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A Short Primer on UQ

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Outline

- Introduction
- Standard VVUQ formalism
- The UQ formalism
- Statistics in UQ
- Applied math in UQ
- Inverse problems and UQ
- Machine learning and UQ
- Discussion

Introduction

- UQ as a discipline originated to address the problem of determining uncertainties in the predictions made by deterministic models.
- The enterprise was originally an effort by applied mathematicians; numerical analysis, probability, proving convergence of error terms, etc.
- Statisticians more concerned with making inferences (including quantifying uncertainty) directly from data, and without knowledge of the underlying deterministic models.

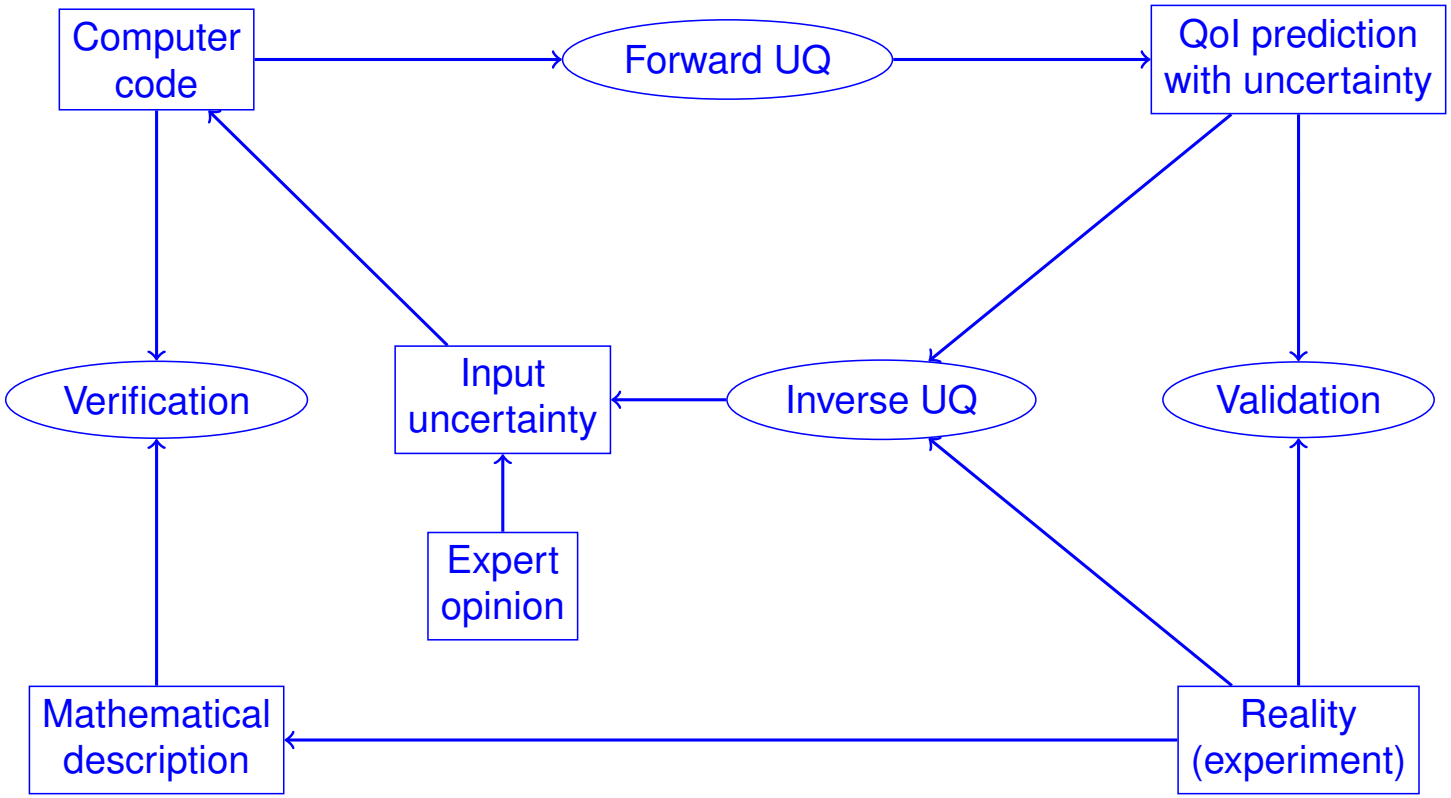
Introduction

- In the late 1980's some statisticians *did* start thinking about the output of deterministic models as "data", giving rise to the design and analysis of computer experiments literature.

- The two communities have moved towards each other over time, and are beginning to discard the domain labels. UQ is now a cohesive, identifiable discipline area strongly driven by applications.

- Emergence of data science and machine learning have brought new tools and capabilities to exploit massive volumes of observational/experimental data and massive model output.

Standard VVUQ formalism



Adapted from Wu et al, (2018). DOI: 10.1016/j.nucengdes.2018.06.004.

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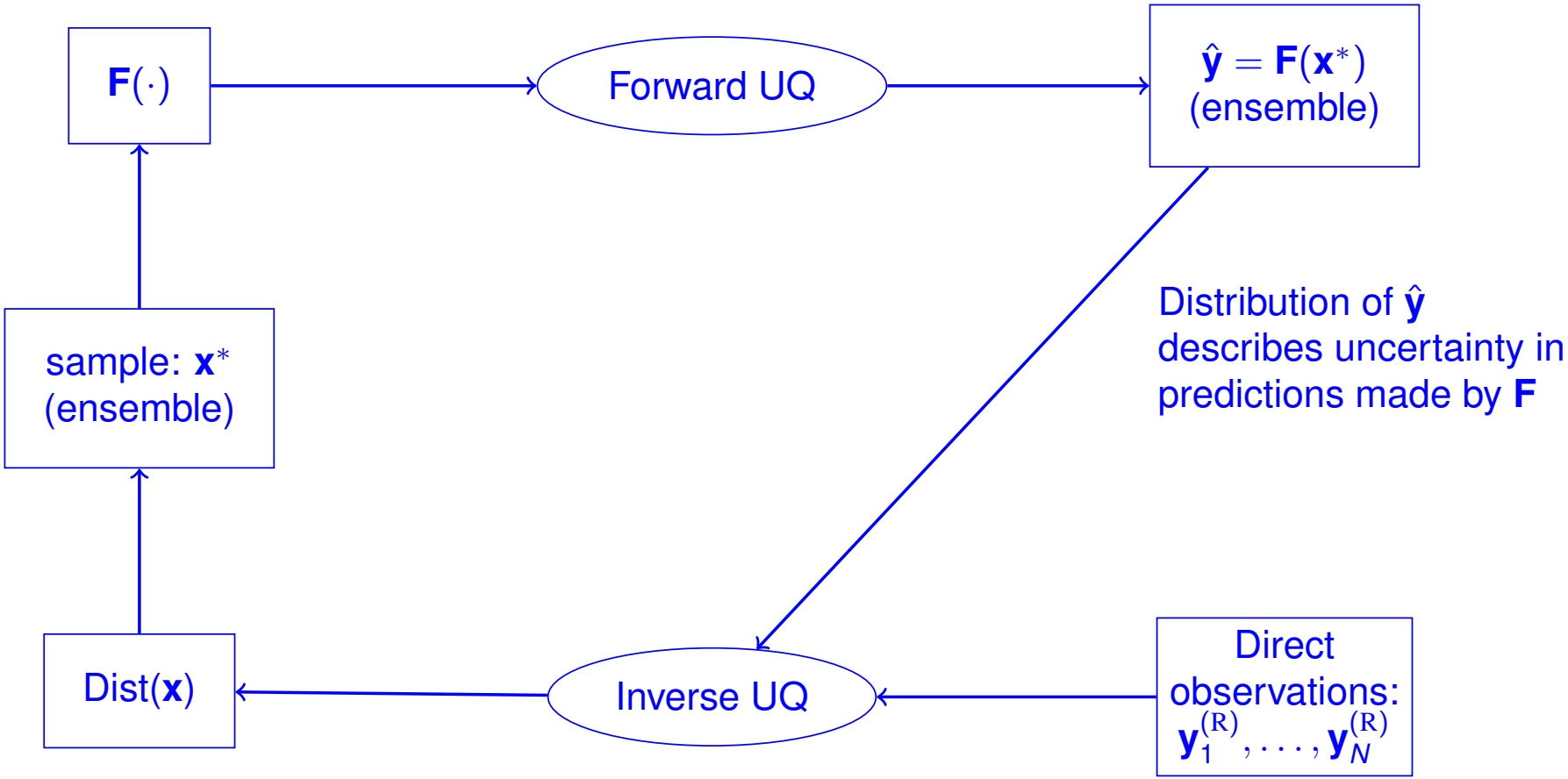
UQ formalism



Statistics in UQ

- Statistical methods: inference from observations using probabilistic models.
  - estimation and hypothesis testing
  - exploratory data analysis, density estimation, unsupervised learning
  - regression, supervised learning, to uncover significant relationships
  - uncover, test, and quantify relationships from data
  - use estimated model to make statistical predictions with uncertainty
  - Design of Experiments (DOE)
- Statistical models inherently carry uncertainties with them.

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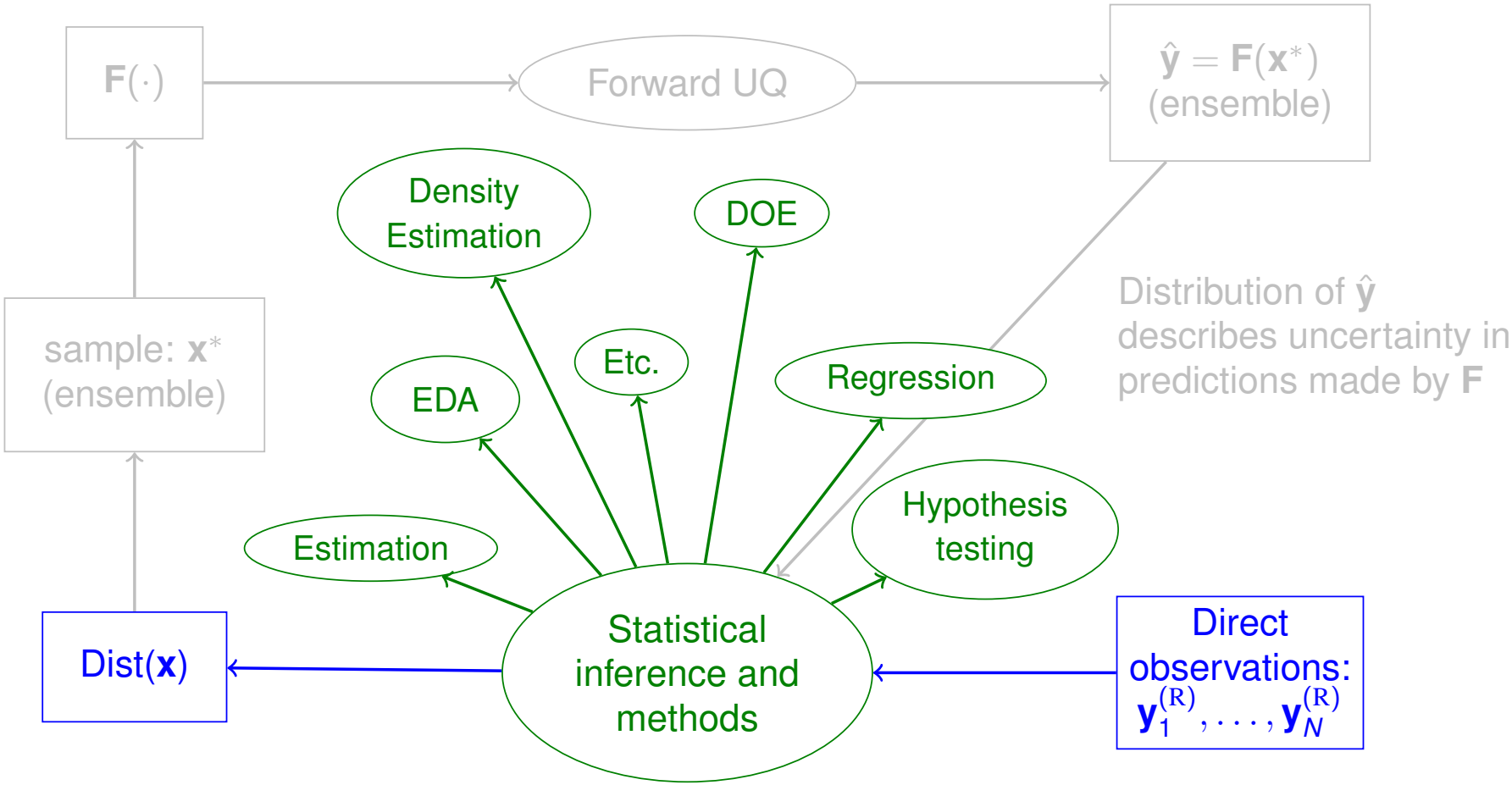
Statistics in UQ



Applied math in UQ

- Mathematical UQ: mathematical approaches for understanding sources of uncertainty in **F** and facilitating efficient forward UQ.
  - exploit structure and properties of **F** to guide forward UQ
  - alternatives to brute-force Monte Carlo forward UQ
  - numerical and other approximations for speed and efficiency
  - optimization!
- Uncertainty expressed through probability distributions, and driven by probabilistic description of input uncertainties.

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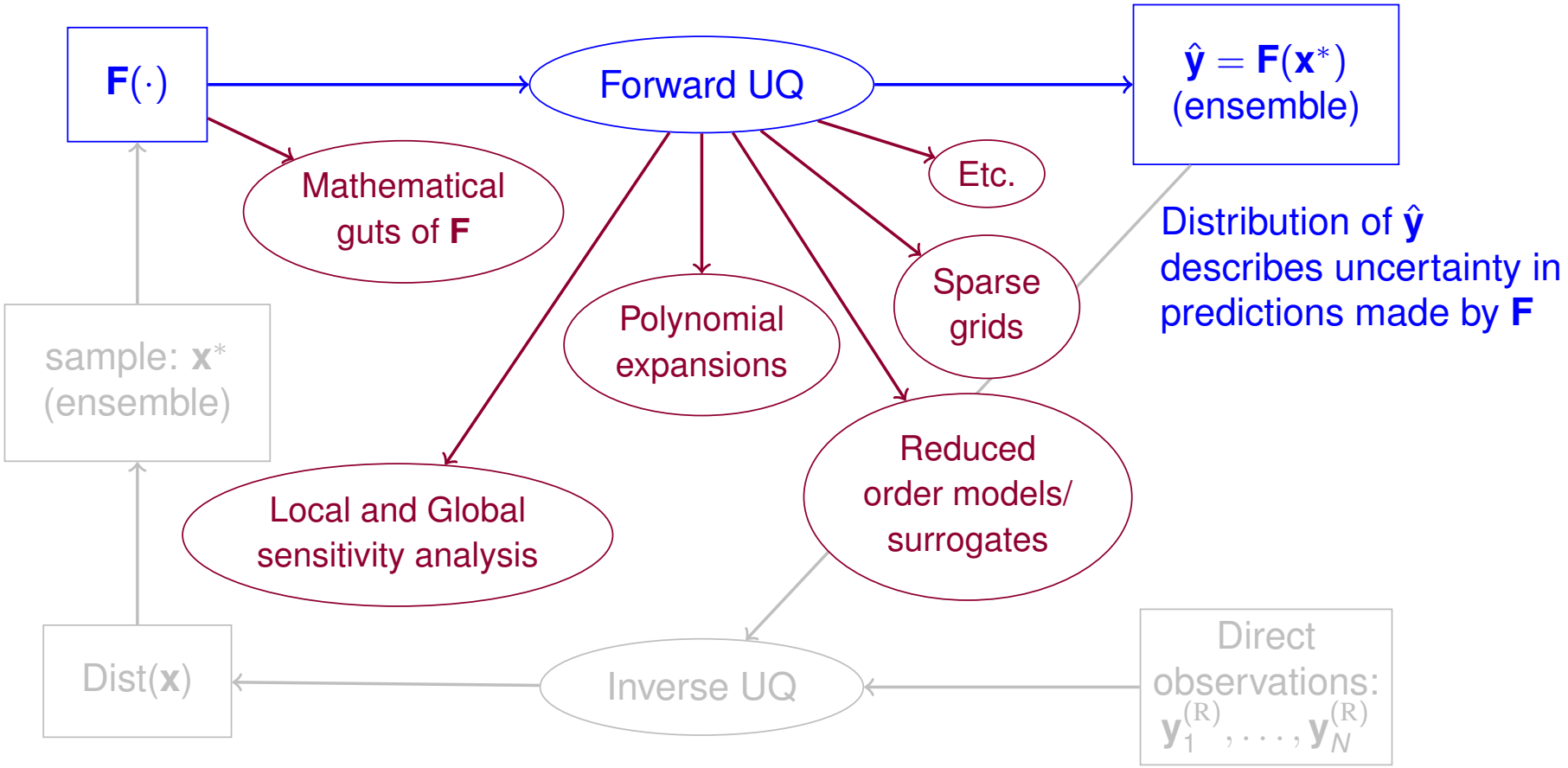
Applied math in UQ



Inverse problems and UQ

- Inverse problems: infer the state of a system from noisy, indirect measurements.
  - heavy use of Bayesian methods
  - overlaps substantially with statistics, but more focussed on this class of problems
  - emphasis on algorithms/samplers
  - because result is a distribution, easy forward propagation

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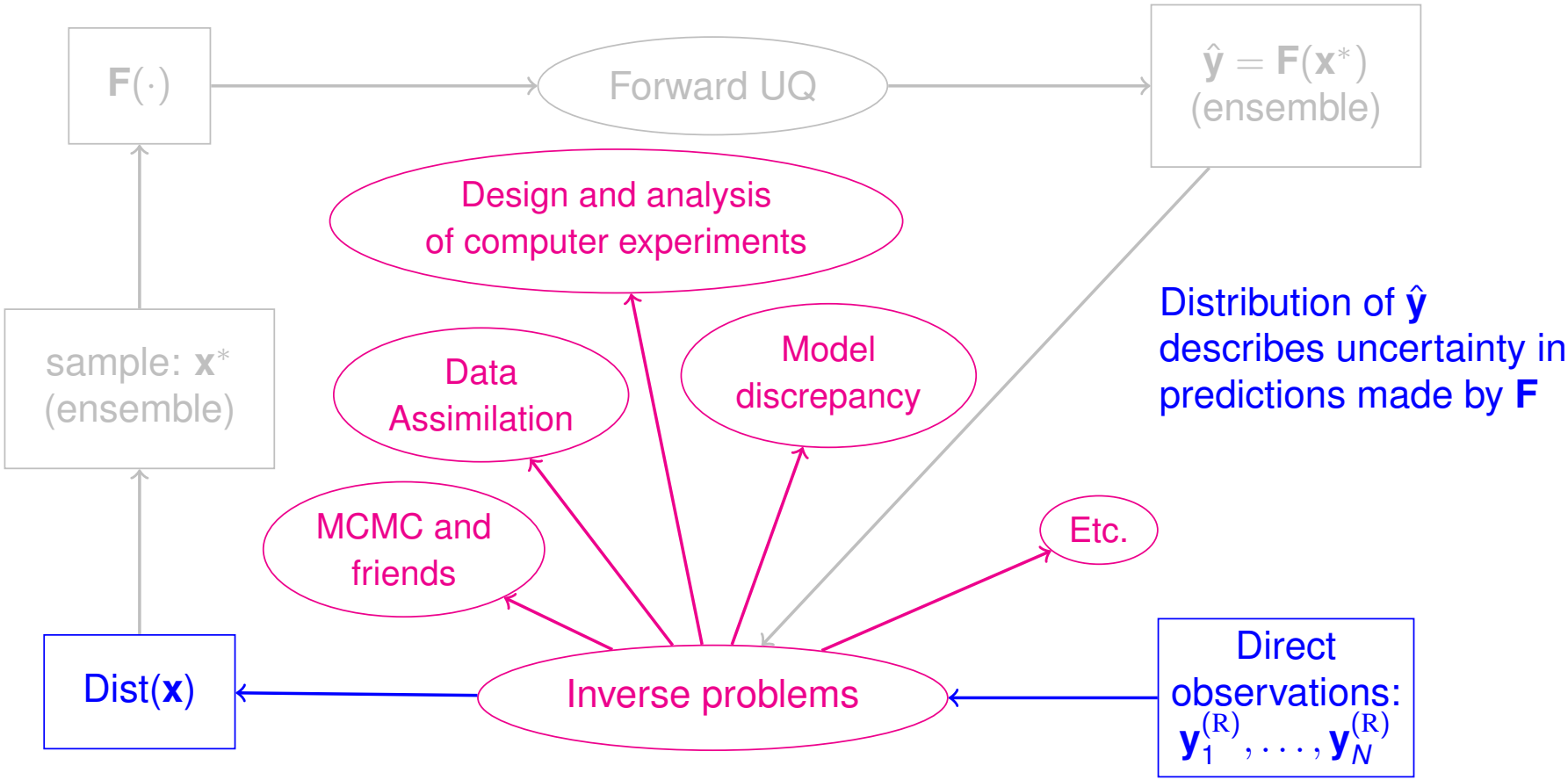
Inverse problems and UQ



Machine learning and UQ

- Machine learning: learning complex relationships in data, and making predictions using those relationships.
  - Classification and regression (linear, non-linear), support vector machines
  - Cluster analysis, generative modeling
  - neural networks (NN) and friends: UQ is a challenge, but conformal inference to the rescue
  - Gaussian Processes (GP) provide UQ but how good is it?
  - Major role in UQ is emulation of complex models

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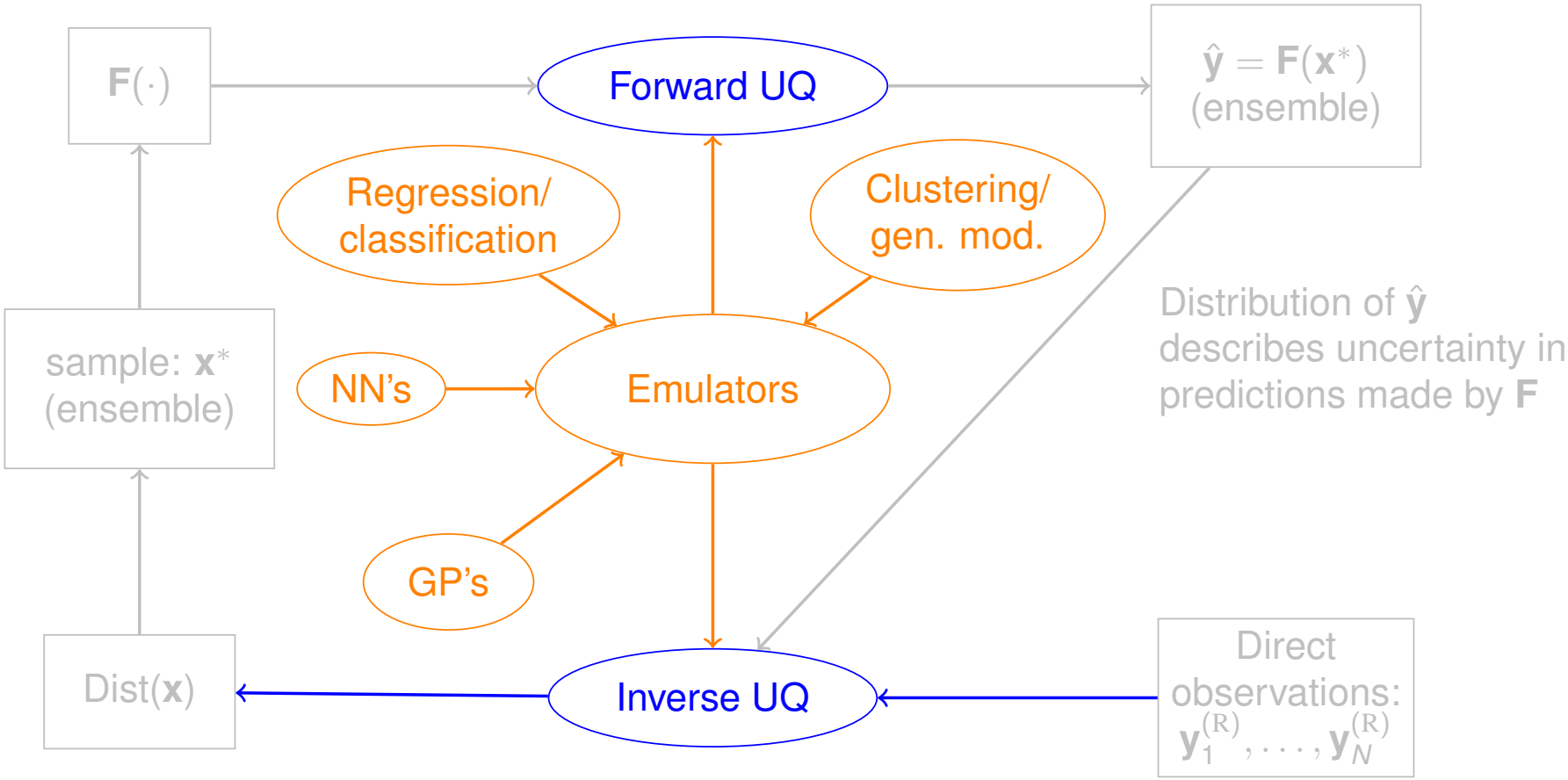
Machine learning in UQ



Discussion

- Aligning a specific application with components of this formalism may be harder than it looks.
- Role of ML in UQ is still being understood. What about the role of UQ in ML?
- UQ is now its own discipline, inheriting theory and methods from statistics, applied math, and inverse problems communities.
- When someone talks about UQ, ask yourself: who they are and what they mean!
- New contributions arise from new problems, data types, modeling capabilities, and science questions. Your insights are needed!

Acknowledgments