My research over Bayesian Optimization and Gaussian Processes

Eduardo C. Garrido–Merchán
PhD student. Teacher Assistant. Universidad Autónoma de Madrid

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Challenges in Engineering Design

The society demands new products of better quality, functionality, usability, etc.!

   

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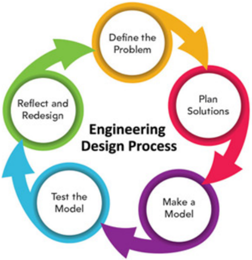

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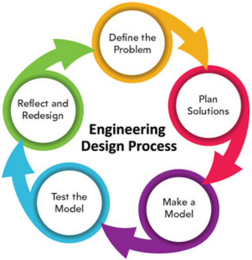

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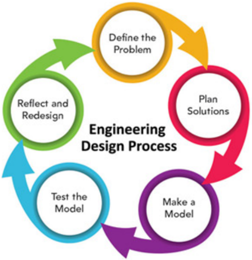

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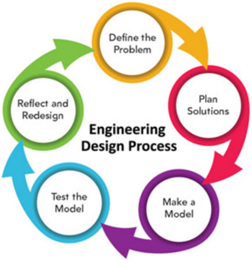

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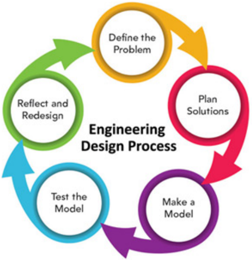

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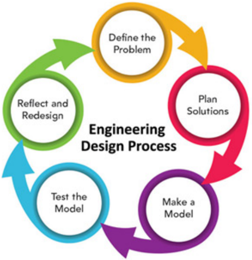

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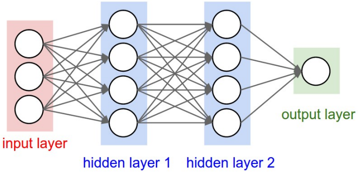
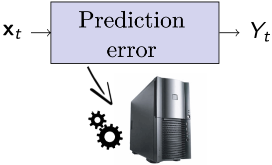
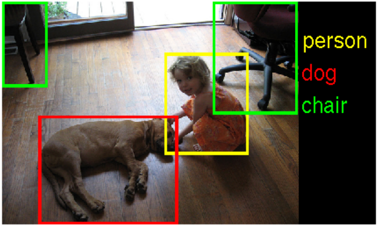
Optimization is a challenging task in new products design!

Example: **Deep Neural Network** for object recognition.







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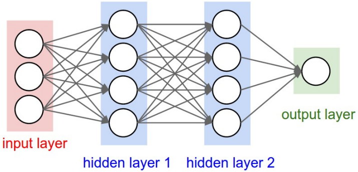

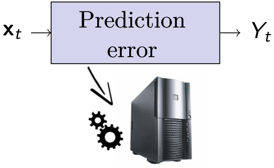

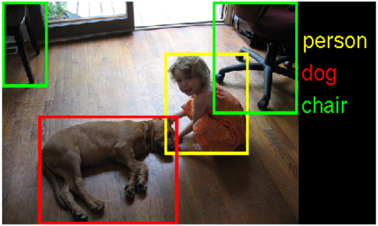

Parameters to tune: Number of neurons (Integer-Valued), number of layers (Integer-Valued), learning-rate, activation function (Categorical-Valued), etc.

Optimization Problems: Common Features

- Very expensive evaluations.

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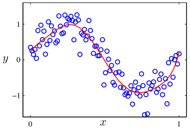
$$y = f(\mathbf{x}) + \epsilon$$



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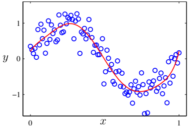
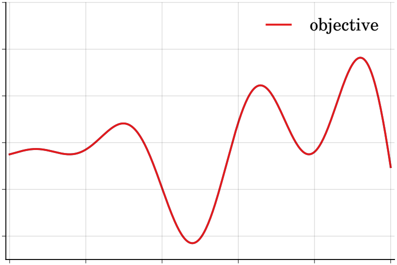


Bayesian optimization methods can be used to solve these problems!

Bayesian Optimization in Practice



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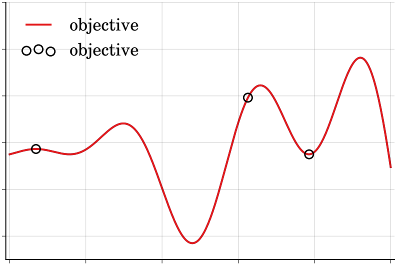

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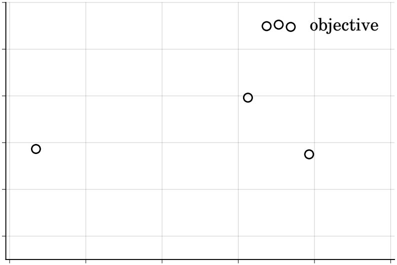

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2. Fit a model to the data:

$$p(y|\mathbf{x}, \mathcal{D}_n) \,.$$

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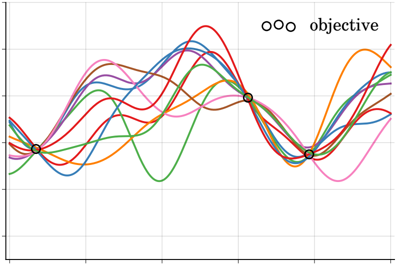

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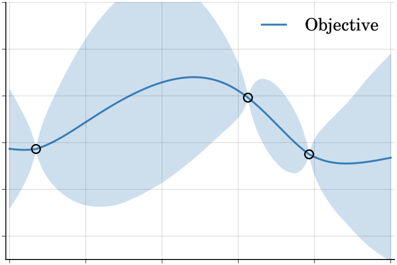

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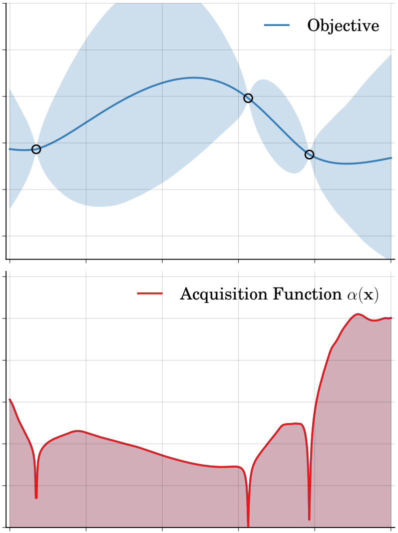

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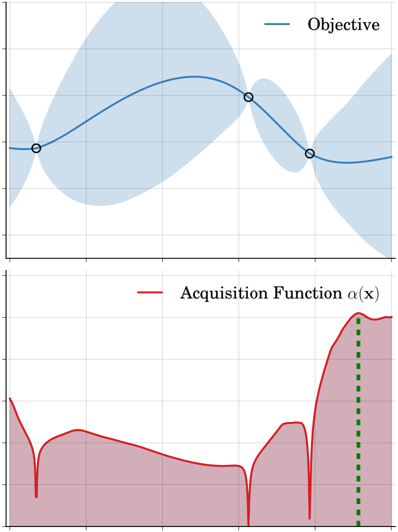

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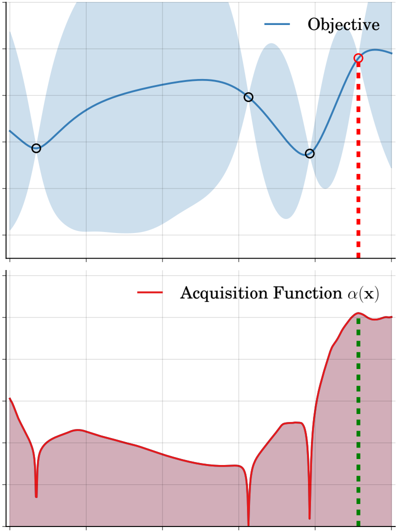

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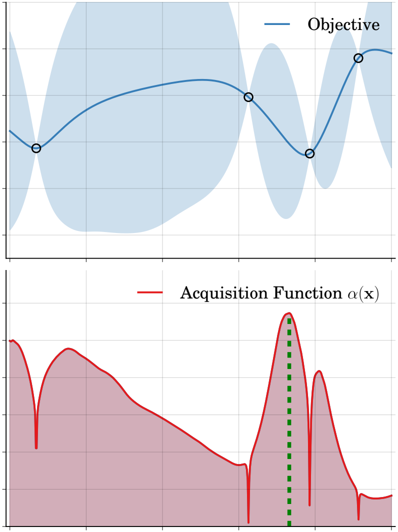

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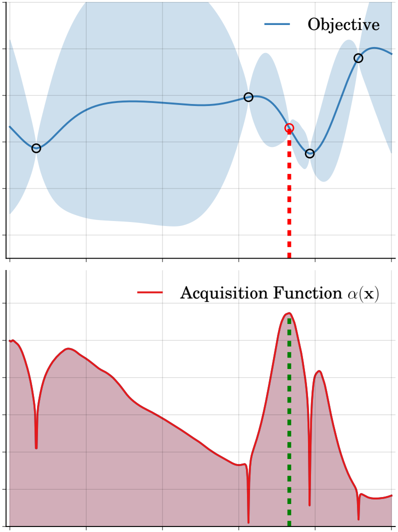

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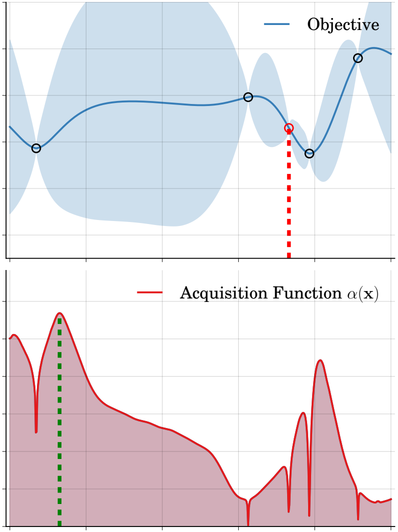

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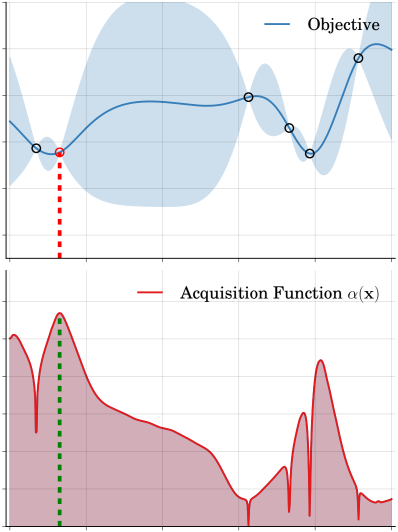

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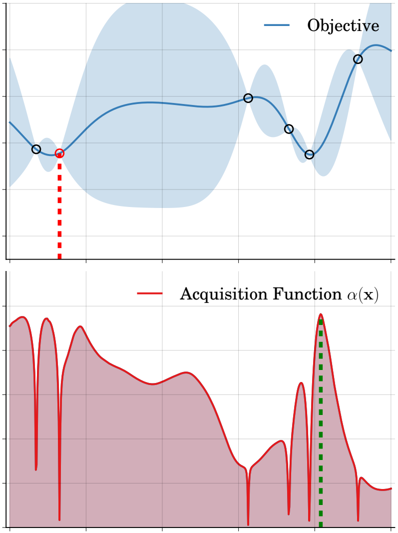

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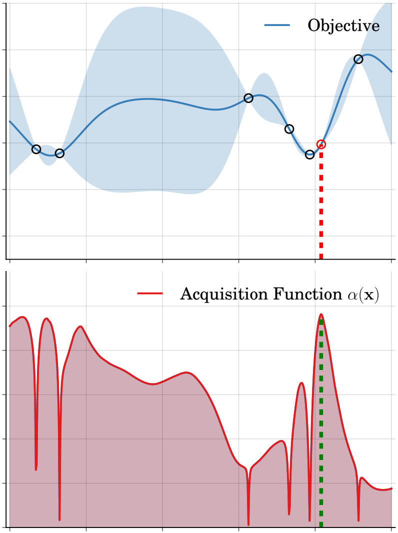

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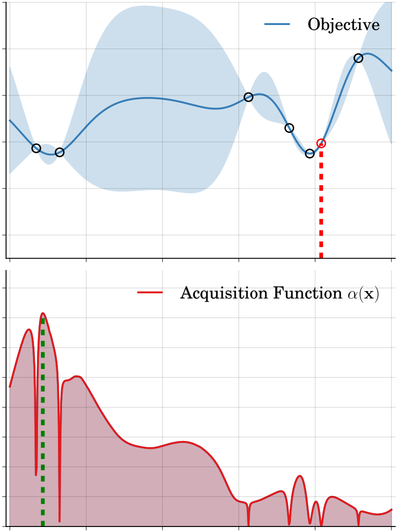

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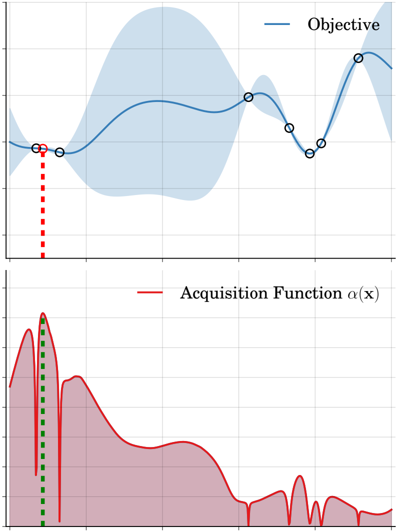

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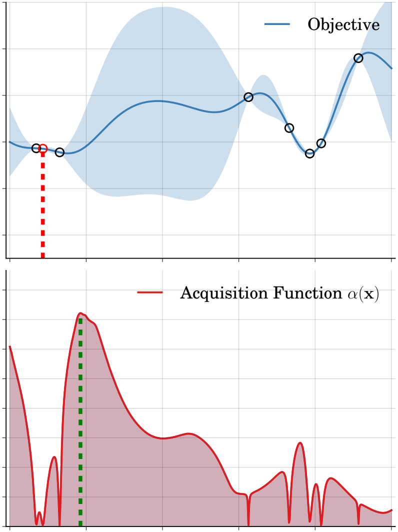

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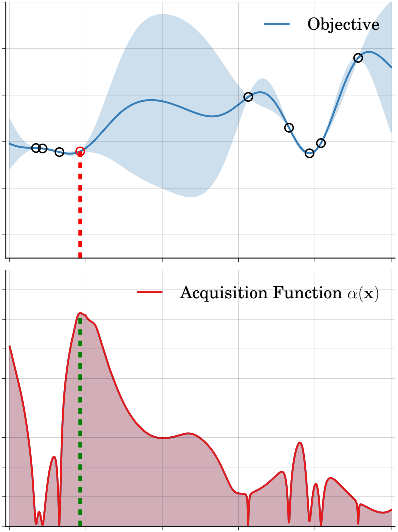

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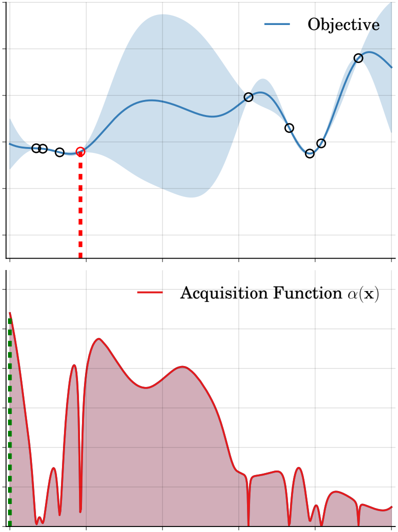

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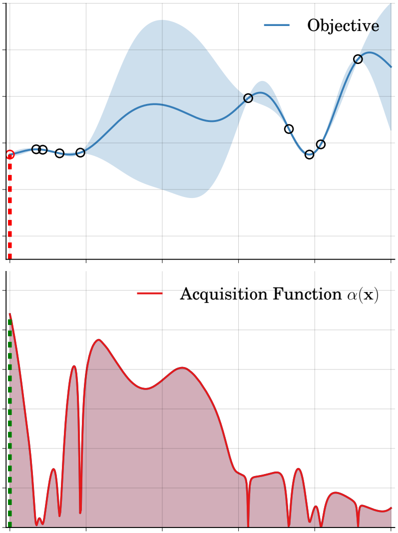

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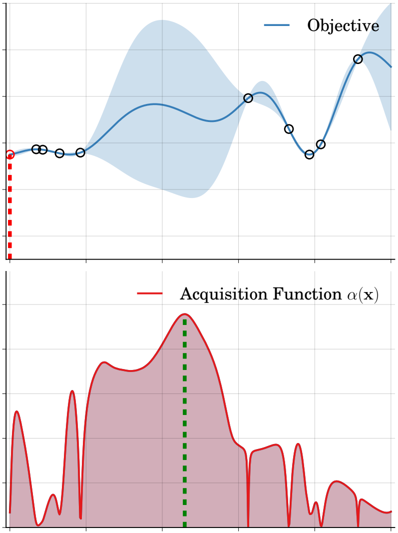

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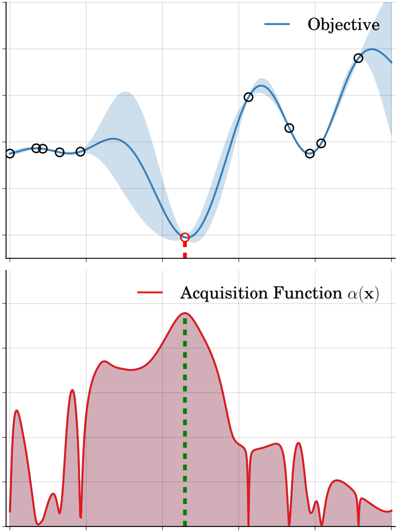

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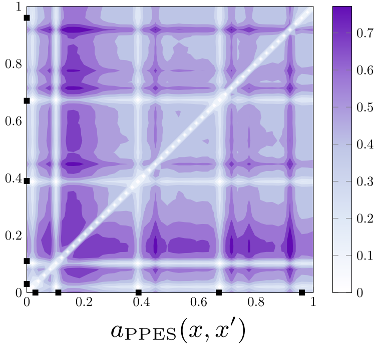

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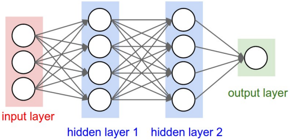
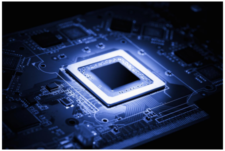
Several Objectives and Constraints

Optimal design of **hardware accelerator** for neural network predictions.





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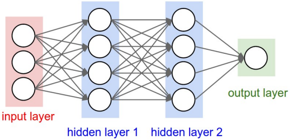

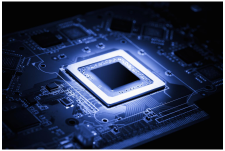

Goals:

- Minimize **prediction error**.
- Minimize **prediction time**.

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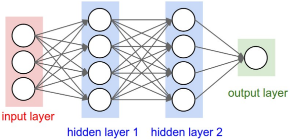

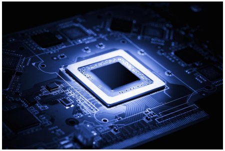

Goals:

- Minimize **prediction error**.
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Several Objectives and Constraints

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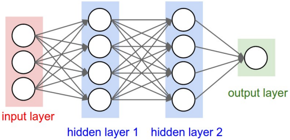

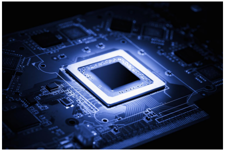

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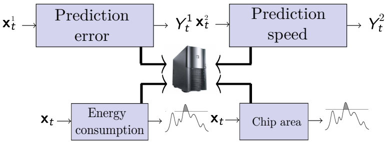

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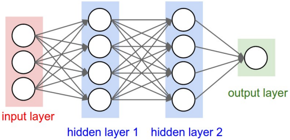

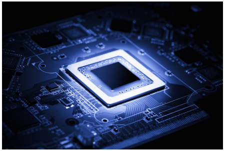

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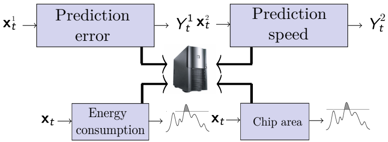
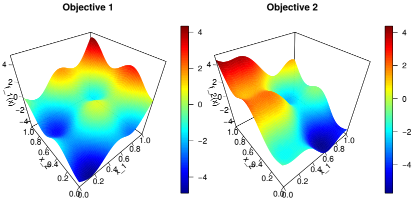


Challenges:

- **Complicated** constraints.
- **Conflictive** objectives.

Constrained Multi-Objective Optimization



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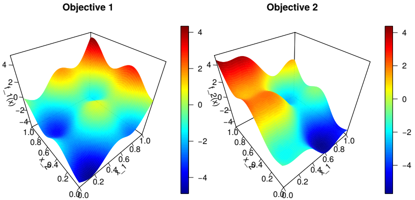

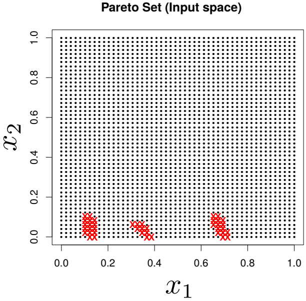

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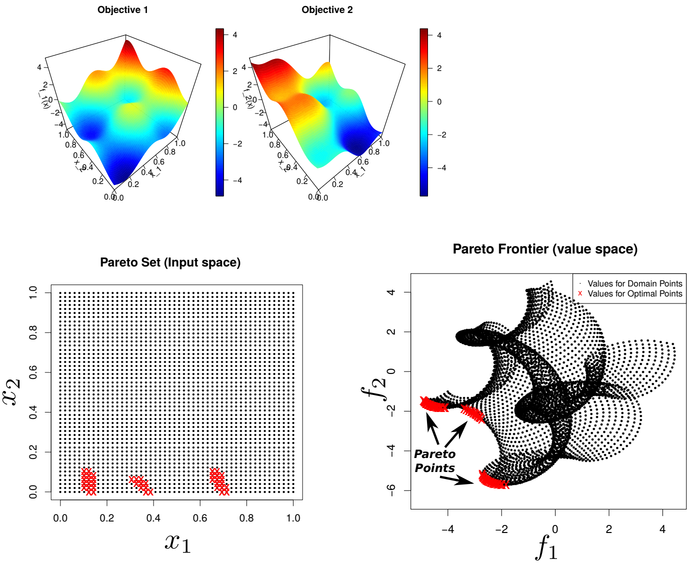

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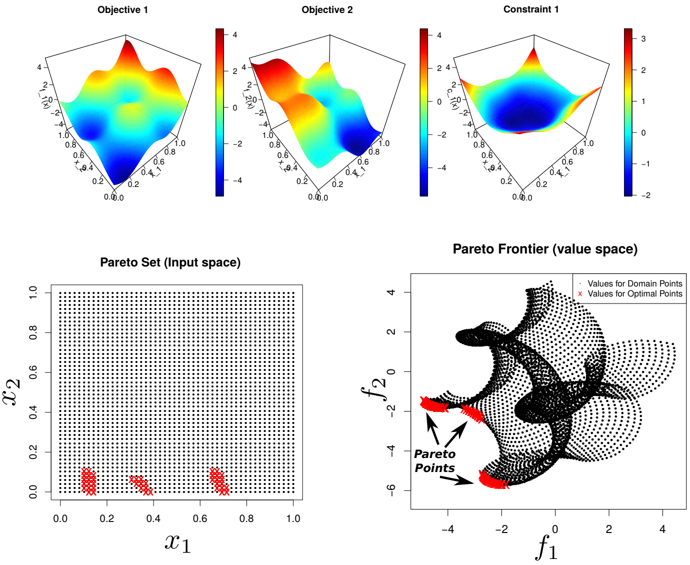

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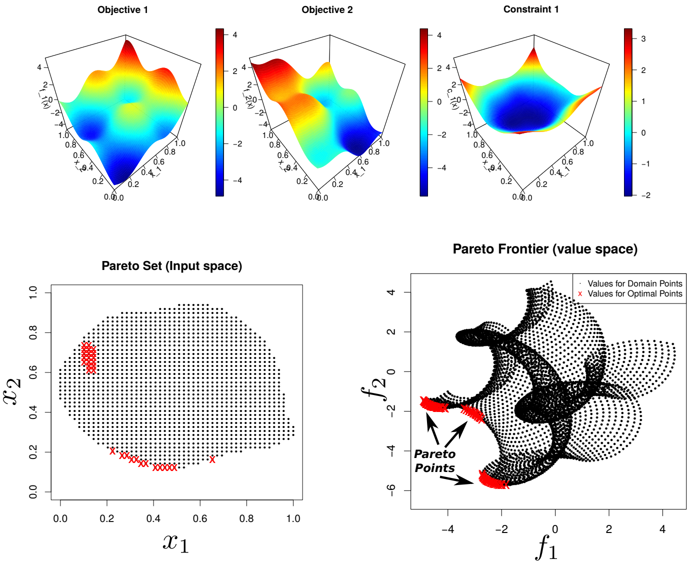

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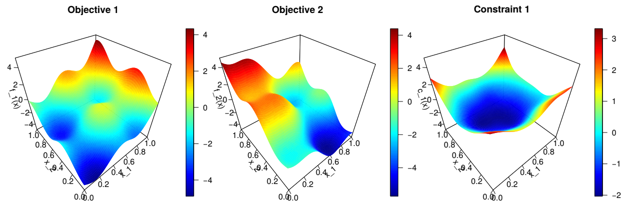
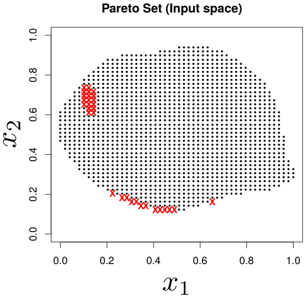
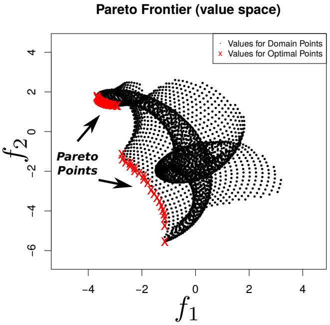
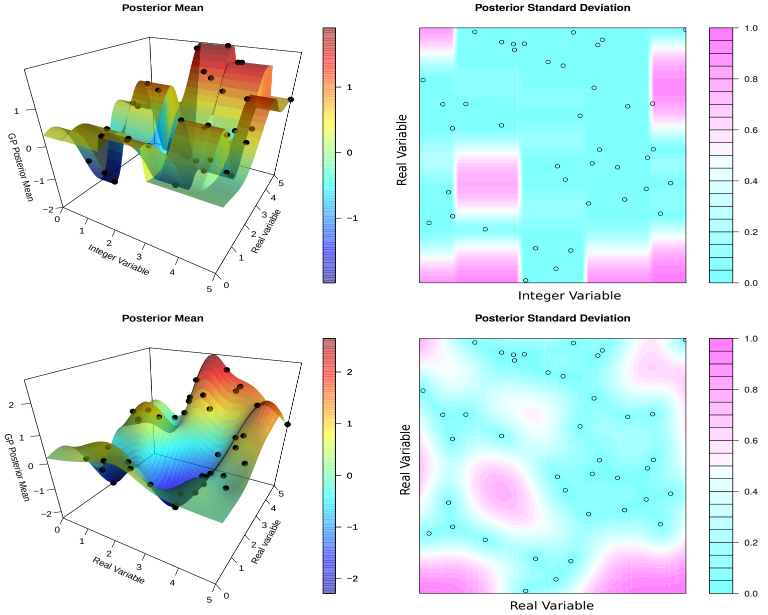






Visualizing a GP under the *proposed approach*



Applications of Bayesian Optimization

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- I have used BO in an optimization of a Genetic Algorithm to optimize the wave energy retrieved in a real experiment in USA.
- I have also applied it in an undergraduate thesis in cooking recipes with amazing results!

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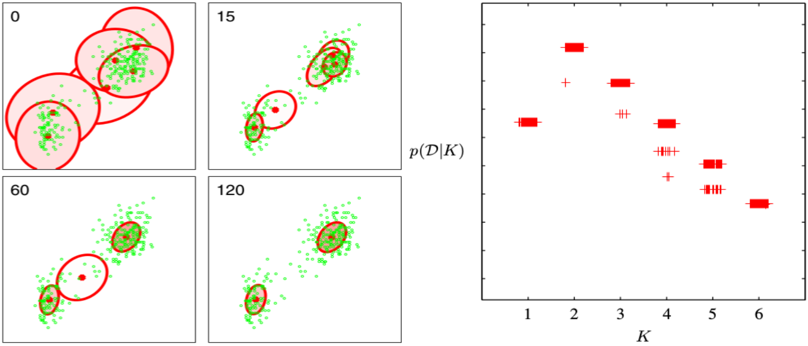

- **Bayesian inference** automatically makes the **trade-off between model complexity and fitting the data**. **No overfitting** by considering a large K and **maximizing the lower bound**!

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Ideas for DarkMachines unsupervised learning project

- This technique could be refined using **Bayesian Optimization** having in count not only one but several objectives and constraints.
- **Gaussian Processes** have also been applied for unsupervised learning with amazing results with the **Gaussian Process Latent Variable Model** (and related approaches) that I think that would be a more advanced approach than the **Variational Mixture of Gaussians**.

References

- Proposed initial Approach: **Variational Mixture of Gaussians**. Nasrabadi, Nasser M. "Pattern recognition and machine learning." Journal of electronic imaging 16.4 (2007): 049901. Section 10.2. Recommended: Read chapter 10.

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- Proposed Approach: **Gaussian Process Latent Variable Model**. Lawrence, Neil. "Probabilistic non-linear principal component analysis with Gaussian process latent variable models." Journal of machine learning research 6.Nov (2005): 1783-1816.
- Enhanced Proposed Approach, **Bayesian Gaussian Process Latent Variable Model**. Titsias, Michalis, and Neil D. Lawrence. "Bayesian Gaussian process latent variable model." Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics. 2010.

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