo Simulation





Polynomial Chaos

$$Y = \sum_{j=0}^{p} y_j \psi_j(\Xi) = \eta(x) \qquad X_P = \sum_{j=0}^{p} x_j \psi_j(\Xi)$$

The Koopman Operator

$$g : \mathbb{R}^n \to \mathbb{R}$$

Observable

$$S : \mathbb{R}^n \to \mathbb{R}^n$$

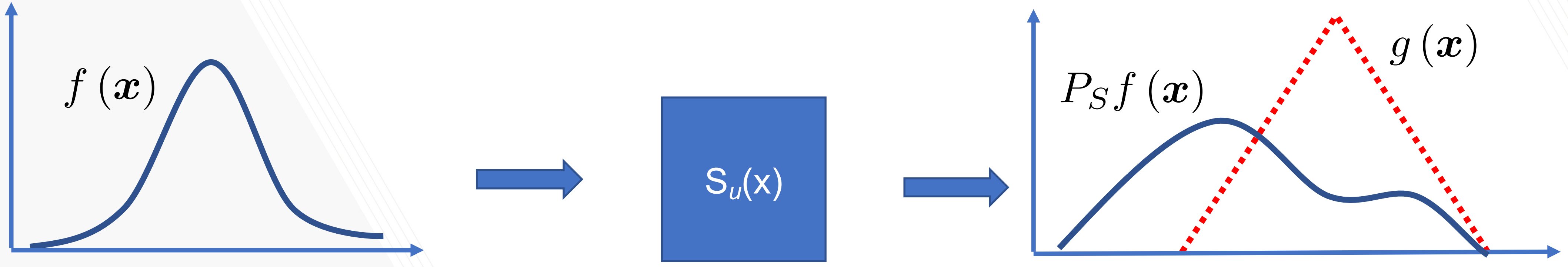
State Map

$$\mathcal{K}_S g\left(\boldsymbol{x}\right) = g\left(S\left(\boldsymbol{x}\right)\right)$$

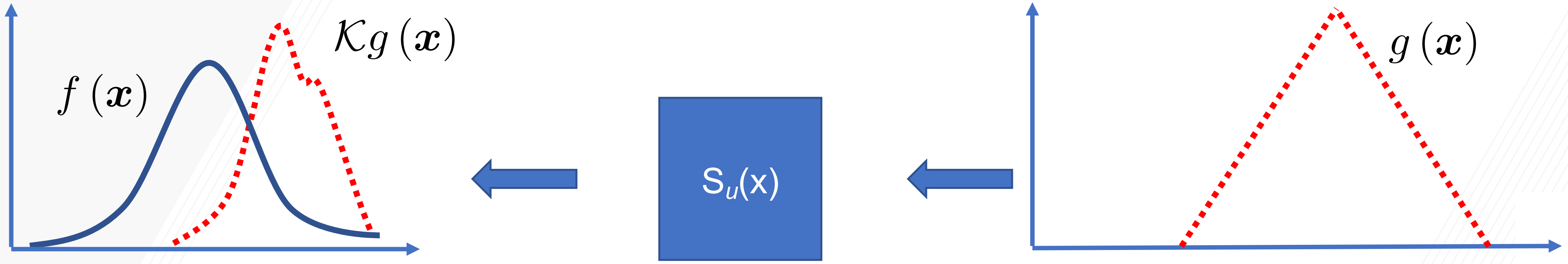
Koopman Operator

- Properties of Koopman operator of a system reveals properties of the underlying system
- Recent advancement in the literature for approximating via data-driven methods
  - Extended Dynamic Mode Decomposition (Williams *et al.* 2014, Korda and Mezic 2018)

Relationship with Uncertain Systems



$$\mathbb{E}\left[\mathcal{K}g(X)\,|X \sim f\right] = \int_{\Omega} f(\boldsymbol{x})\,\mathcal{K}g(\boldsymbol{x})\,d\boldsymbol{x} \quad = \quad \mathbb{E}\left[g(X)\,|X \sim P_S f\right] = \int_{S(\Omega)} P_S f(\boldsymbol{x})\,g(\boldsymbol{x})\,d\boldsymbol{x}$$



Benefits of the Koopman Expectation

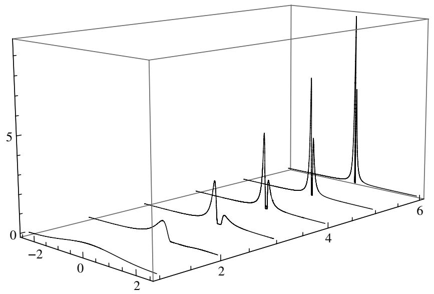
$$\mathbb{E}\left[\mathcal{K}g\left(X\right)|X\sim f\right]=\int_{\Omega}f\left(\boldsymbol{x}\right)\mathcal{K}g\left(\boldsymbol{x}\right)d\boldsymbol{x}$$

vs.

$$\mathbb{E}\left[g\left(X\right)|X\sim P_{S}f\right]=\int_{S(\Omega)}P_{S}f\left(\boldsymbol{x}\right)g\left(\boldsymbol{x}\right)d\boldsymbol{x}$$

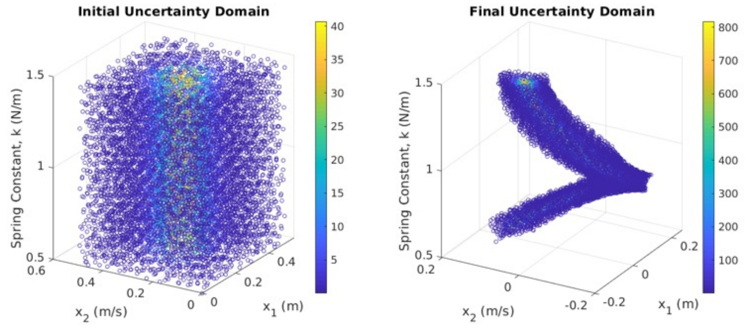
Pull-Back (Koopman) Expectation

Push-Forward (FP) Expectation



Halder and Bhattacharya, 2011

- Improved numerical stability
- Simpler evaluation
  - Domain of integration is initial domain Ω vs its image $S(\Omega)$
  - Provides well-defined structure of data, leading to simpler solution approaches (e.g., quadrature integration)



Meyers *et al.*, ACC 2019.

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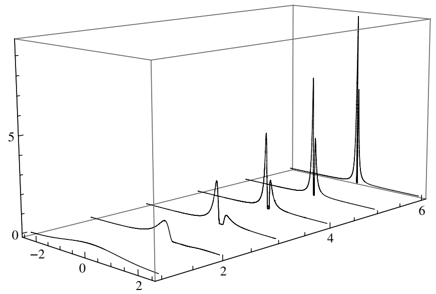

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- Improved numerical stability
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  - Provides well-defined structure of data, leading to simpler solution approaches (e.g., quadrature integration)
- Computing expectation of multiple observables with varying supports in space-time
  - Pull-back each to a common domain domain ➞ Single, vector-valued expectation calculation

Meyers *et al.*, ACC 2019.

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$$\mathbb{E}\left[\mathcal{K}g\left(X\right)|X\sim f\right]=\int_{\Omega}f\left(\boldsymbol{x}\right)\mathcal{K}g\left(\boldsymbol{x}\right)d\boldsymbol{x}$$

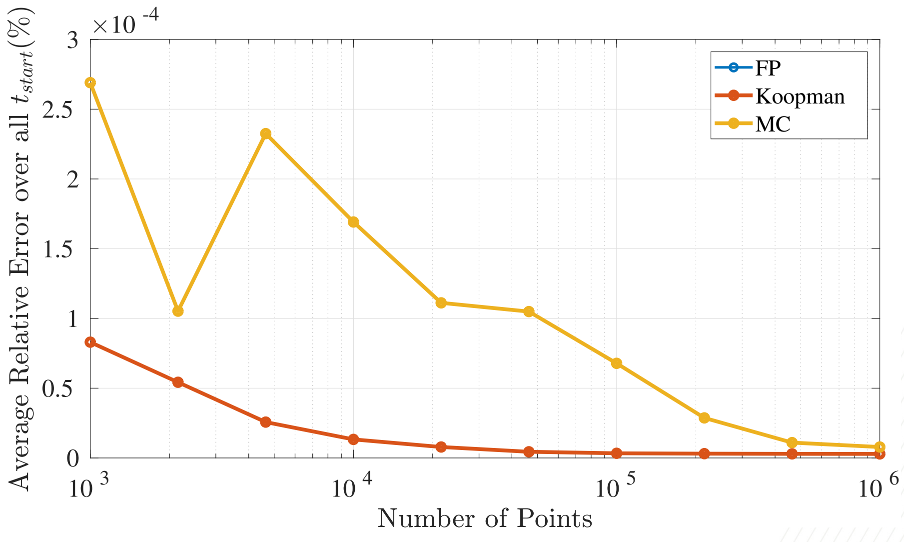
vs.

Monte Carlo Simulation

Pull-Back (Koopman) Expectation

- Faster convergence
- Error bounds / tolerancing via quadrature integration

- Downside: Koopman expectation assumes no process noise.
  - Application limited to systems which have only parametric uncertainty



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Pull-Back (Koopman) Expectation

vs.

Generalized Polynomial Chaos (gPC)

- In general, they are not the same
- However, there is an equivalence between the Koopman expectation and non-intrusive gPC when computing the mean value of an observable function $g(\boldsymbol{x})$

1

Koopman Expectation

$$\int_{\Omega}\mathcal{K}g(\boldsymbol{x})f(\boldsymbol{x})d\boldsymbol{x}=\int_{\Omega}\underbrace{\eta\left(f_p(\boldsymbol{\xi})\right)}_{g\left(S\left(f_p(\boldsymbol{\xi})\right)\right)=\mathcal{K}g(\boldsymbol{x})}\psi_0(\boldsymbol{\xi})p(\boldsymbol{\xi})d\boldsymbol{\xi}$$

gPC computation of mean of transformed RV

Benefits of the Koopman Expectation

$$\mathbb{E}\left[\mathcal{K}g\left(X\right)|X \sim f\right] = \int_{\Omega} f\left(\boldsymbol{x}\right)\mathcal{K}g\left(\boldsymbol{x}\right)d\boldsymbol{x}$$

Pull-Back (Koopman) Expectation

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Generalized Polynomial Chaos (gPC)

- In general, they are not the same
- However, there is an equivalence between the Koopman expectation and non-intrusive gPC when computing the mean value of an observable function $g(\boldsymbol{x})$
- **Koopman** advantage: When computing higher-order moments, Koopman method (redefining observable) requires a lot less integrals than gPC
- **gPC** advantage: You can sample from transformed distribution (Koopman expectation only provides expected values)

Using the Koopman Expectation for Probabilistic Optimization

- In practice, we do not compute Koopman operator $\mathcal{K}_S$
- Instead, we compute *action* of the Koopman operator on observable functions of interest at discrete points in state space $\mathcal{K}_S g(x_i)$
  - Then integrals can be approximated via quadrature

$$\int_{\Omega} \mathcal{K}_S g(x) f_0(x) dx \approx \sum_{i=1}^{N} \mathcal{K}_S g(x_i) f_0(x_i) w_i$$

Note: We can also use other methods such as Monte Carlo integration to compute this as well.

$\mathcal{K}_S g(x_i)$: From each discrete sample x_i, forward simulate and compute observable function

$f_0(x_i)$: Initial uncertainty PDF evaluated at sample x_i

w_i: Quadrature weight

Meyers *et al.*, ACC 2019.

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Probabilistic Optimization via the Koopman Expectation

- We wish to solve the following optimization problem:

$$\boldsymbol{u}^* = \underset{\boldsymbol{u}\in\mathcal{U}}{\arg\min} \int_{\Omega} \mathcal{K}_S g(\boldsymbol{x},\boldsymbol{u}) f_0(\boldsymbol{x}) d\boldsymbol{x}$$

Minimize expected value of cost

subject to:

$$\int_{\Omega} \mathcal{K}_S \boldsymbol{c}(\boldsymbol{x},\boldsymbol{u}) f_0(\boldsymbol{x}) d\boldsymbol{x} < \boldsymbol{r}$$

Satisfy chance constraints

Meyers *et al.*, ACC 2019.

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subject to:

$$\int_{\Omega} \mathcal{K}_S \boldsymbol{c}(\boldsymbol{x}, \boldsymbol{u}) f_0(\boldsymbol{x}) d\boldsymbol{x} < \boldsymbol{r}$$

Key point: Because cost and constraint functions pulled back to initial time via Koopman operator, $f_0(\boldsymbol{x})$ is never explicitly propagated forward in time.

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Example 1: Bouncing Ball

Bouncing ball in 2D with uncertain coefficient of restitution.
Compute expected cost value (no optimization).

System:

$$\ddot{\boldsymbol{x}} = \begin{bmatrix} \ddot{x} \\ \ddot{z} \end{bmatrix} = \begin{bmatrix} 0 \\ -g \end{bmatrix}, \qquad x_0 = 2\,\mathrm{m}, \dot{x}_0 = 2\,\mathrm{m/s}, z_0 = 50\,\mathrm{m}, \dot{z}_0 = 0\,\mathrm{m/s}$$

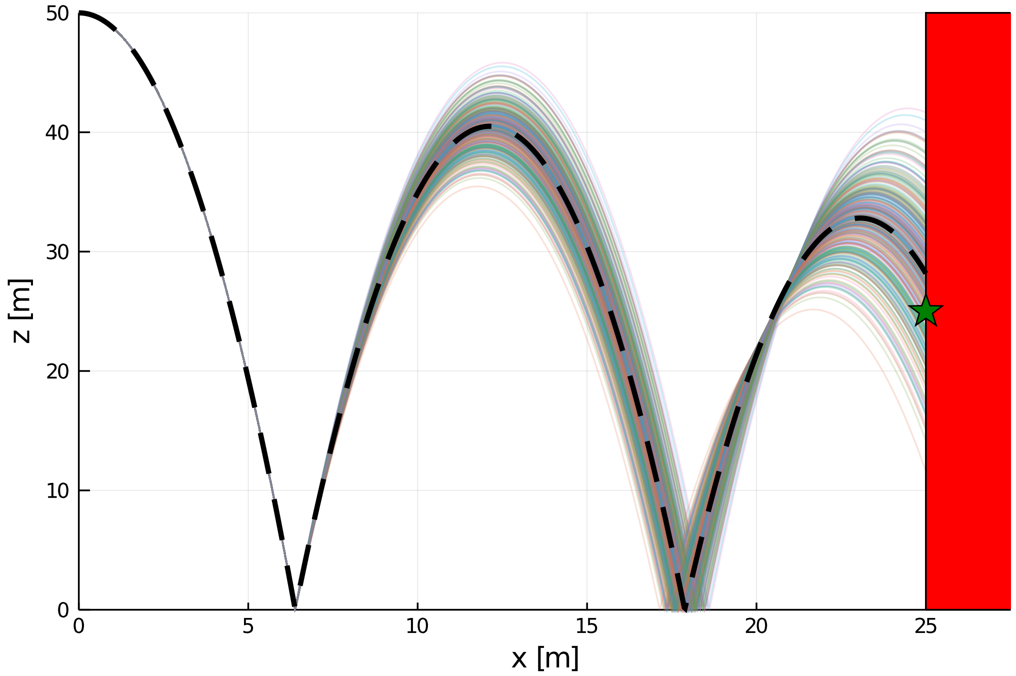
$$\dot{z}^+ = -\alpha\dot{z}^- \qquad \text{when } z = 0$$

Uncertainty:

$$\alpha \sim \mathcal{N}(0.9, 0.02) \qquad \text{truncated at 0.84 and 1}$$

Cost:

$$g(\boldsymbol{x}) = (z - z^*)^2$$



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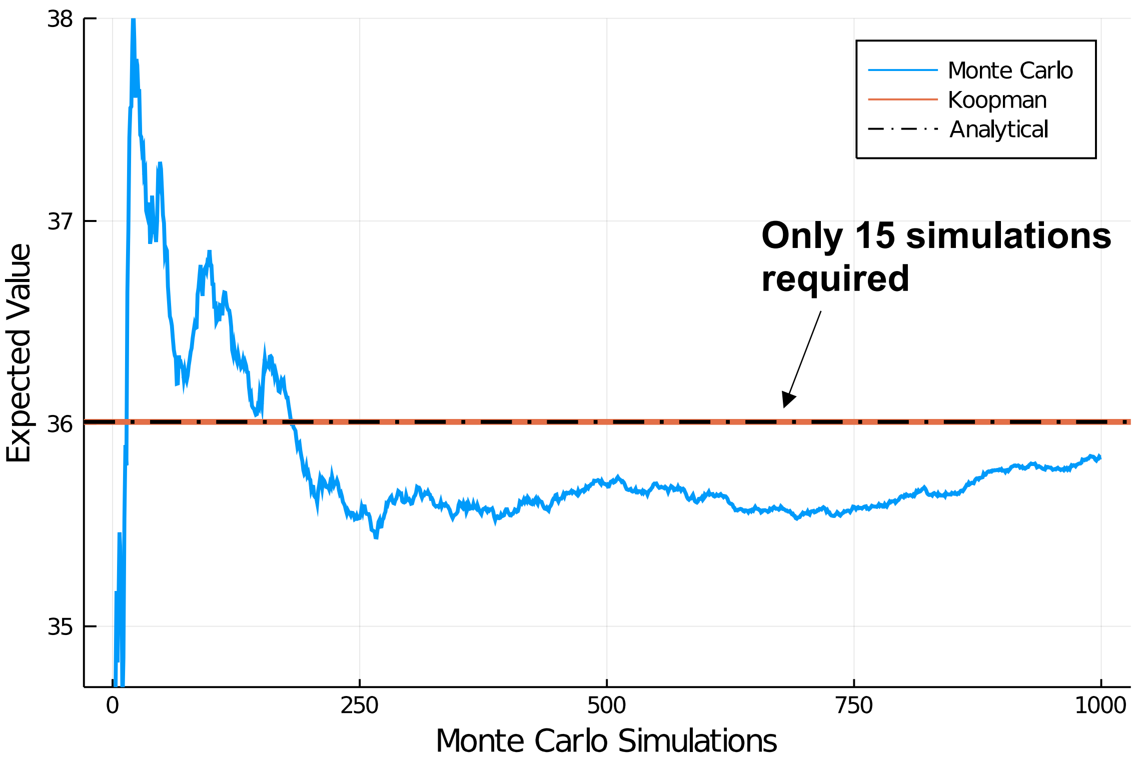

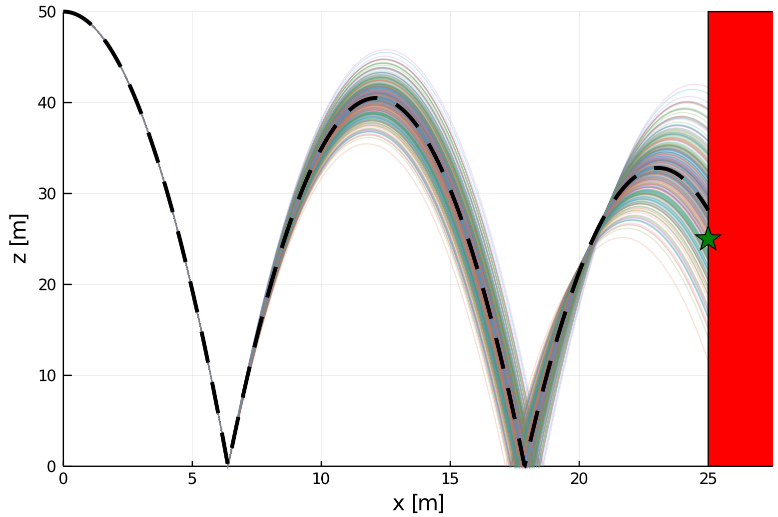

	Analytical	Monte Carlo	Koopman
No. of Simulations	-	100,000	**15**
Exp. Value (m^2)	**36.008**	35.782	**36.008**
Computation Time (s)	-	2.060	0.0012

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Initial Conditions to Optimize:

$$x_0 \in [-100\,\mathrm{m}, 0\,\mathrm{m}]$$

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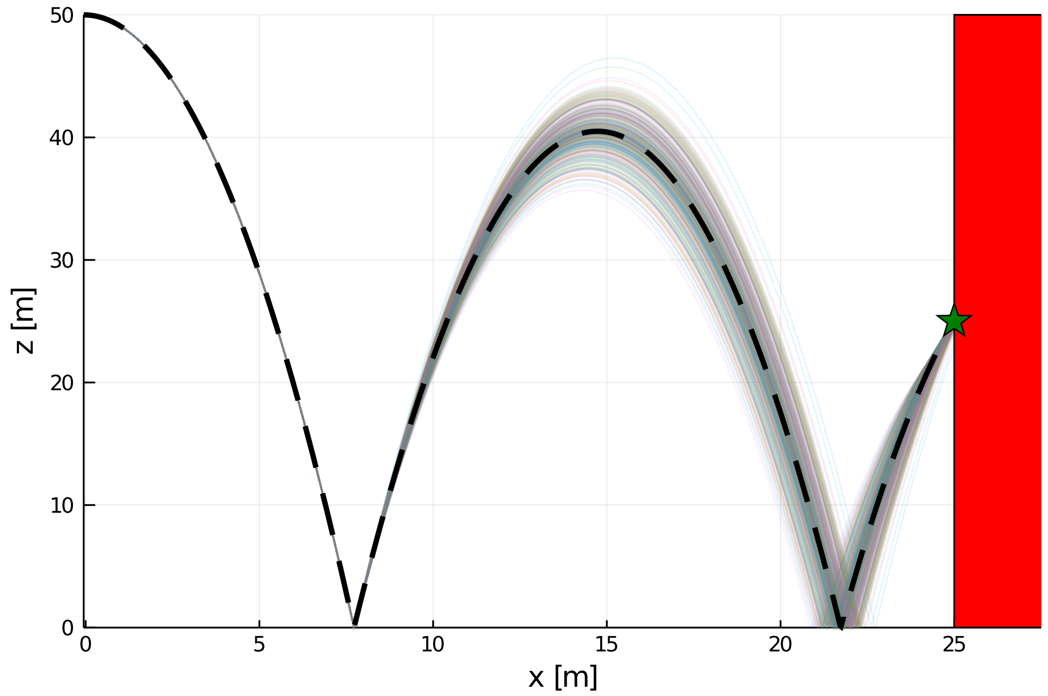

Gradient-Based optimization to solve $\boldsymbol{u}^* = \underset{\boldsymbol{u} \in \mathcal{U}}{\arg\min} \int_{\Omega} \mathcal{K}_S\, g(\boldsymbol{x}, \boldsymbol{u}) f_0(\boldsymbol{x}) d\boldsymbol{x}$

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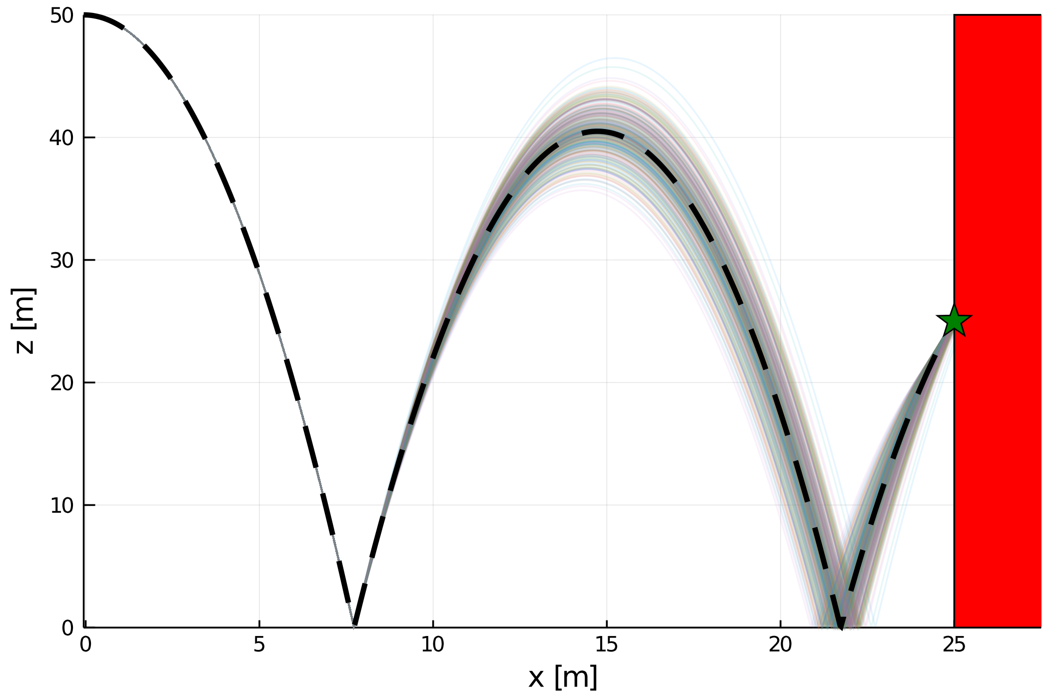

Optimal Solution produces expected cost of 8.3×10^{-2} in 0.12 sec (Julia implementation)

Gerlach *et al.*, 2020, https://arxiv.org/pdf/2008.08737.pdf

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Example 1: Bouncing Ball

Particular observable functions defined to “extract” raw moments (which can then be converted to central moments)

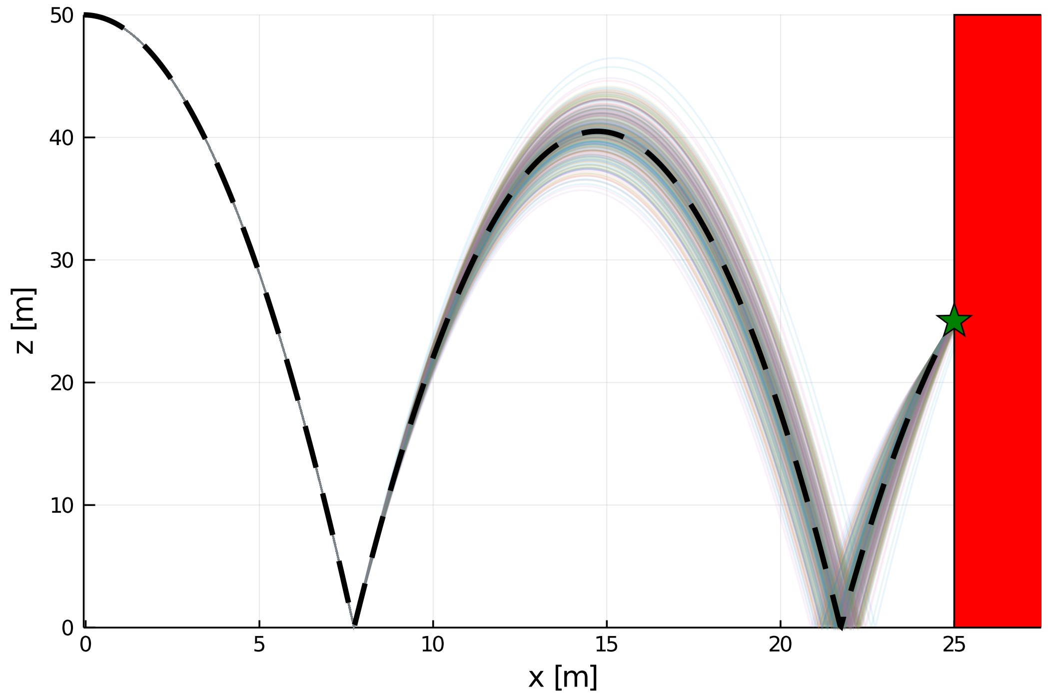
$g_1(x) = x$ mean

$g_2(x) = x^2$ 2nd raw moment

$g_3(x) = x^3$ 3rd raw moment

$\vdots$

$$\int_{\Omega} \mathcal{K}_S g_i(\boldsymbol{x}, \boldsymbol{u}) f_0(\boldsymbol{x}) d\boldsymbol{x}$$



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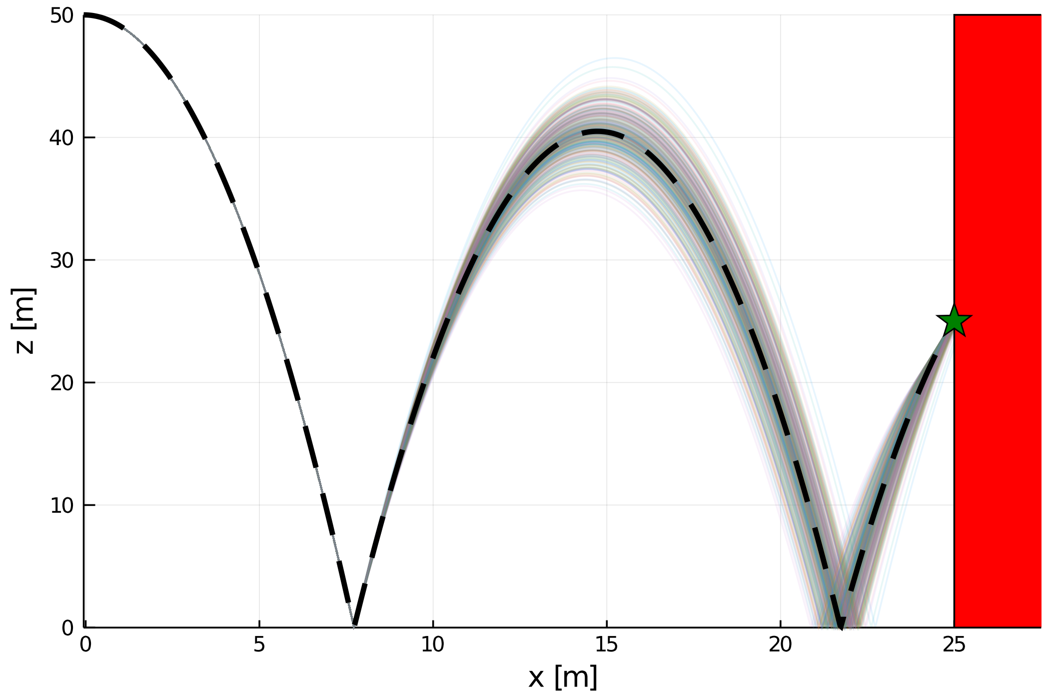
$$\int_{\Omega} \mathcal{K}_S g_i(\boldsymbol{x}, \boldsymbol{u}) f_0(\boldsymbol{x}) d\boldsymbol{x}$$

Central Moment	Monte Carlo	Koopman
2	9.030e−2	9.007e−2 ± 3.878e−5
3	3.878e−1	3.924e−1 ± 1.776e−3
4	3.214	3.428 ± 1.536e−3
5	38.116	44.536 ± 3.733e−3
	10M simulations, 264 sec	225 simulations, 3.4 ms



Koopman-based method produces solution with same accuracy but runs 77,000x faster.

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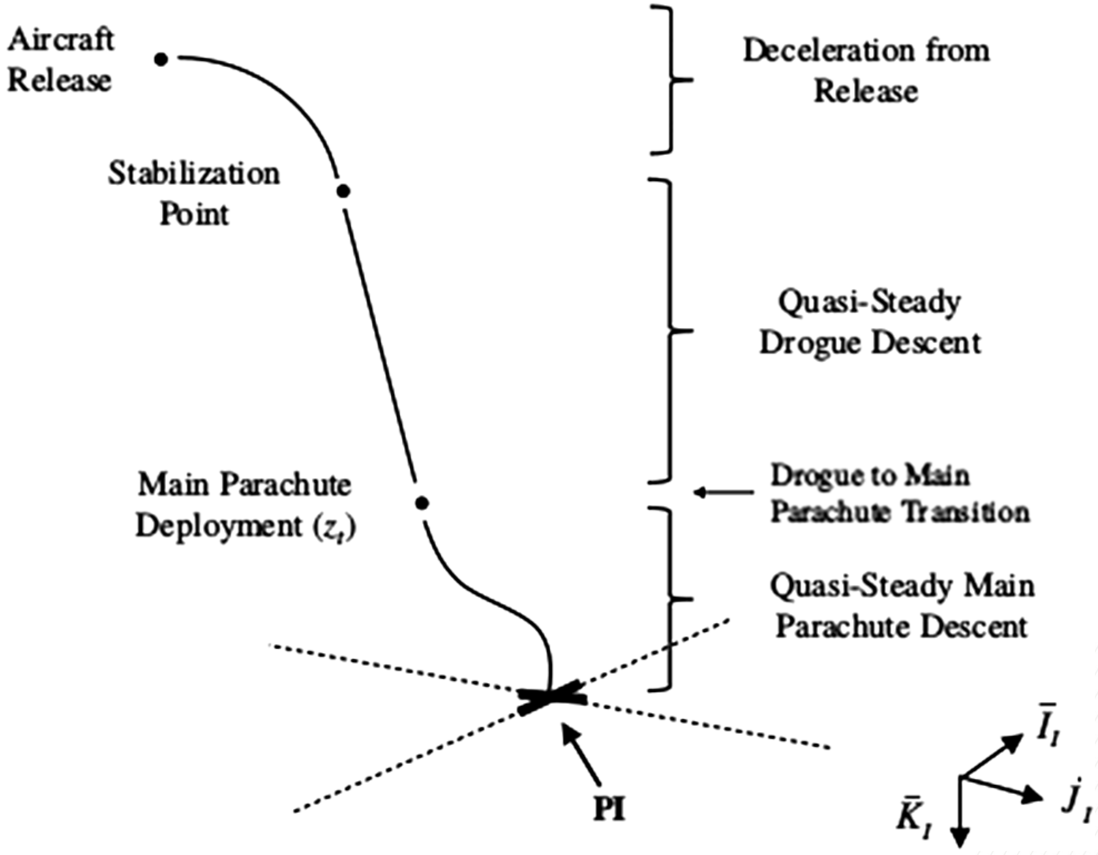
Example 2: Airdrop Mission Planning

High-Altitude Low-Opening (HALO) Airdrop



Uncertainty: Winds, parachute drag, package release dynamics

Optimize: Release point, aircraft heading, opening altitude

Leonard *et al.*, J. Guidance, Control, and Dynamics, 2020.

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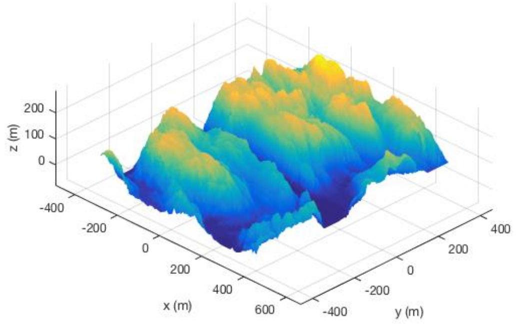
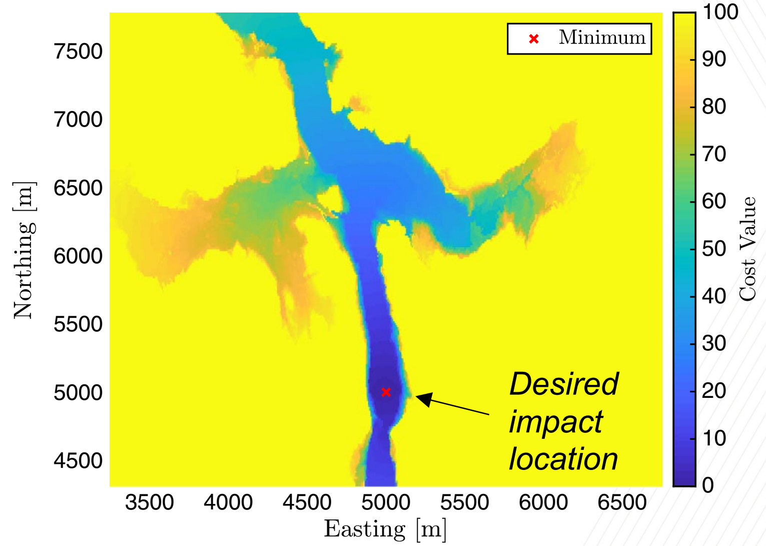


Cost Function $g(x, y)$



$$\mathbb{E}_{\mathcal{D}}[G(\boldsymbol{X})|\boldsymbol{u}] = \int_{\Omega} G(\boldsymbol{x}) f_{xy}(x, y|\boldsymbol{u}) f_{C_d}(C_d) f_{\hat{w}_m}(\hat{w}_m) f_{\hat{x}_\psi}(\hat{w}_\psi)\, \mathrm{d}\boldsymbol{x}$$

Choose drop location (x, y) that minimizes this expected value

Leonard *et al.*, J. Guidance, Control, and Dynamics, 2020.

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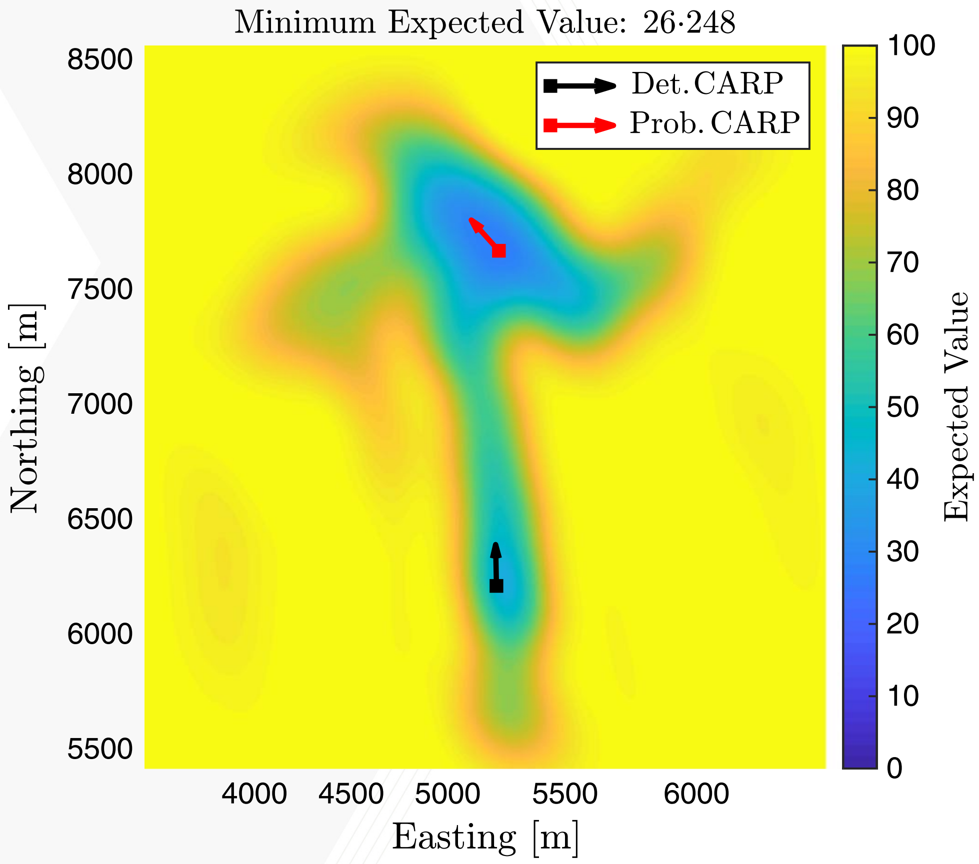
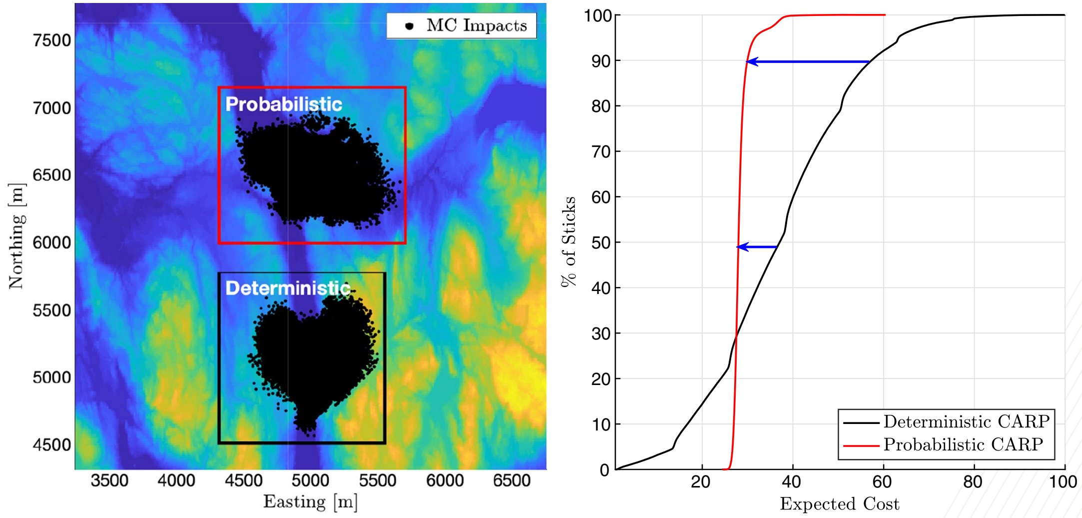


Leonard *et al.*, J. Guidance, Control, and Dynamics, 2020.

- **Deterministic planner** does not account for uncertainty, drops straight into canyon (lots of bad outcomes)
- **Probabilistic planner** drops in flatter region – gives up best-case performance to protect against lots of poor outcomes



Example 3: Maneuver-Based Trajectory Planning

Use library of (uncertain) maneuvers to construct path that minimizes expected cost while satisfying chance constraints

$$\min_{\mu \in U} E\left[J\left(H_\mu(x_0, t_0)\right)\right]$$

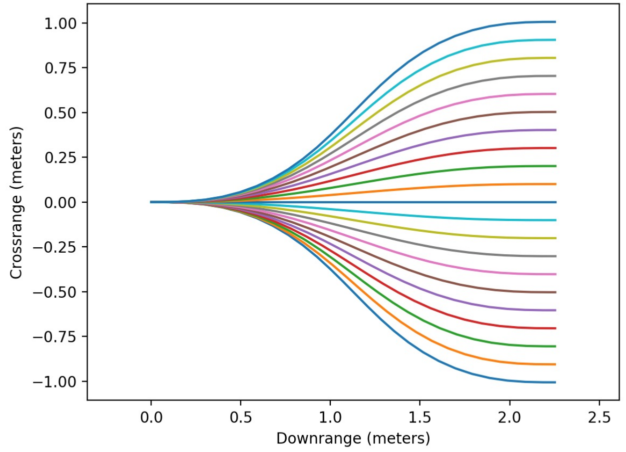
s.t. $P\left(H_\mu(x_0, t_0) \notin F\right) \leq r$

H_μ gives the state history under the controller μ

Koopman operator used to pull-back expected cost and constraint values for each maneuver

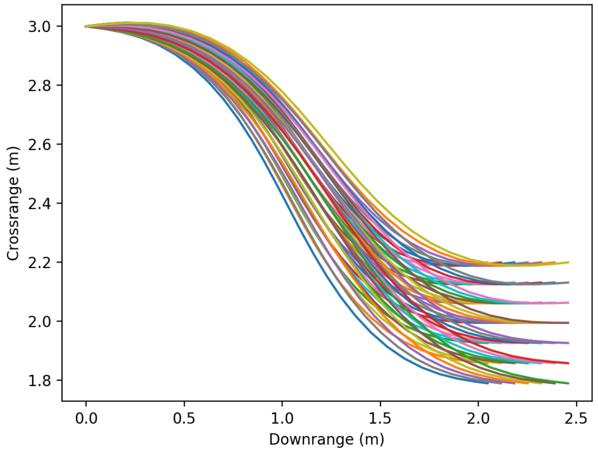
Gutow and Rogers, IEEE RAL, 2020.

Library:



Single Maneuver Under Parameter Uncertainty:

Each realization has probability of occurring given joint distribution on parameters or ICs



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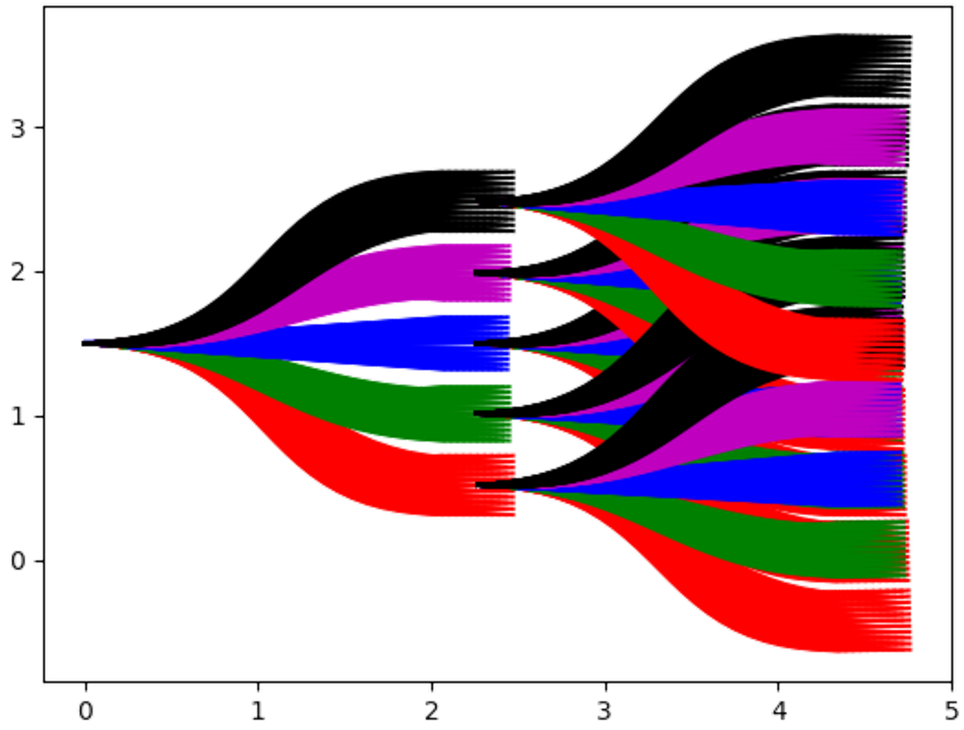
Example 3: Maneuver-Based Trajectory Planning

"Expected State Planner"

- Chain together next primitive from expected state of last one
- Use Koopman operator to pull back expected costs and constraint violations of candidate paths
- Use of primitives + Koopman allows UQ without real-time simulation

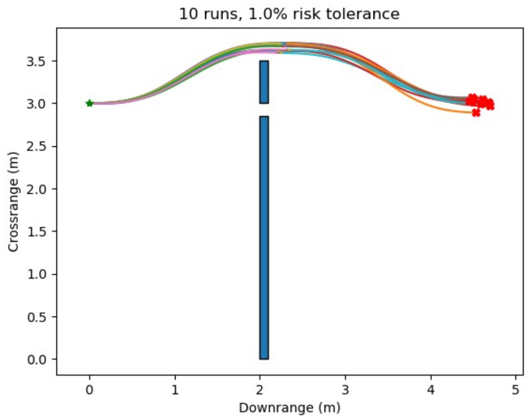


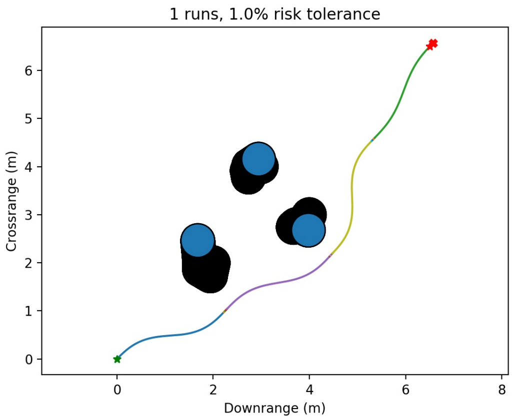
A* or dynamic programming can be used to solve for optimal path.

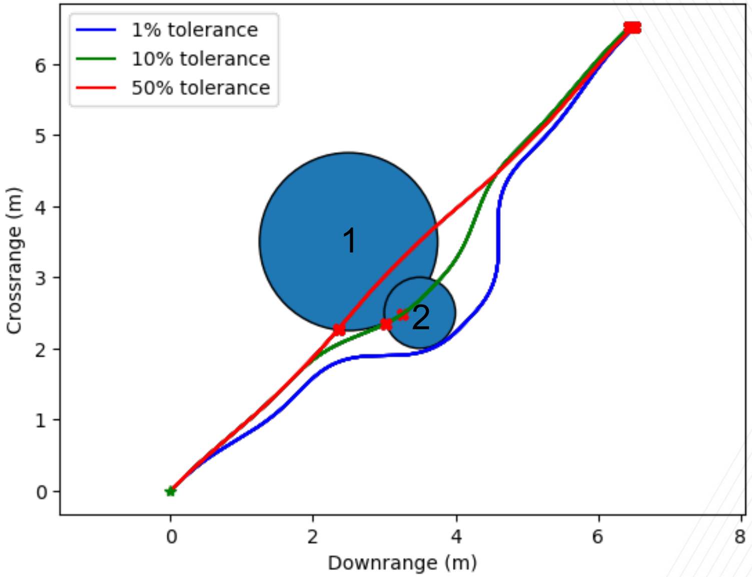
Gutow and Rogers, IEEE RAL, 2020.

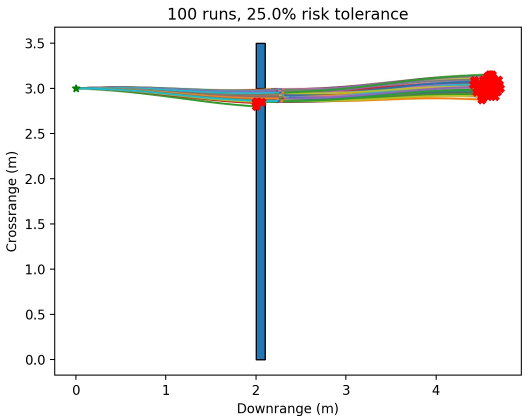
Example 3: Maneuver-Based Trajectory Planning

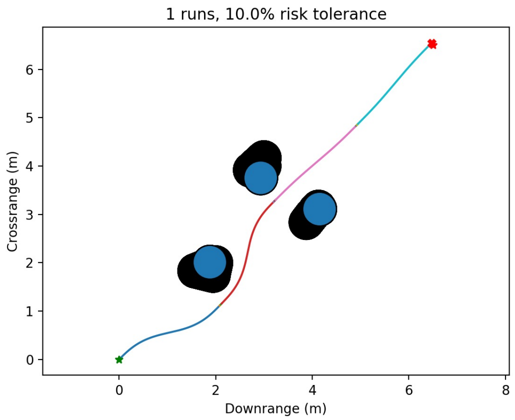
Yields planner with tunable risk thresholds











- Vehicle has 40% chance of being destroyed every 0.25 sec inside region 1
- Vehicle has 2.5% chance of being destroyed every 0.025 sec inside region 2
- Trajectory adapts based on risk tolerance

Gutow and Rogers, IEEE RAL, 2020.

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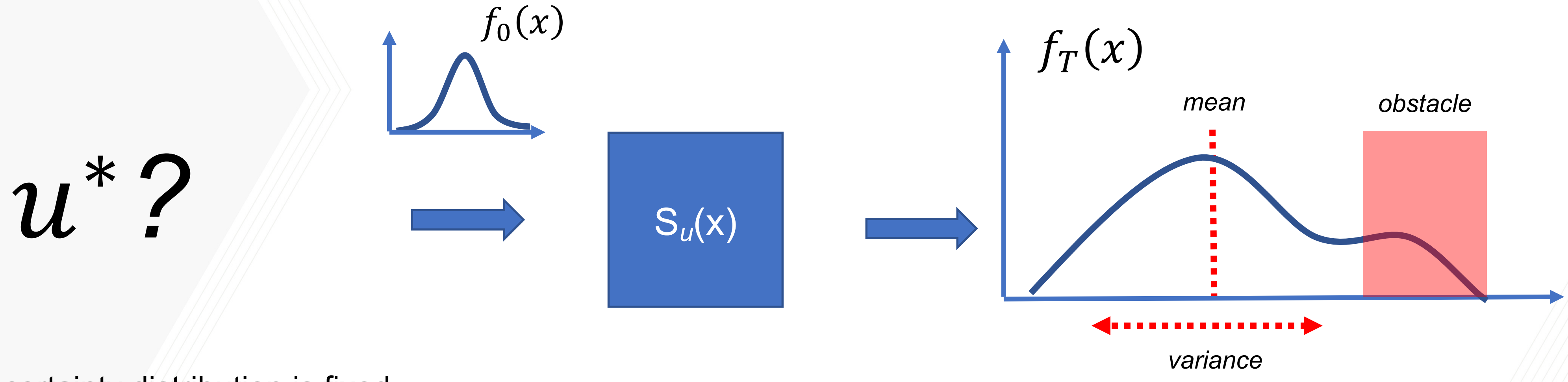
Probabilistic Inverse Problems

So far, we have tried to optimize vector of initial inputs given desired expected values of observables



- Initial uncertainty distribution is fixed
- We are allowed to pick the system

OR

- Form of initial uncertainty distribution is fixed
- We are allowed to set its parameters

$$\int_\Omega g_1(x,u) f_T(\boldsymbol{x}) d\boldsymbol{x} - c_1 = 0$$

$$\int_\Omega g_2(x,u) f_T(\boldsymbol{x}) d\boldsymbol{x} - c_2 = 0$$

$$\vdots$$

Probabilistic Inverse Problems

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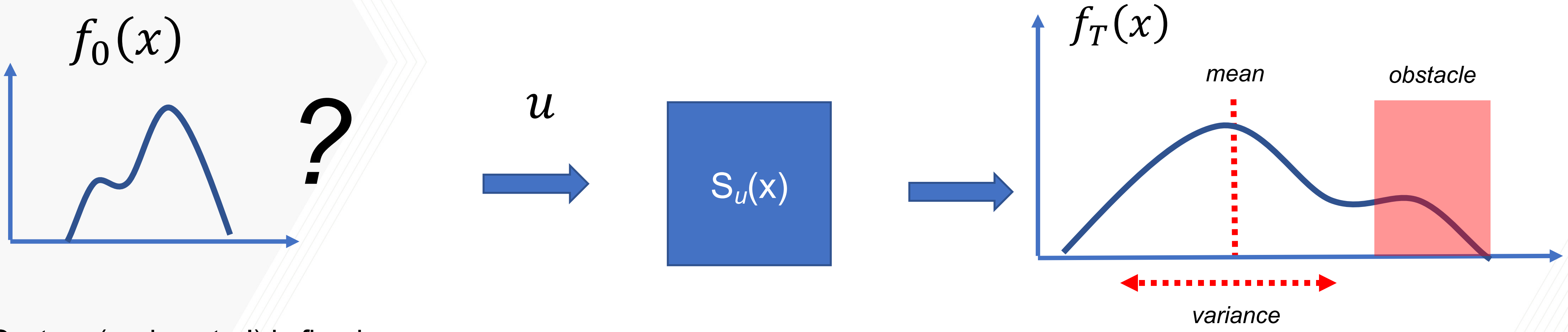


- System (and control) is fixed
- What is the initial uncertainty distribution that meets desired expected values?

- Engineering design problems, drug design/dosing, disease modeling, biological population modeling…

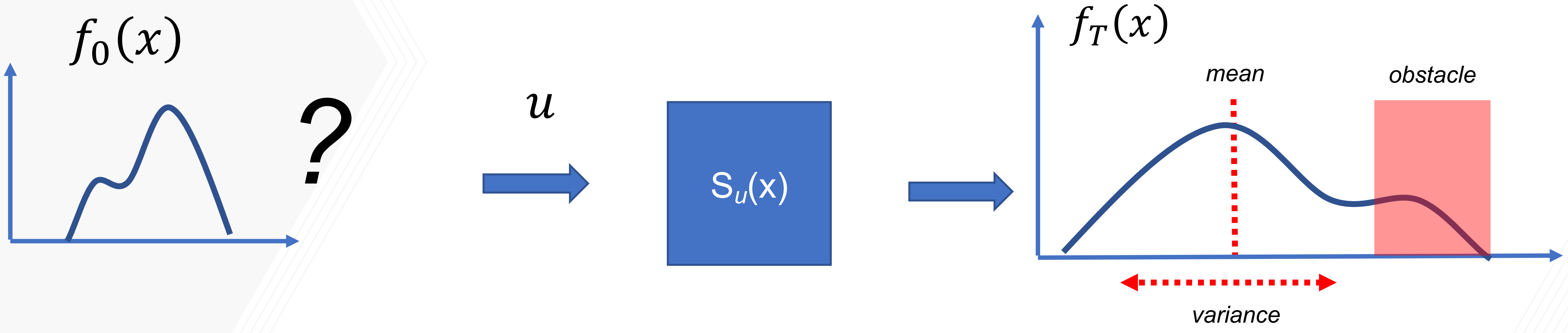
$$\int_{\Omega} g_1(x,u) f_T(\boldsymbol{x}) d\boldsymbol{x} - c_1 = 0$$

$$\int_{\Omega} g_2(x,u) f_T(\boldsymbol{x}) d\boldsymbol{x} - c_2 = 0$$

$$\vdots$$

Probabilistic Inverse Problems

So far, we have tried to optimize vector of initial inputs given desired expected values of observables



Probabilistic inverse problem: Given expectations of observables of the output, what is a valid input distribution?

$$\int_{\Omega} g_1(x,u) f_T(\boldsymbol{x}) d\boldsymbol{x} - c_1 = 0$$

$$\int_{\Omega} g_2(x,u) f_T(\boldsymbol{x}) d\boldsymbol{x} - c_2 = 0$$

$$\vdots$$

Probabilistic Inverse Problems

Problem statement:

Find $f_0(\boldsymbol{x})$ s.t.:

$$1 = \int_{supp(f_0)} f_0(\mathbf{x})\, d\mathbf{x}$$

Integrate to 1 constraint

$$c_i = \int_{supp(f_0)} f_0(\mathbf{x}) U_i g_i(\mathbf{x})\, d\mathbf{x} \qquad i = 1, \ldots, p$$

EV equality constraints

$$c_j < \int_{supp(f_0)} f_0(\mathbf{x}) U_j g_j(\mathbf{x})\, d\mathbf{x} \qquad j = p+1, \ldots, K$$

EV inequality constraints

U_i is Koopman operator that pulls observable function back from time t_i to t_0

Meyers *et al.*, J. Comp. Phys., 2021.

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Optimize over the space of L^1 functions…this is hard.

Meyers *et al.*, J. Comp. Phys., 2021.

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EV inequality constraints

Optimize over the space of L^1 functions…this is hard.

This is an ill-posed problem.
So we will need regularization.

Meyers *et al.*, J. Comp. Phys., 2021.

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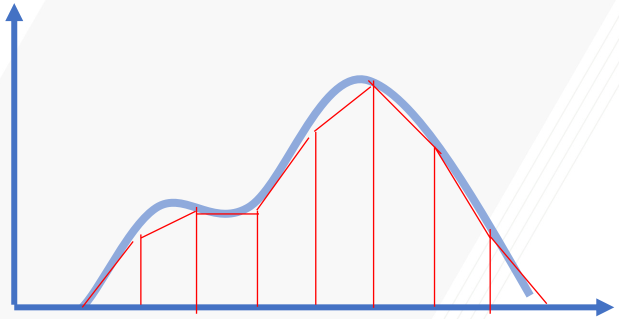
Probabilistic Inverse Problems

Formulation as a quadratic program:

Approximate $f_0(\boldsymbol{x})$ as piecewise linear over grid



$$\hat{c}_i \approx \sum_{k=0}^{n} w_k \hat{f}_0(\mathbf{x}_k) g_i(S_i(\mathbf{x}_k))$$

Quadrature approximation of desired EVs

$$\underset{\mathbf{f}\in\mathbb{R}^n}{\operatorname{argmin}} ||G\mathbf{f} - \mathbf{c}||_2^2 + \lambda^2 ||L\mathbf{f}||_2^2$$

EV targets (LS cost)

Regularization

$$\mathbf{w}^T\mathbf{f} = 1$$ Integrate to 1 constraint

$$G_{eq}\mathbf{f} = \mathbf{c}_{eq}$$ EV equality constraints

$$G_{ineq}\mathbf{f} \geq \mathbf{c}_{ineq}$$ EV inequality constraints

$$\mathbf{f} \geq \mathbf{0}$$

Meyers *et al.*, J. Comp. Phys., 2021.

Probabilistic Inverse Problems

Formulation as a quadratic program:

- Non-negative constrained least-squares problem
- Cast as a convex quadratic program
- Use QP solver to find vector **f** which approximates initial distribution

$$\underset{\mathbf{f}\in\mathbb{R}^n}{\operatorname{argmin}} ||G\mathbf{f}-\mathbf{c}||_2^2 + \lambda^2||L\mathbf{f}||_2^2$$

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$\mathbf{w}^T\mathbf{f} = 1$	Integrate to 1 constraint
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Meyers *et al.*, J. Comp. Phys., 2021.

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$\mathbf{f} \geq \mathbf{0}$	

Made possible because we formulated problem using Koopman expectations!

Meyers *et al.*, J. Comp. Phys., 2021.

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Inverse Problem Example: Reentry Vehicle

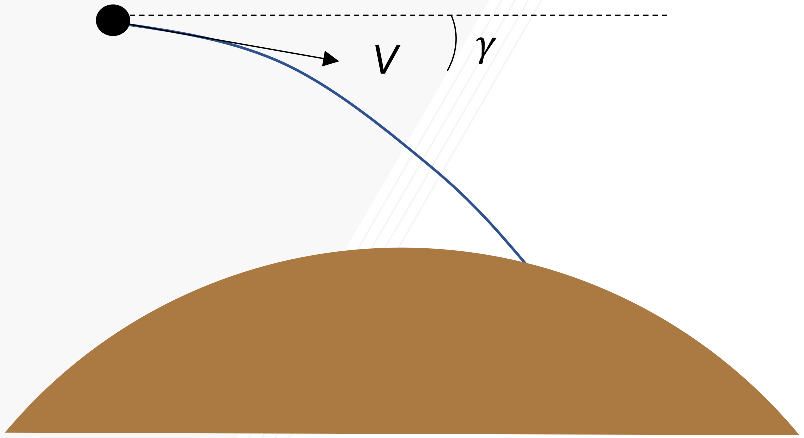
- Vinh's Equations

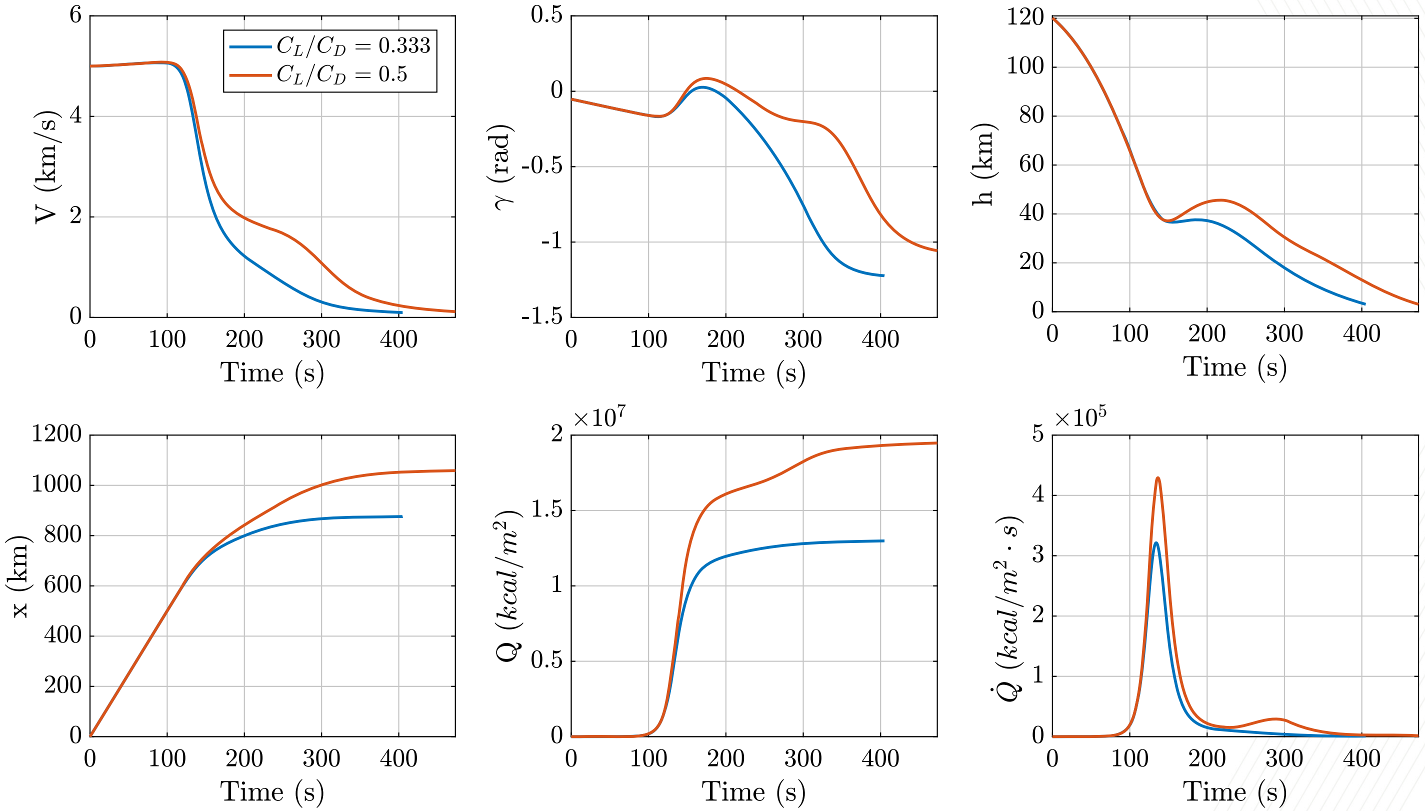
$$\dot{x} = V\cos\gamma\,,$$

$$\dot{r} = V\sin\gamma\,,$$

$$\dot{V} = \frac{-\rho S C_D}{2m}V^2 + g_0\left(\frac{r_0}{r}\right)^2\sin\gamma\,,$$

$$\dot{\gamma} = \frac{\rho S C_L}{2m}V + \left(\frac{V}{r} - \frac{g_0}{V}\left(\frac{r_0}{r}\right)^2\right)\cos\gamma$$





Meyers *et al.*, J. Comp. Phys., 2021.

Inverse Problem Example: Reentry Vehicle

Case	Expected Value	Constraint	
Case 1	$Pr(1000 \le x(T) \le 1150\ \mathrm{km})$	≥ 0.99	Final **position** constraint
	$Pr(0.09 \le V(T) \le 0.11\ \mathrm{km/s})$	≥ 0.99	Final **velocity** constraint
	$Pr(Q(T) < 1.5\times10^7\ \mathrm{kcal/m})$	≥ 0.99	Final **integrated heat load** constraint
	$Pr\left(\max \dot{Q}(T) < 3\times10^5\ \mathrm{kcal/m^2/s}\right)$	≥ 0.99	Maximum **heating rate** constraint (allowable range)
Case 2	$Pr(1000 \le x(T) \le 1150\ \mathrm{km})$	≥ 0.99	
	$Pr(0.09 \le V(T) \le 0.11\ \mathrm{km/s})$	≥ 0.99	
	$E\left[\max \dot{Q}(T)\right]\quad (\mathrm{kcal/m^2/s})$	$= 3\times10^5$	Maximum **heating rate** equality constraint

Uncertainty in lift coefficient (C_L), drag coefficient (C_D), heating coefficient (C_f)

What are allowable distributions for them?

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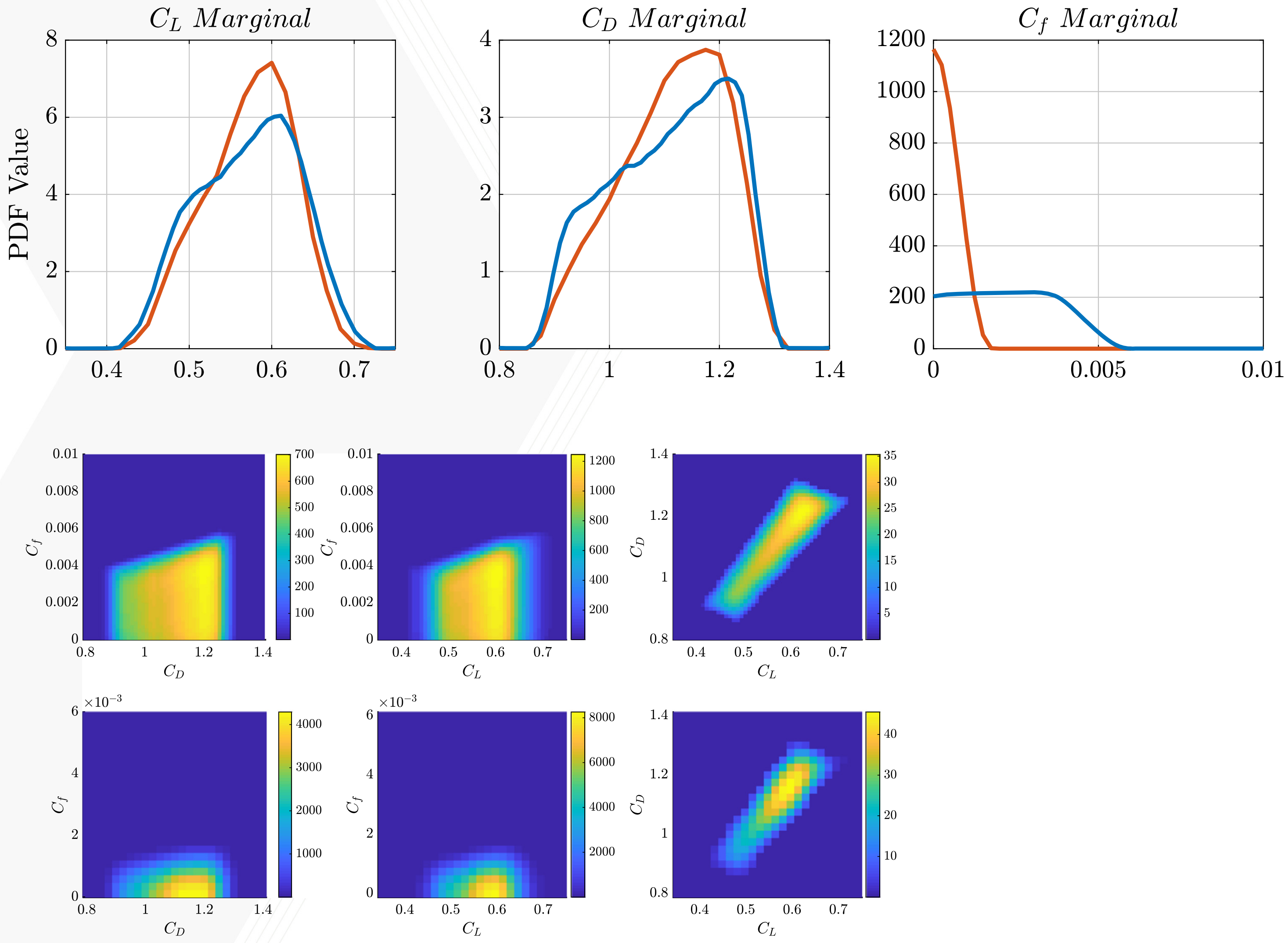
Inverse Problem Example: Reentry Vehicle



Case 1: Allowable range of heating rates

Case 2: Maximum heating rate enforced

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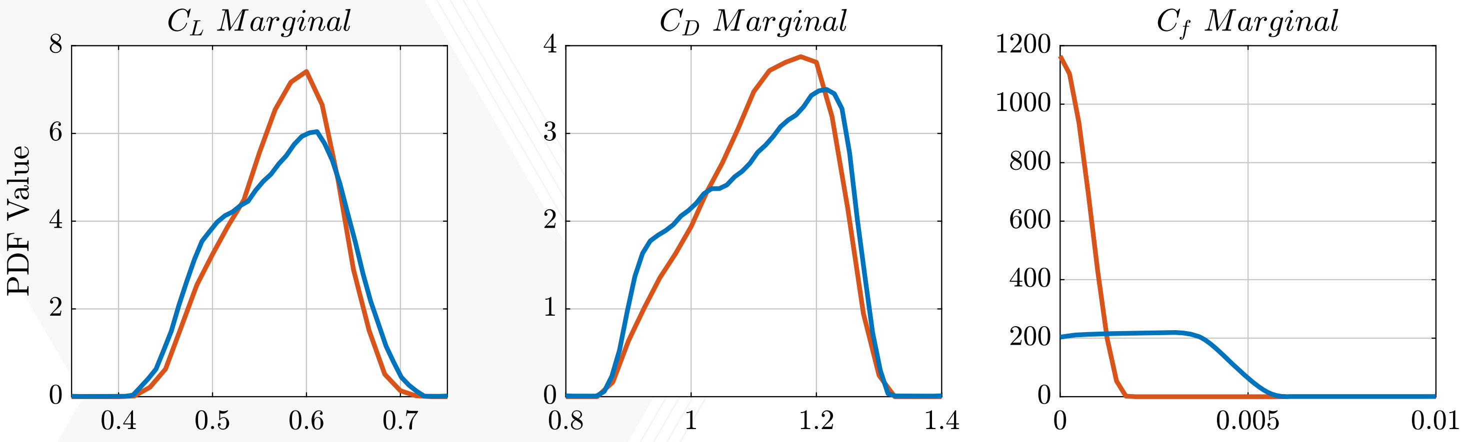
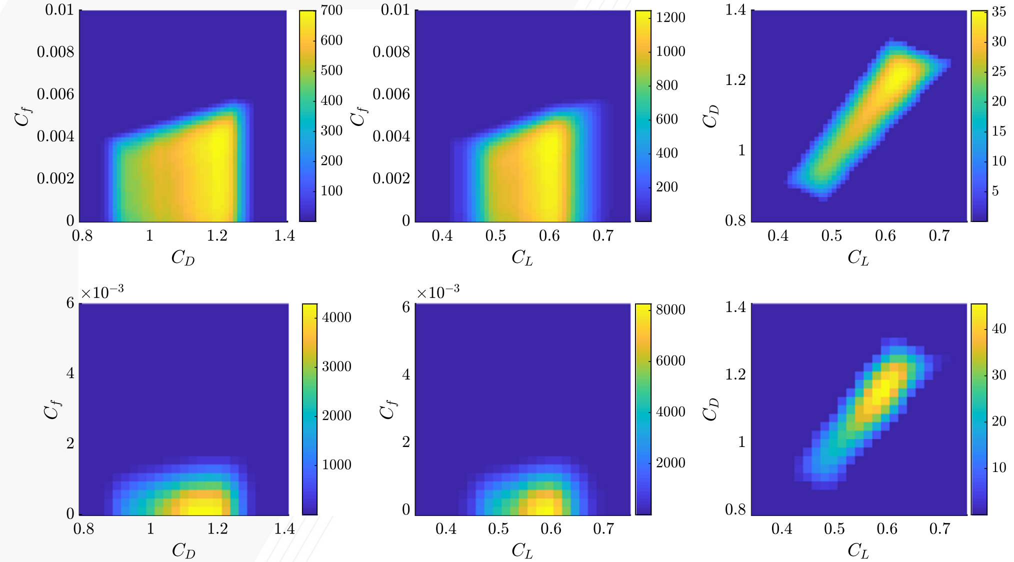
Inverse Problem Example: Reentry Vehicle



Case 1: Allowable range of heating rates

Case 2: Maximum heating rate enforced



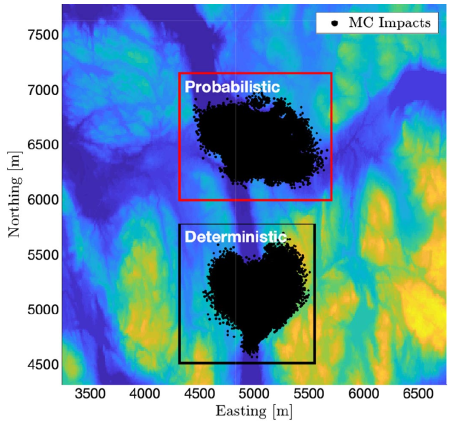
- Multi-dimensional distributions computed using 125,000 points (Case 1) and 15,625 points (Case 2)
- Monte Carlo simulations verify that desired EV constraints were met using computed distributions

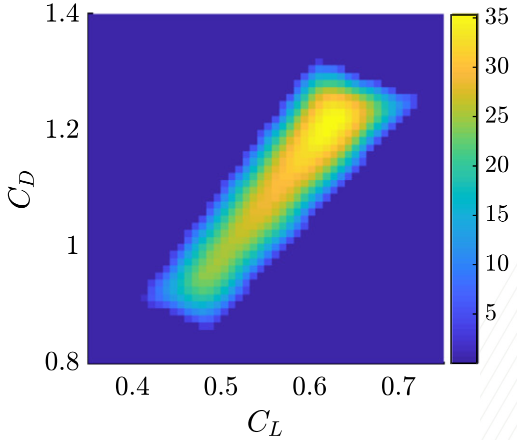
Meyers *et al.*, J. Comp. Phys., 2021.

Conclusion

- Koopman operator provides powerful mechanism for optimization under parametric uncertainty
- Unique computational advantages compared to MC and other explicit UQ methods
- Approach has been demonstrated in optimization of discrete control decisions and initial uncertainty distributions
- Potential extensions to systems with process noise and cases involving optimization of continuous-time controllers

$$\int_{\Omega} \mathrm{P_S} f(\boldsymbol{x}) g(\boldsymbol{x}) d\boldsymbol{x} = \int_{\Omega} f(\boldsymbol{x}) \mathrm{U_S} g(\boldsymbol{x}) d\boldsymbol{x}$$





Relevant Publications

A. Gerlach, A. Leonard, J. Rogers, C. Rackauckas, The Koopman Expectation: An Operator Theoretic Method for Efficient Analysis and Optimization of Uncertain Hybrid Dynamical Systems," Arxiv Preprint, https://arxiv.org/abs/2008.08737

J. Meyers, J. Rogers, A. Gerlach, "Koopman Operator Method for Solution of Probabilistic Inverse Problems," *Journal of Computational Physics*, Vol. 428, 2021, pp. 1-21.

G. Gutow, J. Rogers, "Koopman Operator Method for Chance-Constrained Motion Primitive Planning," *IEEE Robotics and Automation Letters*, Vol. 5, No. 2, 2020, pp. 1572-1578.

J. Meyers, A. Leonard, J. Rogers, A. Gerlach, "Koopman Operator Approach to Optimal Control Selection Under Uncertainty," 2019 American Control Conference, Philadelphia, PA, July 10-12, 2019.

A. Leonard, J. Rogers, A. Gerlach, "Koopman Operator Approach to Airdrop Mission Planning Under Uncertainty," *Journal of Guidance, Control, and Dynamics*, Vol. 42, No. 11, 2019, pp. 2382-2398.

A. Leonard, J. Rogers, A. Gerlach, "Probabilistic Release Point Optimization for Airdrop with Variable Transition Altitude," *Journal of Guidance, Control, and Dynamics*, Vol. 43, No. 8, 2020, pp. 1-11.

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