Machine Learning Course
basic track

Lecture 6: Ensembles

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Outline

1. Bagging & Random Forest
2. Stacking.
3. Blending.
4. Gradient boosting

Bootstrap

Consider the errors unbiased and uncorrelated:

$$\mathbb{E}_x \varepsilon_j(x) = 0;$$
$$\mathbb{E}_x \varepsilon_i(x)\varepsilon_j(x) = 0, \quad i \neq j.$$

The final model averages all predictions:

$$a(x) = \frac{1}{N}\sum_{j=1}^{N} b_j(x).$$

$$E_N = \mathbb{E}_x\left(\frac{1}{N}\sum_{j=1}^{n} b_j(x) - y(x)\right)^2 =$$
$$= \mathbb{E}_x\left(\frac{1}{N}\sum_{j=1}^{N} \varepsilon_j(x)\right)^2 =$$
$$= \frac{1}{N^2}\mathbb{E}_x\left(\sum_{j=1}^{N} \varepsilon_j^2(x) + \underbrace{\sum_{i\neq j} \varepsilon_i(x)\varepsilon_j(x)}_{=0}\right) =$$
$$\boxed{= \frac{1}{N}E_1.}$$

Error decreased by N times!

Bootstrap

Consider the errors ~~unbiased and uncorrelated~~:

Because this is a lie

$$\mathbb{E}_x \varepsilon_j(x) = 0;$$
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The final model averages all predictions:

$$a(x) = \frac{1}{N}\sum_{j=1}^{N} b_j(x).$$

Error decreased by N times!

$$\boxed{= \frac{1}{N}E_1.}$$

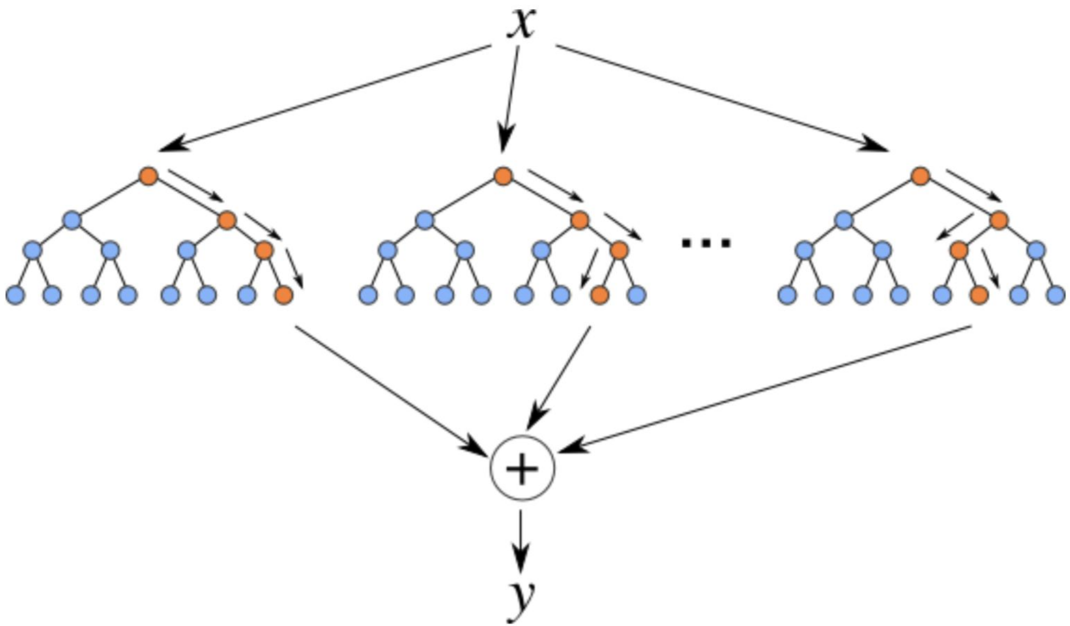
Bagging = Bootstrap aggregating

Decreases the variance if the basic algorithms are not correlated.

RSM - Random Subspace Method

Same approach, but with features.

Bagging + RSM = Random Forest



Random Forest

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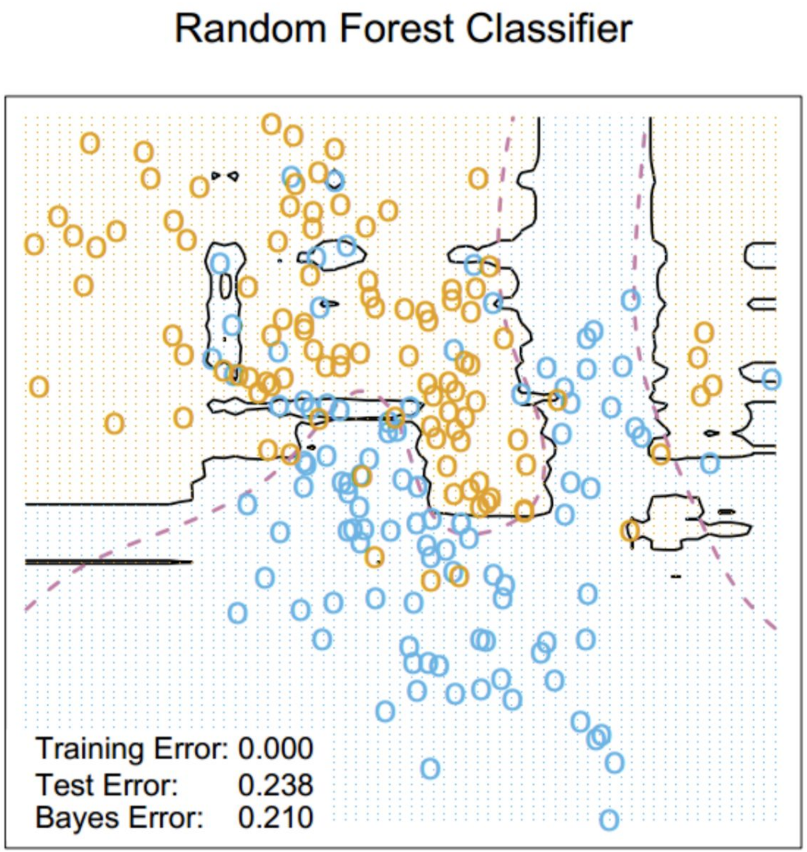
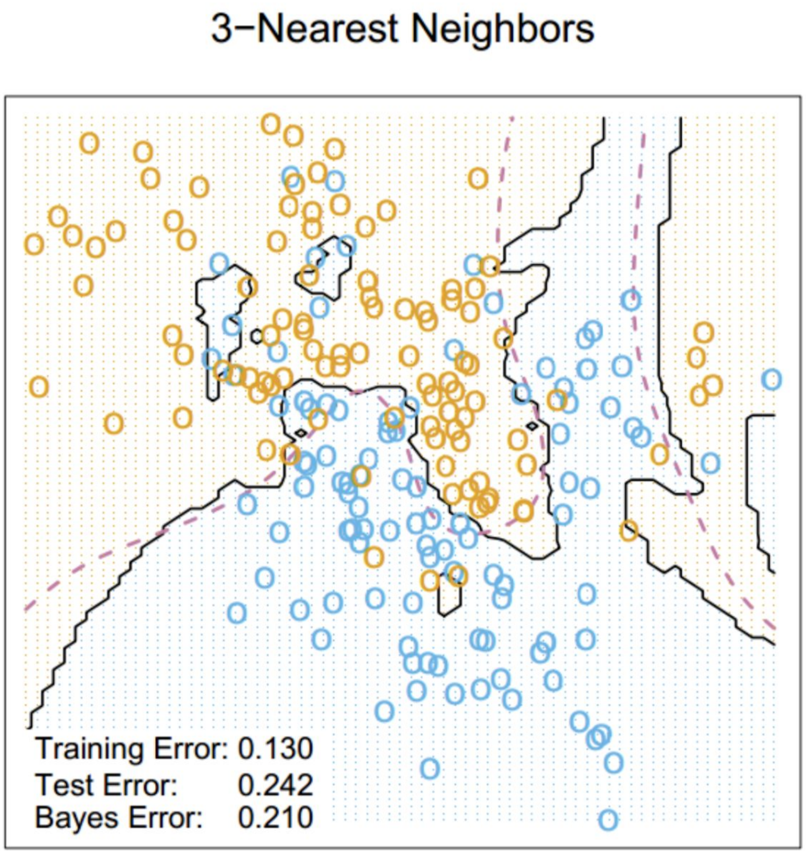
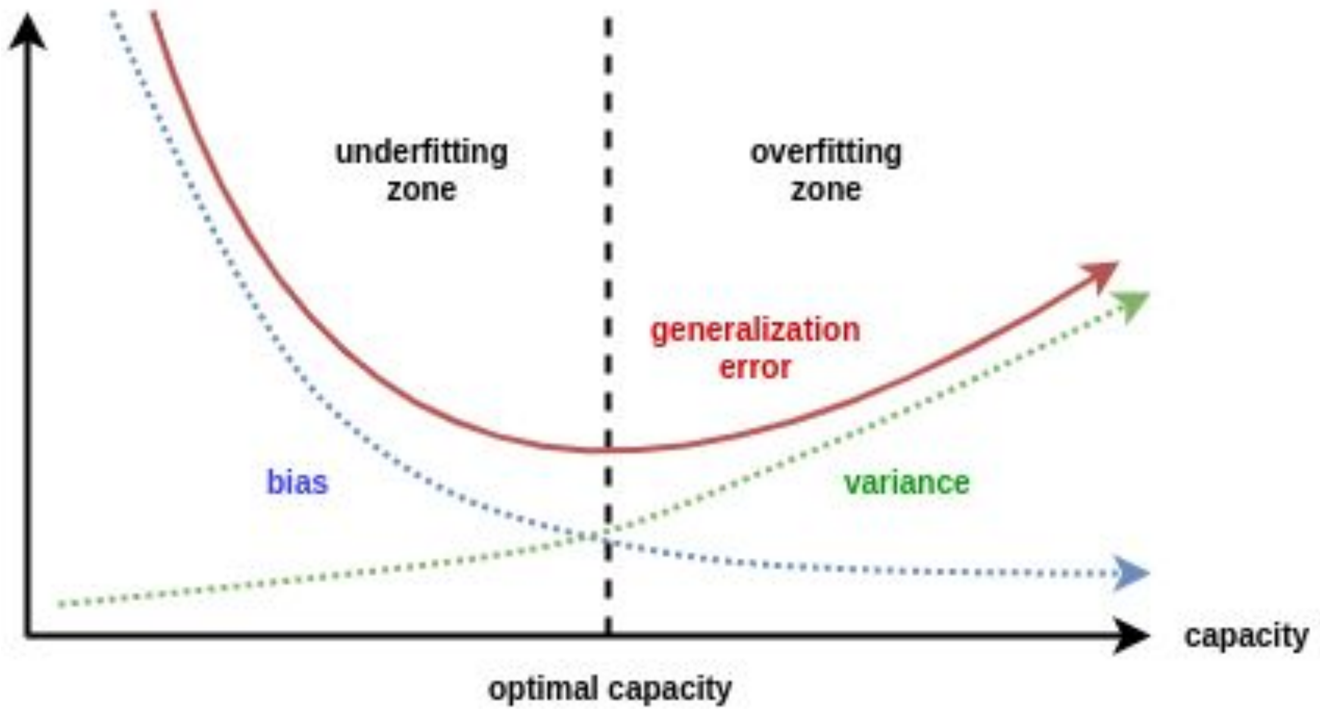
- Allows to use train data for validation: OOB

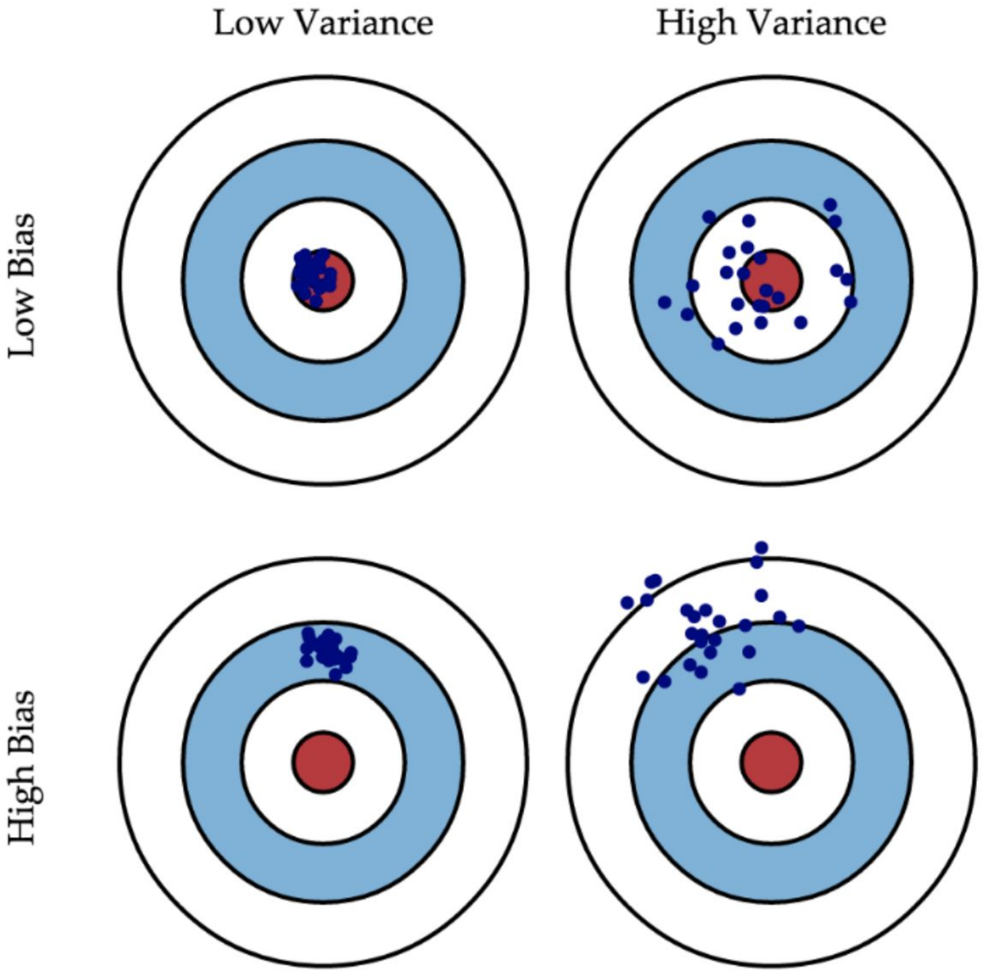
$$\mathrm{OOB} = \sum_{i=1}^{\ell} L\left(y_i, \frac{1}{\sum_{n=1}^{N}[x_i \notin X_n]} \sum_{n=1}^{N}[x_i \notin X_n] b_n(x_i)\right)$$


Random Forest Classifier
Training Error: 0.000
Test Error: 0.238
Bayes Error: 0.210


3−Nearest Neighbors
Training Error: 0.130
Test Error: 0.242
Bayes Error: 0.210

Bias-variance tradeoff




Low Variance
High Variance
Low Bias
High Bias

Bias-variance decomposition

The dataset $X = (x_i, y_i)_{i=1}^{\ell}$ with $y_i \in \mathbb{R}$ for regression problem.

Denote loss function $L(y, a) = \big(y - a(x)\big)^2$

The corresponding risk estimation is

$$R(a) = \mathbb{E}_{x,y}\Big[\big(y - a(x)\big)^2\Big] = \int_{\mathbb{X}}\int_{\mathbb{Y}} p(x, y)\big(y - a(x)\big)^2 dx dy.$$

Denote $\mu : (\mathbb{X} \times \mathbb{Y})^\ell \to \mathcal{A}$, where $\mathcal{A}$ is some family of algorithms.

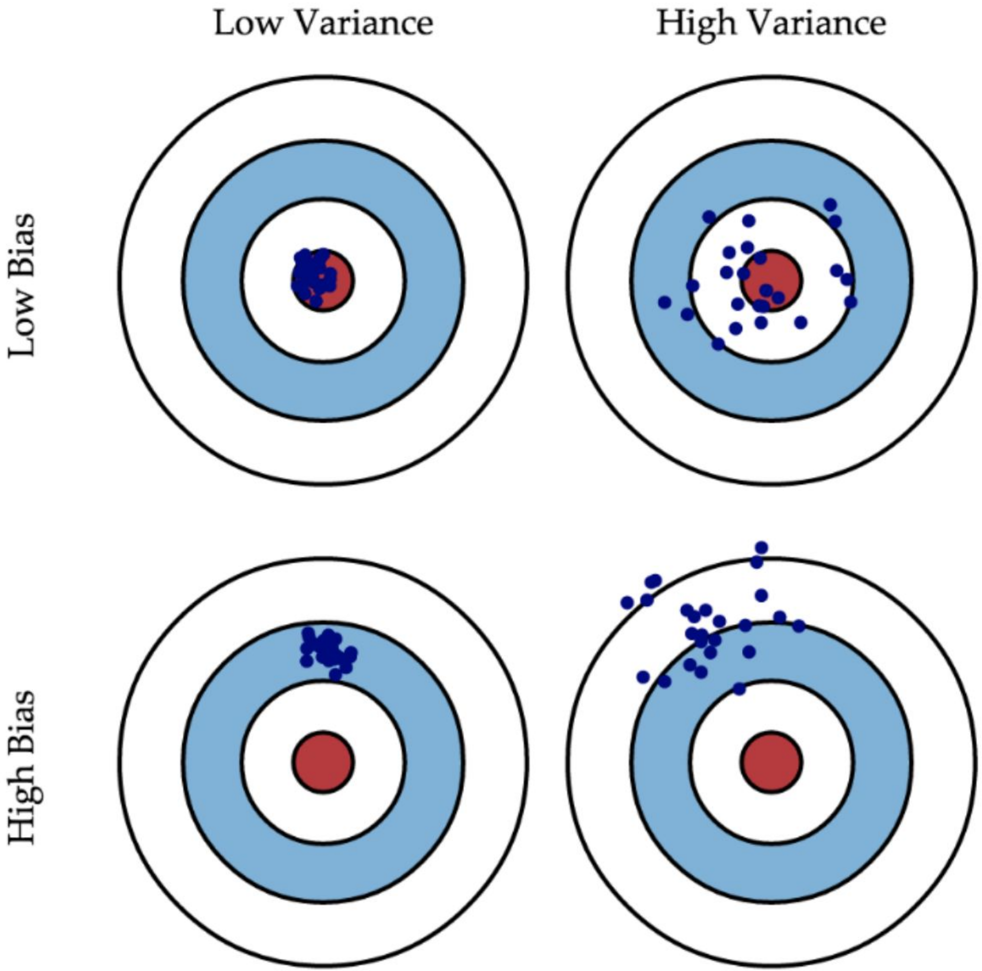
So $L(\mu) = \mathbb{E}_X\left[\mathbb{E}_{x,y}\left[\left(y - \mu(X)(x)\right)^2\right]\right]$, where X dataset.

$$L(\mu) = \underbrace{\mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \mid x]\right)^2\right]}_{\text{noise}} +$$

$$+ \underbrace{\mathbb{E}_x\left[\left(\mathbb{E}_X\left[\mu(X)\right] - \mathbb{E}[y \mid x]\right)^2\right]}_{\text{bias}} + \underbrace{\mathbb{E}_x\left[\mathbb{E}_X\left[\left(\mu(X) - \mathbb{E}_X\left[\mu(X)\right]\right)^2\right]\right]}_{\text{variance}}.$$

This exact form of bias-variance decomposition is correct for square loss in regression.

However, it is much more general. See extra materials for more exotic cases.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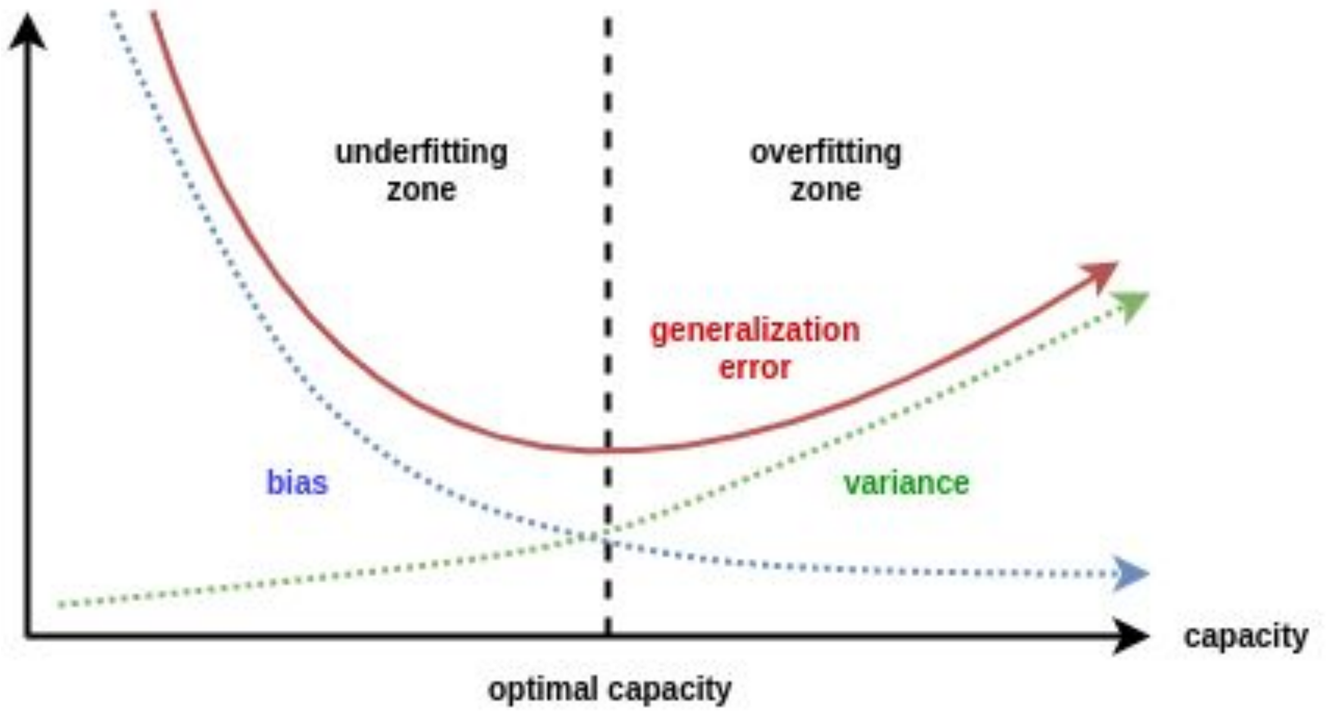
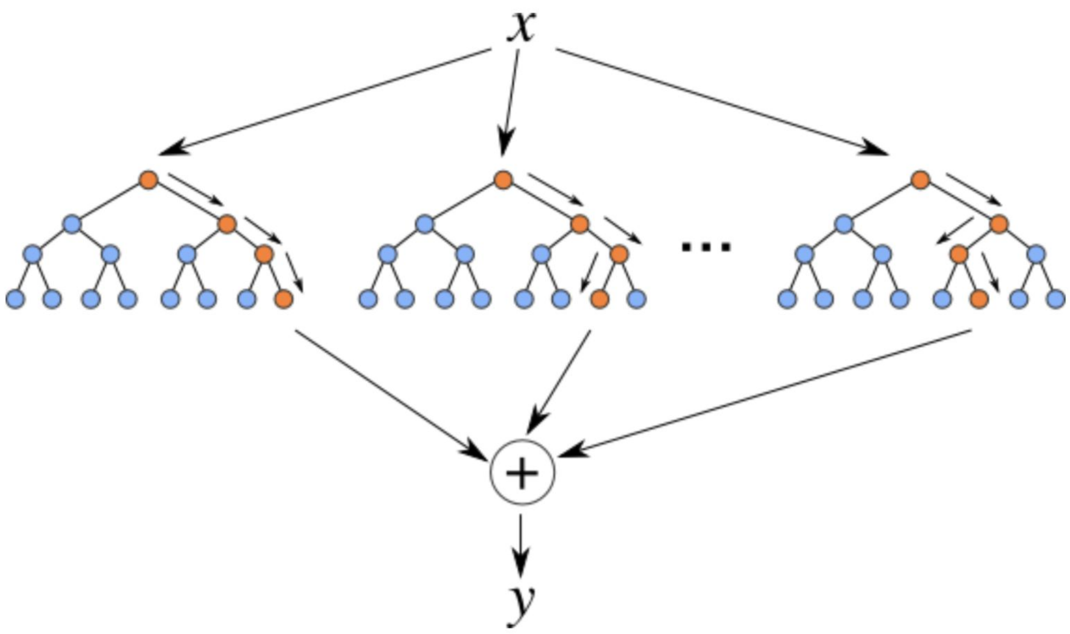
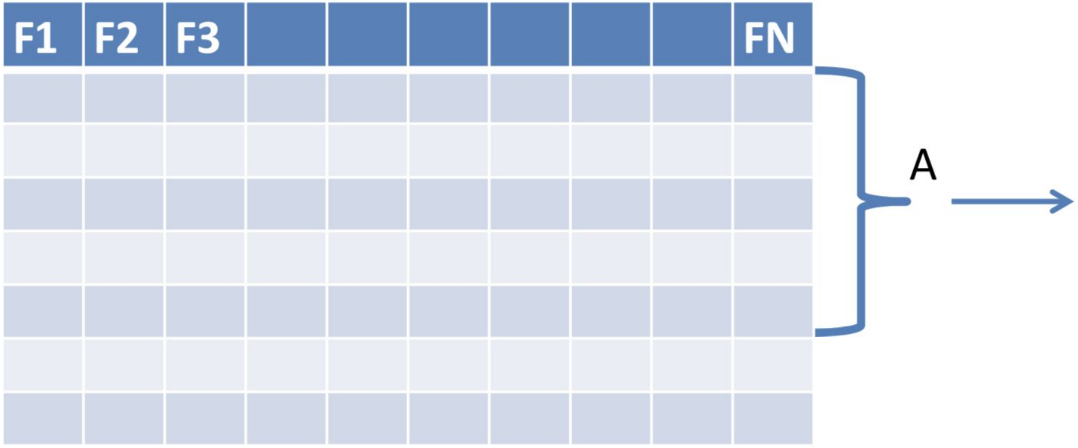


Bagging + RSM = Random Forest



Stacking

How to build an ensemble from *different* models?



Tune M basic algorithms

Stacking

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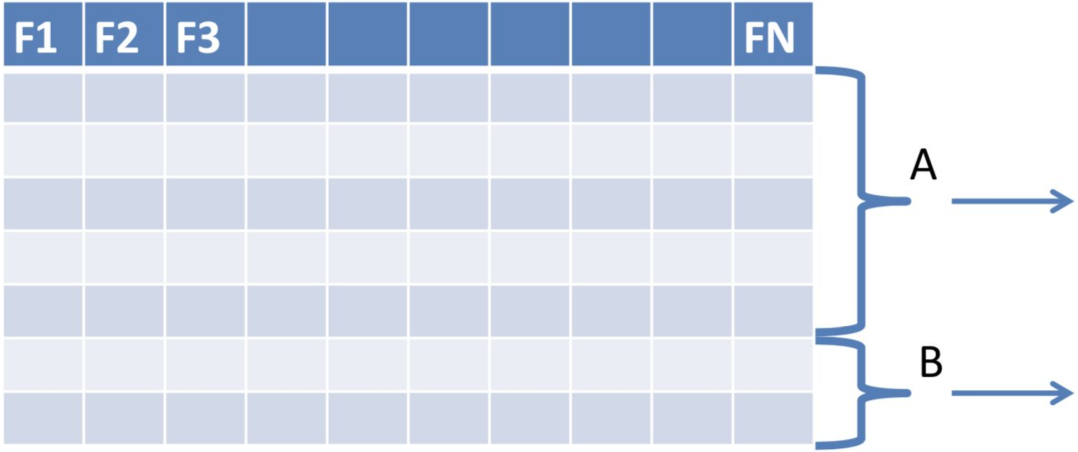

Tune M basic algorithms

Tune new model on the outputs of the basic algorithms

Stacking

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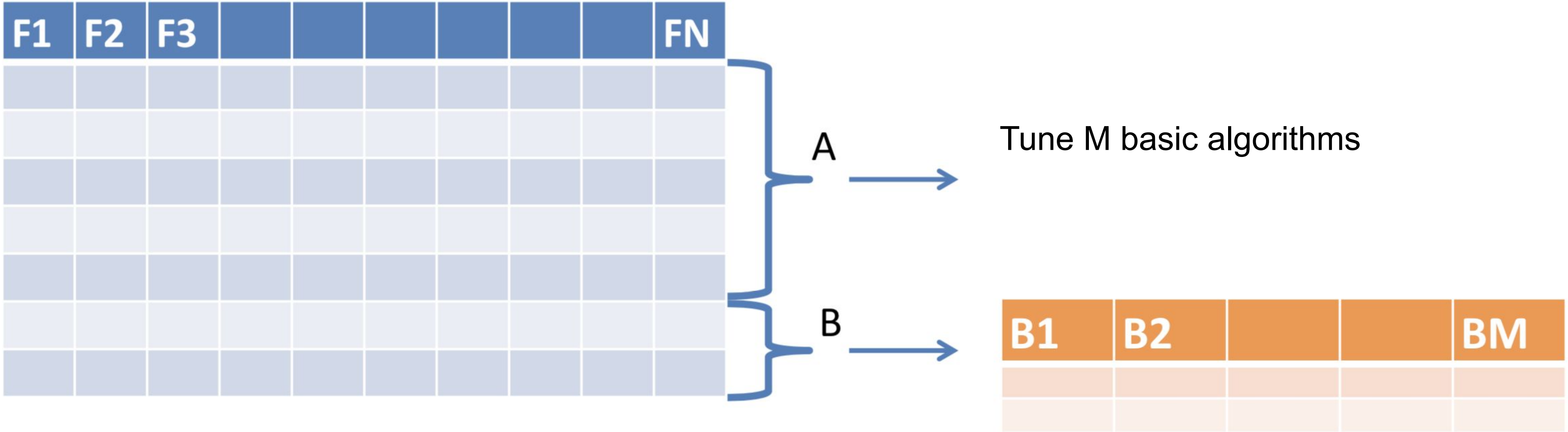

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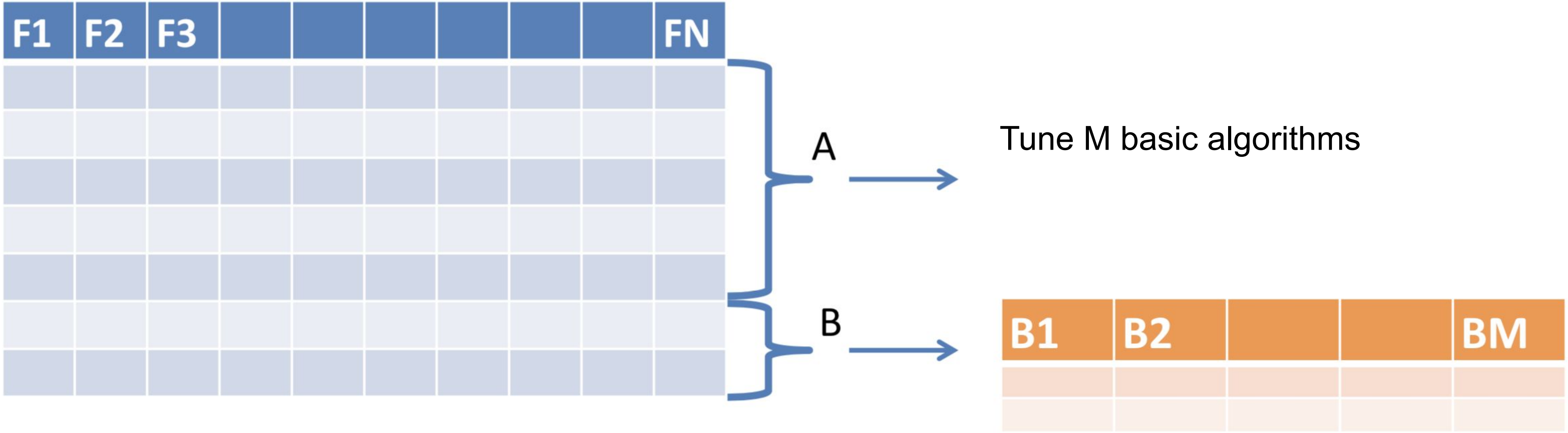

$$a(x) = \sum_{t=1}^{T} \alpha_t b_t(x)$$

e.g.

Stacking

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- Use different datasets (or datasets parts) for different level models.

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- Experiment with different models (linear, trees ensembles, simple networks, etc.)

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How to build an ensemble from *different* models?

- Use different datasets (or datasets parts) for different level models.
- Experiment with different models (linear, trees ensembles, simple networks, etc.)
- Or just different GBT ensembles (hola, kaggle :)

Blending

Just combine several *strong/complex* models.

Weights should sum up to 1
and come from [0; 1]

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- Finding optimal weights could be tricky.

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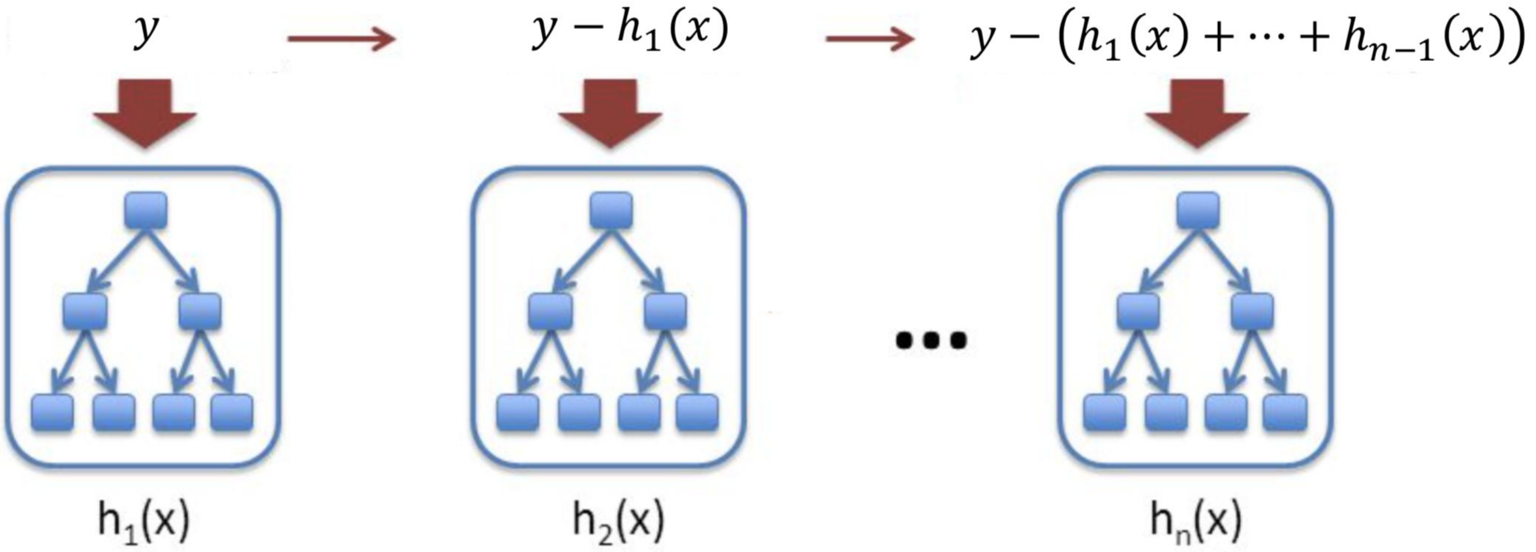
$$a(x) = \sum_{t=1}^{T} \alpha_t b_t(x)$$

- Simple and intuitive ensembling method.
- Finding optimal weights could be tricky.
- Linear composition is not always enough.

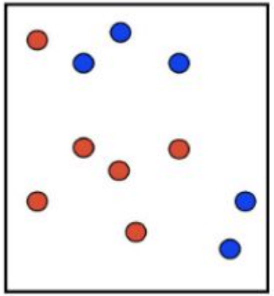
Gradient boosting

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

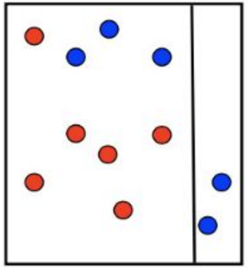


Boosting: intuition

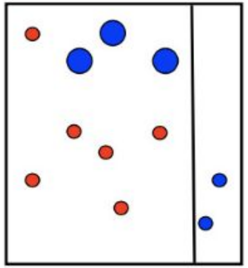
Binary classification problem.
Models - decision stumps.

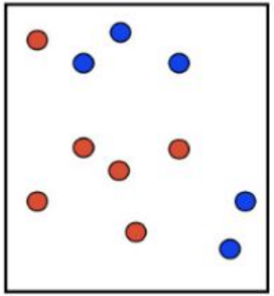


Boosting: intuition



t = 1





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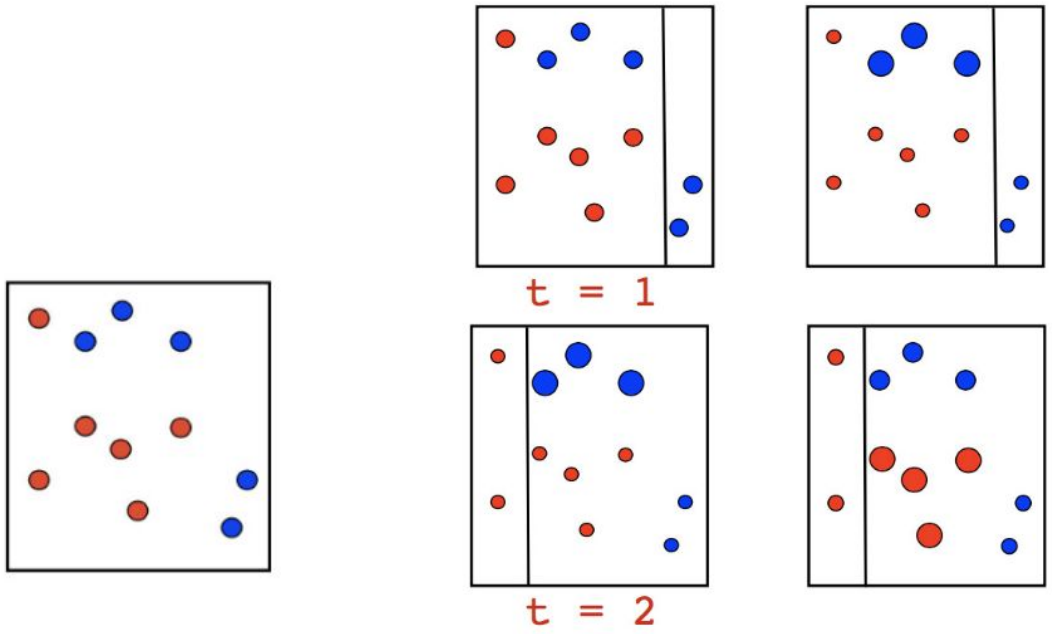

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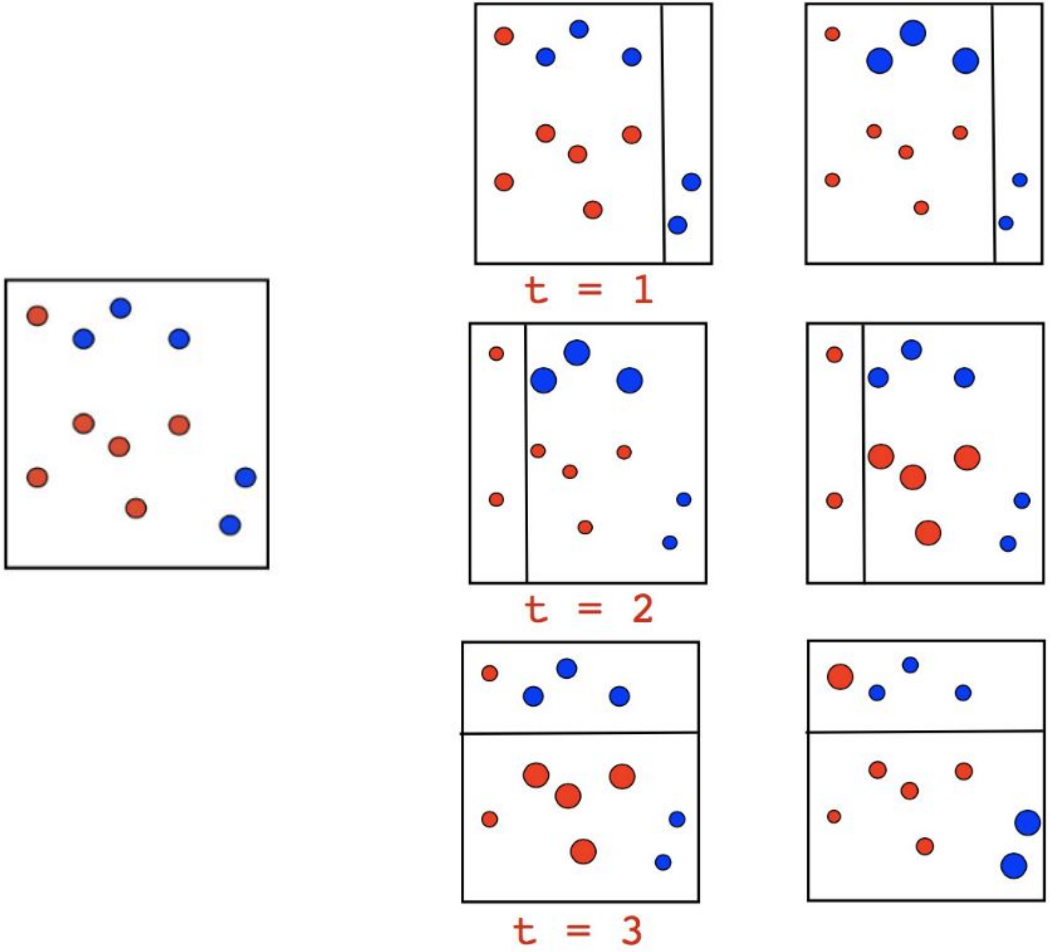

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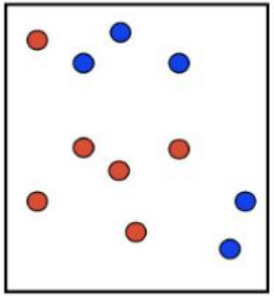

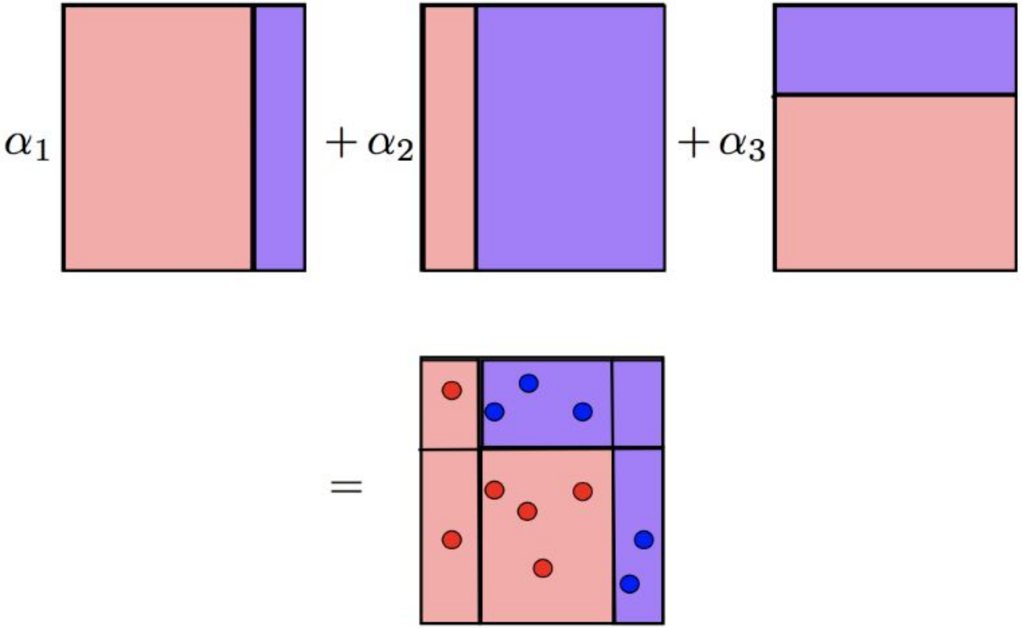

Gradient boosting: theory

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

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Optimal model:

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

Gradient boosting: theory

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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

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

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

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

Gradient boosting: theory

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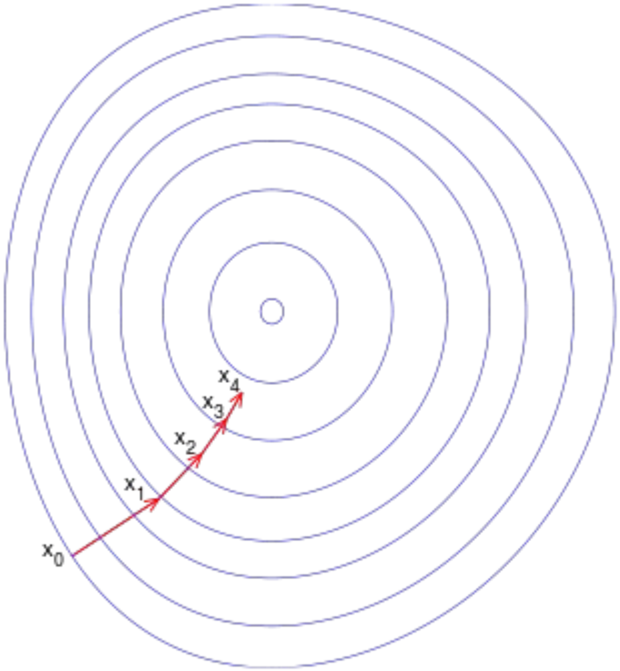
What if we could use gradient descent in *space of our models*?

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:

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

Gradient boosting: theory

What we need:

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

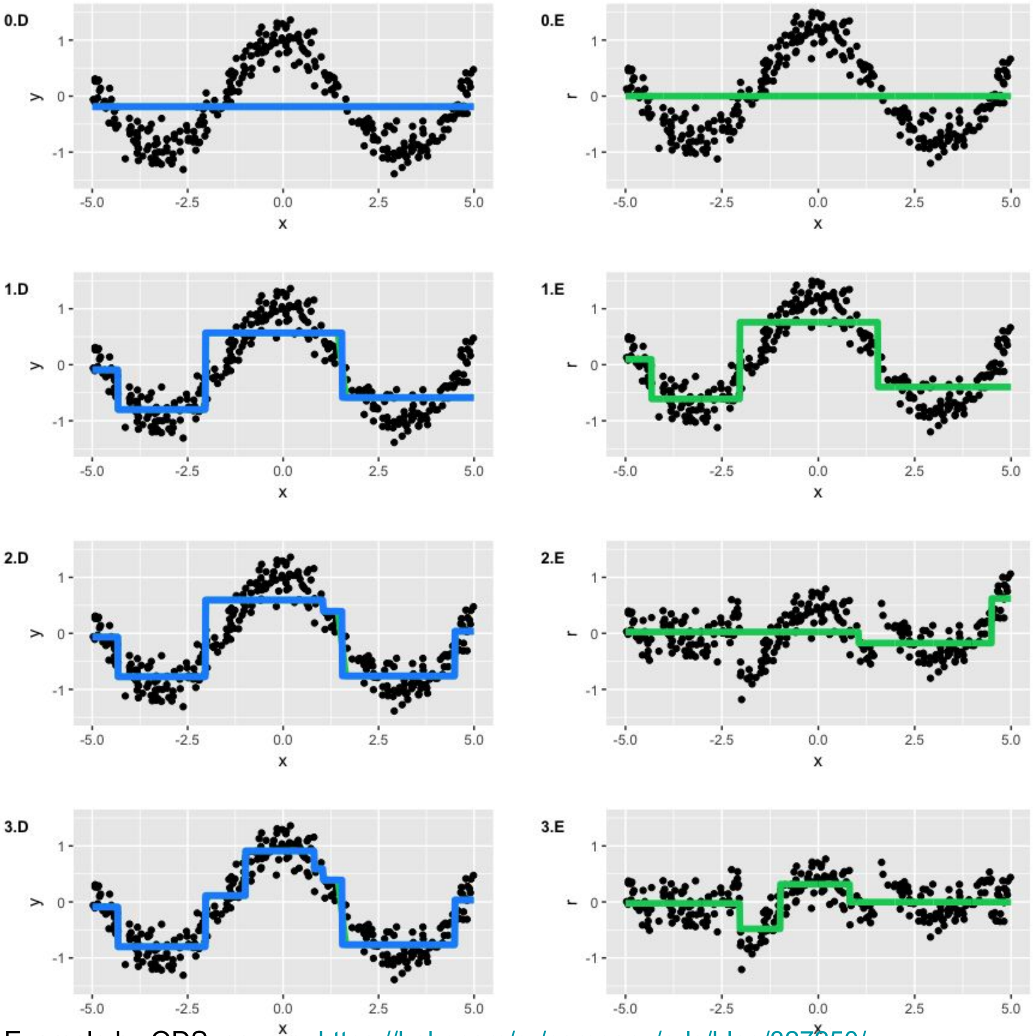
Gradient boosting: example

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 value

Example by ODS; source: https://habr.com/ru/company/ods/blog/327250/

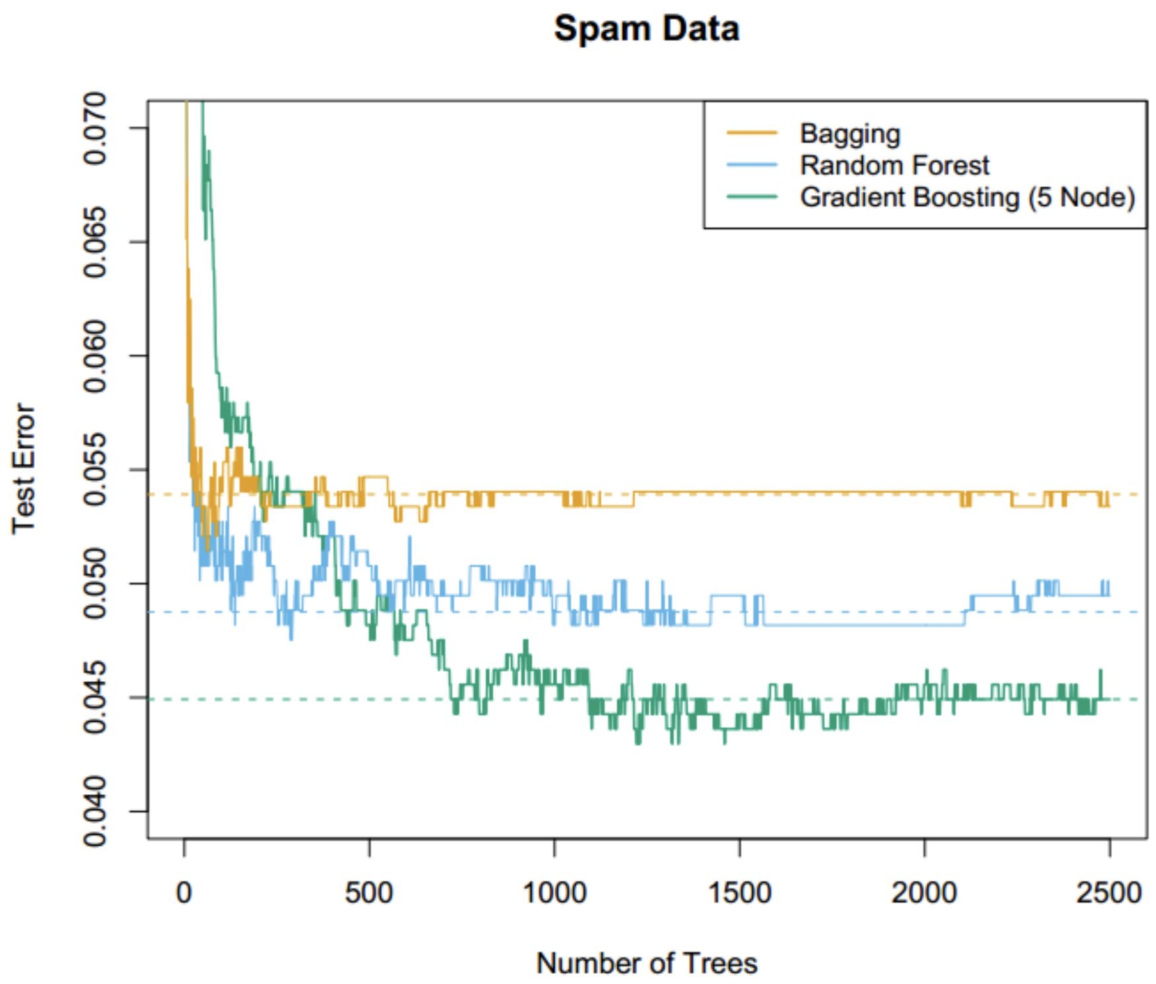
Gradient boosting: example

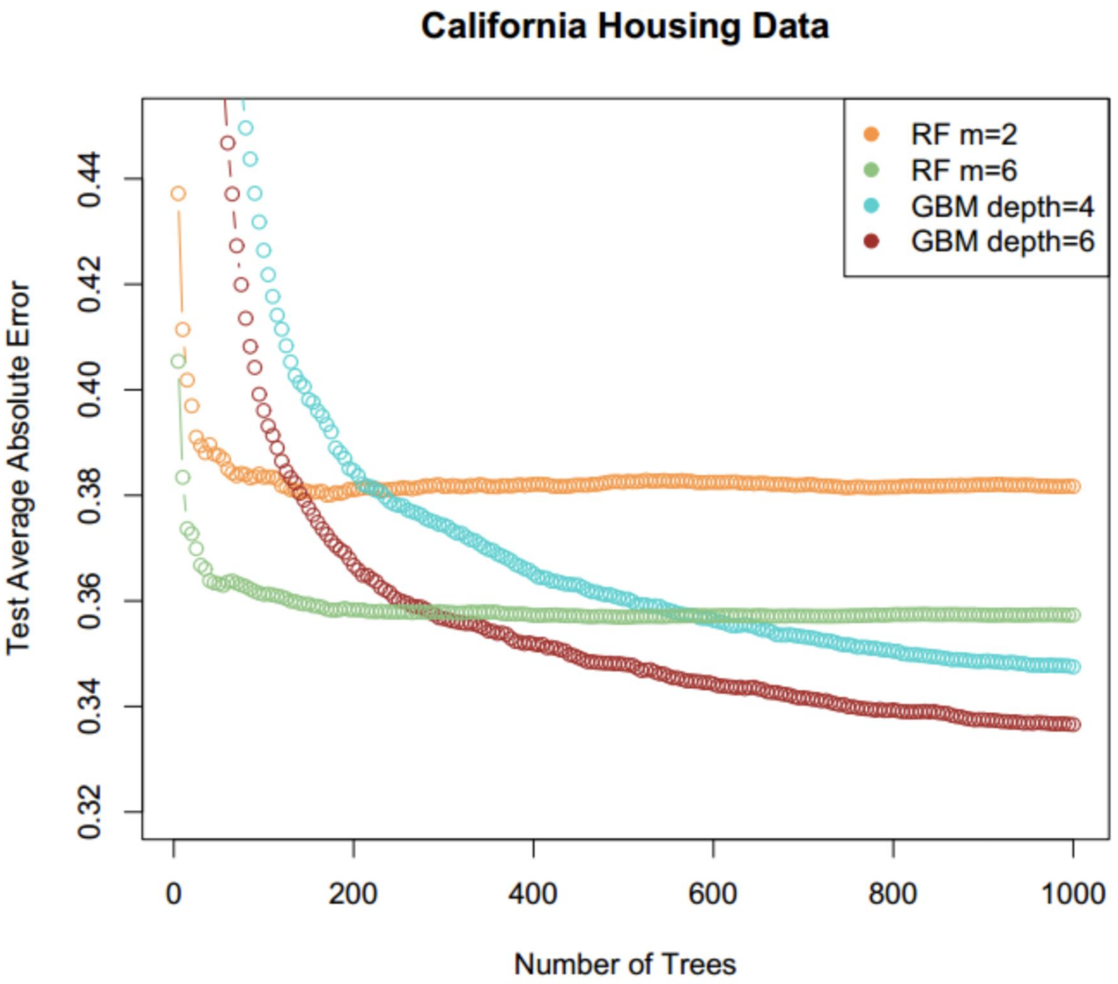


Left: full ensemble on each step.

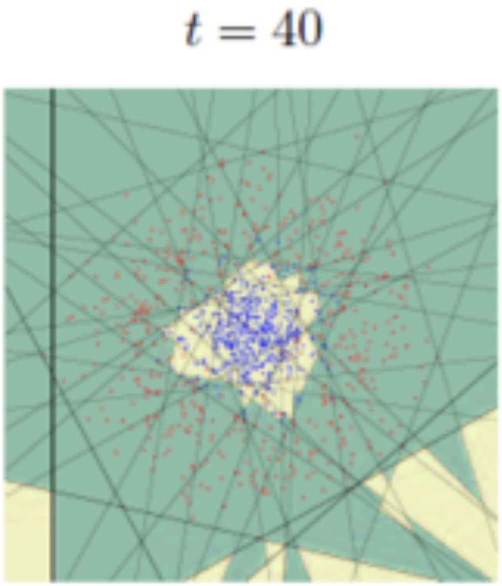
Right: additional tree decisions.

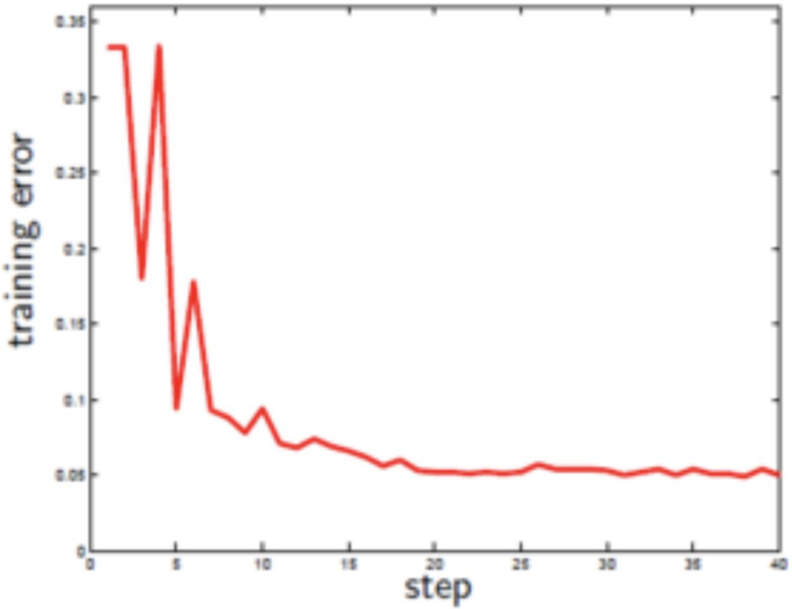
Example by ODS; source: https://habr.com/ru/company/ods/blog/327250/


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

Boosting with linear classification methods





Technical side: training in parallel

Which of the ensembling methods could be parallelized?

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- Random Forest: parallel on the forest level (all trees are independent)

Technical side: training in parallel

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

Recap: ensembling methods

1. Bagging.
2. Random subspace method (RSM).
3. Bagging + RSM + Decision trees = Random Forest.
4. Gradient boosting.
5. Stacking.
6. Blending.

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

Extra lecture about feature engineering and ML techniques is coming next week. Stay tuned.