Multi-objective Bayesian optimisation for design of Pareto-optimal current drive profiles in STEP

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Introduction

JETTO is a high-fidelity plasma modelling code that solves coupled core transport and equilibrium equations[1].
It is used to **evaluate plasma scenarios** as part of the STEP design process[2].
JETTO is initialised with the parameters of a candidate design, and the simulation is run until the plasma reaches a steady state.
The steady-state properties of the plasma are used to assess the **impact of design choices** and the **suitability** of a given design.

However, JETTO takes **several hours** to run, which severely limits the extent to which the design space can be explored.

We demonstrate **multi-objective Bayesian optimisation**, a method for design optimisation that delivers **higher-quality solutions** in significantly **fewer iterations** than previous methods used in STEP, using techniques from **machine learning** and **surrogate modelling**. Our approach also offers **improved interpretability**, allowing design engineers to **quantify the tradeoffs** between different objectives.

Our example application is the optimisation of electron cyclotron resonance heating profiles to achieve desirable safety factor properties.

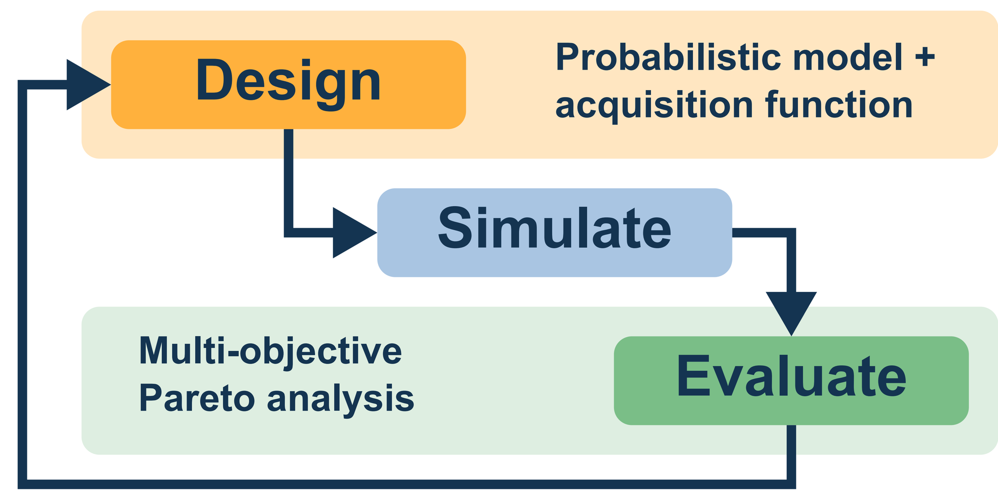

Figure 1: Overview

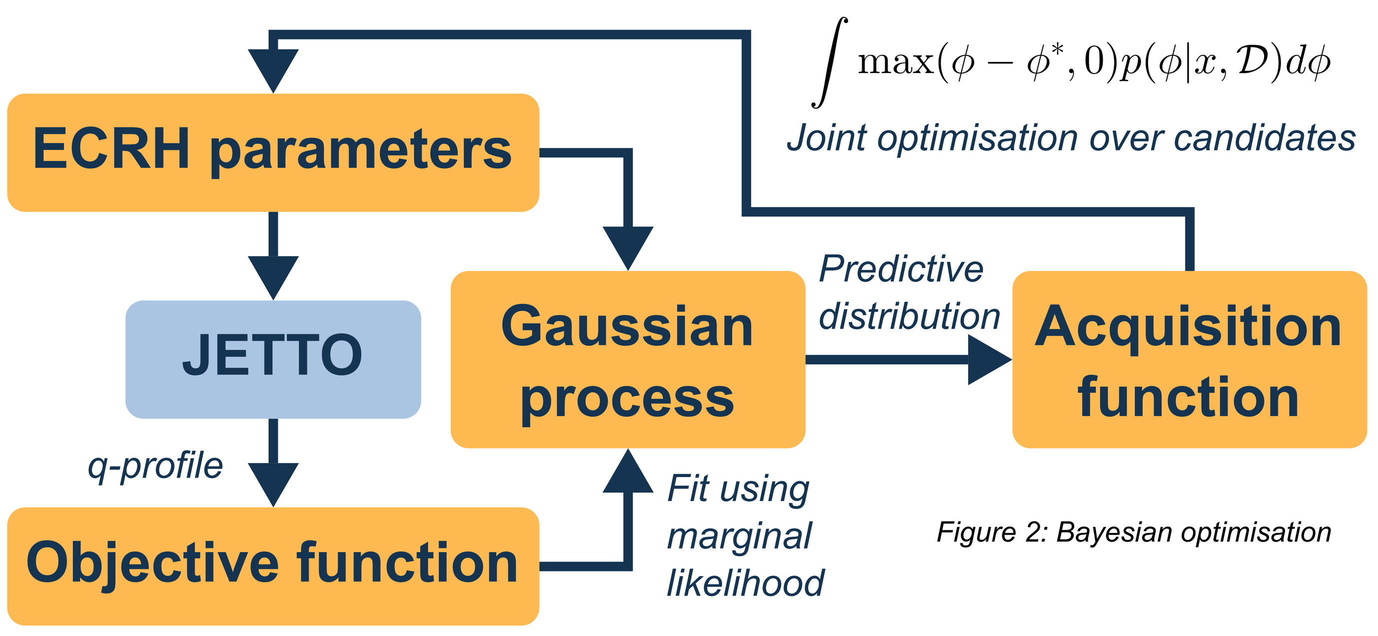

Figure 2: Bayesian optimisation

What is Bayesian optimisation?

Bayesian optimisation is built upon a **probabilistic model**, such as a **Gaussian Process** (GP).
The model is fit to the **previous observations** (inputs and objective values).
It is used to generate **predictions** about the **performance of unseen points**.
An inner optimisation loop uses the predictions to find the **most promising** points to try next.

This method:
- a) **reduces** the number of runs '**wasted**' on trying suboptimal points
- b) ensures that all the **information** gained at each step is **propagated** to future steps

As a result, BO gives **vastly improved performance** compared to stochastic search methods[2].

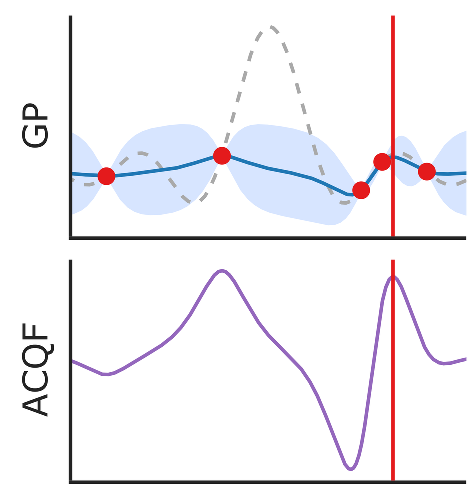

Figure 3: Using a GP model to select next candidates

What is Pareto optimality?

Single-objective optimisation tasks involve finding **one solution** that maximises a **scalar objective**.
Comparing solutions is easy, as each solution is either better or worse than the others.

In **multi-objective** settings, there is normally no solution that simultaneously maximises every objective.
Instead, we seek to find a **set of solutions** that represent the **tradeoffs** between each objective.
The set is made up of all points that are **Pareto optimal**.

A point is Pareto optimal if it is impossible to improve its performance under one objective without reducing its performance under another objective.

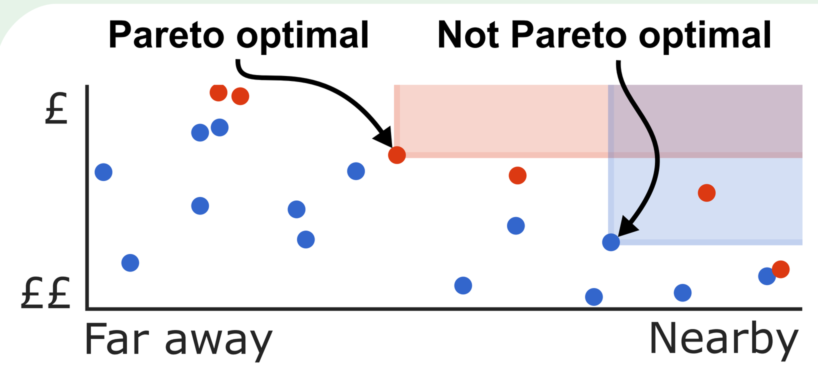

Figure 4: Pareto optimality criterion

Target metrics for safety factor profile[2,3,4]

Property	Rationale	Formulation
Minimise shear at centre	Improve β	$q(0) - \min q \qquad \arg\min_{\rho} q$
Minimum q above 2	Avoid NTMs	$\lVert \min q - (2 + \epsilon) \rVert$
Monotonic *q*	Improve stability	$\int_0^1 q\, \mathbf{1}\left(\frac{dq}{d\rho} \leq 0\right) d\rho$
Monotonic gradient of *q*	Reduce fast ion losses	$\int_0^1 \frac{dq}{d\rho}\, \mathbf{1}\left(\frac{d^2q}{d\rho^2} \leq 0\right) d\rho$
High shear at integer *q*	Mitigate NTMs	$q^{-1}(n),\ n \in \mathbb{N}$

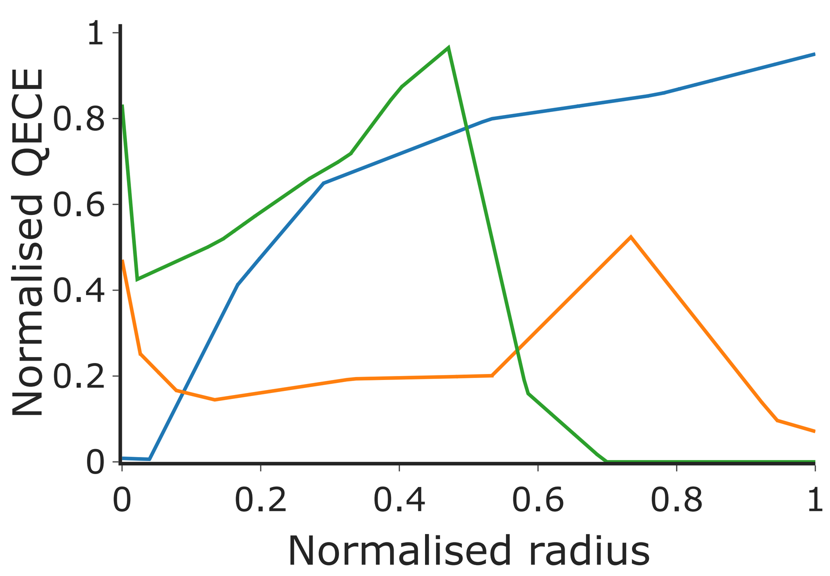

Figure 5: Example piecewise linear ECRH profiles

Parameterisation of ECRH profile

The choice of input parameterisation affects the **rate of convergence** and **quality of results**.
Ideally, the parameterisation would be **general**, so that every possible profile can be represented.
However, this can mean that the search space is **too large** to explore effectively.

Previously, the ECRH profile has been represented as a piecewise linear function[3] (Fig. 5), with manually tuned constraints on the parameters. We also experimented with using a **sum-of-Gaussians representation** (Fig. 6), where each Gaussian represents an EC beam launcher.

The SoG parameterisation produces smooth ECRH profiles, and leads to a simpler mapping from input space to objective space: **small changes in parameters result in small changes in objective value**. This ensures that the mapping can be well-represented by a GP model.

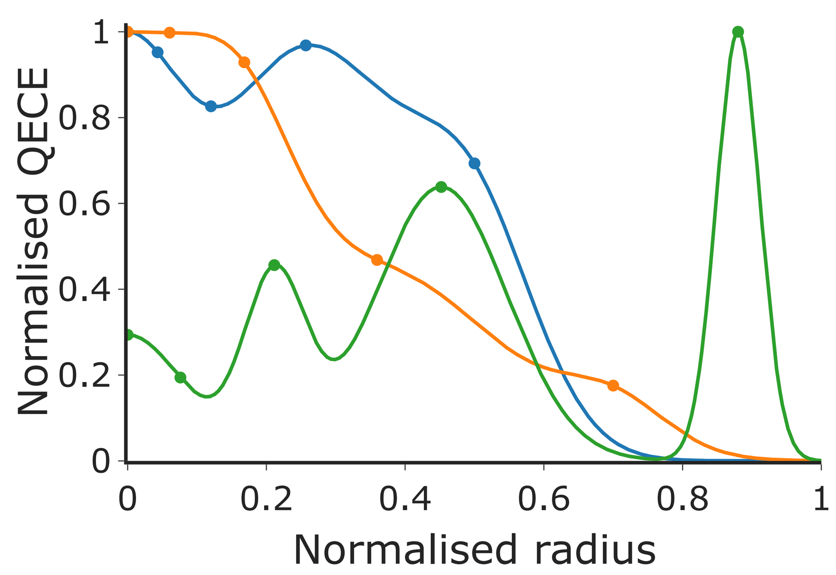

Figure 6: Example sum-of-Gaussians ECRH profiles

Results with piecewise linear ECRH

Running the multi-objective Bayesian optimisation loop using the piecewise linear ECRH function for 5 steps with 5 candidates at each step produces 8 Pareto optimal solutions.

The solutions are split into two groups: **monotonically decreasing ECRH** profiles (e.g. Solution 1) and **double-peaked ECRH** profiles (e.g. Solution 8). STEP designs currently use monotonically decreasing ECRH, as previous optimisation methods[1] failed to find good double-peaked solutions.

Results with sum-of-Gaussians ECRH

Running the multi-objective Bayesian optimisation loop using the sum-of-Gaussians ECRH function for 10 steps with 30 candidates at each step produces 8 Pareto optimal solutions. **More steps** are required because the parameterisation is **more general**.

The ECRH parameterisation we used has up to 4 Gaussians logarithmically-spaced in [0, 1].
Achieving the **monotonicity objectives** are much more challenging with this representation.

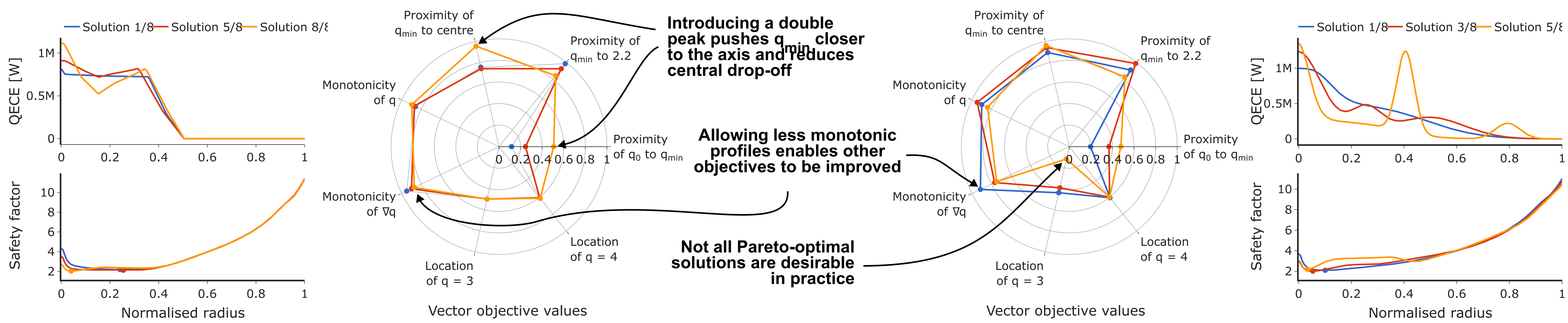

Figure 7: A selection of Pareto-optimal solutions generated by MOBO with piecewise linear ECRH (L) and sum-of-Gaussians ECRH (R)

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References:
[1] Romanelli et al. "JINTRAC: A System of Codes for Integrated Simulation of Tokamak Scenarios", Plasma and Fusion Research 9 (2014).
[2] Tholerus et al. "Flat-top plasma operational space of the STEP power plant", preprint at arxiv:2403.09460.
[3] Marsden et al. "Using Genetic Algorithms to Optimise Current Drive in STEP", 48th European Conference on Plasma Physics (2022).
[4] Menard et al. "Aspect Ratio Scaling of Ideal No-wall Stability Limits in High Bootstrap Fraction Tokamak Plasmas", Physics of Plasmas 11.2 (2004).

Future work
- Better objective and ECRH functions
- MOBO analysis of **ballooning stability**
- Trained models for **transfer learning**