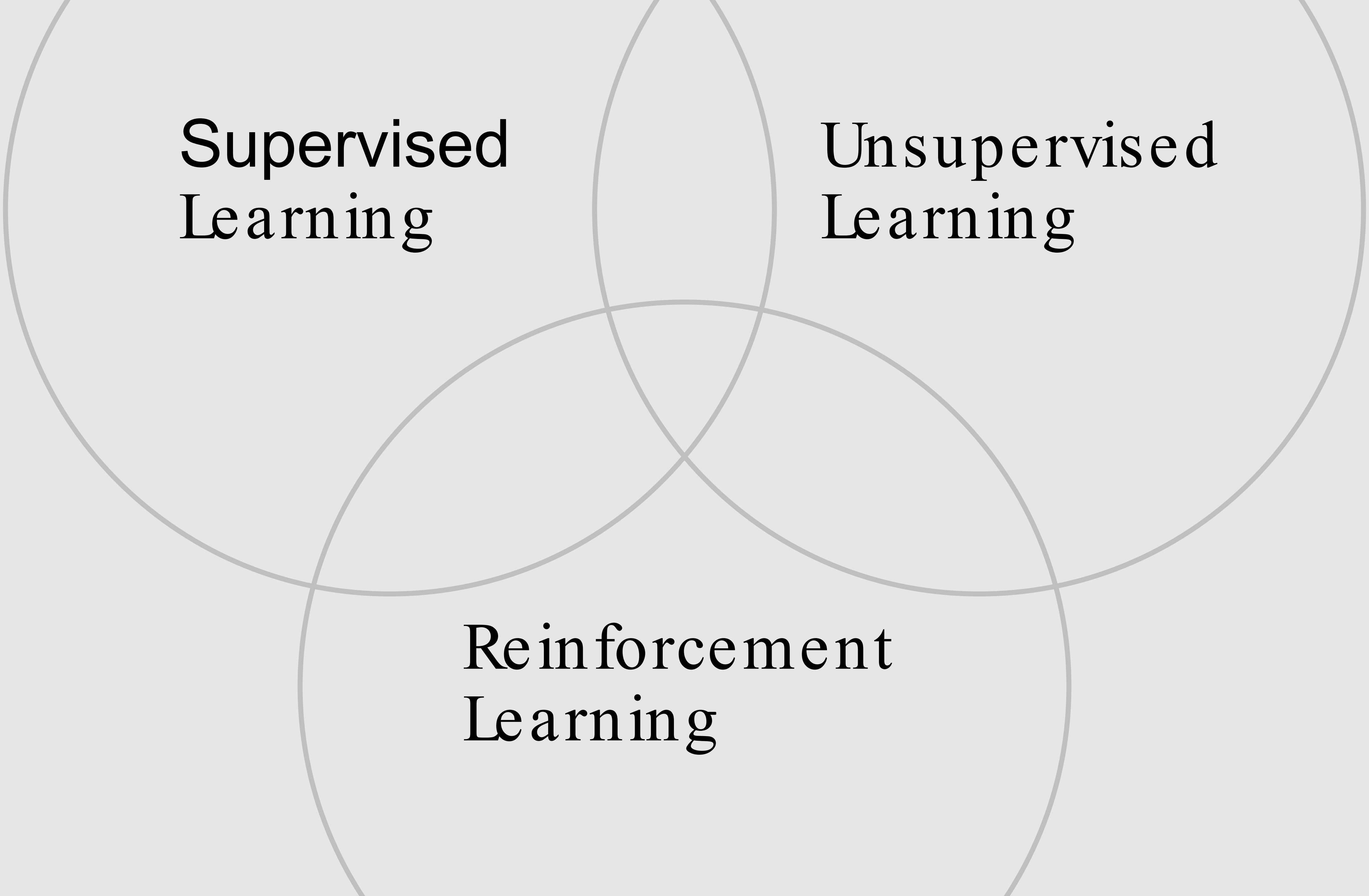
Introduction to Machine Learning

Dr. Mark Fuge
Univ. of Maryland, College Park
(301) 405-2558
fuge@umd.edu
ideal.umd.edu

What I hope you get from today:

1. What is Machine Learning?
2. When is it helpful?
3. When is it not helpful?
4. Where do you go from here?


Supervised Learning
Unsupervised Learning
Reinforcement Learning

Types of ML

Supervised Learning

Unsupervised Learning

Reinforcement Learning

Typical Engineering or Science Tasks

Reduced Order Models

Multi-Fidelity / Coarse-graining

Inverse Problems/ Design

Forecasting/ Prognostics

Generative Design

Anomaly Detection

System identification

Optimal Control

Optimization

Types of ML

Supervised Learning

Unsupervised Learning

Reinforcement Learning

Typical Engineering or Science Tasks

Reduced Order Models

Multi-Fidelity / Coarse-graining

Inverse Problems/ Design

Forecasting/ Prognostics

Generative Design

Anomaly Detection

System identification

Optimal Control

Optimization

1. What is the problem that needs solving?
2. How can machine learning help?
3. How do we know it is working?
4. When does it break down?

Types of ML

Supervised Learning

Unsupervised Learning

Reinforcement Learning

Typical Engineering or Science Tasks

Reduced Order Models

Multi-Fidelity / Coarse-graining

Inverse Problems/ Design

Forecasting/ Prognostics

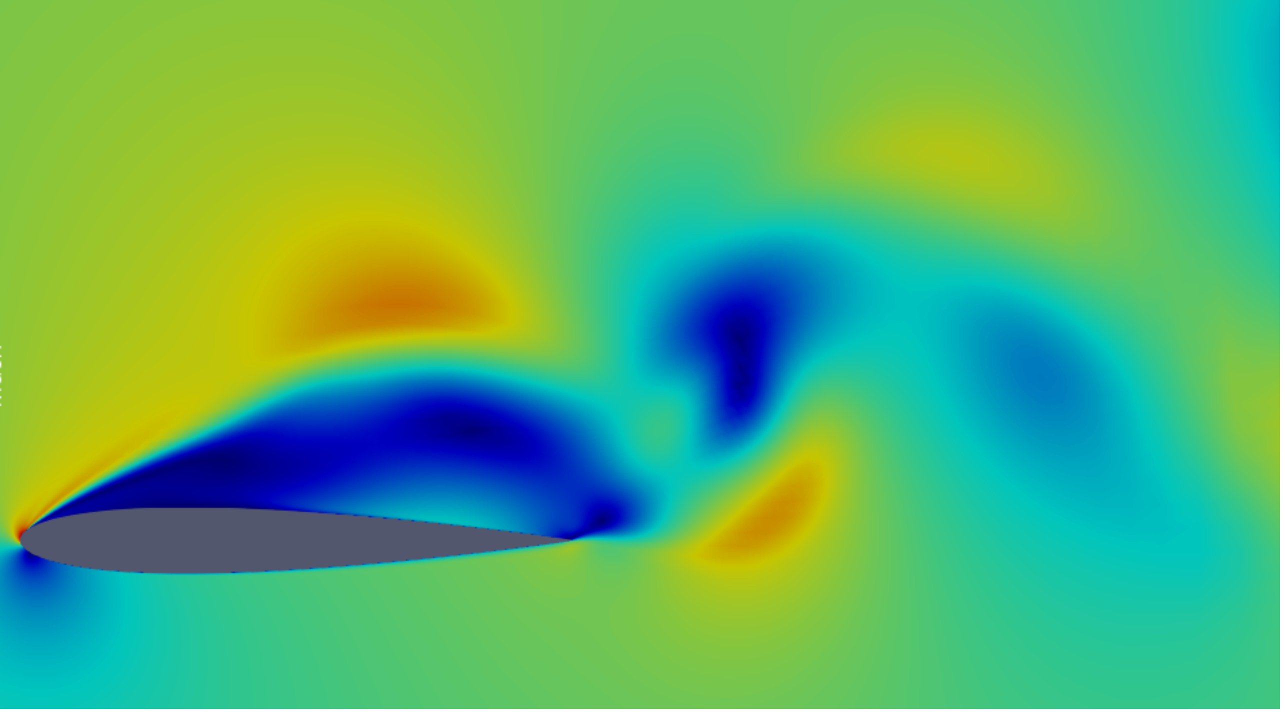
Generative Design

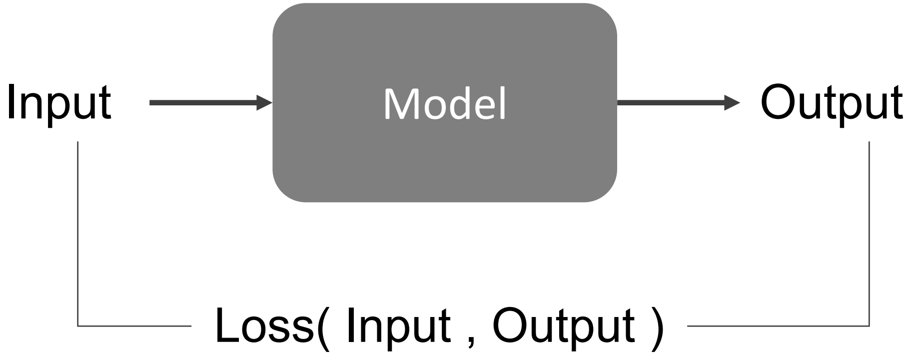
Anomaly Detection

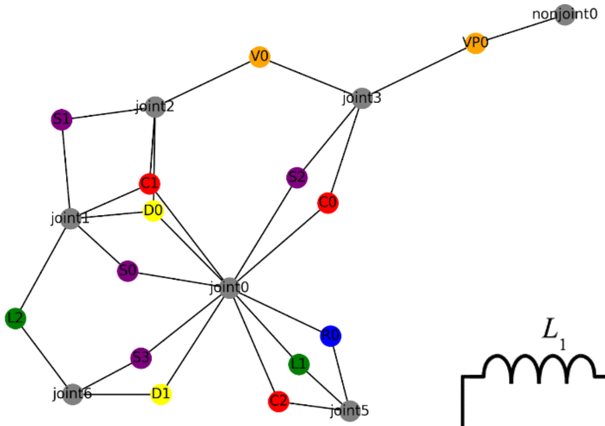
System identification

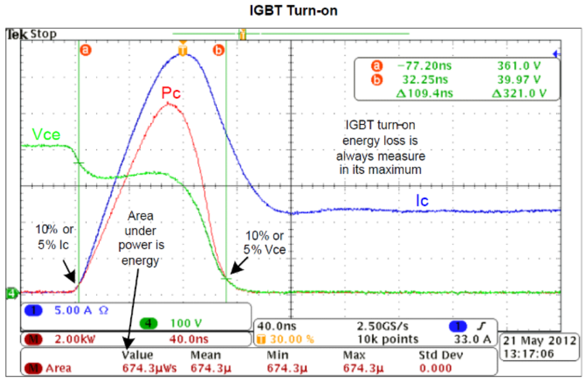
Optimal Control

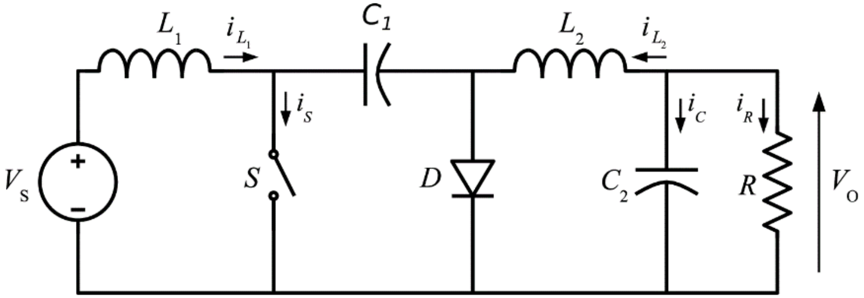
Optimization

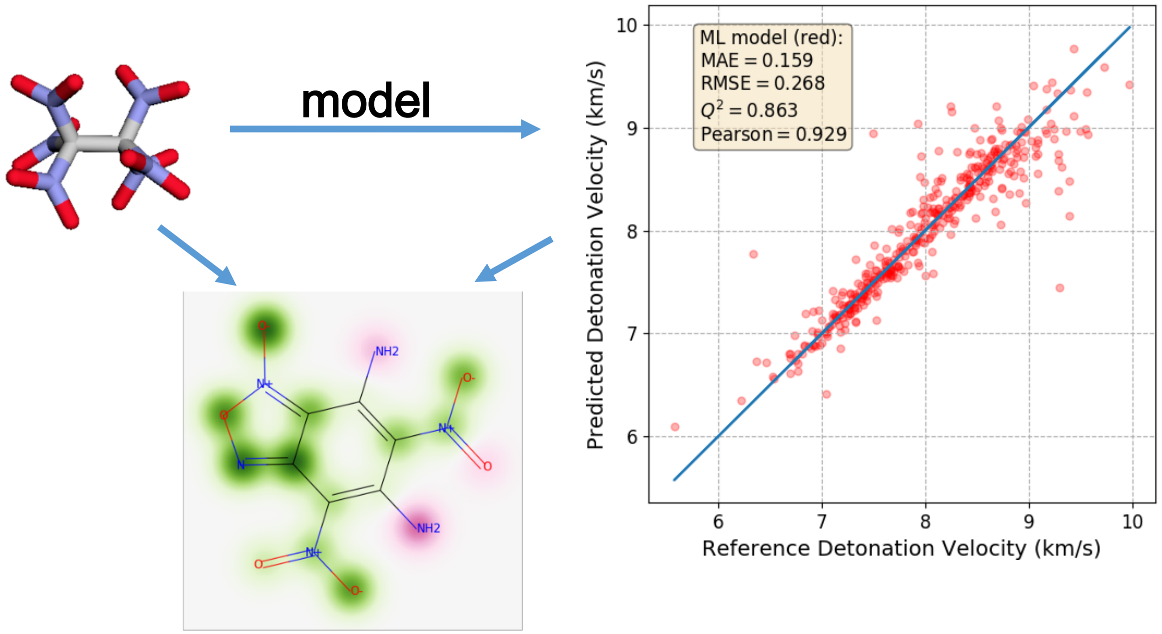



Input
Model
Output
Loss(Input , Output)


nonjoint0
VP0
V0
joint2
joint3
S1
C1
D0
joint1
S2
C0
S0
joint0
L2
B0
S3
L1
joint6
D1
C2
joint5


IGBT Turn-on
Vce
Pc
Ic
IGBT turn-on
energy loss is
always measure
in its maximum
10% or
5% Ic
Area
under
power is
energy
10% or
5% Vce
21 May 2012
13:17:06


L_1
i_{L_1}
C_1
L_2
i_{L_2}
i_S
i_C
i_R
V_S
S
D
C_2
R
V_O


model
NH2
N+
O-
O
N
NH2
ML model (red):
MAE = 0.159
RMSE = 0.268
Q^2 = 0.863
Pearson = 0.929
Predicted Detonation Velocity (km/s)
Reference Detonation Velocity (km/s)
6
7
8
9
10

Types of ML

Supervised Learning

Unsupervised Learning

Reinforcement Learning

Typical Engineering or Science Tasks

Reduced Order Models

Multi-Fidelity / Coarse-graining

Inverse Problems/ Design

Forecasting/ Prognostics

Generative Design

Anomaly Detection

System identification

Optimal Control

Optimization

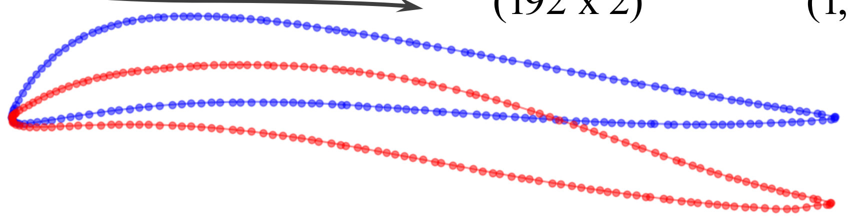
Example: ARPA-E DIFFERENTIATE Program

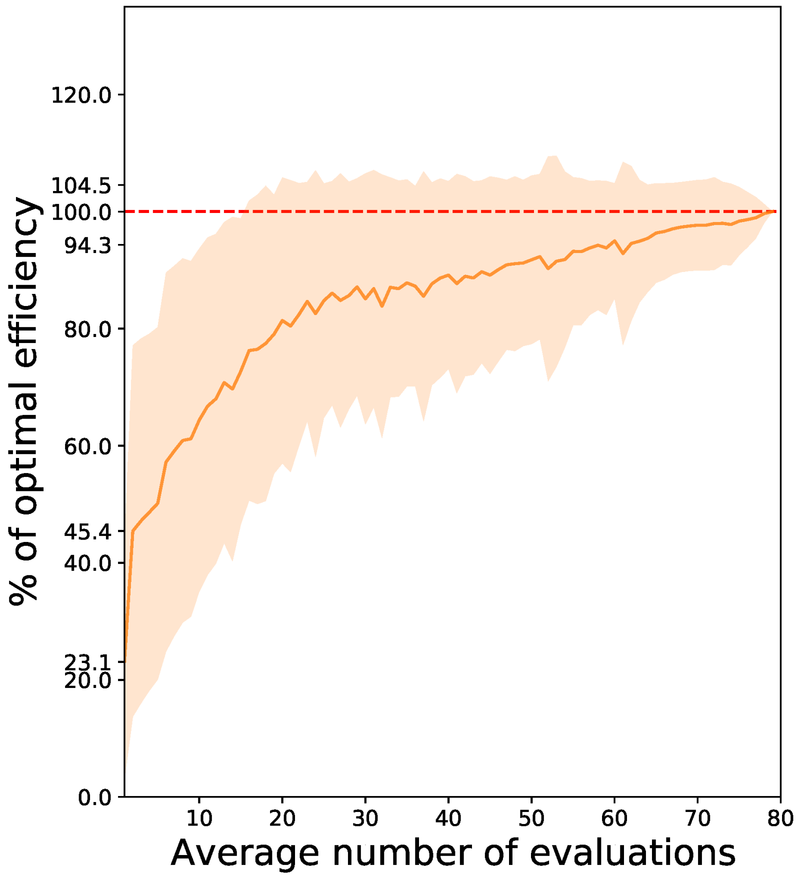
Inverse Design of Aero & Heat Transfer Surfaces

Mach number, Ma
Reynolds number, Re
Target lift coefficient, C_l

CFD + Supercomputer

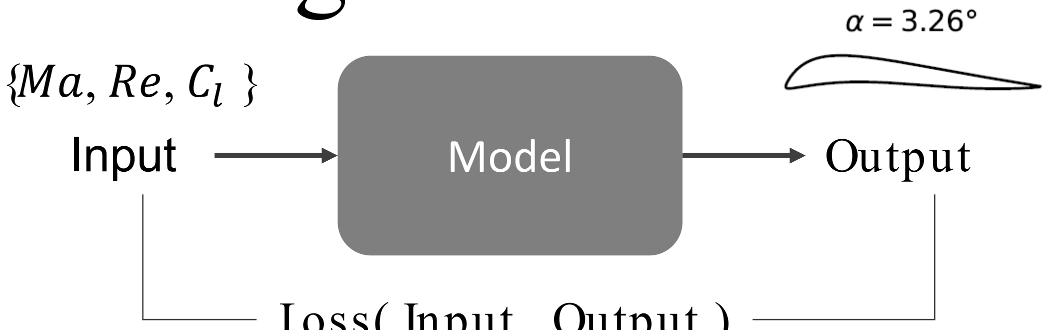
Optimized airfoil coordinates + Angle of attack, α
(192 x 2) (1, a scalar)

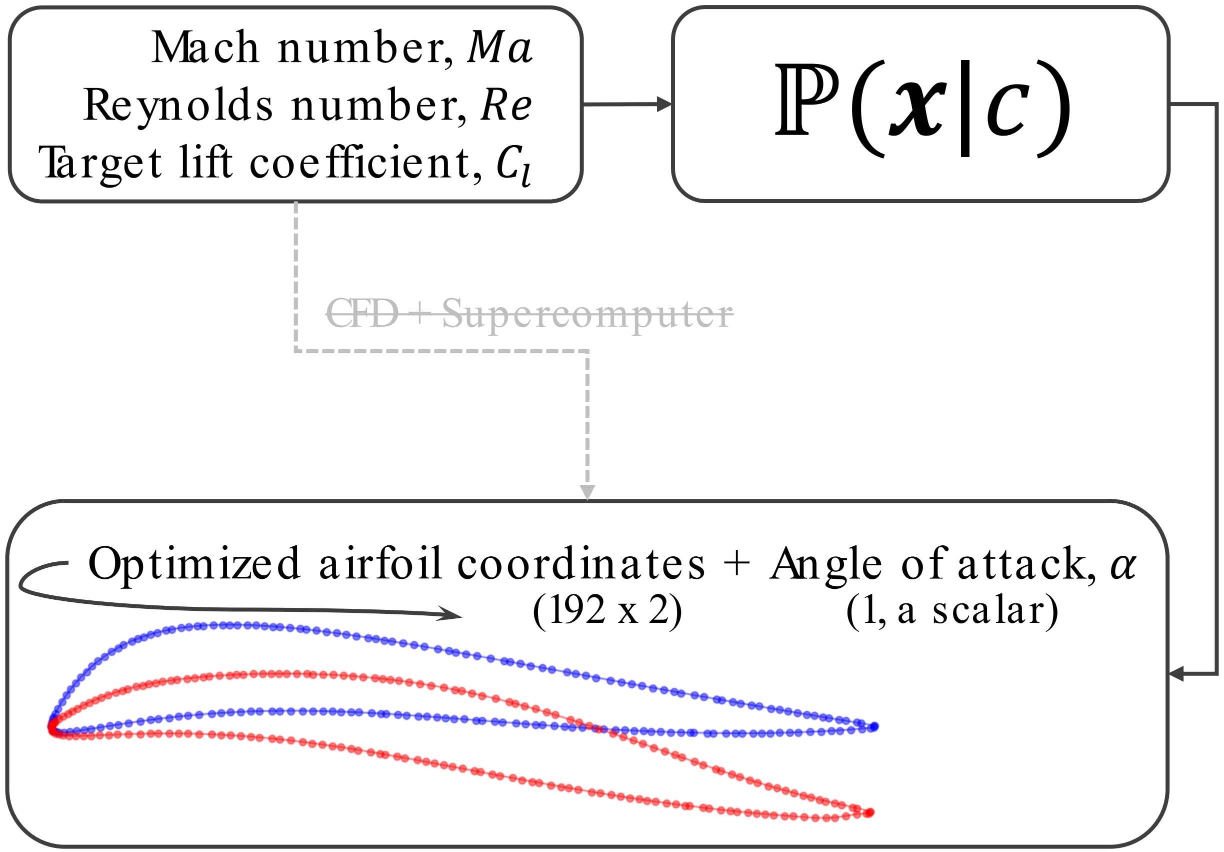


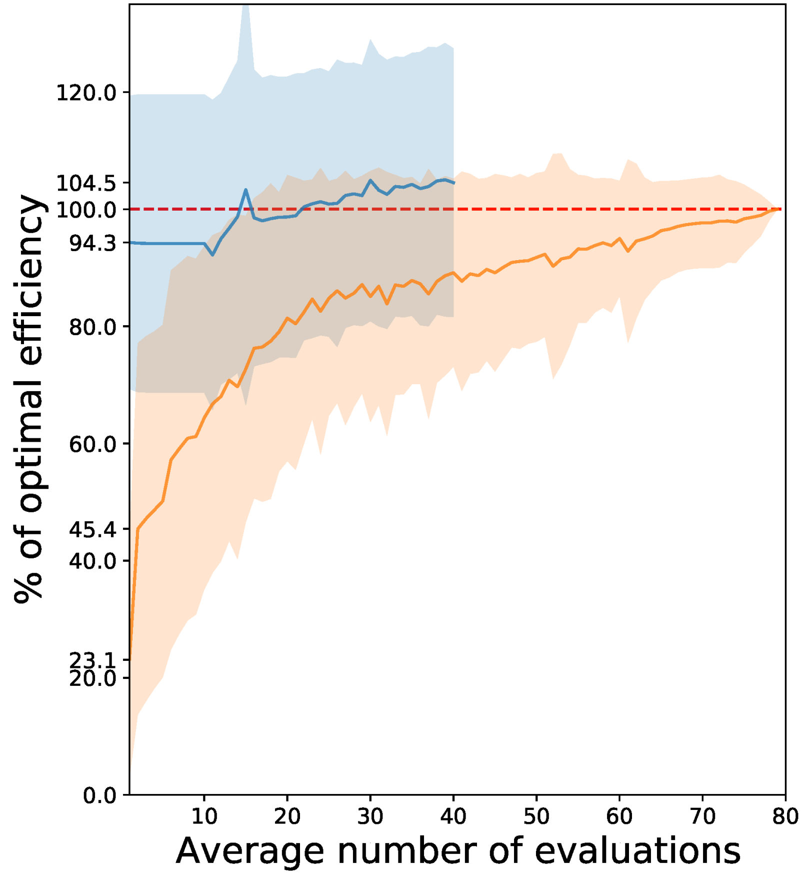


Example: ARPA-E DIFFERENTIATE Program

Inverse Design of Aero & Heat Transfer Surfaces







Types of ML

Supervised Learning

Unsupervised Learning

Reinforcement Learning

Typical Engineering or Science Tasks

Reduced Order Models

Multi-Fidelity / Coarse-graining

Inverse Problems/ Design

Forecasting/ Prognostics

Generative Design

Anomaly Detection

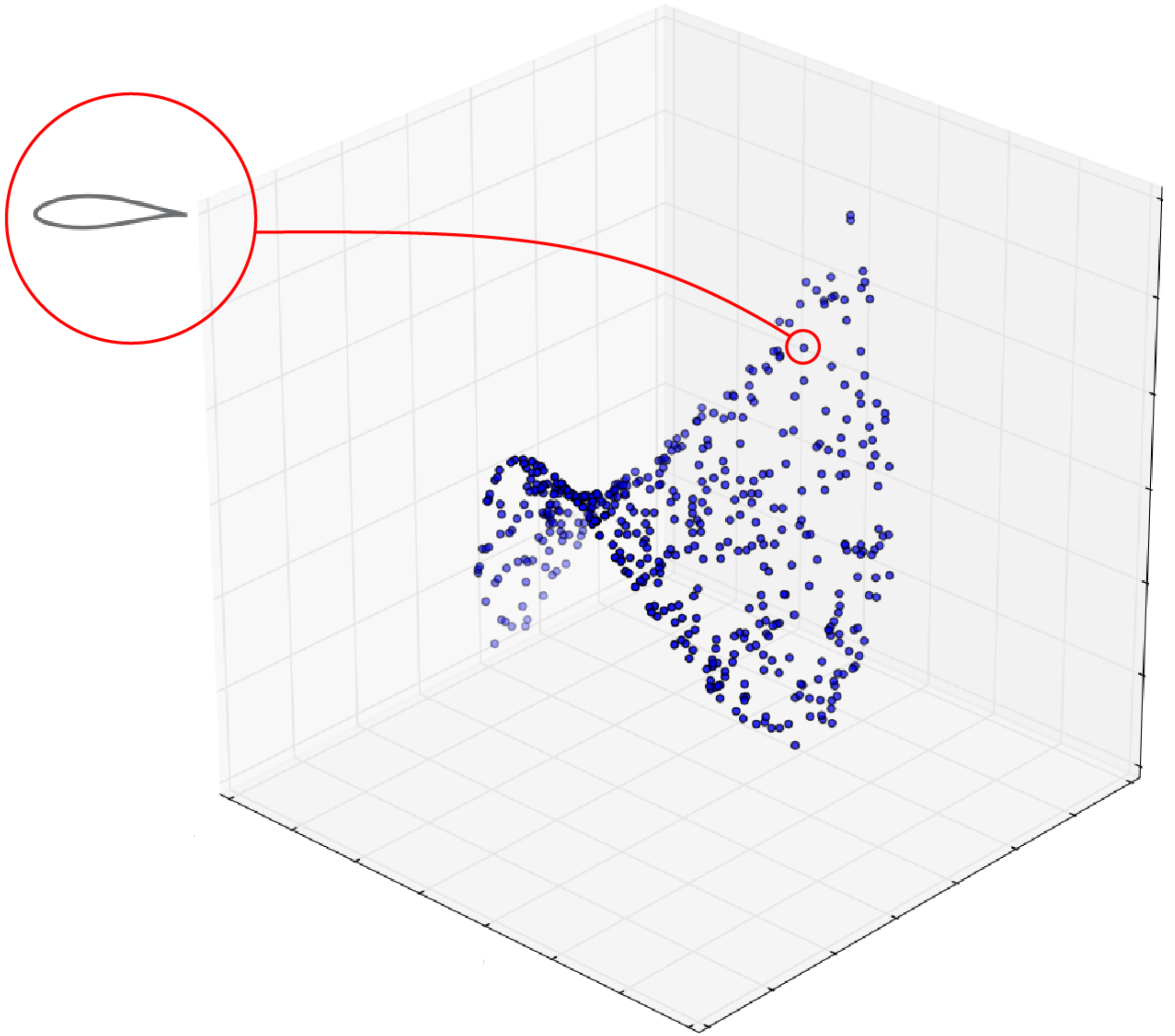
System identification

Optimal Control

Optimization

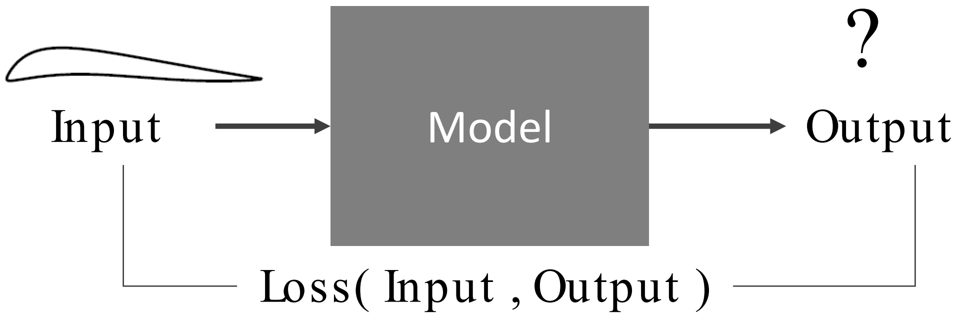
Problem: Original airfoil representation (~100 coordinates)
is too large to be useful.

The Manifold Hypothesis

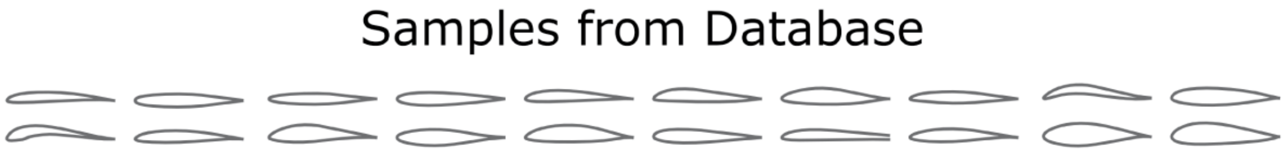


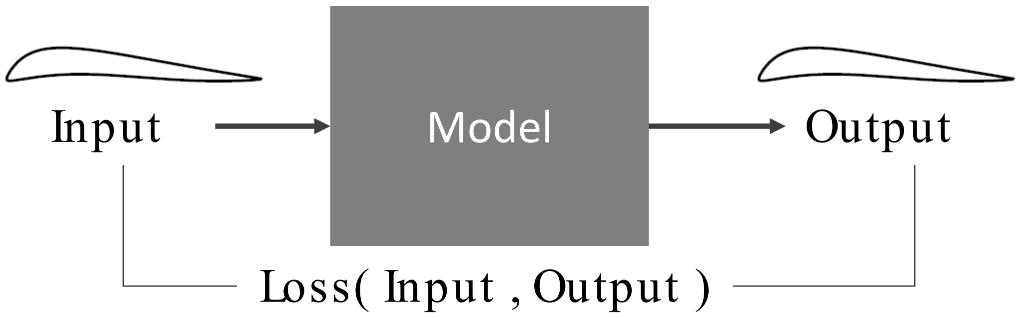
Example: Learning Airfoil Manifolds

Samples from Database

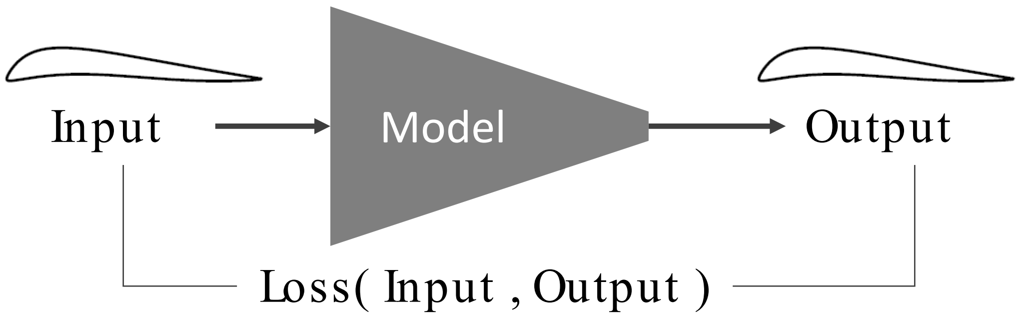


Example: Learning Airfoil Manifolds

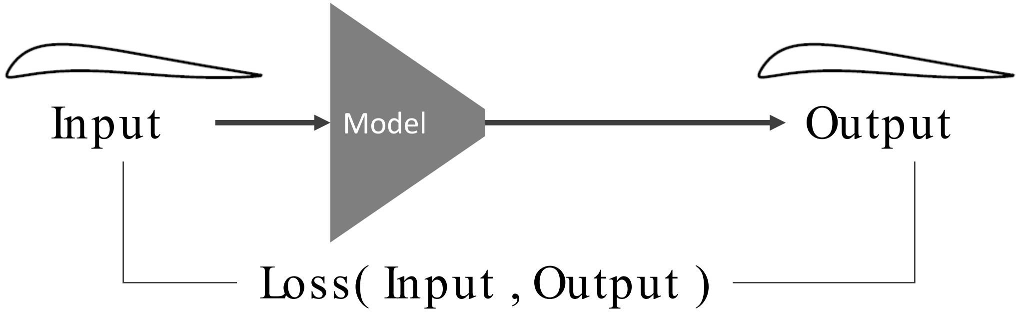




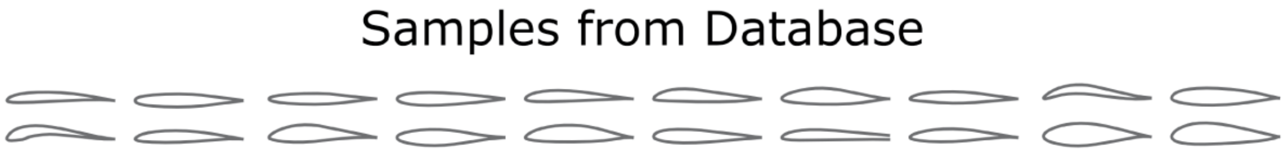
Example: Learning Airfoil Manifolds

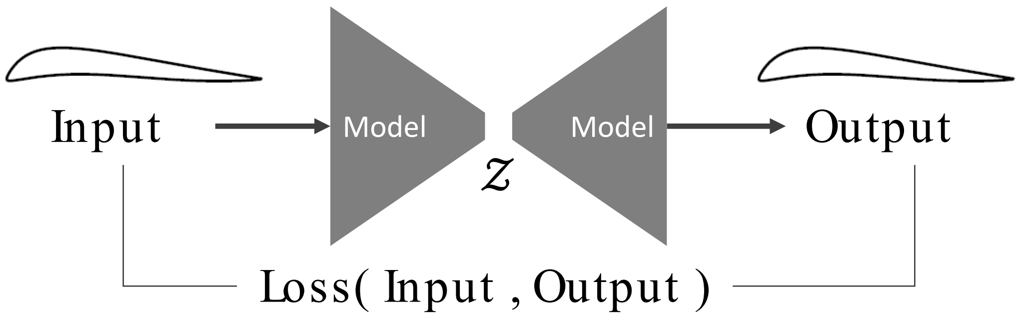


Example: Learning Airfoil Manifolds

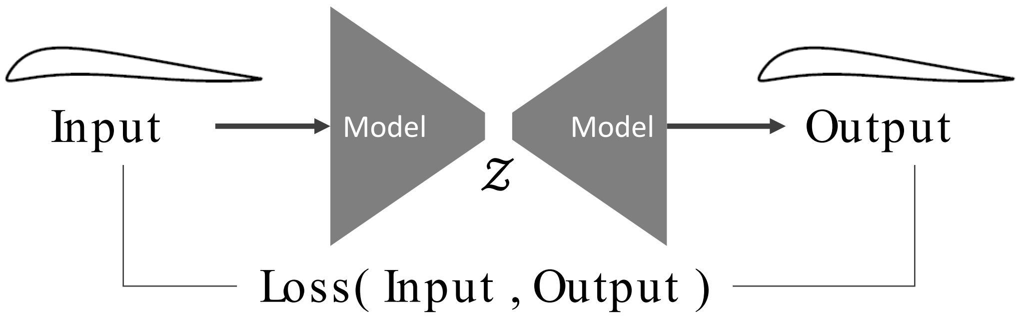


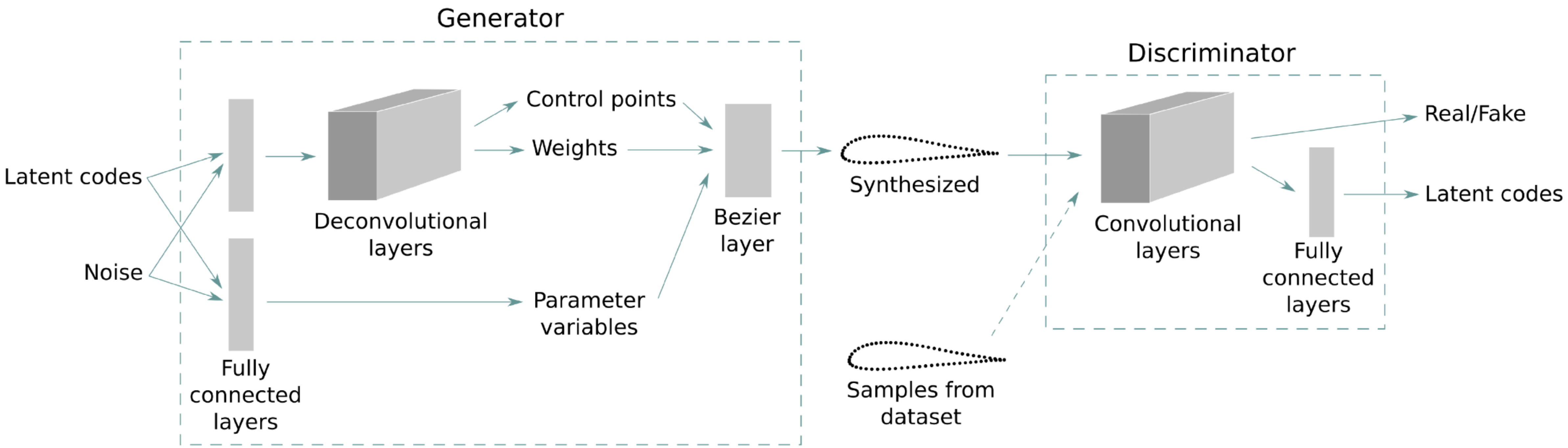
Example: Learning Airfoil Manifolds





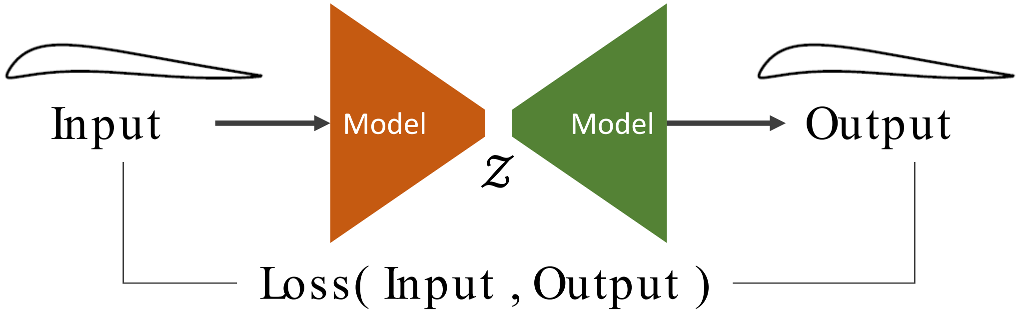
Example: Learning Airfoil Manifolds

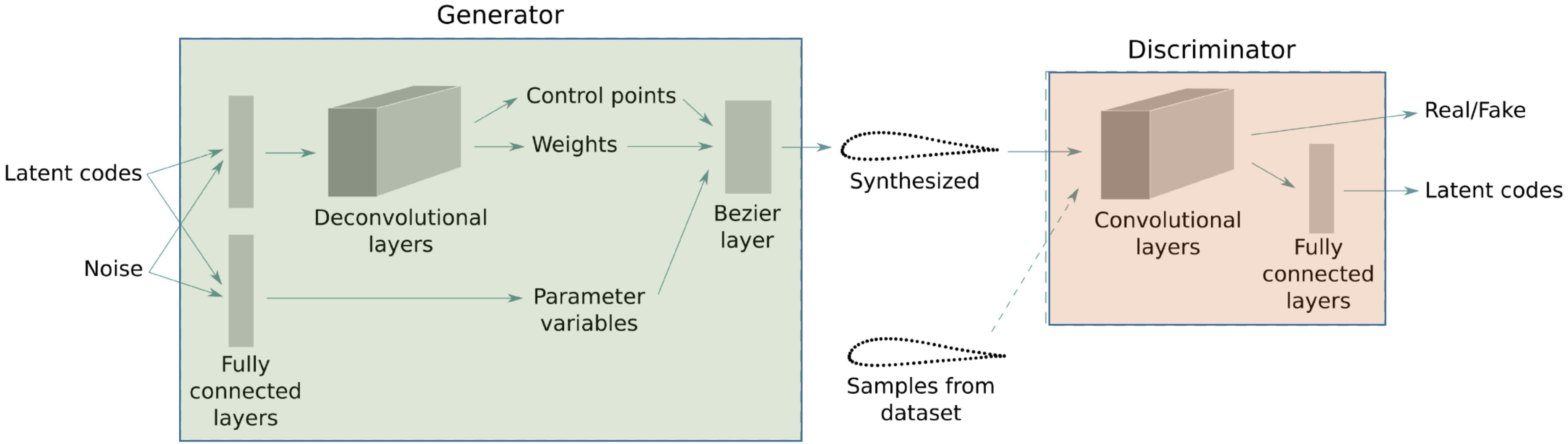




Example: Learning Airfoil Manifolds

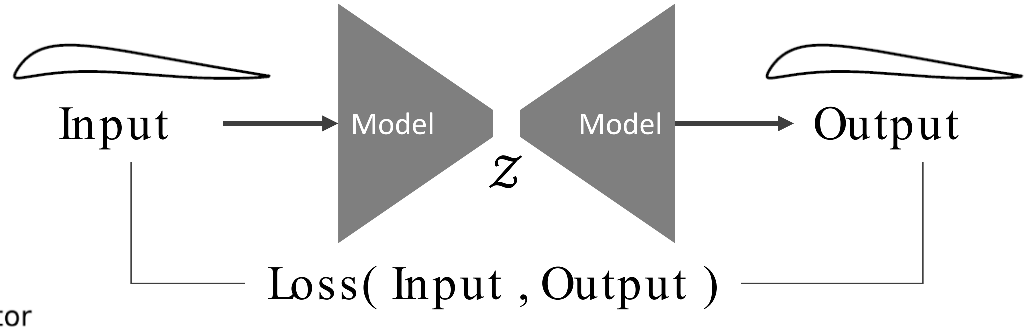
Samples from Database

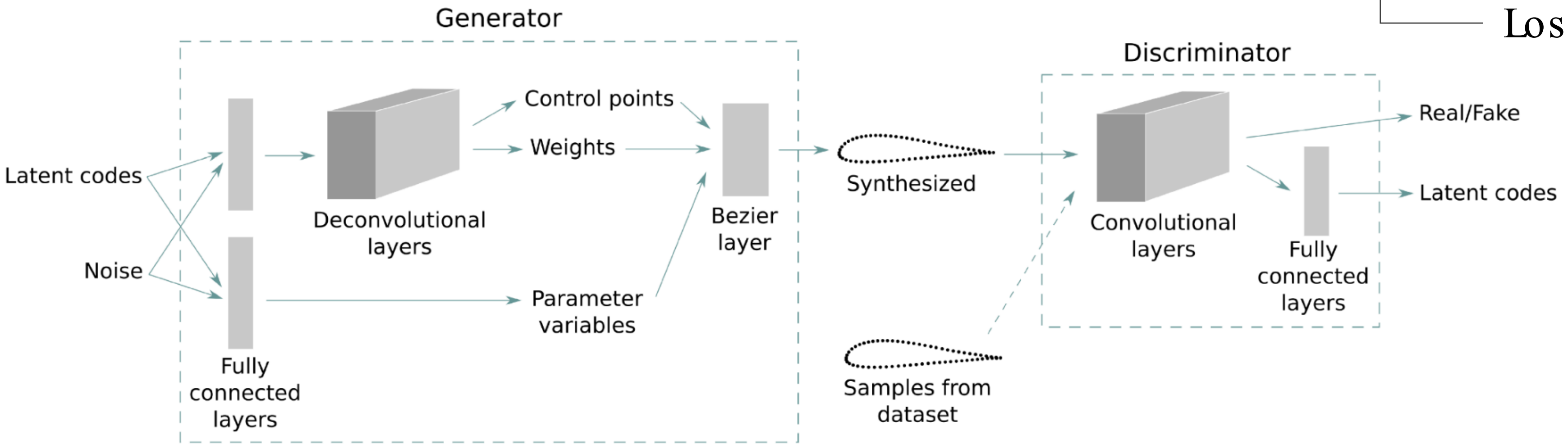




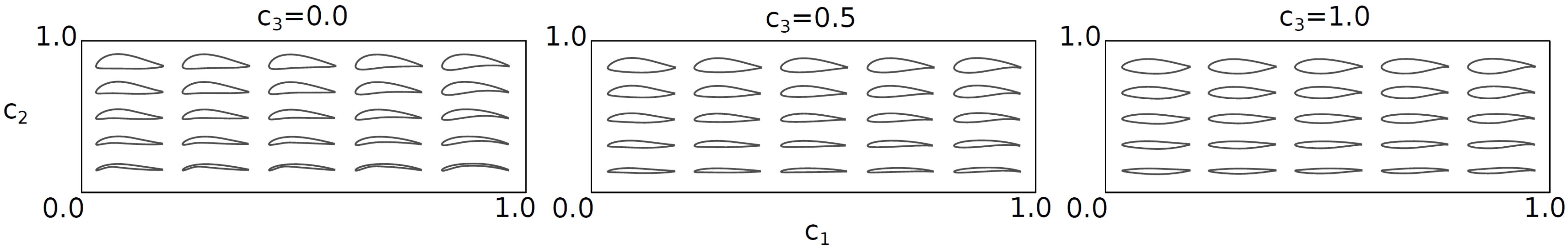
Example: Learning Airfoil Manifolds

Samples from Database

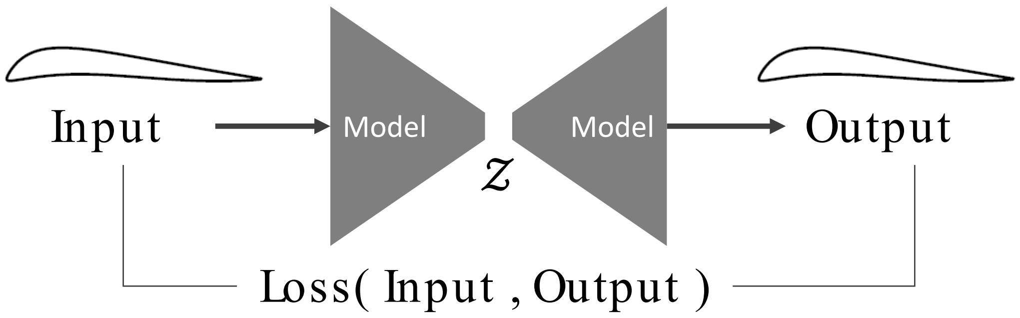


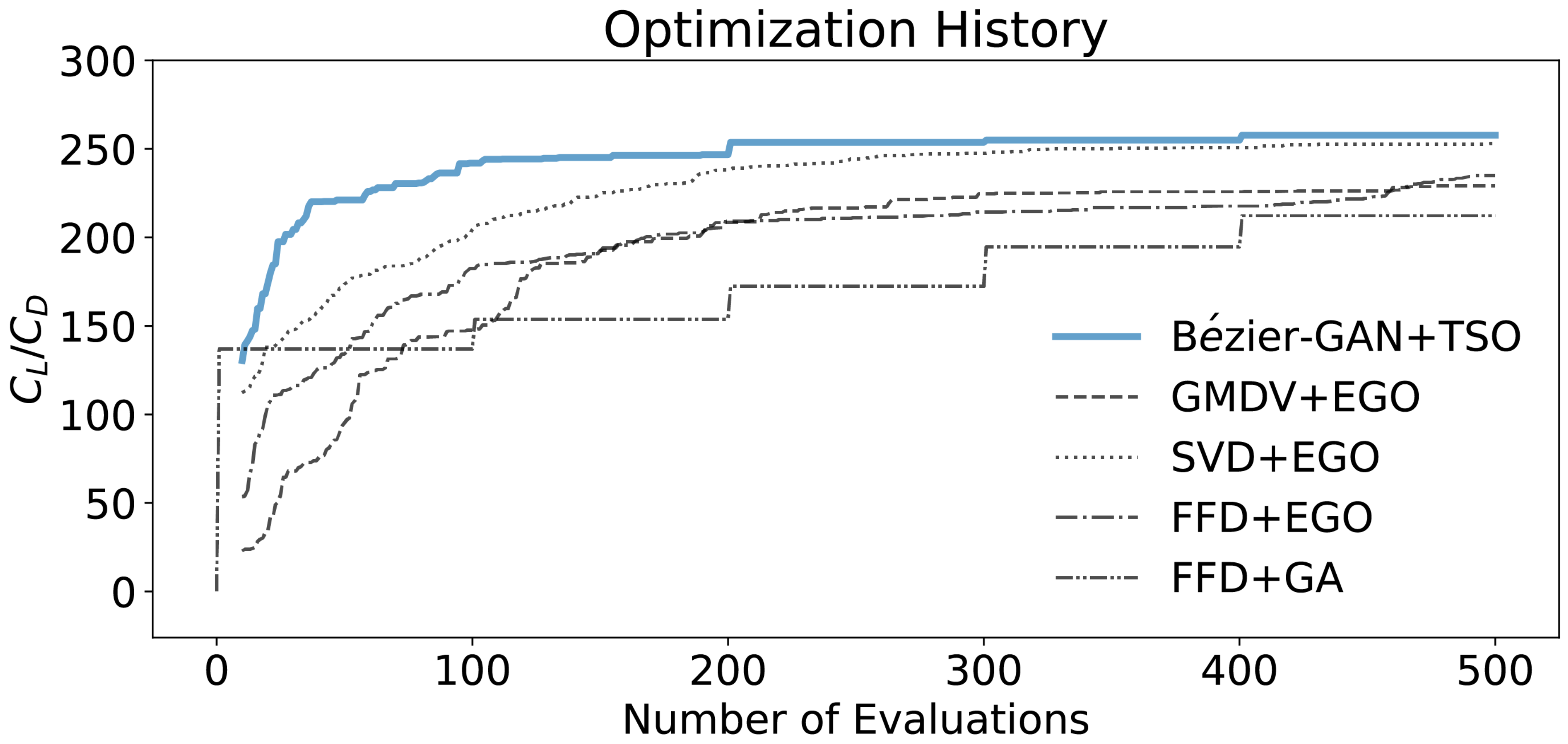


Latent space



Example: Learning Airfoil Manifolds





Types of ML

Supervised Learning

Unsupervised Learning

Reinforcement Learning

Typical Engineering or Science Tasks

Reduced Order Models

Multi-Fidelity / Coarse-graining

Inverse Problems/ Design

Forecasting/ Prognostics

Generative Design

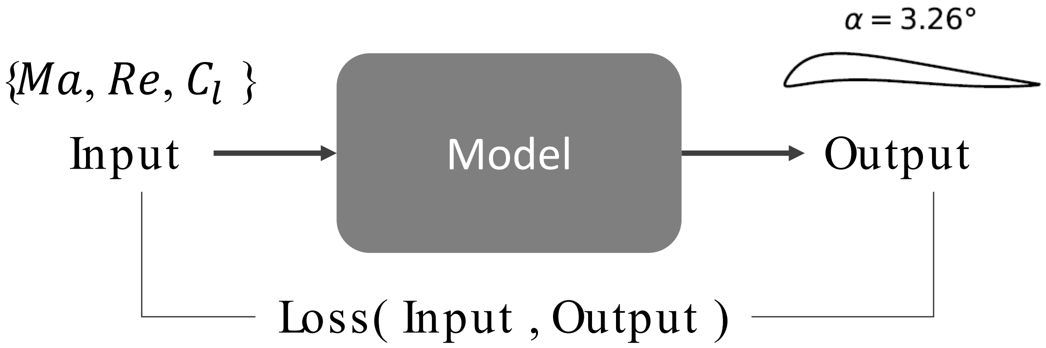
Anomaly Detection

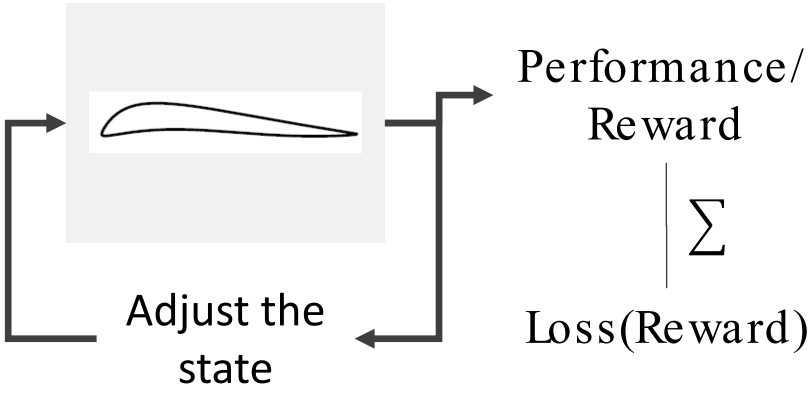
System identification

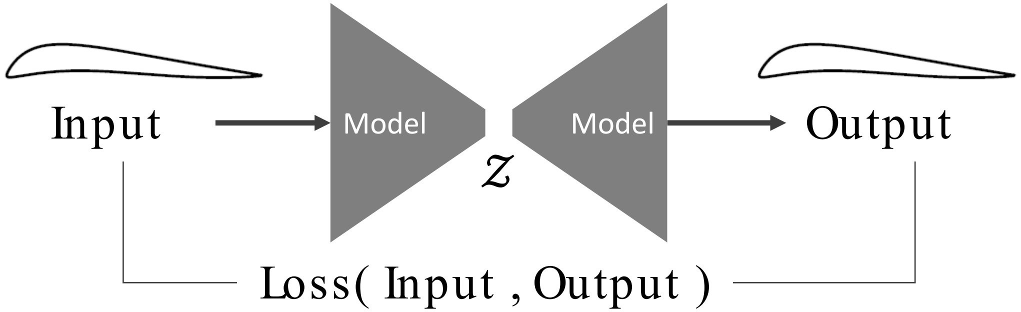
Optimal Control

Optimization

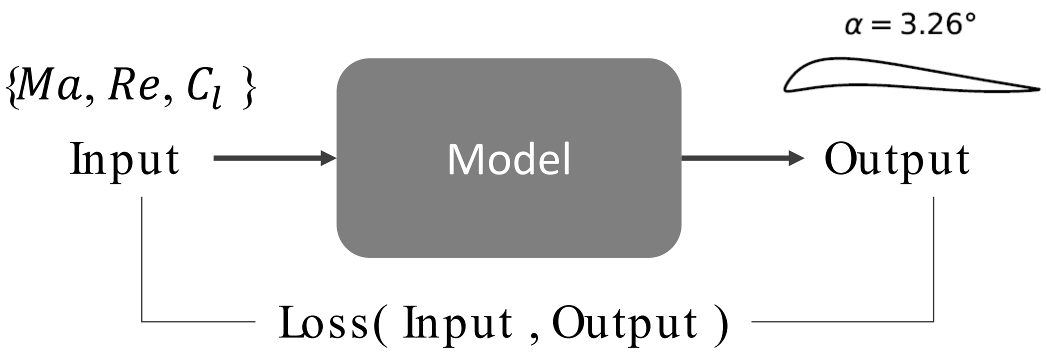
Reinforcement Learning vs Other models

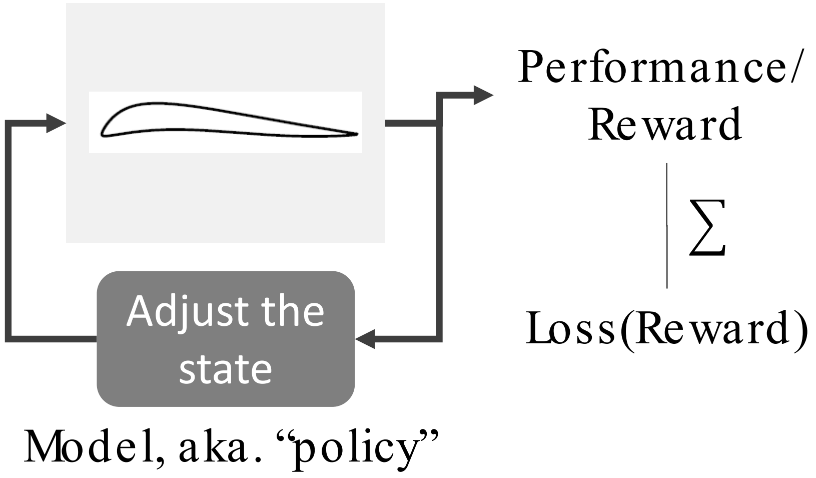


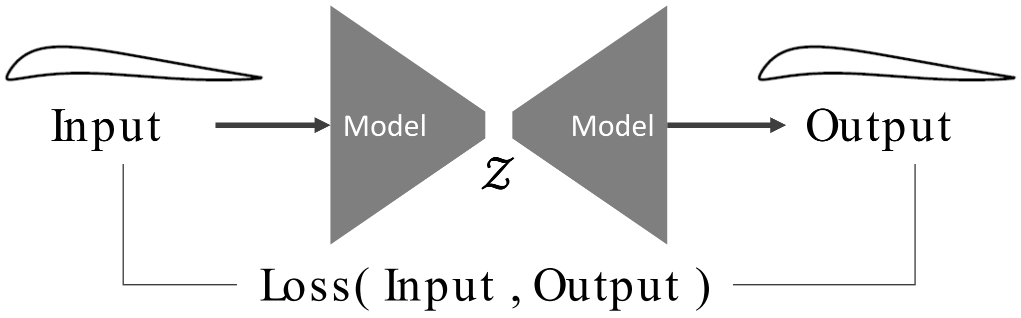




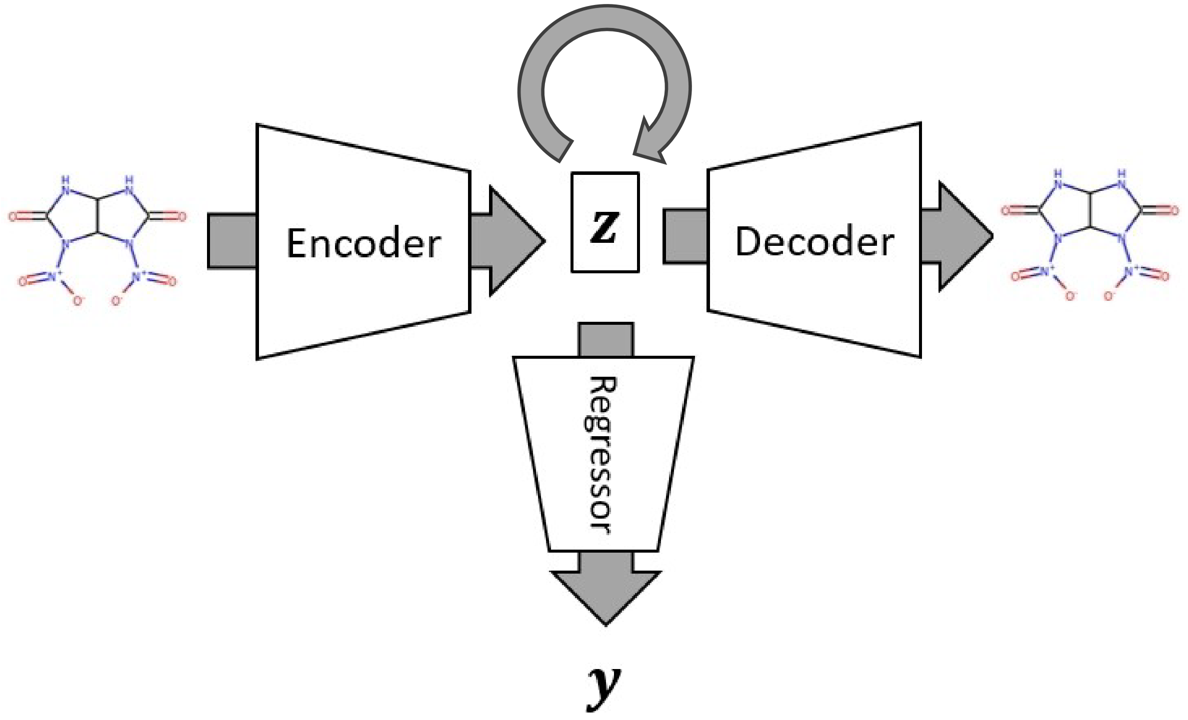
Reinforcement Learning vs Other models

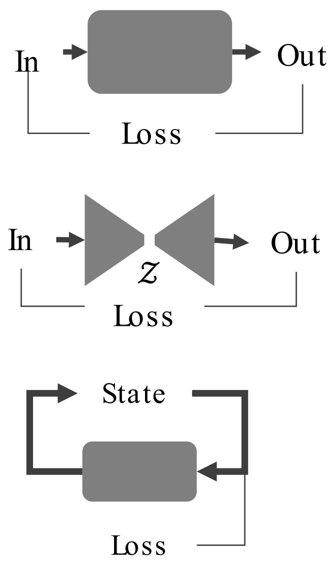




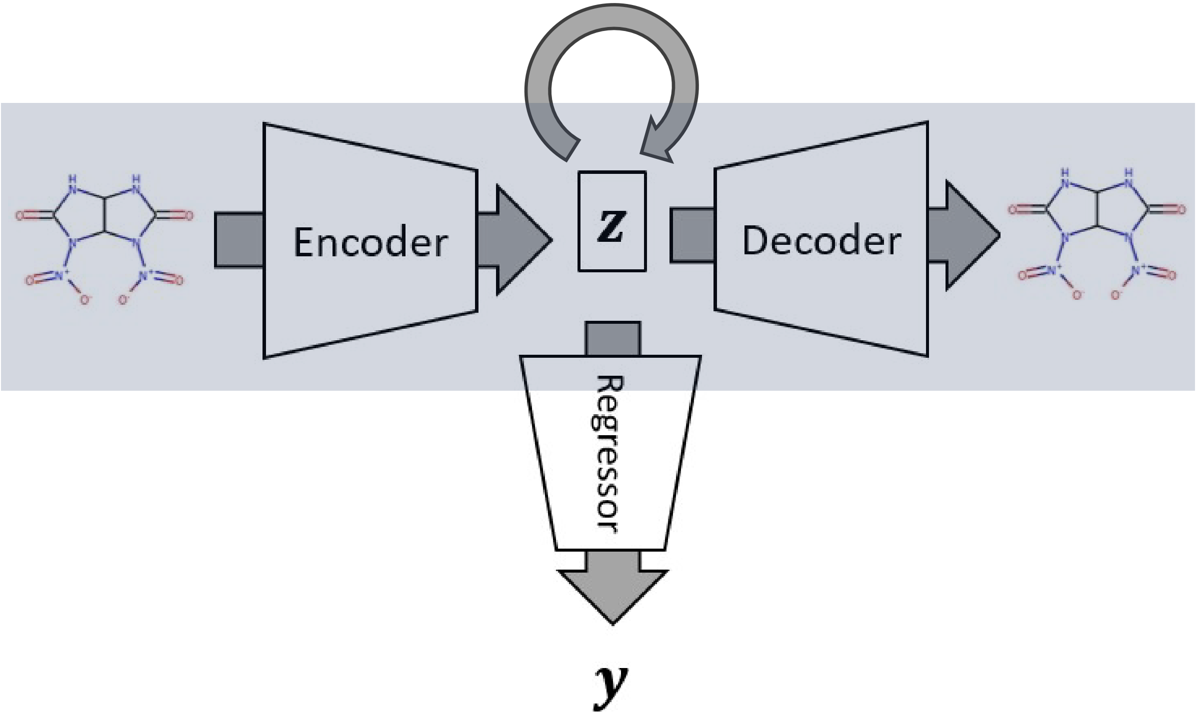


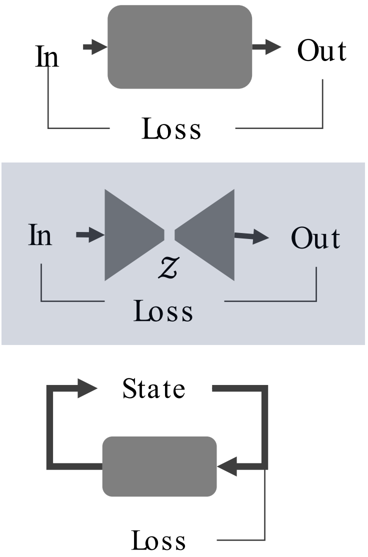
Example: Optimizing Molecular Properties



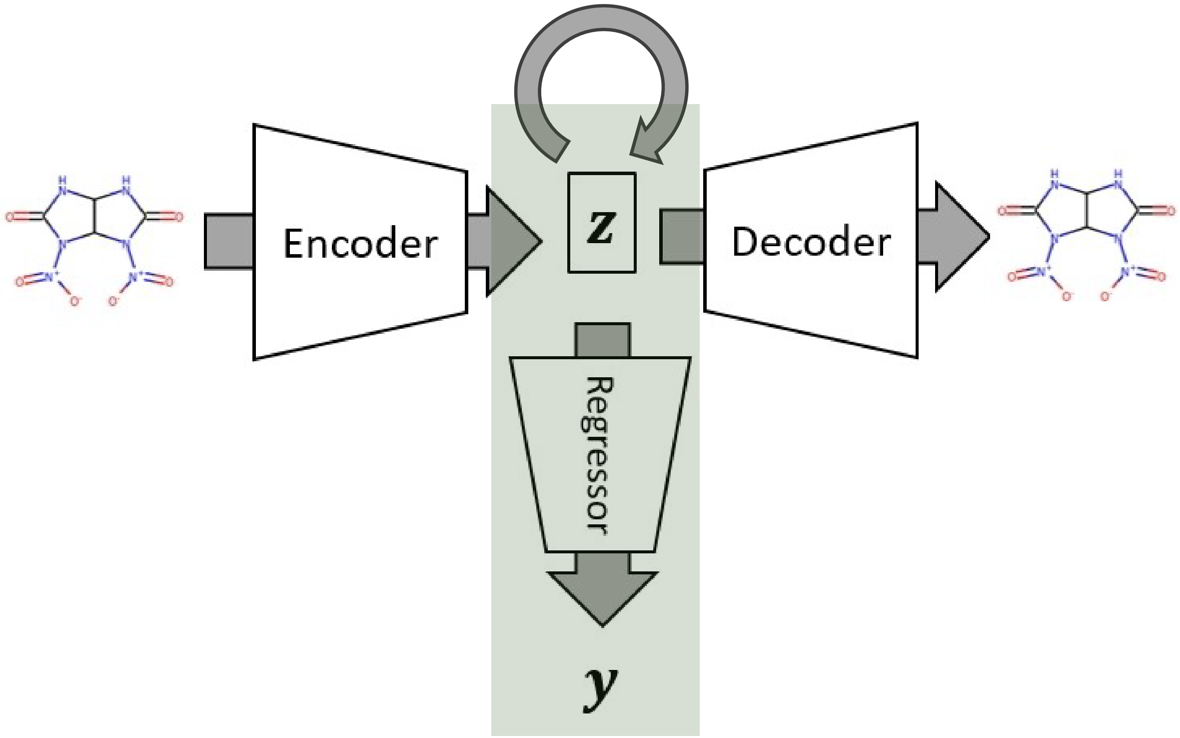


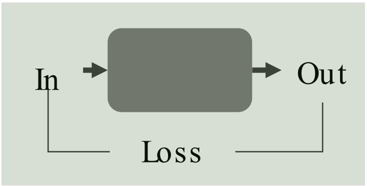
Example: Optimizing Molecular Properties

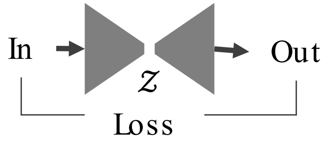


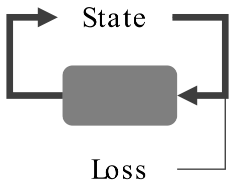


Example: Optimizing Molecular Properties

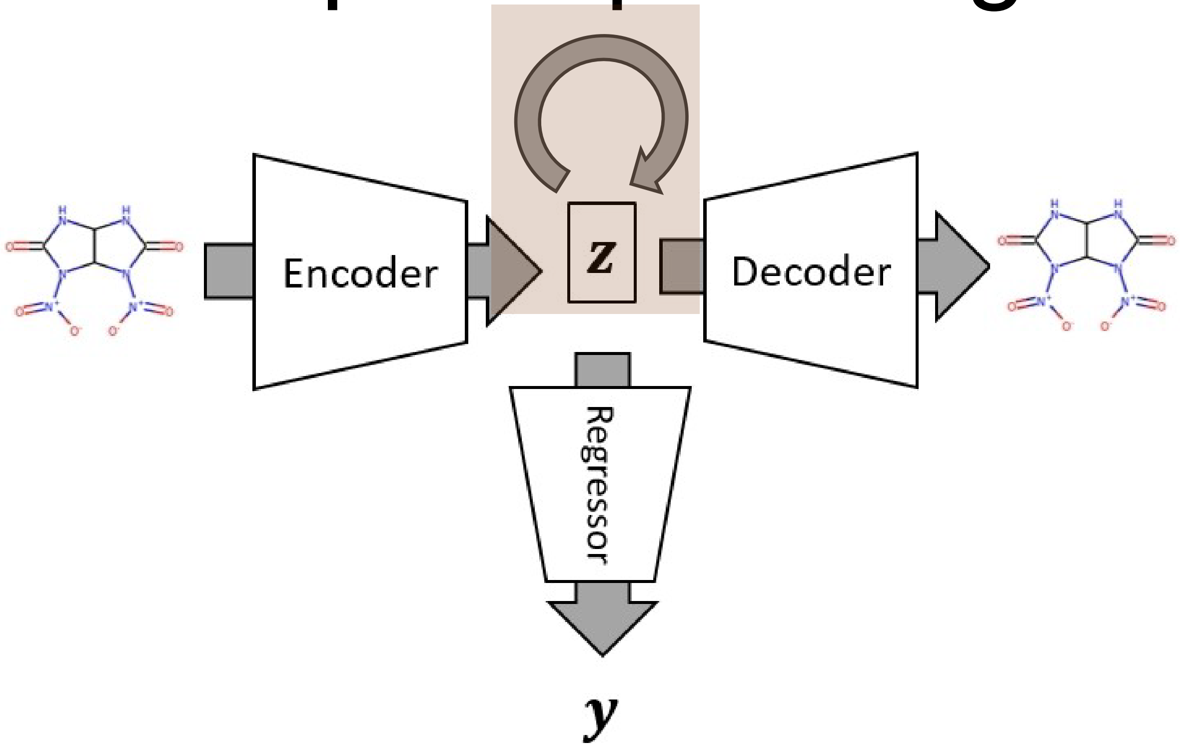


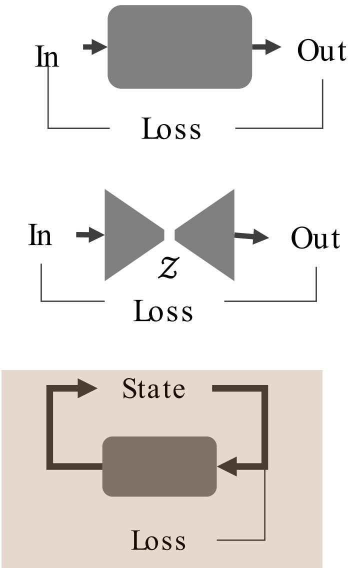




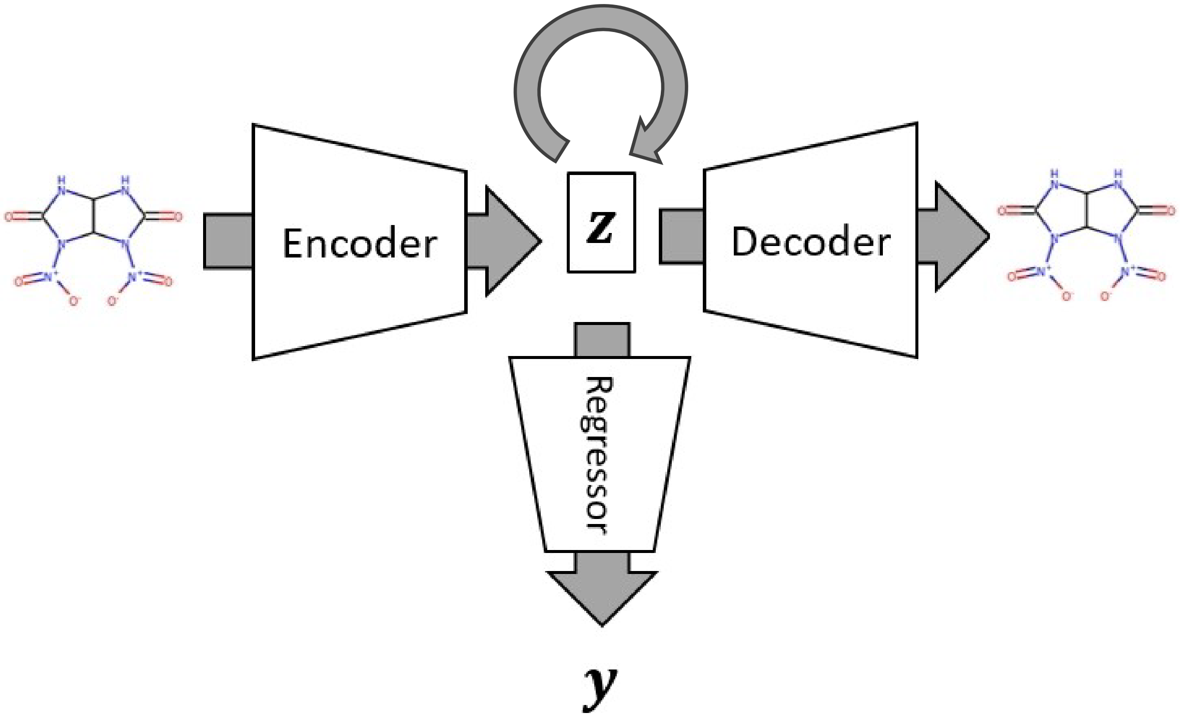


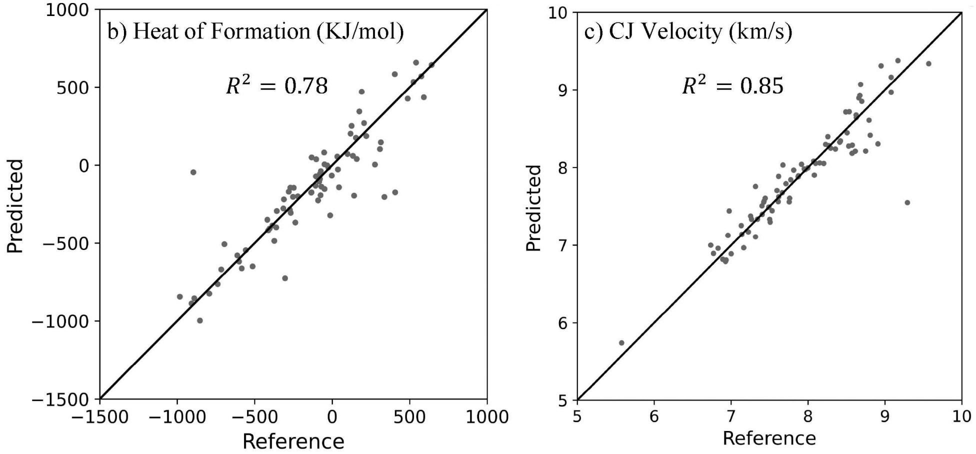
Example: Optimizing Molecular Properties

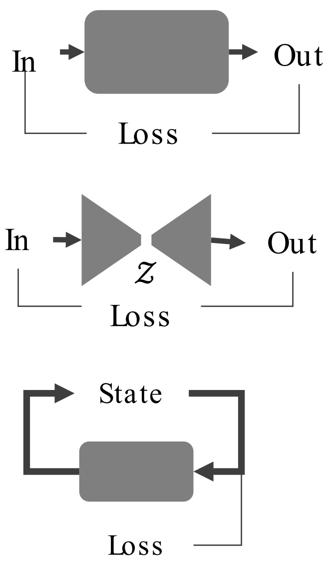


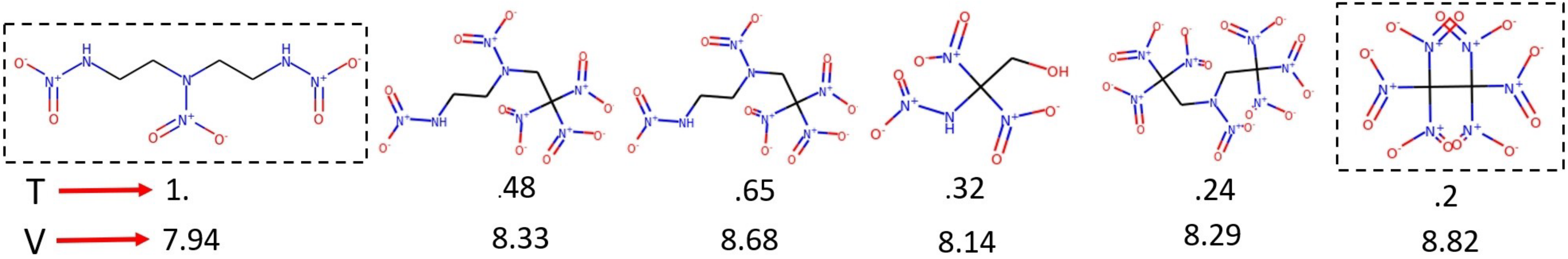


Example: Optimizing Molecular Properties









Types of ML	Typical Engineering or Science Tasks
Supervised Learning	Reduced Order Models Multi-Fidelity / Coarse-graining Inverse Problems/ Design Forecasting/ Prognostics
Unsupervised Learning	Generative Design Anomaly Detection System identification
Reinforcement Learning	Optimal Control Optimization

Where do you go from here?

Technical Challenges

How do we create, collect, and share benchmark datasets?

How do we best combine existing Engineering knowledge with ML techniques?

How do we perform Verification and Validation?

What are appropriate Standards for such models?

What are the key Figures of Merit we should be optimizing in such systems?

Socio-Economic Challenges

How do we estimate the economic Return on Investment for ML techniques or datasets?

How do we protect IP or Privacy in trained models?

What regulatory frameworks do we need for verification of safety critical or other systems?

How should we train our workforce differently to leverage these techniques?

For more details see:

- JMD Editorial: ML in Engineering Design: http://ideal.umd.edu/papers/paper/ml-eng-design-jmd
- Summary of Data-Driven Design workshop: http://ideal.umd.edu/papers/paper/d3-implications

Where do you go from here?

What can you do?

Continue your education in these areas, or for those of your workforce.

Reach out to researchers and domain experts for new technical challenges we can resolve in these areas.

Provide guidance to policy and regulatory bodies on how these techniques might be managed.

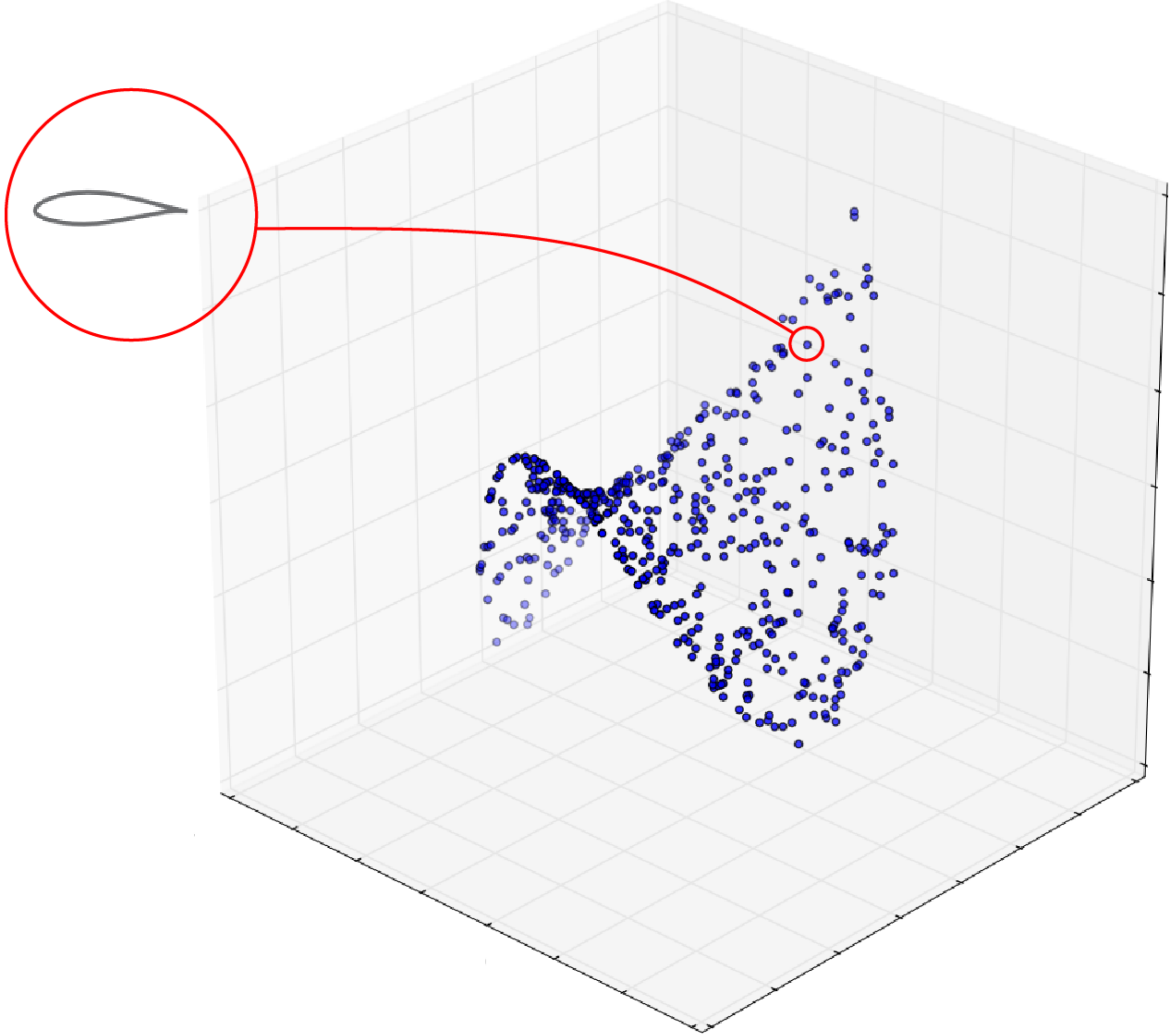
Advocate for additional studies of impact in these areas.

Thank you

Dr. Mark Fuge
Univ. of Maryland, College Park
(301) 405-2558
fuge@umd.edu
ideal.umd.edu

Backup Slides

What are Generative Models doing?

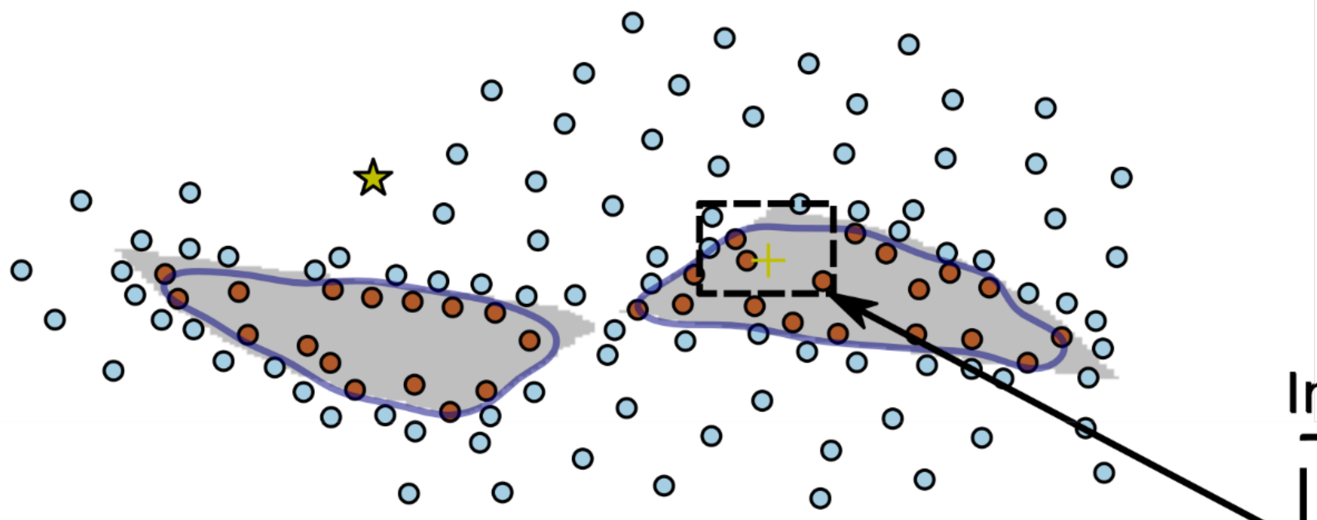


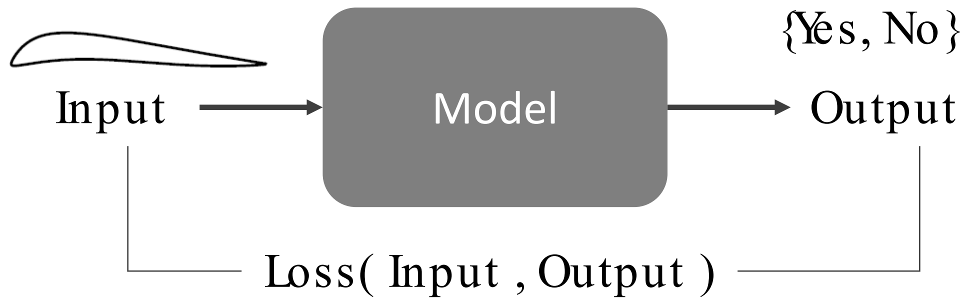
$$f : \mathcal{Z} \to \mathcal{X} \qquad \mathbb{P}(\boldsymbol{x}|\boldsymbol{z})$$

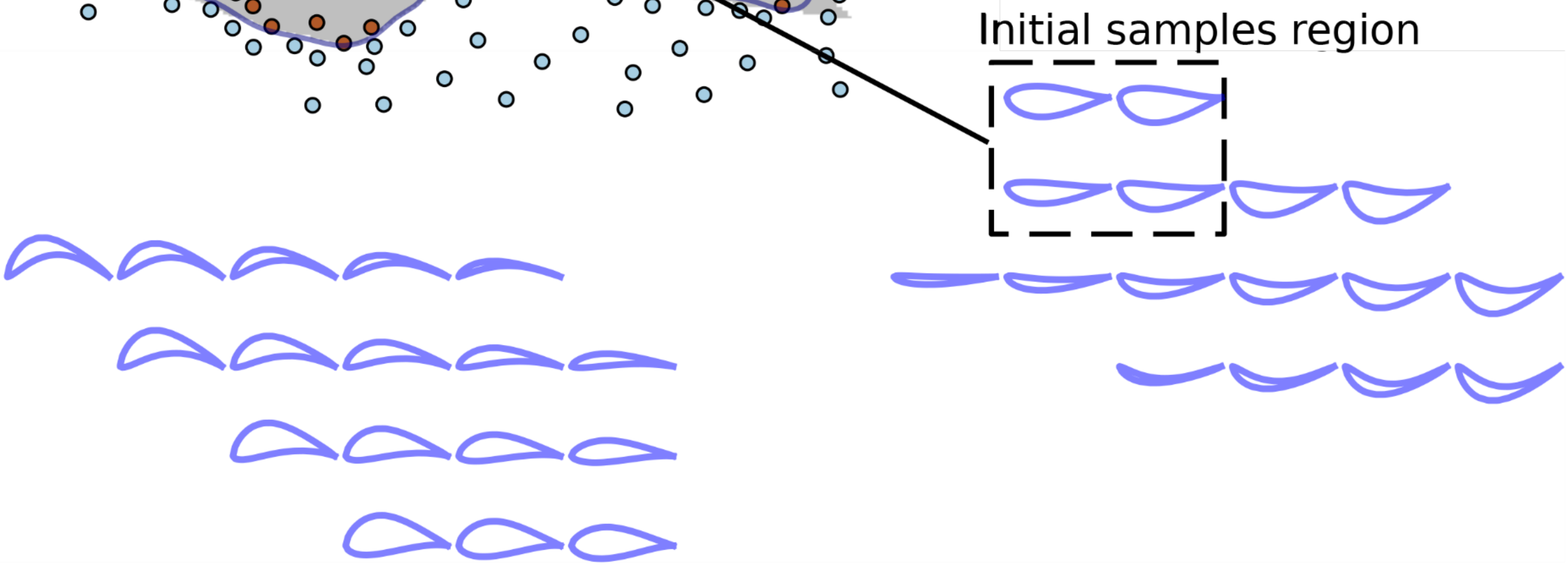
$$f^{-1} : \mathcal{X} \to \mathcal{Z} \qquad \mathbb{P}(\boldsymbol{z}|\boldsymbol{x})$$

$$\log \mathbb{P}(\boldsymbol{x}) = \log \mathbb{P}(\boldsymbol{z}) + \log |\det \nabla_{\boldsymbol{x}} f^{-1}(\boldsymbol{x})|$$

Example: Identifying Feasible Performance Regions

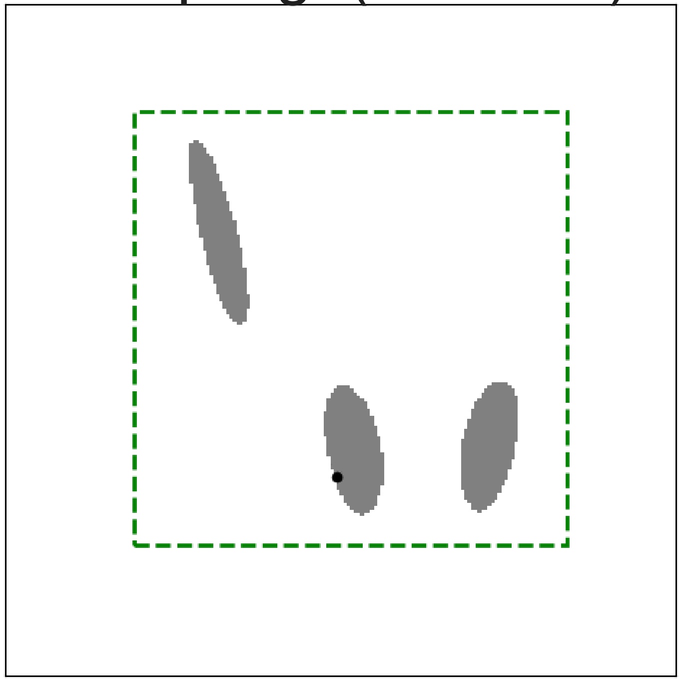






Example: Identifying Feasible Performance Regions

Conventional adaptive sampling (Straddle)



Active Expansion Sampling