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MU Training Challenges relating to Machine Learning

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Overview

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TRAINING FOR THE METROLOGY COMMUNITY

- Current applications of ML uncertainty evaluation
- Framing the uncertainty evaluation task
- Regression models
  - Uncertainty propagation through training models
  - Taking uncertainty related to model training into account
    - Classical statistical modelling approaches
    - Modern ML approaches
- Classification models

TRAINING FOR THE WIDER COMMUNITY

CONCLUSIONS

Training for the metrology community

Some applications of ML uncertainty evaluation in the metrology community

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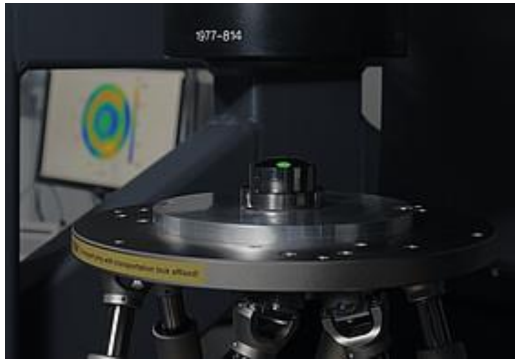
18HLT07 MedalCare

Qumphy

MAIB AI

Battery state-of-health

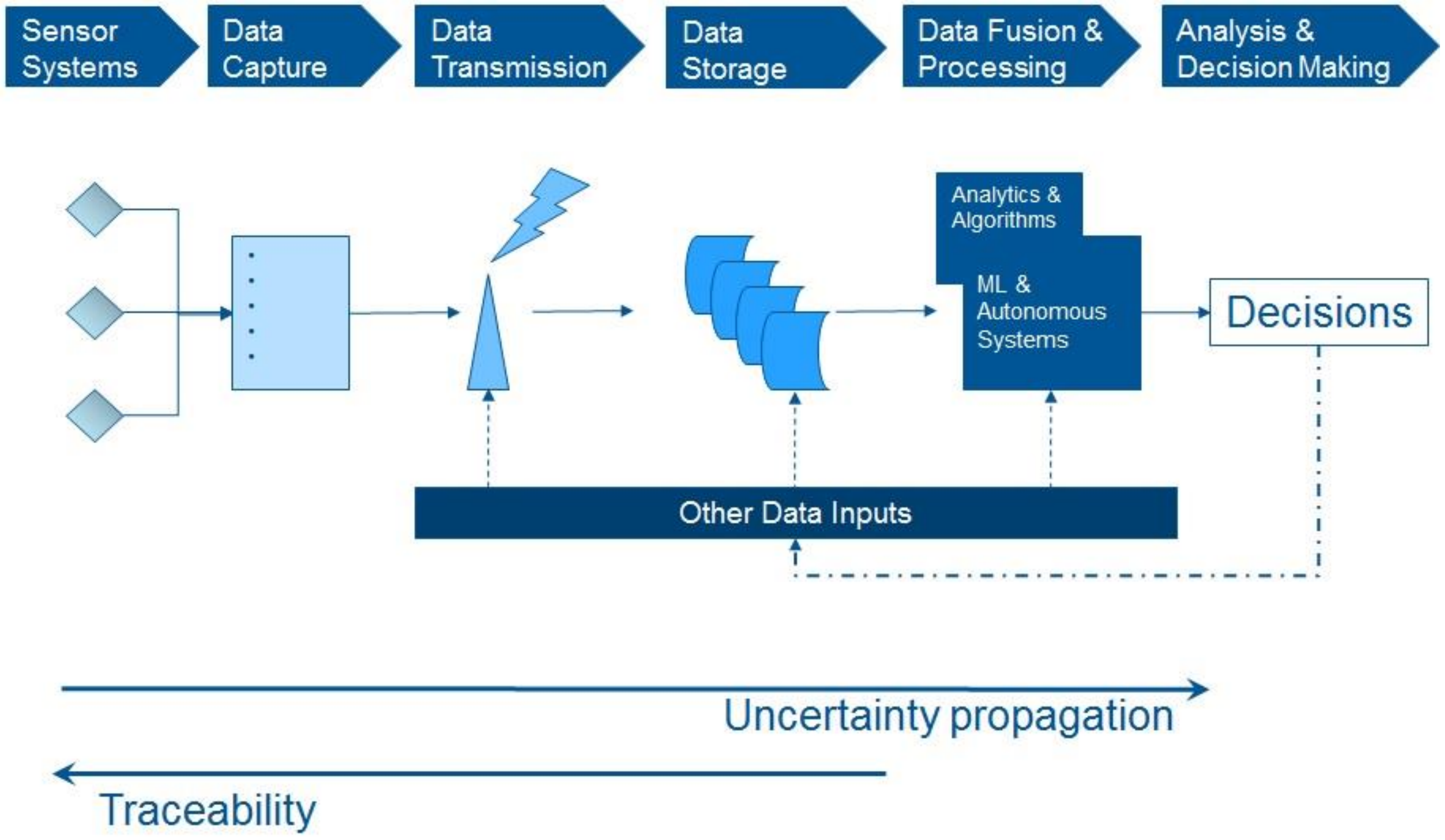
Critical care
[image from PTB]



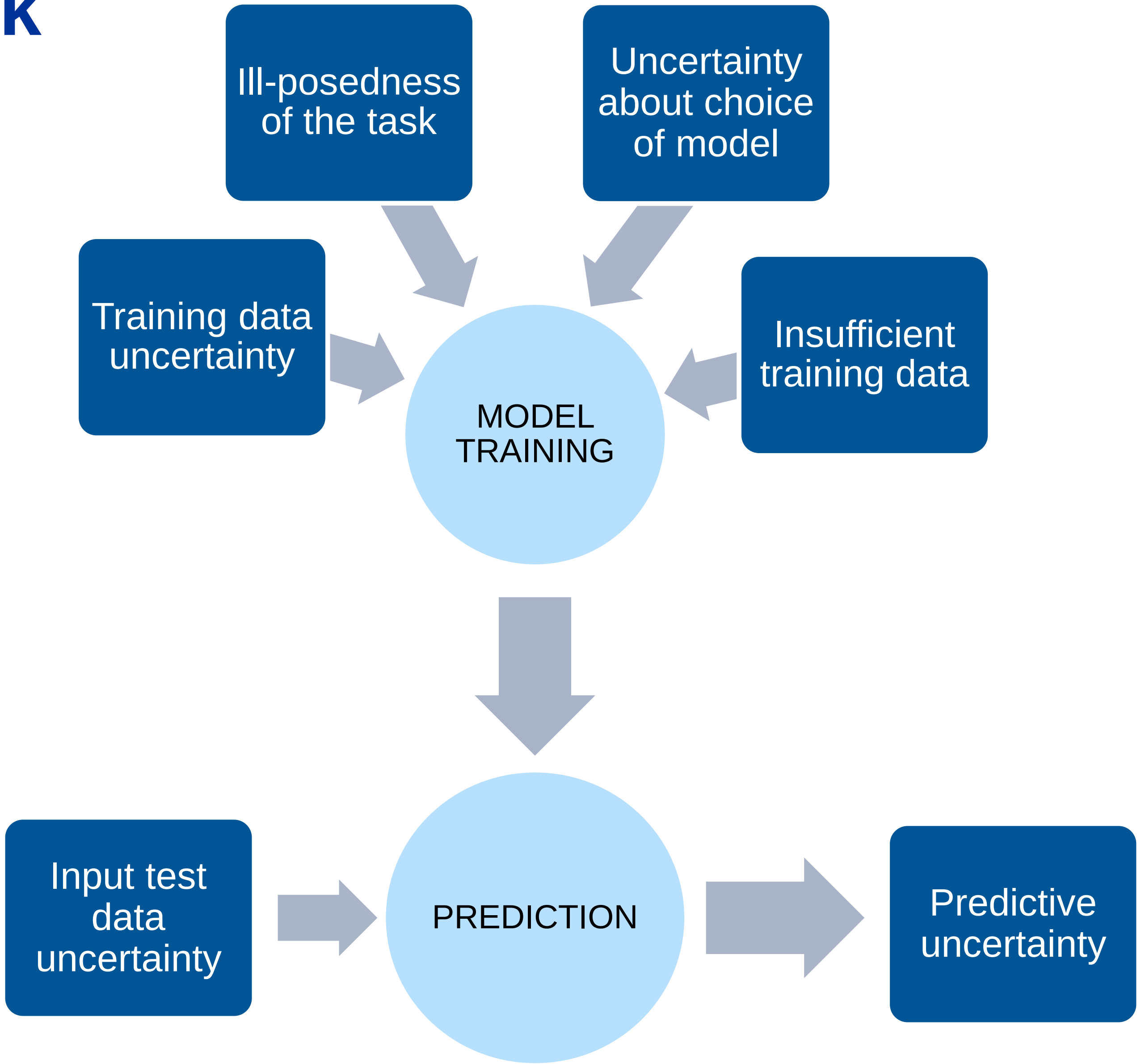
Optical form measurements
[image from PTB]

Landcover classification

Uncertainty evaluation in machine learning: framing the task

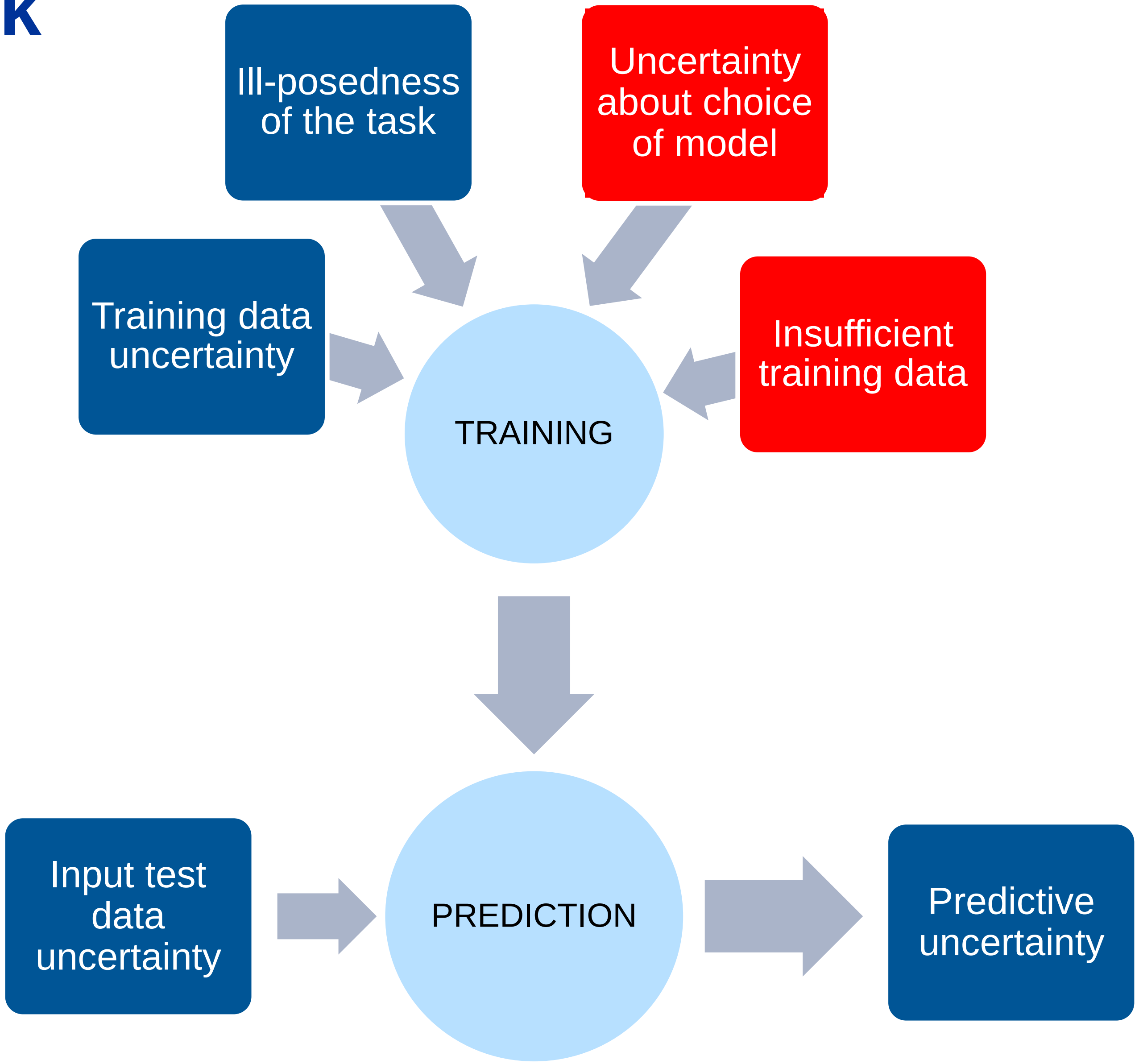


Uncertainty evaluation in machine learning: framing the task



Uncertainty evaluation in machine learning: framing the task

Sources of uncertainty in blue cannot be removed (aleatoric); sources of uncertainty in red can be potentially be removed (epistemic)



Uncertainty evaluation in machine learning: framing the task

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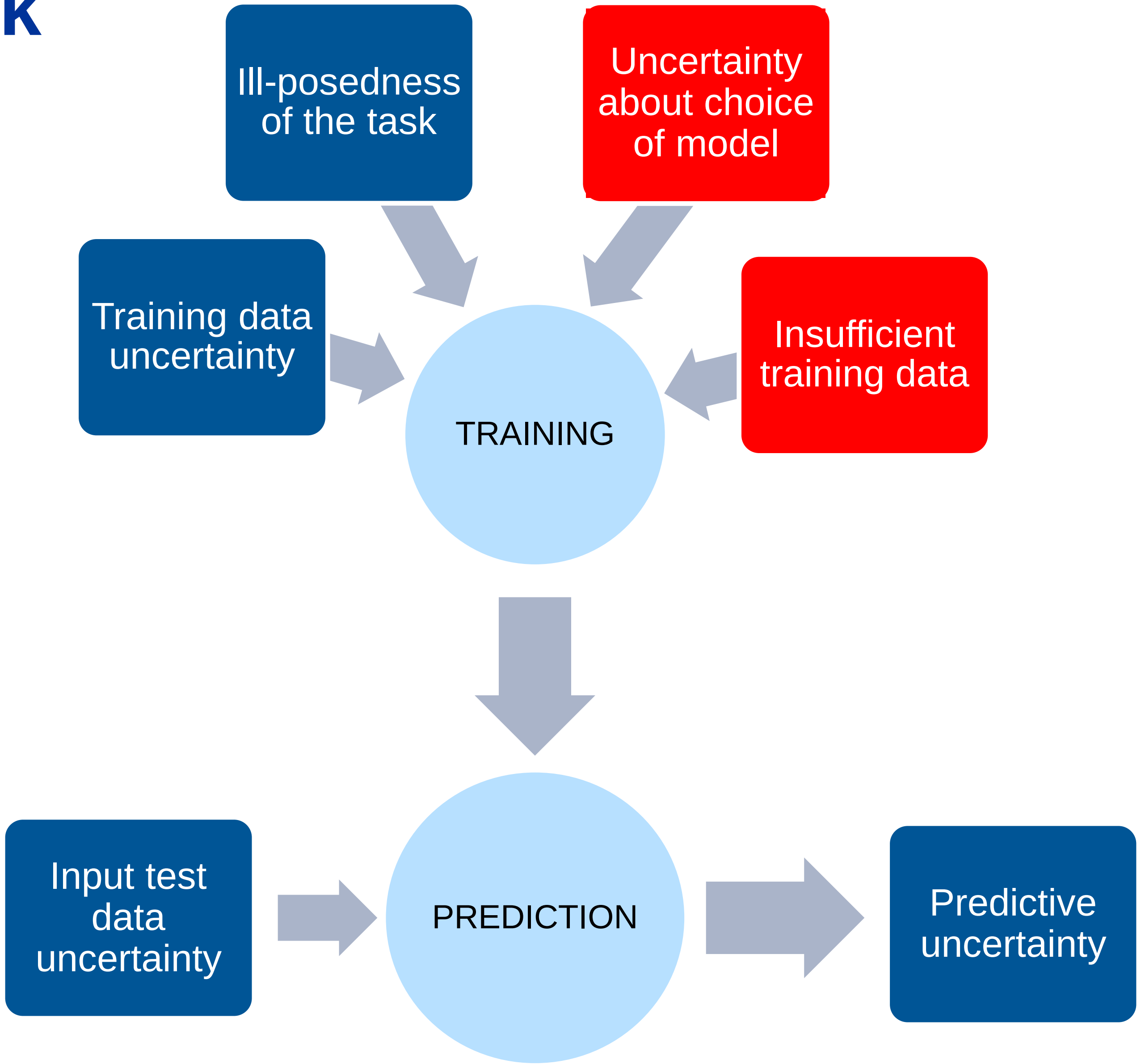

It is sources of uncertainty relating to the training of the model which take us beyond the GUM

Expression of predictive uncertainty

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- ML models are typically either **regression** (numeric output) or **classification** (categorical output).

- For **regression** models, A GUM approach to expressing uncertainty can essentially be used: standard errors, credible/confidence intervals, etc.

- For **classification**, it is less straightforward:
  - What is the measurand?
    - The class assignment (uncertainty is probabilities, entropy)
    - The class probabilities (a regression approach can be taken)
  - A metrology framework is needed for the expression of uncertainty for classification problems, and ML models in particular.

Uncertainty propagation through fixed ML regression models

- **Analytical approach**
  - Linear models
    - Input distribution → Output distribution
    - Input moments → Output moments
  - Kernel-based models
    - Input distribution → Output moments

    Analytical Results for Uncertainty Propagation through Trained Machine Learning Regression Models (AT, 2023, under review).

- **Monte Carlo sampling approach**
  - Can be used with all ML regression models

Uncertainty-aware regression using classical statistical modelling

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- Analytical approaches exist for linear and kernel-based models
  - ✓ Ordinary least squares, ridge regression
  - χ Sparse linear regression (requires a numerical approach)
  - ✓ Gaussian Processes
  - χ Support vector machines
- They tend to assume simplistic i.i.d. Gaussian noise models
- Extensions are needed to take input data uncertainties into account:
  - Errors-in-variables for linear models
  - Input-uncertainty aware GPs *(Quinonera-Candela et al., 2003)*
  - Monte Carlo sampling and variance decomposition

Uncertainty-aware regression using modern ML models

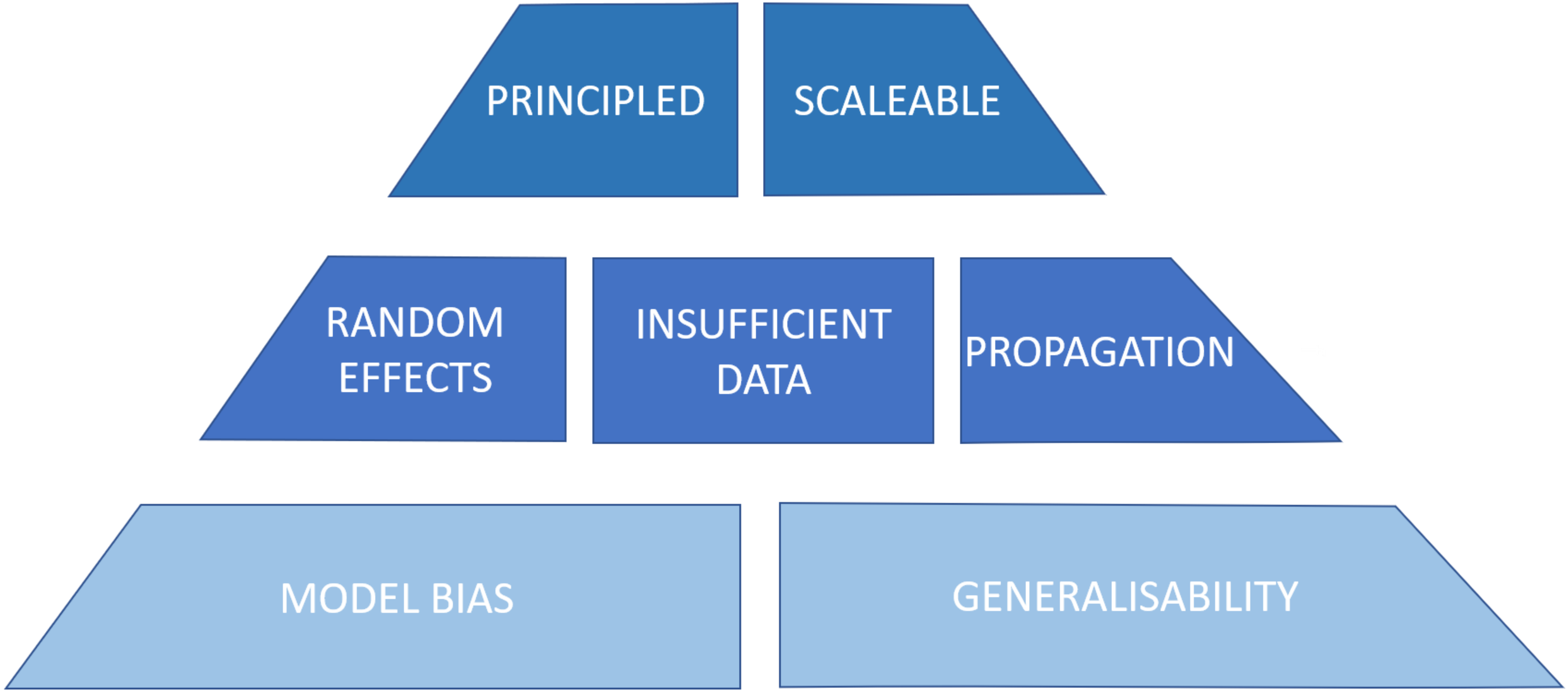
- Most notably **neural networks** and **tree-based models**…
- Techniques from the ML community need to be used.
- These methods involve changing the way ML models are trained – and so require all the computational skills associated with ML model development.
- Examples for **neural networks**: Deep Ensembles, Monte Carlo Dropout.
- Examples for **tree-based models**: Jackknife-after-Bootstrap, Quantile Regression Forests.

Uncertainty-aware regression using modern ML models: considerations

- These methods do not take into account uncertainty about the choice of model → **empirical model validation** good practice from the ML community are important.

- These methods often sacrifice mathematical rigour for the sake of scaleability…
  - → It is important that metrologists **understand** the assumptions/approximations made.
  - → **Empirical validation of uncertainties** using techniques from the ML community (e.g. calibration analysis) is important.
  - → It is possible to combine with frequentist **recalibration** techniques.

A metrology framework for uncertainty-aware ML regression models



Uncertainty evaluation for machine learning, AT et al., 2021, NPL Report MS 34

Uncertainty evaluation for ML classification

- Classification problems are usually significantly ill-posed → we should focus on **probabilistic** classification approaches in metrology.
- Developments in the ML community have focused on neural networks.
- Neural networks for classification typically have a final *softmax* layer which outputs probabilities.
- These probabilities are often poorly calibrated.
- Methods for regression can also be used to explore the effect of aleatoric and epistemic uncertainty on the probabilities and their uncertainties.

Calibration of classifiers

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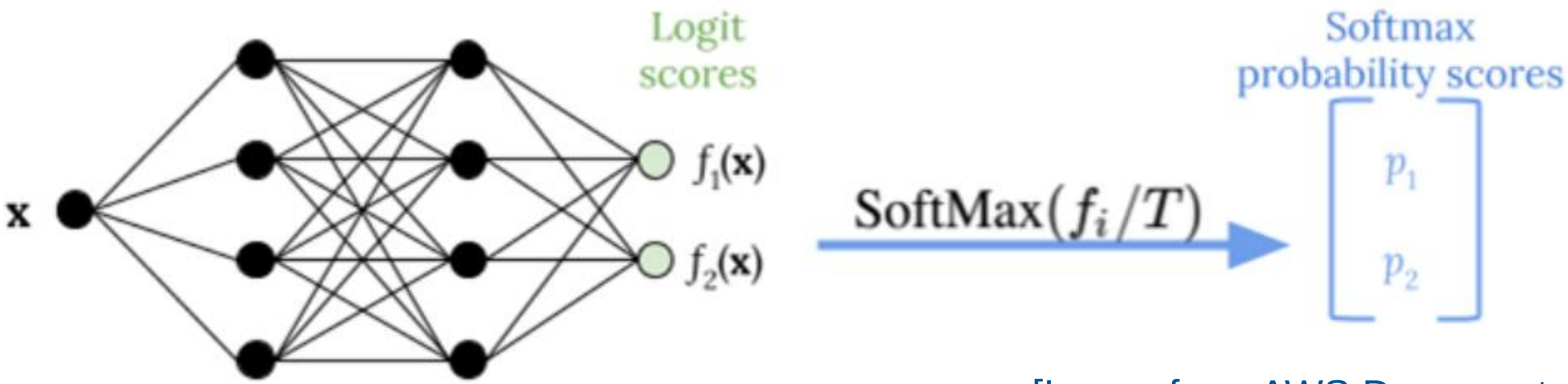
- Deep classifiers typically output ‘scores’ which are interpreted as probabilities.
- But these probabilities cannot necessarily be trusted…
- **Well-calibrated**: *“If an image is assigned a 60% probability of being in a certain class, then it should actually be in that class 60% of the time.”*
- There are various post-hoc techniques for improving calibration, such as temperature scaling.



[Image from AWS Documentation]

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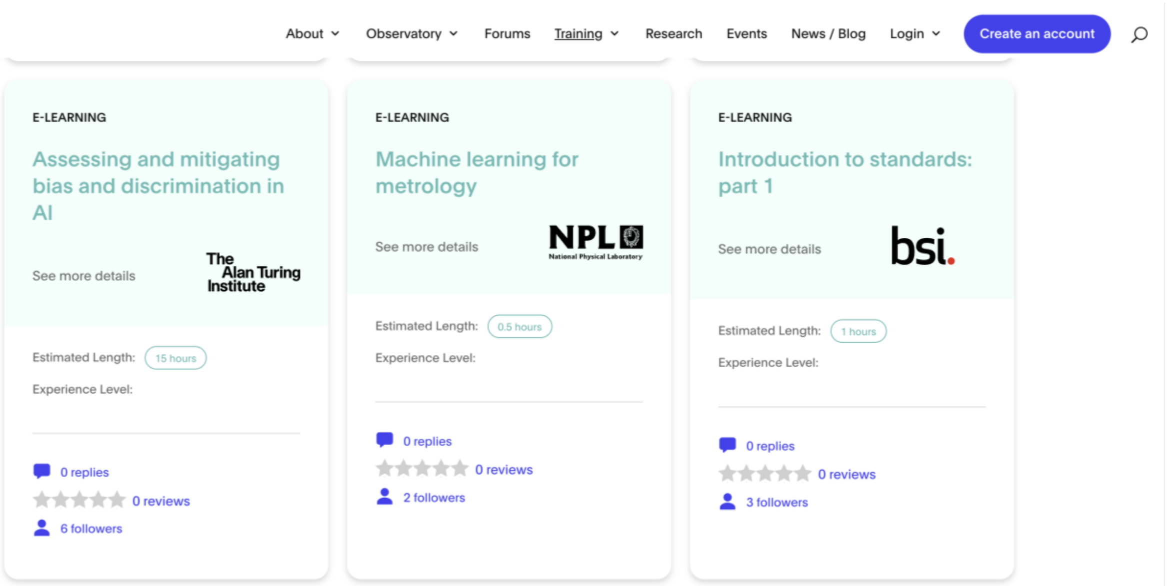
Training for the wider community

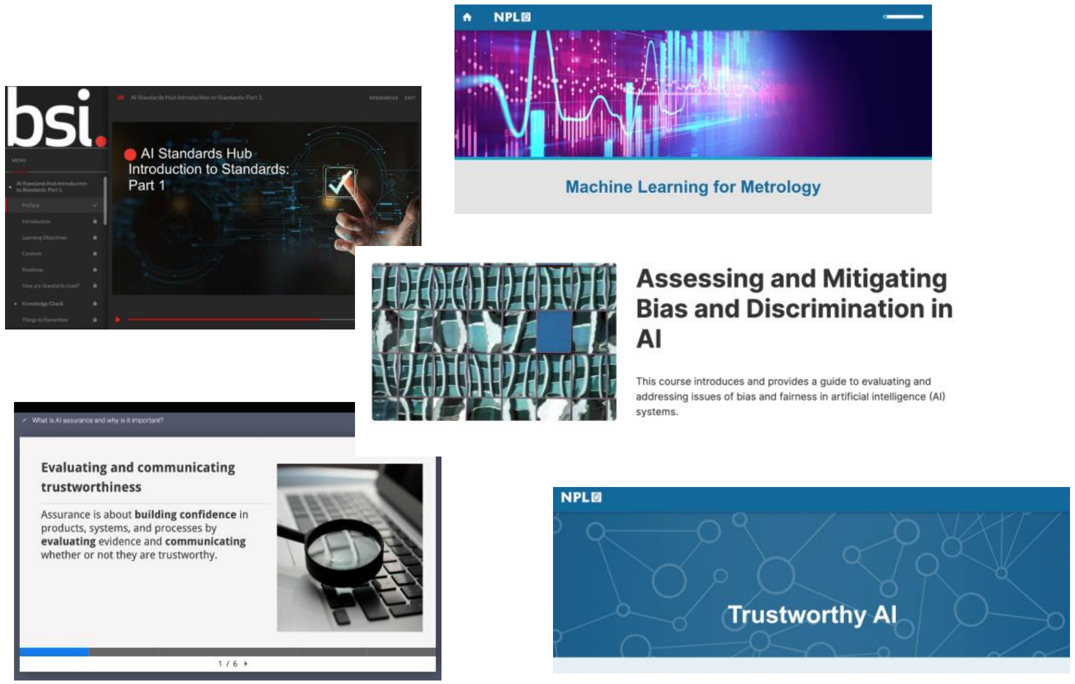
AI STANDARDS HUB

The Hub's online training offering

Course catalogue



e-learning platform



ML training courses produced by NPL

E-LEARNING

Machine learning for metrology

See more details

Estimated Length: 0.5 hours

Experience Level:

0 replies

0 reviews

2 followers

Introduction to trustworthy AI

See more details

Estimated Length: 1 hours

Experience Level:

2 replies

0 reviews

8 followers

Conclusions

Conclusions – training needs

Dissemination of knowledge and skills originating from the ML community:

- Theory background and computational skills for modern machine learning approaches
- The aleatoric/epistemic framework
- Knowledge and know-how relating to the implementation of state-of-the-art uncertainty evaluation methods

→ Use of external training courses produced by the ML community

→ Knowledge sharing across NMIs as part of EPM projects etc.

Conclusions – training needs

Development and dissemination of metrologically-specific good practice:

- Agreed vocabulary and framework for sources of uncertainty and expressions of uncertainty in both regression and classification
- Agreed good practice on uncertainty evaluation for metrology when using modern machine learning approaches (e.g. neural networks and tree-based methods):
  - choice of method
  - implementation of methods
  - validation of methods

→ This should be developed partly through collaborative projects, e.g. QUMPHY

→ Vehicles are needed for (within MATHMET?)

  - bringing together good practice
  - disseminating this good practice

Eventual dissemination to the wider community through standards etc.

Thank you for your attention!

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