Hyperparameter Optimization using Hyperopt

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About us

Yassine

- Data Scientist @ Qucit
- Centrale Paris & Cambridge
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Paul

- Data Scientist @ Qucit
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- Market finance in London
- Horse riding

Outline

1. Hyperparameters in Machine Learning
2. How to Choose Hyperparameters ?
3. Tree-structured Parzen Estimation Approach
4. Live-coding Example

1. Hyperparameters in Machine Learning

What are hyperparameters ?

Parameters:

Rent = $a_1 \times$ surface +

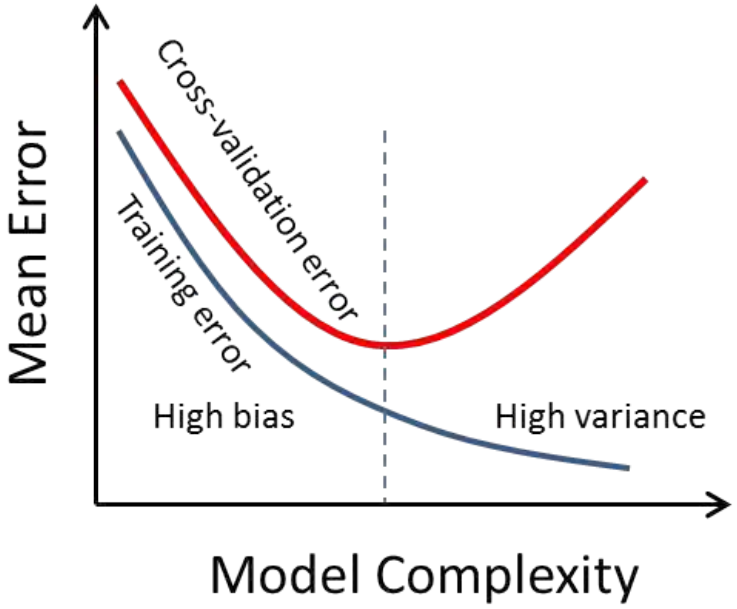
$a_2 \times$ distance to city center +

...

Hyperparameters:

$RMSE_{LASSO} = RMSE + \alpha \times (|a_1| + ...)$

The impact of hyperparameters



2. How to choose hyperparameters ?

Cross validation

Enable to choose the hyperparameter(s) with the best generalization capabilities making an efficient use of the data

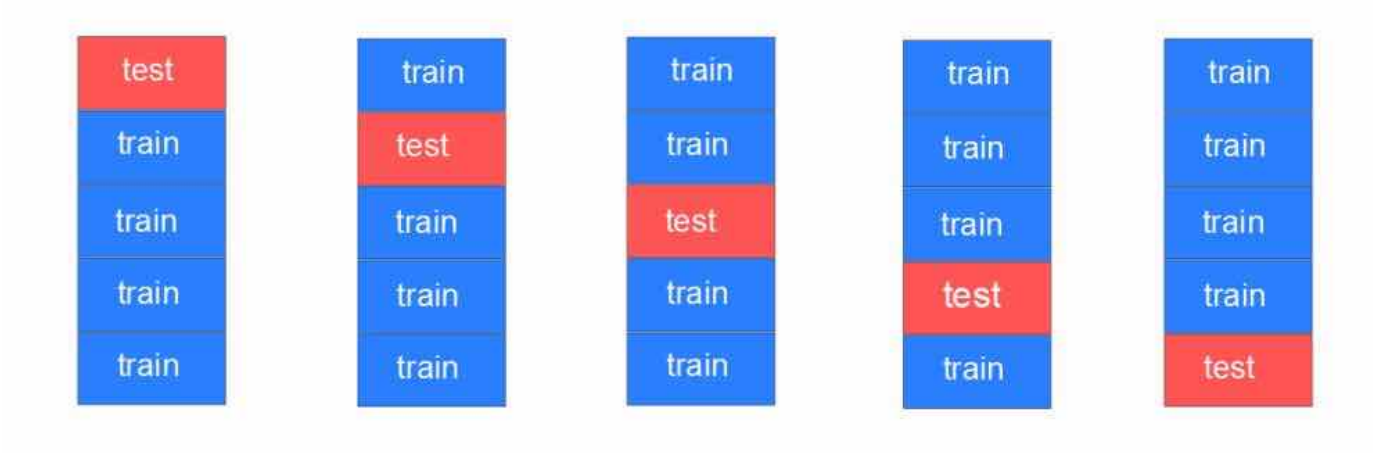
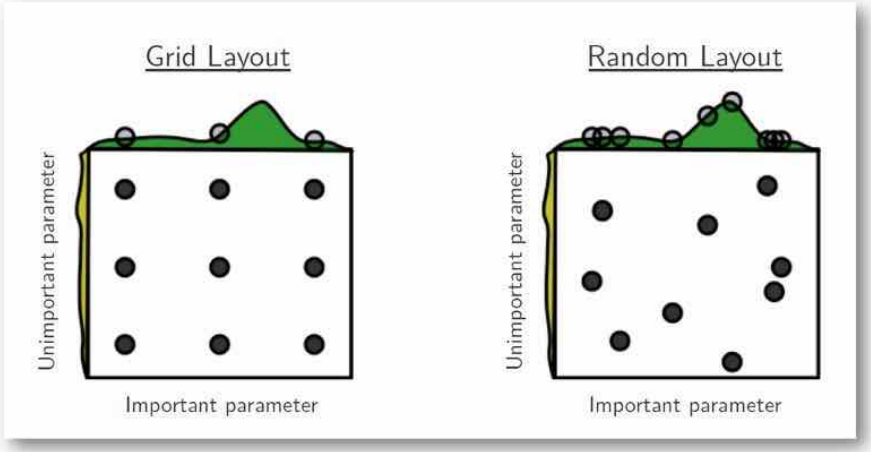


Figure credit: http://vinhkhuc.github.io/2015/03/01/how-many-folds-for-cross-validation.html

How to choose the points to cross-validate?

Grid search

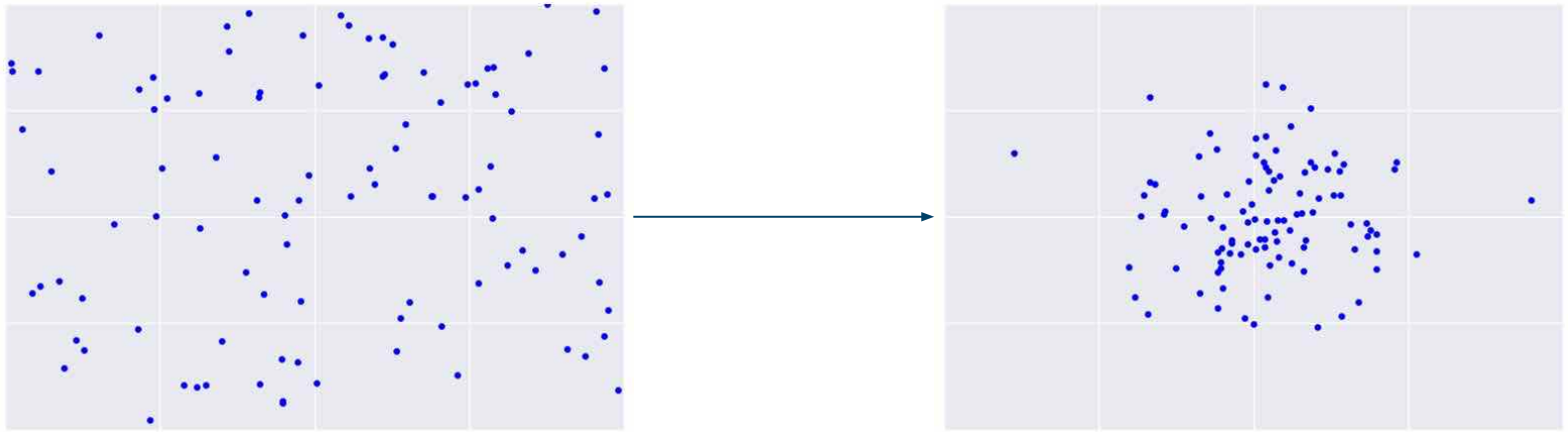
Random search



Credits: https://medium.com/rants-on-machine-learning/smarter-parameter-sweeps-or-why-grid-search-is-plain-stupid-c17d97a0e881#.db7060phq
https://districtdatalabs.silvrback.com/visual-diagnostics-for-more-informed-machine-learning-part-3

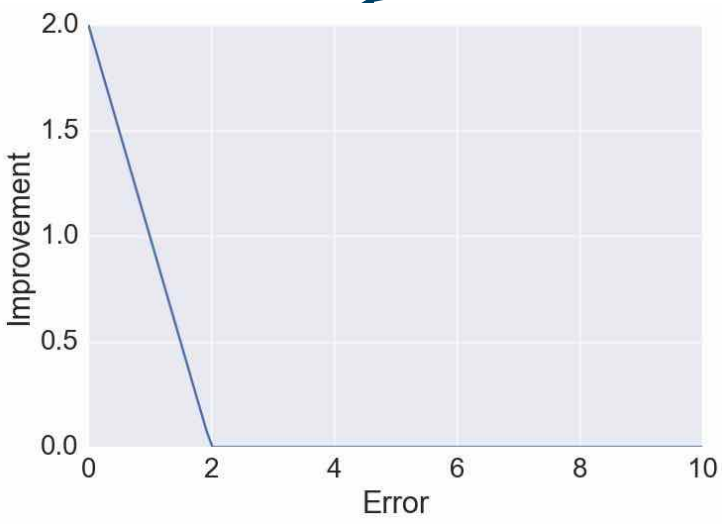
3. Tree-structured Parzen Estimation Approach

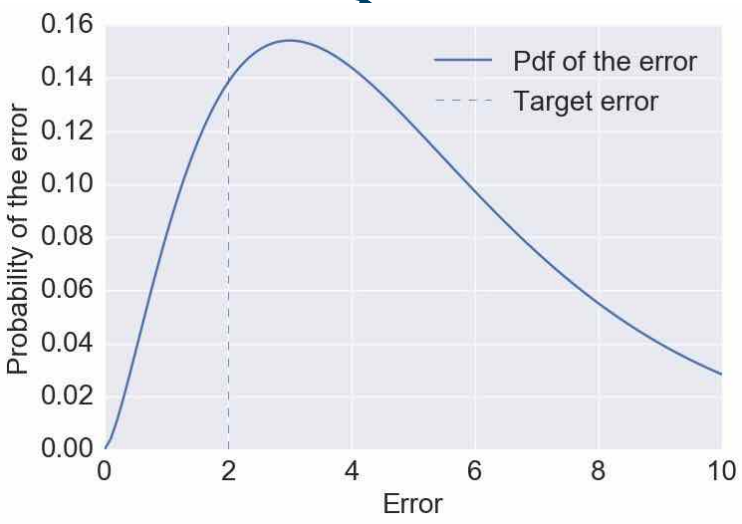
Sequential Model-based Global Optimization



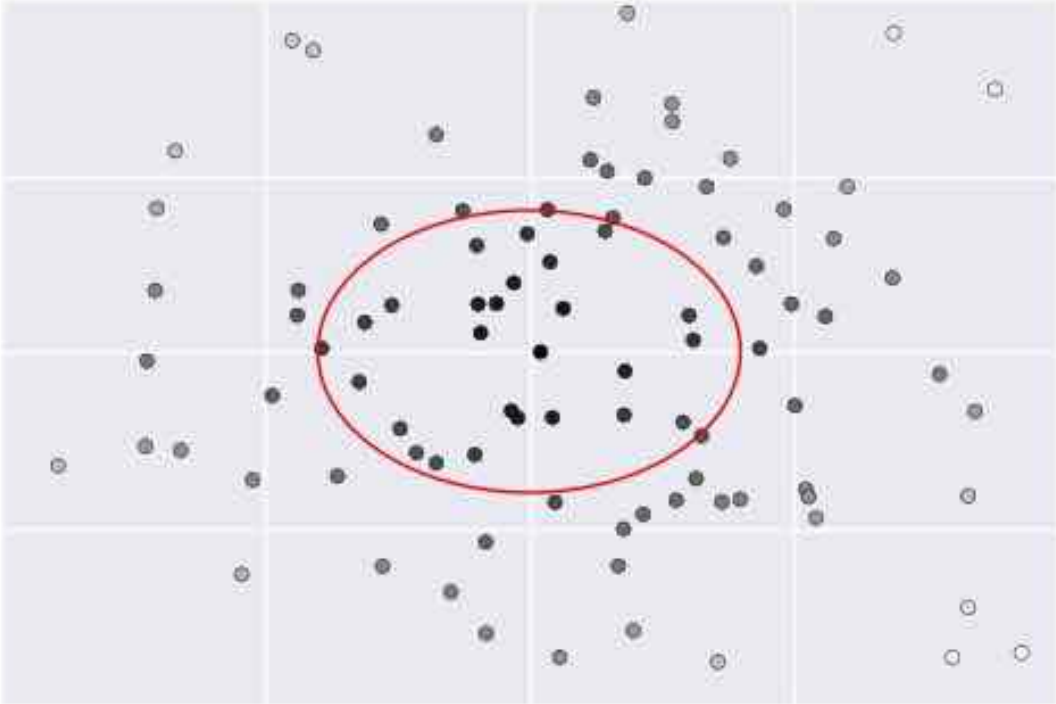
The Expected Improvement

$$EI_{\varepsilon^*}(a) = \int max(\varepsilon^* - \varepsilon, 0) p_M(\varepsilon|a) d\varepsilon$$



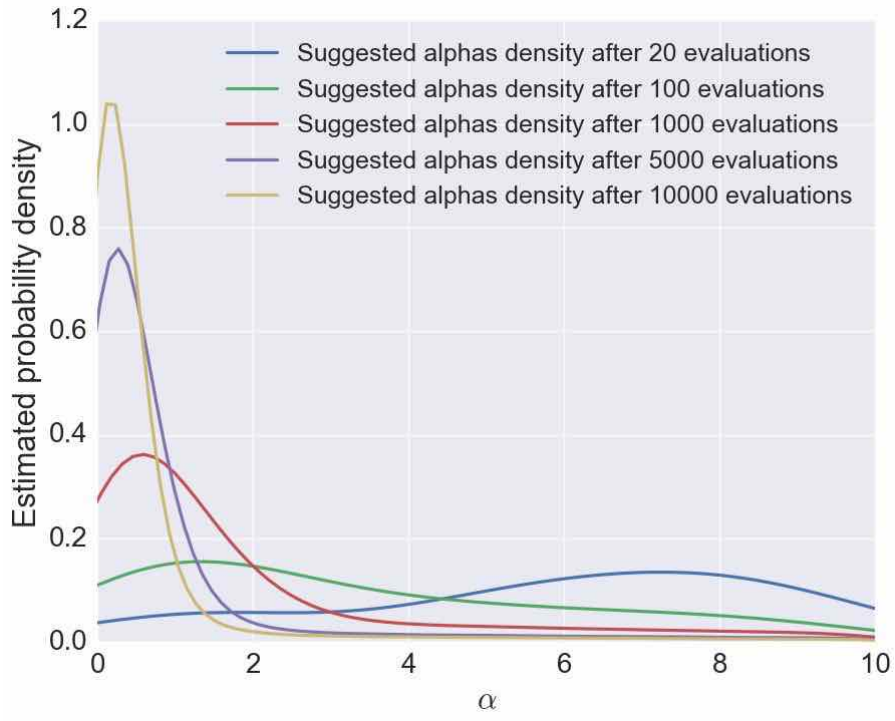


How to Optimize the EI ? (1)



How to Optimize the EI ? (2)

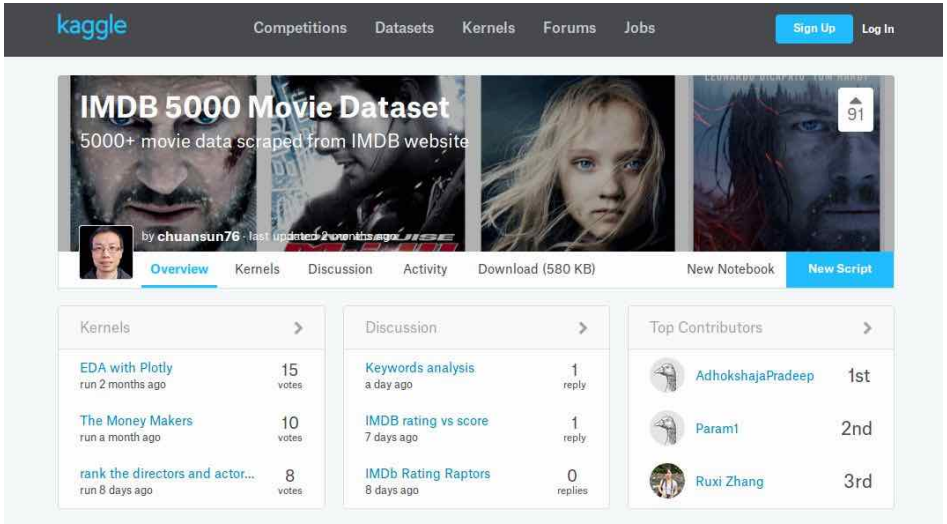
- Lasso model on the Boston Housing Dataset
- Distribution of the suggested αs



4. Live-coding Example

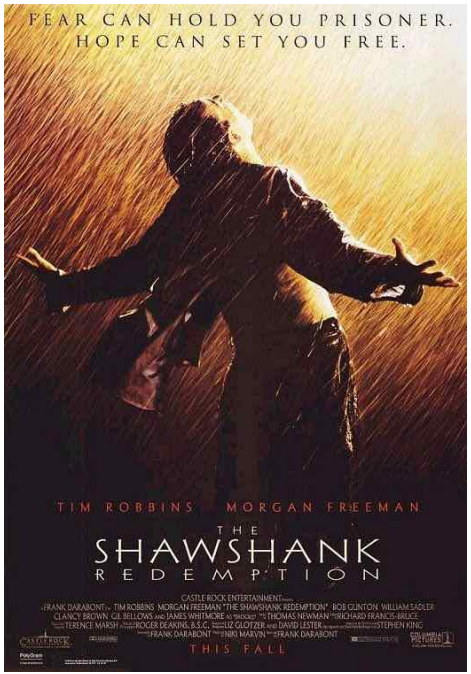
Description of the dataset

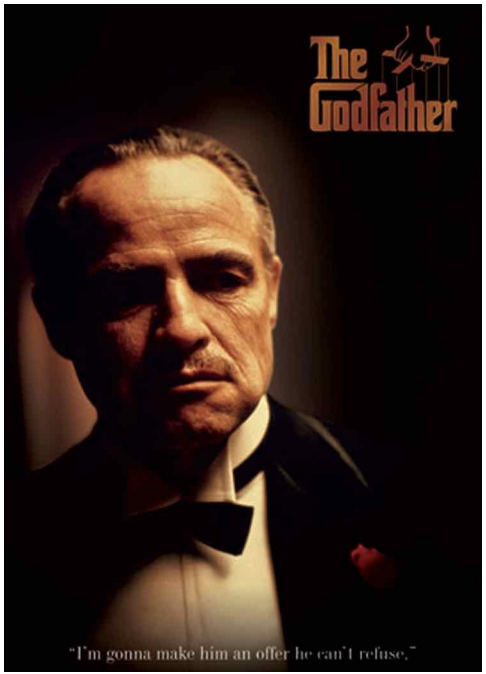
- IMDb dataset
- Dataset publicly available (from Kaggle)



Credits: screenshot, 24/10/2016, https://www.kaggle.com/deepmatrix/imdb-5000-movie-dataset

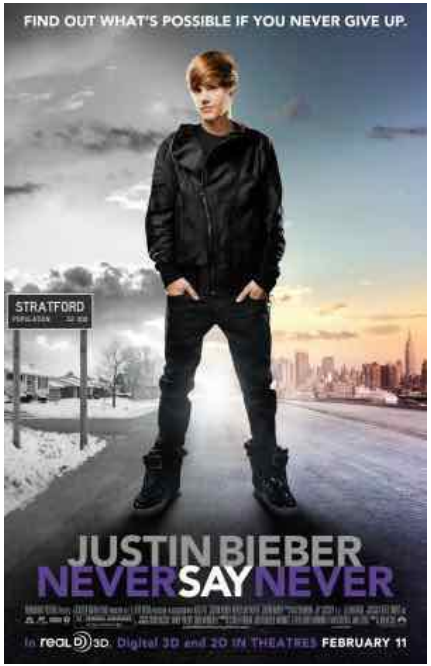
Movies having the best score

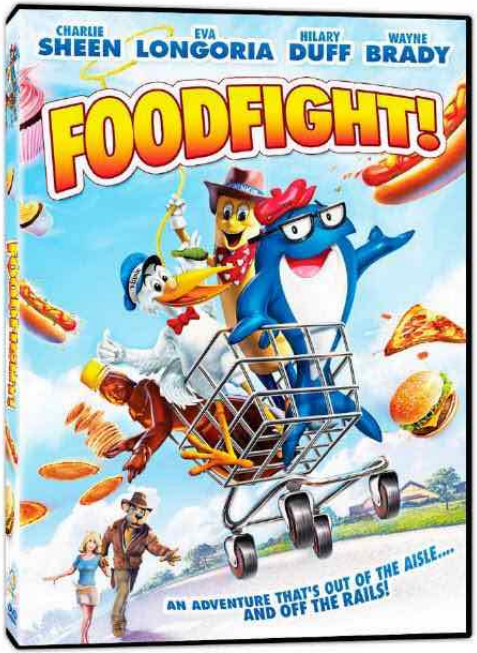


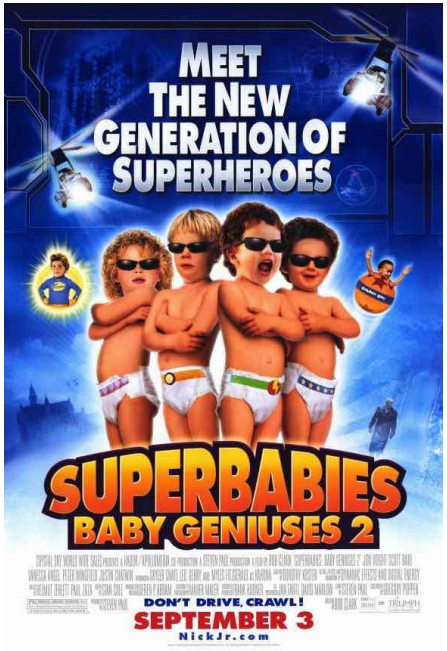


Credits: http://www.impawards.com/1974/towering_inferno.html, http://www.impawards.com/1994/shawshank_redemption_ver1.html, http://ruthusher.com/wordpress/wp-includes/js/godfather-poster

Movies having the worst score



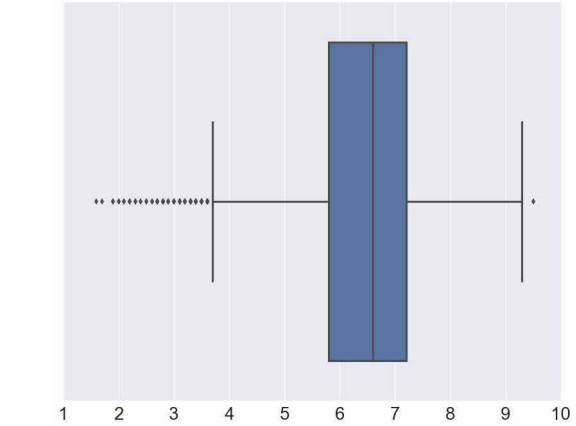


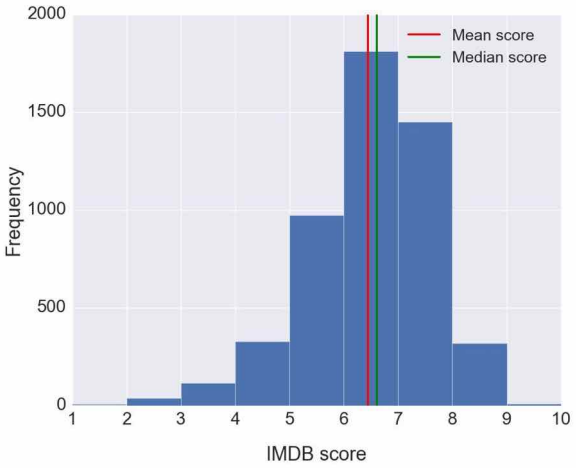


Credits: https://en.wikipedia.org/wiki/Justin_Bieber:_Never_Say_Never, http://www.movieinsider.com/m766/foodfight, http://www.moviepostershop.com/superbabies-baby-geniuses-2-movie-poster-2004

Task

- Predict the IMDB movie score
- Gradient Boosting algorithm (XGBoost package)
- 3 hyperparameters optimization strategies
  - A *naive* grid search
  - An *expert* grid search (*)
  - The TPE algorithm (hyperopt package)

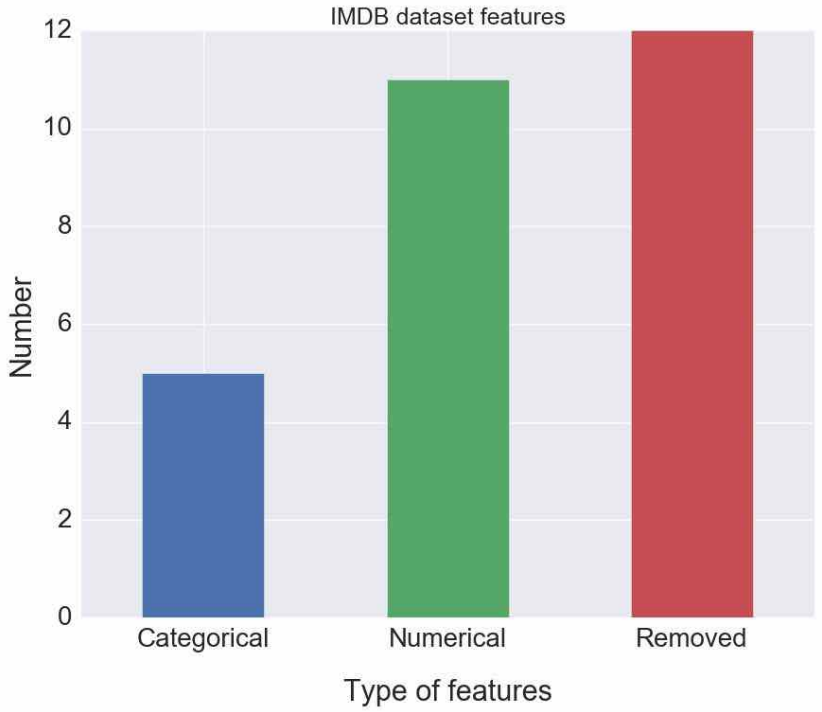




(*) http://blog.kaggle.com/2016/07/21/approaching-almost-any-machine-learning-problem-abhishek-thakur/

Features description

- **28 features:**
  - 14 movie-related
  - 4 review-related
  - 10 cast-related
- **16 kept:**
  - 11 numerical
  - 5 categorical
- **12 removed**



Live demo

Our code is available here:
https://github.com/yassineAlouini/hyperparameters-optimization-talk

Conclusion

- Outperforms the standard methods in most cases
- Search space matters
- Other Python libraries: Spearmint, BayesOpt, Scikit-Optimize
- Distributed optimization (using MongoDB)

Thanks for your attention.
Question time

Qucit is hiring!

References

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- https://conference.scipy.org/proceedings/scipy2013/pdfs/bergstra_hyperopt.pdf
- https://github.com/scikit-optimize
- http://jaberg.github.io/hyperopt/
- https://github.com/JasperSnoek/spearmint
- https://github.com/fmfn/BayesianOptimization
- http://xgboost.readthedocs.io/en/latest/
- http://www.cs.ubc.ca/~hutter/papers/13-BayesOpt_EmpiricalFoundation.pdf