

FY2021-0702/Optimizing Machine Learning Predictions with Prediction Uncertainty

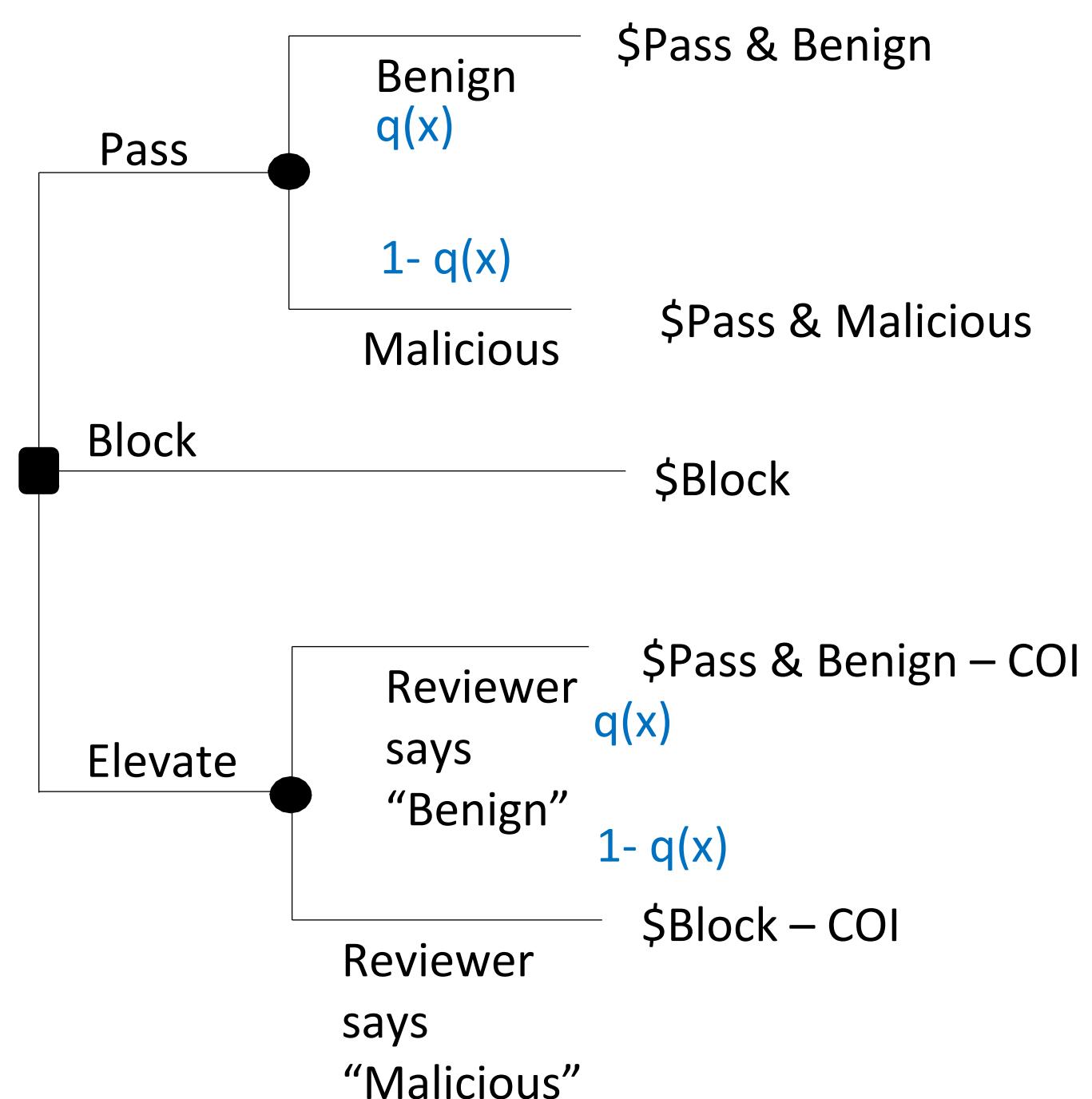


Introduction / Motivation

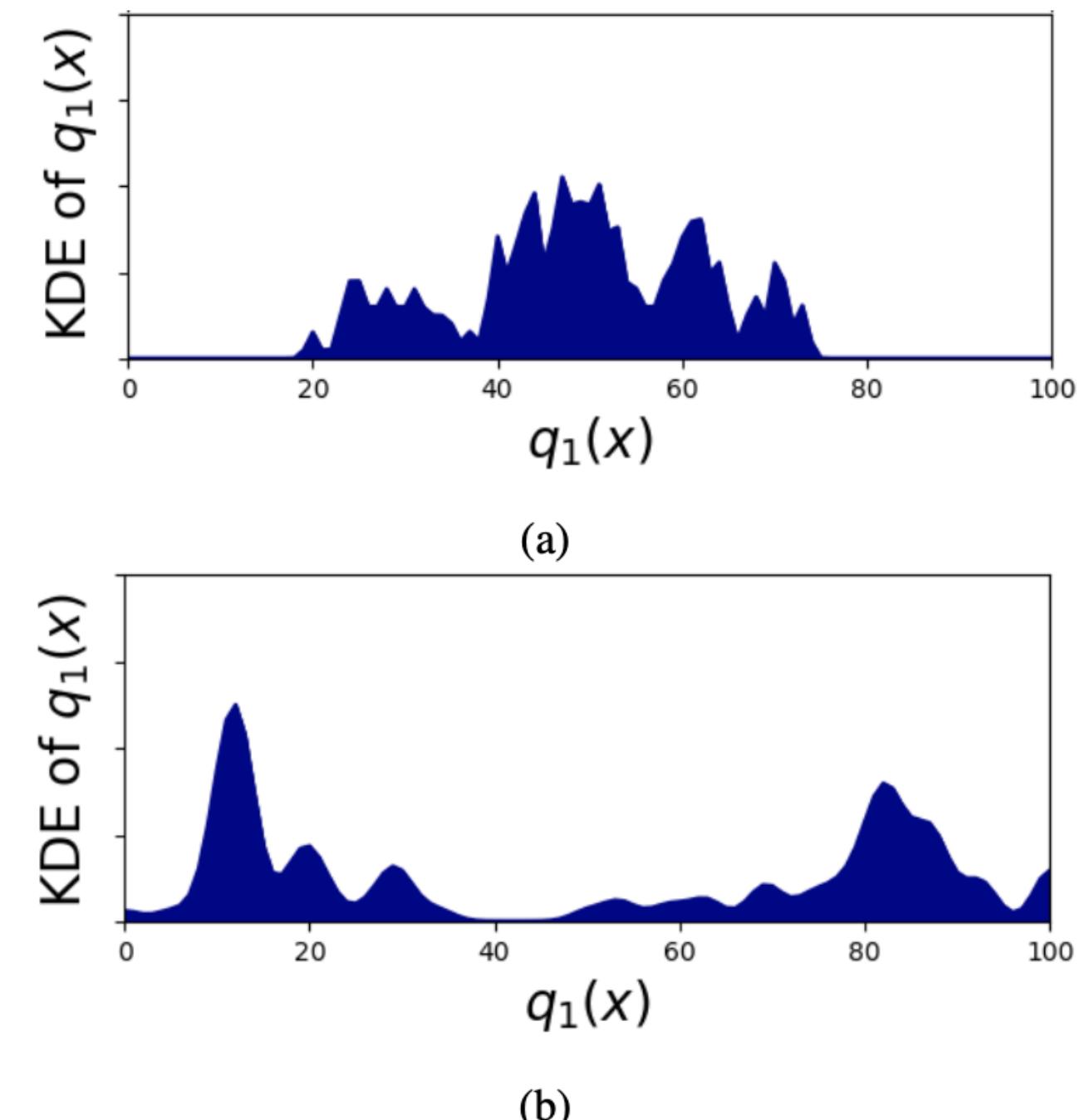
- Question: Can we improve machine learning models in the context of decision making under uncertainty?
- In decision analysis, probability distributions (along with costs) are inputs to a decision problem
- These distributions could be estimated using a machine learning model
- Previous work at Sandia suggests analyzing the outputs of a machine learning model using Uncertainty Quantification metrics. UQ measures confidence in individual predictions made by the model
- Primary goal is to understand how model uncertainty (captured in the UQ analysis) should be used in the context of a decision problem

Approach

Decision problem - URL screening

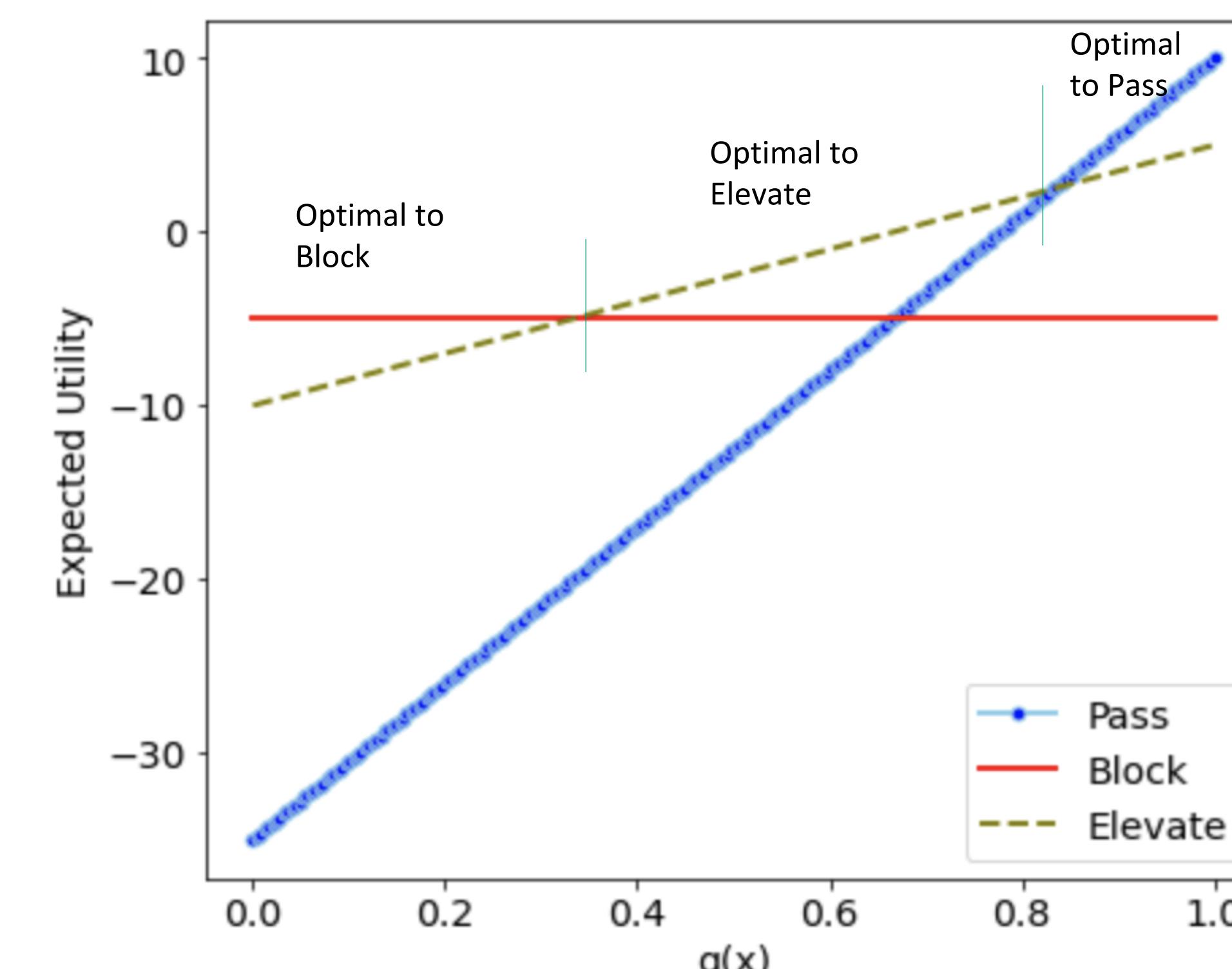


UQ metrics - bootstrap forecast distributions



Current Status/ Results

- Determine what type of machine learning model is best-suited for the decision problem
- Determine appropriate UQ metrics based on chosen model
- Quantify when “too much uncertainty” around ML prediction should change a decision (or prompt addition information acquisition)

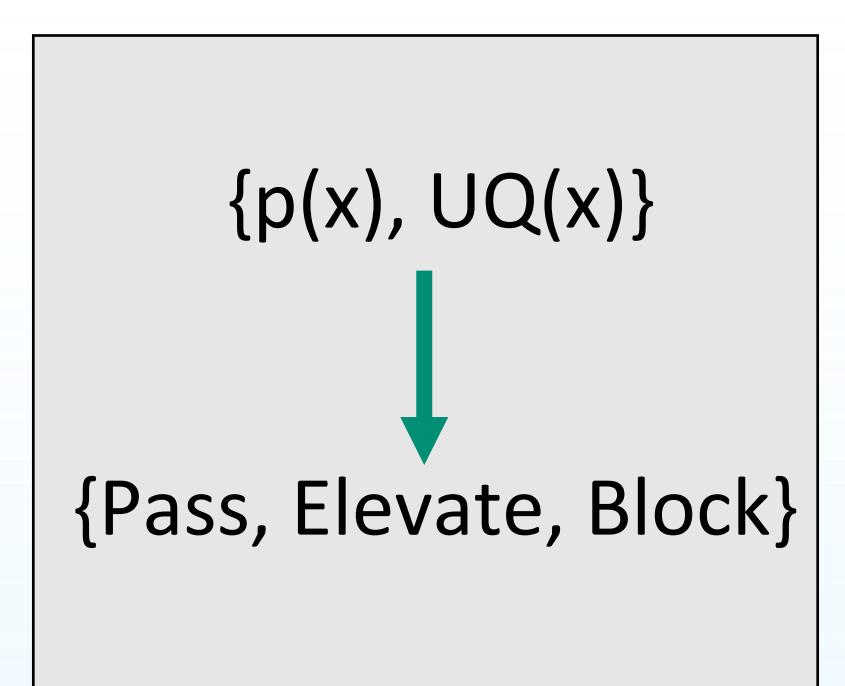


Challenges

In experiments, significant computation time required for bootstrapping with complex models



Can be difficult to determine when to change a decision from the model's initial recommendation



Next Steps/ Future Work

Computational experiments on ‘learning’ how to incorporate UQ into better decisions

Incorporating out-of-distribution (OOD) analysis

