Aalto University
School of Science

Enhancing Optimization Under Uncertainty with Neural Networks

and biography

Oliver Lundqvist 30/09/2024

Biography
Oliver Lundqvist

1990 – Born in San Diego U.S.A

1992 – Moving “back” to Finland

2010 – starting mechanical engineering studies at Aalto university

Studying in Aalto 1st time (2010–2015)

2013 – **B.Sc. in mechanical engineering**

2015 – **M.Sc. in mechanical engineering**

Working in Andritz Oy as a structural engineer (2015–2018)

2018 – Switching from Andritz to Sweco

Working full time in Sweco as a FEM-analyst, project manager and department manager (2018–2024)

2019 – Starting math OR masters

founding a medical device/AI company

Studying in Aalto 2nd time (2019–2023)

2022 – My son Benjamin is born

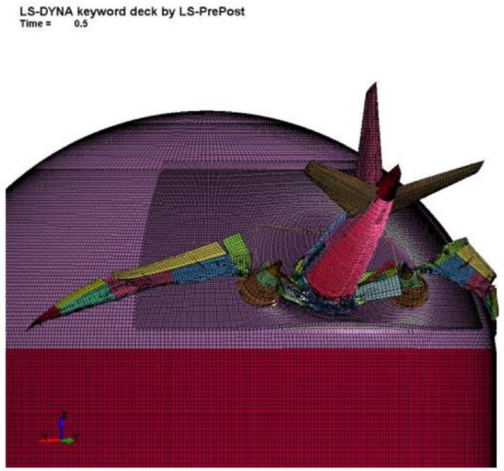
2023 – **M.Sc. in Math OR**

2024 – PHD student

A!

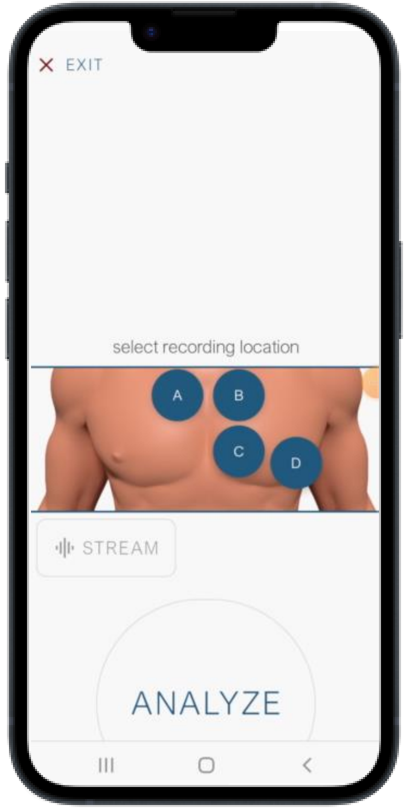
Biography
Working career

- **Andritz Oy 2012-2018:**
  - Structural engineer doing FEM-analysis for thin-plated structures for recovery and power boilers
  - Internships in Vienna, Graz and Stockholm during studies
  - Full time employment 2015-2018
- **Sweco Finland Oy 2018-2024:**
  - 2018-2020 FEM-analyst for demanding analysis (explosions, earthquakes, impacts etc.)
  - 2020-2022 Project manager. Leading different FEM-analysis projects for different customers
  - 2022-2024 Department manager. Leading a team of 6-8 people from various nationalities



AusculThing
Reinventing auscultation

- **AusculThing Oy**, Medical device company with the aim of introducing AI-powered screening tools for heart sounds.
- Currently **FDA-cleared** product and starting sales in the U.S.
  - Accuracy 93%   Sensitivity 91%   Specificity 96 %
- Recently (21.9.2024) published article:
  Automated analysis of heart sound signals in screening for structural heart disease in children
  https://link.springer.com/article/10.1007/s00431-024-05773-3
- Currently looking for the first seeding round…
  → if you know any rich and easy-going investors let me know…



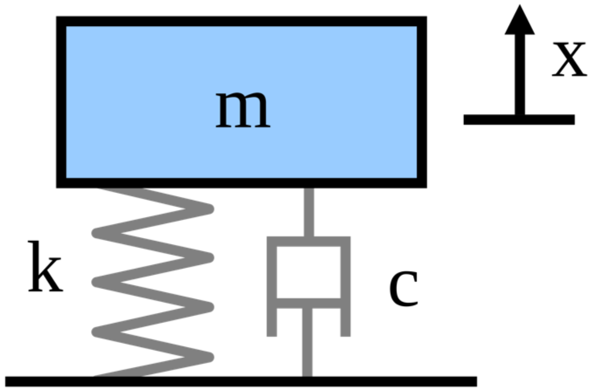
Enhancing Optimization Under Uncertainty with Neural Networks

Optimization under uncertainty with neural networks

Pre-example

- Consider damped harmonic oscillator with the following dynamics

$$x''(t) + 2\xi\omega x'(t) + \omega^2 x(t) = 0$$
$$x(0) = u$$
$$x'(0) = 0$$
$$\omega = 1$$



- **We want** the oscillator to have an amplitude of $x = -0.4$ at time $T = 5s$
- Critical damping ξ, $\xi \sim f(\xi) = \mathcal{N}(\xi \mid \mu = 0.1, \sigma = 0.02)$

- **Target:** From what initial condition u should we release the system so at $t = 5$ we "most likely" end up at $x = -0.4$
→ **Minimize on the expectation and observe the squared missed distance**

Optimization under uncertainty with neural networks

Pre-example

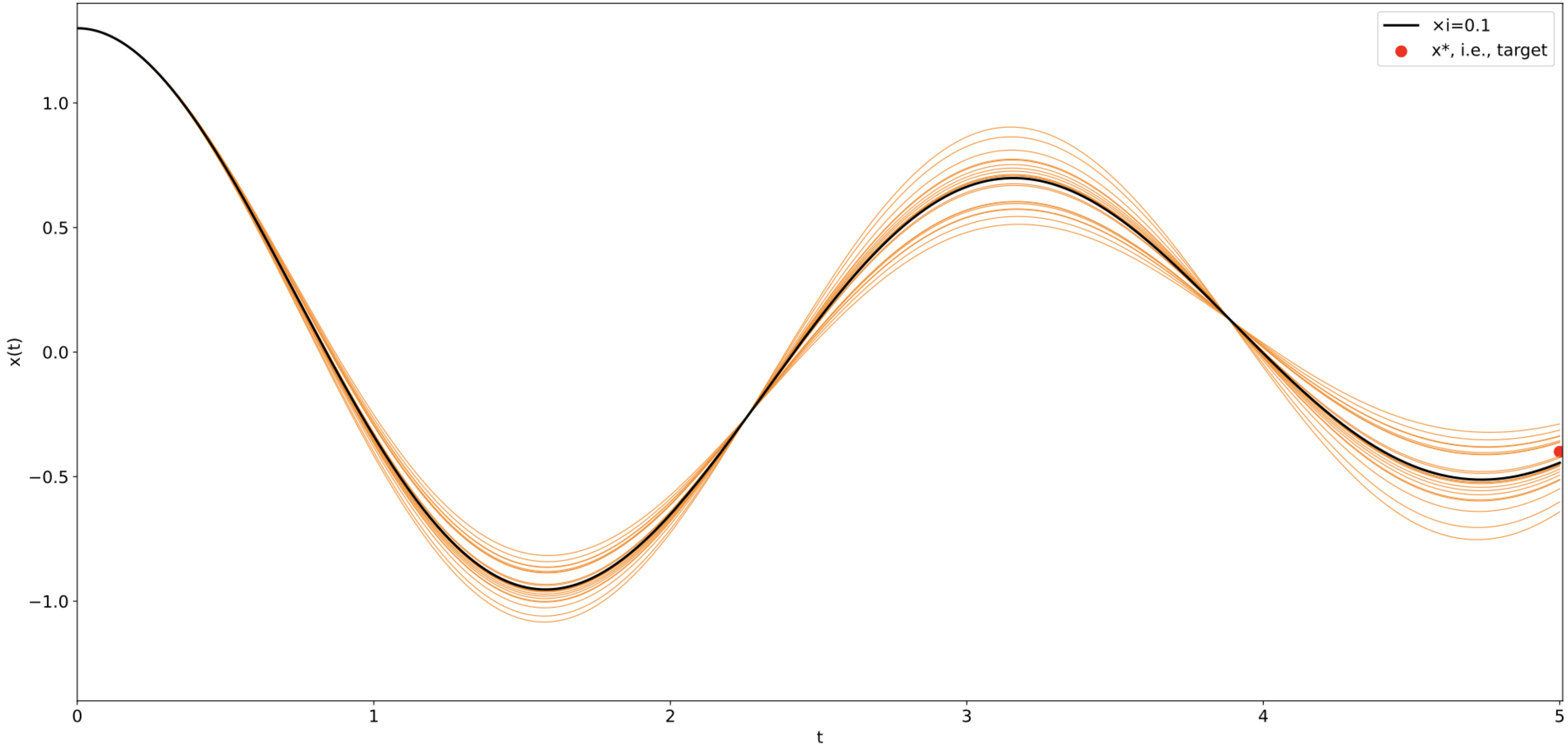
- Define map $S(x) = x(T)$
- Our observable, the square missed distance $g(S(x)) = (x(T) - x^*)^2$ and target $x^* = -0.40$
- Target is to decide on u such that it minimizes the expected squared miss on the target

$$\min_u \mathbb{E}[(x(T) - x^*)^2 | x(T) \sim P_S f(\xi)]$$

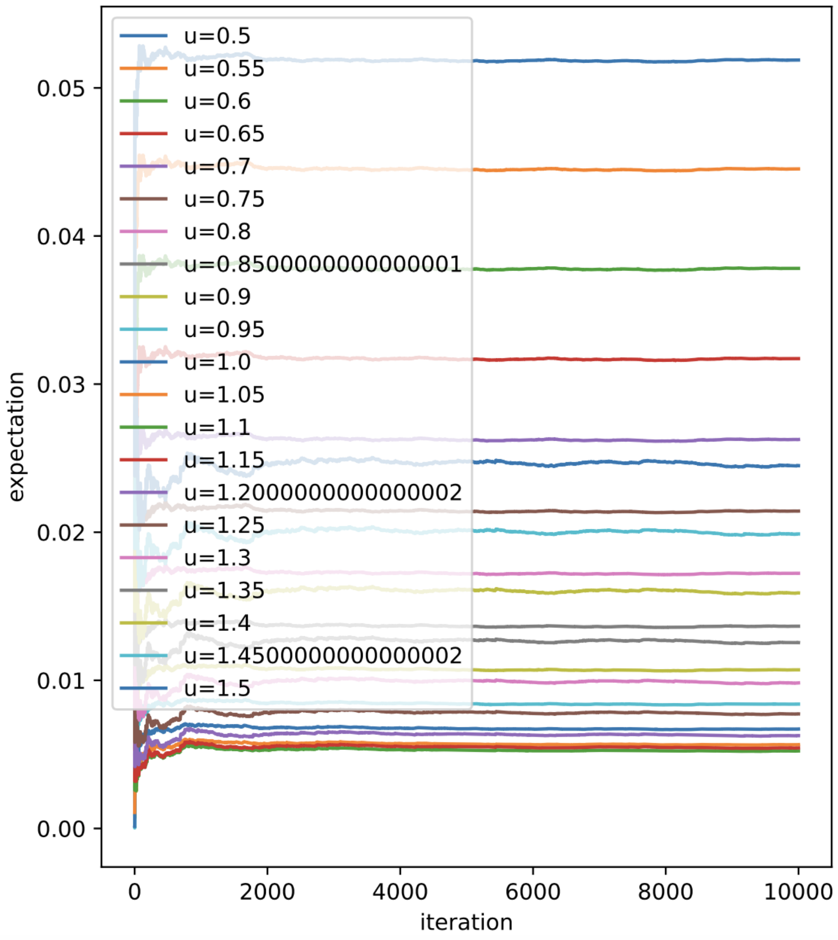
where $P_S f(\xi)$ is the density pushed forward through the system (more later…).

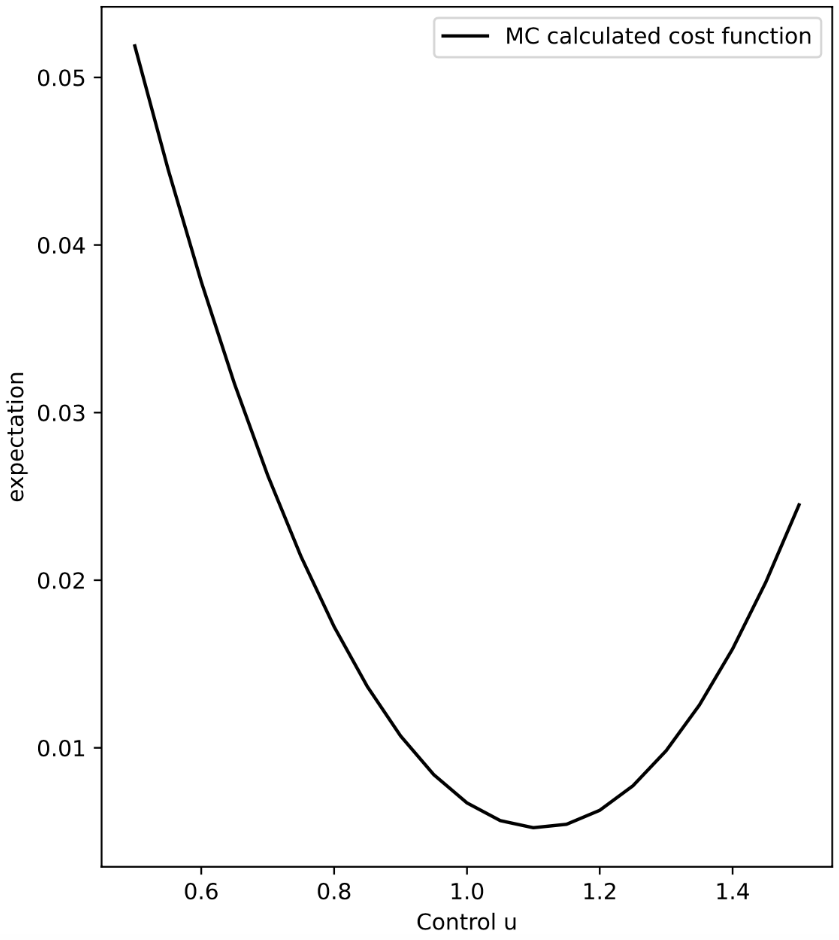
- What approaches do we have?

Optimization under uncertainty with neural networks
Pre-example



Optimization under uncertainty with neural networks
Pre-example





Optimization under uncertainty with neural networks

Background

- **General case:**

Dynamical system

observable

control

$$\min_{u} \mathbb{E}[g(S(x(t,u|\alpha)) \,|x\sim P_s f(\alpha)]$$

Uncertain parameter

Mapping or description of dynamical system

Pushed forward distribution through the dynamical system

Target: minimize the expectation of an observable $g(x)$ depending on some dynamical system $x(t,u|\alpha)$ for some parametric uncertainty $\alpha \sim f(\alpha)$ with respect to control u.

Optimization under uncertainty with neural networks

Background

- **Question:** How does the uncertainty distribution evolve through the dynamical system? I.e., given an initial distribution what is the output distribution?

- **Simple example:** how does the distribution develop from $t = 0$ to $t = 5$ when $x(0) = 1$, i.e. what is the distribution of $x(5)$?

$$S(x) \coloneqq -\alpha \frac{dx(t)}{dt} = x(t)$$

$$x(0) = 1$$

$$\alpha \sim \mathcal{N}(0,1)$$

Optimization under Uncertainty with neural networks
Background

- **Approaches:**

1. **Direct sampling and solving (Monte Carlo methods)**
   + simple implementation
   - Computational cost
   - no direct way to compute gradients(?) → how to optimize?

2. **Frobenius-Perron (FP) Operator**
   → Analytical framework to study development of distributions of mappings (dynamical systems)

3. **Koopman Operator**
   → Adjoint to Frobenius-Perron operator

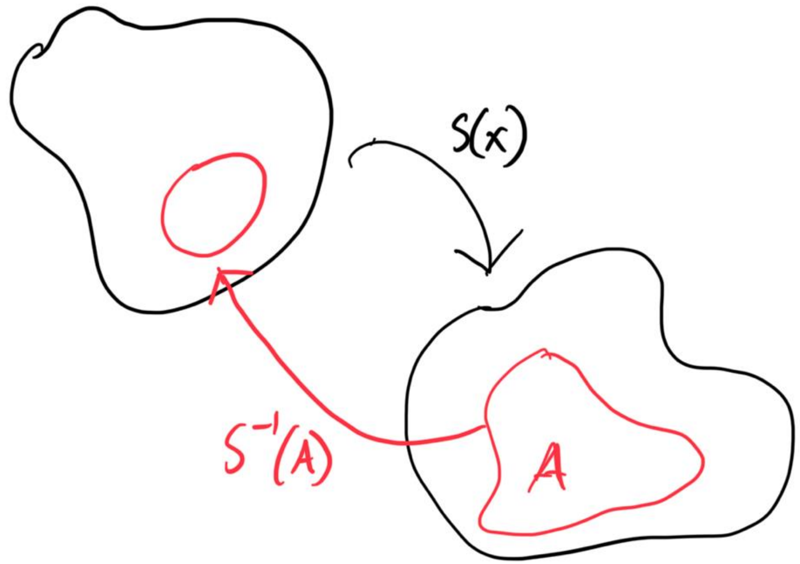
Optimization under Uncertainty with neural networks

Background

- **Frobenius-Perron (FP) Operator :** Operator P_S pushes the uncertainty (distribution) through the system to the output and is defined as:

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

  - $f(x)$ is the probability distribution and $x \sim f(x)$
  - $S(x)$ describes the system dynamics (diff. equation for example)



- If $S(x)$ is differentiable and invertible then:

$$P_S f(x) = f\left(S^{-1}(x)\right)\left|\frac{dS^{-1}(x)}{dx}\right|$$

(= “Change-of-variable” in probability theory)

A!

Optimization under Uncertainty with neural networks
Background

- The FP Operator on the observable can be interpreted as an expectation for some function (observable) $g(x)$ as:

$$\mathbb{E}[g(x)|x \sim P_S f(x)] = \int_{S(\Omega)} P_S f(x) g(x) dx = < P_S\, f(x), g(x) >$$

- One would like to optimize some decision u on the expectation of the dynamical system's outcome uncertainty in the:
  - **Input or initial** values of the system
  - **Parameters** of the dynamical system

  Thus maximize/minimize on the expectation: $\min_u \mathbb{E}\left[g\big(S(x)\big)\middle|x \sim P_S f(x)\right]$

- **Problems:**
  - FP operator difficult to determine and S(x) needs to be invertible and differentiable
  - Numerical stability, original density domain might grow exponential when pushed through the system (explode)

Optimization under Uncertainty with neural networks
Background

- **Koopman Operator :** Defined as:
  $$K_S g(x) = g\big(S(x)\big)$$
  where $g(x)$ is some observable
- FP operator transports densities through maps of dynamical systems, Koopman operator provides a mechanism to ***pull-back*** functions.
- The Koopman Operator is adjoint to the FP operator, thus:

$$< P_S f(x), g(x) > = < f(x), K_S g(x) >$$

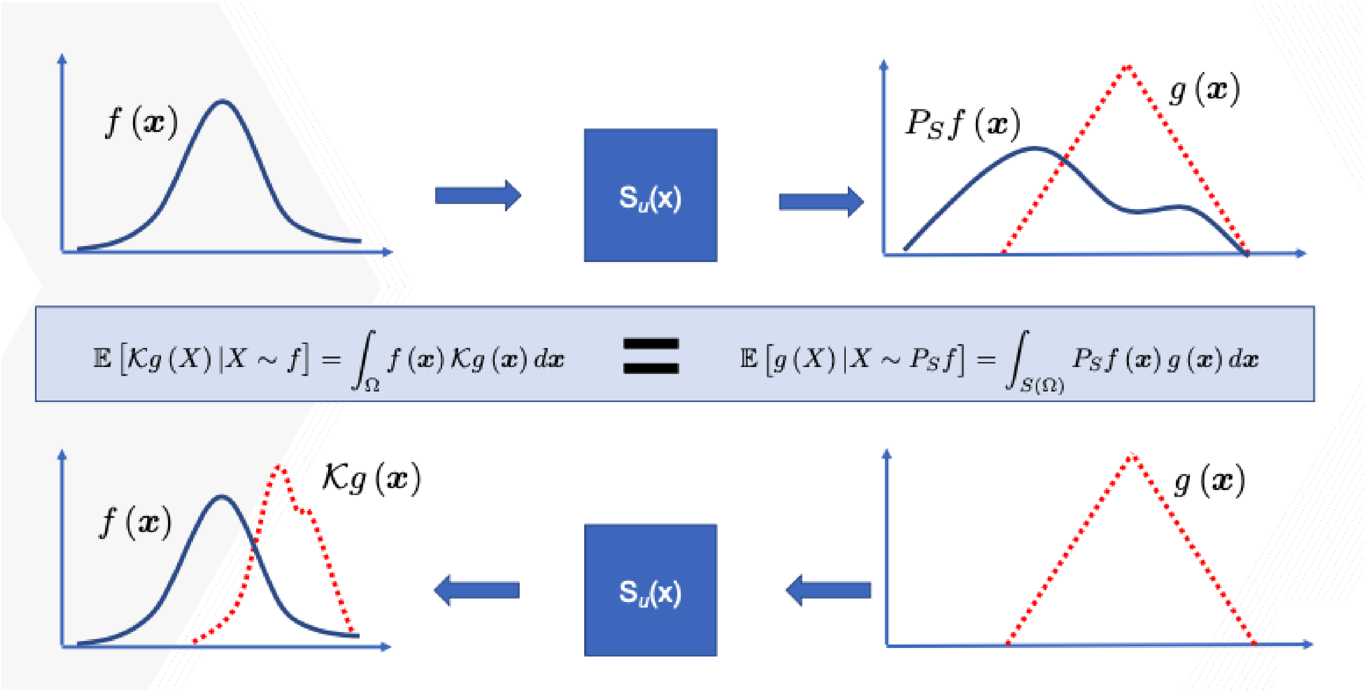
$$\mathbb{E}[g(x)|x \sim P_S f(x)] = \mathbb{E}[K_S g(x)|x \sim f(x)]$$

- Provides a way to ”Pull-back” the system to the original domain of the density and do the integration there

Optimization under Uncertainty with neural networks
Background

Frobenius-Perron expectation aka *"push-forward"*

Koopman expectation aka *"pull-back"*



- Benefits:
  - Numerically stable
  - Integration over known domain
  - Fast to integrate (quadrature or other method)

Optimization under Uncertainty with neural networks
Background

- Optimization problem is transferred to:

$$\min_u \mathbb{E}\left[g\big(S(x)\big)\middle|x \sim P_S f(x)\right] = \min_u \mathbb{E}[K_s g(x)|x \sim f(x)]$$

- The Koopman operator K_S does not need to explicitly known but it’s action is needed to be known, i.e.,

$$K_S g(x) = g\big(S(x)\big)$$

- So we have

$$\min_u \mathbb{E}\left[g\big(S(x)\big)\middle|x \sim f(x)\right]$$

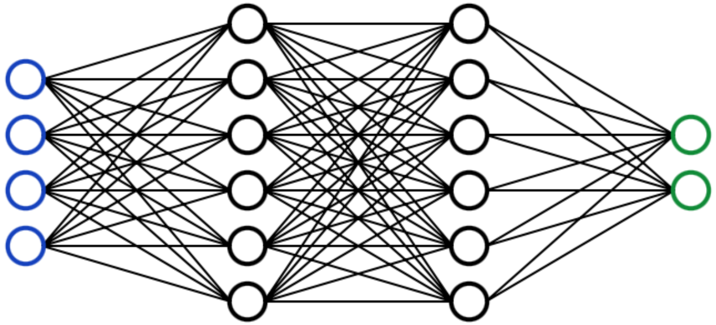
- So solving this can be done with by coupling different solvers (ODE or PDE) and explicitly calculating the dynamics and doing the numerical integration

Optimization under Uncertainty with neural networks

Background

- **NOW THE “RESEARCH”:** Possible to replace ODE or PDE solver with a Physics Informed Neural Network (PINN)

$in: [t, \xi, u]$



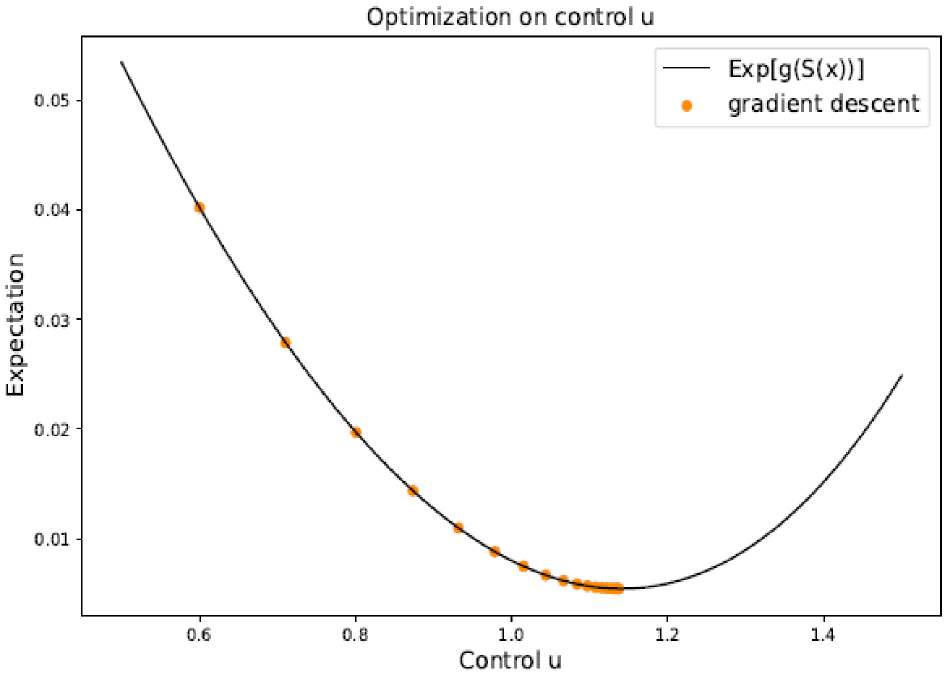
$out: x(t)$

$$SOLVE:\ x''(t) + 2\xi\omega x'(t) + \omega^2 x(t) = 0$$

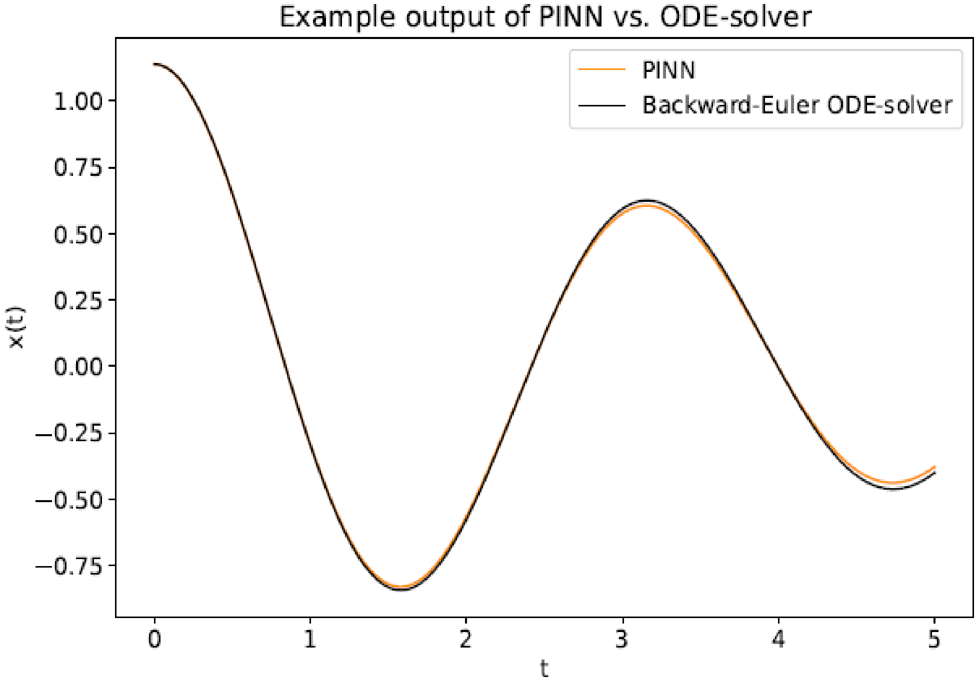
- **Faster forward/computation times**
- **Possible to easily calculate gradient on control variables**
- **PINNs run efficiently in “batch mode” → one forward pass for multiple points → efficient integration of expectations or higher order statistics**

Optimization under Uncertainty with neural networks
Example

- Optimum at $u^* = 1.138277$



Cost function and gradient descent with NN



PINN and ODE solution for $\xi = 0.1$ and $u^* = 1.138277$

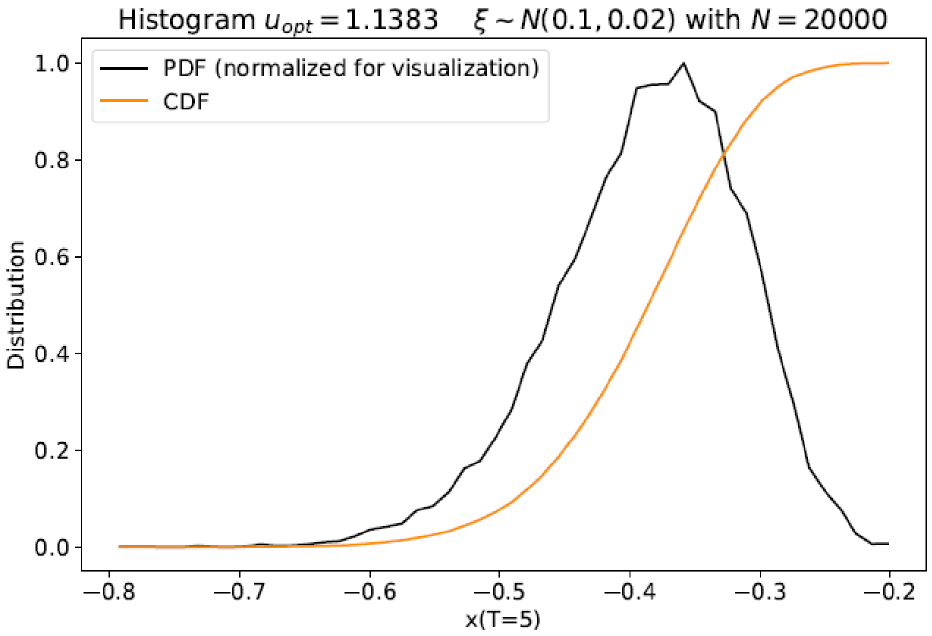
Optimization under Uncertainty with neural networks
Example

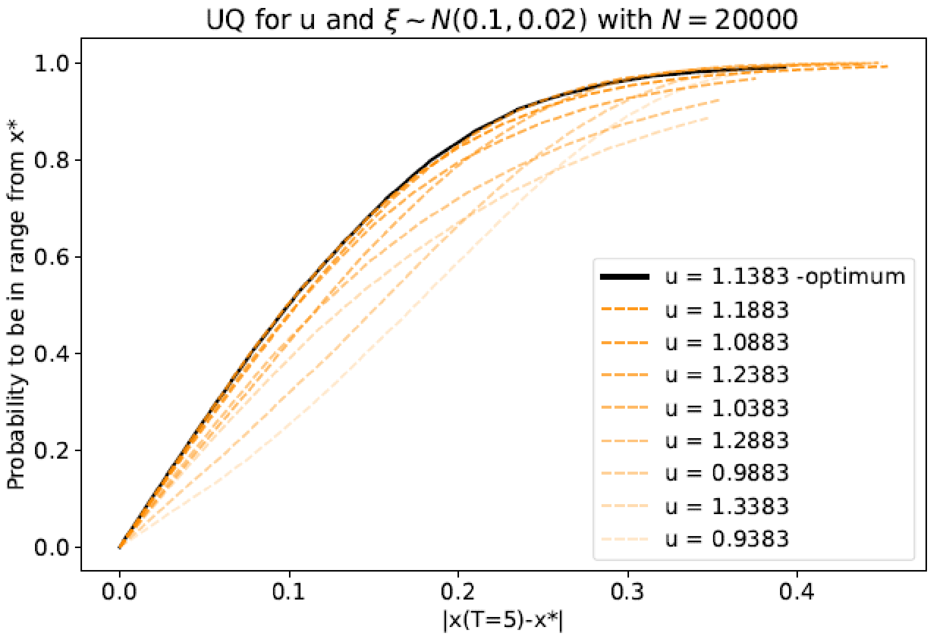
- **Further question:** How certain are we that our policy is the best and with what uncertainty? If we use our optimum how certain are we end up close to the target?

→ Use PINN to do MC-sampling and estimate some uncertainties

Optimization under Uncertainty with neural networks
Example

Sampling ξ with N=20 000 samples from $N(0.1{,}0.02)$ and do forward passes (solve ODE) on the PINN and plot the distribution

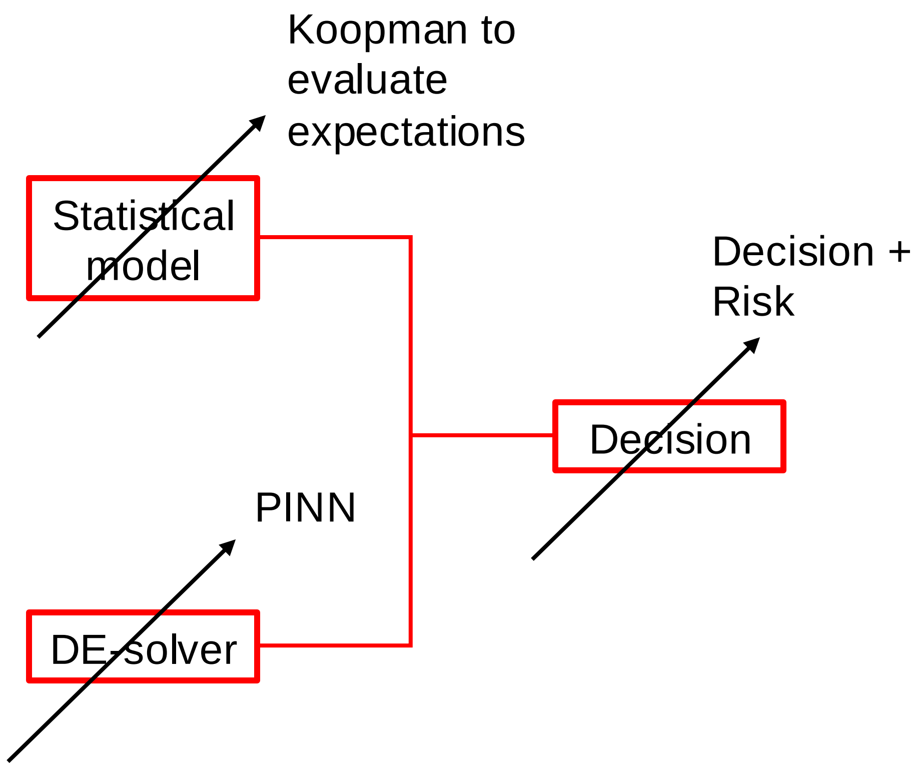




Optimization under uncertainty with neural networks
Conclusion

Conclusion:

1. **PINNs** can replace ODEs/PDEs for optimization tasks
   → Efficient batch mode evaluation
   → Gradients can be easily calculated from the PINN
2. **Koopman Expectation** seems to work
3. **Uncertainty quantification** can efficiently be done with PINNs if distributions are known by direct sampling
   → Risk quantification



Further question: Now the uncertainty quantification is done a-posteriori can we done it a-priori or during the optimization process?