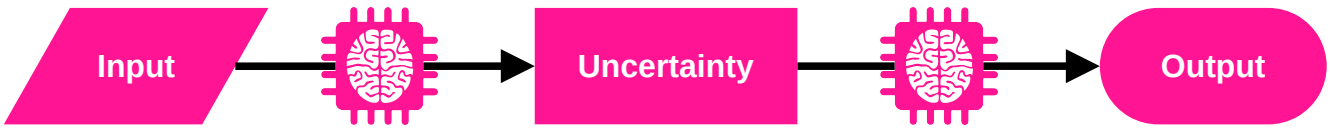
Understanding the unexpected: exposing information hidden in noise

Bogdan Zviazhynski & Gareth Conduit bz267@cam.ac.uk

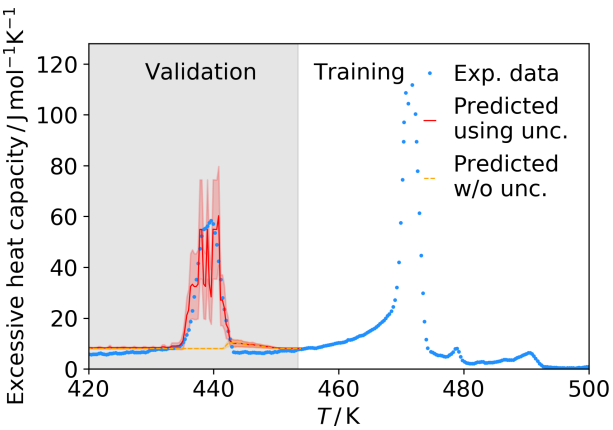
We present a machine learning architecture that computes uncertainty in one target variable to extrapolate a second target variable. We exploit this architecture to predict phase transitions in a $PbZr_{0.7}Sn_{0.3}O_3$ ferroelectric and a 10OBA liquid crystal.

The methodology is shown below. The two machine learning models are depicted by the brain embedded in the microchip.

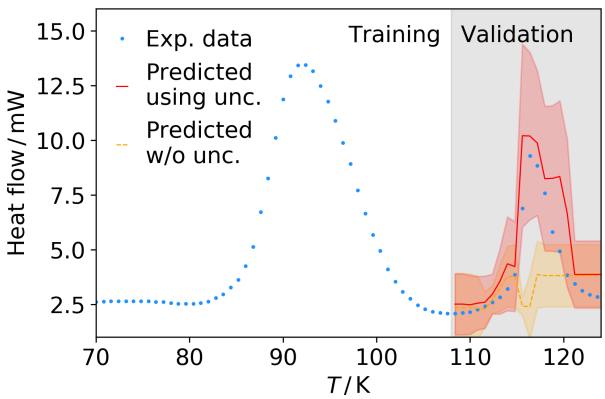


Results

$PbZr_{0.7}Sn_{0.3}O_3$ ferroelectric [1]
Uncertainty in dielectric constant
Predicts heat capacity



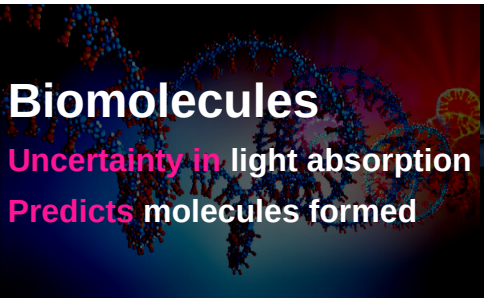
10OBA liquid crystal [2]
Uncertainty in texture contrast
Predicts heat flow

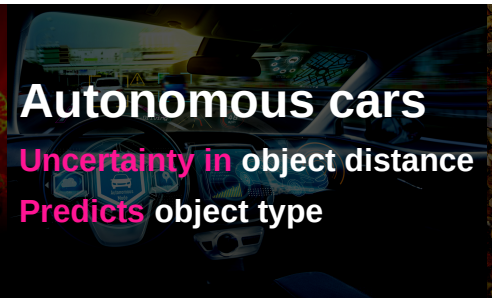


In both cases, the peak inside the grey shaded area corresponds to a phase transition that was discovered by machine learning.

Future opportunities

The methodology can be applied to a broad range of areas including:





[1] J. Therm. Anal. Calorim. 128, 713-719 (2017)
[2] Advances in Condensed Matter Physics 2012, 527065 (2012)