Bayesian optimization - Lecture 1

Hrvoje Stojic

May 25, 2017

The roadmap

The problem

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- What are (dis)advantages of the usual approaches?

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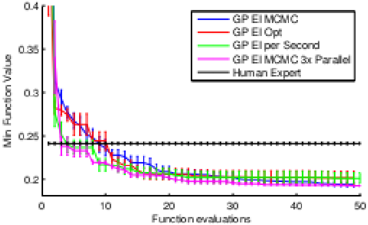
  - Optimizing SMBO can be a hard problem
  - Hence, when optimizing costly models, i.e. when time or number of evaluations is very valuable

The main goal - Automated statistician and hyperparameter tuning

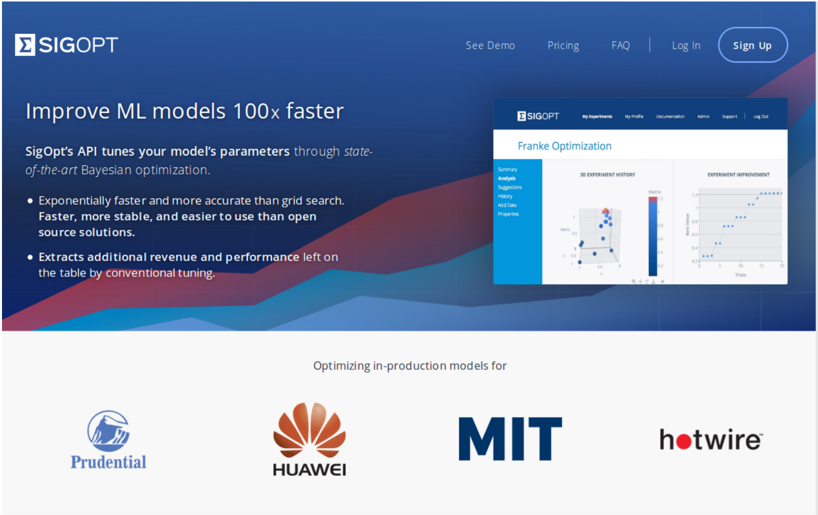


	convex	MRBI
TPE	**14.13** ± 0.30 %	**44.55** $\pm 0.44\%$
GP	$16.70 \pm 0.32\%$	$47.08 \pm 0.44\%$
Manual	$18.63 \pm 0.34\%$	$47.39 \pm 0.44\%$
Random	18.97 ± 0.34 %	$50.52 \pm 0.44\%$

Table 2: The test set classification error of the best model found by each search algorithm on each problem. Each search algorithm was allowed up to 200 trials. The manual searches used 82 trials for **convex** and 27 trials **MRBI**.

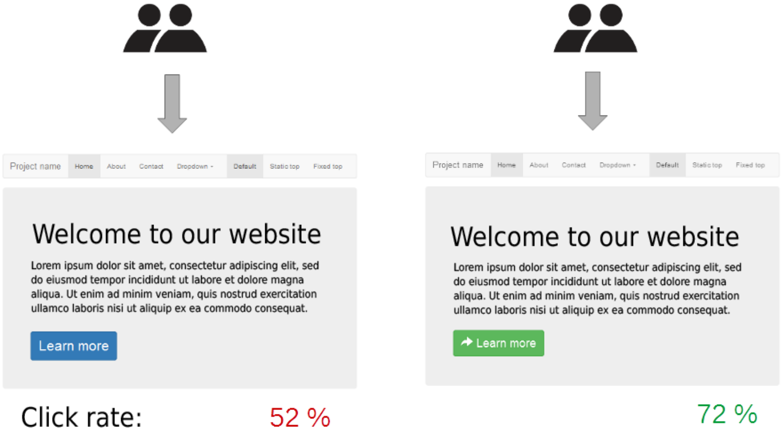
Source: Snoek et al 2012; Bergstra et al 2011

Entrepreneurship



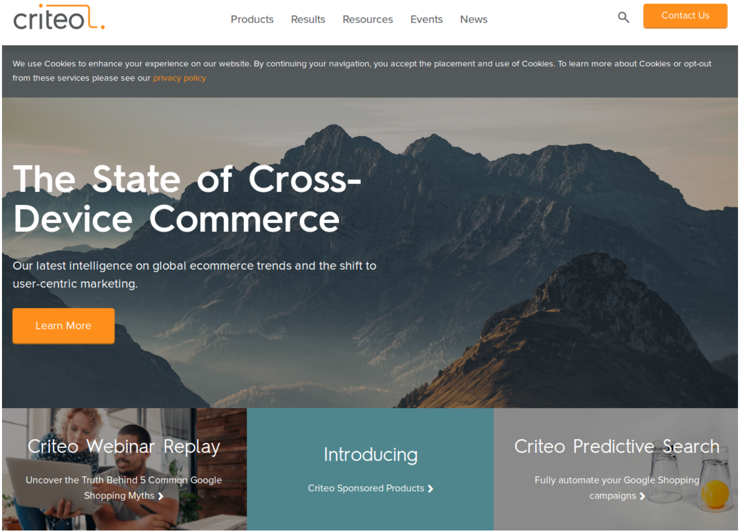
Source: SigOpt webpage

Bonus - A/B testing



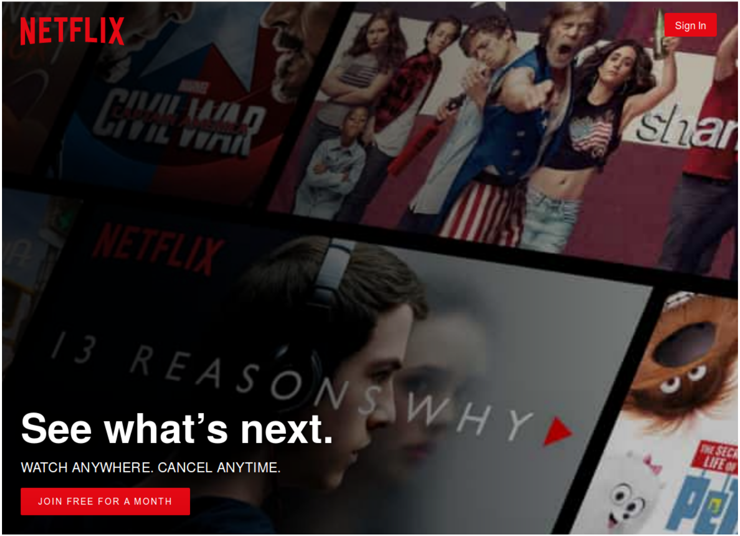
Source: Wikipedia

Bonus - Recommender systems and ad placement



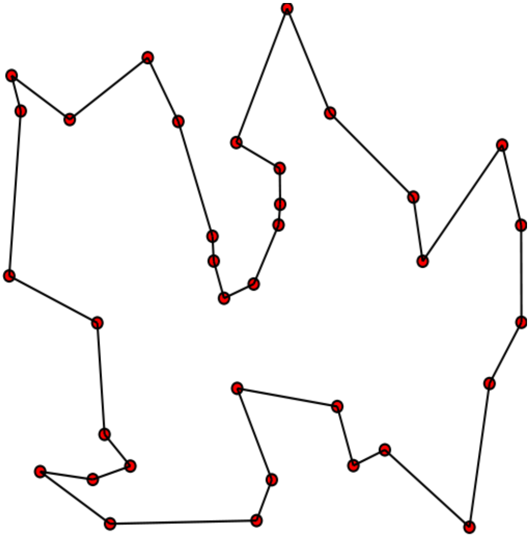
Source: Criteo webpage

Bonus - Preference learning and interactive user interfaces



Source: Netflix webpage

Bonus - Combinatorial optimization



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  - Agents, environments, rewards, states, MDPs
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- Extensions and applications

References

- Reinforcement learning
  - Sutton, R., & Barto, A. (2017). Introduction to Reinforcement Learning (book free of charge: www.incompleteideas.net/sutton/book/the-book.html)
  - D. Silver's lectures (videos and slides: www0.cs.ucl.ac.uk/staff/D.Silver/web/Teaching.html)
- Gaussian Processes
  - Rasmussen, C. E., & Williams, C. K. I. (2006). Gaussian processes for machine learning. MIT Press. (book free of charge: www.gaussianprocess.org/gpml/)
  - Karl Rasmussen's lectures
  - Nando De Freitas' lectures (videos and slides: www.youtube.com/user/ProfNandoDF/videos)

References

- Bayesian optimization

  - Shahriari, B., Swersky, K., Wang, Z., Adams, R. P., & de Freitas, N. (2016). Taking the Human Out of the Loop: A Review of Bayesian Optimization. Proceedings of the IEEE, 104(1), 148–175.
  - Snoek, J., Larochelle, H., & Adams, R. P. (2012). Practical Bayesian Optimization of Machine Learning Algorithms. Advances in Neural Information Processing Systems, 2951-2959.

Software

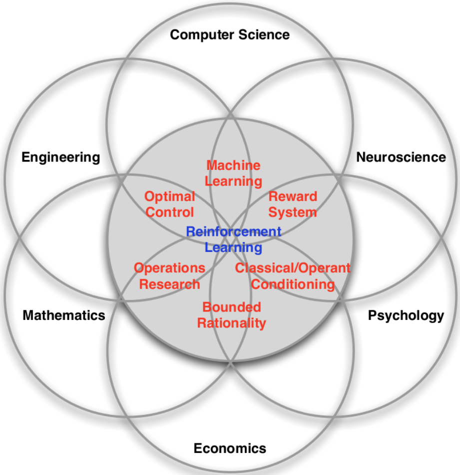
- R packages
  - GPfit, gptk, FastGP
  - rBayesianOptimization (Yan)
  - DiceOptim (Roustant et al., 2012)
- Python libraries
  - scikit-learn
  - Hyperopt (Bergstra et al., 2011)
  - Spearmint (Snoek et al., 2014)
- Matlab
  - GPML (Rasmussen)
- C++
  - BayesOpt (Martinez-Cantin, 2014)
- Java
  - SMAC (Hutter et al., 2011)

Practicalities

- Contact:
  - h.stojic_at_ucl.ac.uk
  - Office hours by video calls
- Evaluation:
  - No exam
  - Individual problem set (two coding exercises): 40%
  - Group projects: 60%
  - Deadline: June 20

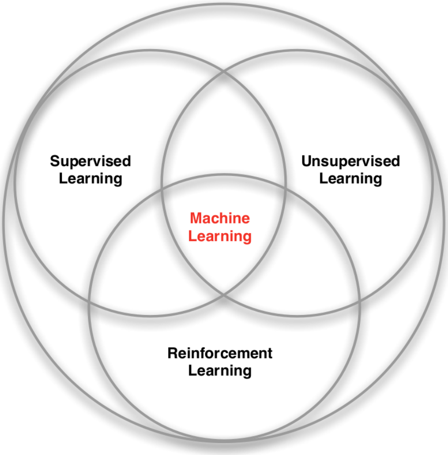
Introduction to Reinforcement Learning

Interdisciplinary area



Source: David Silver lectures

Relation to other types of learning



Source: David Silver lectures

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- Agent receives rewards
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- Examples
  - Robots, autonomous vehicles
  - Managing investment portfolio
  - Optimizing the data centres

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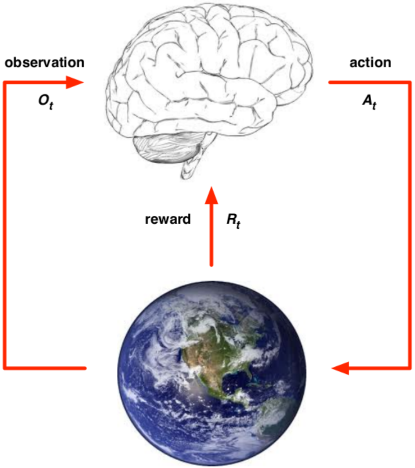
- Examples
  - Pain if you lose a body part, satisfaction from food
  - Negative reward for moving in the gridworlds
  - Positive/negative reward for increasing/decreasing score in Atari videogames

Agent and environment



Source: David Silver lectures

History and State

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- **The history** is the sequence of observations, actions, rewards

$$H_t = O_1, R_1, A_1, ..., A_{t-1}, O_t, R_t$$

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    - E.g. estimate function in parametric way and keep parameters

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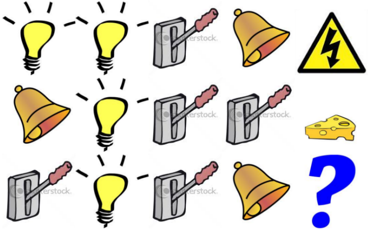

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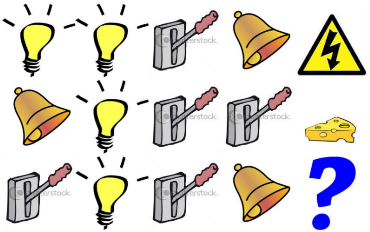

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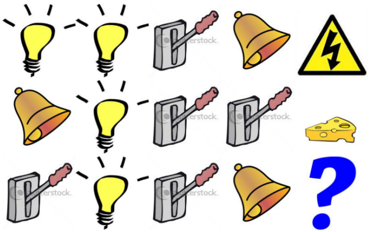

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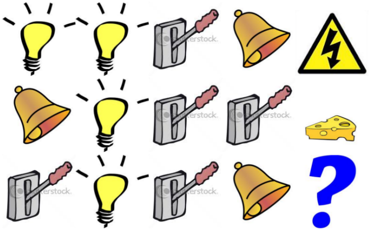

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  - Agent can observe environment state $O_t = S_t^a = S_t^e$
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  - E.g. investment agent observes prices, but not trends etc

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- **Model**: agent's representation of the environment, predicts
  - What the environment will do next
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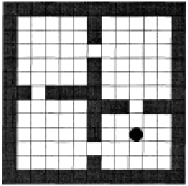
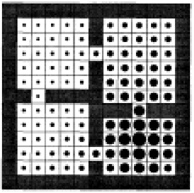
  - The next reward: $\mathcal{R}^a_s = E[R_{t+1}|S_t = s, A_t = a]$

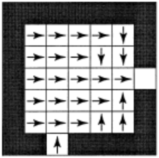
Gridworld example



Initial values



Iteration #5



Target Hallway

Source: Sutton, Precup & Singh (1999). Between MDPs and semi-MDPs: A framework for temporal abstraction in reinforcement learning. Artificial Intelligence, 112 (1-2), 181-211.

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- Examples:
  - Going to a favourite restaurant (**exploitation**), or try a new restaurant (**exploration**)
  - Show the most successful ad (**exploitation**), or show a new ad (**exploration**)

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3. **Information state space search**
   - Considering agent's information in its state space
   - Lookahead to determine how information helps in maximizing rewards
   - Examples: Gittins indices (see Whittle, 1980), tractable approximation with Bayesian Adaptive Monte Carlo Planning (Guez, Silver, Dayan, 2012; 2014)