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

Theodore Brown[1,2], Stephen Marsden[1], Francis Casson[1], Alexander Terenin[2] and Vignesh Gopakumar[1]

[1]United Kingdom Atomic Energy Authority, Oxford, UK OX14 3EB
[2]Department of Engineering, University of Cambridge, UK CB2 1PZ

UK Atomic Energy Authority

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.
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.
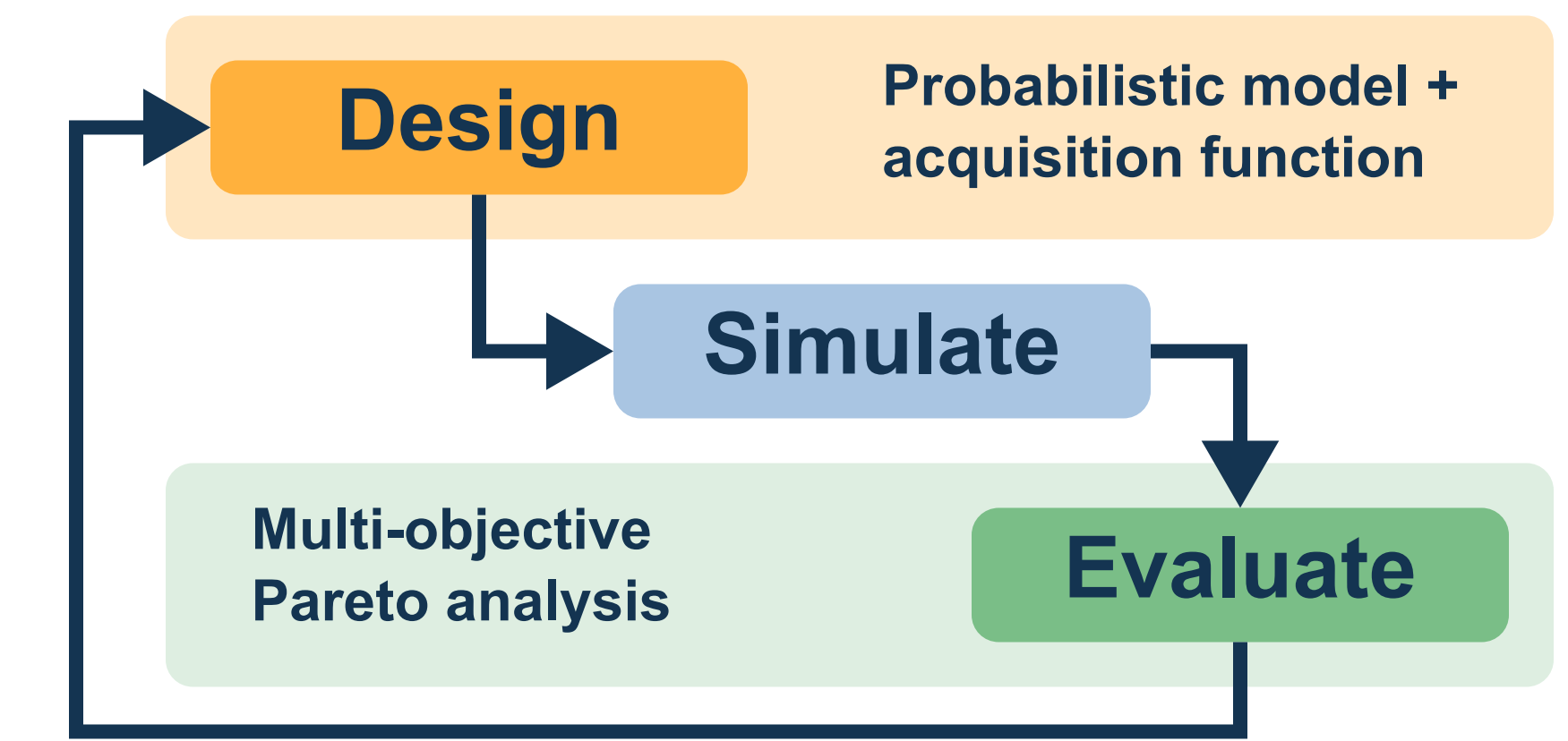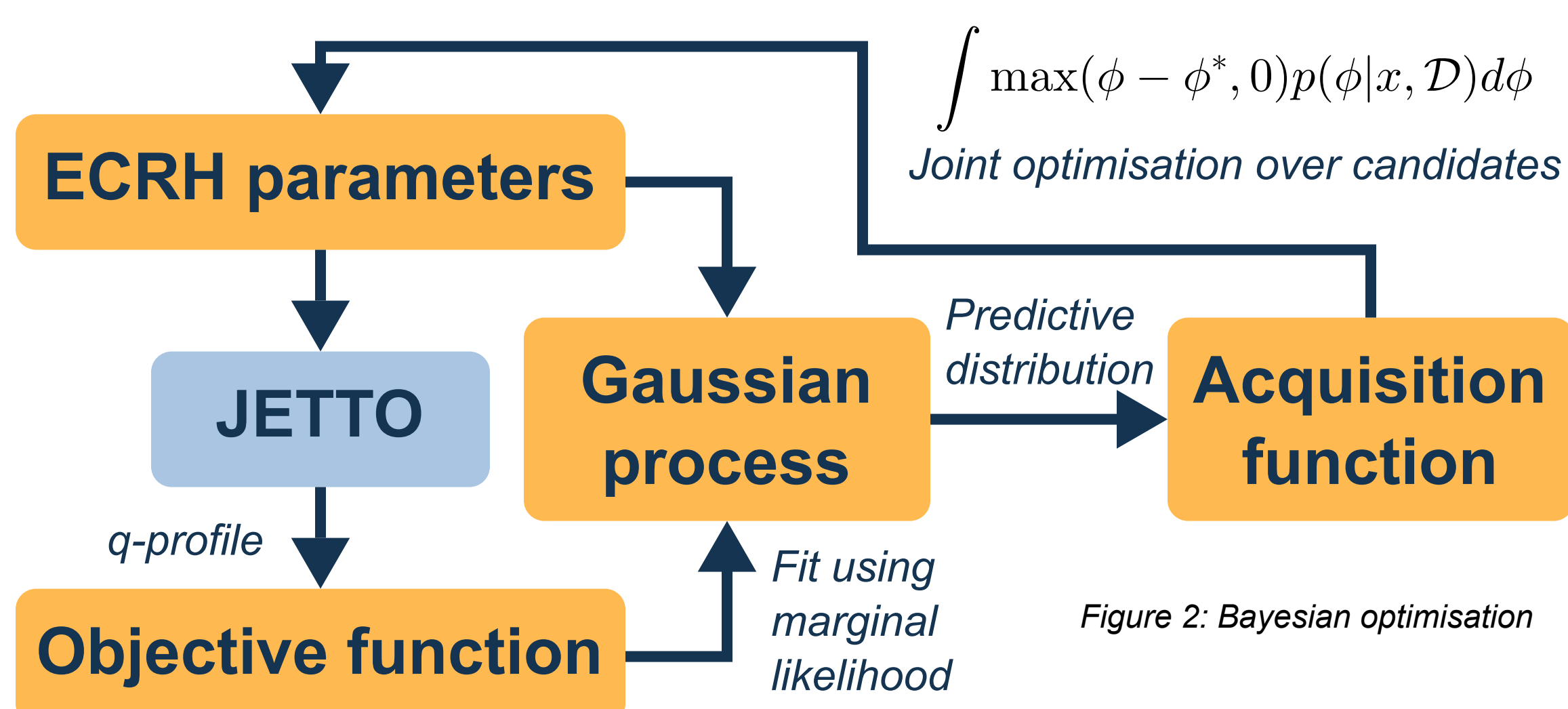
Figure 1: Overview

What is Bayesian optimisation?

$$\int \max(\phi - \phi^*, 0)p(\phi|x, \mathcal{D})d\phi$$
Joint optimisation over candidates

Figure 2: 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].
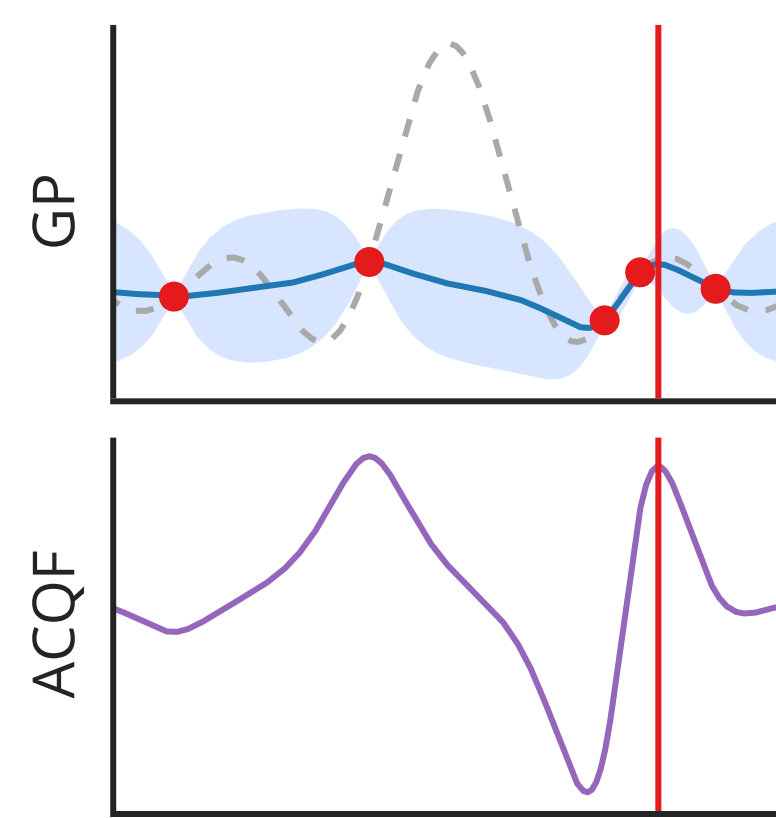
*Figure 3: Using a GP model to select next candidates*

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
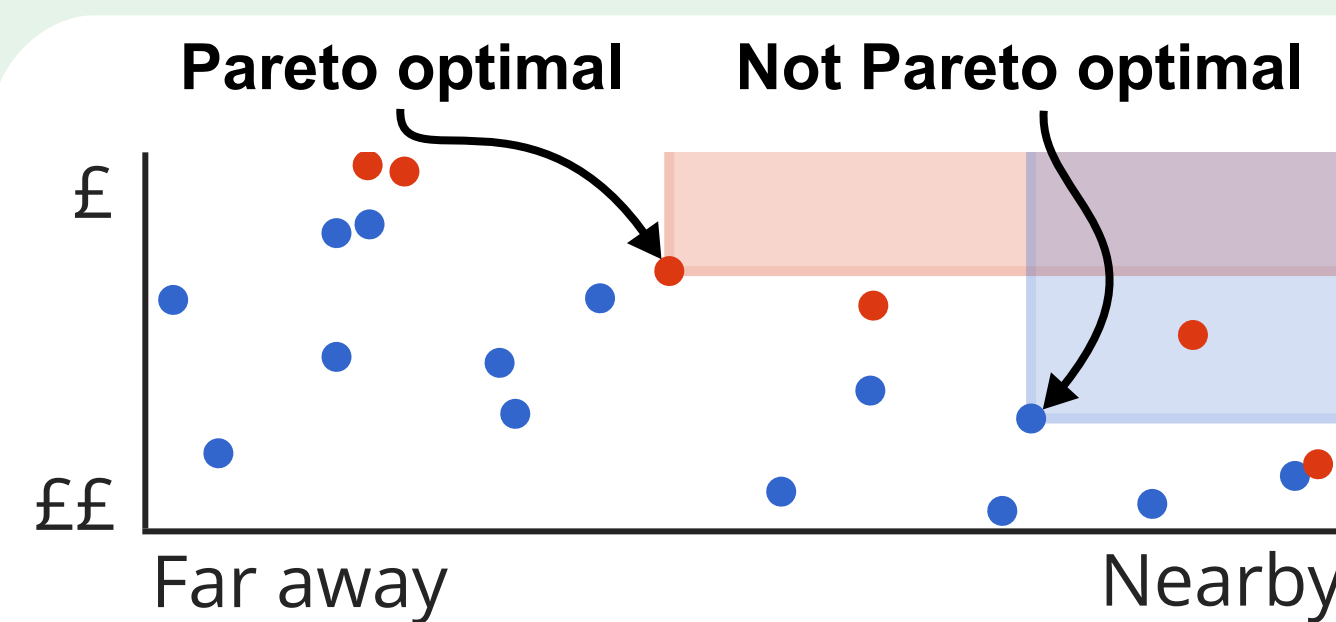
Target metrics for safety factor profile[2,3]

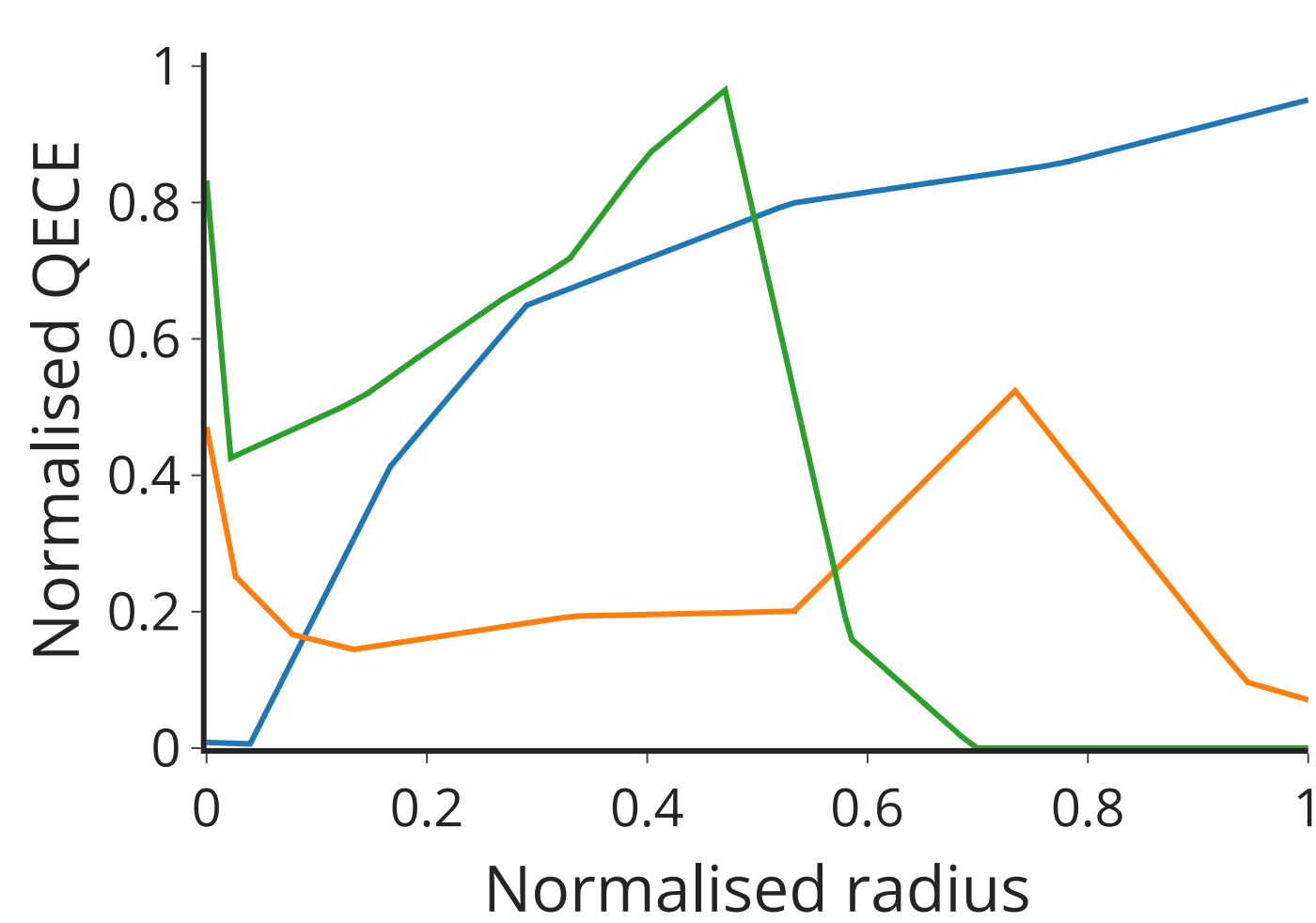| Property	Rationale	Formulation
Minimise shear at centre	Improve β	$q(0) - \min q$ $\quad \arg\min_{\rho} q$
Minimum q above 2	Avoid NTMs	$\| \min q - (2 + \epsilon) \|$
Monotonic q	Improve stability	$\int_0^1 q\, \mathbf{1}\left(\frac{dq}{d\rho} \leq 0\right)d\rho$
Monotonic gradient of q	Reduce fast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

Parameterisation of ECRH profile

Figure 5: Example piecewise linear ECRH profiles

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[2] (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.
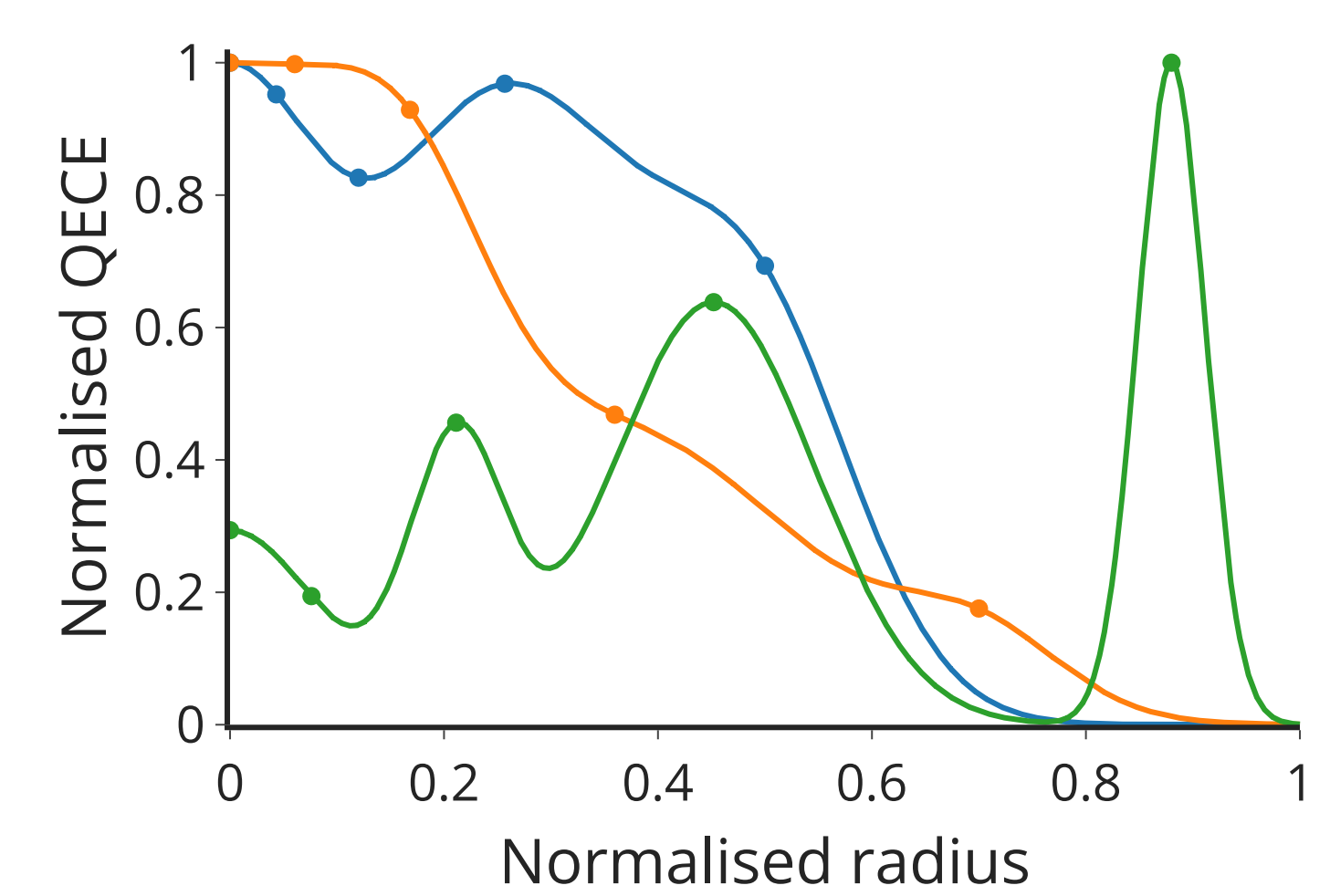
Figure 6: Example sum-of-Gaussians ECRH profiles

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.

Introducing a double peak pushes q_min closer to the axis and reduces central drop-off

Allowing less monotonic profiles enables other objectives to be improved

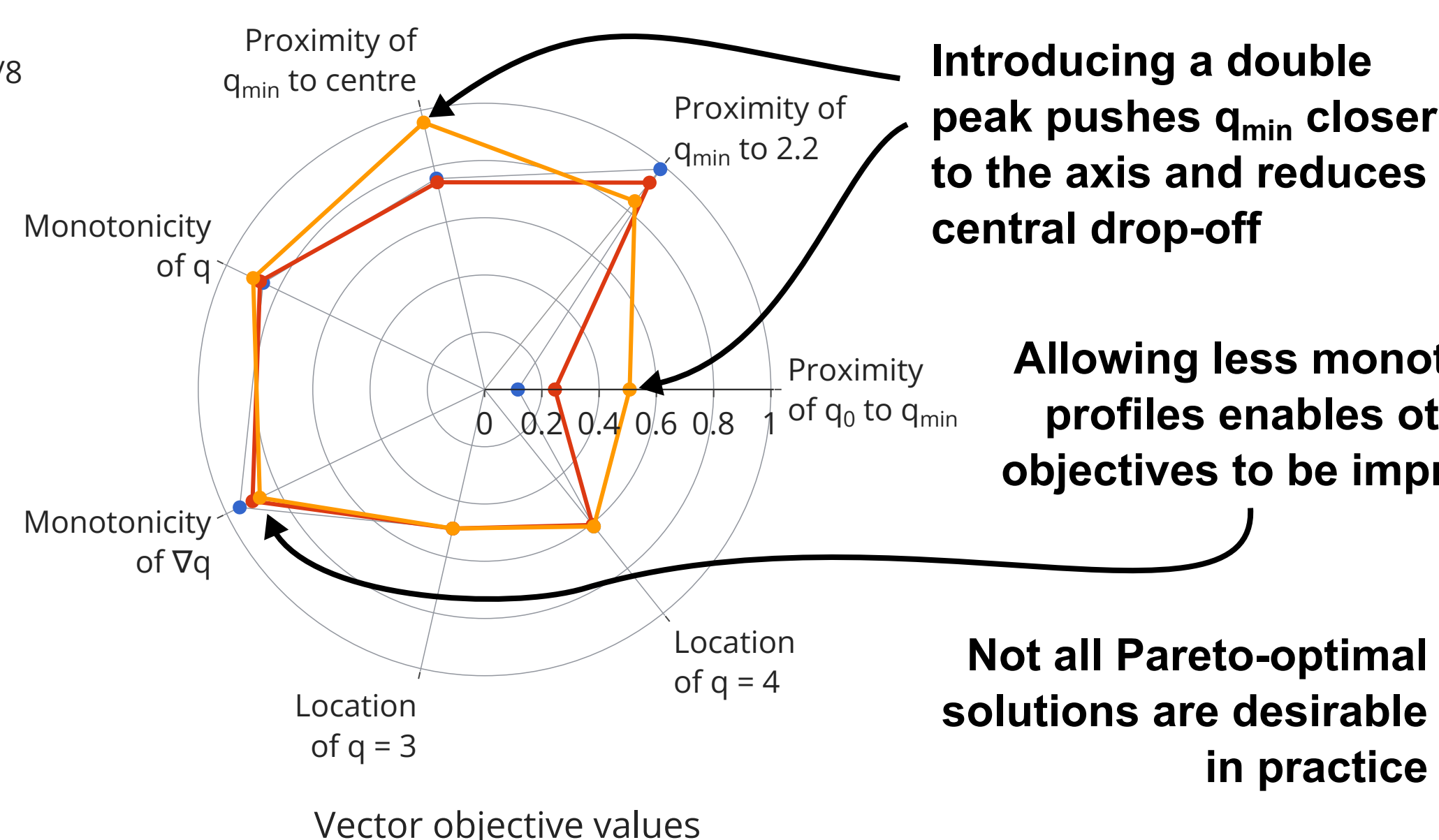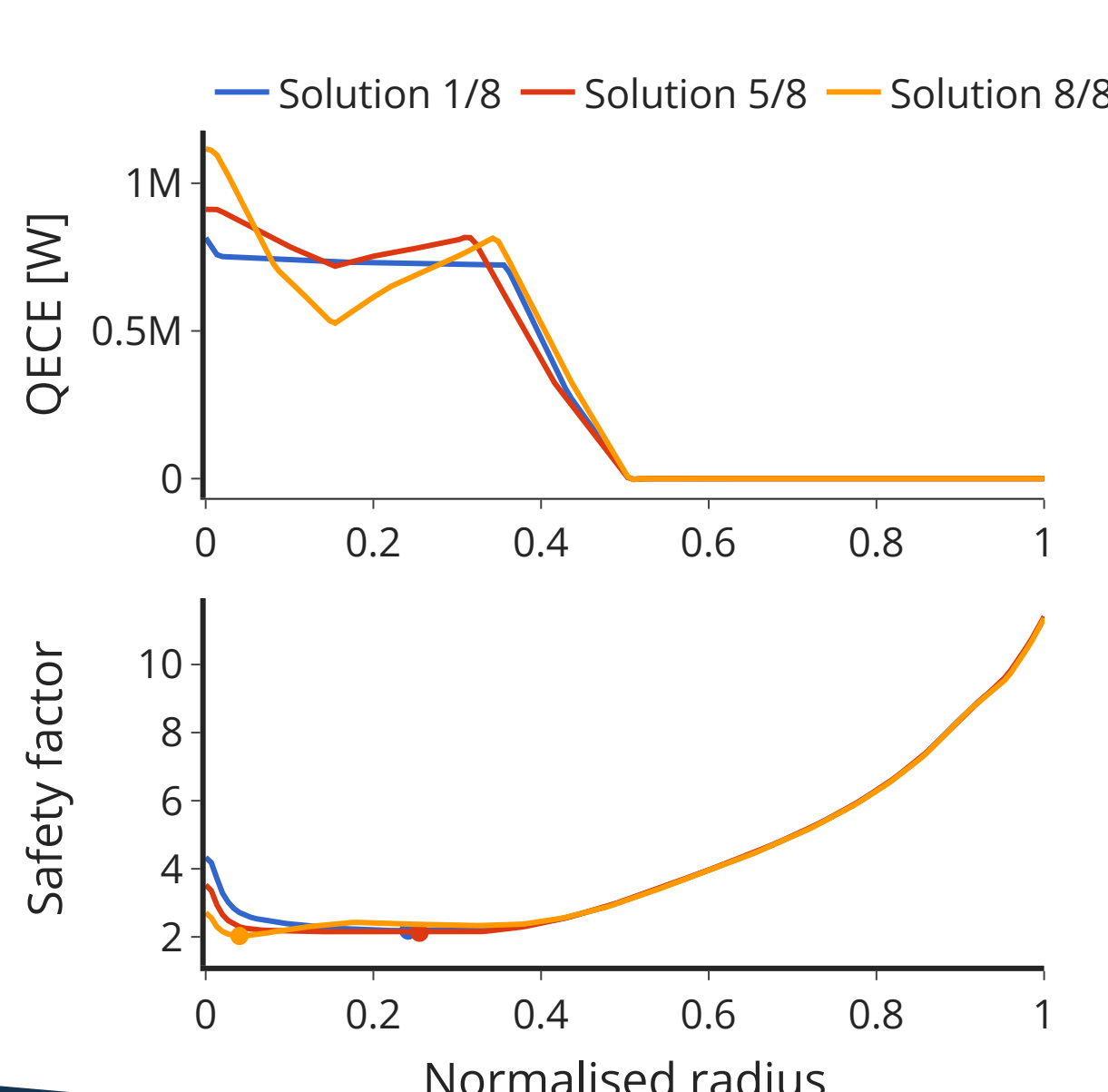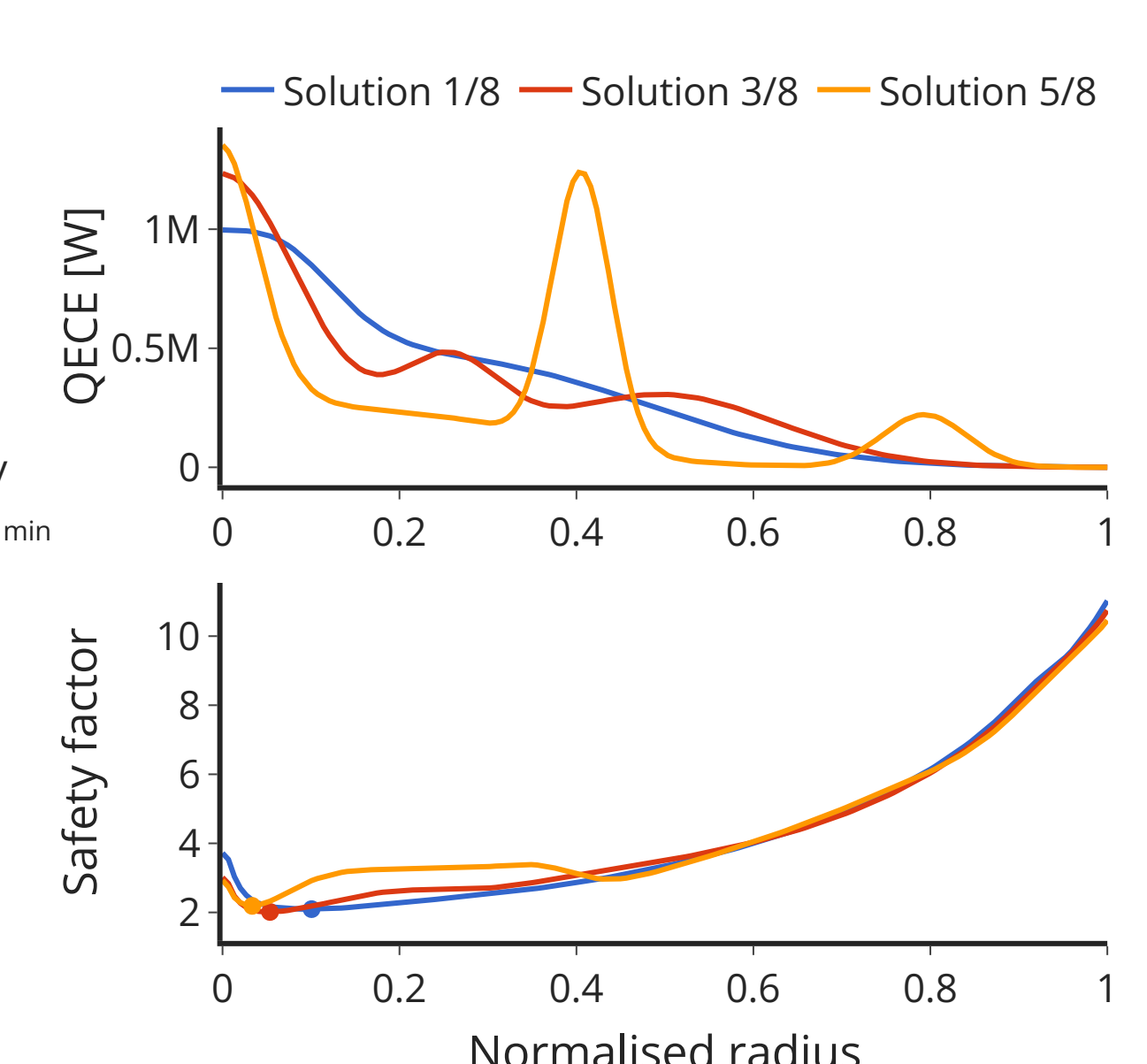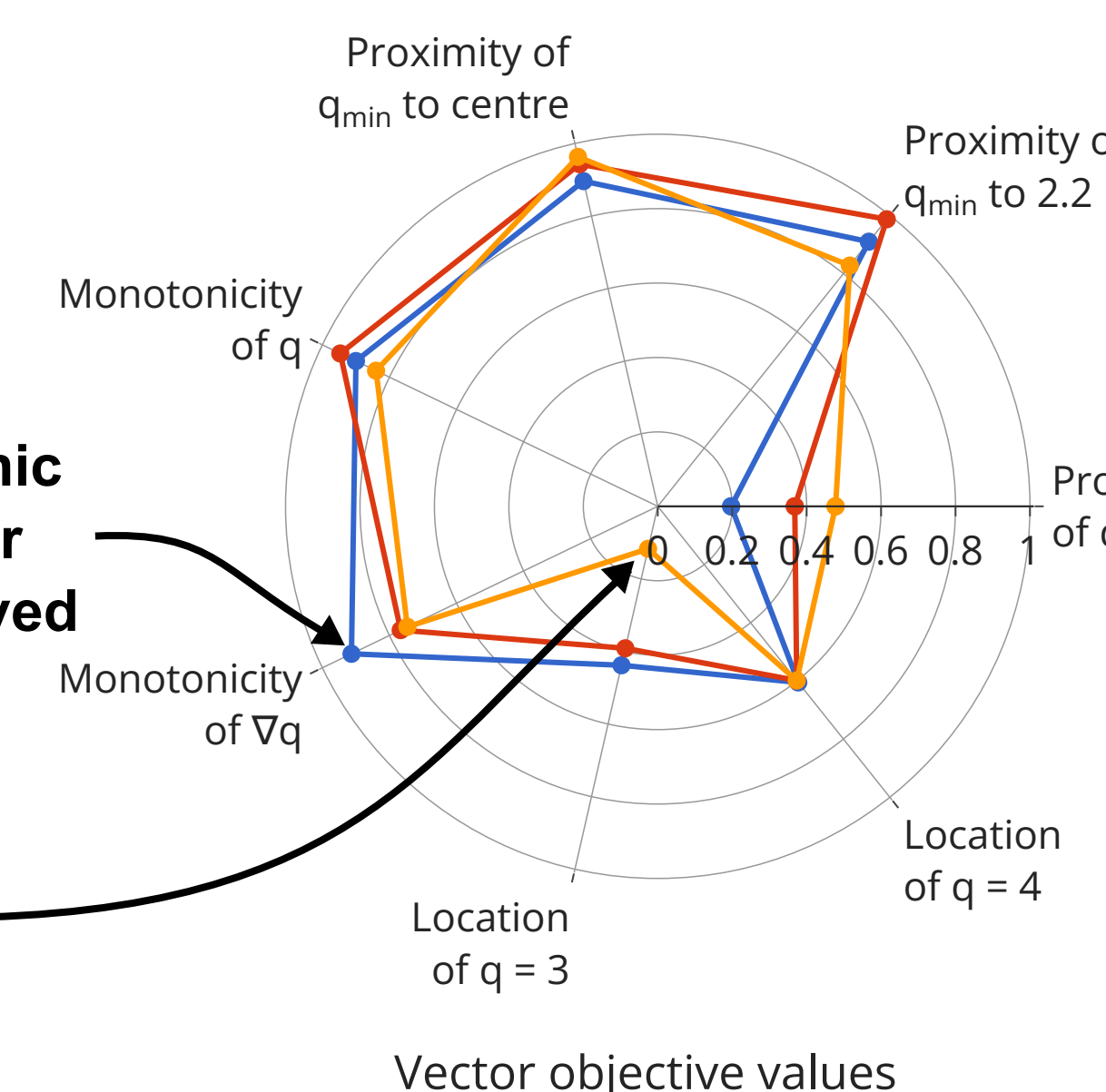Not all Pareto-optimal solutions are desirable in practice

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

References:
[1] Romanelli et al. "JINTRAC: A System of Codes for Integrated Simulation of Tokamak Scenarios", Plasma and Fusion Research 9 (2014).
[2] Marsden et al. "Using Genetic Algorithms to Optimise Current Drive in STEP", 48th European Conference on Plasma Physics (2022).
[3] 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**

Contact: tab3@cam.ac.uk

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