Accelerating the Convergence of Optimisation Procedures for Parameter Estimation in Left Ventricular Models via Bayesian Optimisation

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Outline

1. Motivation
2. Left ventricular modelling
3. Bayesian Optimisation
4. Current work
   - Synthetic data
   - Real data
5. Conclusions

Motivation

Overall goal

To find and implement a fast, reliable and systematic approach to estimating the material properties of the left ventricular biomechanical model

Motivation

Estimating the heart material properties from in-vivo clinical measurements

- Central problem in biomechanical studies of personalized human left ventricular (LV) modelling.
- Important: these properties provide insight into heart function or dysfunction and help to inform on the effectiveness of different treatments post heart attack (myocardial infarction).

Context

Mathematical modelling

- The myocardium (muscular tissue) of the heart can be described by differential equations represented by the Holzapfel–Ogden constitutive law (HO law, Holzapfel and Ogden, 2009).
- In order to assess LV function, it is necessary to determine HO law parameters (e.g. passive myocardial stiffness) ⇒ not in vivo!
- HO law: possible to be solved numerically (finite-element method) ⇒ Problem: the numerical solution is computationally expensive (relies on simulating from the LV model).
- Hence: not suitable for designing personalised treatments within clinics (real time decisions).

Optimisation

Aim: to find the parameters best matching the observed measurements and the model.

1. "Brute force optimisation"?
   - i.e. using standard gradient based optimisers
   - infeasible: time consuming, identification issues
2. Gao et al. (2015): optimisation schemes for LV models
   - based on heuristics (expert knowledge)
   - no joint optimisation
   - several steps based on rescaling of the "original parameter" in different directions
   - still time-consuming
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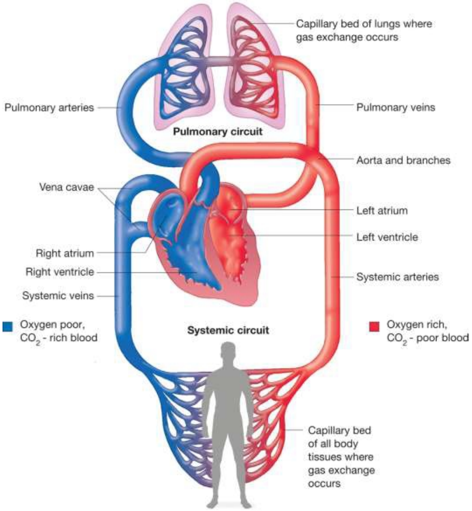
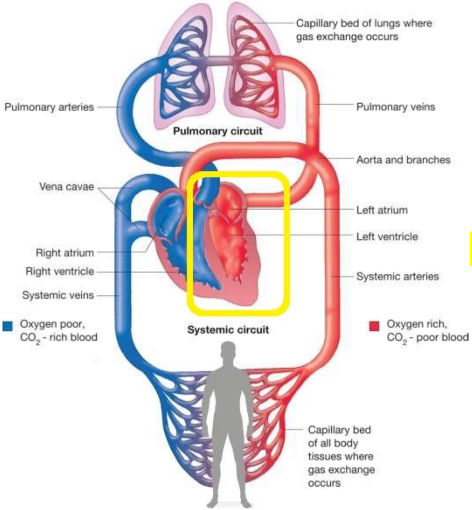
Left ventricular modelling

Left ventricle



Left ventricle



$\Leftarrow$ Left ventricular disfunction

Left ventricular modelling

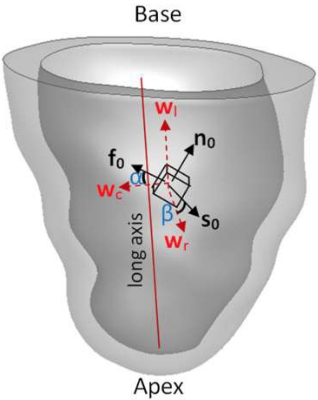


Figure 1: From Wang et al., 2013.

The LV fibre structure = fibre-aligned material axes:

- $\mathbf{f_0}$ – the fibre axis,
- $\mathbf{s_0}$ – the sheet axis,
- $\mathbf{n_0}$ – the sheet-normal axis.

Holzapfel–Ogden constitutive law

- Can give a detailed description of the myocardium response, including the effects of fibre structure (accounts for a layered myofibre architecture).
- Responses: circumferential strains and LV cavity volume (end-diastolic).
- The strain energy function for the myocardium:

$$\Psi(I_1, I_{4f}, I_{4s}, I_{8fs}) = \frac{a}{2b}\{\exp[b(I_1 - 3)] - 1\} + \sum_{i\in\{f,s\}} \frac{a_i}{2b_i}\{\exp[b_i(I_{4i} - 1)^2] - 1\} + \frac{a_{fs}}{2b_{fs}}[\exp(b_{fs}I_{8fs}^2) - 1],$$

where:
I_i, $i \in \{1, 4f, 4s, 8fs\}$ – quantities describing the deformation;

$\phi = (a, b, a_f, b_f, a_s, b_s, a_{fs}, b_{fs})^T$ – (unknown) constitutive parameters to be inferred.

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Constitutive parameters

$\phi = (a, b, a_f, b_f, a_s, b_s, a_{fs}, b_{fs})^T$

E.g. the reference parameters from Wang et al. (2013):

a [kPa]	b	a_f [kPa]	b_f	a_s [kPa]	b_s	a_{fs} [kPa]	b_{fs}
0.236	10.810	20.037	14.154	3.724	5.164	0.411	11.300

Not in vivo!

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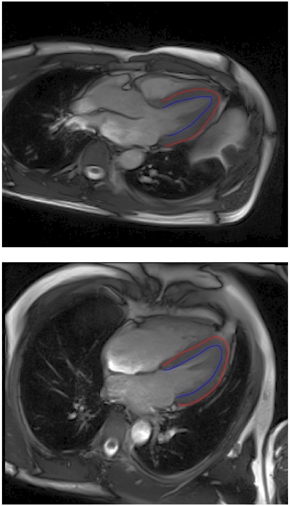
Data: CMR images



Cardiovascular Magnetic Resonance images

Extracted:

- circumferential strains
- LV cavity volume

(Blue and red lines: LV segmentation)

Objective function

The objective function for **minimisation**:
matching the simulated values (depending on the constitutive parameter θ) to the measurements:

$$f_{O2} = \sum_{i=1,\dots,24} (\varepsilon_i - \varepsilon_i^*)^2 + \frac{(V - V^*)^2}{V^*},$$

where ε_i^*, $i = 1, \dots, 24$ and V^* – measurements of the 24 circumferential strains and the volume, respectively.

Bayesian Optimisation

Bayesian Optimisation

Bayesian Optimisation: a sequential model-based method for performing global optimisation of unknown "black box" objectives, particularly useful when their evaluations are expensive (cf. Shahriari et al., 2016).

Key idea: to approximate the costly objective by a cheaper surrogate function and to evaluate the uncertainly of the approximation to quantify the exploitation–exploration trade-off.

Bayesian approach: to update our initial beliefs (prior distribution) about the object of interest after observing the data (likelihood), with sequential updates possible.

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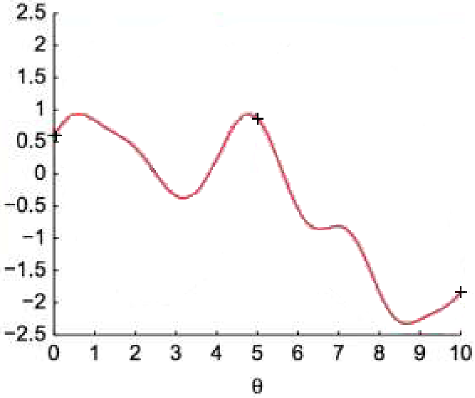
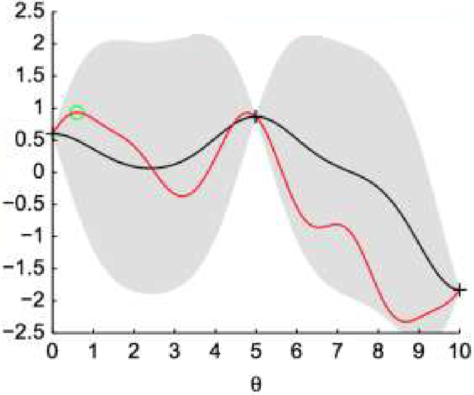


– Unknown objective function (expensive!)

+ Data points

Here:
likelihood maximisation

Illustration



- Surrogate function, typically a Gaussian Process (GP, cf. Rasmussen and Williams, 2006) (cheap!)
- Approximation uncertainty: determines the acquisition function

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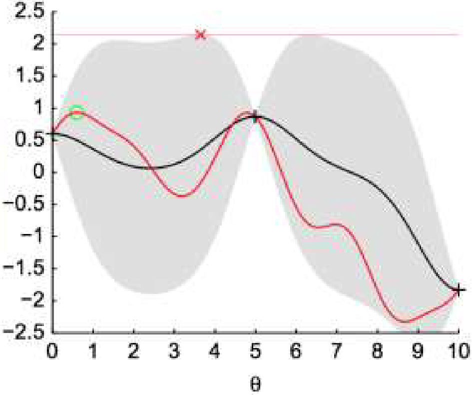

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- × Maximum of acquisition function: exploration–exploitation trade-off

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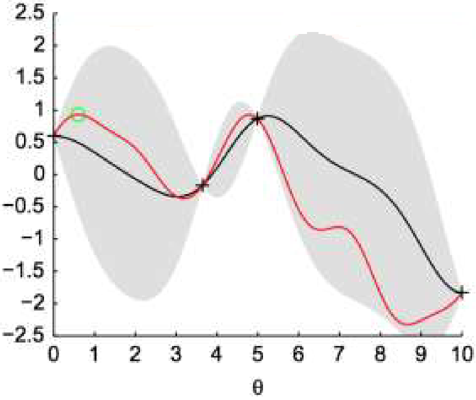

+ Query at the previous maximum ×
  ⇒ uncertainty gets reduced

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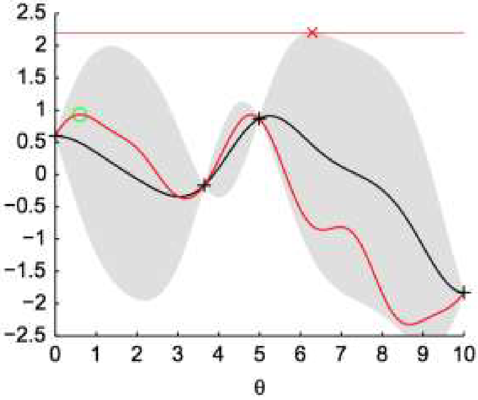

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× Find a new maximum of acquisition function

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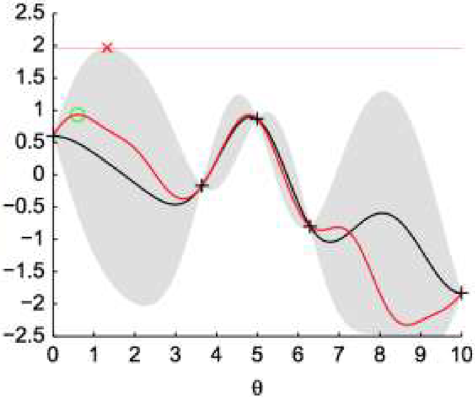

Iterate:

- + Evaluate the objective at the current maximum × (expensive!)
- – Update the surrogate model (cheap!)
- × Find a new maximum of the acquisition function (cheap!)

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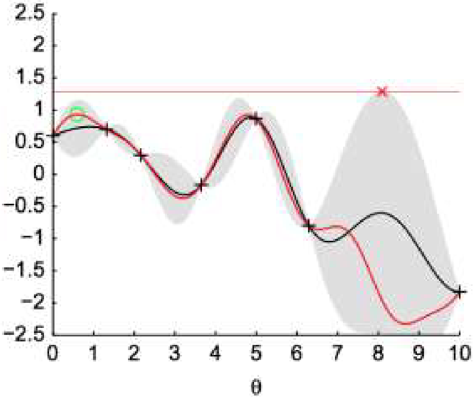

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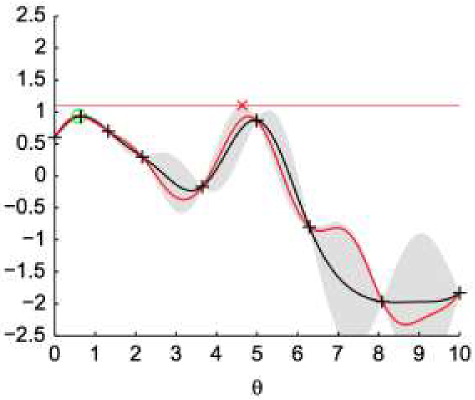

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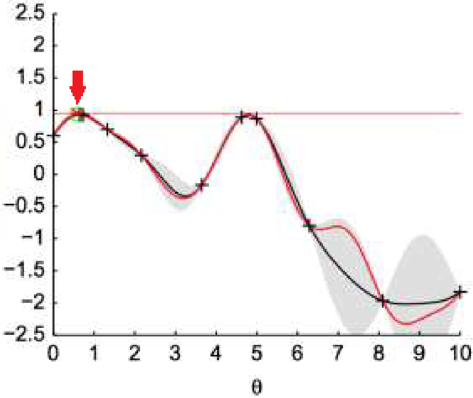

Continue until:
global maximum ⇓

Acquisition functions

- Dictate where to query next
  (i.e. where to carry out the expensive evaluation step)
- Are being optimised (instead of the true objective function)
  (as they are cheap themselves)
- Determine the exploration-exploitation trade-off
- There exist several different types
  (improvement based, information based, etc.)
  - In the figure: Upper-Confidence Bound (UCB)
    (easy to visualise)
  - In our studies: Expectation of Improvement (EI)
    ((presumably) most popular but more complex than UCB)
- For GPs often available in closed form

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Current work

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a &= x_1 a_0, & b &= x_1 b_0, \\
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- Meaning: rescaling of the reference parameters (original parameters) from Wang et al. (2013) in 4 dimensions to match the data.

General settings

- End-diastolic pressure: set to 8 mmHg (for forward simulation in ABAQUS)
- GP for Bayesian Optimisation (BO)
  - Standard squared exponential kernel
  - Initialised using Latin Hypercube Sampling (at $4 \cdot 10$ points)
  - Updated every iteration
- Acquisition function: Expected Improvement
- Comparison with the updated algorithm of Gao et al. (2015) (GLCBL) – 4 Steps:
  1. Initialisation: grid search (10×10 2-dim scaling of 8 parameters)
  2. Klotz curve fitting
  3. `fmincon` of 2-dim scaling of a_f, b_f
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Synthetic data

Ground truth values:

- Parameters (realistic for the chosen mesh):

  $$\theta = (0.1000, 1.2443, 2.0059, 3.1184, 0.3356, 0.9928, 0.1000, 1.3007)^T$$

- Volume: 142.588 mL
- Mean strain (std): -0.195 (0.052)

Synthetic data (cont'd)

Results:

- After 7 iterations of BO [8 hrs] (excl. 40 initial invocations):

  $f_{O2}^{\min,\mathrm{BO}} = 0.0037$

  $\theta^{\min,\mathrm{BO}} = (0.040, 1.816, 1.449, 3.540, 0.269, 1.292, 0.084, 2.318)^T$

  $\Rightarrow \mathrm{RMSE}(\theta^{\min,\mathrm{BO}}) = 0.493$

- After $74 + 26 + 51 = 151$ iterations of GLCBL [31.5 hrs] (excl. 100 initial invocations):

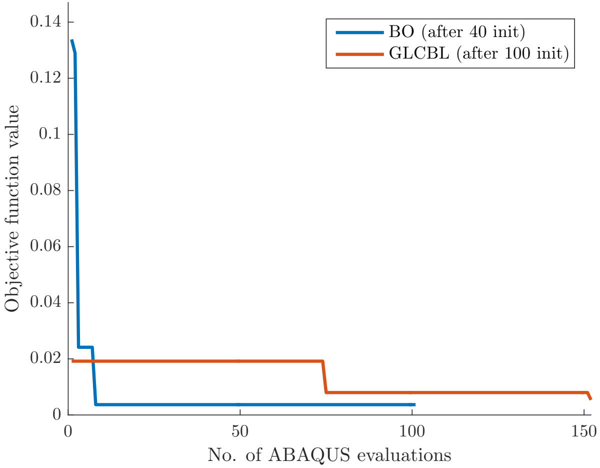
  $f_{O2}^{\min,\mathrm{GLCBL}} = 0.0054$

  $\theta^{\min,\mathrm{GLCBL}} = (0.100, 1.693, 1.305, 3.2586, 0.243, 1.189, 0.100, 2.602)^T$

  $\Rightarrow \mathrm{RMSE}(\theta^{\min,\mathrm{GLCBL}}) = 0.554$

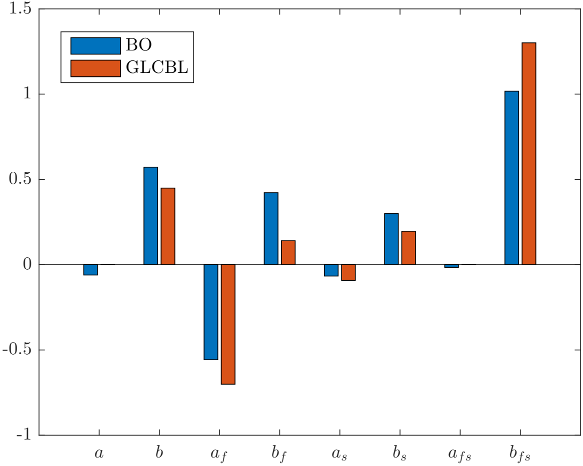
Synthetic data (cont'd)

Best (=min) value of the objective function in subsequent iterations



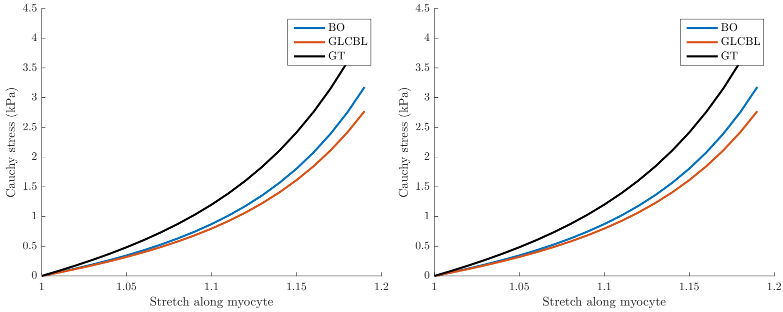
Synthetic data (cont'd)

Errors in parameter estimates (wrt the ground truth)



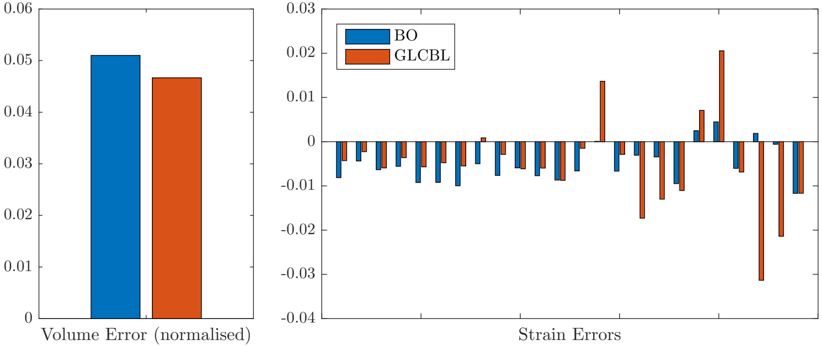
Synthetic data (cont'd)

Stress-strain curves



Synthetic data (cont'd)

Response errors



Real data

Measurements:

- Volume: 116.134 mL
- Mean strain (std): -0.162 (0.047)

Real data (cont'd)

Results:

- After 58 iterations of BO [14 hrs] (excl. 40 initial invocations):

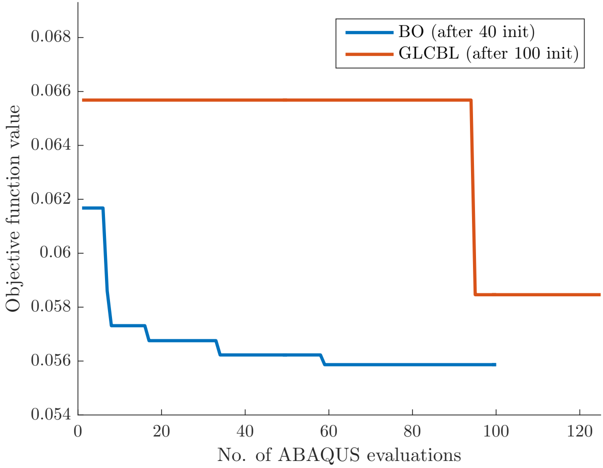
  $f_{O2}^{\text{min,BO}} = 0.0559$

- After $38 + 56 + 30 = 124$ iterations of GLCBL [25.5 hrs] (excl. 100 initial invocations):

  $f_{O2}^{\text{min,GLCBL}} = 0.0585$

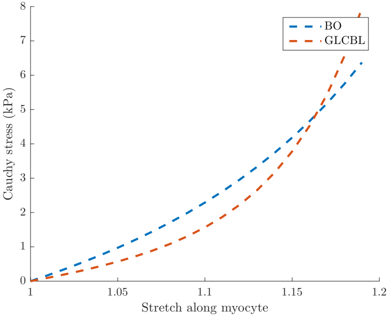
Real data (cont'd)

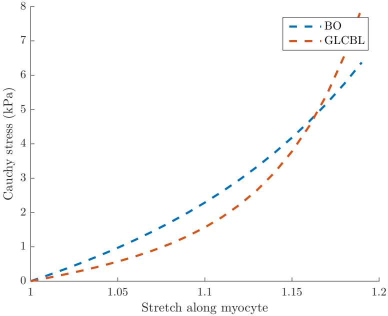
Best (=min) value of the objective function in subsequent iterations



Real data (cont'd)

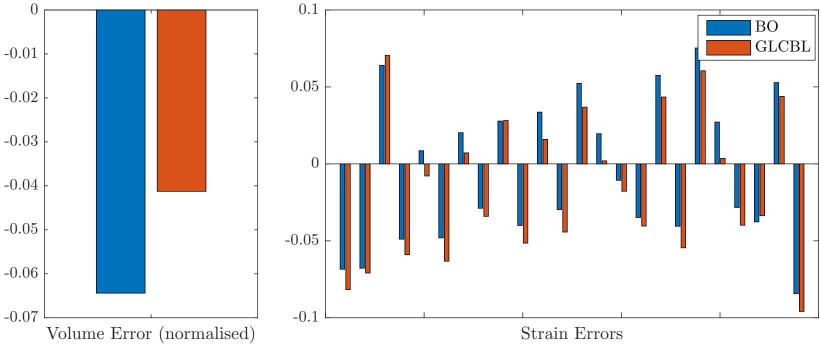
Stress-strain curves





Real data (cont'd)

Response errors



Conclusions

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- Personalised treatment of LV requires inferring of the myocardium properties in a viable clinical time frame using in-vivo LV data.
- Previous methods: infeasible for real time problems.
- Bayesian Optimisation provides a fast, reliable and systematic approach to parameter inference in LV models.
- With Bayesian Optmisation: slightly better results but obtained in much shorter time.

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Further research

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2. Investigate the impact of the choice of the acquisition function and explicitly control the exploration–exploitation trade-off (better to be greedy or not?).
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