Constrained Bayesian Optimisation with Knowledge Gradient

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Constrained KG

Non-constrained KG:

$$KG(x) = \mathbb{E}[\max_{x'}\{\mu^{n+1}(x')\}|x^{n+1} = x]$$

Constrained KG with Probability of Feasibility (pf):

$$c - KG(x) = \mathbb{E}[\max_{x'}\{pf^{n+1}(x')\mu^{n+1}(x')\}|x^{n+1} = x]$$

Constrained KG corrected*:

$$c - KG(x) = \mathbb{E}[\max_{x'}\{pf^{n+1}(x')\mu^{n+1}(x') + (1 - pf^{n+1}(x'))M\}|x^{n+1} = x]$$

where $M \in \mathbb{R}$ is the penalisation for sampling points in an infeasible region. It's commonly assumed to be zero.

Constrained KG

Benefits

- Takes into account that constraints change for each possible x^{n+1} considered.
- Assuming $M = 0$ may give "benefit" to infeasible regions. A more general approach avoids that problem.

Limitations

- Computationally expensive compared to constrained Expected Improvement. However, it's possible to make an efficient implementation by using gradients.
- M may be need to chosen by the decision maker.

Results

benchmark Method:

- Constrained Expected Improvement. i.e. Expected Improvement times Probability of feasibility.

Test Functions:

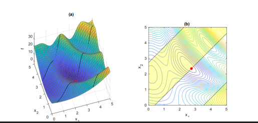
- New Branin, test function 2, and Mistery function. Non-noisy and constrained test functions.

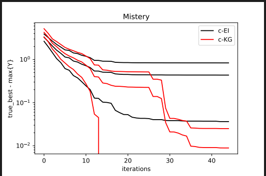
Important Remark:

- In the last evaluation of our approach, the function is sampled according to Expected Improvement times the probability of feasibility.

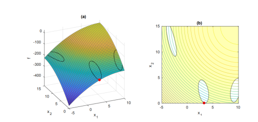
Plots

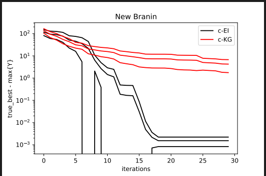
Mistery



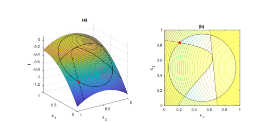


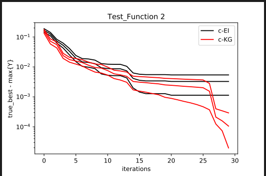
New Branin





Test function 2





Gradient Information

- Numerical methods to optimise KG rely on ∇KG. Quantity can be obtained either by Finite Difference or Analytically.

$$\nabla cKG(x) = \nabla \mathbb{E}[\max_{x'}\{pf^{n+1}(x')\mu^{n+1}(x')\}|x^{n+1} = x]$$

Once solved, the inner optimisation problem,

$$\nabla cKG(x) = \mathbb{E}[\nabla\{pf^{n+1}(x^*; x^{n+1})\mu^{n+1}(x^*; x^{n+1})\}|x^{n+1} = x]$$

Potential issue with Finite Differences:

- Since the expectations is calculated only over a few values slight deviations of x^* affect greatly the outer gradient estimation.

Results with Analytical Gradients

Multi-Objective Constrained Optimisation

- Multi-Objective formulation using linear scalarisation.

$$KG(x';\theta) = \mathbb{E}_y[\max_{x'} \theta\mu^{n+1}(x')|x^{n+1} = x', \theta]$$

where the policy is,

$$maKG(x') = \mathbb{E}_\theta[KG(x';\theta)]$$

- Multi-Objective constrained formulation

$$KG(x';\theta) = \mathbb{E}_y[\max_{x'} \theta\mu^{n+1}(x')pf^{n+1}(x')|x^{n+1} = x', \theta]$$

where the policy is,

$$maKG(x') = \mathbb{E}_\theta[KG(x';\theta)]$$

Work to do

Main line of work

- Constrained Multi-Objective problem

Secondary line of work

- Include noisy test functions.
- Set dynamically the M penalization.