Bias-variance decomposition Gradient boosting

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girafe ai

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Outline

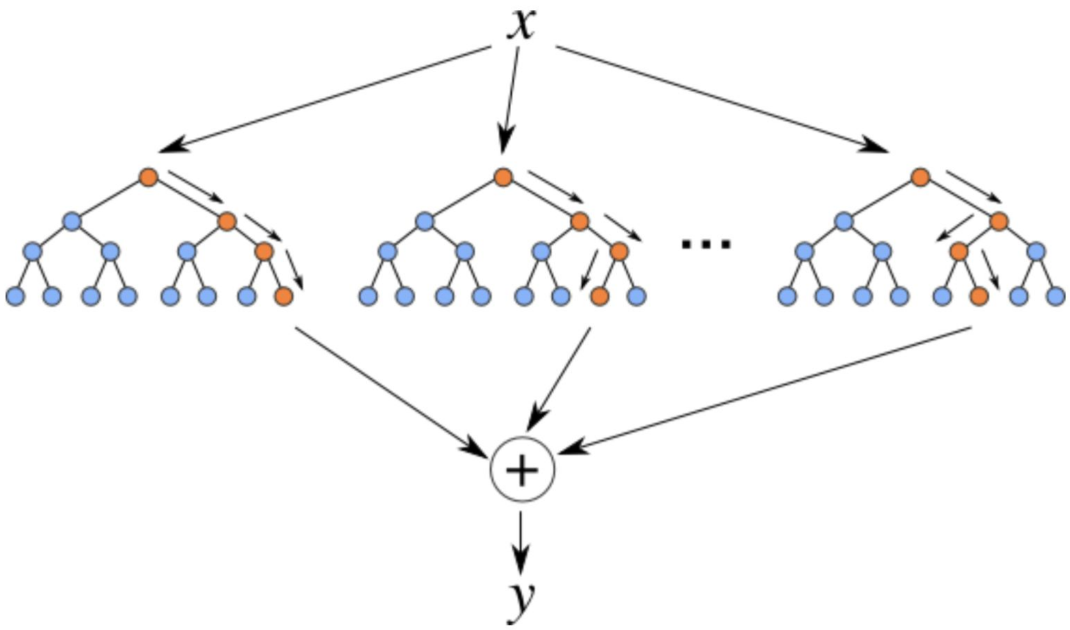
1. Intuitions
2. Gradient boosting theory
3. Examples
4. Libraries
5. Feature importances
6. Hyperparameter optimization

Ensembling recap

00

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 decomposition

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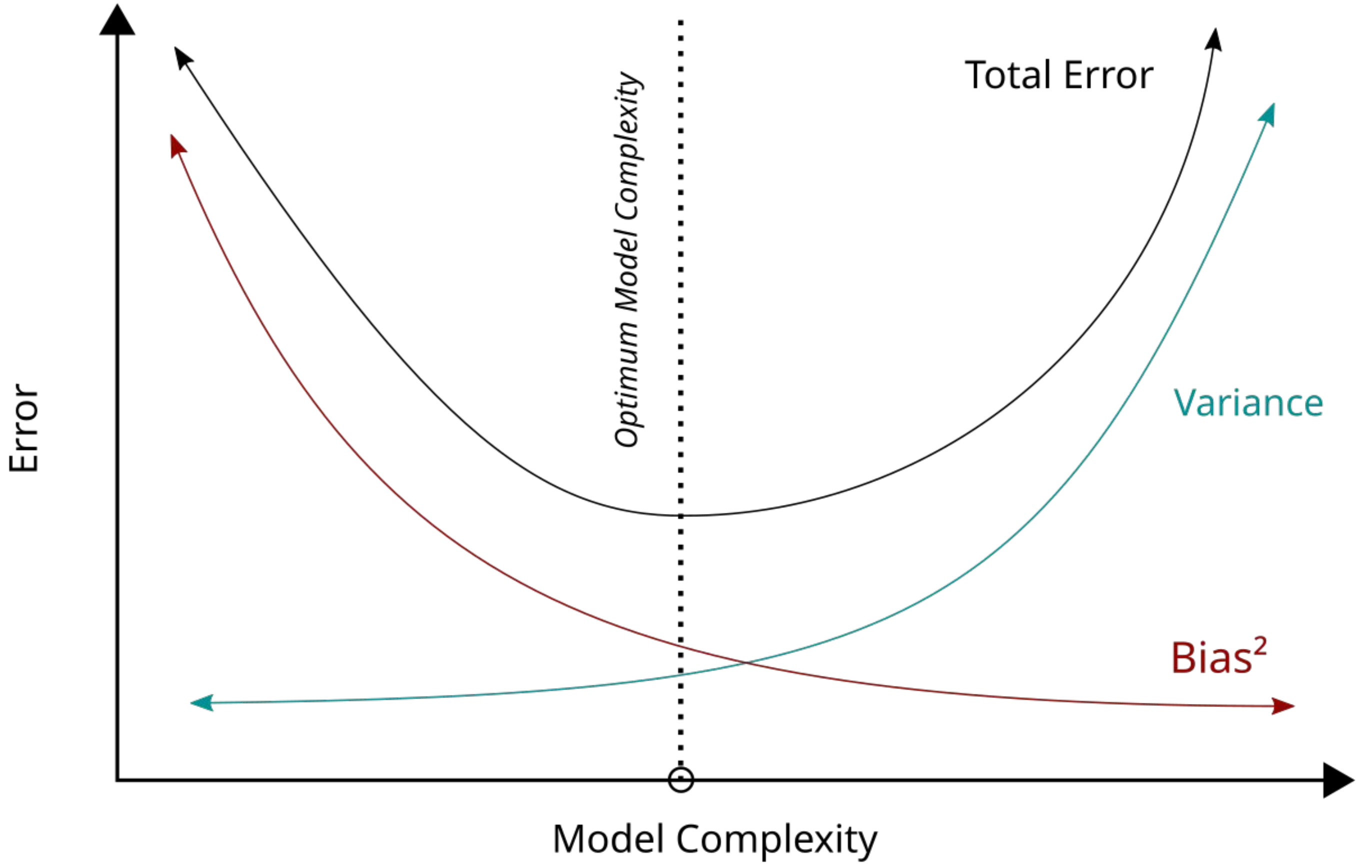
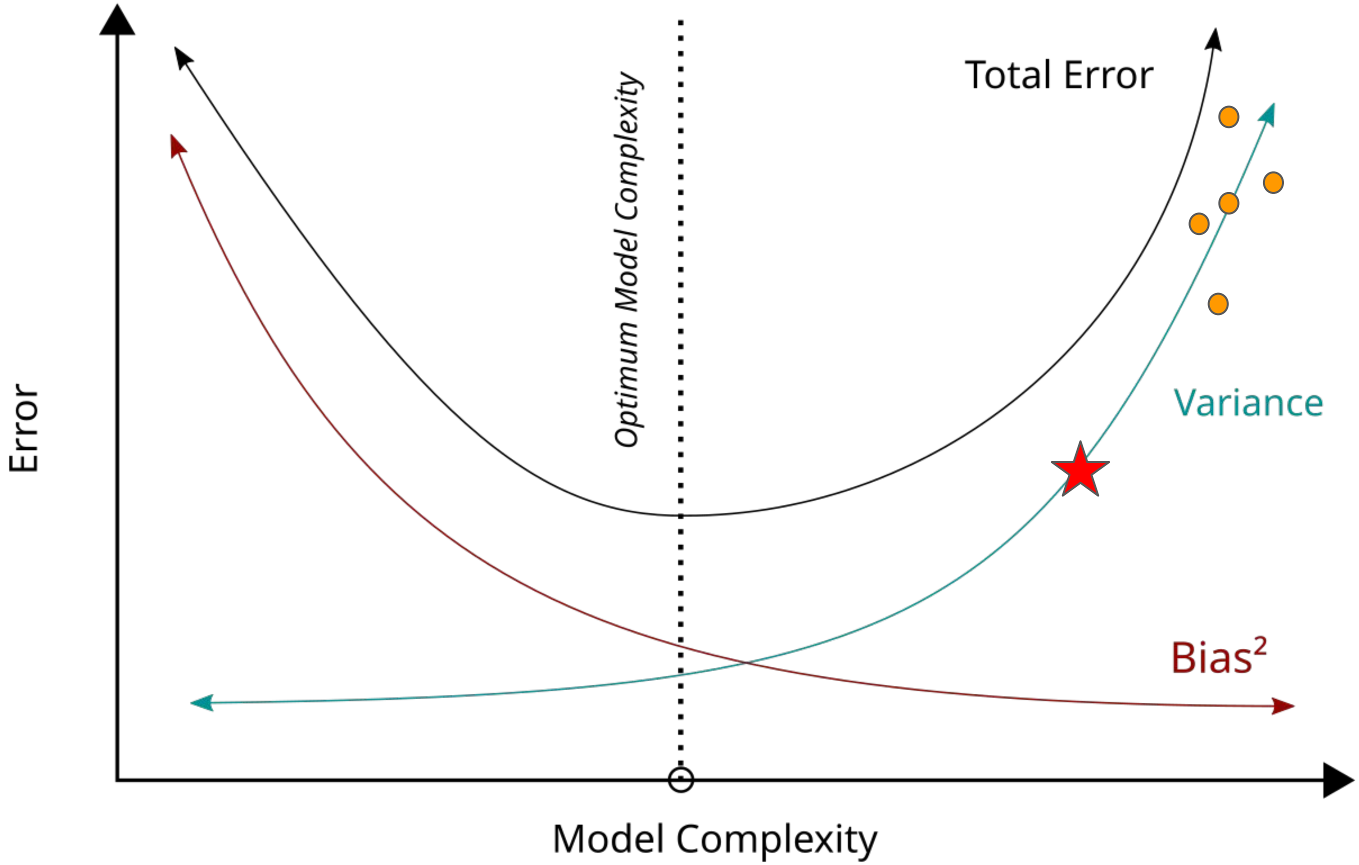
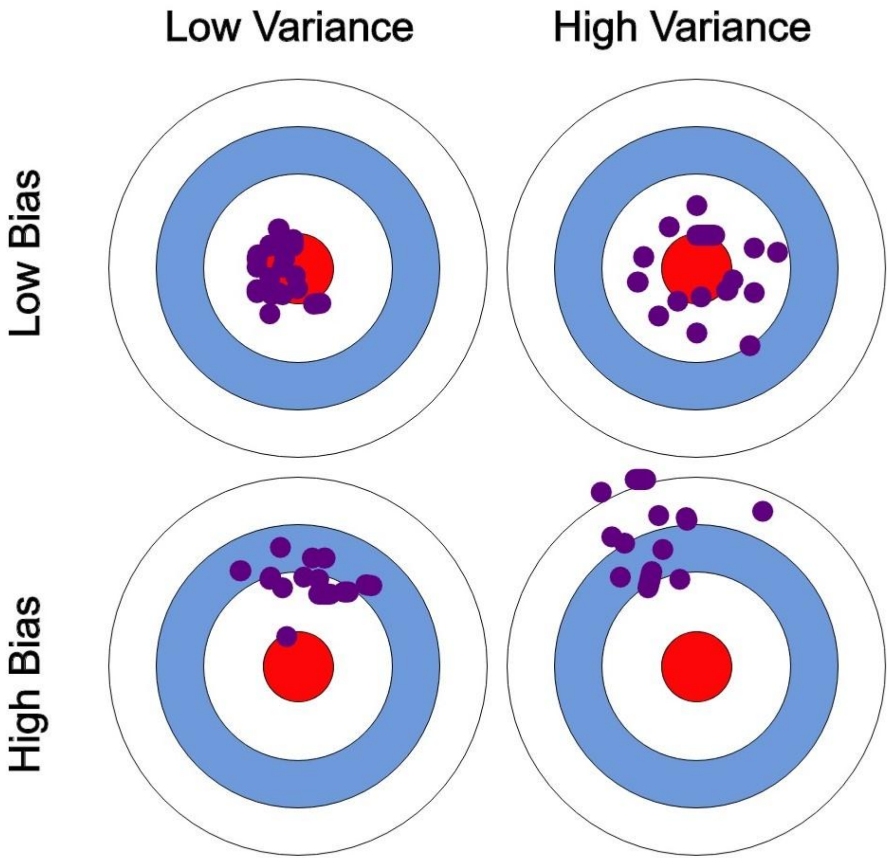
Bias-variance tradeoff



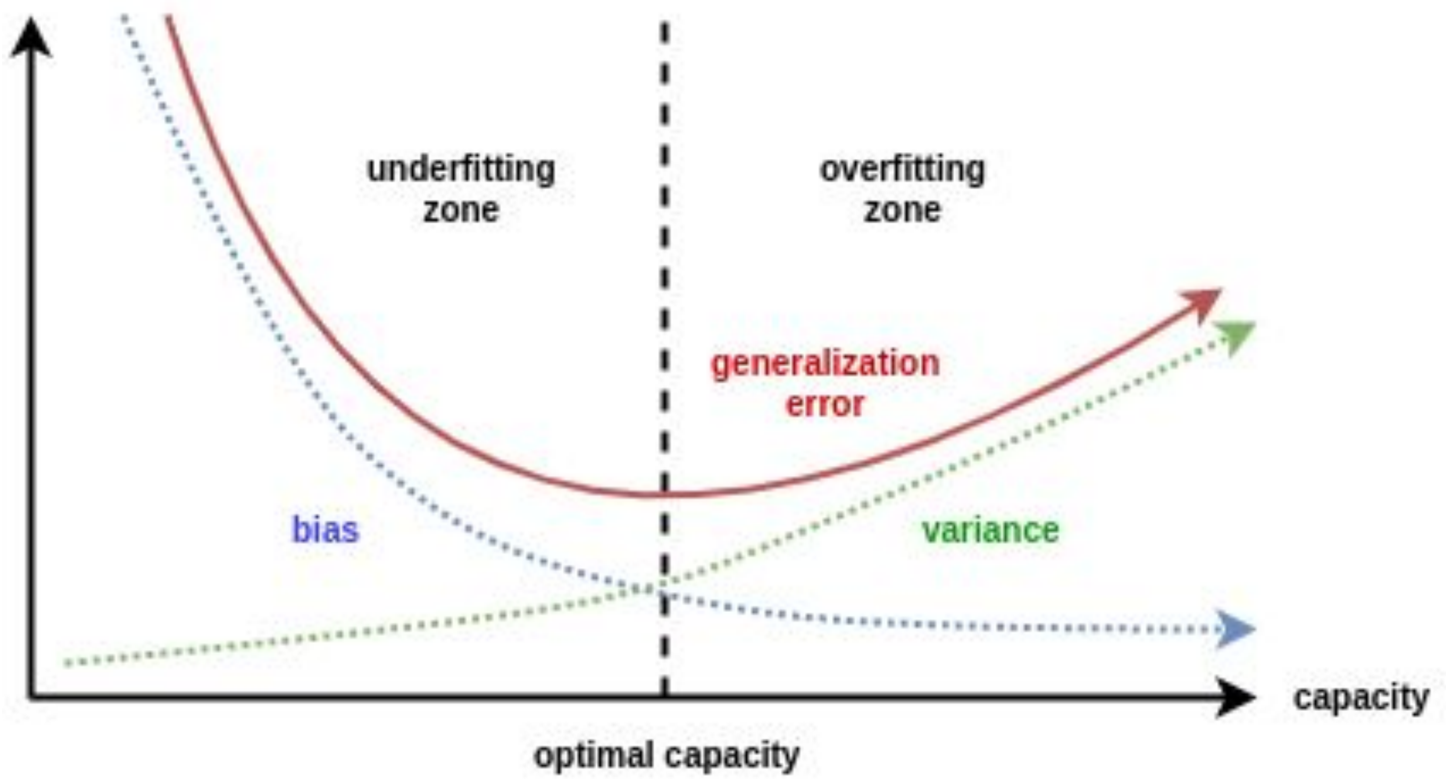
Bagging motivation



Bias-variance tradeoff



Bias-variance tradeoff



Randomness in error

1. Random sampling in training procedure
   a. for Linear model - initial weights
   b. for Tress - feature and threshold sampling
   c. for SGD - sampling of batches
2. Computational errors due to limited precision arithmetics
3. Target noise
   a. epsilon in regression model
4. Objects sampling

GB derivation for MSE

$$L \in R; y \in R^n; p \in R^n$$

$$

\textstyle{\frac{\partial}{\partial{p}}} L(y, p) = [{\frac{\partial}{\partial{p_1}}} L(y, p), {\frac{\partial}{\partial{p_2}}} L(y, p), ...]

$$

$$

1/n \cdot \textstyle{\frac{\partial}{\partial{p}}} \sum_i (y_i - p_i)^2 = 1/n [-2 (y_1 - p_1), -2 (y_2 - p_2), ...]

$$

GB derivation for MSE

$$f_1(x) = fit(x; \bar{y}); \quad g_i = \sum_{k=1}^{i} f_i(x)$$

$$\bar{f}_1 = \begin{pmatrix} f_1(x_1) \\ f_2(x_2) \\ \vdots \end{pmatrix}; \quad \bar{g}_i = \begin{pmatrix} g_i(x_1) \\ g_i(x_2) \\ \vdots \end{pmatrix}$$

$$L(\bar{y}; \bar{g}_2) \to \min$$

$$\frac{\partial L(\bar{y}; \bar{g}_2)}{\partial \bar{f}_2} = \frac{\partial L(\bar{y}; \bar{g}_1 + \bar{f}_2)}{\partial \bar{f}_2} =$$

$$= \frac{\partial L(\bar{y}; \bar{q})}{\partial \bar{q}} \cdot \frac{\partial (\bar{g}_1 + \bar{f}_2)}{\partial \bar{f}_2} =$$

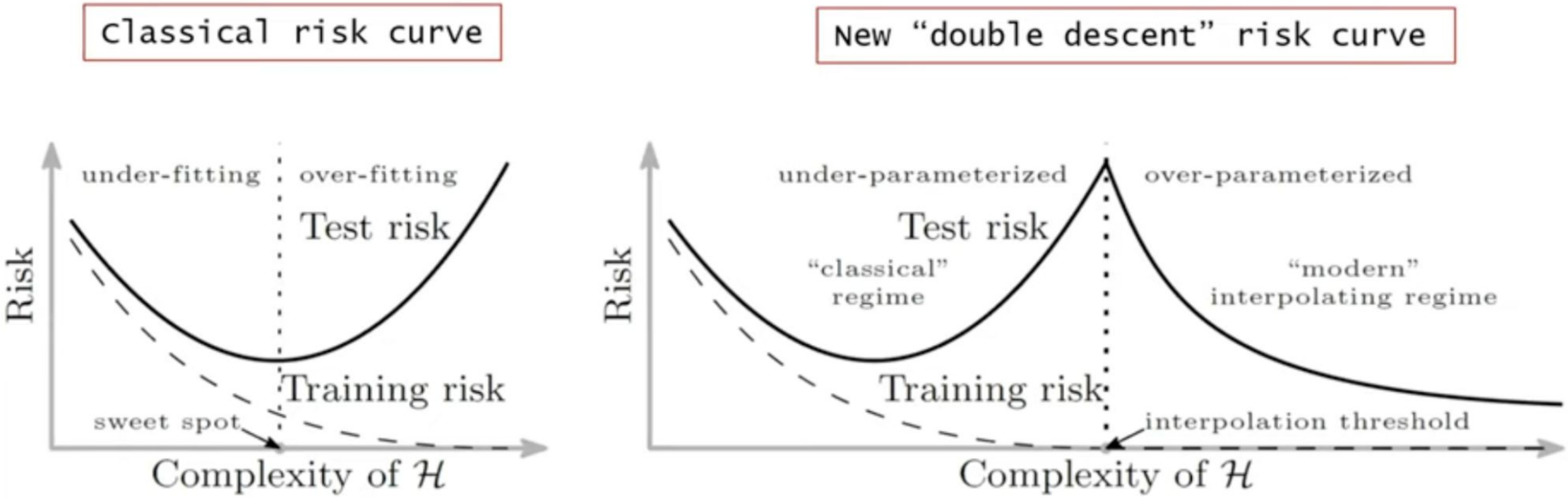
$$= \left. \frac{\partial L(\bar{y}; \bar{q})}{\partial q} \right|_{q = g_1}$$

Bias-variance decomposition

$$\mathrm{MSE} = \left(f(x) - \mathbb{E}\left[\hat{f}\,(x)\right]\right)^2 + \mathbb{E}\left[\left(\mathbb{E}\left[\hat{f}\,(x)\right] - \hat{f}\,(x)\right)^2\right] + \sigma^2$$

$$= \mathrm{Bias}\left(\hat{f}\,(x)\right)^2 \; + \; \mathrm{Var}\left[\hat{f}\,(x)\right] \; + \; \sigma^2$$

Contemporary hypothesis



For contemporary LLMs and other big models "double descent" theory is being developed, see https://www.youtube.com/watch?v=waJOSLNhHII or https://www.youtube.com/watch?v=5-QjjOYfeSI

Boosting intuition

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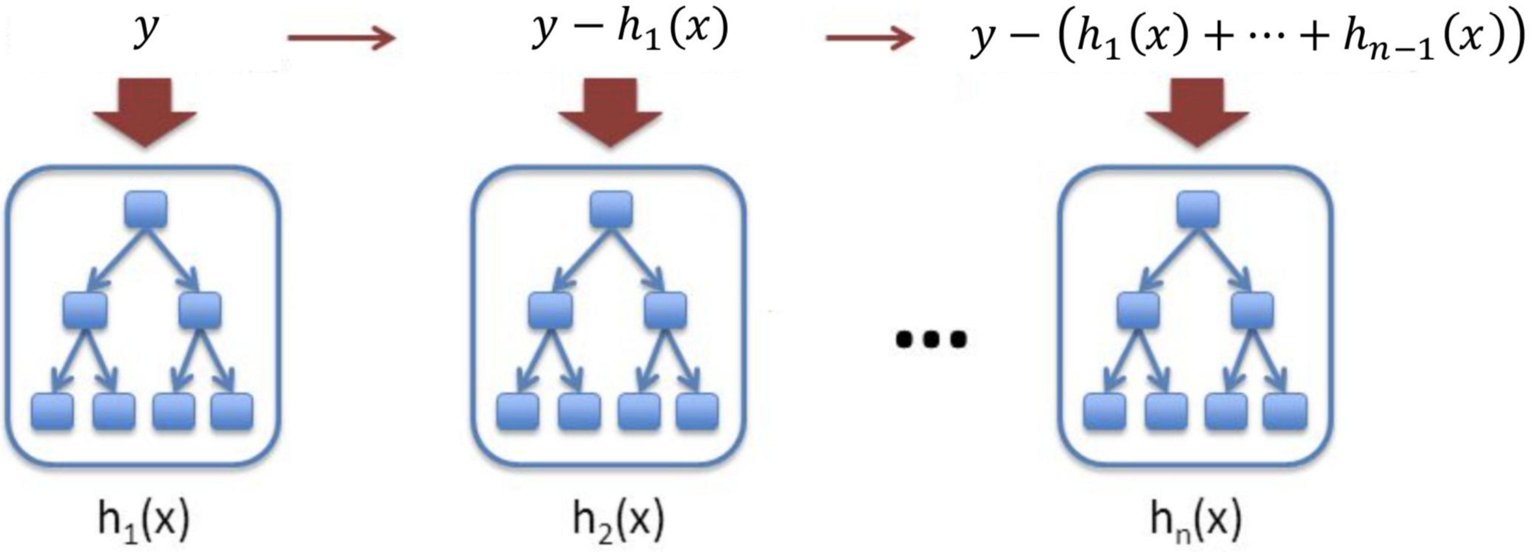
Boosting for _MSE_

$$a_n(x) = h_1(x) + \dots + h_n(x)$$

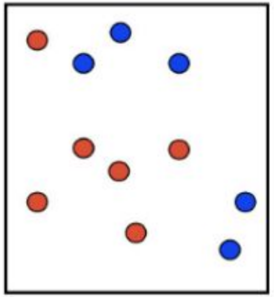


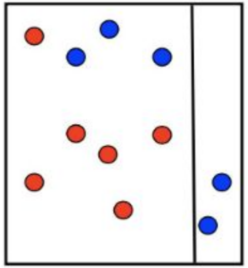
* in case of MSE loss

Boosting: intuition

Binary classification

Use decision stumps



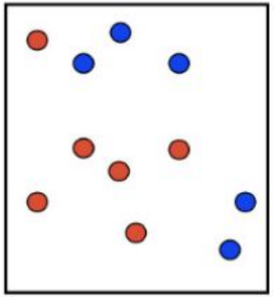


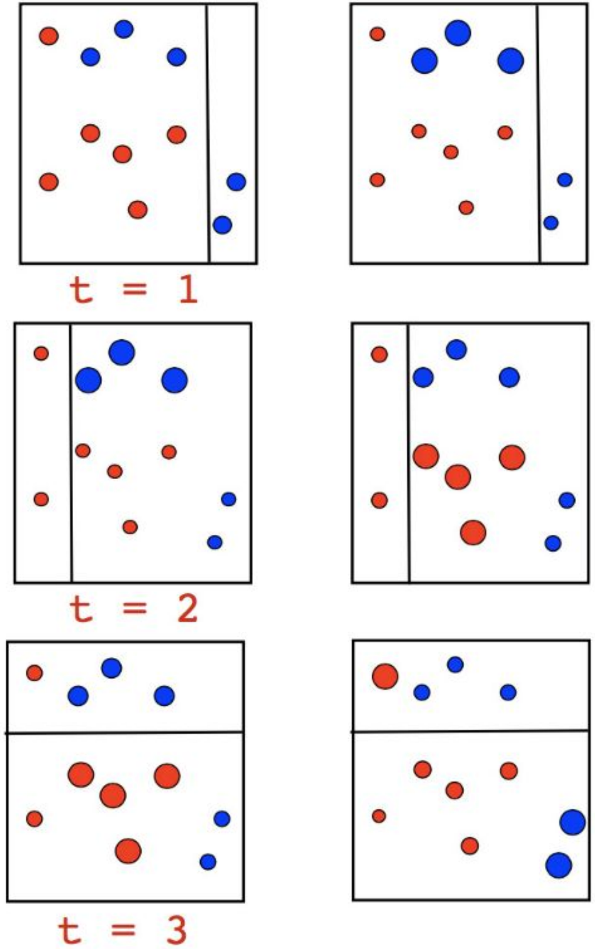
t = 1

Boosting: intuition

Binary classification

Use decision stumps.

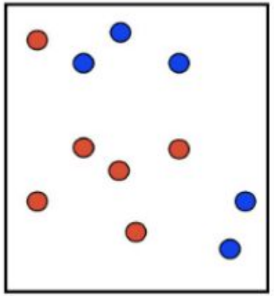


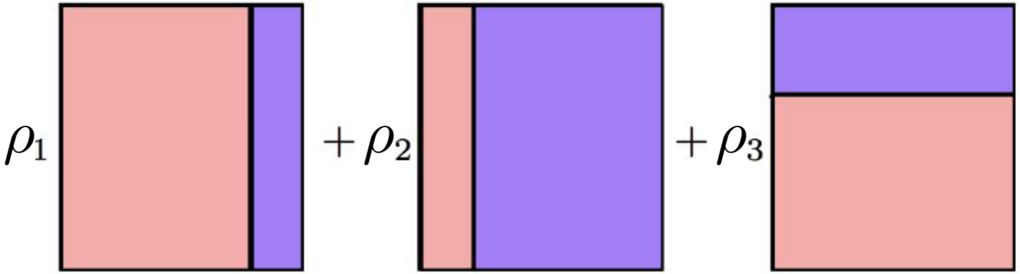


Boosting: intuition

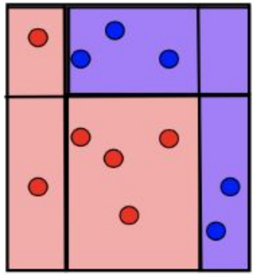
Binary classification

Use decision stumps.





$$\hat{f}_T(x) = \sum_{t=1}^{T} \rho_t h_t(x) \quad =$$



Gradient boosting theory

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Gradient boosting: theory

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

Optimal model:

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

Let it be from parametric family:

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

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

Gradient boosting: theory

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

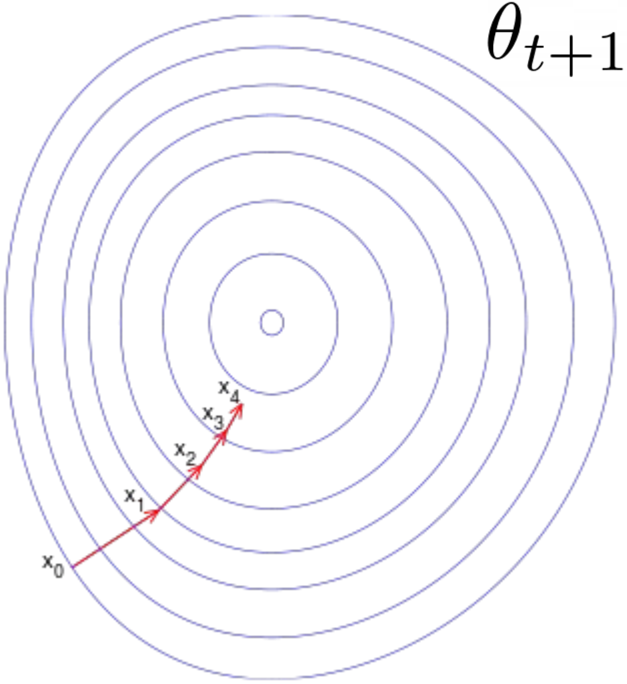
$$(\rho_t, \theta_t) = \arg\min_{\rho,\theta} \mathbb{E}_{x,y}[L(y, \hat{f}(x) + \rho \cdot h(x, \theta))],$$

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

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

Gradient boosting: theory

$$\theta_{t+1} = \theta_t - \text{learning rate} \cdot \frac{\partial}{\partial \theta} Loss$$



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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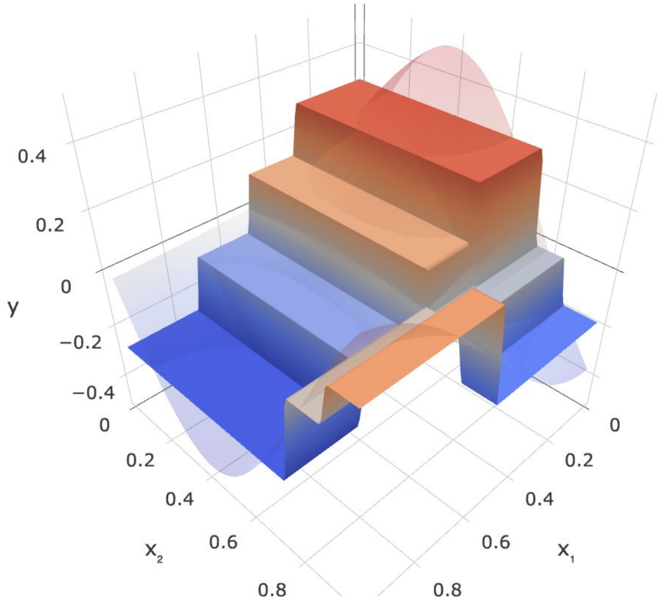
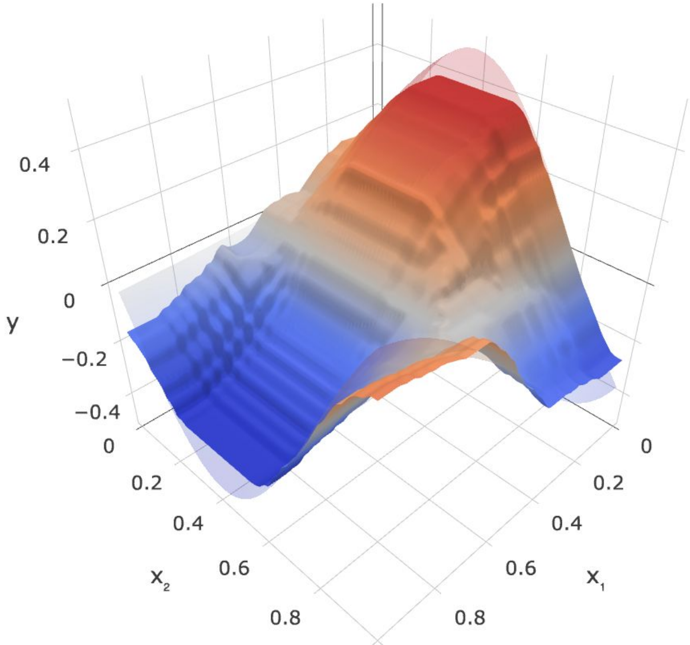
Tree vs GB demo



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

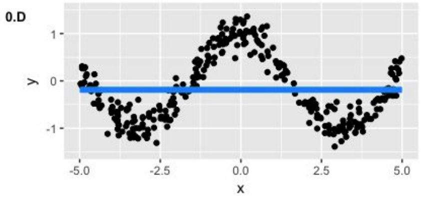
Gradient boosting: example

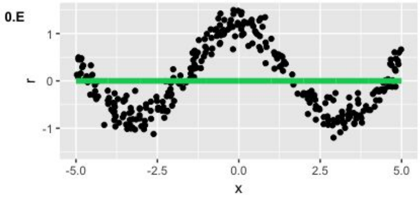
What we need:

- 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

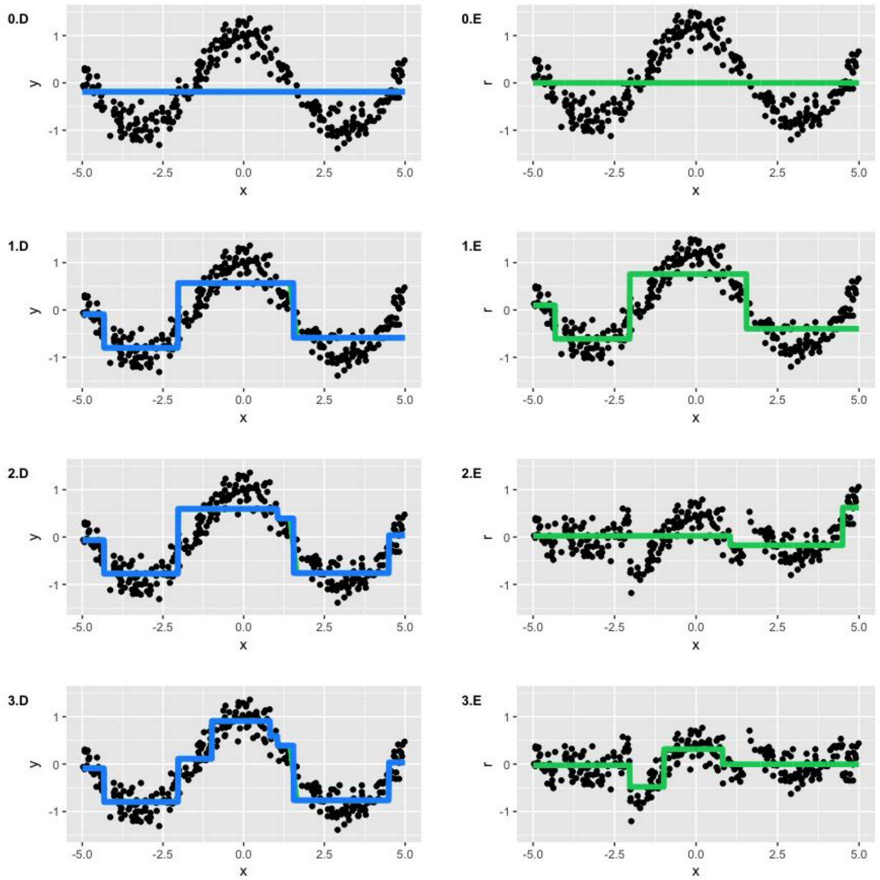




Left: full ensemble on each step.

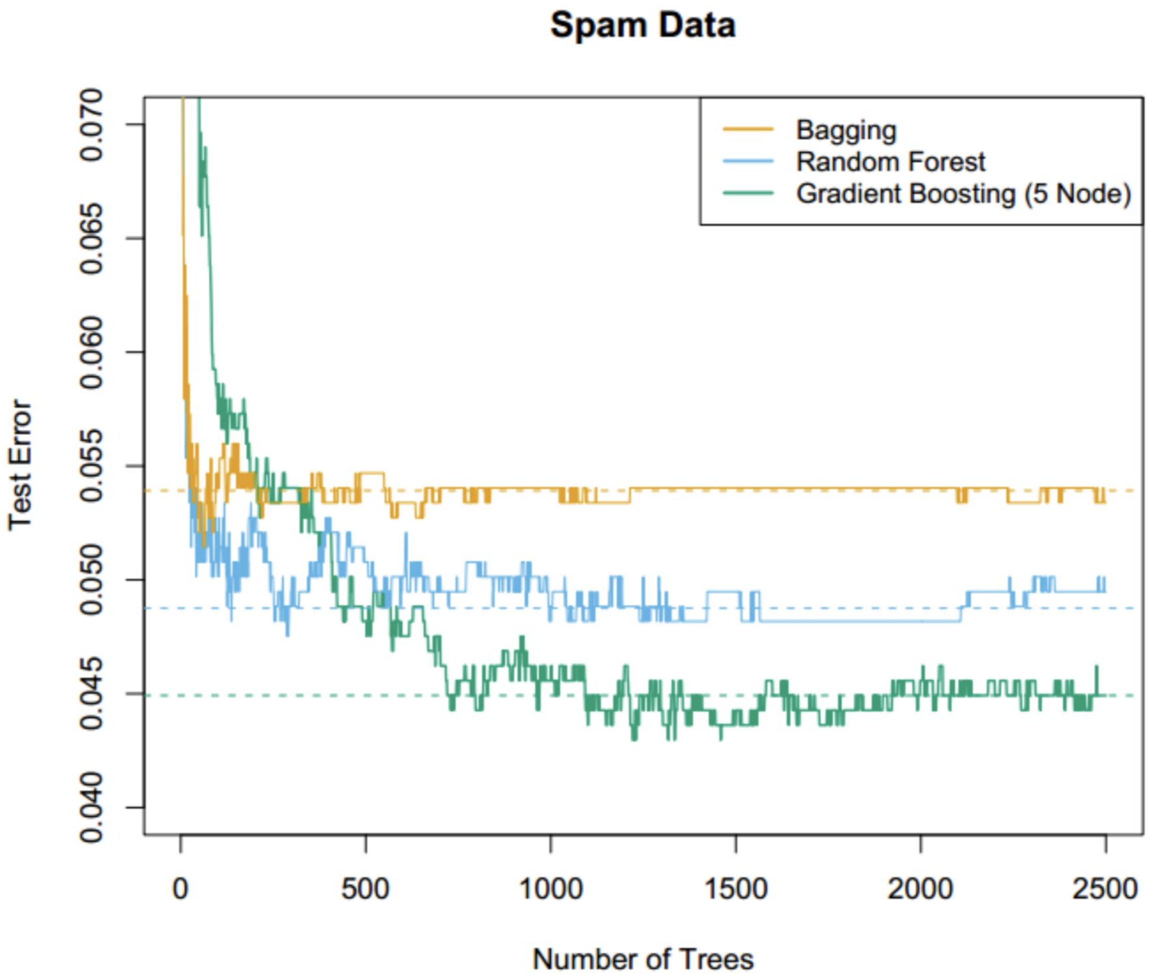
Right: additional tree decisions.

Gradient boosting: example



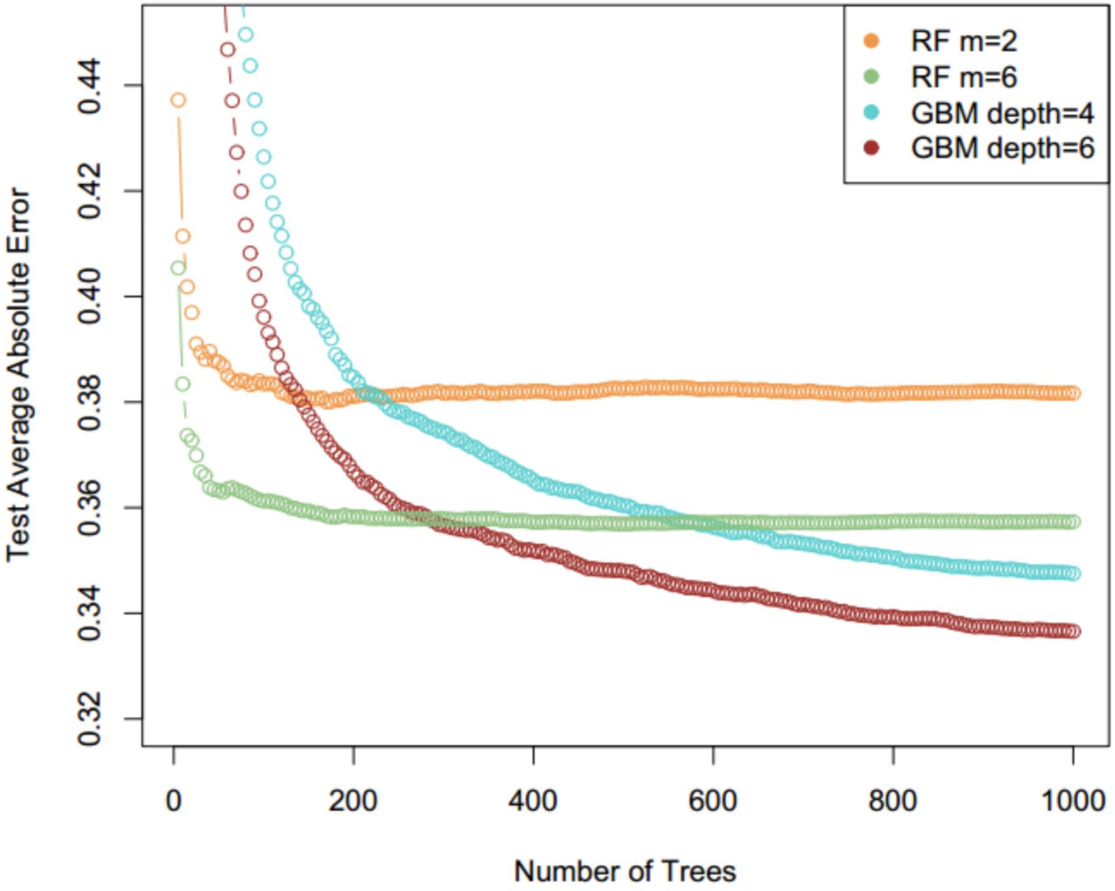
Left: full ensemble on each step.

Right: additional tree decisions



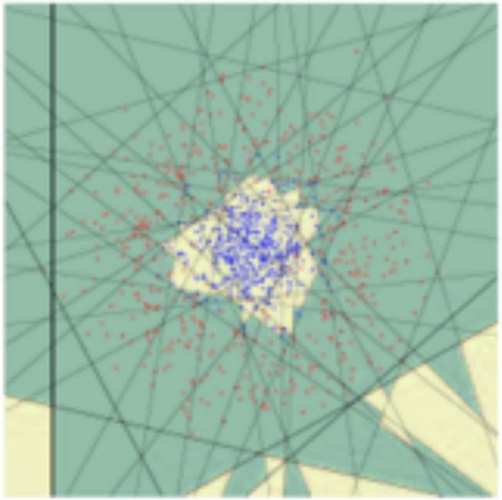
Spam Data
Bagging
Random Forest
Gradient Boosting (5 Node)
Test Error
0.040
0.045
0.050
0.055
0.060
0.065
0.070
0
500
1000
1500
2000
2500
Number of Trees

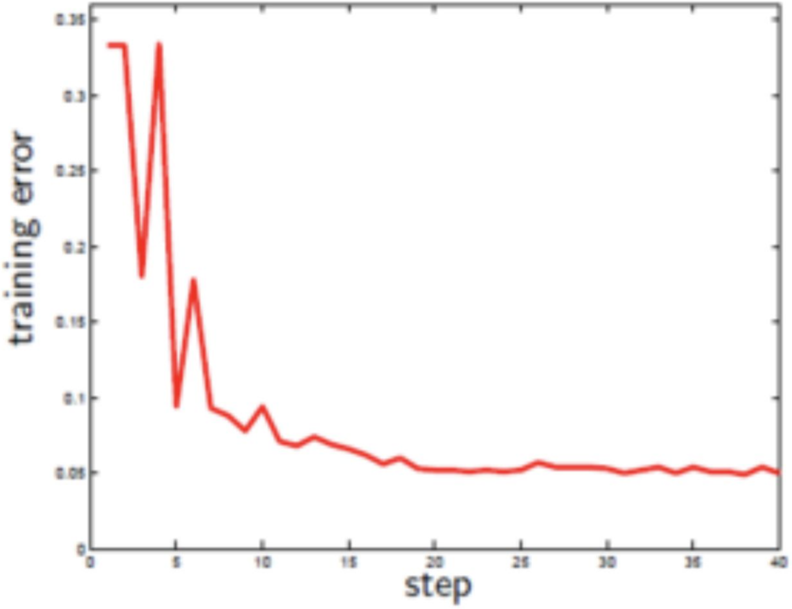
California Housing Data



Boosting with linear classification methods

$t = 40$





Ensembles parallelization

	Training	Inference
Bagging	parallel	parallel
Boosting	sequential	parallel

Libraries for GB

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04

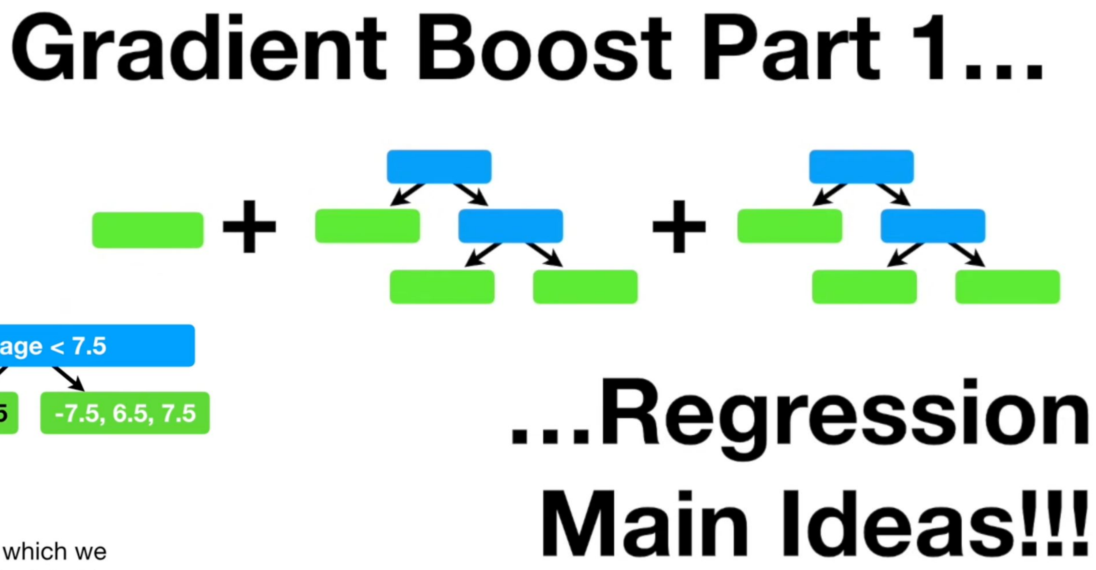
Main contemporary instruments

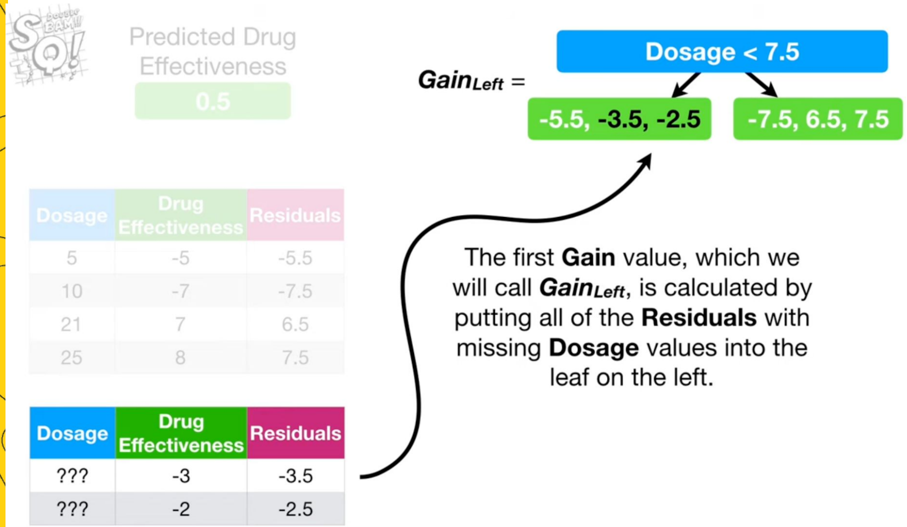
1. Catboost by Yandex
   https://catboost.ai/
   a. Explained by core developer for girafe-ai slides
2. LightGBM by Microsoft
   https://lightgbm.readthedocs.io/en/latest/index.html
3. XGboost by community
   https://xgboost.readthedocs.io/en/stable/

Definitely not sklearn!

Boosting explained in verse!

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

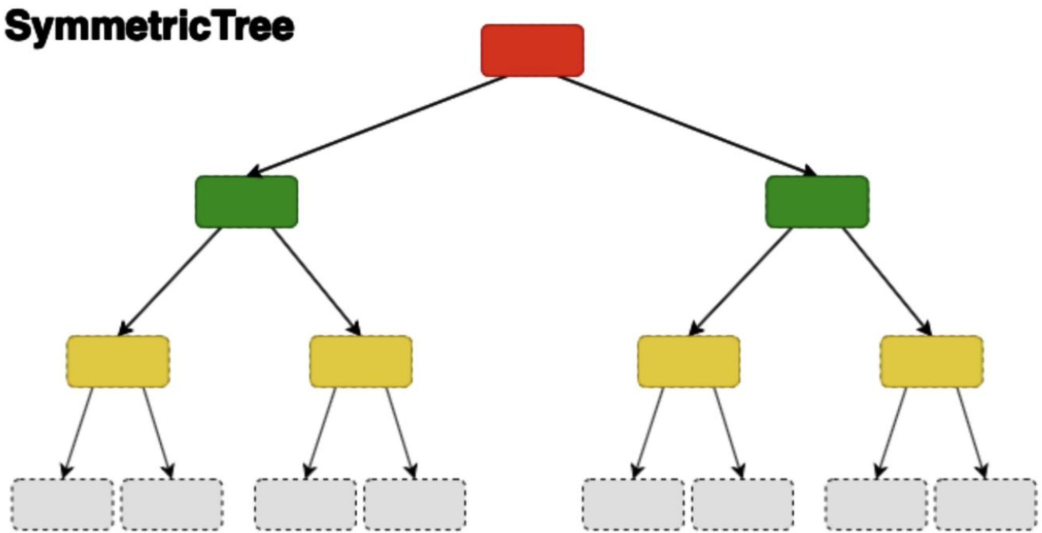




Dive to Catboost

- https://www.youtube.com/watch?v=s4GWmfB9VTA
- https://github.com/girafe-ai/journal-club/blob/master/slides/08%20CatBoosting.pdf

Форма дерева – CatBoost – SymmetricTree



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

Feature importances

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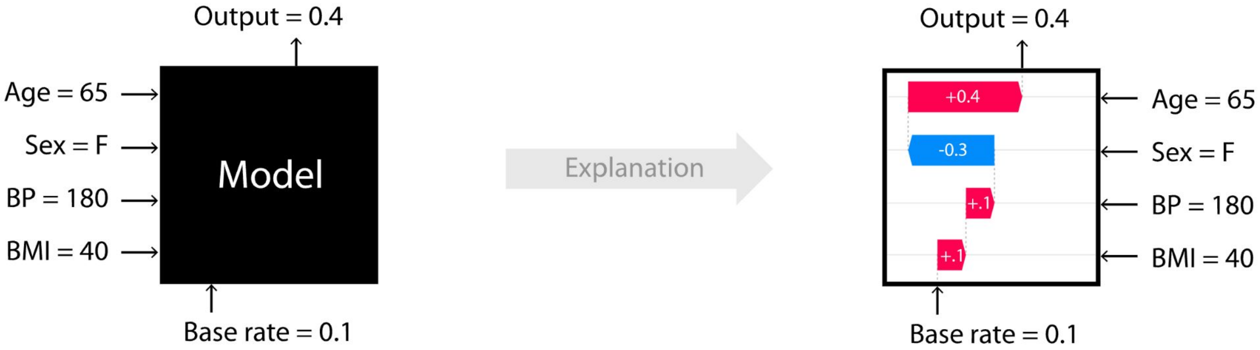
05

Shap values



https://github.com/shap/shap

Shap values

$$\phi_i = \sum_{S \subseteq \{1,\ldots,p\}\{i\}} \underbrace{\frac{|S|!(p-|S|-1)!}{p!}}_{\text{Weight}} \underbrace{[val(S \cup \{i\}) - val(S)]}_{\text{Marginal contribution of player i to coalition S}}$$

p! = number of ways to form a coalition of p players

|S| = number of players in coalition S

|S|! = number of ways coalition S can form

(p-|S|-1)! = number of ways players can join after player i joins

https://youtu.be/UJeu29wq7d0

Shap values calculation

Coalition values

$C_{12} = 10{,}000$
$C_{1} = 7{,}500$
$C_{2} = 5{,}000$
$C_{0} = 0$

Marginal contribution

The increase in a coalition's value due to a player joining that coalition

$C_{12} - C_{2} = 5{,}000$
$C_{1} - C_{0} = 7{,}500$

$(5{,}000+7{,}500)/2$
$=$ **\$6,250**

$C_{12} - C_{1} = 2{,}500$
$C_{2} - C_{0} = 5{,}000$

$(2500+5000)/2$
$=$ **\$3,750**

Shap values calculation

$$C_{123} = 10,000$$
$$C_{0} = 0$$

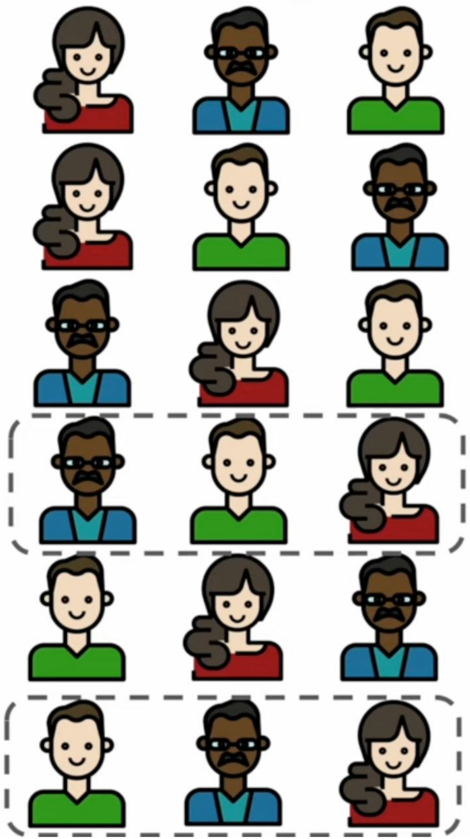
$$C_{12} = 7,500$$
$$C_{13} = 7,500$$
$$C_{23} = 5,000$$

$$C_{1} = 5,000$$
$$C_{2} = 5,000$$
$$C_{3} = 0$$

$$C_{123} - C_{23} = 5,000$$
$$C_{12} - C_{2} = 2,500$$
$$C_{13} - C_{3} = 7,500$$
$$C_{1} - C_{0} = 5,000$$

$$5,000^*(\tfrac{1}{3}) + 2,500^*(\tfrac{1}{6}) + 7,500^*(\tfrac{1}{6}) + 5,000^*(\tfrac{1}{3})$$
$$= \mathbf{\$5,000}$$

Shap values calculation



$C_{123} - C_{23} = 5{,}000$

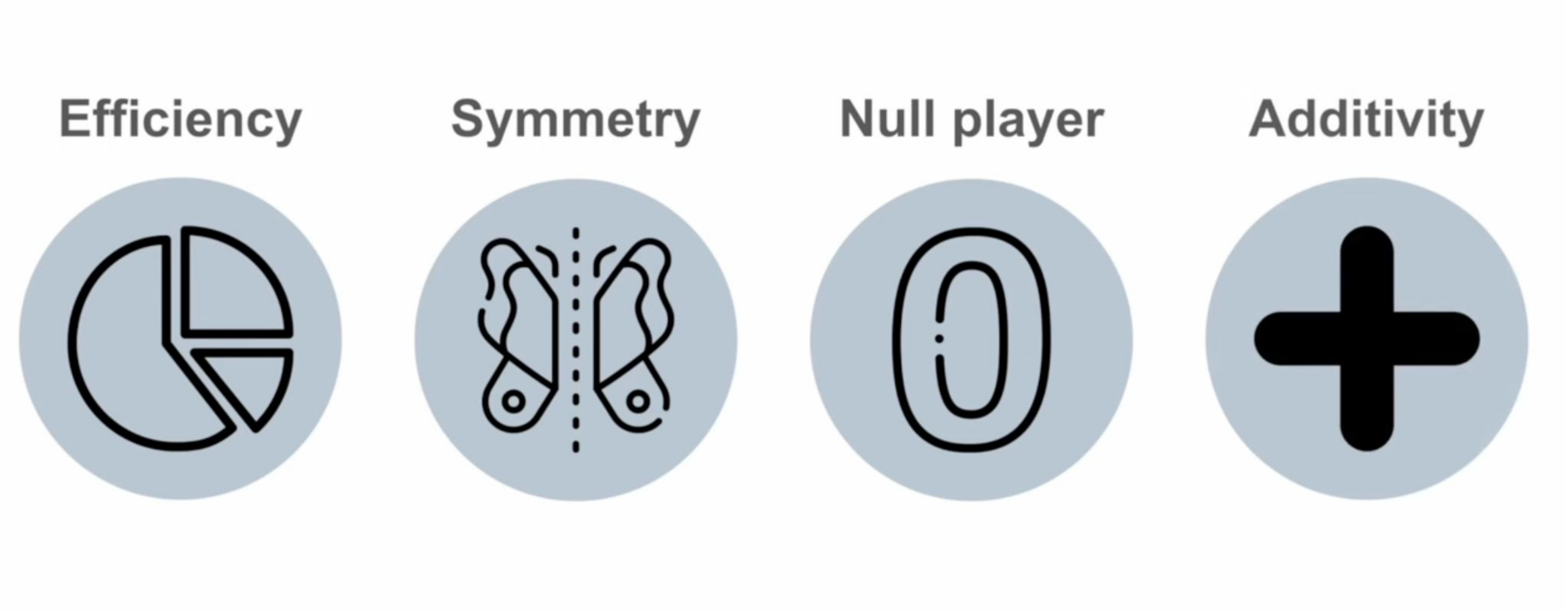
$P(C_{123} - C_{23})$ = probability that player 1 makes a marginal contribution to a coalition of player 2 and 3

$3! = 6$

$2! * 1! = 2$

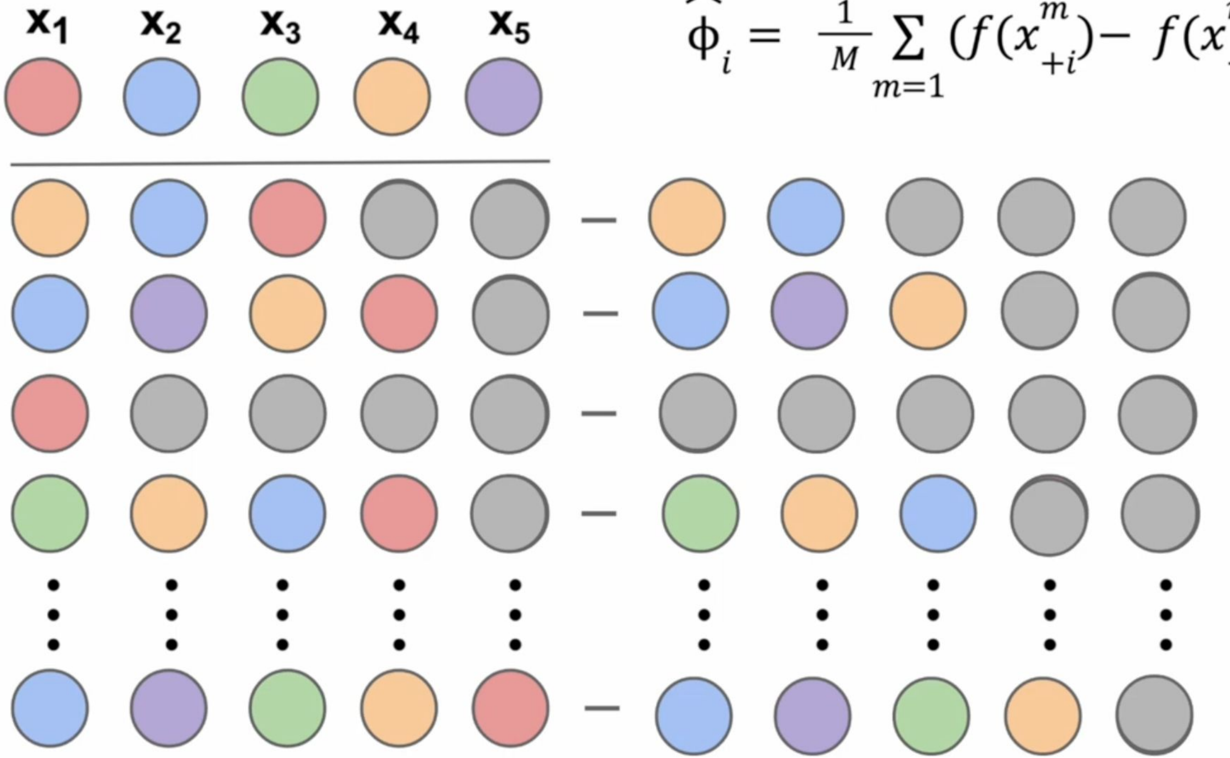
$P(C_{123} - C_{23}) = 2/6 = 1/3$

Shap values axioms

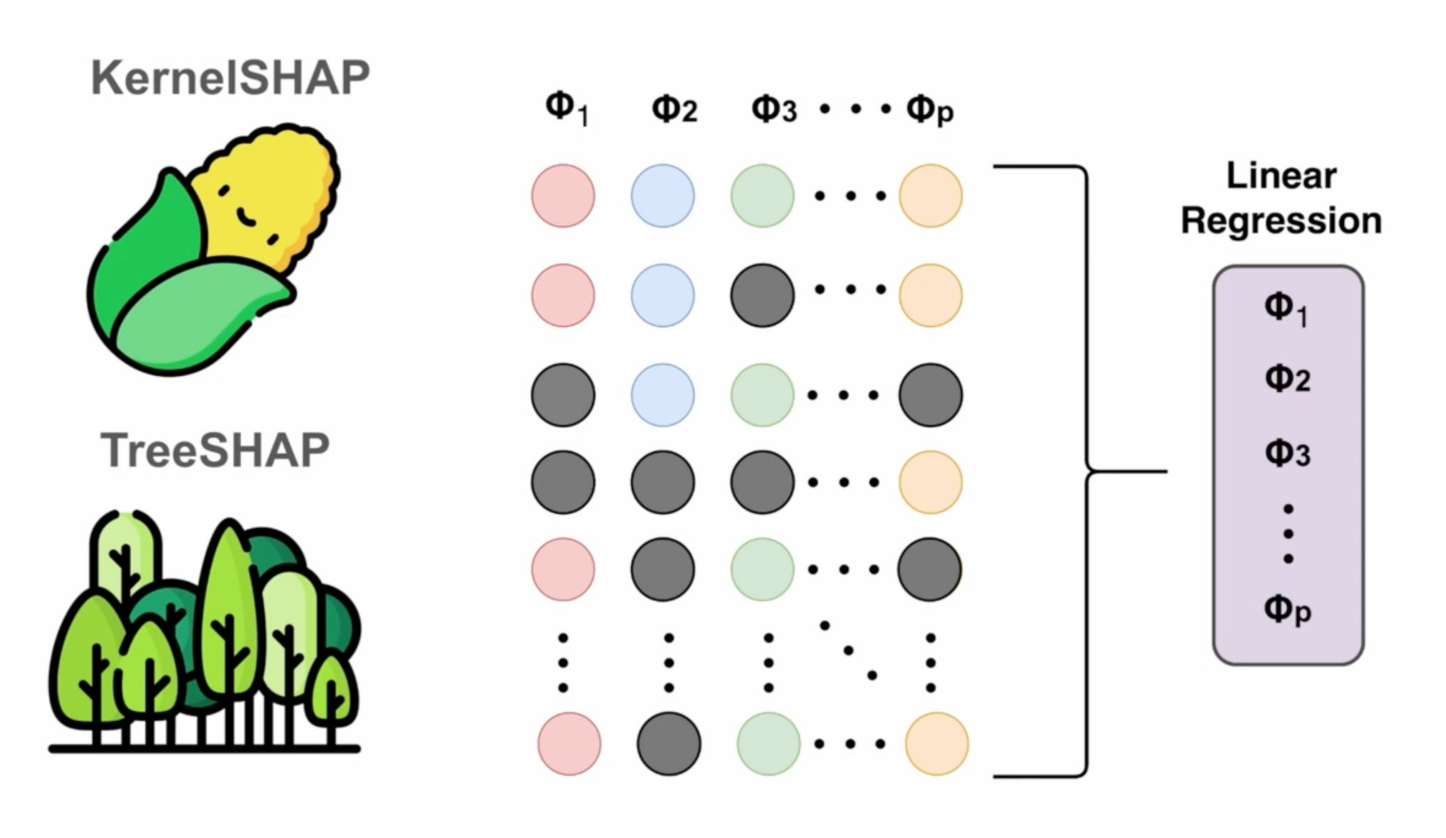


Shap values for ML

$$\widehat{\phi}_i = \frac{1}{M}\sum_{m=1}^{M}\left(f(x_{+i}^{m}) - f(x_{-i}^{m})\right)$$



Shap values for ML



Hyperparameter optimization

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06

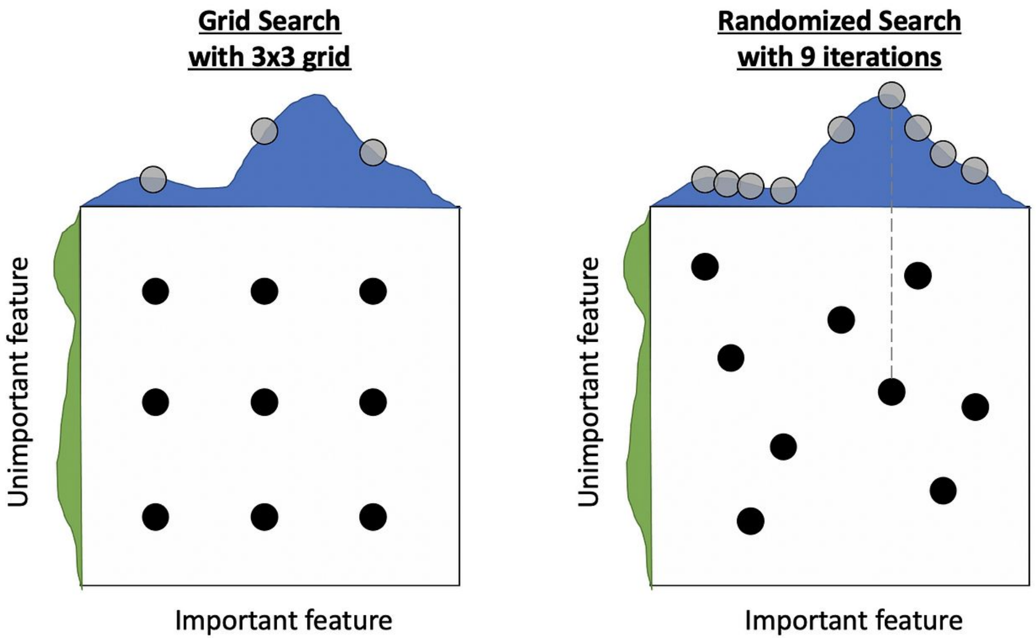
Optimization note

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

- first order optimization (gradient based optimization)
  - use gradient of optimized function
  - e.g. SGD which we discussed
- second order optimization (Newton's method)
  - use Hessian matrix
  - they are quite slow
- zero order (black box optimization)
  - don't need gradient, only values of optimized function
  - that's what we are interested in today

0-order optimization approaches

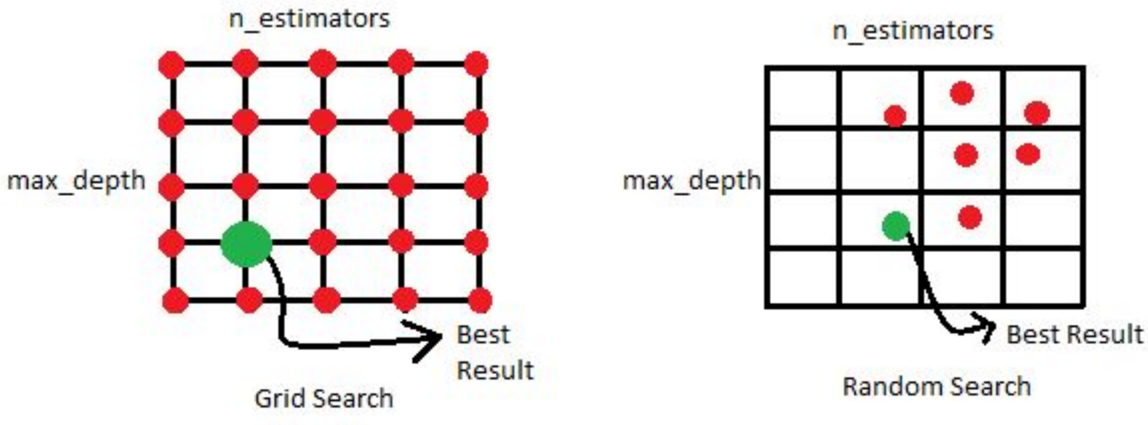
1. Manual trials
2. Grid search
3. Random search



In theory

0-order optimization approaches

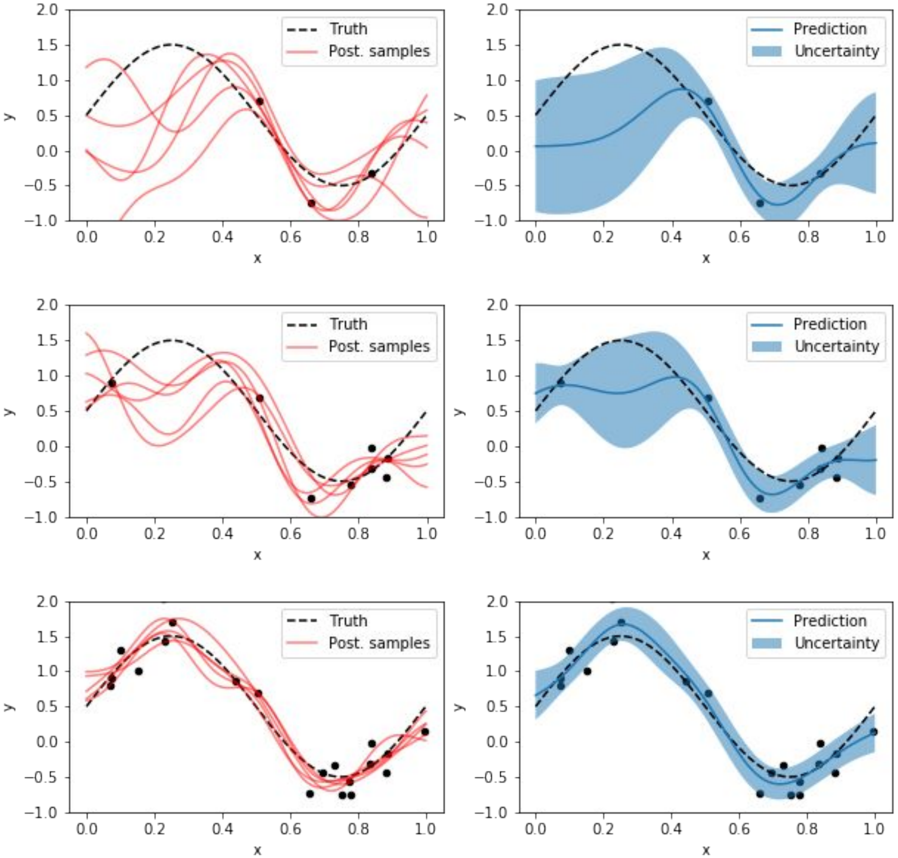
1. Manual trials
2. Grid search
3. Random search



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]()

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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