Can We Make Machine Learning Safe for Safety-Critical Systems?

(and two thesis proposals)

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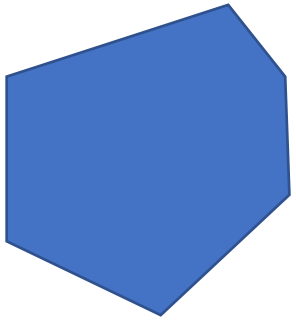
Oregon State University

Outline

- Part 1: Integrating ML into traditional safety engineering processes
  - Scenario-based data collection
  - Verification-based data collection
  - Risk quantification
- Part 2: ML in open worlds: Safety as Control
  - Detecting anomalies, near misses, and departures from the Operational Design Domain
  - Adaptation strategies
- Part 3: Safety as Continual Redesign
  - Design is never finished
  - Resilient systems are “Poised to adapt”

Traditional Safety Engineering

Semi Driving on Freeway



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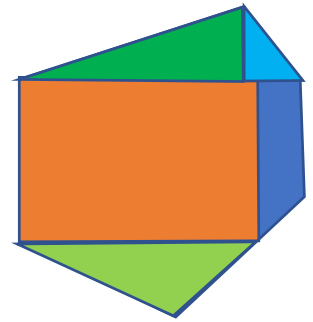

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- Front collision
- Rear collision
- Side collision
- Drive off road

Harms:
- Death
- Severe injury
- Physical damage

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Acceptable Risk of Death:
1 in 10^8 hours

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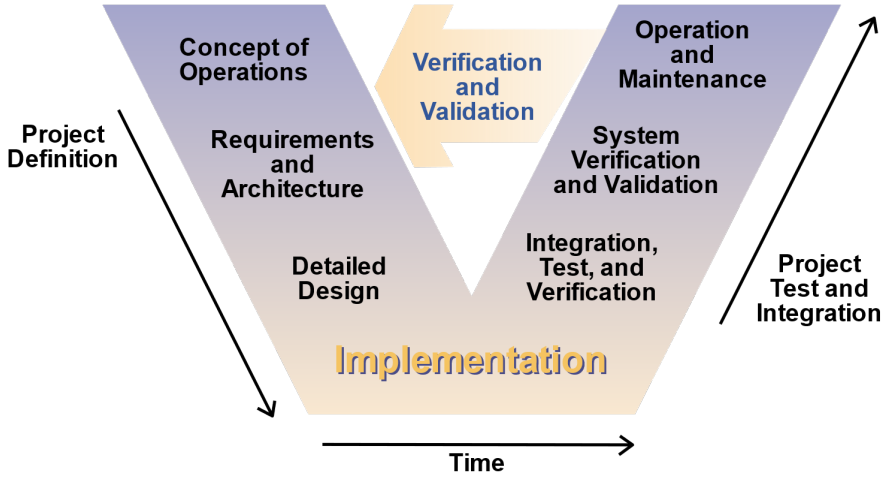

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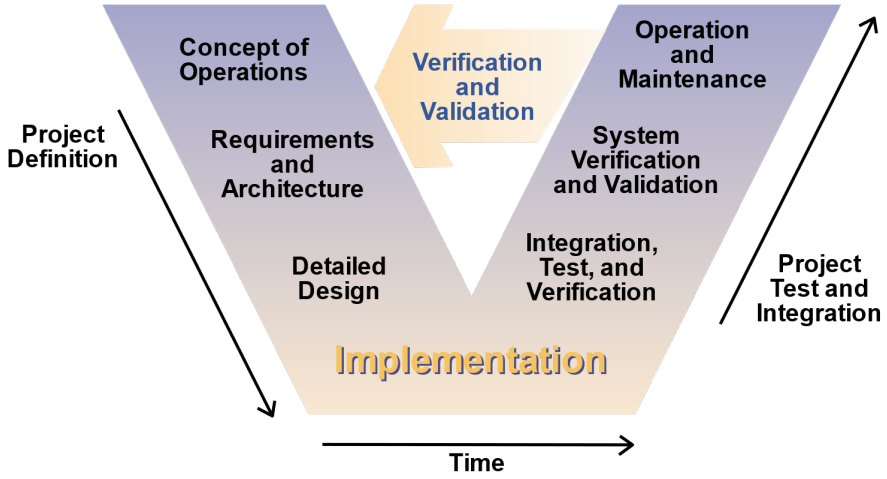

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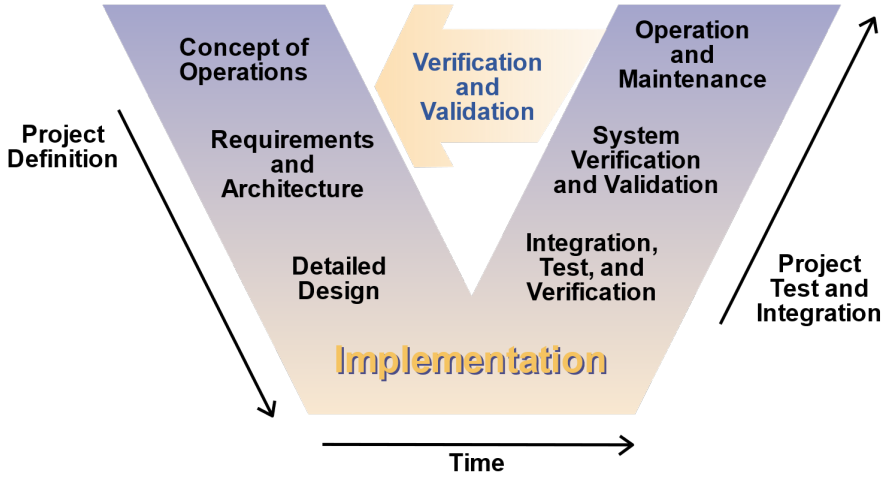

Simulation studies
Real-world system tests

Traditional Safety Engineering

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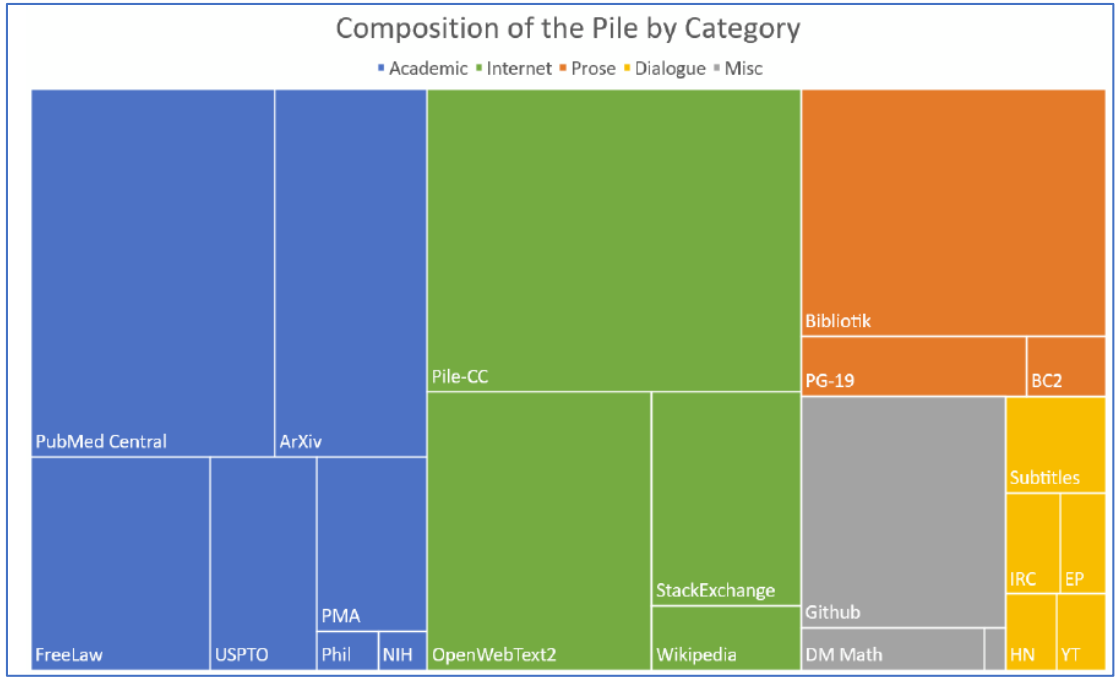
https://waabi.ai/blog/

Contrast: Traditional Machine Learning Methodology

- Aggregate data from as many sources as possible
  - Data was often collected for other purposes
  - “Big Data” is “the new oil”

[Deng, et al, 2009]



[Gao, et al, 2020]

The Pile: An 800GB Dataset of Diverse Text for Language Modeling

Consequences of this Methodology

- No guarantee that the Operational Domain is covered well
- No guarantee that the ML system will learn a model that meets the safety requirements
- Learning Theory only provides statistical guarantees for inputs drawn *from the same distribution* as the training data
- If the actual distribution in operations concentrates on a region of poor coverage, error can be arbitrarily large/serious

We need a new methodology

Achieving Distribution-Independent Accuracy in Machine Learning Components

- Deliberately collect training data to attain good coverage of all cases (including corner cases)
  - Risk-driven sampling techniques (e.g., [Wang, et al., 2023])
- Verify approximation quality of the learned model
  - Collect additional examples as needed

Sampling via Surrogate Model Optimization
(also known as Bayesian Optimization)

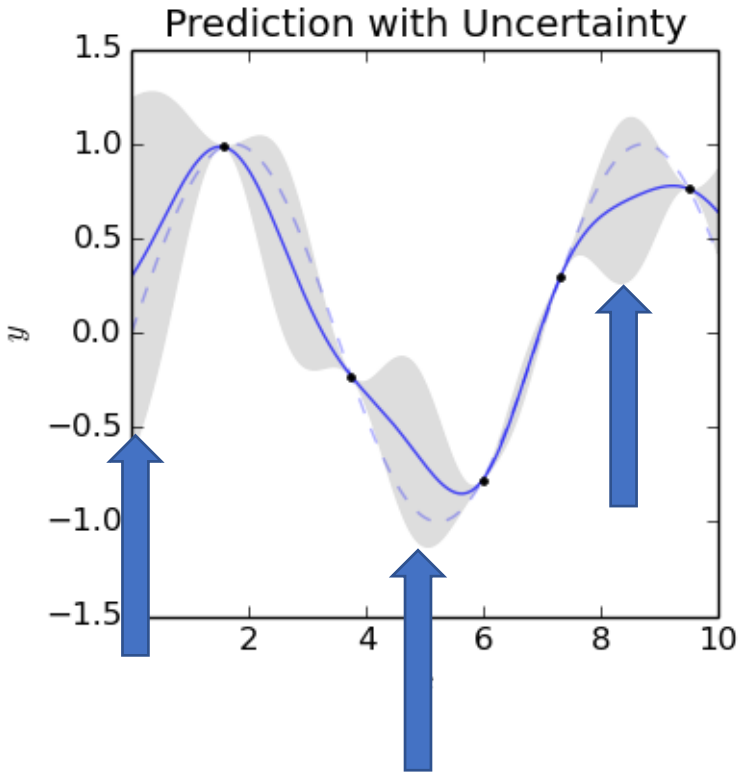
- Collect an initial real-world sample and train the ML component
- Build and validate a simulation model ("digital twin")

Repeat

- Fit the ML model
- Fit surrogate model (e.g., Gaussian Process)
  - Provides estimates of "epistemic uncertainty"
- Select a batch of new cases using an "acquisition function"
  - Collect training example for each case using simulation

Until target metrics are attained

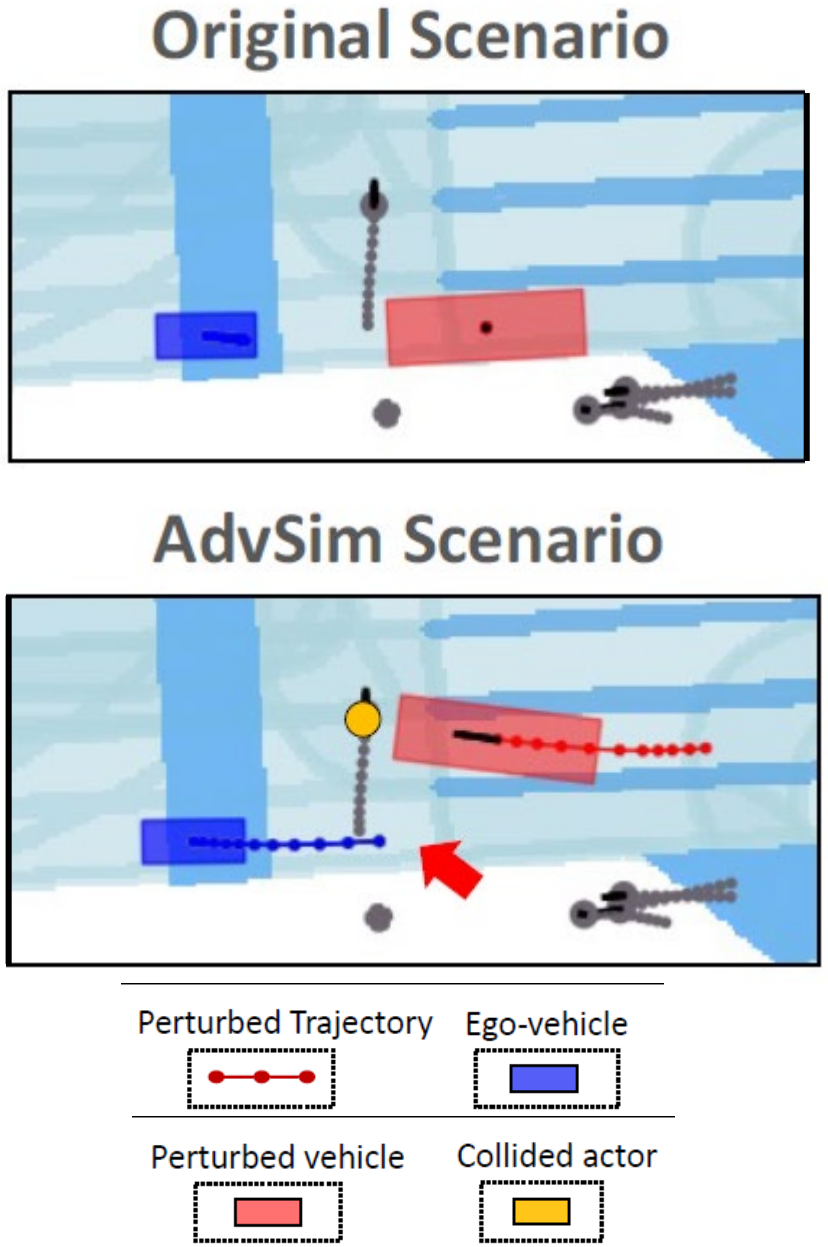
- Metrics of interest:
  - Coverage of the state space
  - Good coverage of hazardous states



Example: Generating an Adversarial Scenario with AdvSim

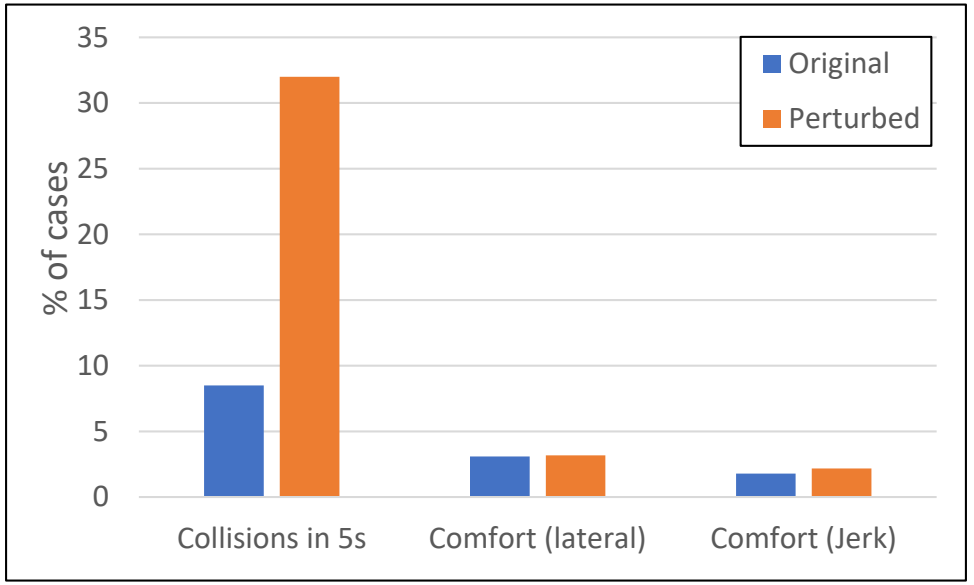
[Wang, et al., 2023]

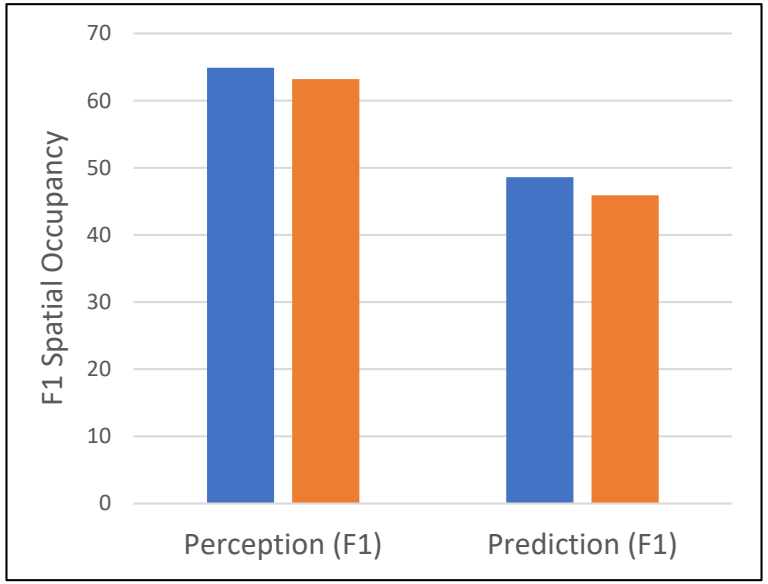
- Given: original trajectory from expert driver
  - trajectories of all "actors" (vehicles, pedestrians, cyclists), LiDAR data, map
- Select one or more vehicles and perturb their behavior to maximize an adversarial loss for the end-to-end system
  - collisions, law violations, passenger discomfort
  - Perturbation is at the level of a kinematic trajectory (acceleration and curvature)
- Simulate the perturbed LiDAR data
- Run the current end-to-end system
- Score the adversarial loss
- Repeat N times and keep the perturbation with the largest adversarial loss



AdvSim Results

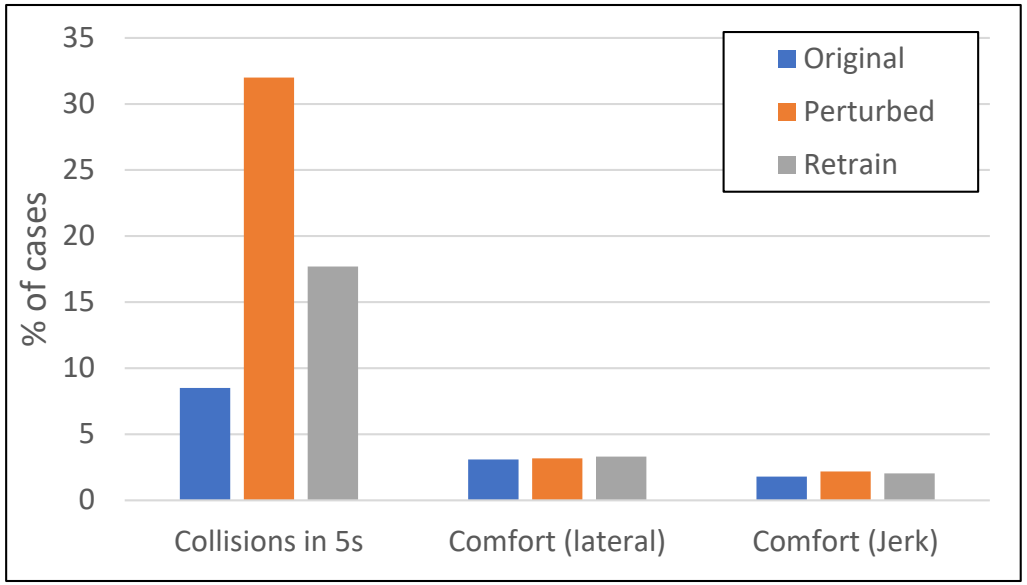
- 376% increase in collisions
- Small increases in discomfort
- Decreases in accuracy of perception and trajectory predictions





Updating the Model

- Retrain on the original data + adversarial cases
- Collisions reduced to 17.7%



- To be determined: What improvement is possible with more iterations?

Notes

- AdvSim operates at the semantic level (agent behavior)
  - Much smaller search space than searching in image space
  - Requires high fidelity simulation of imaging
- Adversarial collision rate is much higher than expected rate under normal driving conditions
  - See below

Verifying Correct Behavior of ML Component

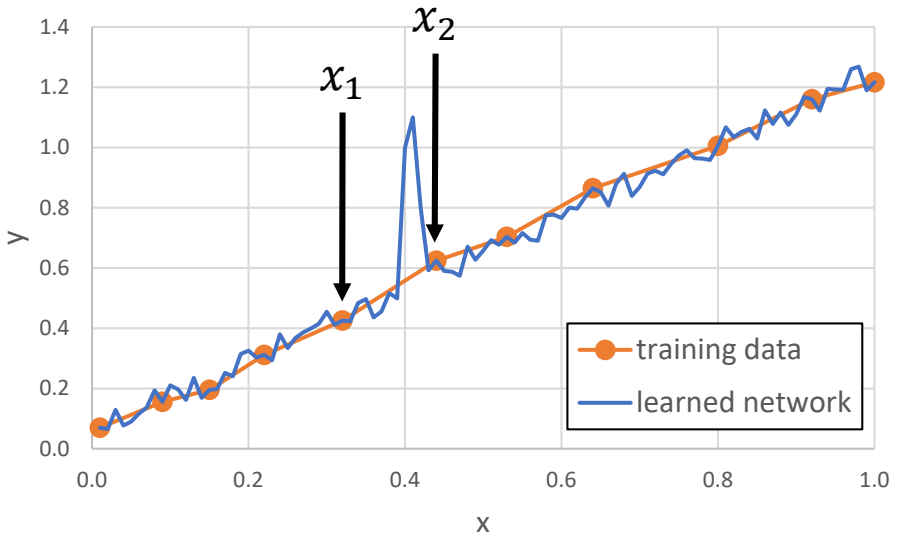
- How can we gain assurance that the ML system has learned the correct function?
- We have no explicit specification of correctness aside from the training data
- Are there regions where the learned function behaves badly?

Thesis proposal 1:

Bound the difference between the fitted function and linear interpolation of the training data

- Consider two adjacent training examples x_1 and x_2
- Let $\alpha \in [0,1]$

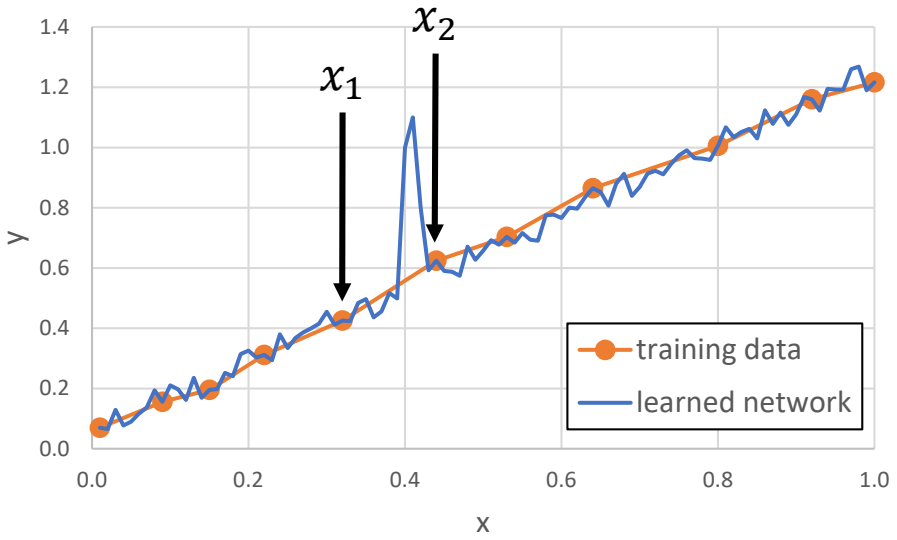
$$\max_{\alpha} \left| \begin{array}{c} f(\alpha x_1 + (1-\alpha)x_2) \\ - \\ \alpha f(x_1) + (1-\alpha) f(x_2) \end{array} \right|$$



- If this is small, the function behaves well in between the training data
- This can be solved by the methods of [Singh, et al. 2021] (but those may not scale)

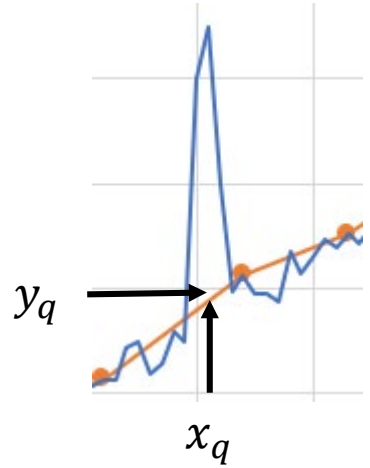
Interpolating in the Right Space

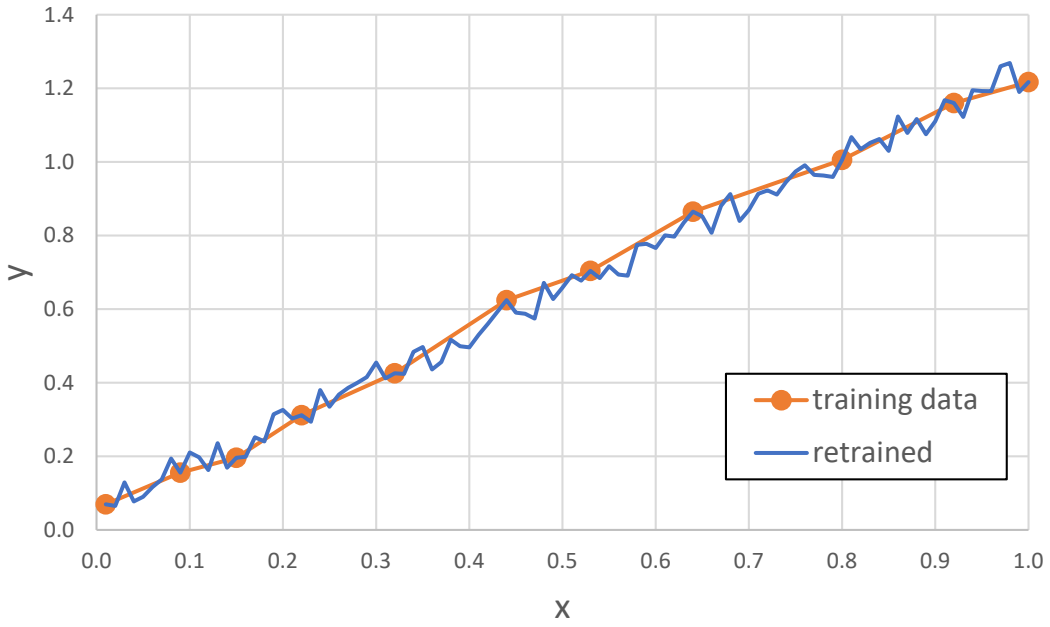
- This looks great in 1 dimension …
- We need to interpolate in a semantic space (like AdvSim)
  - For each known training case, identify the k most similar cases, where $k \approx$ the number of parameters in a scenario
  - Consider all convex combinations of those $k + 1$ cases to find the maximum discrepancy between a linear interpolation and the fitted neural network



Verification-Based Active Learning

- $\alpha_q \coloneqq \underset{\alpha}{\operatorname{argmax}} \left| \begin{matrix} f(\alpha x_1 + (1-\alpha)x_2) \\ - \\ \alpha f(x_1) + (1-\alpha) f(x_2) \end{matrix} \right|$
- Generate a new example at
- $x_q = \alpha_q x_1 + (1-\alpha_q)x_2$
- Obtain y_q
- Retrain the network on (x_q, y_q)
- Repeat until no failure regions can be found





Estimating Risk = Probability of Harm

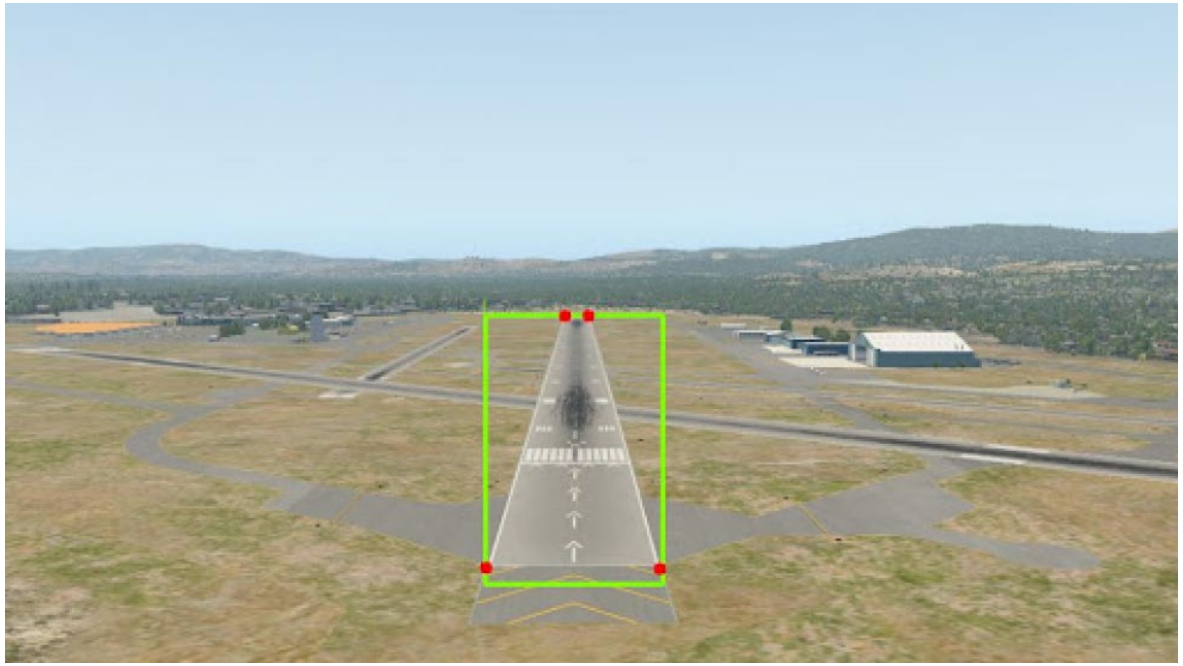
- If we have discarded the data distribution, how can we estimate risk?
- Answer: Simulate system operation and measure the probability of harm
- Challenges:
  - We must be able to simulate system operation
  - Harms are very rare
- Solution:
  - Fit a probabilistic model $P(s)$ of normal operations
    - Probability of initial states
    - Probability of system behavior
    - Probability of the behaviors of other agents
  - Develop a proposal distribution $Q(s)$ that greatly increases the probability of harms
    - Reuse our design data?
  - Simulate according to $Q(s)$
  - Apply importance reweighting $\frac{P(s)}{Q(s)}$ to each hazardous state s that is observed

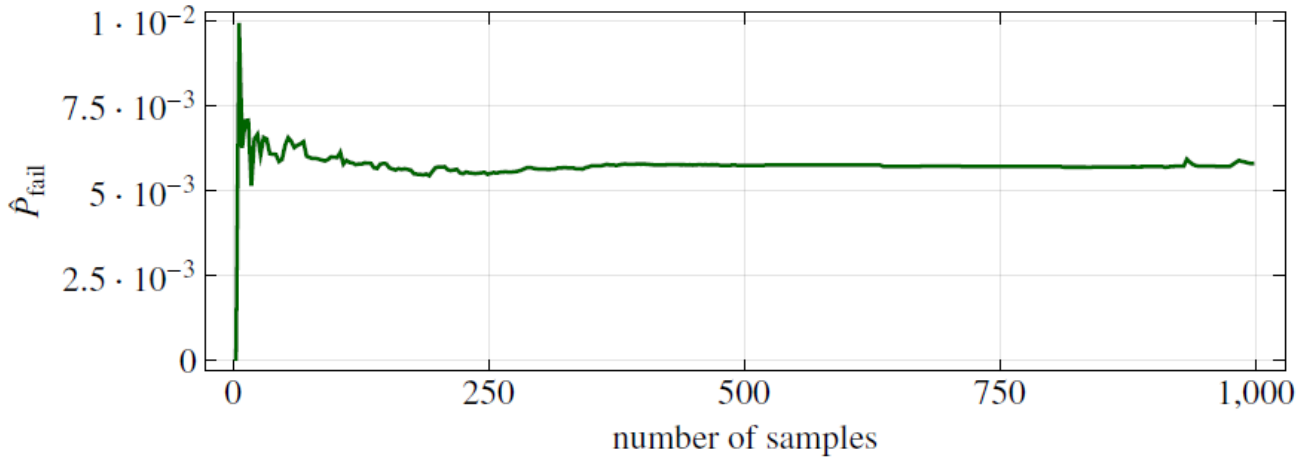
Bayesian Risk Estimation

[Moss, Kochenderfer, Gariel, Dubois, 2024]

- Apply Surrogate Model Optimization to discover failure regions
- Combine three “acquisition functions”
  - Explore regions of high operational likelihood $P(x)$ and high epistemic uncertainty
  - Explore regions near the boundaries of failure regions (hazards)
  - Explore the interiors of the failure regions

Example: Runway Detection





57.2% of samples were in failure regions

$$\hat{p}_{fail} = 5.8 \times 10^{-3}$$

Only 0.6% of Monte Carlo samples are in failure regions

With these tools, ML can be integrated into the safety engineering process

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N.B. No single validation method suffices to ensure safety. See [Kochenderfer, et al., *Algorithms for Validation* (forthcoming)]

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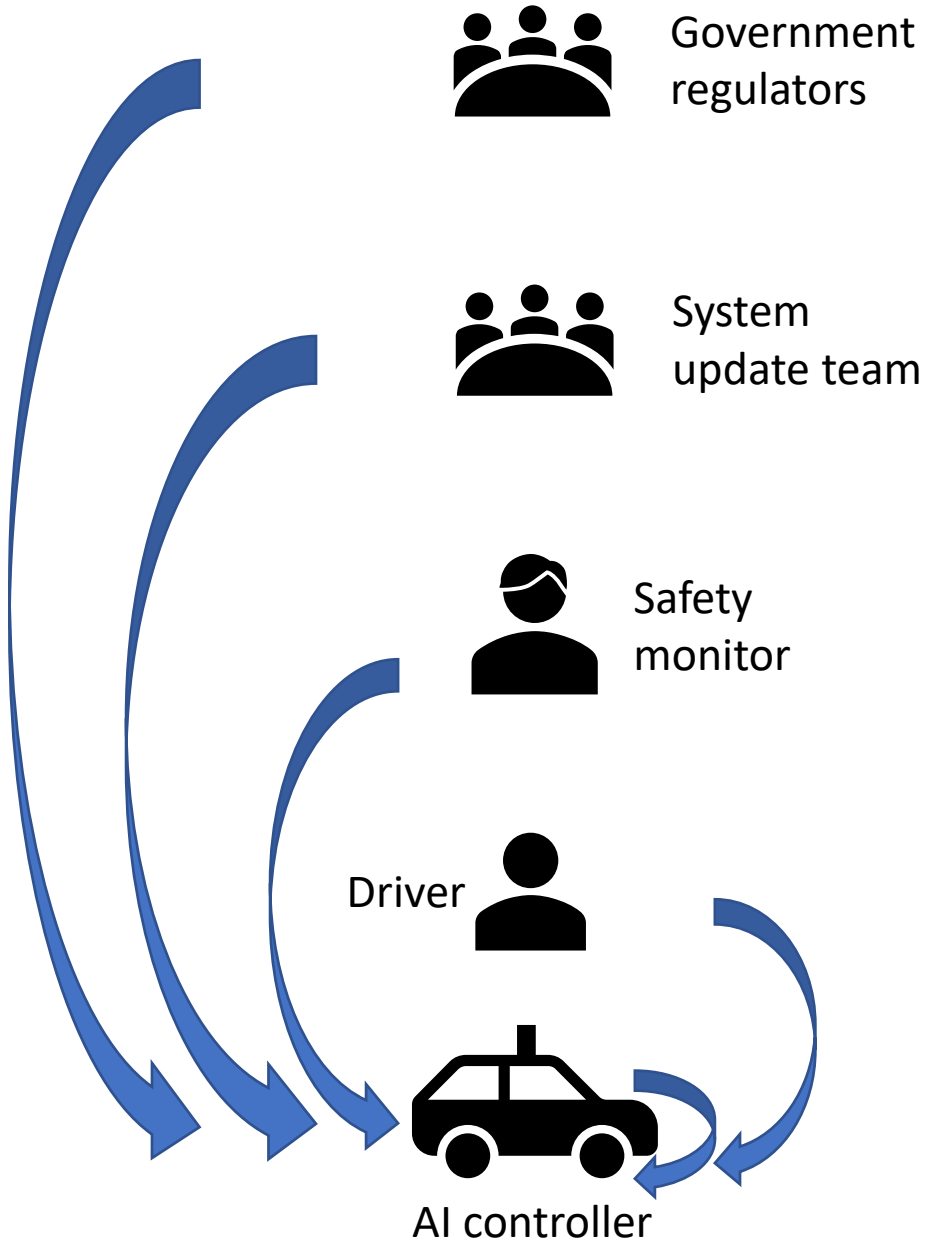
Systems View of Safety

[Leveson 2011: Engineering a Safer World]

- Safety is a control problem
  - Maintain the safety of the system in the presence of disturbances
- What is the “controller”?
  - The human organizations that build, operate, and maintain it
  - Government regulators
  - Elected officials
- What are the “disturbances”?
  - Budget cuts and staff reductions
    - Systems tend to migrate toward the edges of safety
  - Unknown unknowns
    - Environmental Novelty
- The controller must detect and compensate for these disturbances
  - Today: It is the exclusively the humans who do this
  - Can AI help?



Unknown Unknowns: Detecting Novel Failure Modes

- Key performance indicators [Weick, et al., 1999]
  - Number of anomalies detected
  - Number of near misses detected
- These provide evidence of novel failure modes *before* they cause harms

- What is the status of AI methods for detecting anomalies and near misses?

Anomaly Detection in Computer Vision

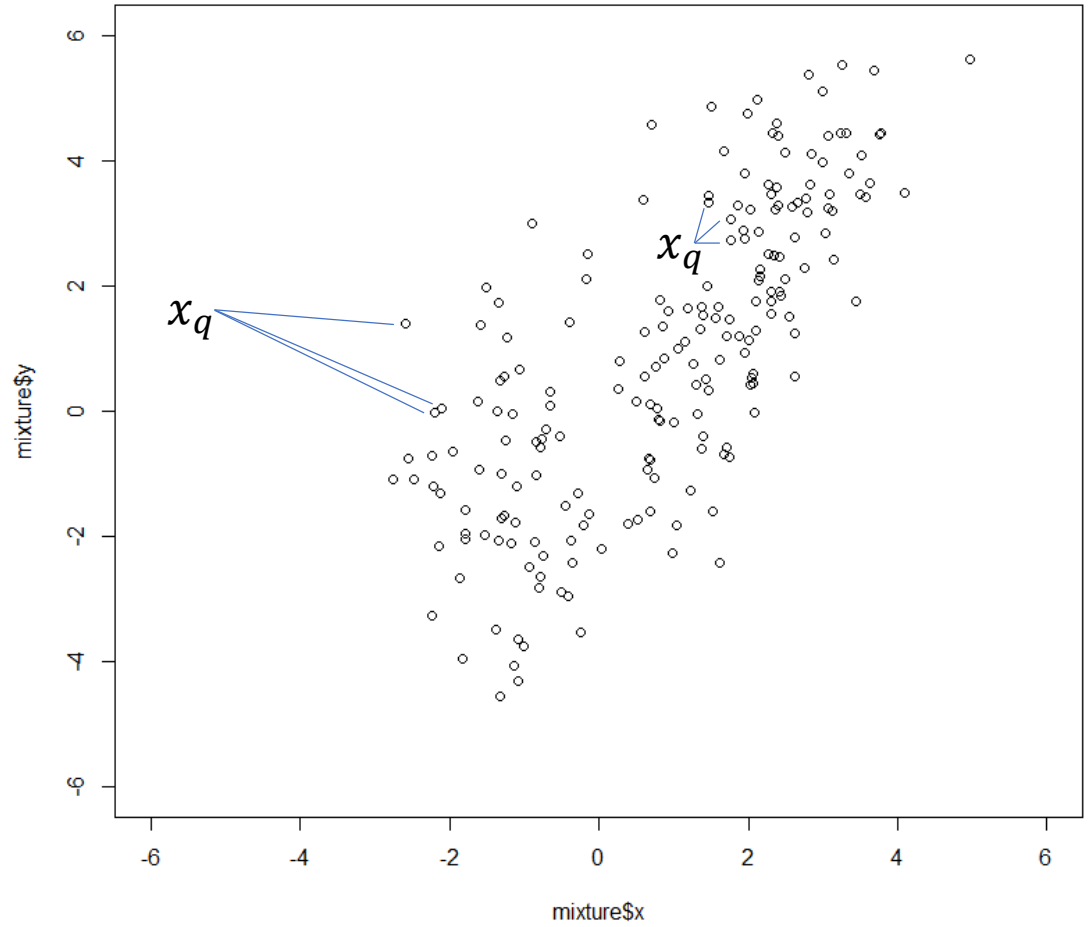
- Extensively studied for the past 10+ years
  - [Ruff, et al., 2021; Dietterich & Guyer, 2022]
- Advances in deep learning and vision foundation models have produced major improvements
- No method can guarantee to detect all novelty

Detecting Novel Hazards

- Perception Failures
  - Novel objects
  - Novel imaging conditions
  - Insufficient sensors
- Control Failures
  - Near misses
  - Collisions

Novelty Detection in Machine Learning

- Distance-Based Methods
  - Define a distance $d(x_i, x_j)$
  - Given a query x_q, compute
$$\min_{x \in D} d(x_q, x)$$
- Density-Based Methods
  - Fit a probability density $P(x_i)$
  - Given a query x_q compute
$$-\log P(x_q)$$
  - Densities are always dependent on distances



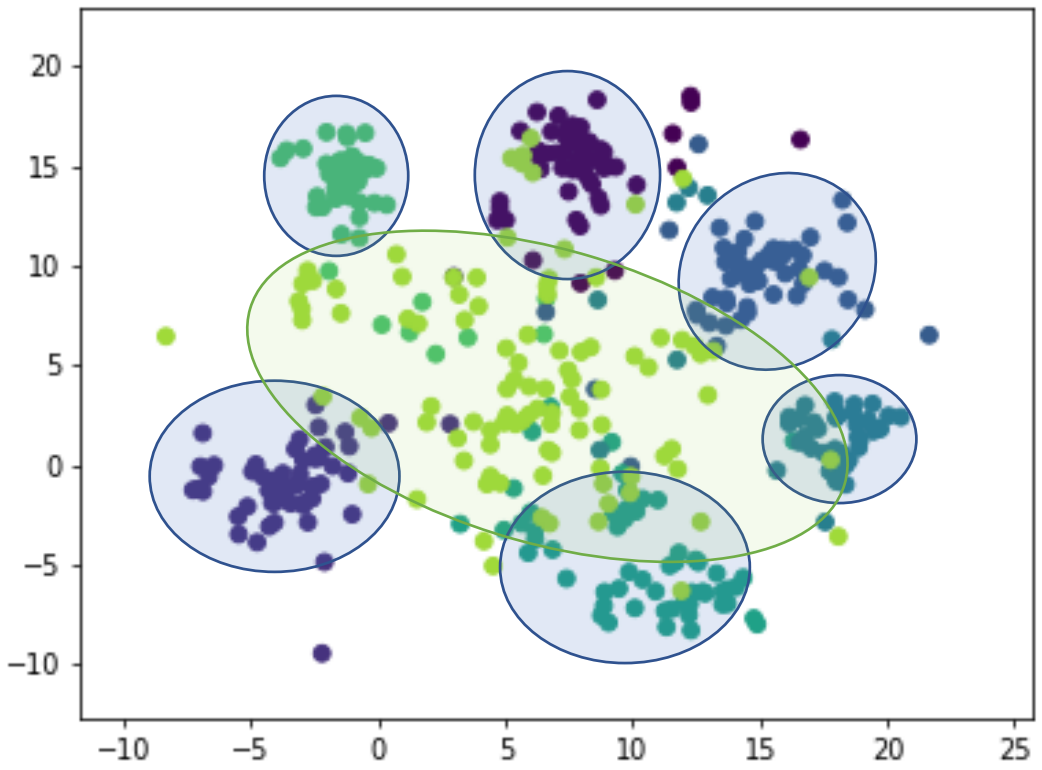
Deep Anomaly Detection

- An important advantage of deep learning is that it learns its own internal features
  - Euclidean distance in pixel space is not useful
- Problem: It only learns the internal features that it needs for the training task. These features may not separate novel queries x_q from nominal data

Experiment:
Deep Learned Features in Computer Vision

- DenseNet with 384-dimensional latent space.
- CIFAR-10: 6 known classes, 4 novel classes
- Light green: novel classes
- Darker greens: known classes

- Images from known classes are “pulled out” from the center of the space
- Most novel-class images stay toward the center of the space; others overlap with known classes
- Novel images are “inliers”



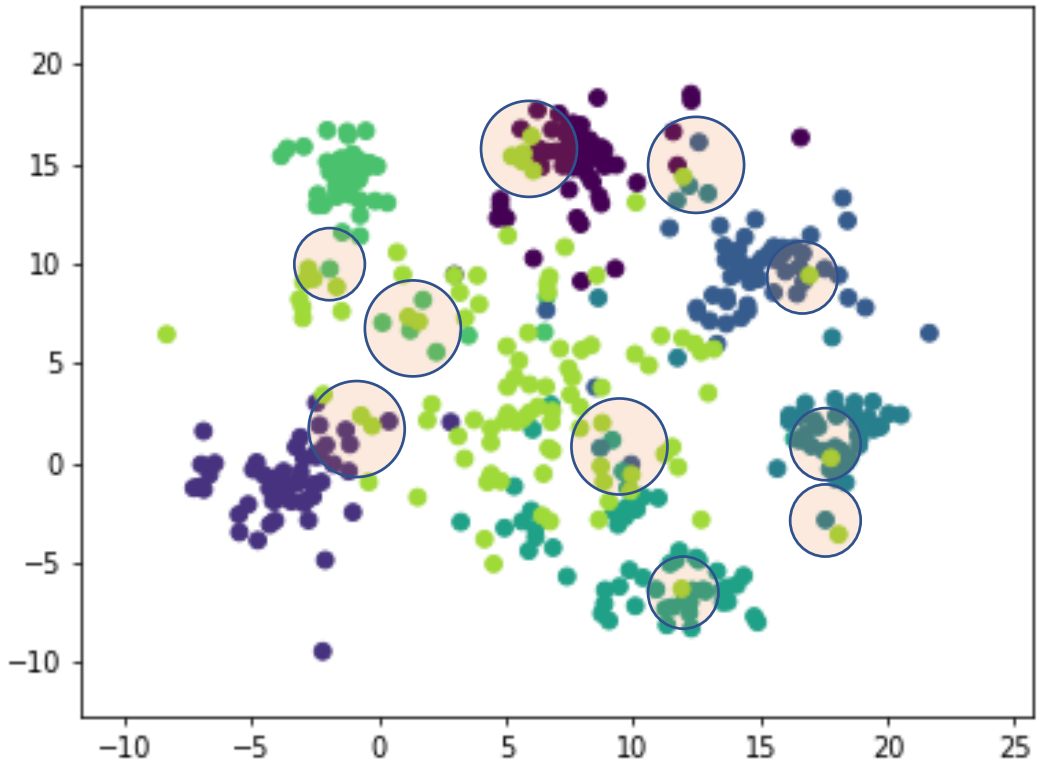
6 Known Classes

4 Novel Classes

Dietterich & Guyer, 2022

The Learned Representation is Promising But Not a Complete Solution

- Many novel-class images are mapped into clusters of known images
- ➔The learned representation can't detect the novelty



How can we learn better features?

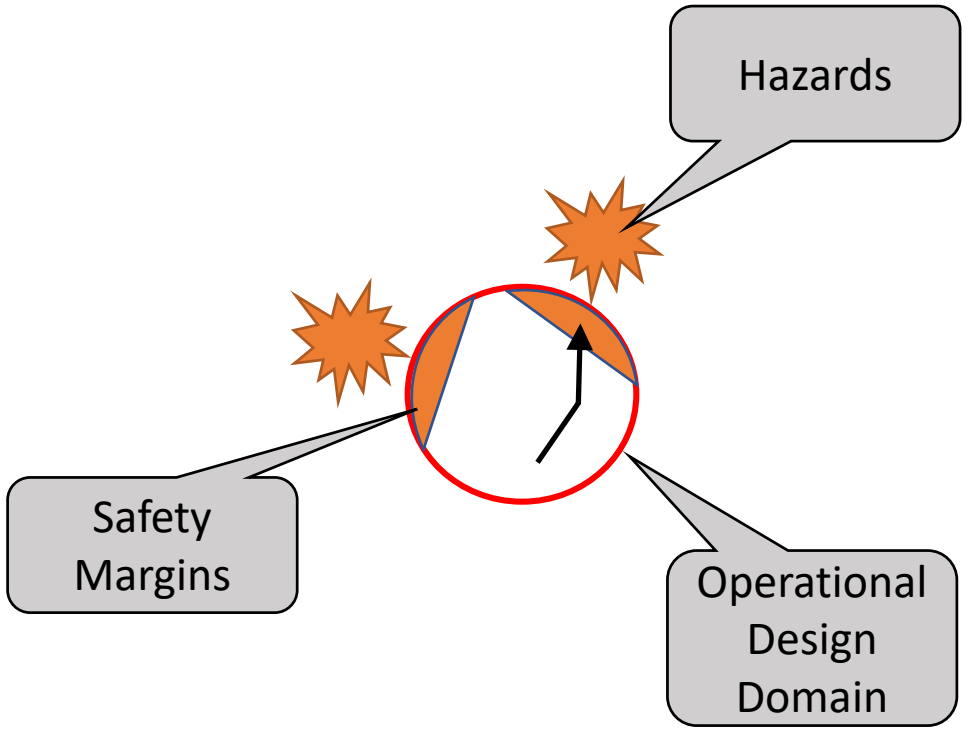
- Foundation Model Approach:
  - Train on all the data we can find
  - Artificially introduce variation through augmentations
    - Rotations, flips, simulated snow, rain, pixel noise, etc.
  - Synthetic data

- The deep representation learns to “see” (represent) the known world
  - A OneWheel will still be novel, but the model should have the right features to represent it and thereby separate it from all known objects

Source: onewheel.com

Detecting Near Misses

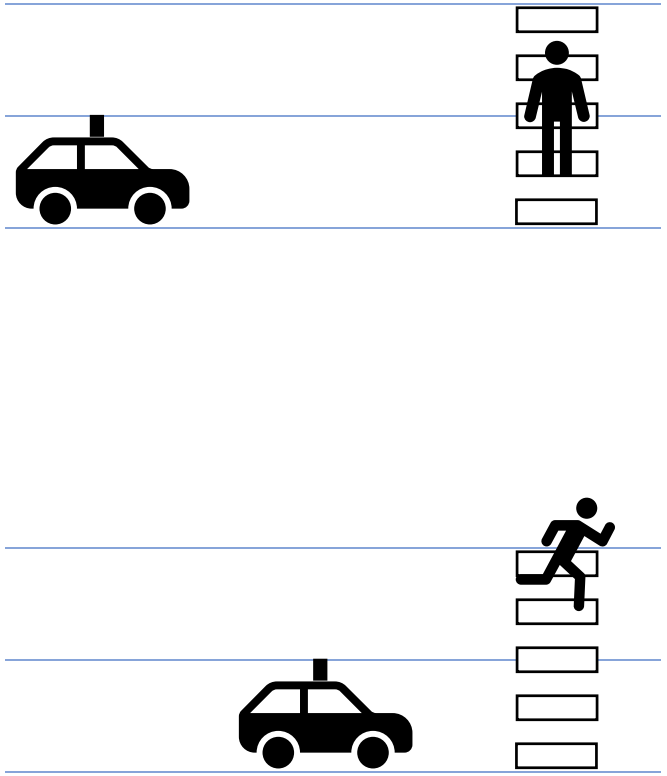
- Case 1: Known Hazards
  - During the design process, we have defined hazardous states and introduced margins of safety around them
    - Come too near to another object
    - Extreme steering and braking
  - Design should include sensors to detect when we enter those safety margin regions



Thesis Proposal 2:

Case 2: Counterfactual Near Misses

- Automatic Vehicle safety conditions
  - At least 2m separation between vehicle and pedestrians, cyclists, stationary obstacles
- Pedestrian sees car coming and jumps out of the way
- Car determines that it met the required 2m separation ➔ “no problem”
- Counterfactual: There would have been a safety violation if the pedestrian had not taken evasive action
- Pearl’s Theory of Causality provides the formal basis for computing counterfactual near misses [Pearl, 2009; Pearl & MacKenzie, 2018]



Automated Diagnosis and Repair

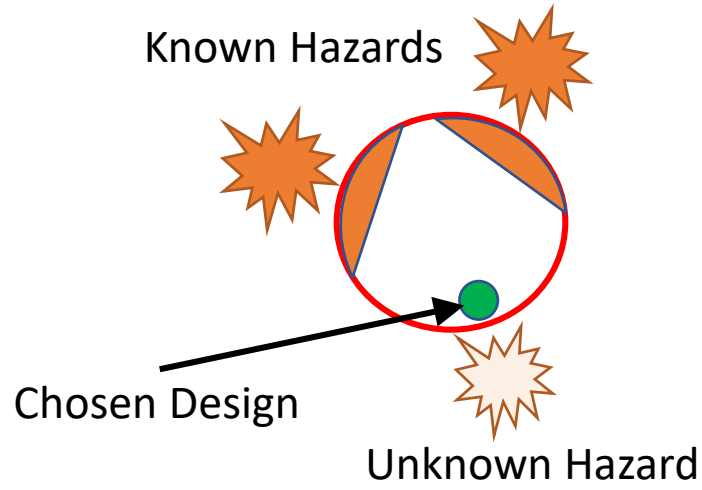
- Given a detected anomaly or hazard, what components contributed and how should they be modified?
- Diagnostic system requires
  - A causal model of the system including information flows
  - Reasoning capability to hypothesize potential contributing components
- Repairs can range from simple retraining of ML components to entire system redesign
  - What repairs can be safely applied by the AI system itself?
    - Adding a new hazard region into the path planner
    - Preparing training data to update the perceptual system and controllers

Outline

- Part 1: Integrating ML into traditional safety engineering processes
  - Scenario-based data collection
  - Verification-based data collection
  - Risk quantification
- Part 2: ML in open worlds: Safety as Control
  - Detecting anomalies, near misses, and departures from the Operational Design Domain
  - Adaptation strategies
- Part 3: Safety as Continual Redesign
  - Design is never finished
  - Resilient systems are “Poised to adapt”

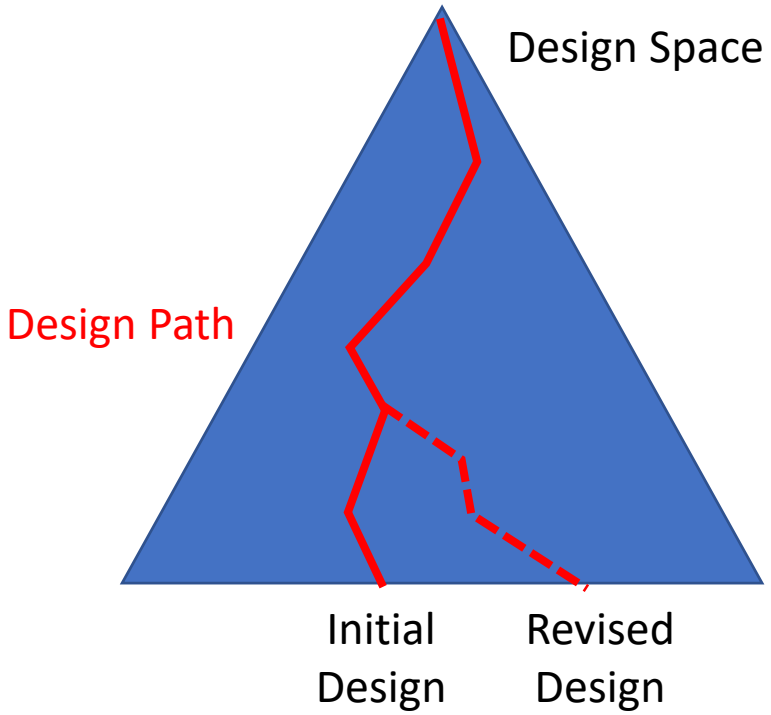
Creating Resilient Systems

- Engineered systems are “robust yet fragile”
  - Robust to the known hazards
  - Vulnerable to novel failure modes
- Optimization for cost, weight, etc. results in designs near the edge of the feasible region
  - Highly Optimized Tolerances (HOT) theory. Carson & Doyle (2002)



Creating Resilient Systems

- David Woods: A resilient system is one that is "poised to adapt"
  - [Woods, 2024a, 2024b]
- An AI perspective:
  - The entire design process should be regarded as one path through a design space
  - Adaptation requires following new paths through that space
  - Build AI tools for continual design



The design space and design process should be "kept on standby" so that they can be resumed whenever adaptation is required

Summary

- ML and traditional safety engineering: Managing Known Hazards
  - High-fidelity simulation
  - Risk-driven generation of training data and test cases
  - Verification methods to ensure distribution-independent generalization
    - Thesis proposal 1: Verification of fitted function properties
  - Importance sampling for risk estimation
- Safety as Control
  - Novel hazards as system disturbances
  - KPIs: Anomalies and Near Misses
  - AI methods for anomaly detection are mature
  - Counterfactual Near Misses: Unstudied
    - Thesis proposal 2: Counter-factual Near Misses
  - AI tools for diagnosis and repair can help
- Safety as Resilience: “Poised to Adapt”
  - The design space and design process “kept on standby” so that they can be invoked whenever adaptation is required

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