Gaussian Processes and Expected Improvement for Fitting Nuclear Models

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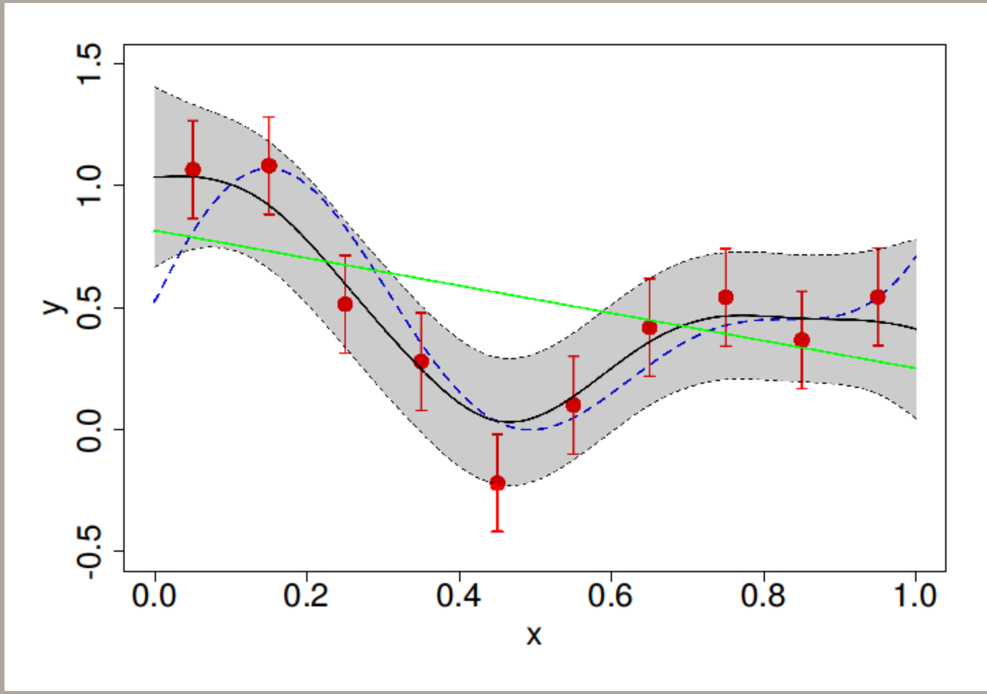
Motivation

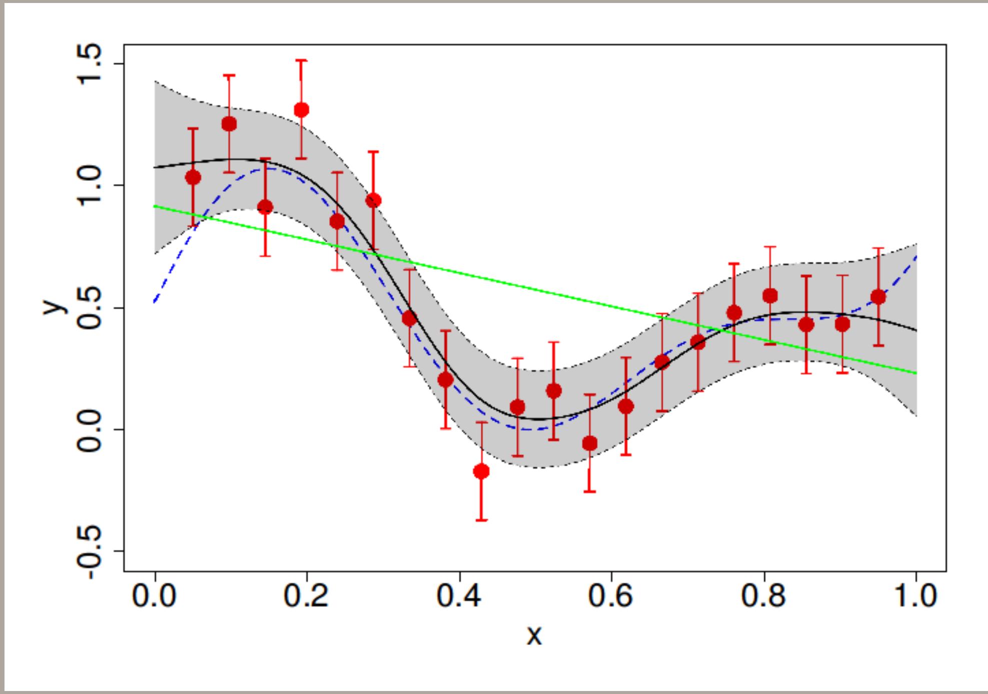
- Fitting complex nuclear physics models
- Models/ functionals can have many parameters
  - Standard Skyrme → 9
    - N2LO → 13
    - N3LO → 17
  - Standard Gogny → 10
- Least squares fitting (χ^2 minimisation) with experimental data (e.g. nuclear masses, radii, ...) is typically used

Gaussian Process Emulation (GPE)

10 training points

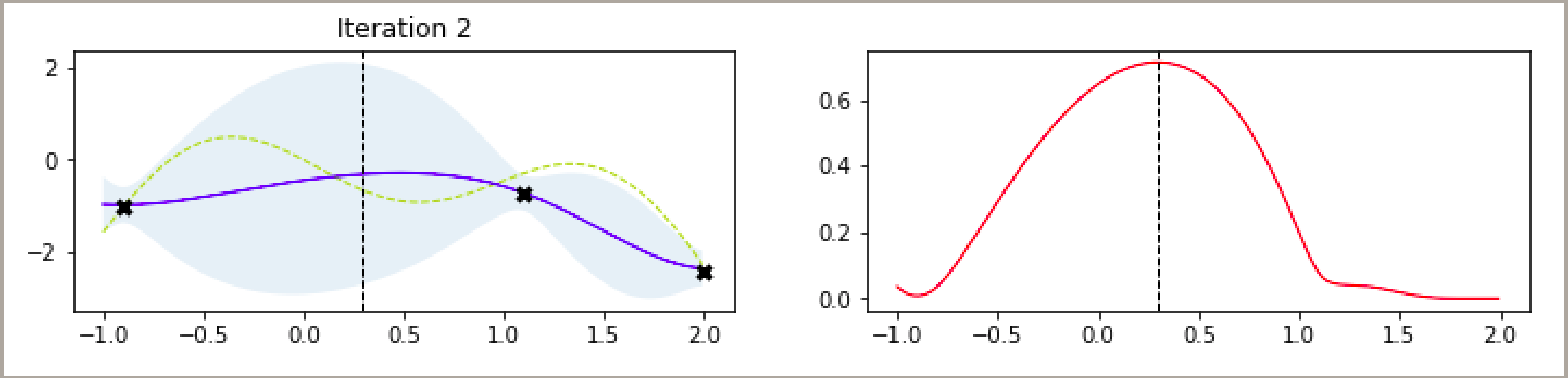


20 training points



- Blue-dotted line: black-box simulator
- Solid black line: emulation
- Solid green line: mean function

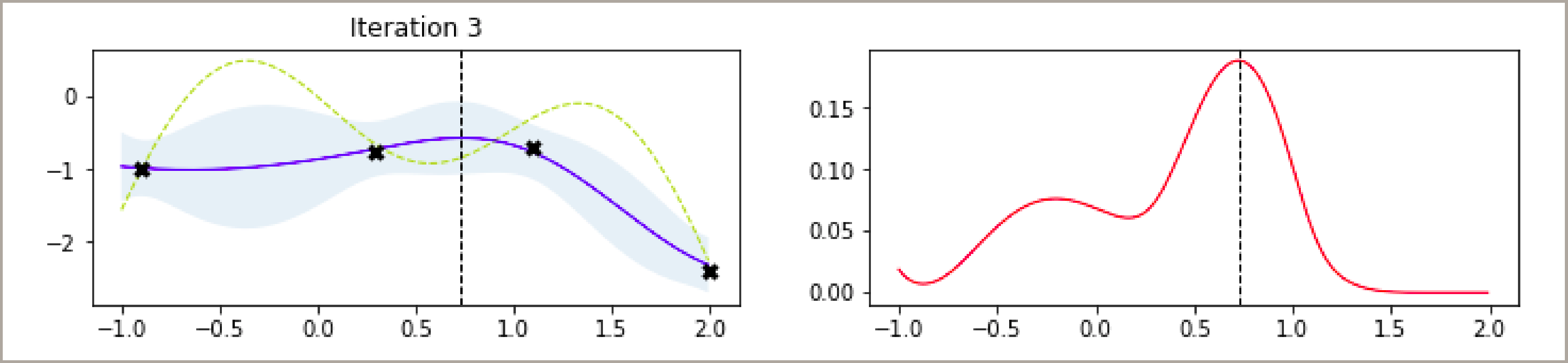
GPE + Expected Improvement (EI)



Left: emulation

Right: acquisition

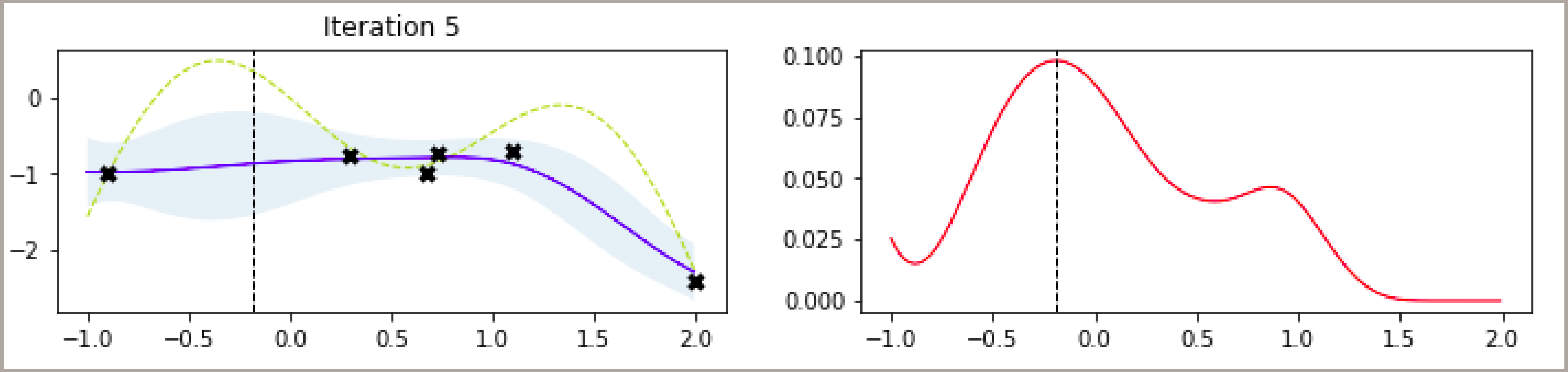
GPE + Expected Improvement (EI)



Left: emulation

Right: acquisition

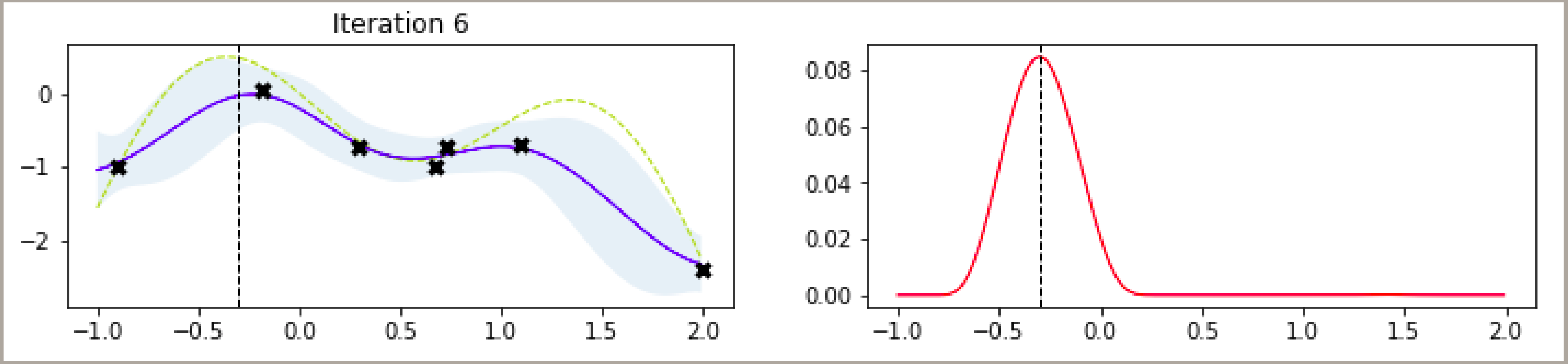
GPE + Expected Improvement (EI)



Left: emulation

Right: acquisition

GPE + Expected Improvement (EI)



Left: emulation

Right: acquisition

Liquid Drop Model (LDM)

- Phenomenological model for nuclear binding energy with 5 parameters:

$$\mathrm{B.E.} = \mathrm{a}_V A - a_S A^{2/3} - a_C \frac{Z(Z-1)}{A^{1/3}} - a_A \frac{(A-2Z)^2}{A} + a_P \delta(A,Z)$$

- Exponent in final term (pairing) can be varied
- AME2012 data, with A>15, and nuclei with error <0.1MeV

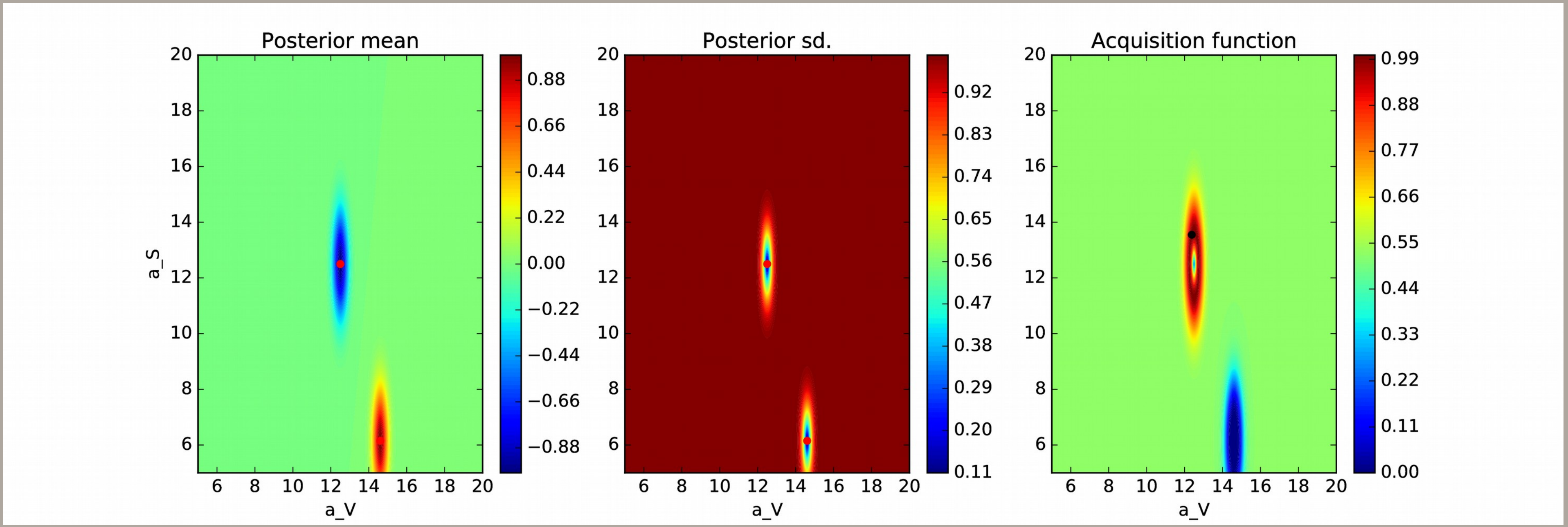
χ^2 fitting

$$\chi^2 = \sum_i (E_i^{th} - E_i^{exp})^2$$

- Aim is to minimise this multi-dimensional function
- Liquid Drop Model is a very fast and simple model, but functionals are slow
  - → need to reduce number of χ^2 evaluations

2D demo: Iterations = 1

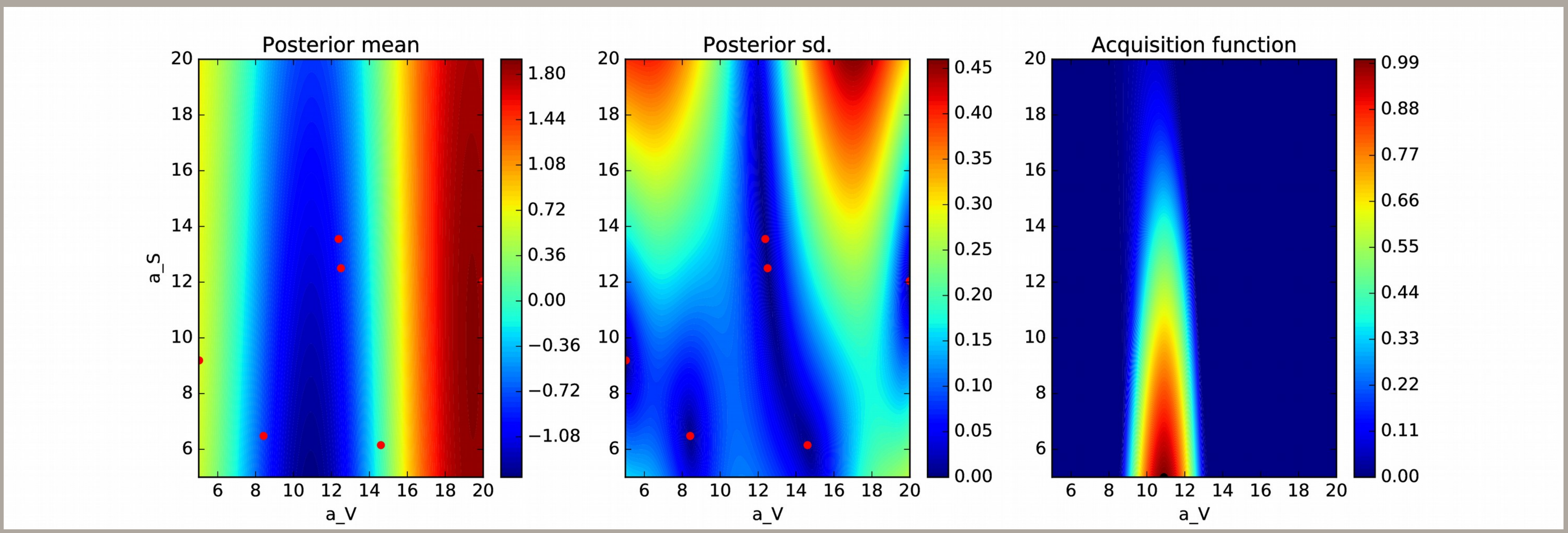
Test with first 2 parameters only: a_V and a_S



- Posterior mean – emulation of χ^2 surface by GPE
- Posterior sd. - confidence intervals provided by GPE
- Acquisition function – maximum gives location for next point

2D demo: Iterations = 5

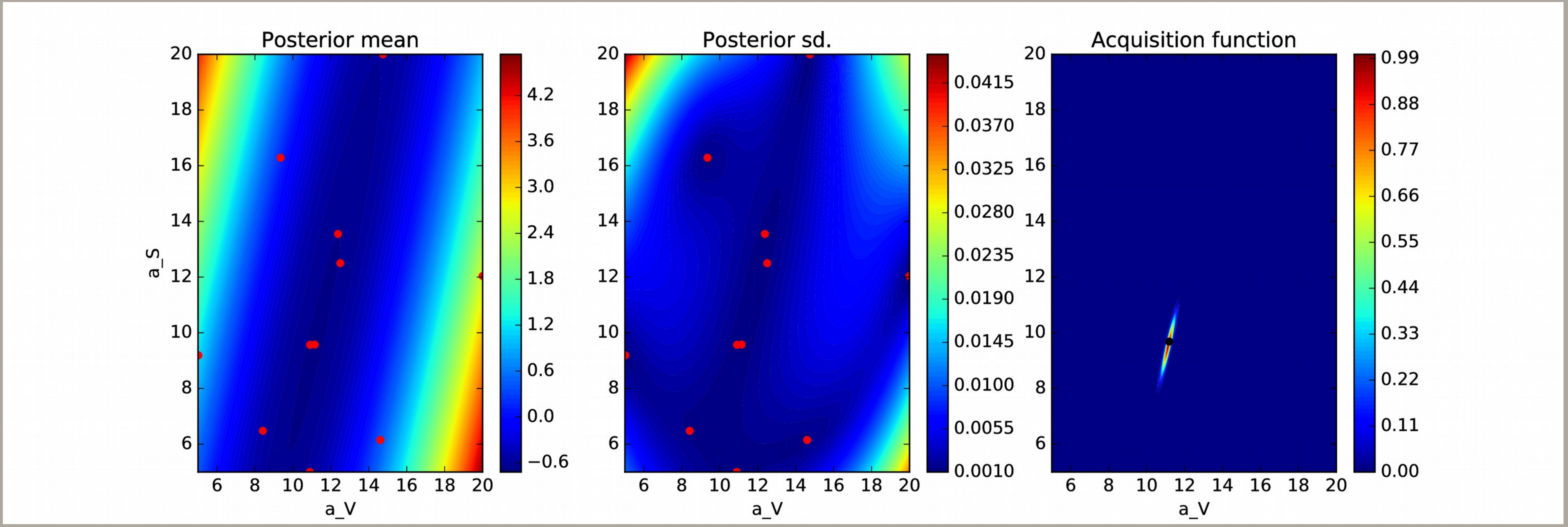
Test with first 2 parameters only: a_V and a_S



- Posterior mean – emulation of χ^2 surface by GPE
- Posterior sd. - confidence intervals provided by GPE
- Acquisition function – maximum gives location for next point

2D demo: Iterations = 10

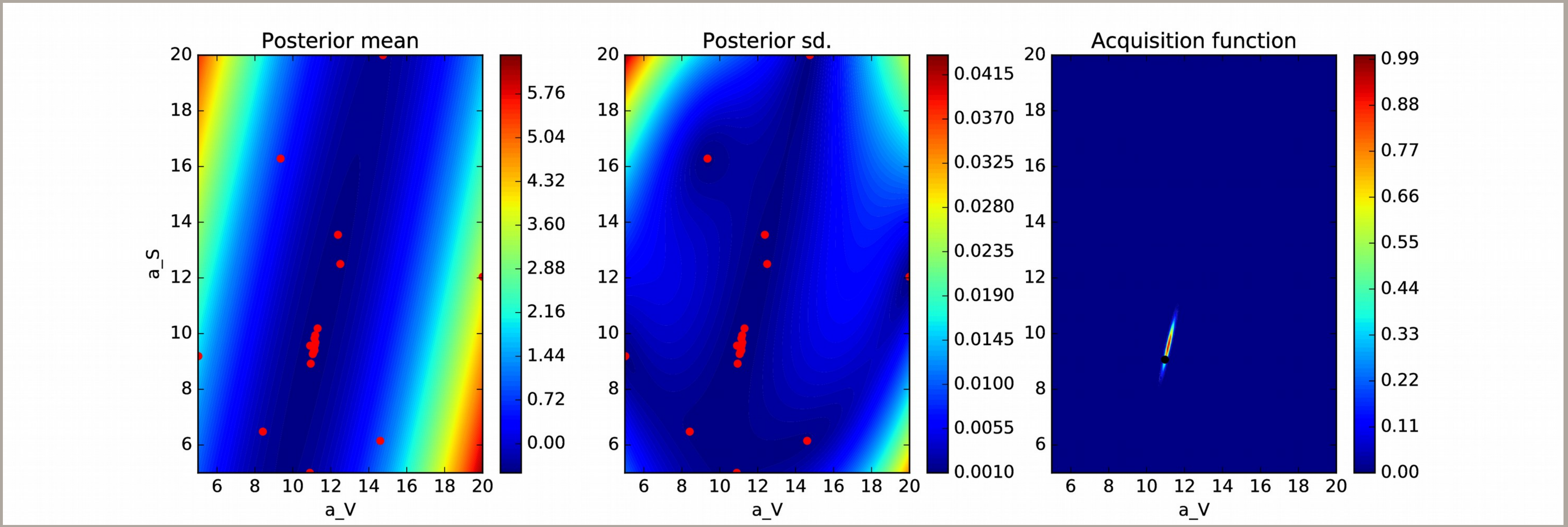
Test with first 2 parameters only: a_V and a_S



- Posterior mean – emulation of χ^2 surface by GPE
- Posterior sd. - confidence intervals provided by GPE
- Acquisition function – maximum gives location for next point

2D demo: Iterations = 20

Test with first 2 parameters only: a_V and a_S

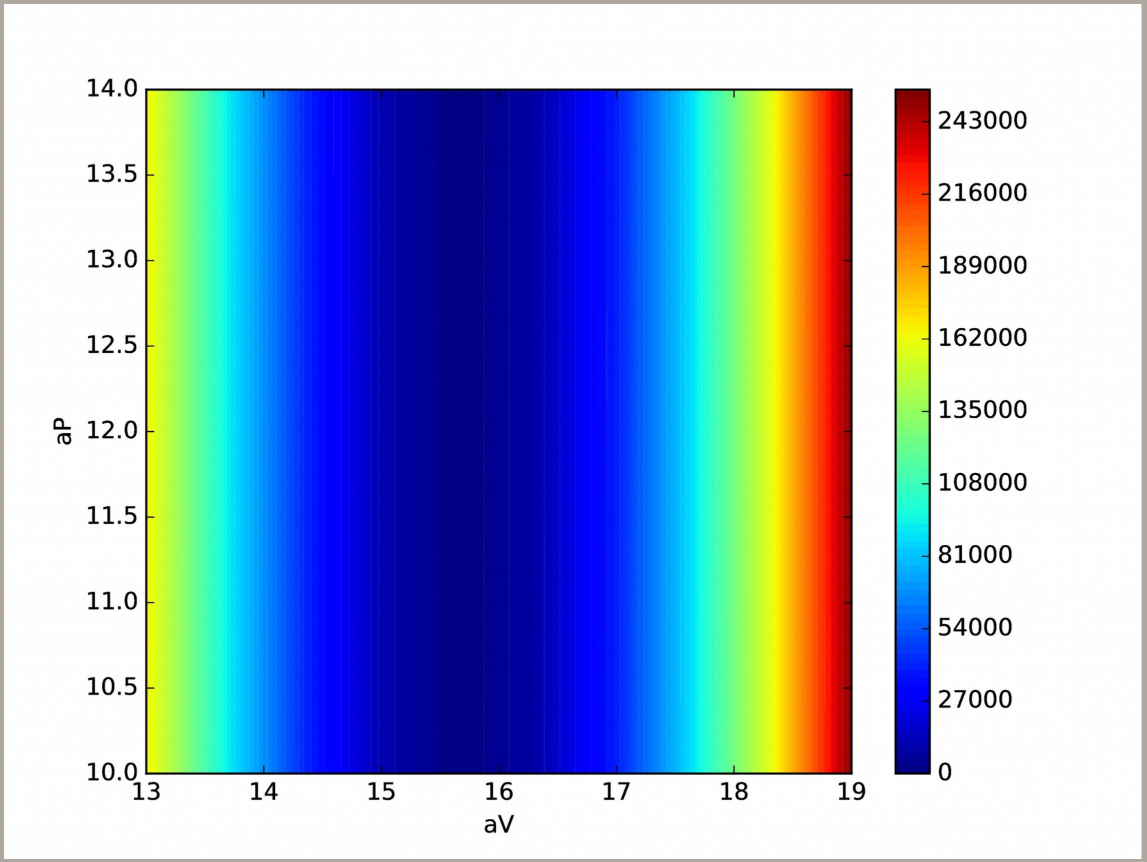


- Posterior mean – emulation of χ^2 surface by GPE
- Posterior sd. - confidence intervals provided by GPE
- Acquisition function – maximum gives location for next point

Full (5D) Liquid Drop Model

- The χ^2 surface is flat along dimension for a_p parameter (pairing term gives very small contribution to binding energies)
- EI algorithm appears to struggle: a_p always last to converge

  → a_p fixed for now, vary other 4 parameters

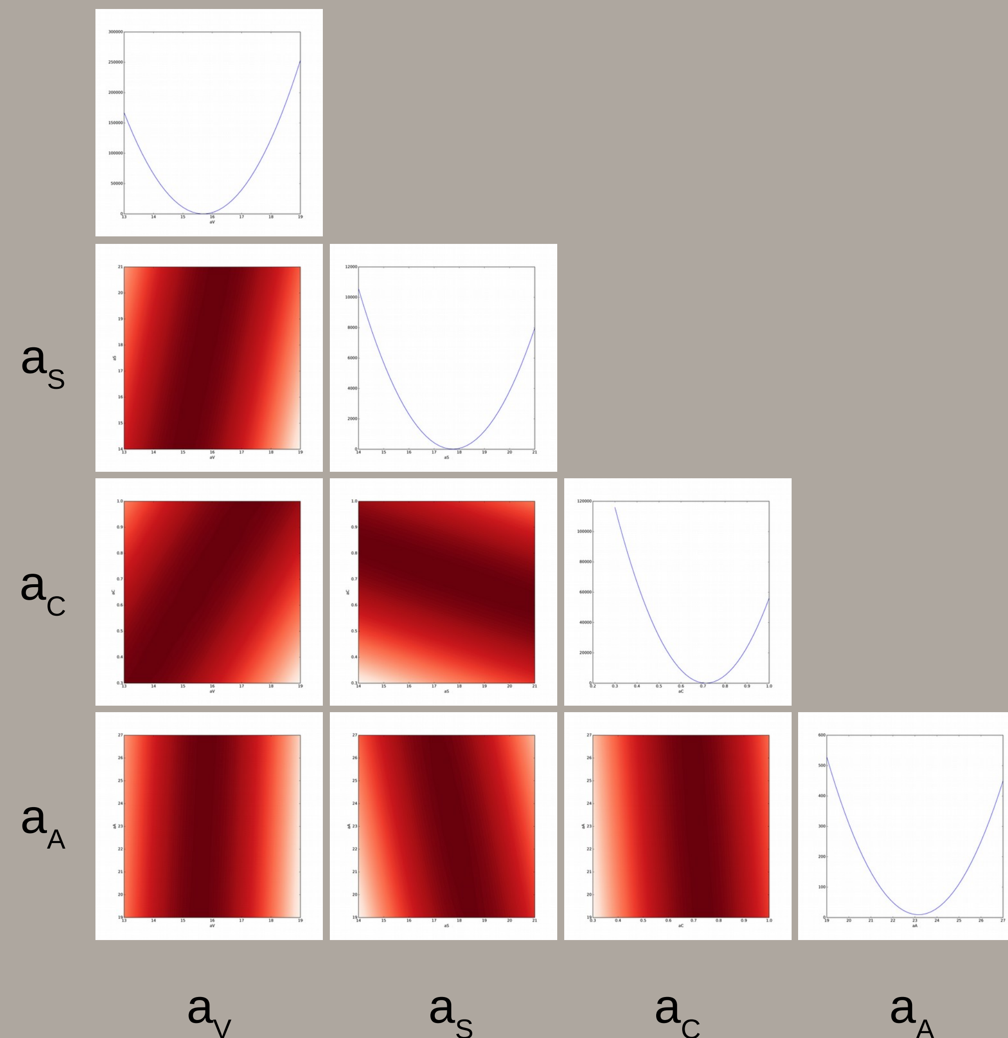


Results (4D)

- After 60 iterations of EI, best minimum found at:

	GPE + EI	True
a_V	15.62	15.69
a_S	17.53	17.76
a_C	0.7103	0.7129
a_A	22.29	23.17

- Corner plot is important tool for examining χ^2 surface around minimum



Summary

- Tested with basic LDM model to become familiar with Expected Improvement (EI) algorithm
- Currently our “simulation” (LDM) is trivially quick
- Real test of EI will be with a non-linear model with multiple local minima, where each simulation run takes minutes → hours
  - Skyrme, Gogny nuclear energy density functionals (NEDFs)