digiLab

When Uncertainty Matters.

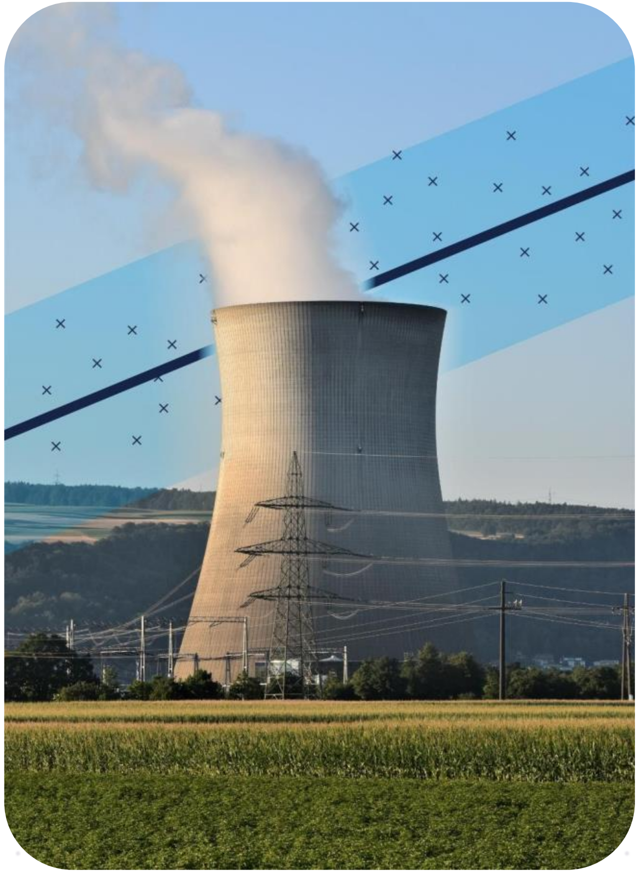
Leveraging Uncertainty Quantification in Complex Environments

- Who are digiLab?
- Our core methods
- Applications in complex environments

Artificial Intelligence When Uncertainty Matters

Many industries have been slow to uptake the benefits of AI, due to a lack of trust needed for important decision making.

However, not all AI methods are untrustworthy - trust can be built through **verification**, **validation**, and **uncertainty quantification** (UQ)



We help people solve the world's biggest challenges with human-in-the-loop AI designed to augment decision making.

- Environment
- Renewables
- Fusion Energy
- Materials
- Aviation & Transport
- Nuclear (Fission)

Born at The University of Exeter

Founded on pioneering high impact research by the UK's leading specialists in uncertainty quantification and explainable AI.

37 Team Members	35% PhDs	100+ peer review papers
8 R&D Team, 11 Product Team	Inhouse Fusion Expert Team	Exeter HQ

Leading companies, Government organisations and Research institutions trust digiLab.

AIRBUS

NATS

UK Atomic Energy Authority

EDF

Jacobs

South West Water

Ofwat

KAUST

YorkshireWater

ARCADIS

UKRI Innovate UK

HENRY ROYCE INSTITUTE

MANCHESTER 1824 The University of Manchester

PSFC MIT Plasma Science & Fusion Center

ROLLS ROYCE

NHS

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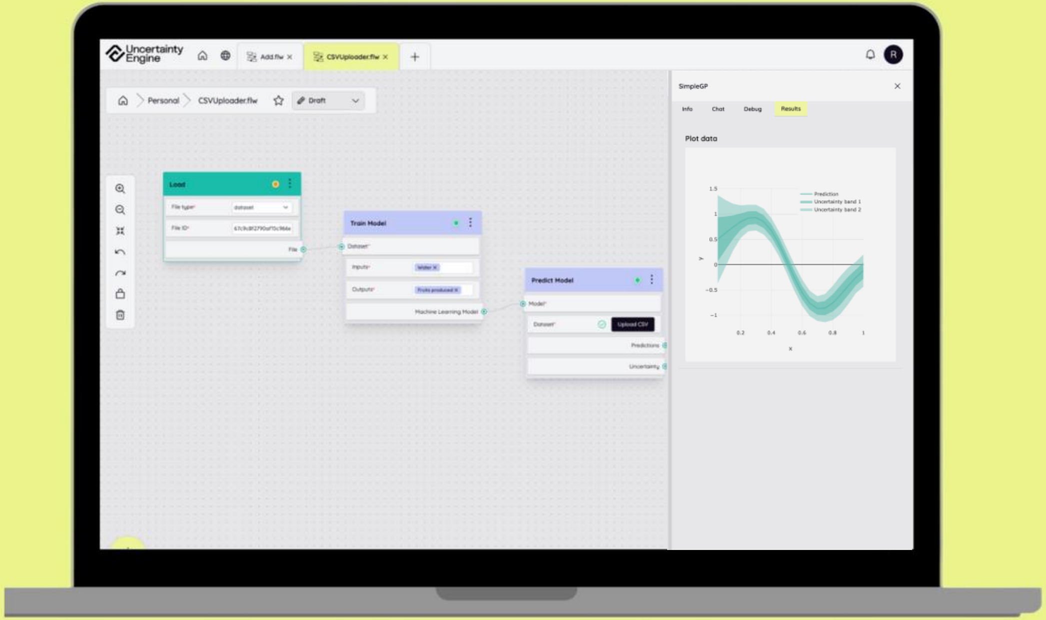
The Uncertainty Engine™



The Machine Learning Platform for Managing Uncertainties:

- No-code agentic AI platform back by uncertainty quantification
- Lower the entry barrier to machine learning
- Get instant access to world-leading data-science workflows
- Get answers from your simulations and experiments, faster
- Secure and auditable platform
- Augment your existing workflows while still applying your domain expertise

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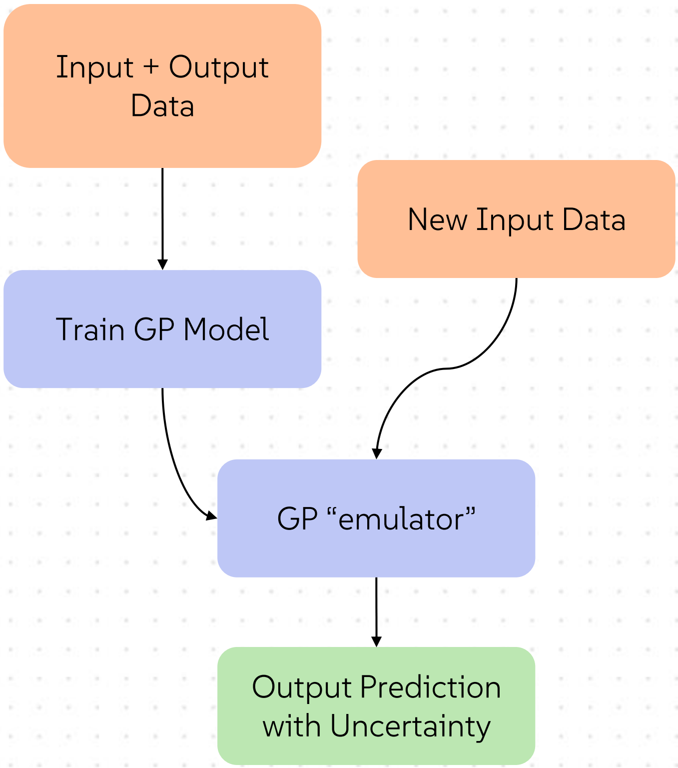
What are Gaussian Processes?

- Gaussian Processes (GPs) are a probabilistic machine learning technique at the core of the Uncertainty Engine.
- GPs model data by sampling likely functions that could fit the data.
- GPs emulate input-output relationships with inherent uncertainty quantification.



Why Gaussian Processes?

Inherent uncertainty quantification:

- Data uncertainty (aleatoric)
- Model uncertainty (epistemic)

Explainable:

- Learn characteristic length scales, amplitudes…

Fast:

- Predictions for trained models typically sub-millisecond

Emulation

Example: Control of Water Treatment

What?

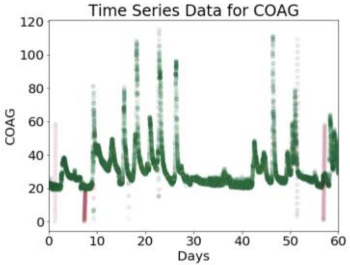
- Sensors used to predict optimal coagulant dosage
- Novel, Zeta potential sensors greatly improve water treatment but are costly

How?

- Gaussian Processes trained to predict Zeta potential sensor data from cheaper sensors

Impact

- Trained emulator gave real-time predictive dosing strategy with uncertainty
- 40% less coagulant and improved water quality.
- Saved approximately £100,000 per annum in coagulant OpEx.

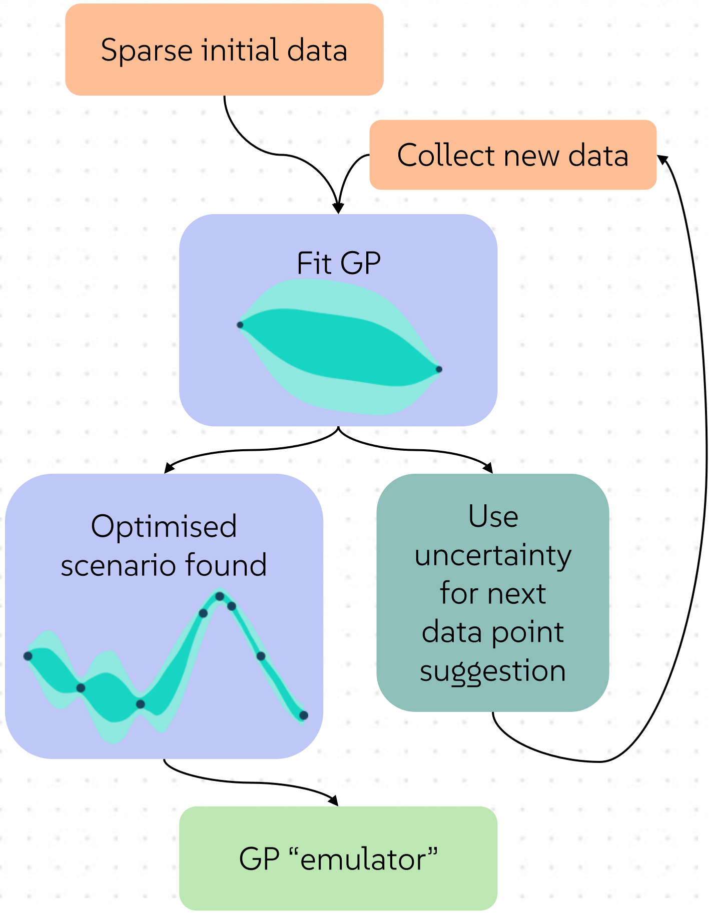


Utilising UQ: Active Learning

Optimization with Limited Data

- Bayesian Optimization:
  - Efficient parameter space exploration
  - Typically 4 times fewer evaluations required

- At digiLab our optimisation:
  - Utilises inherent Uncertainty Quantification (UQ)
  - Is accelerated with efficient-TuRBO (shown to beat particle swarm optimisation)
  - Results in an emulator which is explainable and auditable



Active Learning

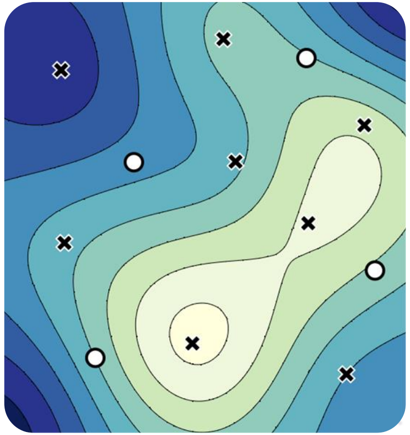
Example: Nuclear Decommissioning

What?

- Current nuclear decommissioning software uses frequentist statistics: slow, costly, ignores prior contamination knowledge.

How?

- Bayesian methods incorporating industry expertise and active learning significantly reduce sampling requirements without compromising safety.



Impact

- Saved partners over £100,000 on a nuclear decommissioning project through efficient, safe sampling.

Active Learning

Outlook: predictive maintenance

Why?

- Identify optimal maintenance tasks and timing through uncertainty quantification
- Effectively handles sparse and incomplete data
- Leverages prior expert knowledge
- Efficiently explores critical areas for early detection of potential damage

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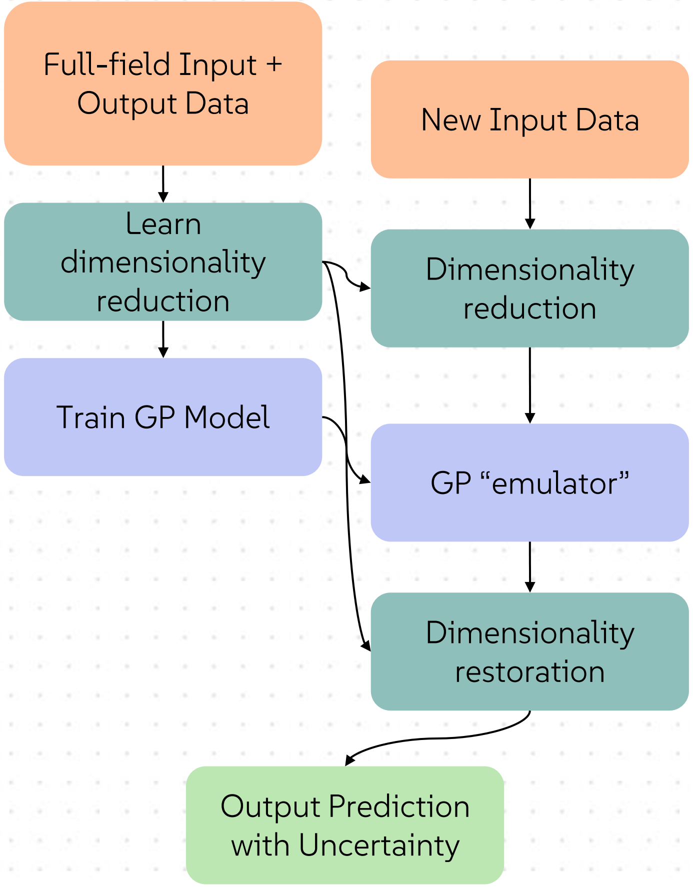
SimAI

Emulators for high-fidelity simulations

- Simulations, including CFD and FEM are often expensive
- Learning patterns to allow emulation highly attractive
- However, brings risk when uncertainties aren’t appreciated

- At digiLab:
  - Transform and condense fields into latent space
  - Advanced algorithms for fitting multi-modal, multi-objective problems
  - Full field emulation with uncertainty

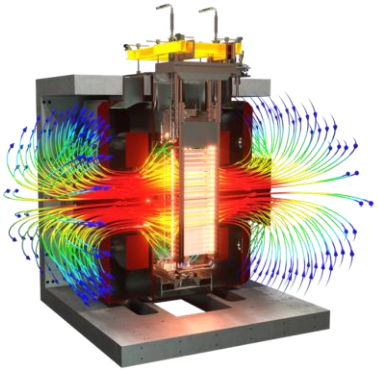


Full-field Emulation

Example: CHIMERA FEM Emulation

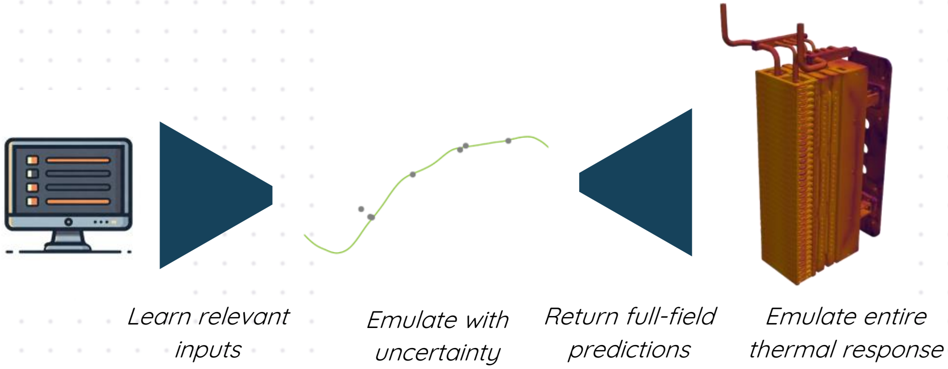
What?

- Wider aim: a digital twin of a thermomechanical system (CHIMERA)
- Subsystem: thermal response to different inputs



How?

- Automated learning and emulation of full thermal field
- FMU: export for use in external system



Full-field Emulation

Outlook: CFD Emulation

Why?

- Bypass expensive simulations in wider system
- Identify largest sources of uncertainty
- Accelerate design choices

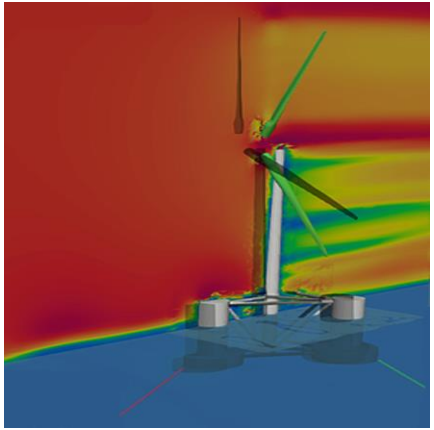


Image from CENER:

cenerFOAM based on OpenFOAM

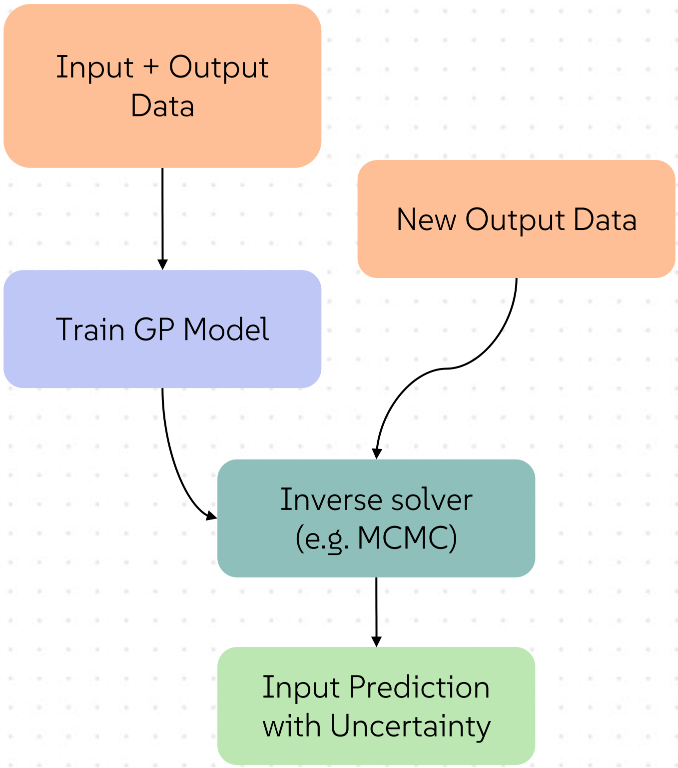
See other talks from the experts!

Inverse Problems

"Given this data, what inputs could have produced it?"

- Often, inverse problems have no analytic solution or are ill-posed
- Markov Chain Monte Carlo (MCMC) explores what inputs are likely, guided by Bayesian inference
- Provides uncertainty quantification

- With GP trained emulators:
    - Efficient exploration



Inverse Problems

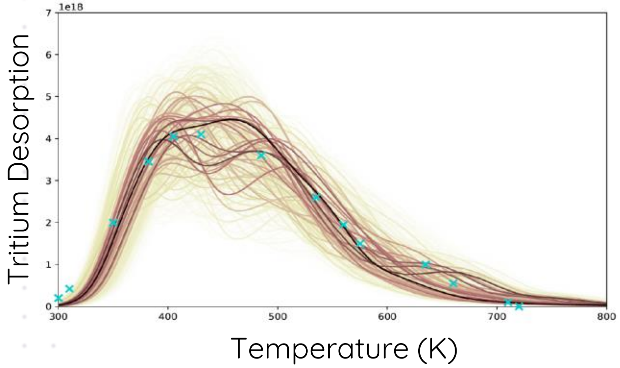
Example: Tritium Transport

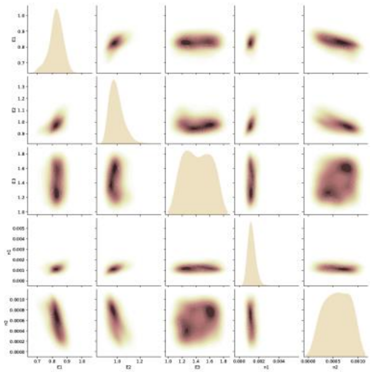
What?

- Emulate expensive tritium desorption simulations for use in tritium transport code
- Tritium desorption spectra are functions of temperature
- These functions depend on key, physical trapping parameters

How?

- Predict full tritium desorption functions for a given set of trapping parameters
- Utilise surrogate models for inverse relationships: given a specific tritium desorption spectra, what were the likely physical trapping parameters?





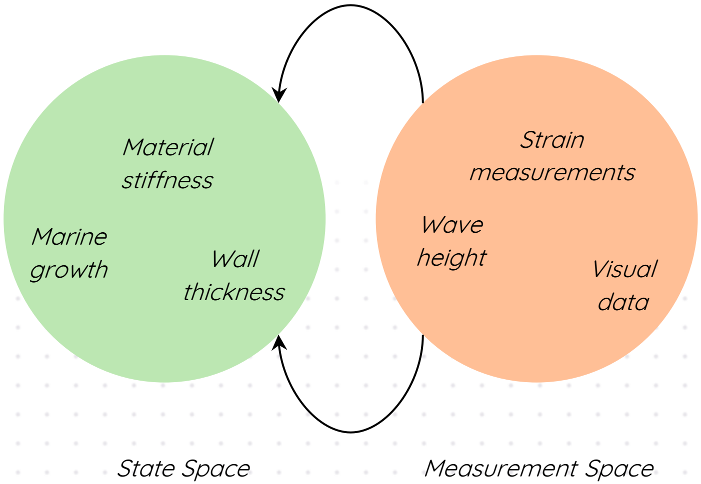
Likelihood of trapping parameters for given measurements from a tritium desorption spectra

Inverse Problems

Outlook: Material properties under corrosion

Why?

- Combine multiple, heterogeneous diagnostics
- Learn complex relationships, aiding simulation <> experimental comparison
- Infer parameter uncertainty -> inform risk reduction strategies

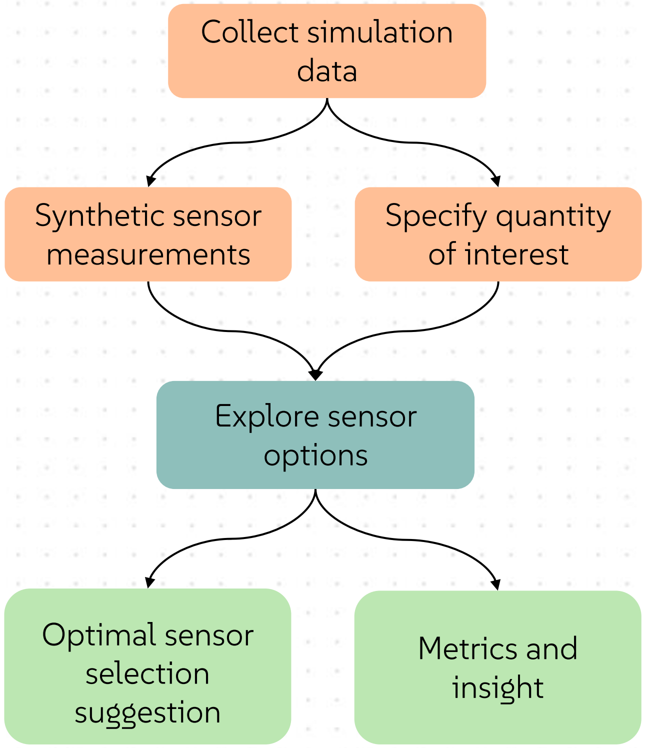


Optimal Sensor Placement

Bayesian Experimental Design

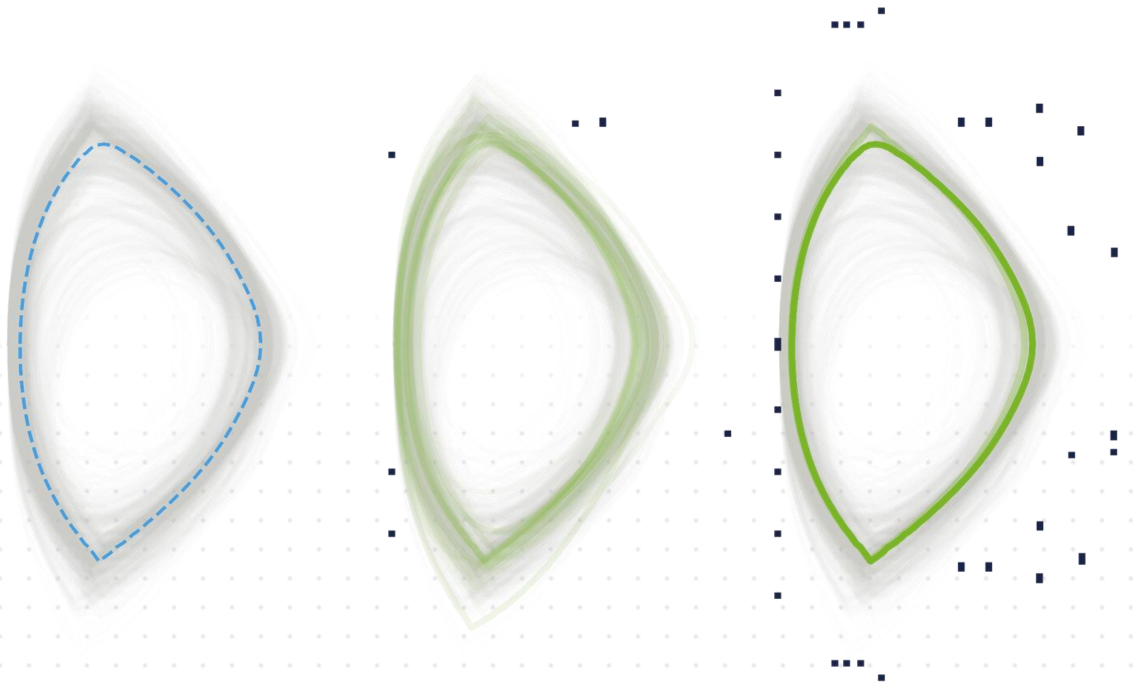
- Bayesian Experimental Design:
  - A generic framework for minimising uncertainty in crucial quantities
  - Rigorous statistical method for optimal asset/sensor placement
  - Can combine different diagnostics

- At digiLab our modern Bayesian experimental design:
  - Has inherent Uncertainty Quantification (UQ)
  - Utilises advanced algorithms to tackle large problems
  - Allows users to specify quantities of interest



Bayesian Experimental Design

A good **sensing system** is one which can, on average, **distinguish** between different events of interest.

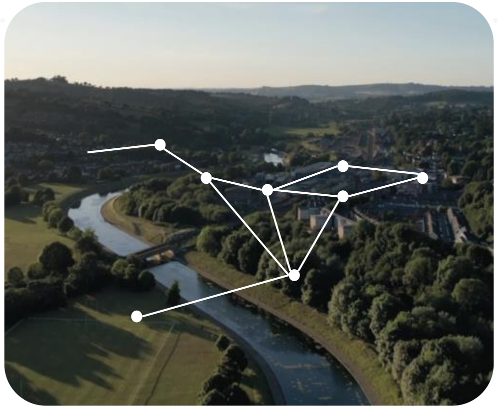


Optimising Sensor Placement

Example: Water Network

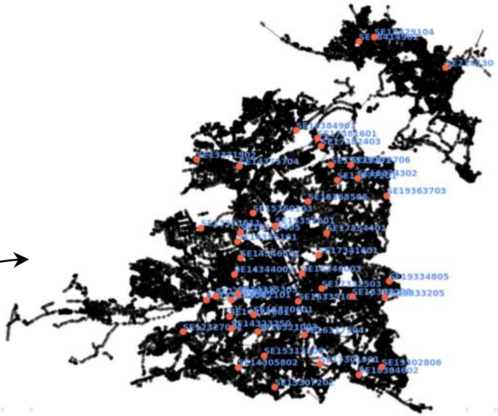
What?

- Water networks struggle with monitoring
- Automate sensor placement for complex networks



How?

- Data collection: historical data -> probabilistic maps of events, such as flooding or pollution
- Advanced optimization algorithms asking: which sensor combination expected to gain the most information?
- Recommended dozens of flow sensor placement to utilities companies



Optimal Sensor Placement

Outlook: Combining Measurements

Why?

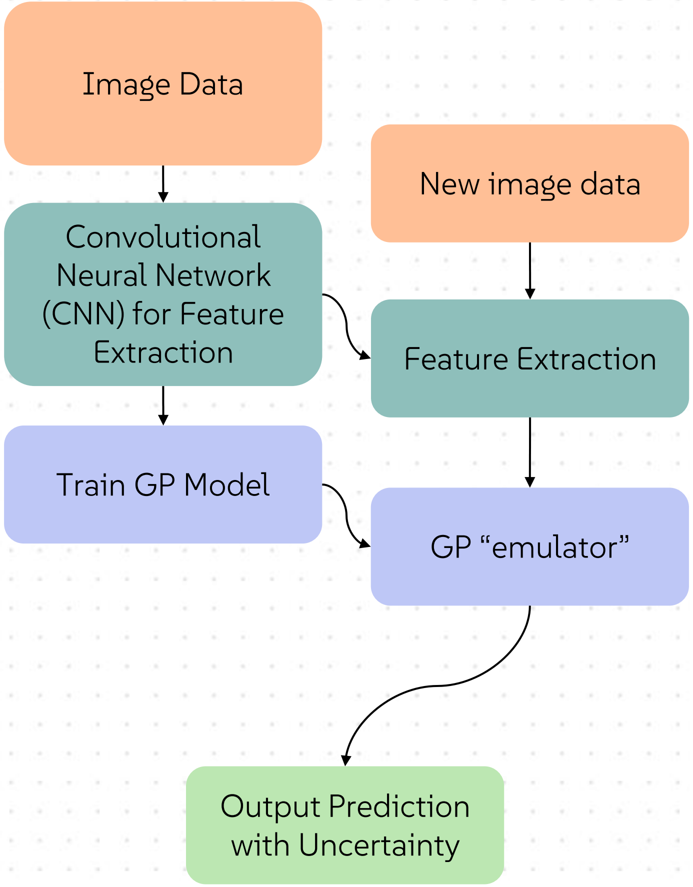
- Generic framework: combine multiple, heterogeneous diagnostics
- Specify quantities of interest to target uncertainty reduction
- Infer parameter uncertainty -> inform risk reduction strategies
- Consider redundancy and diagnostic damage

Full credit/image rights: bachmann.

Computer Vision

Bayesian Experimental Design

- Why?
  - Modelling for resource mapping
  - Automated monitoring,
  - Defect detection
  - Performance optimization
- How?
  - Model with uncertainty
  - Rapid model calling and aggregating



Computer Vision

Example: twinCity Solar

What?

- Rooftop energy capacity information
- Light Detection and Ranging, LiDAR, used to create a 3d map of points

How?

- Deep Convolutional Neural Networks extract rooftops
- Bayesian approach to find roof segments and angles with uncertainty
- Interactive map generated for interrogation and communication

Computer Vision

Outlook: Imaging Diagnostics

Why?

- Image diagnostics hold substantial information and can operate remotely
- Harness this information with uncertainty
- Rapid modelling allows use in other workflows (e.g. sensor placement, active learning...)

Leveraging Uncertainty Quantification in Complex Environments

- Summarised digiLab core methods for leveraging UQ
- Considered how they can be applied to WSI community
- I'd be very interested to hear your thoughts and questions!

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