

# COMBINING MACHINE LEARNING AND REASONING TASKS

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**Curious AI**  
**2019-05-09**



# Prediction and Control

## Case 1: Oil refinery, Neste Engineering Systems







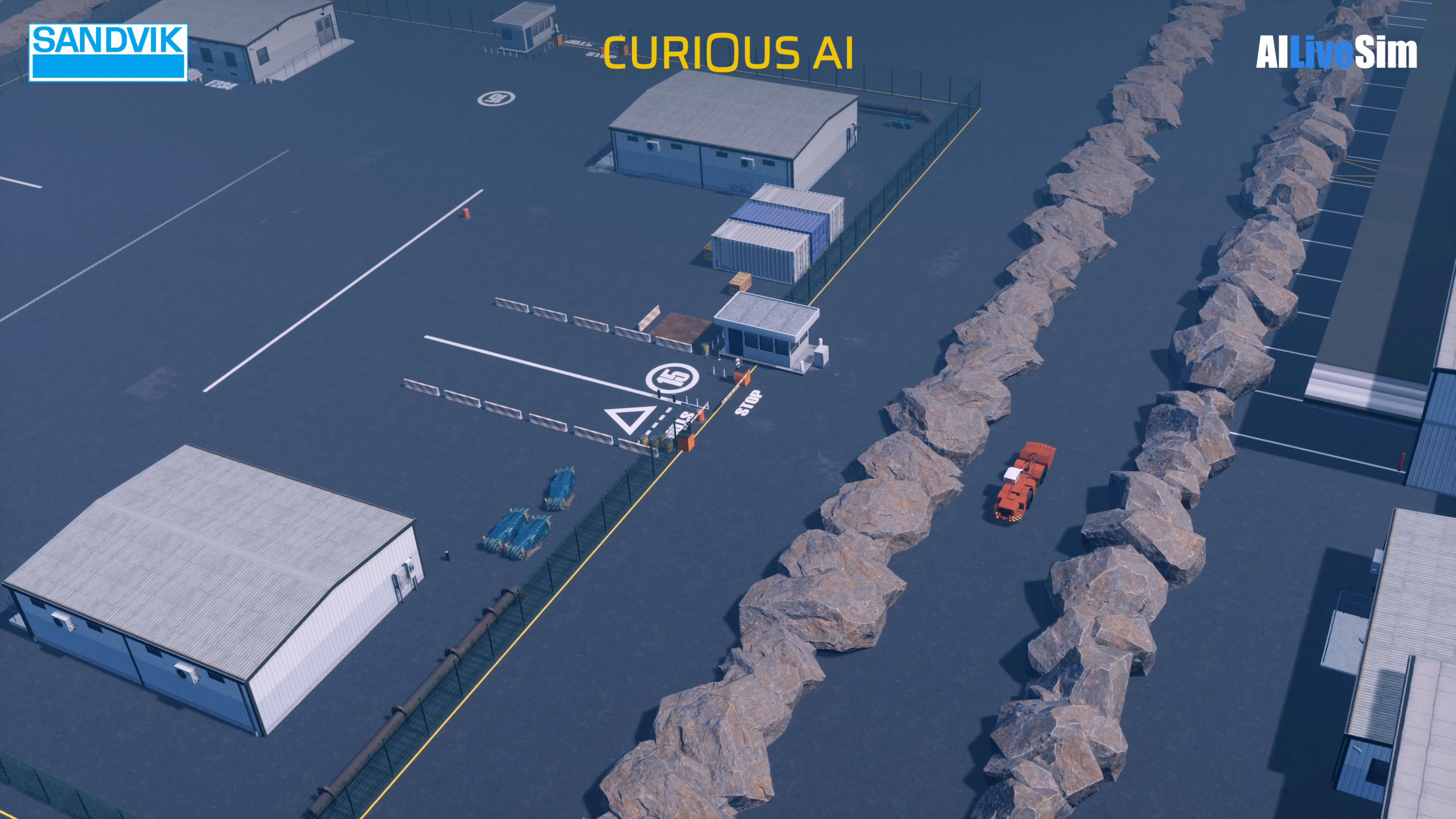
Sandvik LH410 — A loader for underground mining and tunneling



SANDVIK

CURIOUS AI

AlliveSim





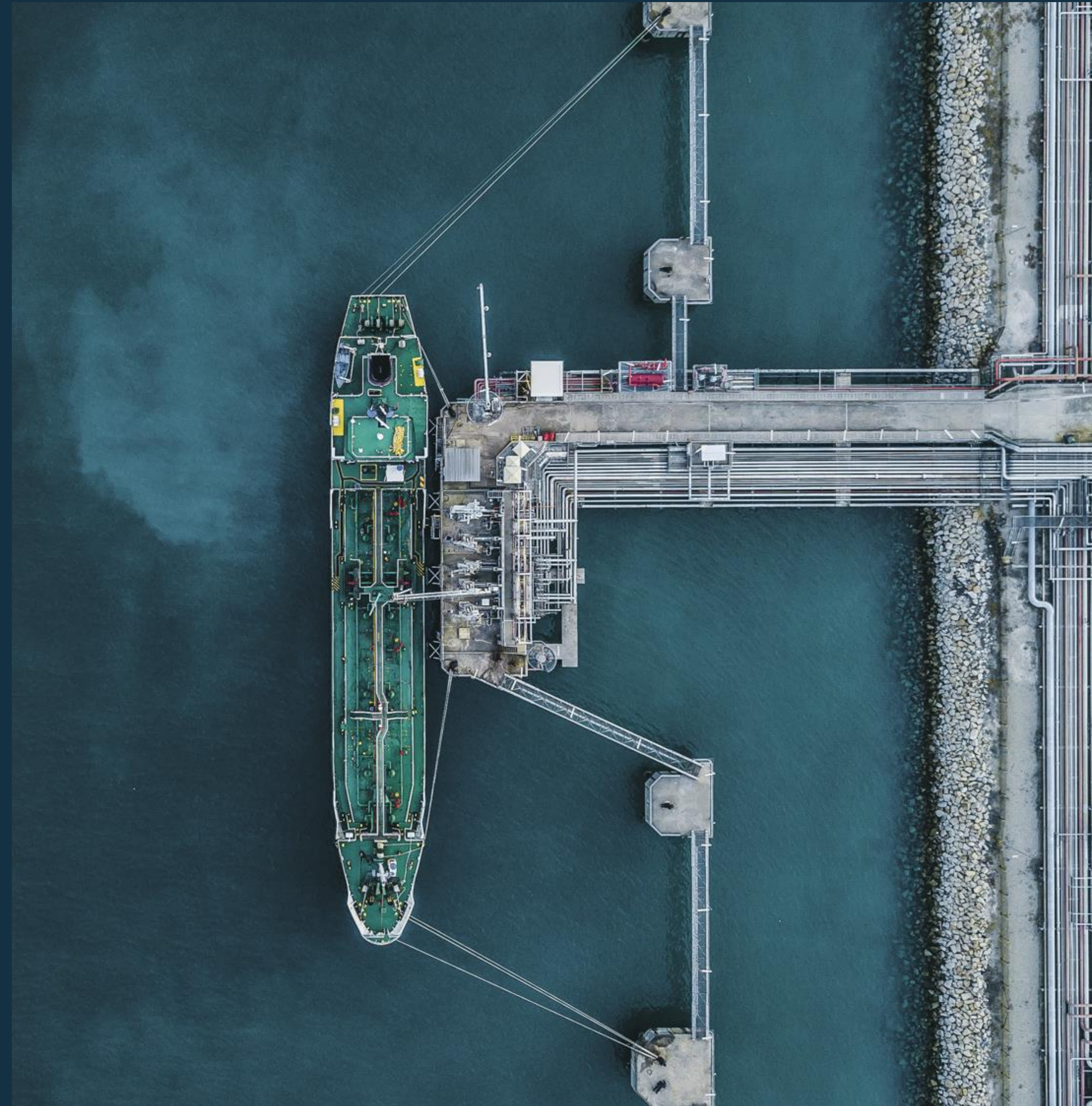
An aerial view of a simulated environment. The scene is a dark blue-grey ground with several grey rectangular buildings of varying sizes. A yellow rectangular boundary encloses a central area containing four grey rectangular blocks and four circular markers with the number '15' inside. To the right of this boundary is a winding track made of brown, rocky terrain. A small red and white car is positioned on the track, moving along a white line. The sky is a clear, light blue.

The Curious AI Autonomous Control learns to drive the machine



# Overview

- 01 MODEL-BASED RL
- 02 WHY IS IT HARD TO USE LEARNED MODELS?
- 03 THE SOLUTION
- 04 RELEVANCE TO MATERIAL SCIENCES





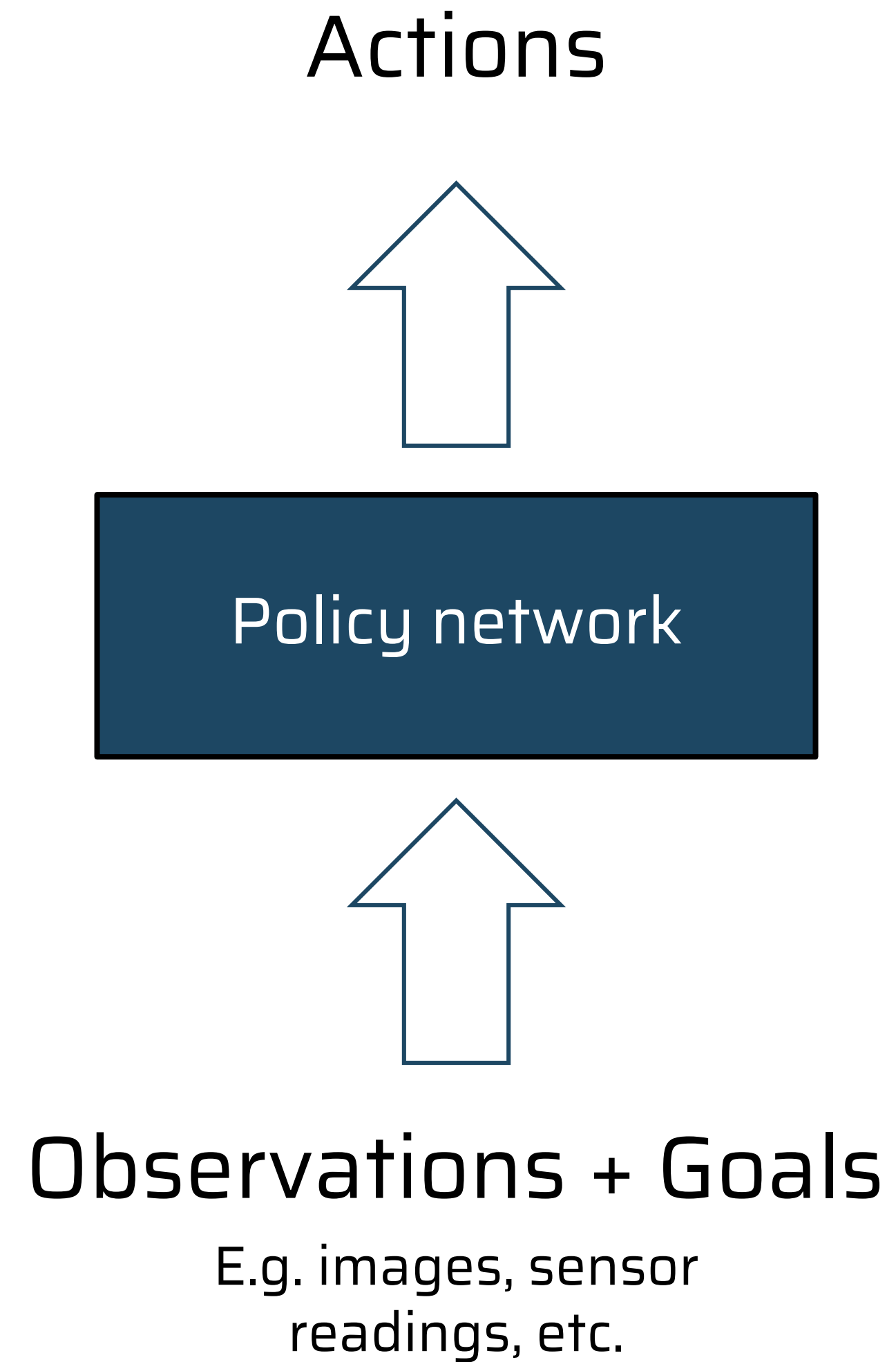
01

MODEL-BASED  
REINFORCEMENT  
LEARNING

# Model-Free RL

## Policy network

- Slow to learn (trial and error or imitation)
- Fast in operation

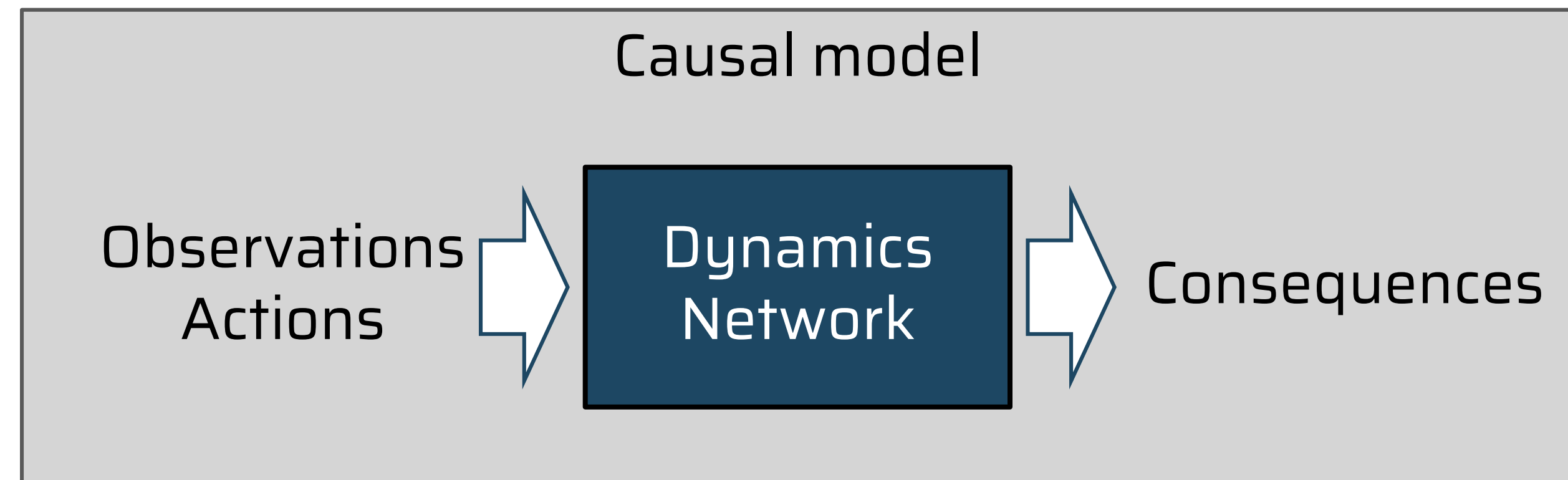




# Model-Based RL

## Model the underlying causal process

- needs much less training data
- applicable to new situations
- offers explanations, can answer “what if” questions





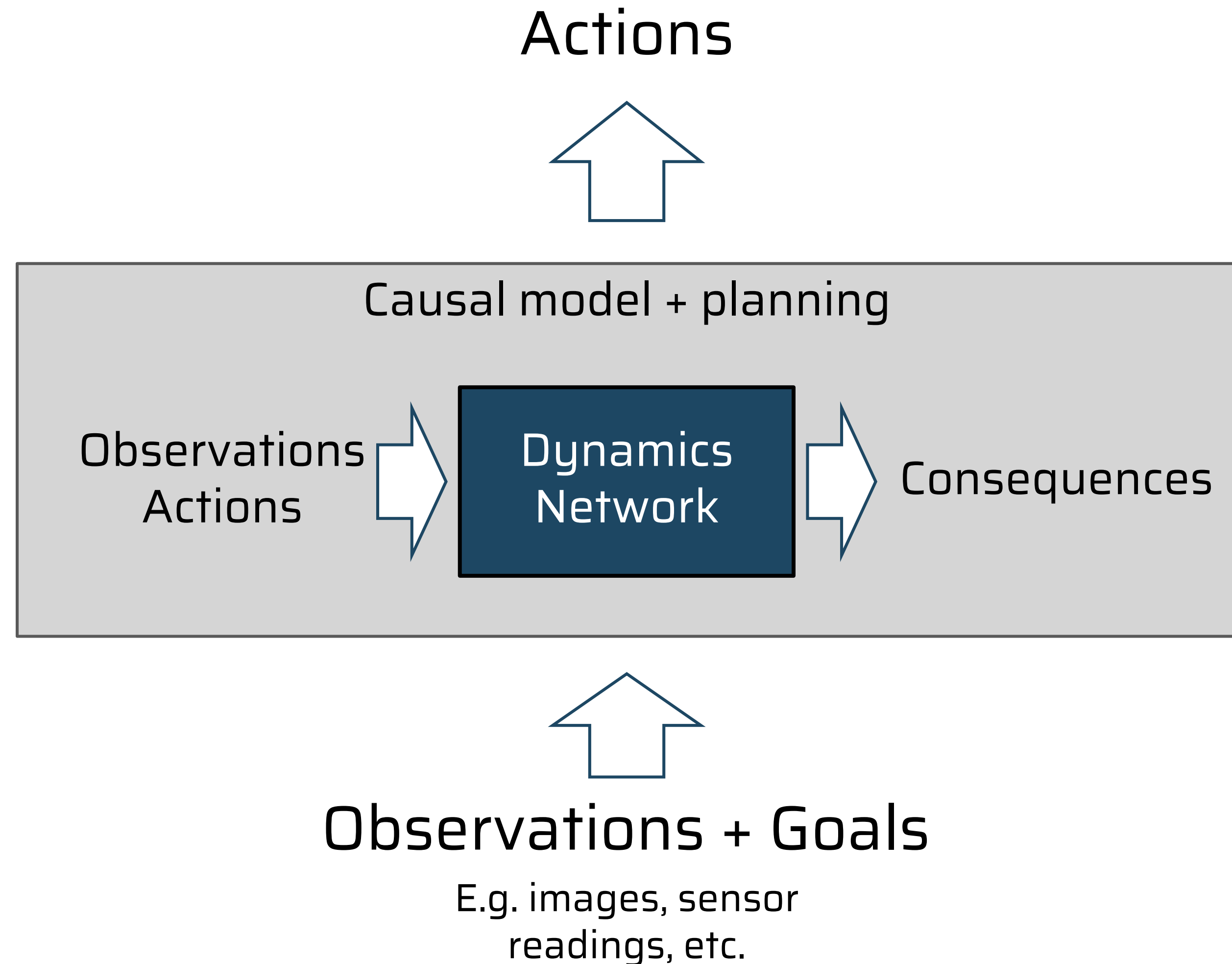
# Model-Based RL

## Model the underlying causal process

- needs much less training data
- applicable to new situations
- offers explanations, can answer “what if” questions

## Just add planning

- the main drawback is that simulations can be costly  $\Rightarrow$  not a replacement of normal stimulus-response but a perfect complement





# Model-Based Control with Simulator as the Model

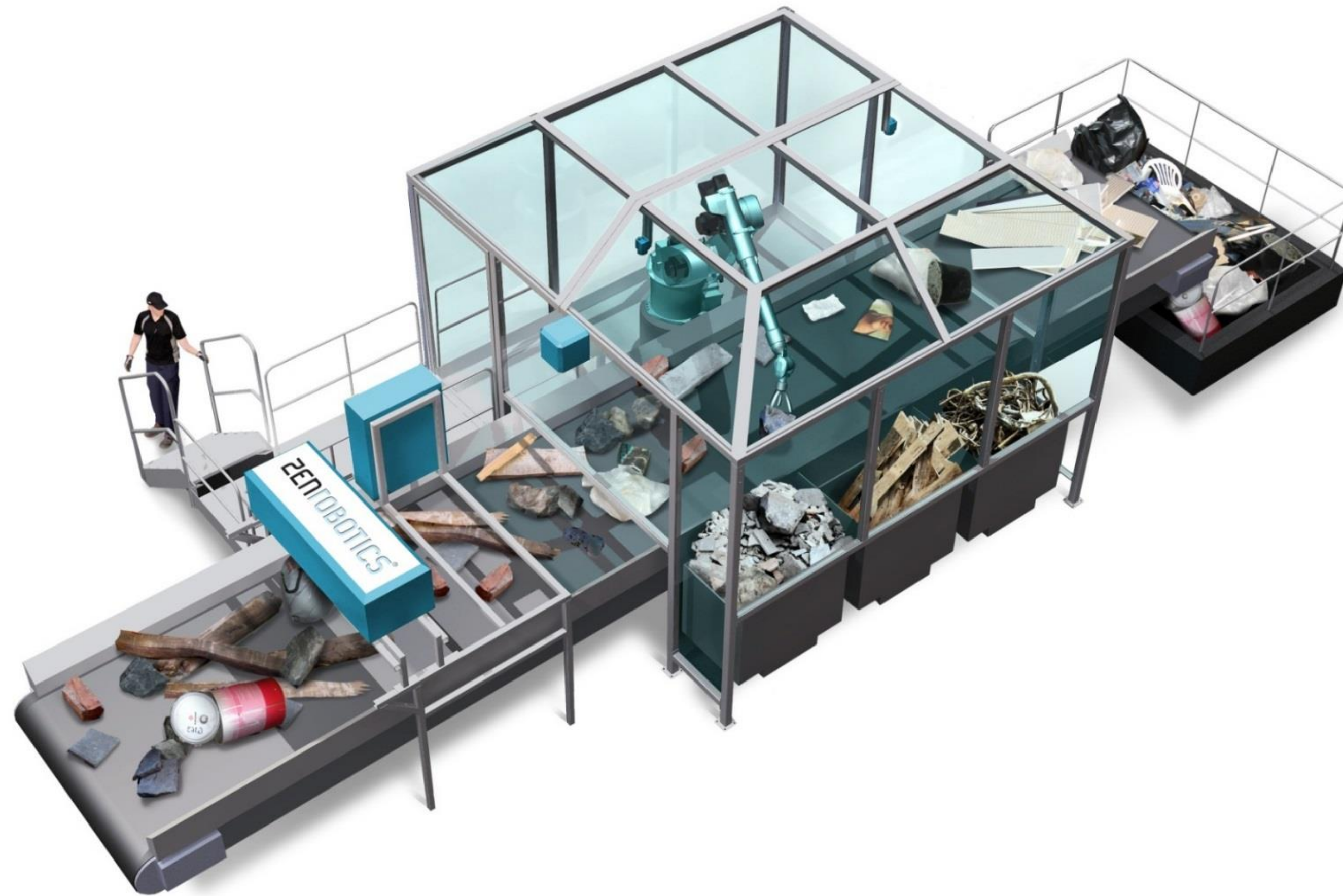
Synthesis of Complex Behaviors  
with  
Online Trajectory Optimization

(preliminary results)

Emanuel Todorov, Tom Erez and Yuval Tassa (2012)



2007 -  
ZenRobotics Ltd.







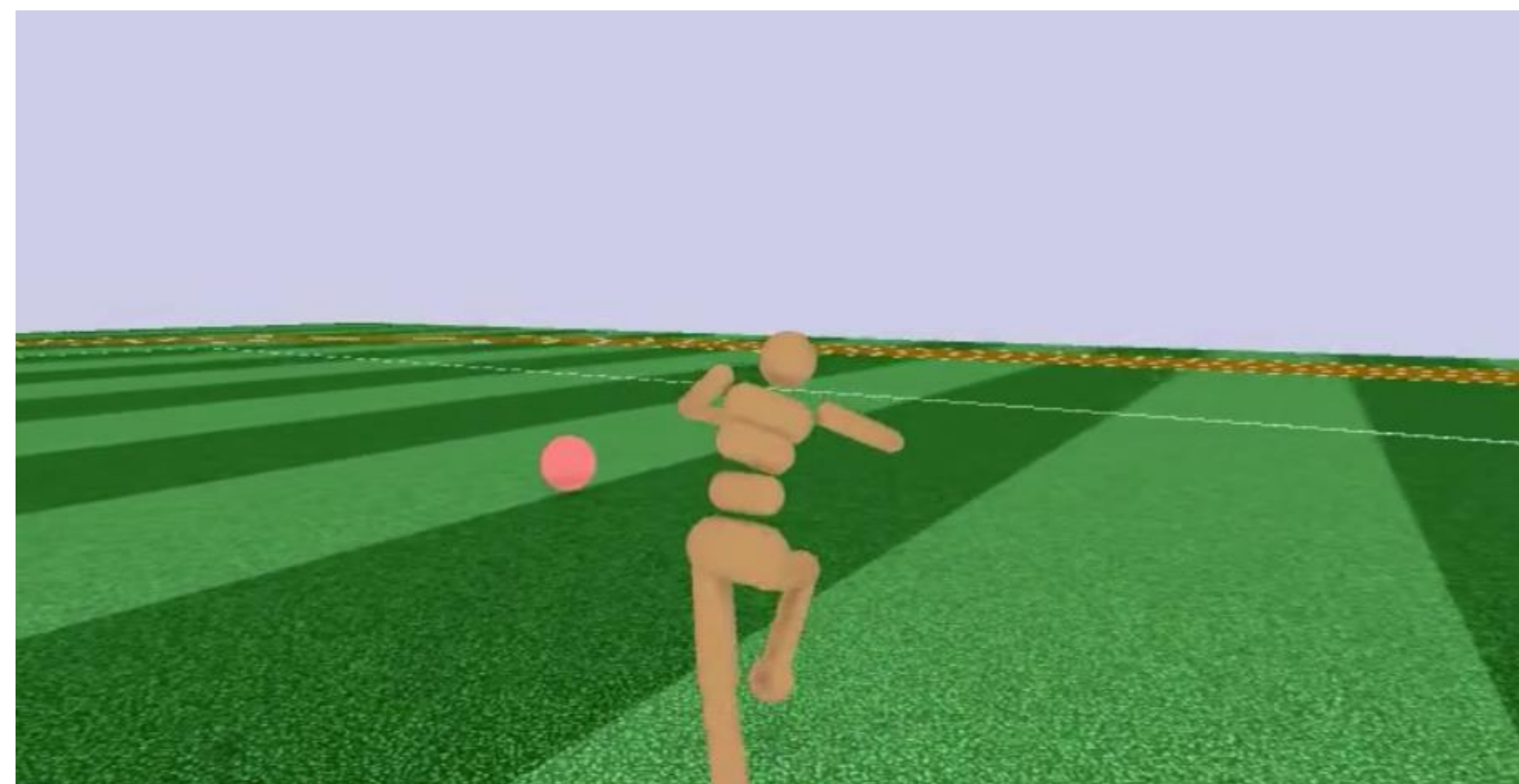
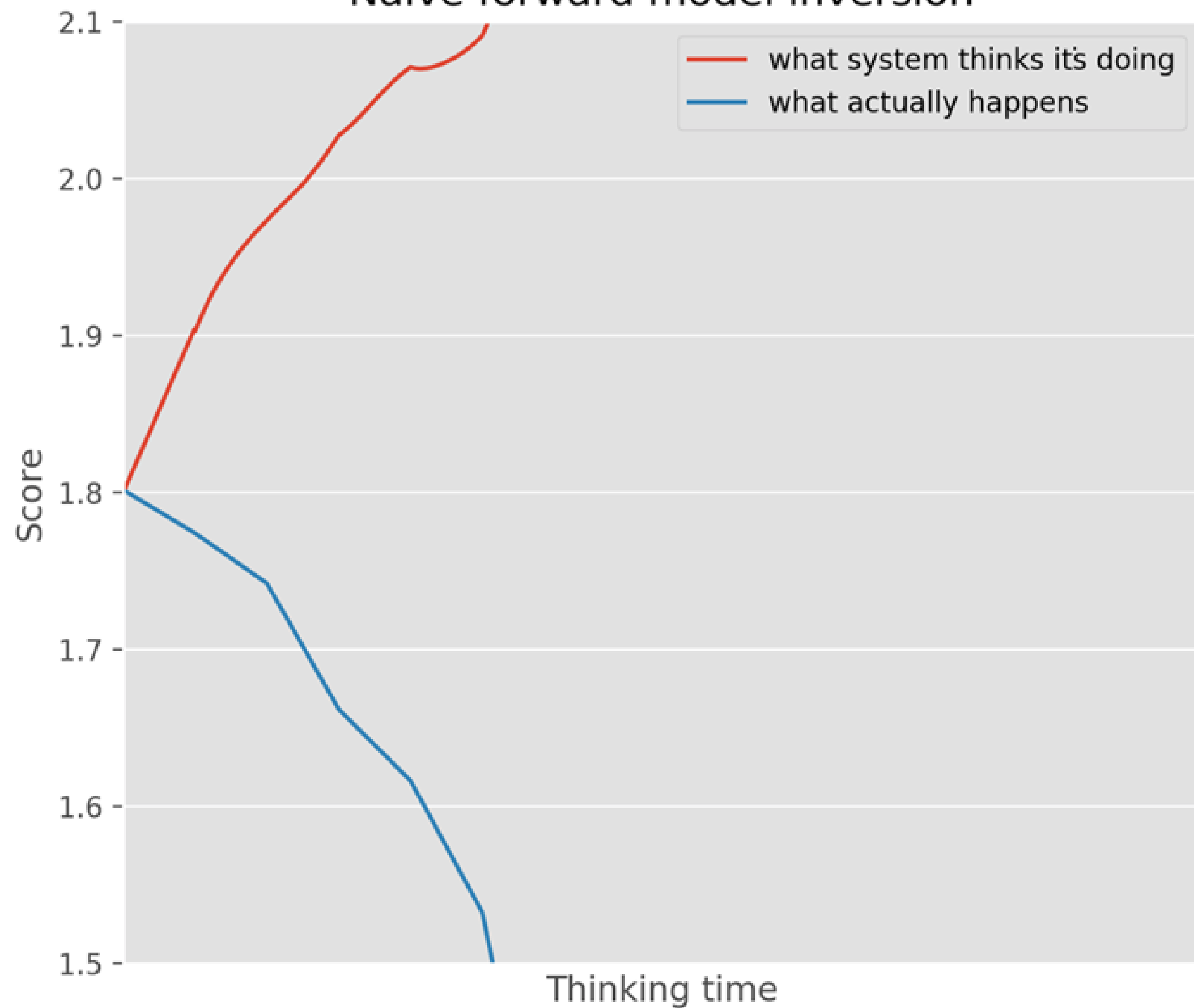


# 02 WHAT'S THE PROBLEM?



# Learned Dynamics Model → Delusional Planning

Naive forward model inversion





# Neural Network Inversion is not Stable

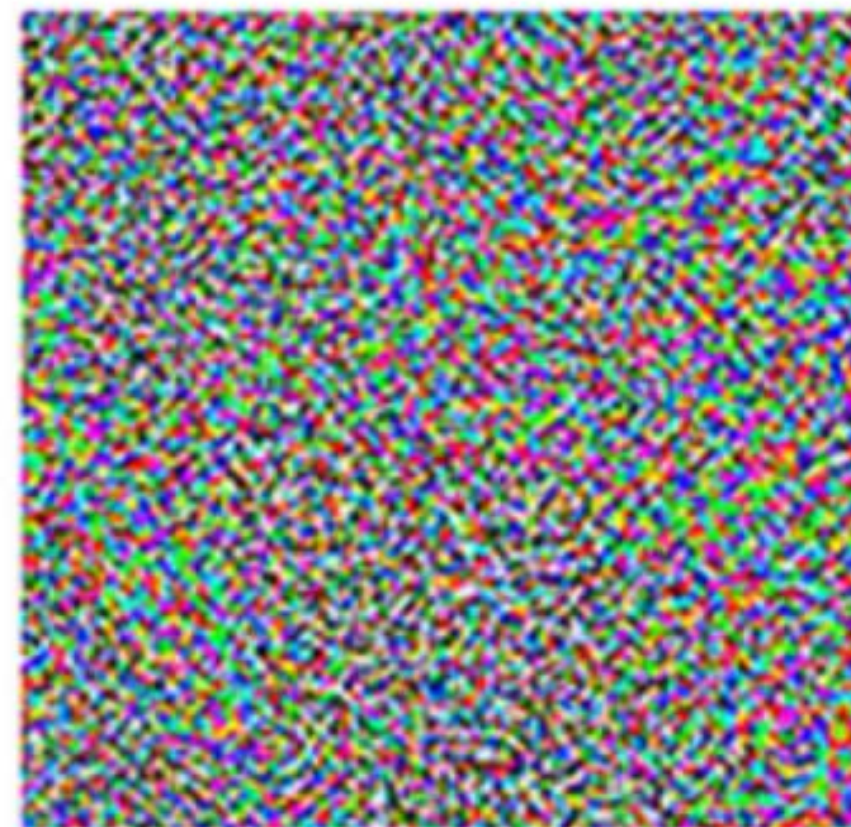
BY SIMPLY OPTIMIZING INPUTS BY GRADIENT DESCENT, NEURAL NETWORKS CAN BE FOOLED



“panda”

57.7% confidence

+  $\epsilon$



=



“gibbon”

99.3% confidence

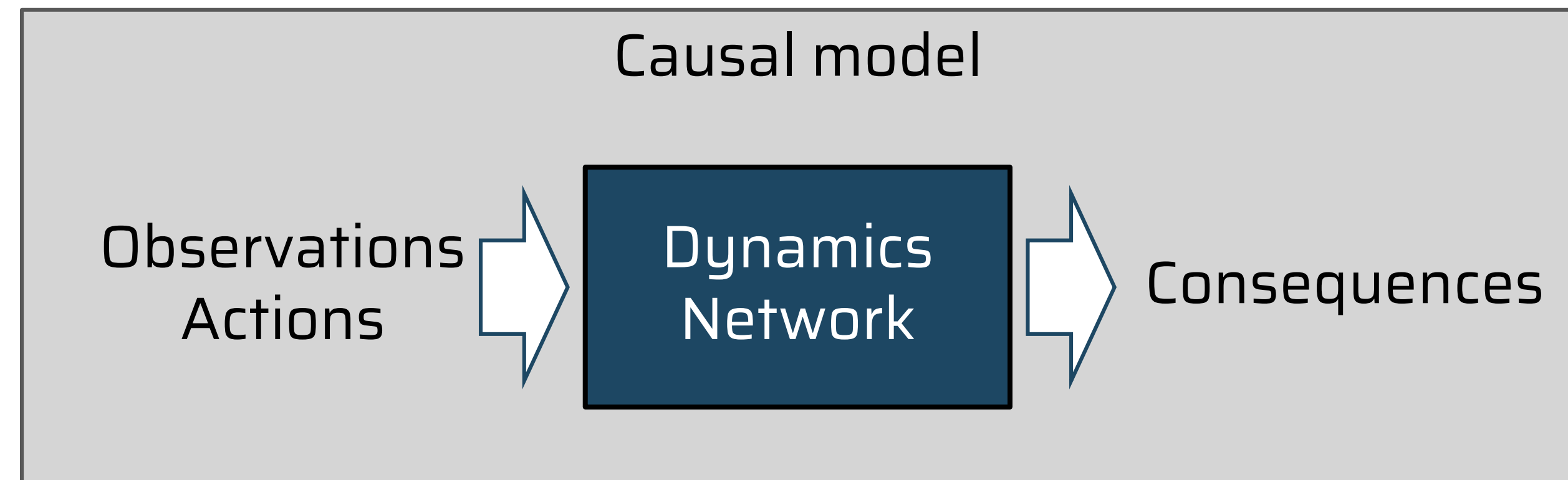


# Model-Based RL

**Backpropagate from  
desired consequences to  
actions**



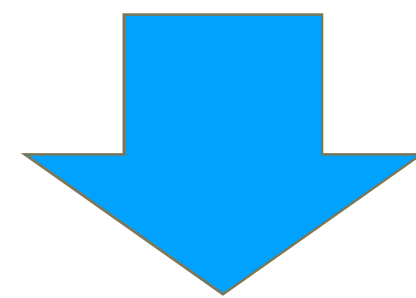
**adversarial examples of  
actions**





# Neural Network Inversion is not Stable

Inverting a neural network gives nonsensical results (so called adversarial examples)



Control does not work if  
dynamics models are learned  
by neural networks



Root Cause:

Neural networks fail without warning  
outside their training manifold

They don't understand their own  
uncertainty



# 03 THE SOLUTION



# First: What Doesn't Work

We tried several ways to estimate the uncertainty

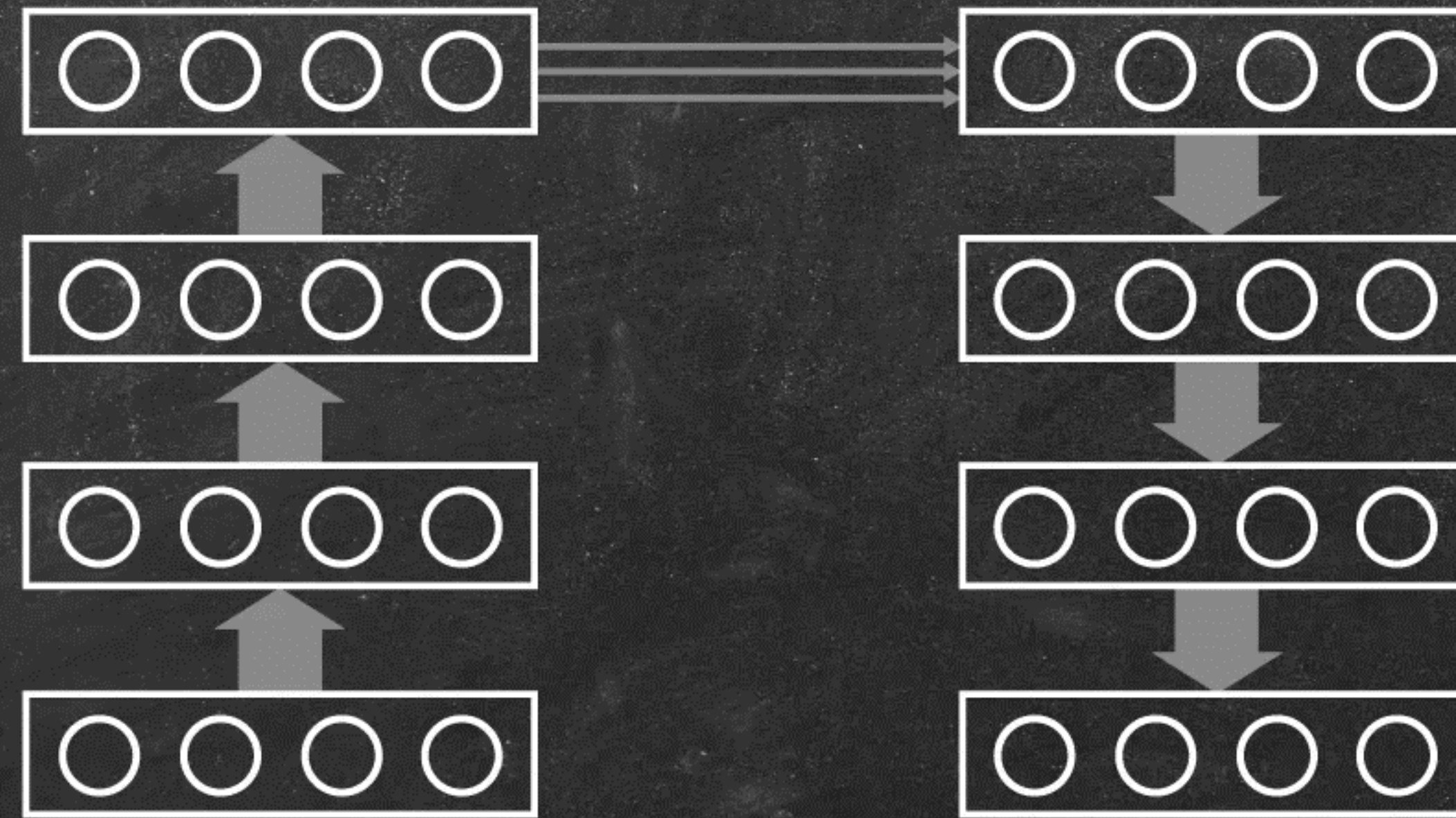
They all work at least somehow when used in ordinary prediction...

... but almost all fail under “adversarial planning attack”

When you model the uncertainty or familiarity directly, optimization finds the weak spots

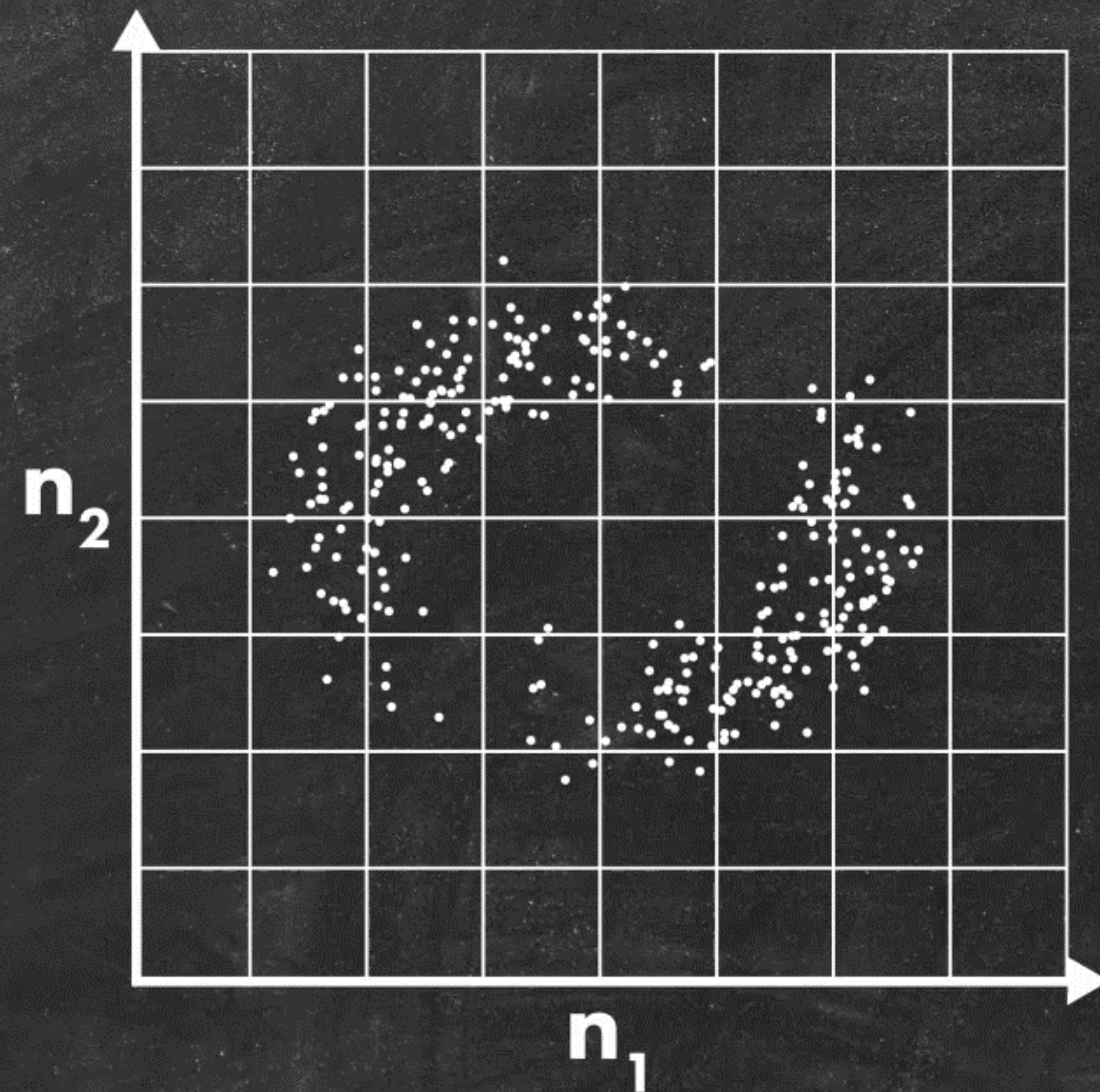


# Denoising Auto-Encoder



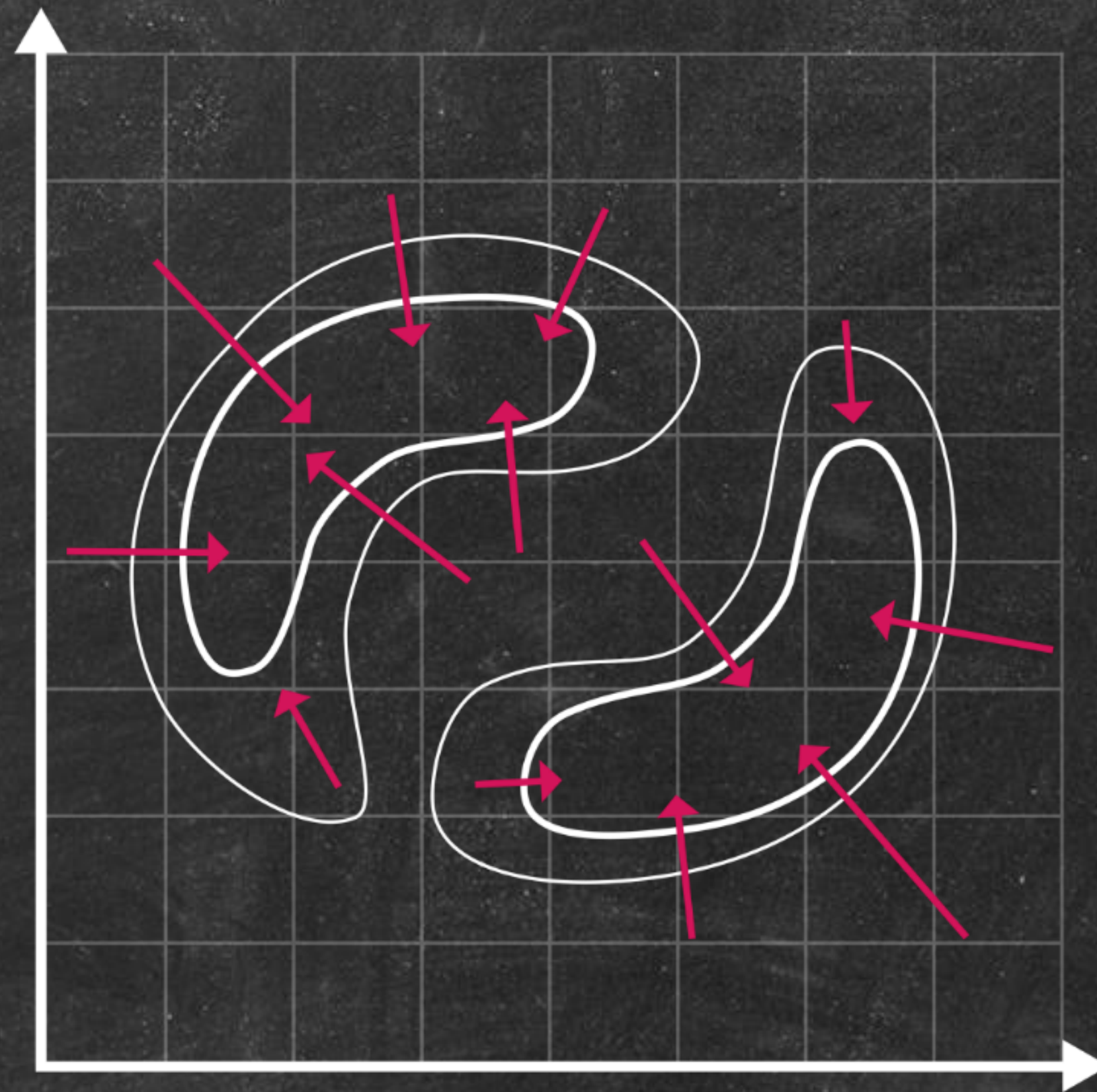


# Original Sample Distribution





# Denoising Auto-Encoders Learn $\nabla \log p(x)$





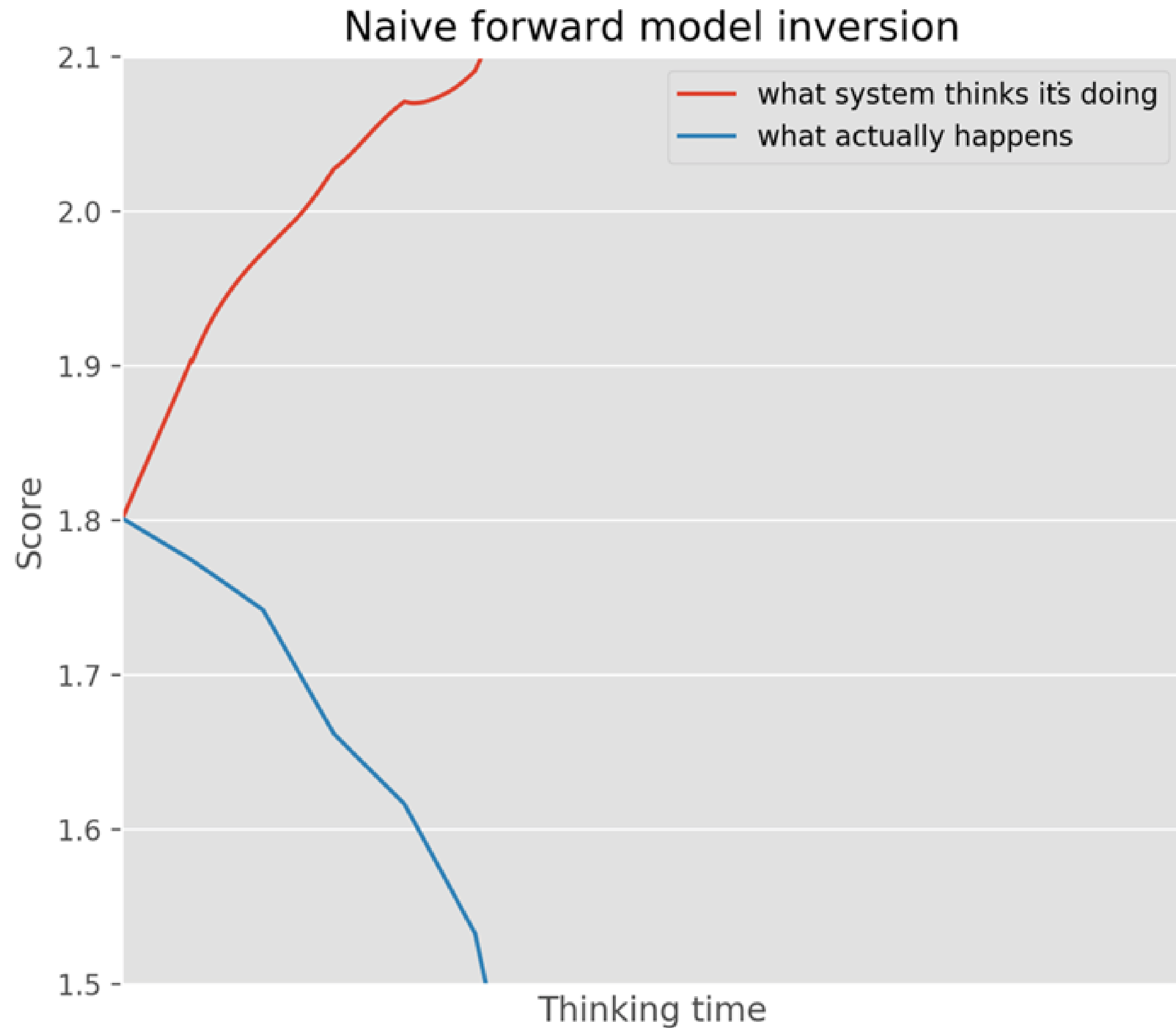
# The Winner

Use denoising autoencoders to explicitly model  $\nabla \log p(x)$



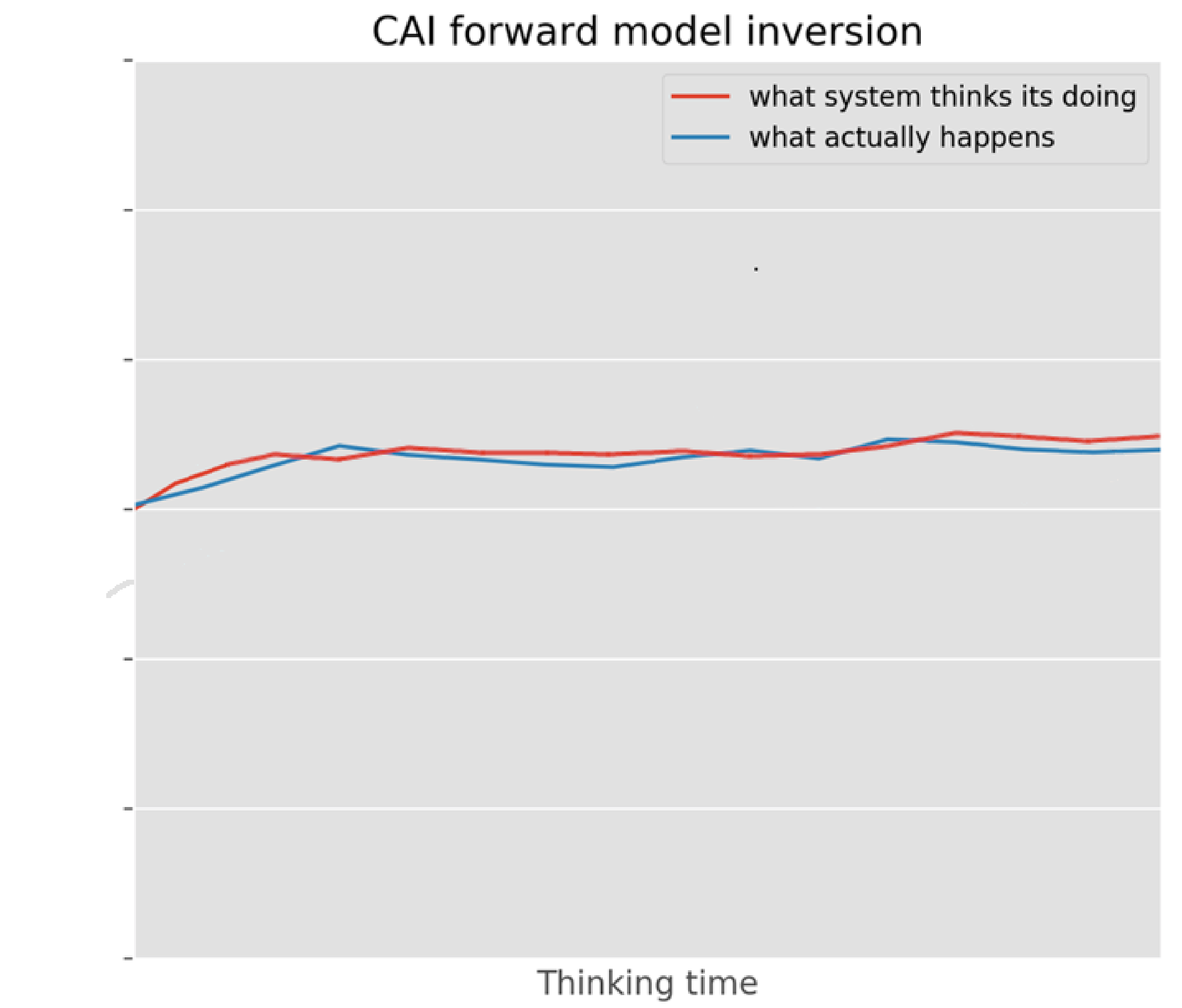
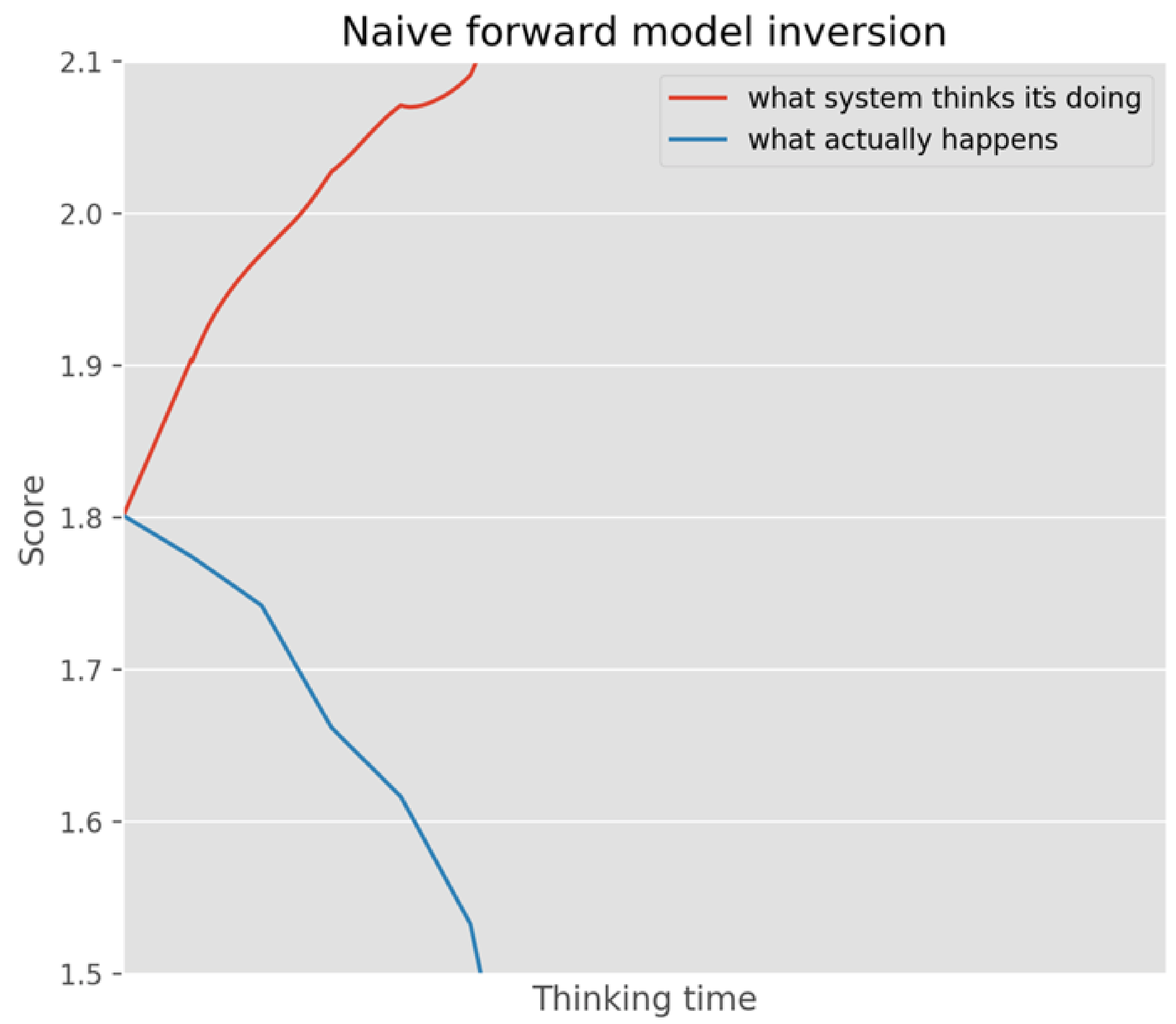
The gradient is sometimes wrong but optimization is not pulled towards these weak spots

# Denoising Autoencoder as a Safety Net → Stable Planning





# Denoising Autoencoder as a Safety Net → Stable Planning



# 04 RELEVANCE TO MATERIAL SCIENCES



# Starting point: blind tinkering

1. Define the desired properties of a new material
2. Try a recipe for cooking up something
3. Measure the properties of the resulting material
4. If not happy, change the recipe and go back to step 2

# Speeding things up

Try a recipe for cooking up something

Simulate the properties of the resulting material

Learn to predict the outcome of the simulation  
and real experiment

ML can help:

Learn the  
predictions

Learn the  
uncertainty

Learn efficient  
search



Thanks!

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