Conformal Prediction

Distribution-Free Uncertainty Quantification

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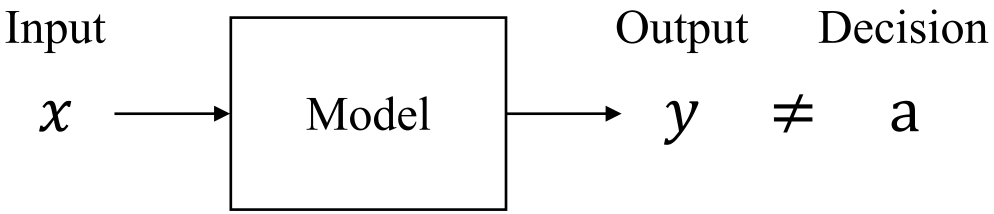
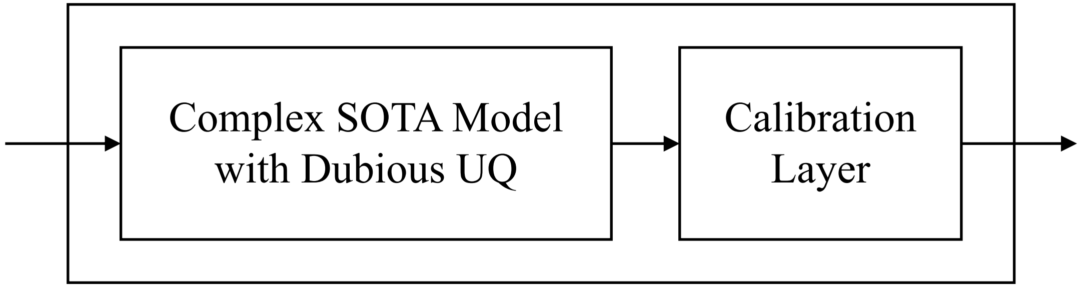
Uncertainty Quantification for Decision-Making



- **Why quantify uncertainty?**
  - **Making good decisions** requires quantification of uncertainty.
    - Raining probability > 30%, bring an umbrella.
    - Mortality rate < 20%, do surgery.
    - Invest more if return rate is $10\pm1\%$ instead of $10\pm20\%$.
- **How to quantify uncertainty?**
  - **Parametric models:** normal assumption is not convincing.
  - **Asymptotic theory:** data volume is not always large enough, convergence may not be guaranteed.
  - **Bayesian statistics:** prior distribution is not convincing, and the posterior distribution is difficult to calculate.
  - **Ensemble learning:** very slow for large datasets.
  - **Monte Carlo drop out:** require special network design and training.
  - **Generative models:** training is computationally expensive.

Conformal Prediction



- Introduce it using the most common **split conformal**:
  - Divide the dataset into training set D_{train}, calibration set D_{cal}, and test set D_{test}.
  - Train the model $\hat{f}$ on D_{train}.
  - For every sample (X_i, Y_i) in D_{cal}, calculate the **nonconformity scores**:

$$S_i = \left|Y_i - \hat{f}(X_i)\right| \text{ (regression) or } S_i = 1 - \hat{\pi}_{Y_i}(X_i) \text{ (classification)}$$

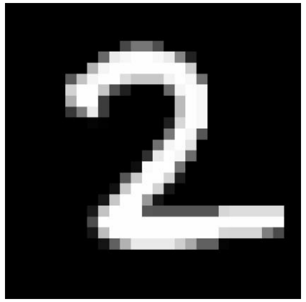
  - Sort the nonconformity scores $\{S_1, S_2, \ldots, S_{n_{cal}}\}$, find the $(1-\alpha)$-quantile $\hat{q}$.
  - Then for a new X_{new} from D_{test}, the interval prediction is

$$C(X_{new}) = \left[\hat{f}(X_{new}) - \hat{q},\ \ \hat{f}(X_{new}) + \hat{q}\right] \text{ (regression) or } \{y: \hat{\pi}_y(X_{new}) \geq 1 - \hat{q}\} \text{ (classification)}$$

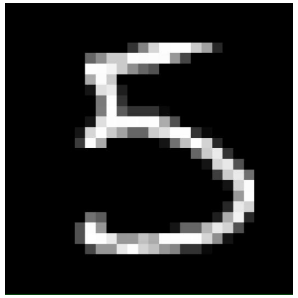
- **Key idea:** Use the distribution of prediction errors on a portion of reserved data (D_{cal}) to quantify the uncertainty range that should be expected when predicting new data.
- **Advantages:** finite-sample coverage, distribution free, model free
- **Disadvantages:** only provide interval or set, too conservative, low data efficiency, rely on data distribution

Experiments

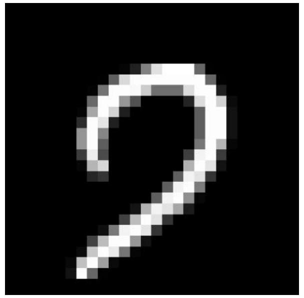
- Train a simple CNN on the MNIST dataset, and set the confidence level $\alpha = 0.05$.



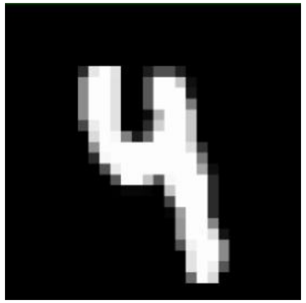
Ground truth: 2
Point prediction: 2
Set prediction: $\{2\}$



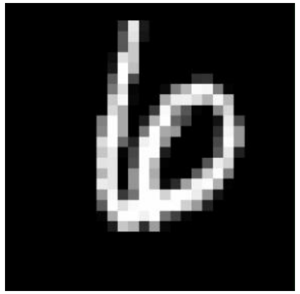
Ground truth: 5
Point prediction: 5
Set prediction: $\{5\}$



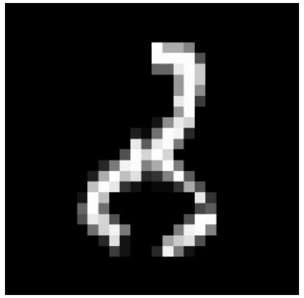
Ground truth: 7
Point prediction: 9
Set prediction: $\{7, 9\}$



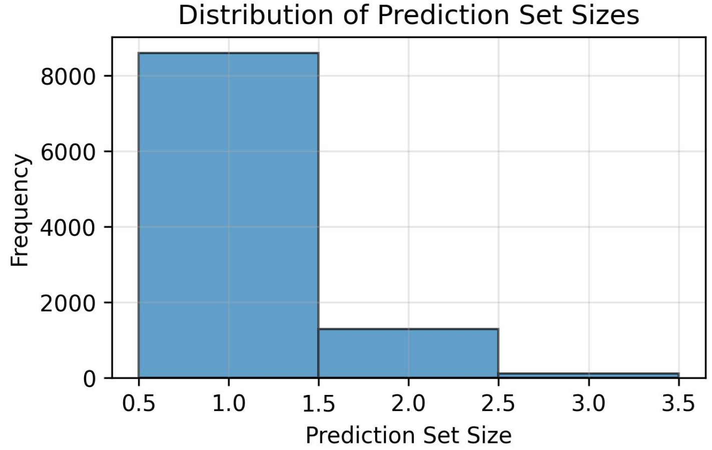
Ground truth: 4
Point prediction: 9
Set prediction: $\{4, 9\}$

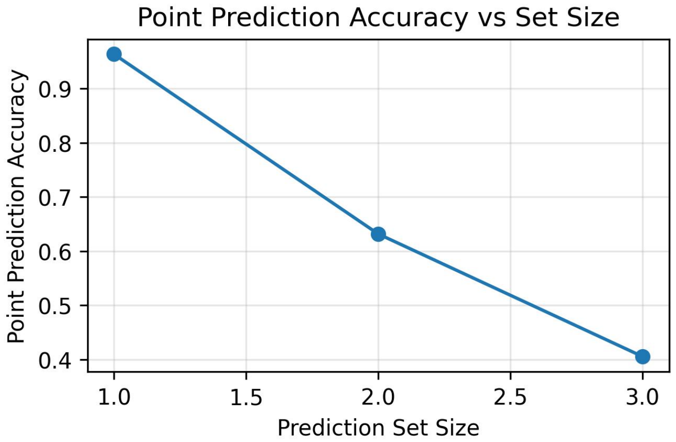


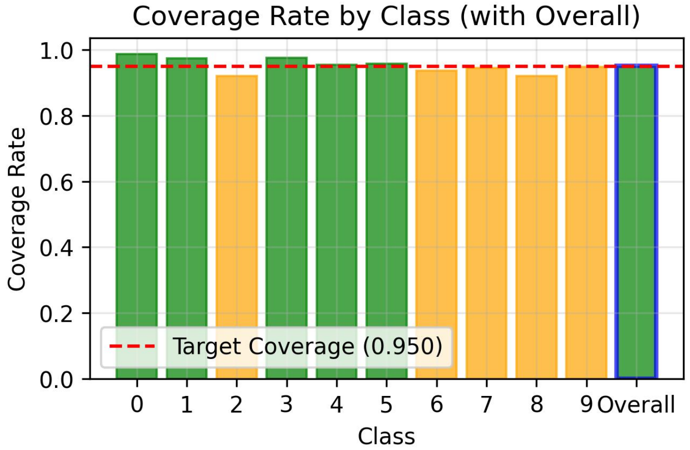
Ground truth: 6
Point prediction: 6
Set prediction: $\{0, 6\}$



Ground truth: 8
Point prediction: 2
Set prediction: $\{2, 3, 8\}$

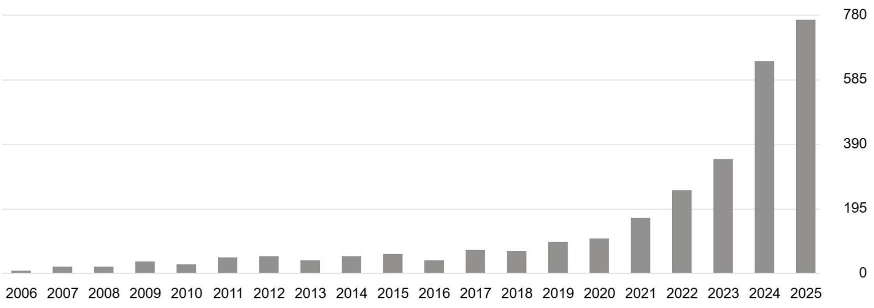


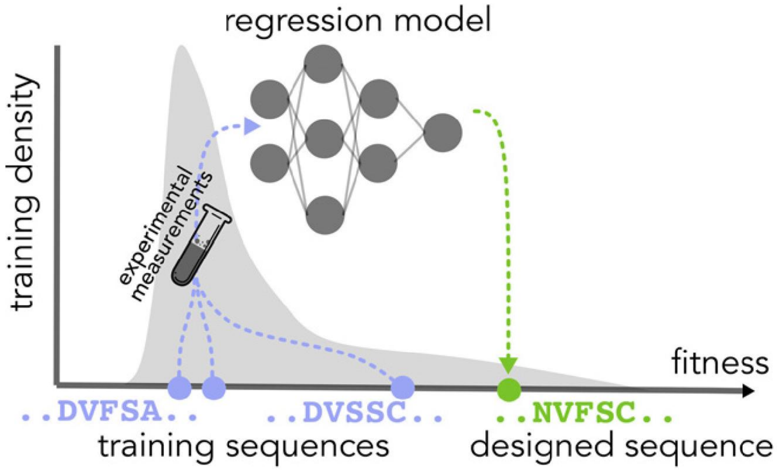




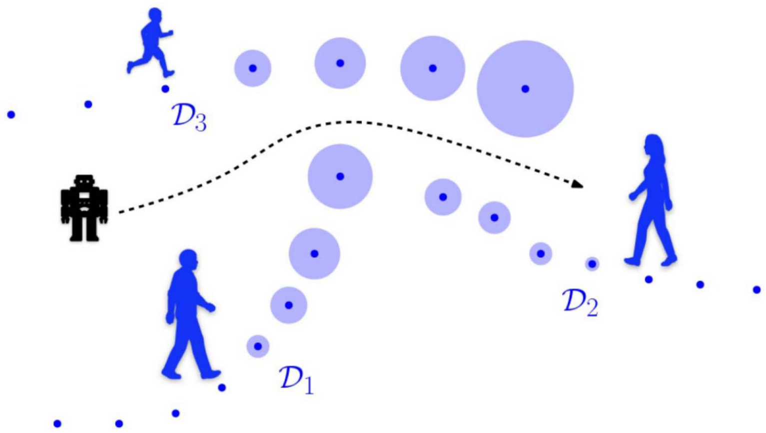
Real World Impacts

- Conformal prediction was first introduced by Gammerman, Vovk, and Vapnik in **1998**[1,2].
  - Originally designed for support vector machines (SVM).
  - It is still being widely used today.

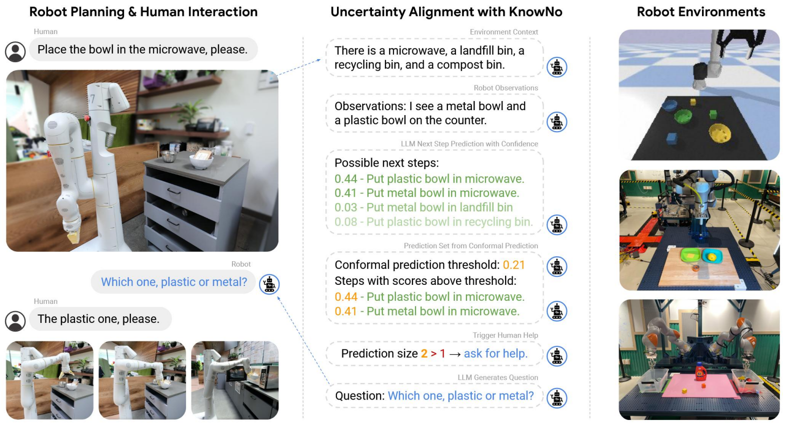




Protein design (2022, PNAS)[3]



Safe planning (2023, IEEE RA-L)[4]



LLM for robotics (2023, CoRL, Best Student Paper)[5]

Additionally: cancer diagnosis (2022, Nat. Commun.)[6], earth observation (2024, Sci. Rep.)[7], disease course prediction (2025, npj Digit. Med.)[8]

[1] A. Gammerman, V. Vovk, and V. Vapnik. 1998. Learning by transduction. In Proceedings of the Fourteenth conference on Uncertainty in artificial intelligence (UAI'98). Morgan Kaufmann Publishers Inc., San Francisco, CA, USA, 148–155.
[2] Vovk, Vladimir, Alexander Gammerman, and Glenn Shafer. *Algorithmic learning in a random world.* Boston, MA: Springer US, 2005.
[3] Fannjiang, Clara, et al. "Conformal prediction under feedback covariate shift for biomolecular design." *Proceedings of the National Academy of Sciences* 119.43 (2022): e2204569119.
[4] Lindemann, Lars, et al. "Safe planning in dynamic environments using conformal prediction." *IEEE Robotics and Automation Letters* 8.8 (2023): 5116-5123.
[5] Ren, Allen Z., et al. "Robots that ask for help: Uncertainty alignment for large language model planners." *arXiv preprint arXiv:2307.01928* (2023).
[6] Olsson, Henrik, et al. "Estimating diagnostic uncertainty in artificial intelligence assisted pathology using conformal prediction." *Nature communications* 13.1 (2022): 7761.
[7] Singh, Geethen, et al. "Uncertainty quantification for probabilistic machine learning in earth observation using conformal prediction." *Scientific Reports* 14.1 (2024): 16166.
[8] Sreenivasan, Akshai Parakkal, et al. "Conformal prediction enables disease course prediction and allows individualized diagnostic uncertainty in multiple sclerosis." *npj Digital Medicine* 8.1 (2025): 224.

Thank you!