Bias-variance decomposition Gradient boosting

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girafe ai

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Outline

1. Intuitions
2. Gradient boosting theory
3. Examples
4. Libraries
5. Feature importances
6. Hyperparameter optimization

Ensembling recap

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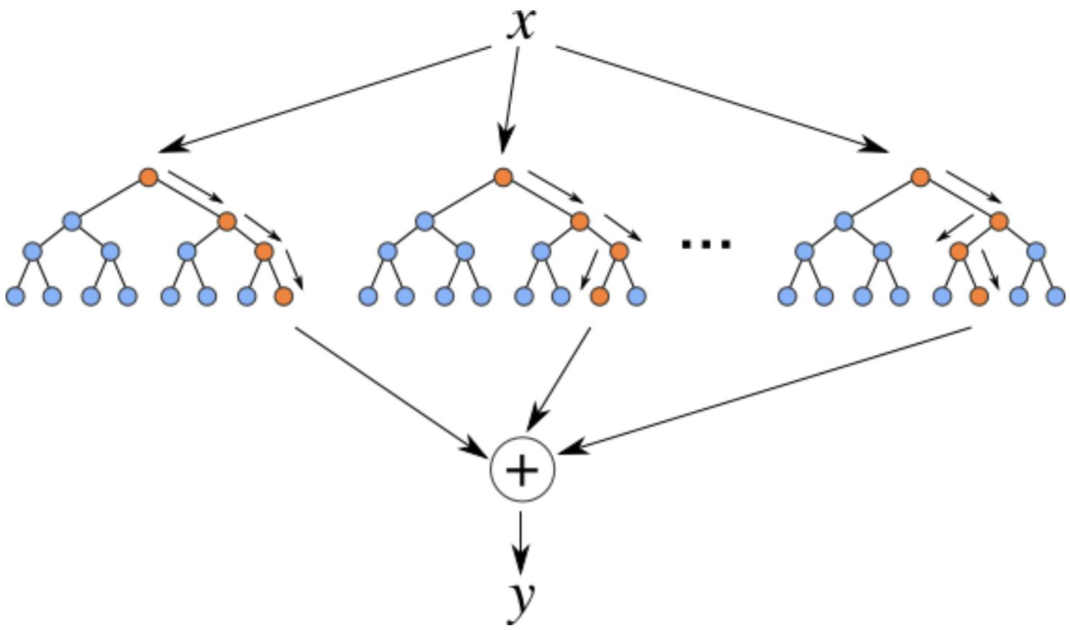
01

Random Forest

Bagging + RSM = Random Forest



Random Forest

- One of the greatest “universal” models
- There are some modifications: Extremely Randomized Trees, Isolation Forest, etc.

Bias-variance tradeoff

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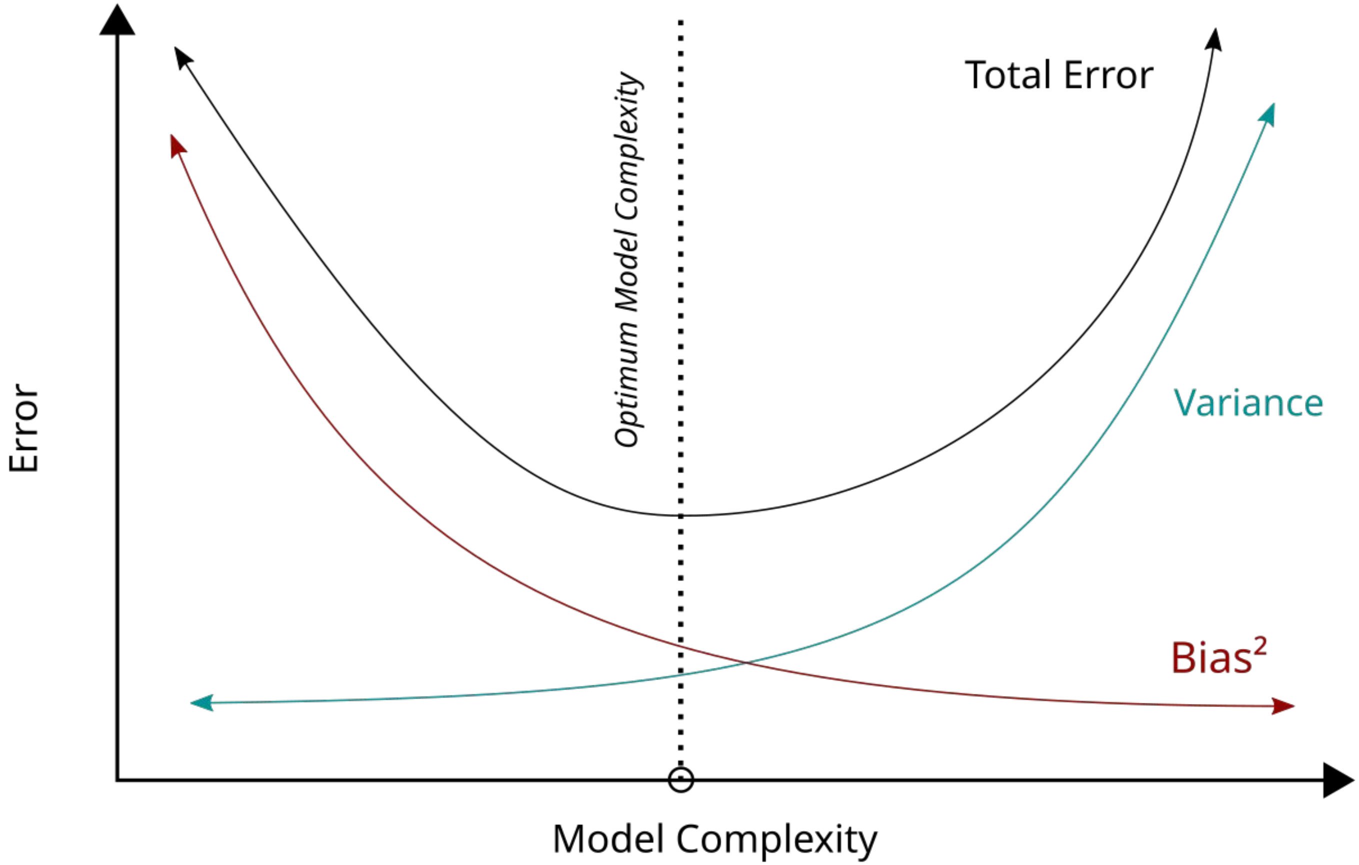
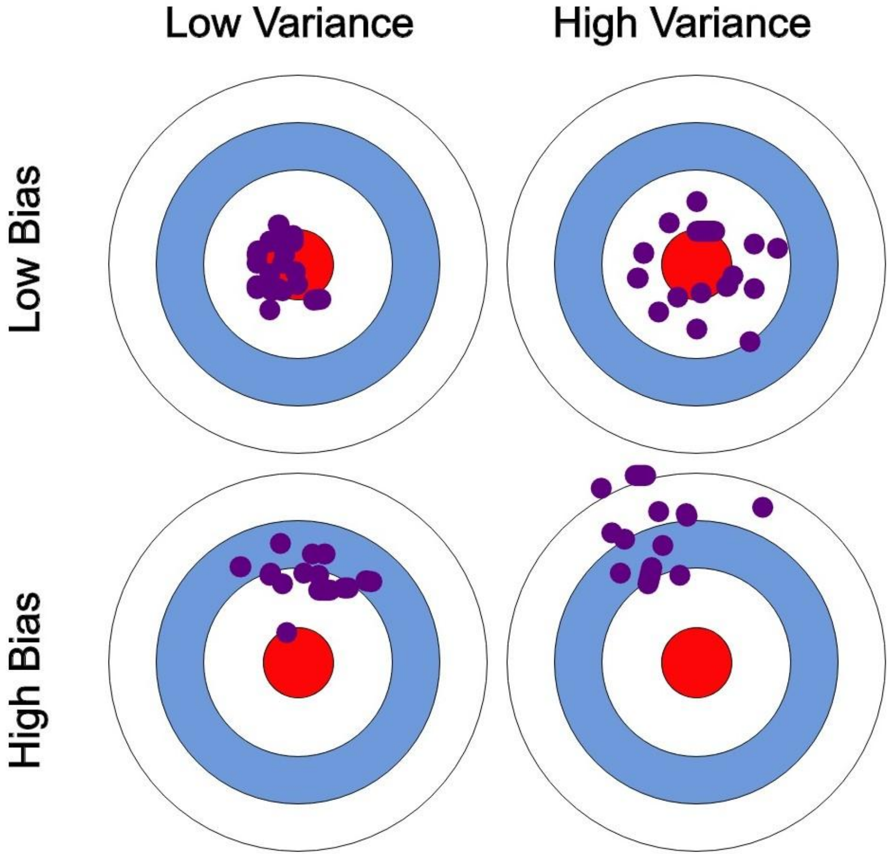
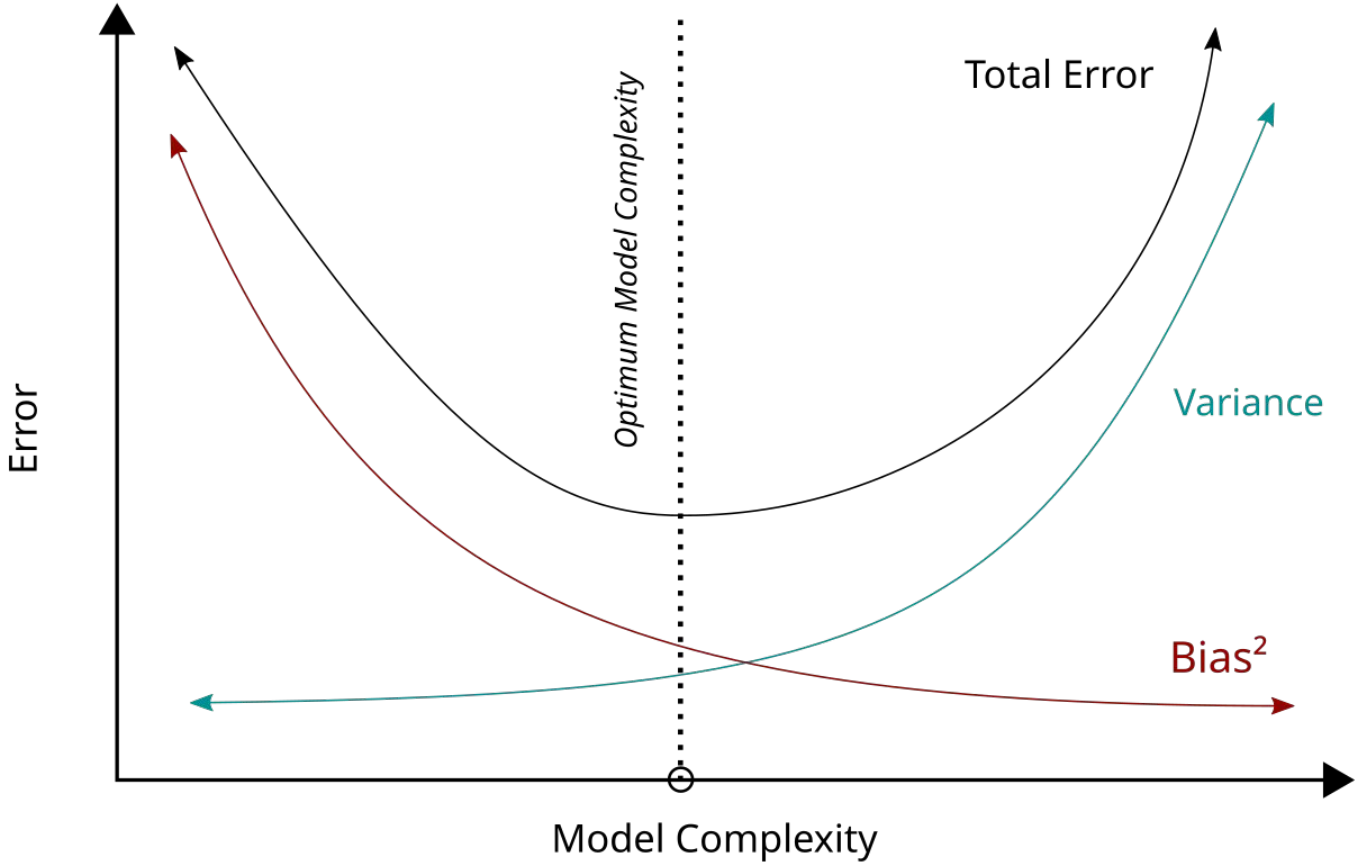
Bias-variance tradeoff



Bias-variance tradeoff



Bias-variance tradeoff



Boosting intuition

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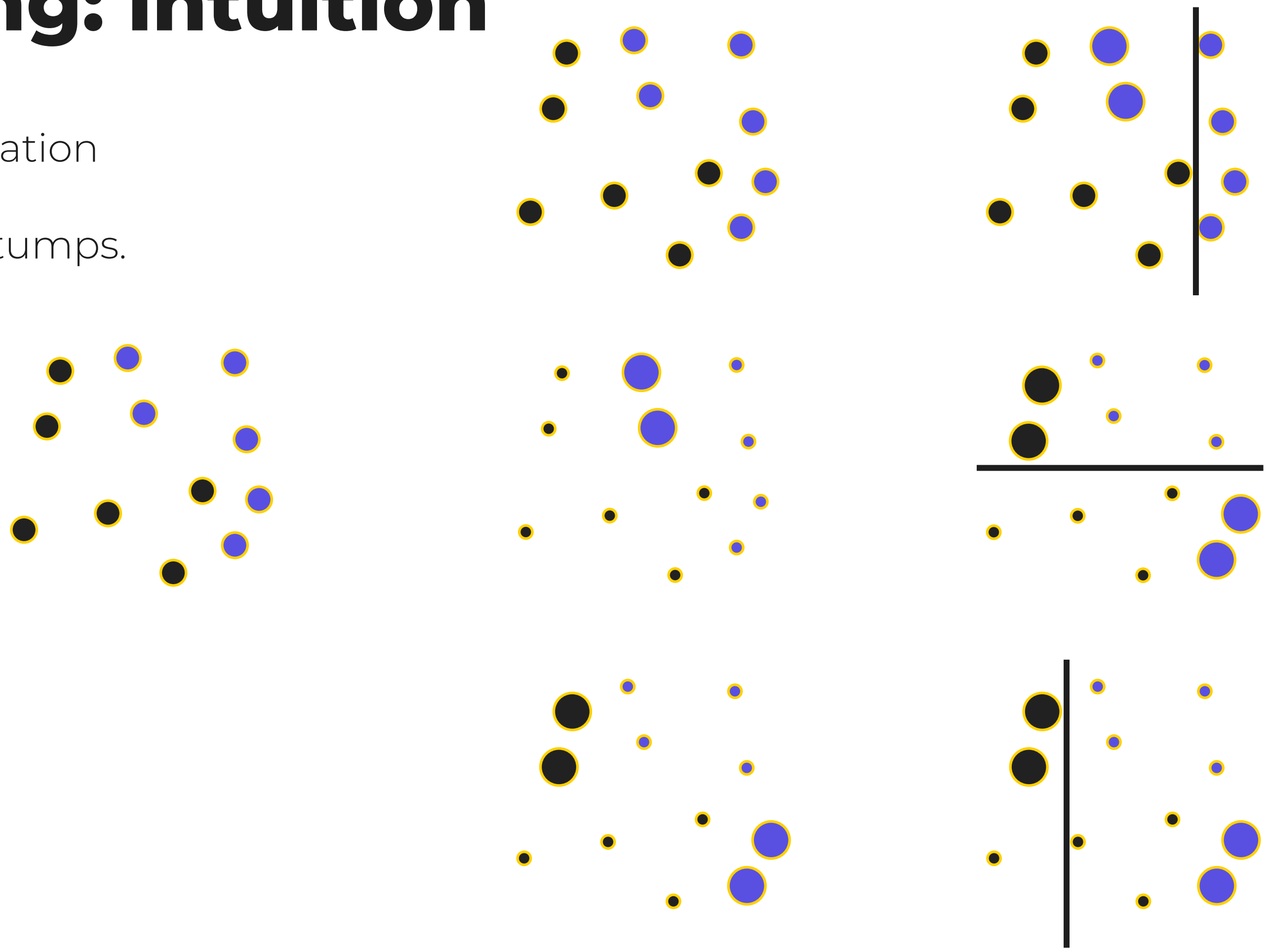
01

Boosting: intuition

Binary classification

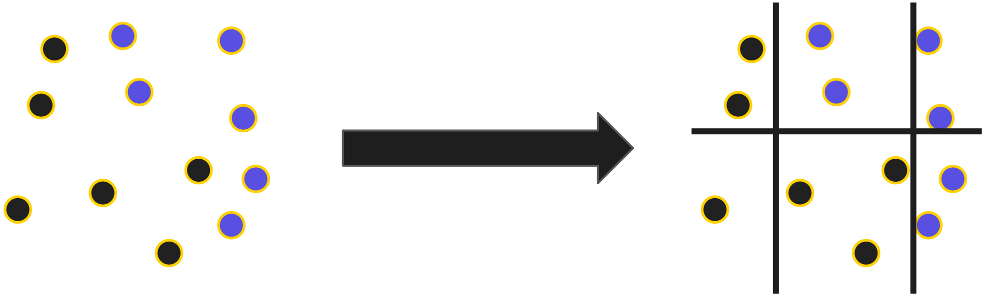
Use decision stumps.



Boosting: intuition

Binary classification

Use decision stumps.



Ensembles computation comparison

	Training	Inference
Bagging	parallel	parallel
Boosting	sequential	parallel

Gradient boosting theory

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Gradient boosting: theory

Denote dataset $\{(x_i, y_i)\}_{i=1,\dots,n}$, loss function $L(y, f)$.

Optimal model:

$$\hat{f}(x) = \underset{f(x)}{\arg\min}\ L(y, f(x)) = \underset{f(x)}{\arg\min}\ \mathbb{E}_{x,y}[L(y, f(x))]$$

Let it be from parametric family:

$$\hat{f}(x) = f(x, \hat{\theta}),$$

$$\hat{\theta} = \underset{\theta}{\arg\min}\ \mathbb{E}_{x,y}[L(y, f(x, \theta))]$$

Gradient boosting: theory

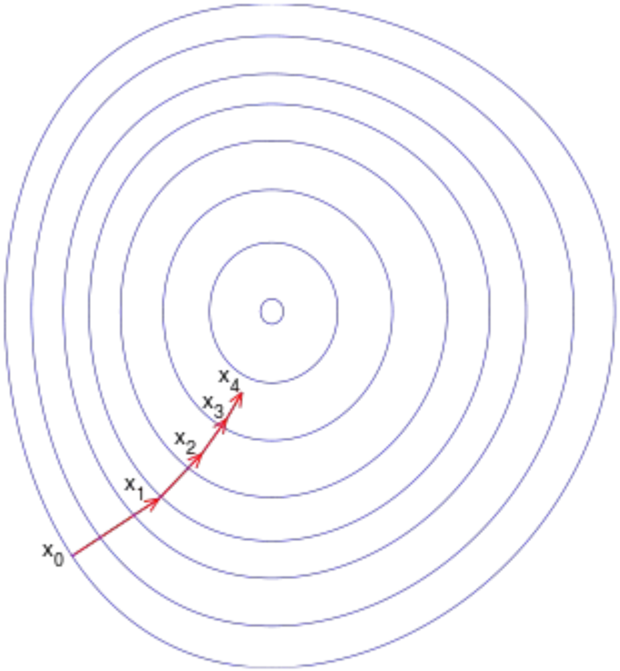
$$\hat{f}(x) = \sum_{i=0}^{t-1} \hat{f}_i(x),$$

$$(\rho_t, \theta_t) = \arg\min_{\rho,\theta} \mathbb{E}_{x,y}[L(y, \hat{f}(x) + \rho \cdot h(x, \theta))],$$

$$\hat{f}_t(x) = \rho_t \cdot h(x, \theta_t)$$

What if we could use gradient descent in space of our models?

Gradient boosting: theory



What if we could use gradient descent in space of our models?

Gradient boosting: theory

$$\hat{f}(x) = \sum_{i=0}^{t-1} \hat{f}_i(x),$$

$$r_{it} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f(x)=\hat{f}(x)}, \quad \text{for } i = 1, \ldots, n,$$

$$\theta_t = \arg\min_{\theta} \sum_{i=1}^{n} (r_{it} - h(x_i, \theta))^2,$$

$$\rho_t = \arg\min_{\rho} \sum_{i=1}^{n} L(y_i, \hat{f}(x_i) + \rho \cdot h(x_i, \theta_t))$$

Gradient boosting: theory

In linear regression case with MSE loss:

$$r_{it} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f(x)=\hat{f}(x)} = -2(\hat{y}_i - y_i) \propto \hat{y}_i - y_i$$

GB examples

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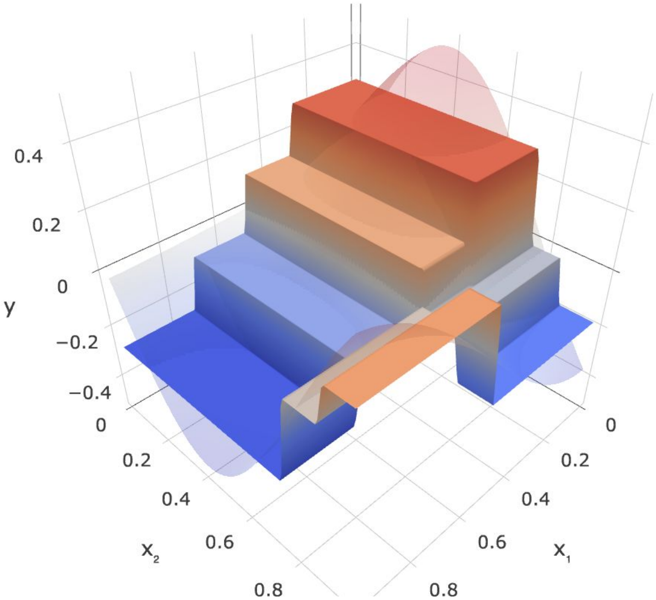
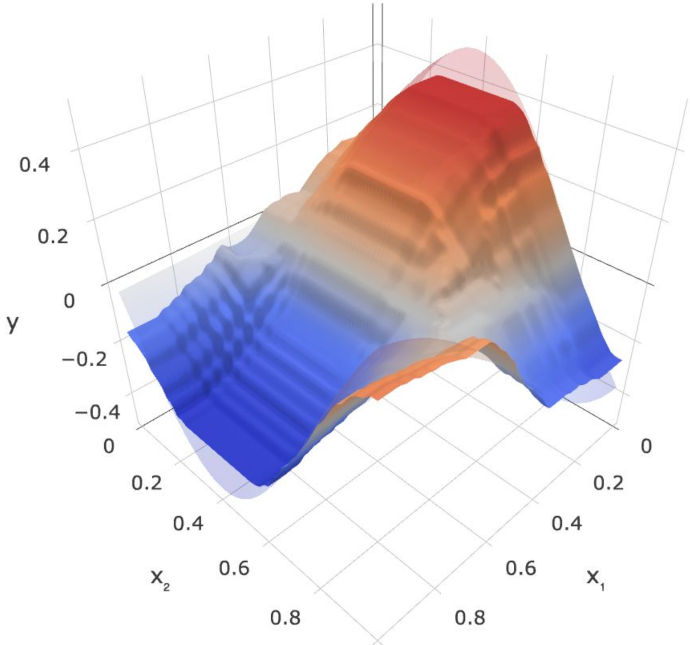
Beautiful demo



One tree



Boosting

http://arogozhnikov.github.io/2016/06/24/gradient_boosting_explained.html

Gradient boosting

What we need:

- Data
- Loss function and its gradient
- Family of algorithms (with constraints if necessary)
- Number of iterations M
- Initial value (GBM by Friedman): constant

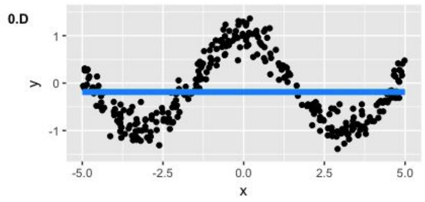
Gradient boosting: example

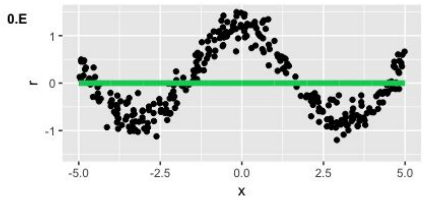
What we need:

- Data: toy dataset $y = cos(x) + \epsilon, \epsilon \sim \mathcal{N}(0, \frac{1}{5}), x \in [-5, 5]$
- Loss function: MSE
- Family of algorithms: decision trees with depth 2
- Number of iterations M = 3
- Initial value: just mean valu

https://habr.com/ru/company/ods/blog/327250/

Gradient boosting: example



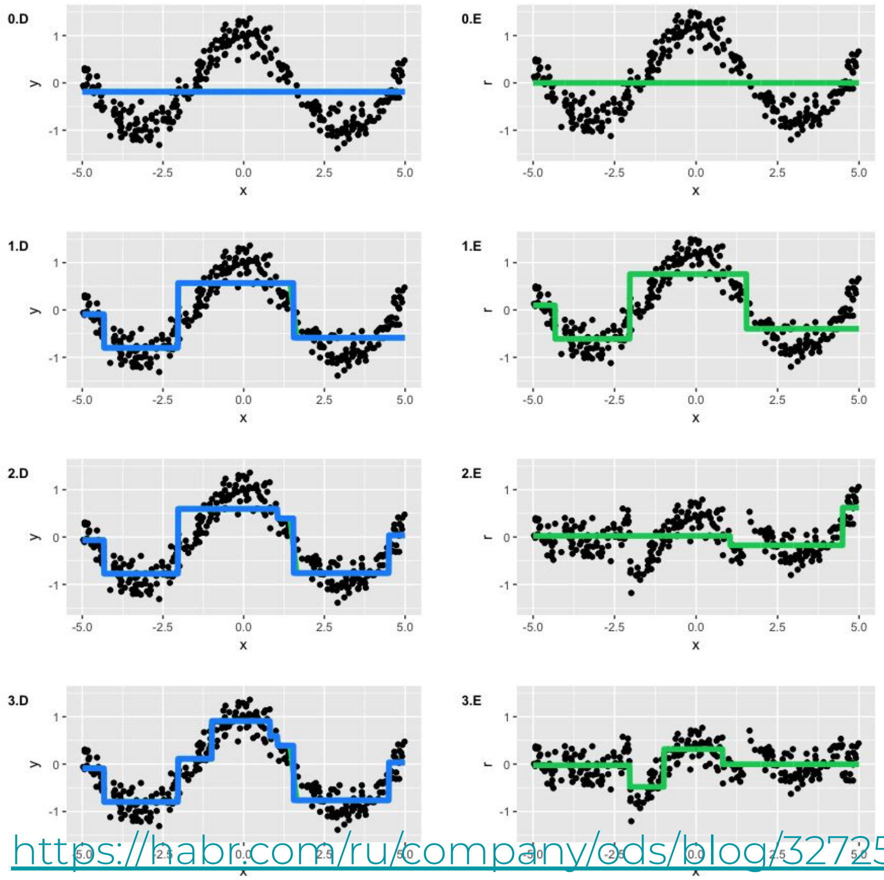


Left: full ensemble on each step.

Right: additional tree decisions.

https://habr.com/ru/company/ods/blog/327250/

Gradient boosting: example



Left: full ensemble on each step.

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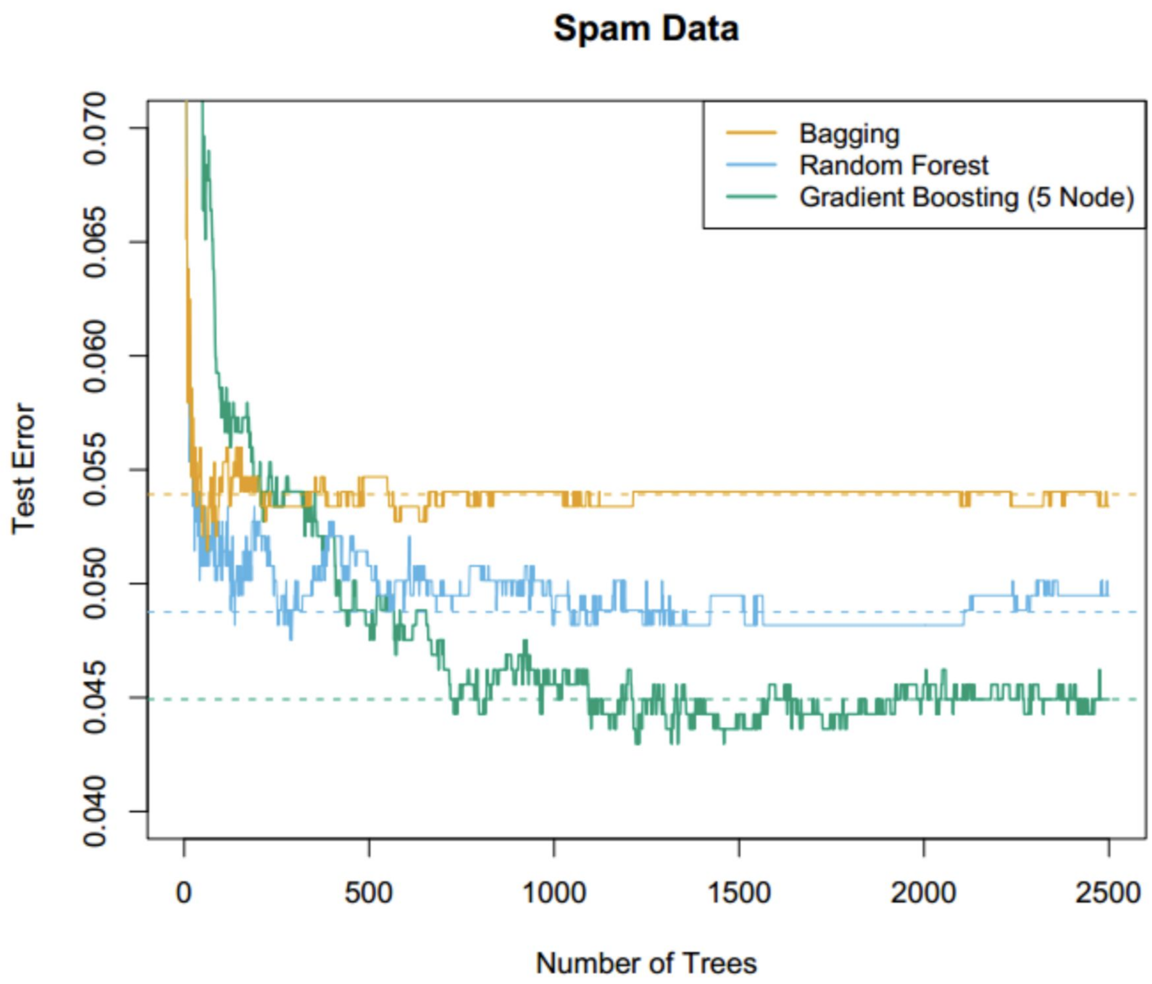
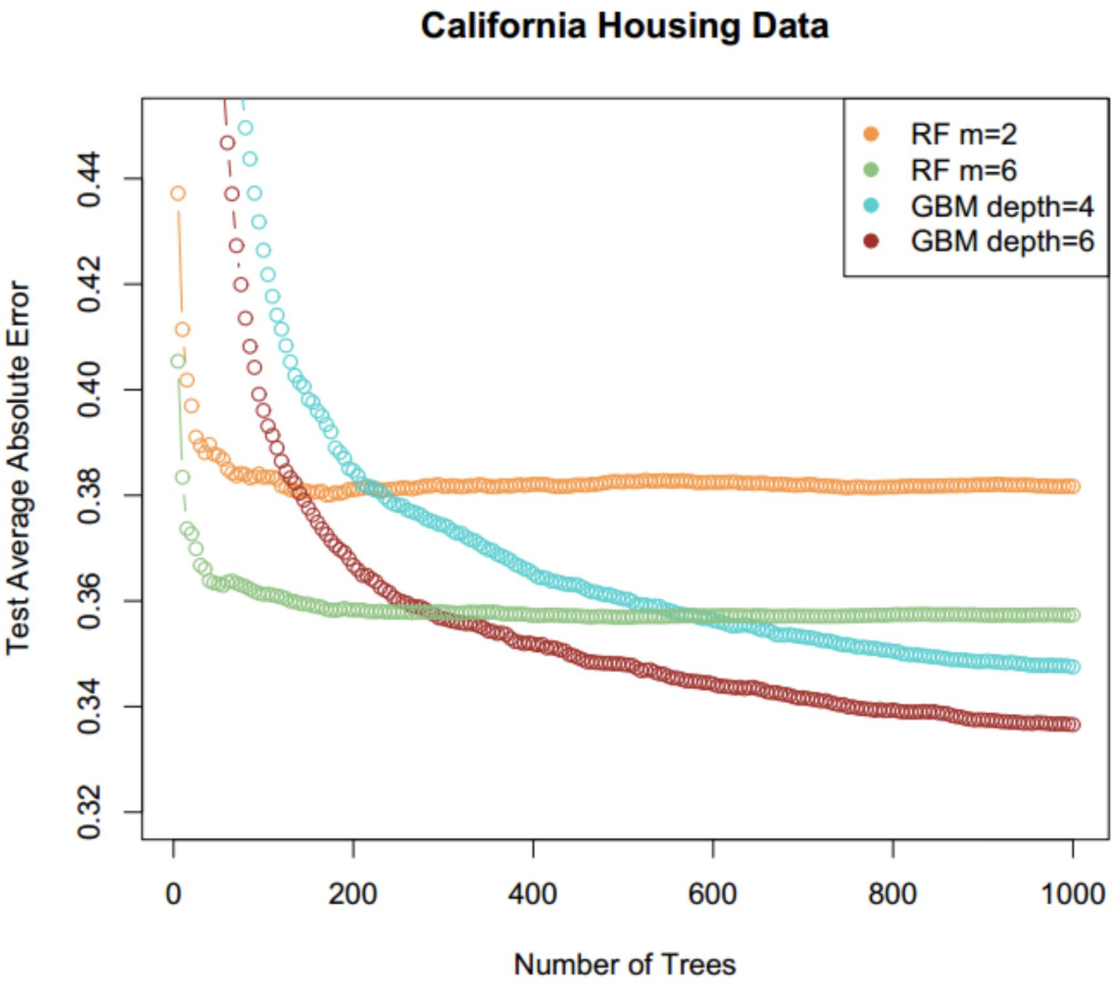

Spam Data
Bagging
Random Forest
Gradient Boosting (5 Node)
Test Error
0.040
0.045
0.050
0.055
0.060
0.065
0.070
0
500
1000
1500
2000
2500
Number of Trees


California Housing Data
RF m=2
RF m=6
GBM depth=4
GBM depth=6
Test Average Absolute Error
0.32
0.34
0.36
0.38
0.40
0.42
0.44
0
200
400
600
800
1000
Number of Trees

Parallelization

Which of the ensembling methods could be parallelized?

- Random Forest: parallel on the forest level (all trees are independent)
- Gradient boosting: parallel on one tree level

Libraries for GB

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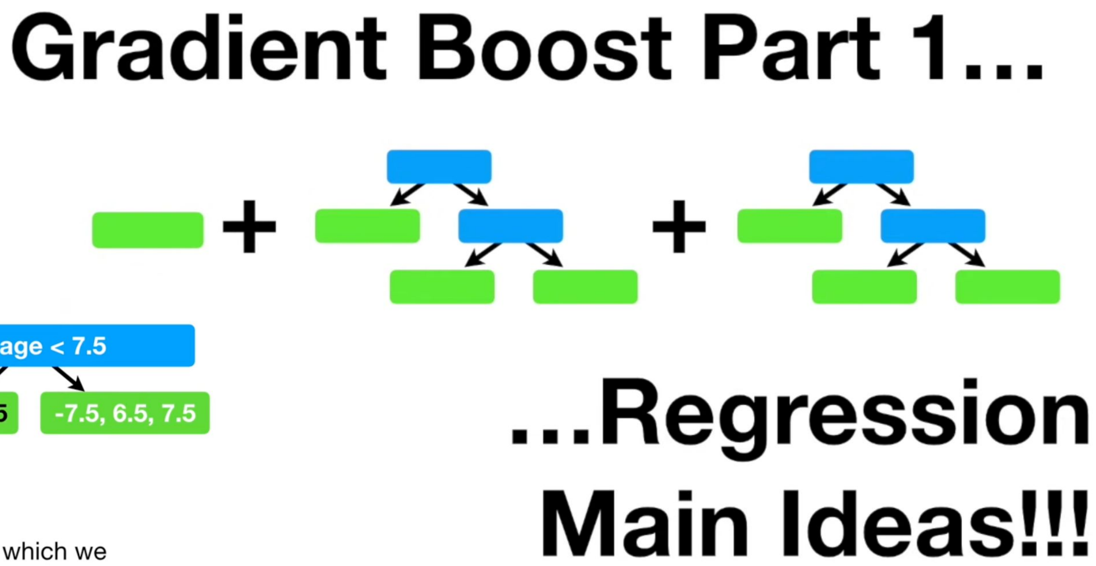
Main contemporary instruments

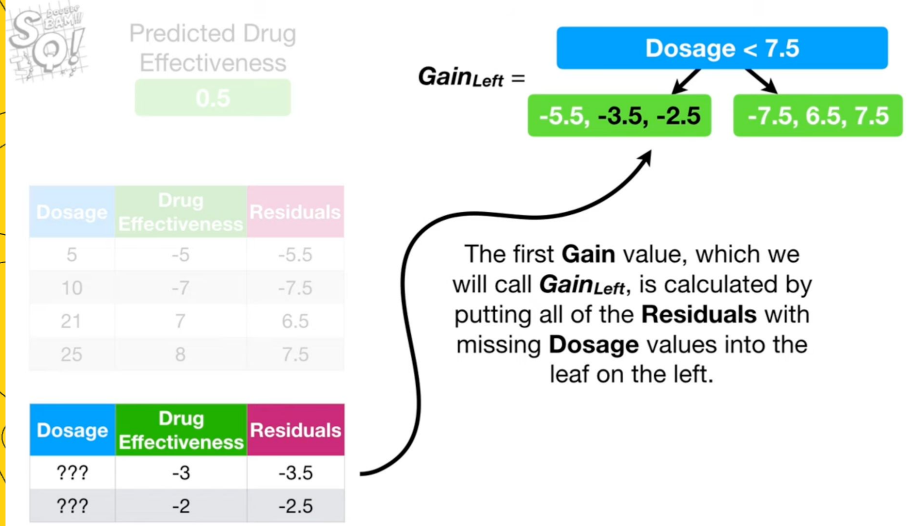
1. Catboost by Yandex
   https://catboost.ai/
   a. Explained by core developer for girafe-ai slides
2. LightGBM by Microsoft
   https://lightgbm.readthedocs.io/en/latest/index.html
3. XGboost by the community
   https://xgboost.readthedocs.io/en/stable/

Definitely not sklearn!

Boosting explained in verse!

1. [Boosting explained]()
2. [XGBoost expained]()





More on boosting

- https://habr.com/ru/companies/ods/articles/645887/
- https://neptune.ai/blog/when-to-choose-catboost-over-xgboost-or-lightgbm
- https://towardsdatascience.com/catboost-vs-lightgbm-vs-xgboost-c80f40662924
- https://www.springboard.com/blog/data-science/xgboost-random-forest-catboost-lightgbm/
- https://towardsdatascience.com/performance-comparison-catboost-vs-xgboost-and-catboost-vs-lightgbm-886c1c96db64

Peak at feature importances!

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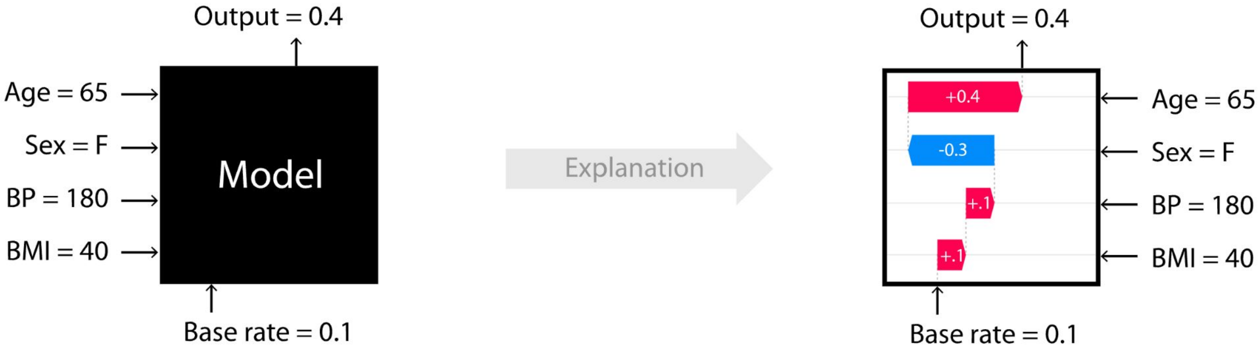
05

Shap values



https://github.com/shap/shap

Hyperparameter optimization

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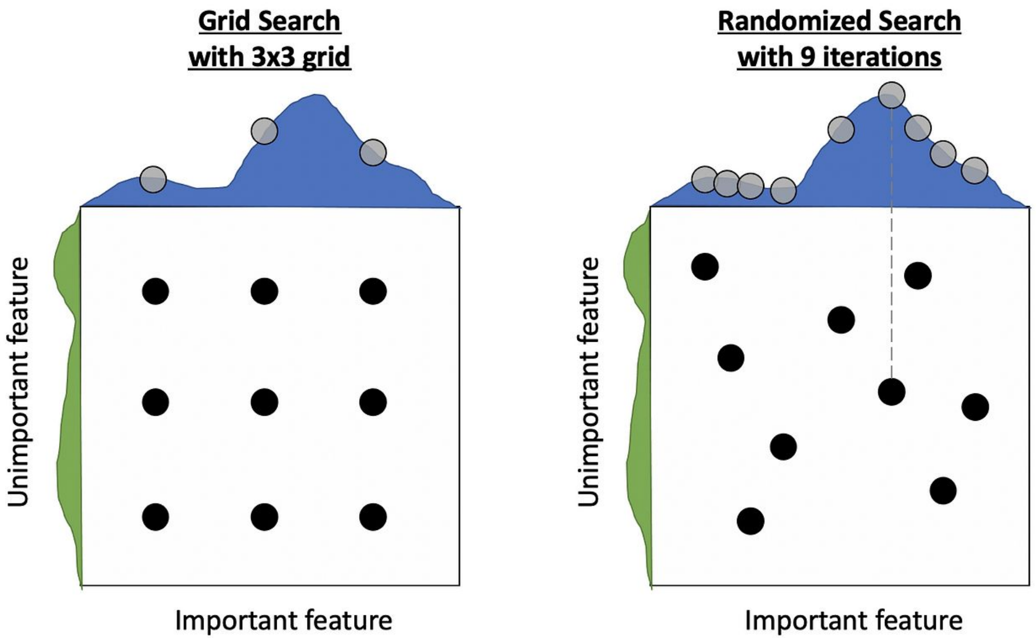
Optimization note

In optimization theory methods are associated with the order of derivatives they use. Main ones are:

- first order optimization
  - use gradient of optimized function e.g. SGD which we discussed
- second order optimization
  - use Hessian matrix. They are qute slow
- zero order
  - don’t need gradient, only values of optimized function
  - that’s what we are interested in today

0-order optimization approaches

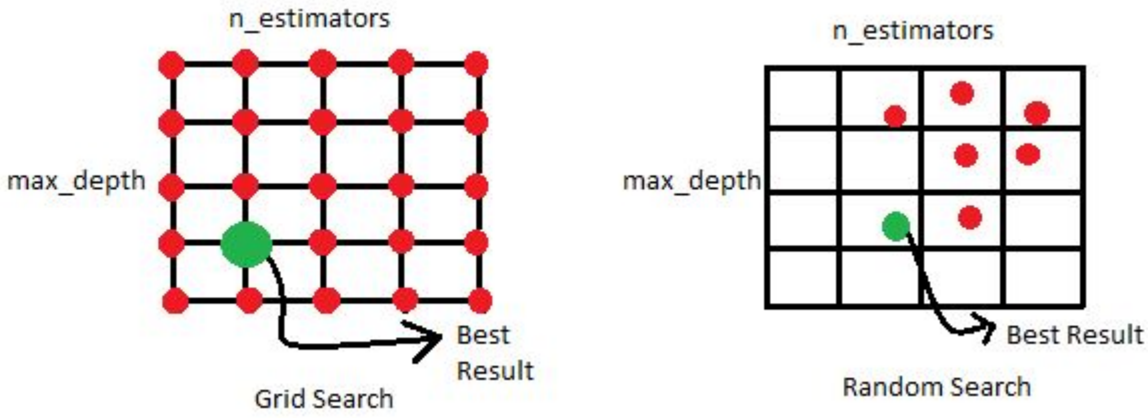
1. Manual trials
2. Grid search
3. Random search



In theory

0-order optimization approaches

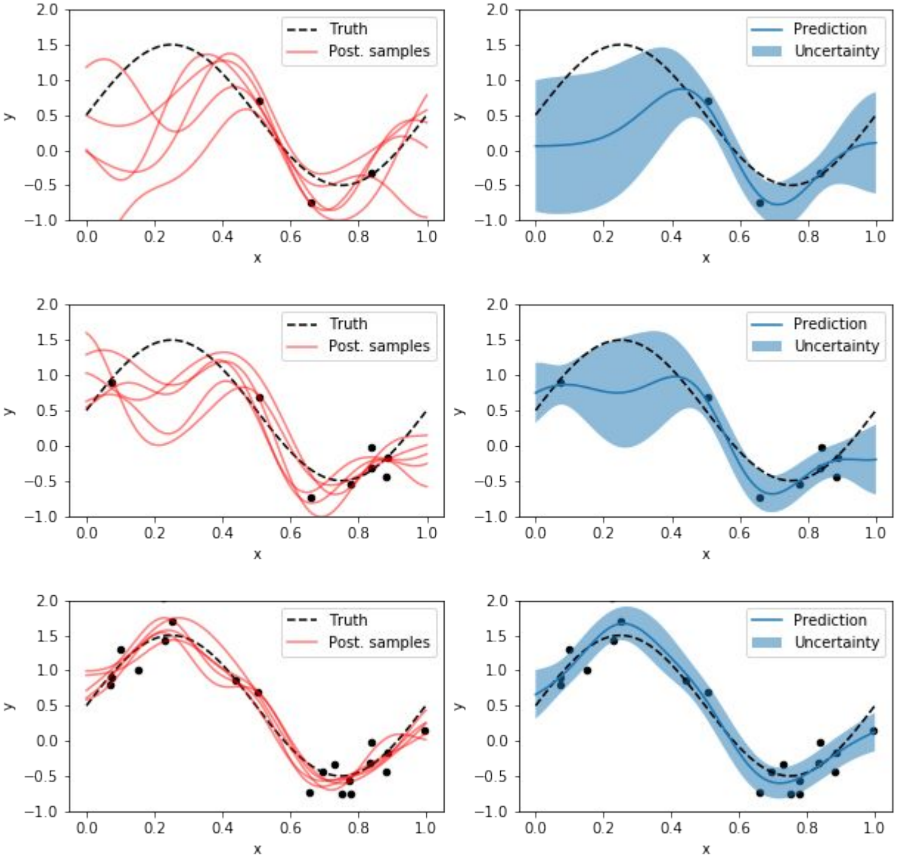
1. Manual trials
2. Grid search
3. Random search



In practice

0-order optimization approaches

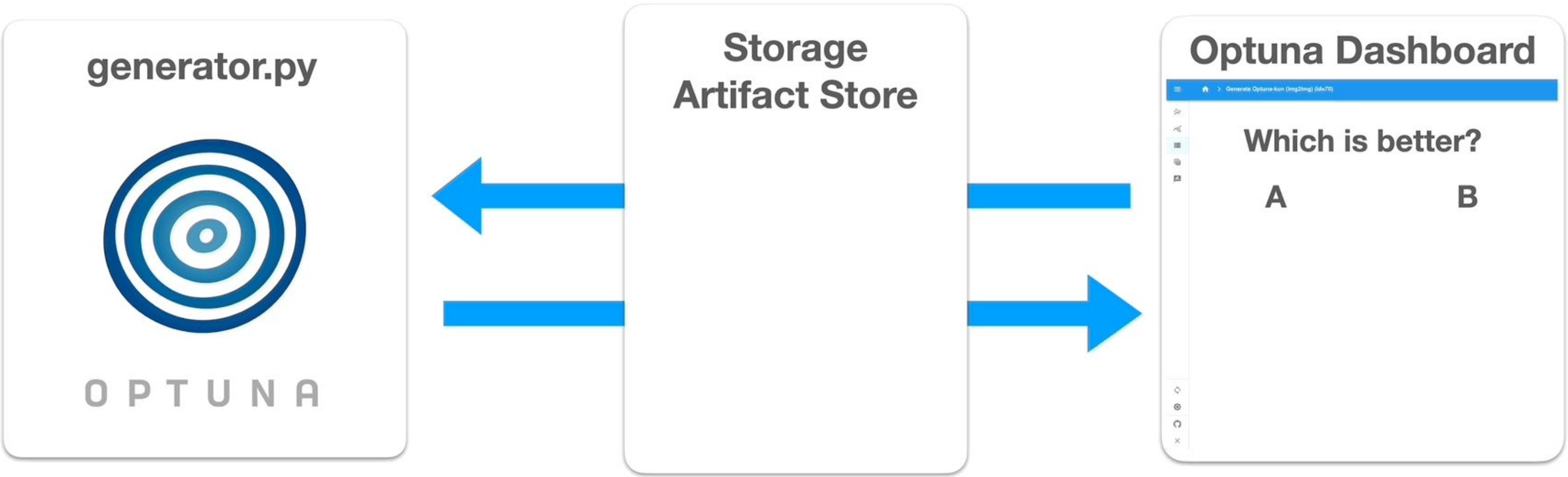
1. Manual trials
2. Grid search
3. Random search
4. Bayesian methods
5. Evolutionary methods



Main libraries

- [Hyperopt]
- [Optuna]

Black box or 0 order optimization



https://optuna.org/ and http://hyperopt.github.io/hyperopt/

Revise

1. Intuitions
2. Gradient boosting theory
3. Examples
4. Libraries
5. Feature importances
6. Hyperparameter optimization

Thanks for attention!

Questions?

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