Bayesian optimization - part 1

Hrvoje Stojic

May 24, 2018

The roadmap

The problem

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- What are the hyperparameters and how do we optimize them?

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

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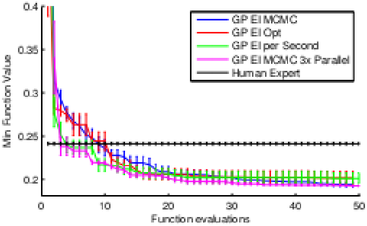
  - Optimizing SMBO can be a hard problem
  - Hence, when optimizing costly models, i.e. when time or number of evaluations is very valuable

The main goal: AutoML and hyperparameter tuning



	convex	MRBI
TPE	**14.13** ±0.30 %	**44.55** ±0.44%
GP	16.70 ± 0.32%	47.08 ± 0.44%
Manual	18.63 ± 0.34%	47.39 ± 0.44%
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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

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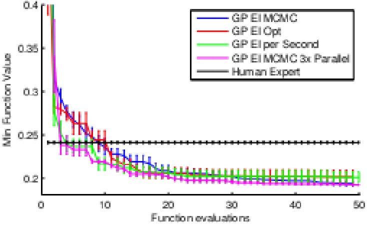

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- CIFAR 10: state of the art was test error of 18%, they achieved 14.98%
- MNIST rotated background images

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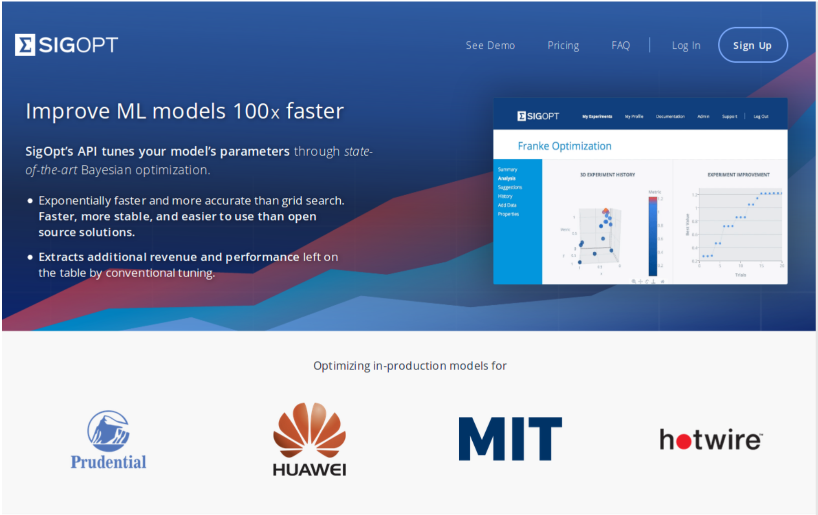
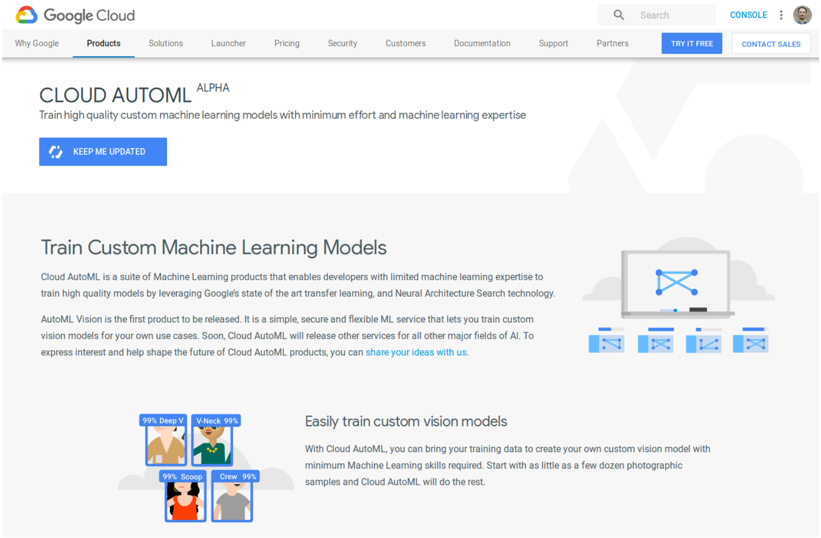
Bayesian optimization going mainstream



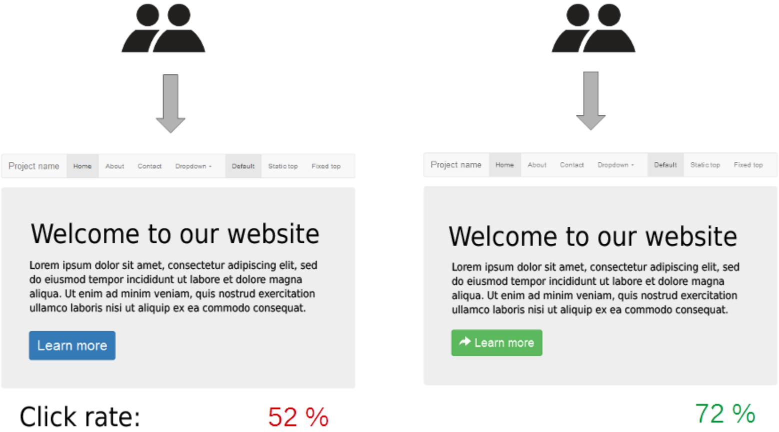
Source: SigOpt webpage

Google Cloud AutoML for computer vision



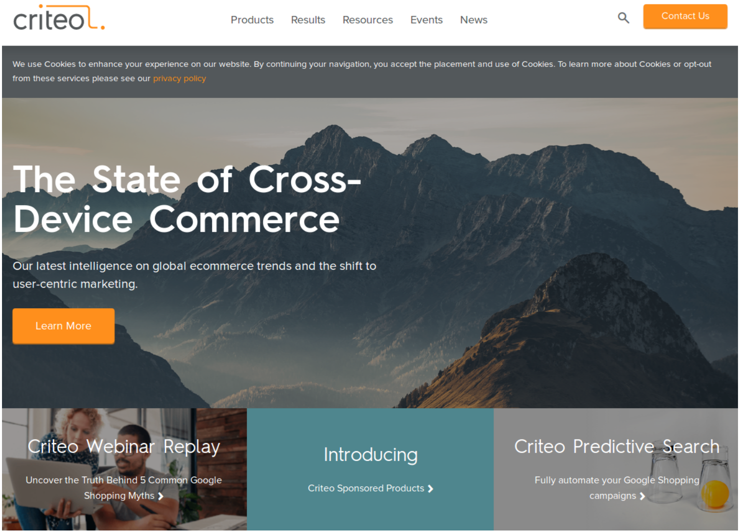
Source: Google AutoML webpage

Bonus - A/B testing



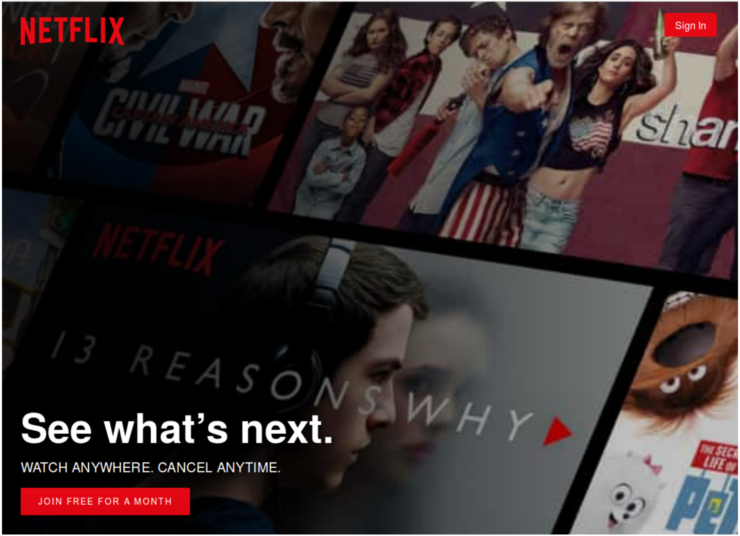
Source: Wikipedia

Bonus - Recommender systems and ad placement



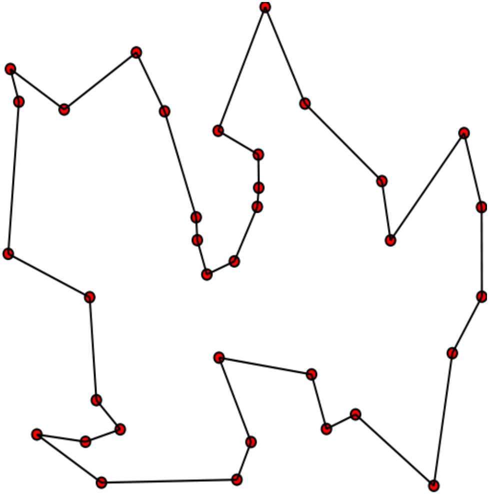
Source: Criteo webpage

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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  - Bayesian non-parametric: GP-UCB
- 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

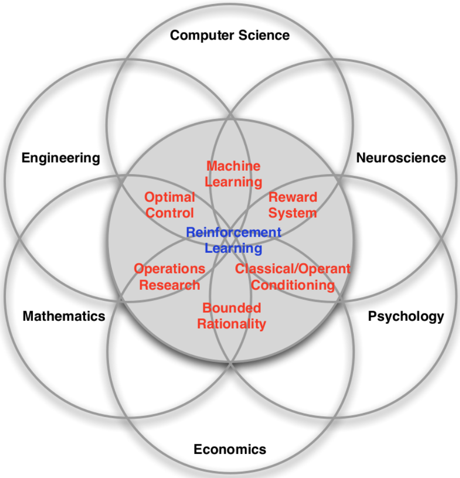
- R packages
  - GPfit, gptk, FastGP
  - rBayesianOptimization (Yan)
  - DiceOptim (Roustant et al., 2012)
- Python libraries
  - scikit-learn, auto-sklearn
  - Hyperopt (Bergstra et al., 2011)
  - Spearmint (Snoek et al., 2014)
- Matlab
  - GPML (Rasmussen)
- C++
  - BayesOpt (Martinez-Cantin, 2014)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

Practicalities

- Contact:
  - h.stojic_at_ucl.ac.uk
  - Office hours by video calls
- Evaluation:
  - No exam
  - Individual coding exercise: 40%
  - Group projects: 60%
  - Deadline: June 20

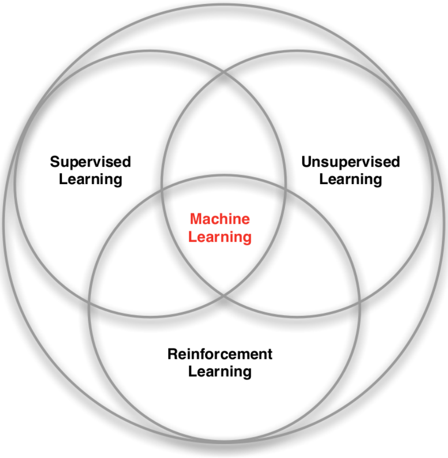
Introduction to Reinforcement Learning

Interdisciplinary area



Source: David Silver lectures

Relation to other types of learning



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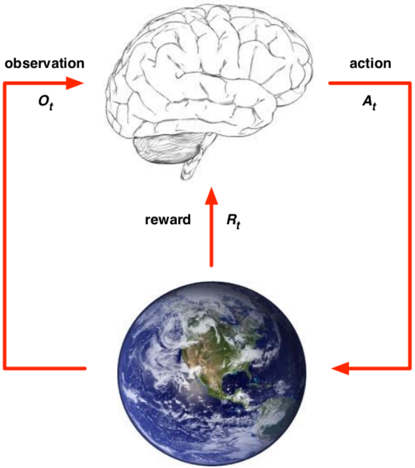
- Examples
  - Pain if you lose a body part, satisfaction from food
  - Negative reward for moving in the gridworlds
  - Positive/negative reward for increasing/decreasing score in Atari videogames

Agent and environment



Source: David Silver lectures

History and State

History and State

- **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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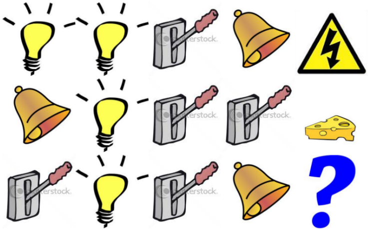

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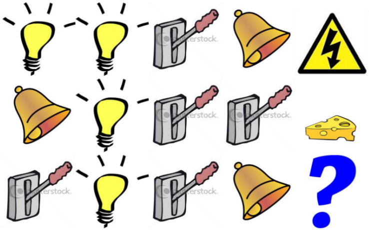

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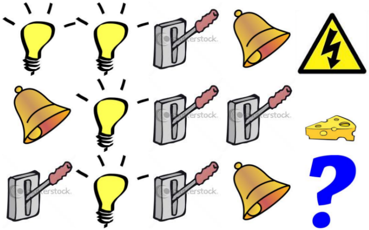

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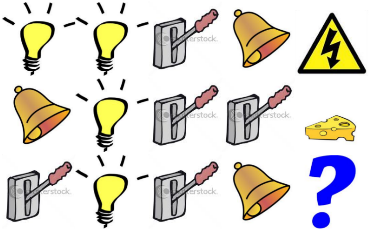

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- Complete sequence?

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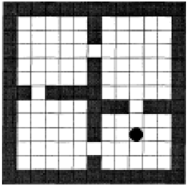
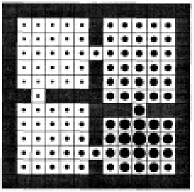
- **Model**: agent's representation of the environment, predicts
  - What the environment will do next
  - The next state: $\mathcal{P}^a_{ss'} = P[S_{t+1} = s'|S_t = s, A_t = a]$
  - The next reward: $\mathcal{R}^a_s = E[R_{t+1}|S_t = s, A_t = a]$

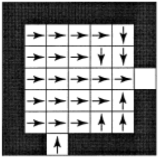
Gridworld example



Initial values



Iteration #5



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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Exploration exploitation problem

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- **Goal**: Gather enough information to make the best overall decisions
- 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)