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Gradient boosting

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MLHEP 2021

NATIONAL RESEARCH UNIVERSITY

LAMBDA • HSE

Yandex

SCHOOL OF DATA ANALYSIS

EPFL

Schaffhausen Institute of Technology

Lecture overview

After this lecture you will be able to:

- Build efficient self-correcting ensembles of models for classification and regression
- Use state-of-the-art techniques to achieve peak performance

Boosting: the idea

> Build a sequence of models, where each model corrects the error of the previous ones

Naive boosting for regression

Boosting for regression

- Consider a regression problem $\frac{1}{2}\sum_{i=1}^{\ell}(h(x_i) - y_i)^2 \to \min\limits_{h}$

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- The **boosting approach:** add weak learners greedily
  1. Start with a "trivial" weak learner $h_0(x) = \frac{1}{\ell}\sum_{i=1}^{\ell} y_i$

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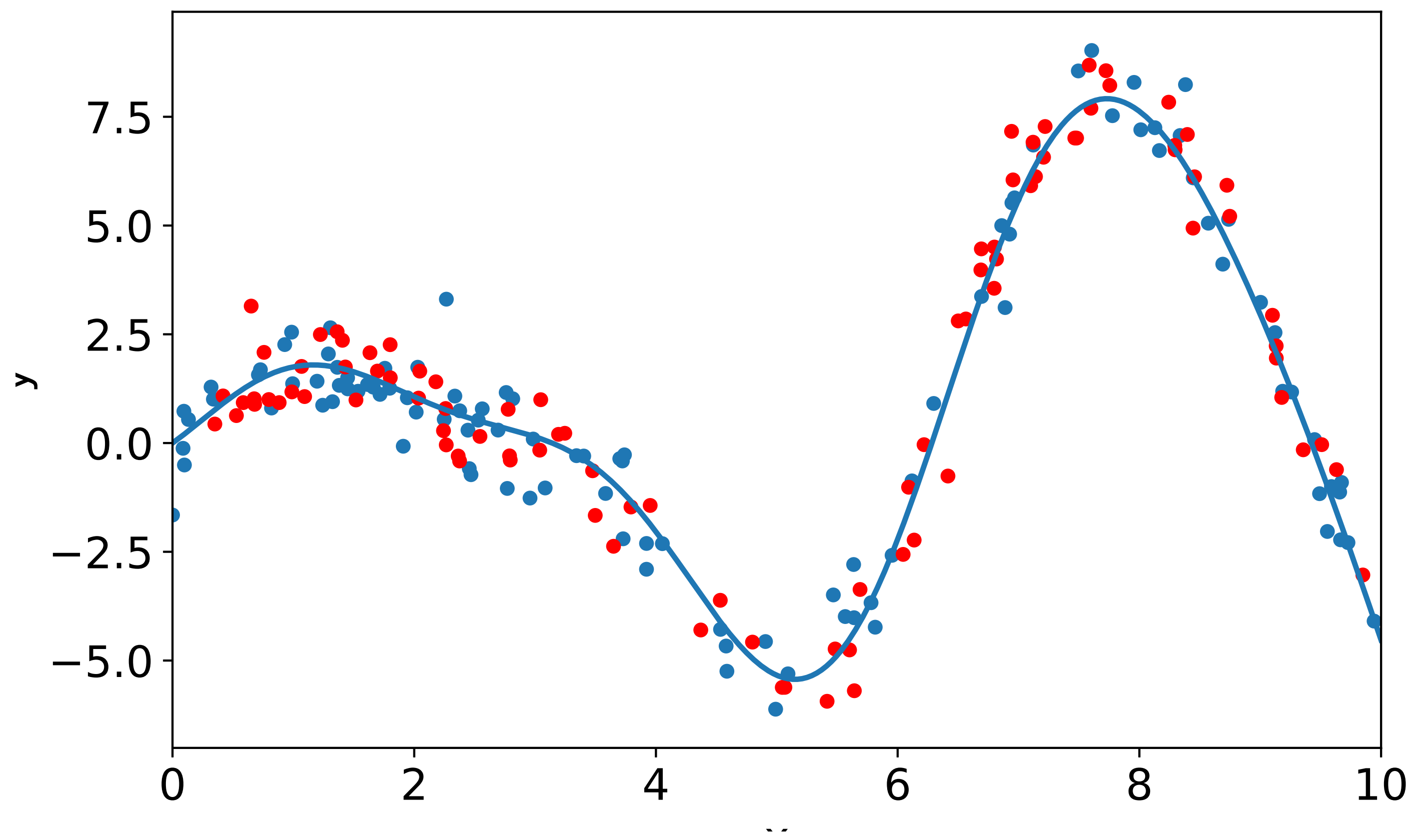
- The **boosting approach:** add weak learners greedily
  1. Start with a "trivial" weak learner $h_0(x) = \frac{1}{\ell}\sum_{i=1}^{\ell} y_i$
  2. At step N, compute the residuals

$$s_i^{(N)} = y_i - \sum_{n=1}^{N-1} h_n(x_i) = y_i - a_{N-1}(x_i), \qquad i = 1, \dots, \ell$$

  3. Learn the next weak algorithm using

$$a_N(x) := \arg\min_{h \in \mathbb{H}} \frac{1}{2}\sum_{i=1}^{\ell}(h(x_i) - s_i^{(N)})^2$$

Boosting: an example regression problem



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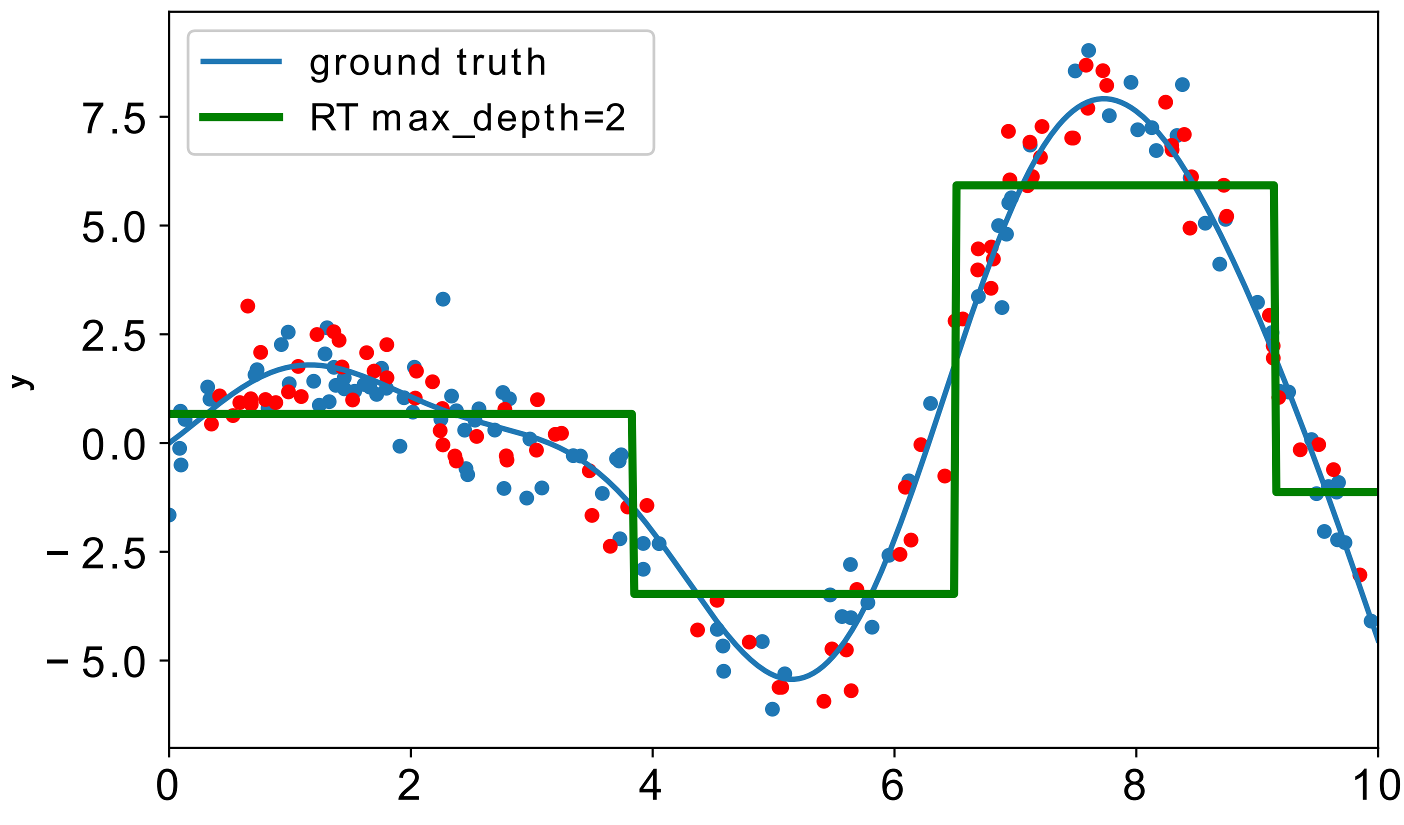

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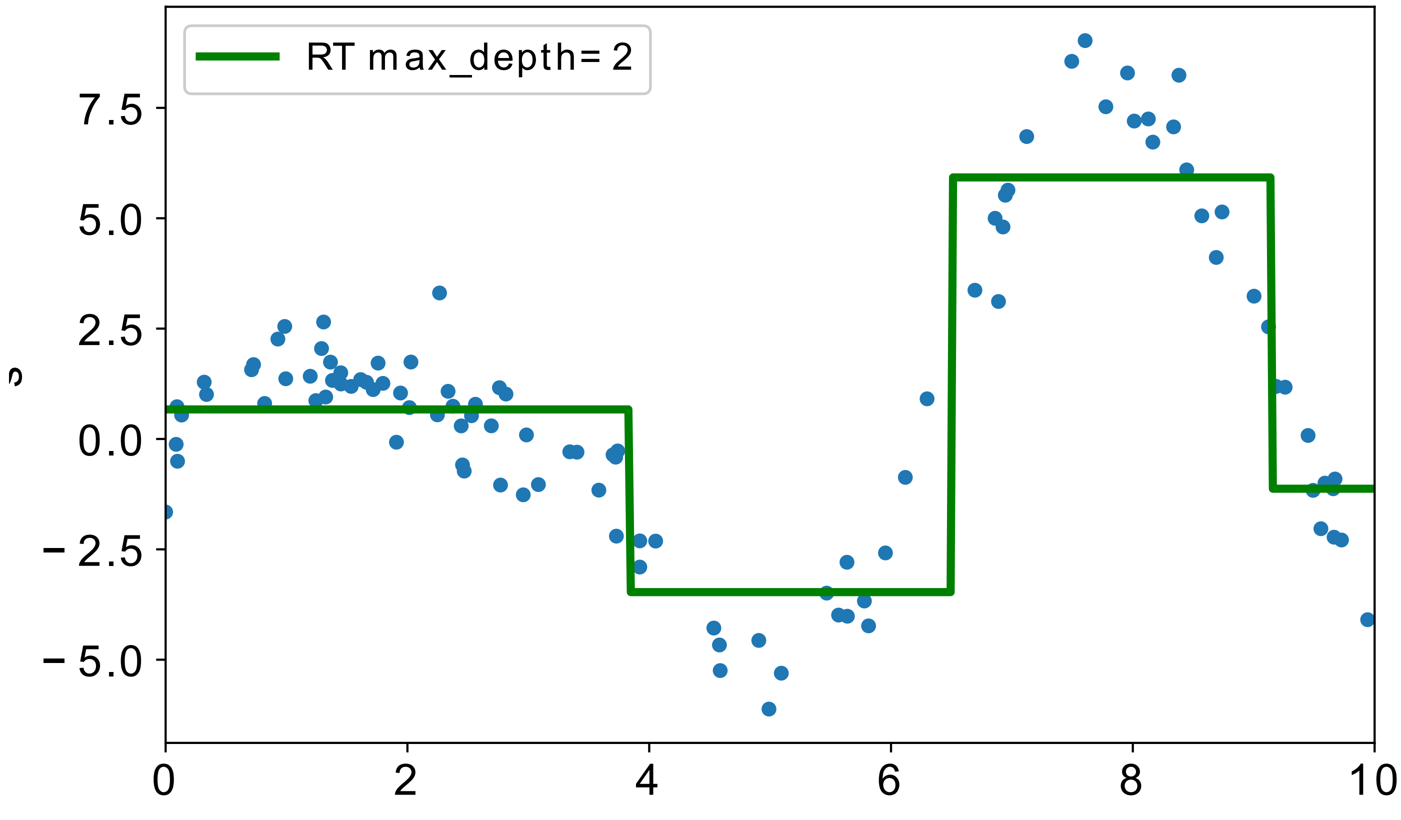

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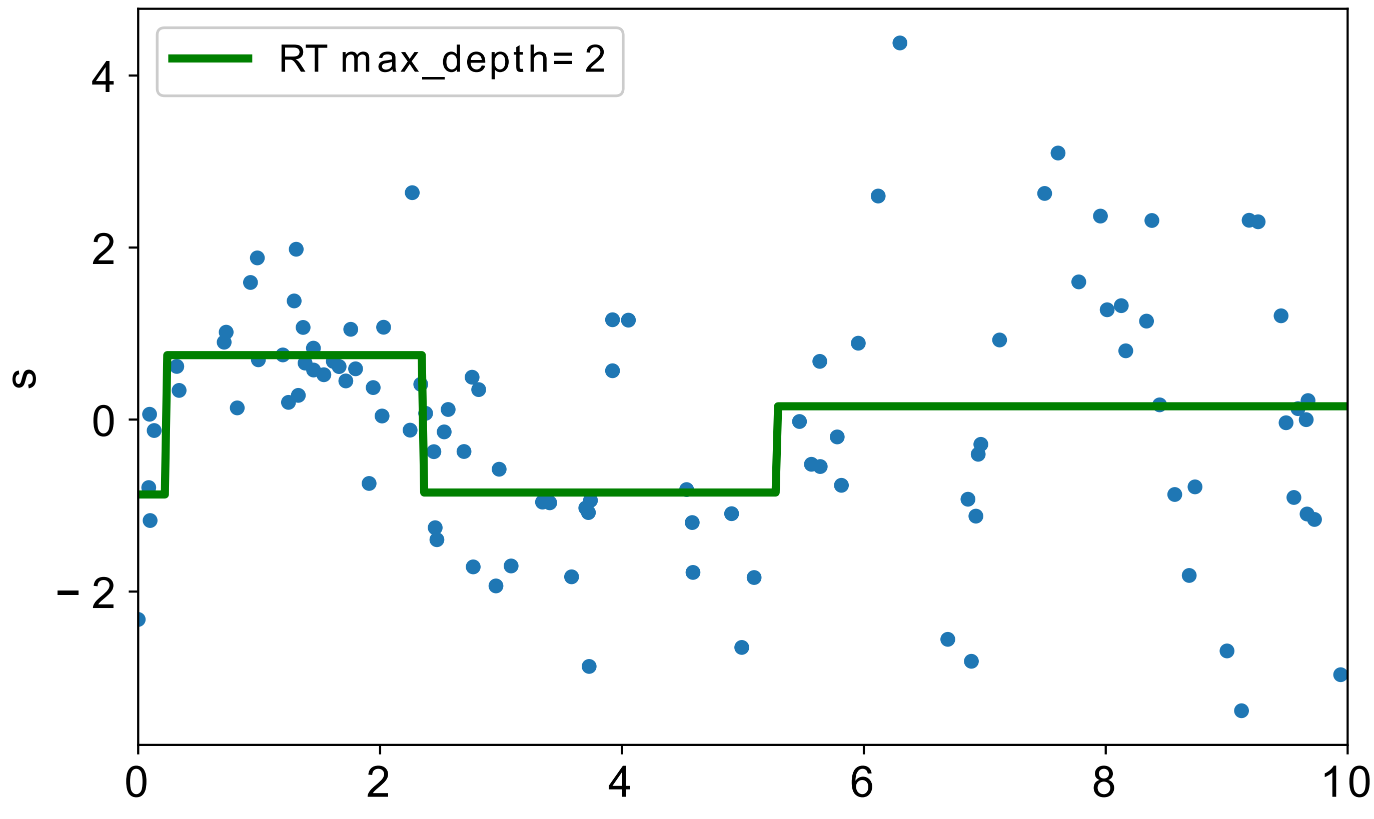

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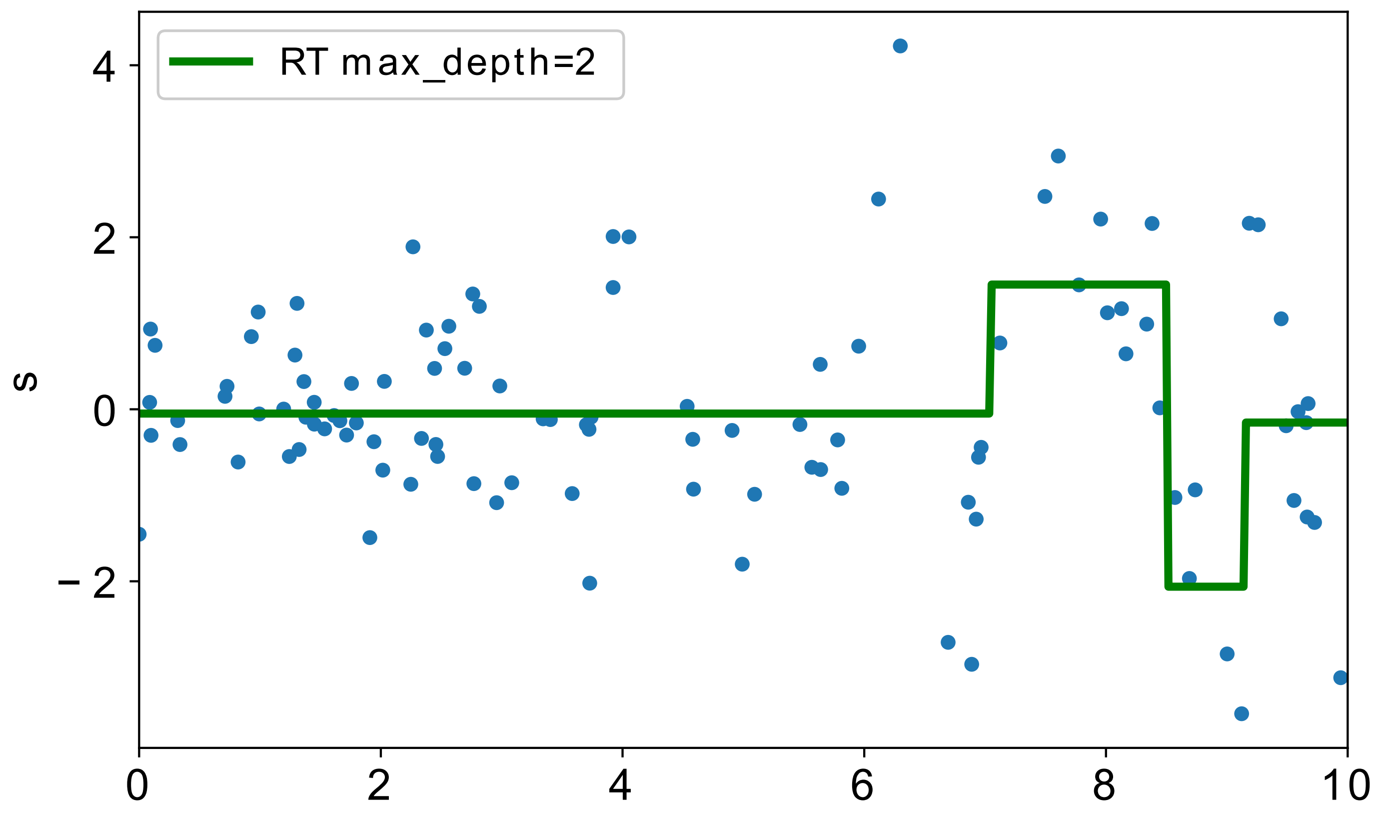

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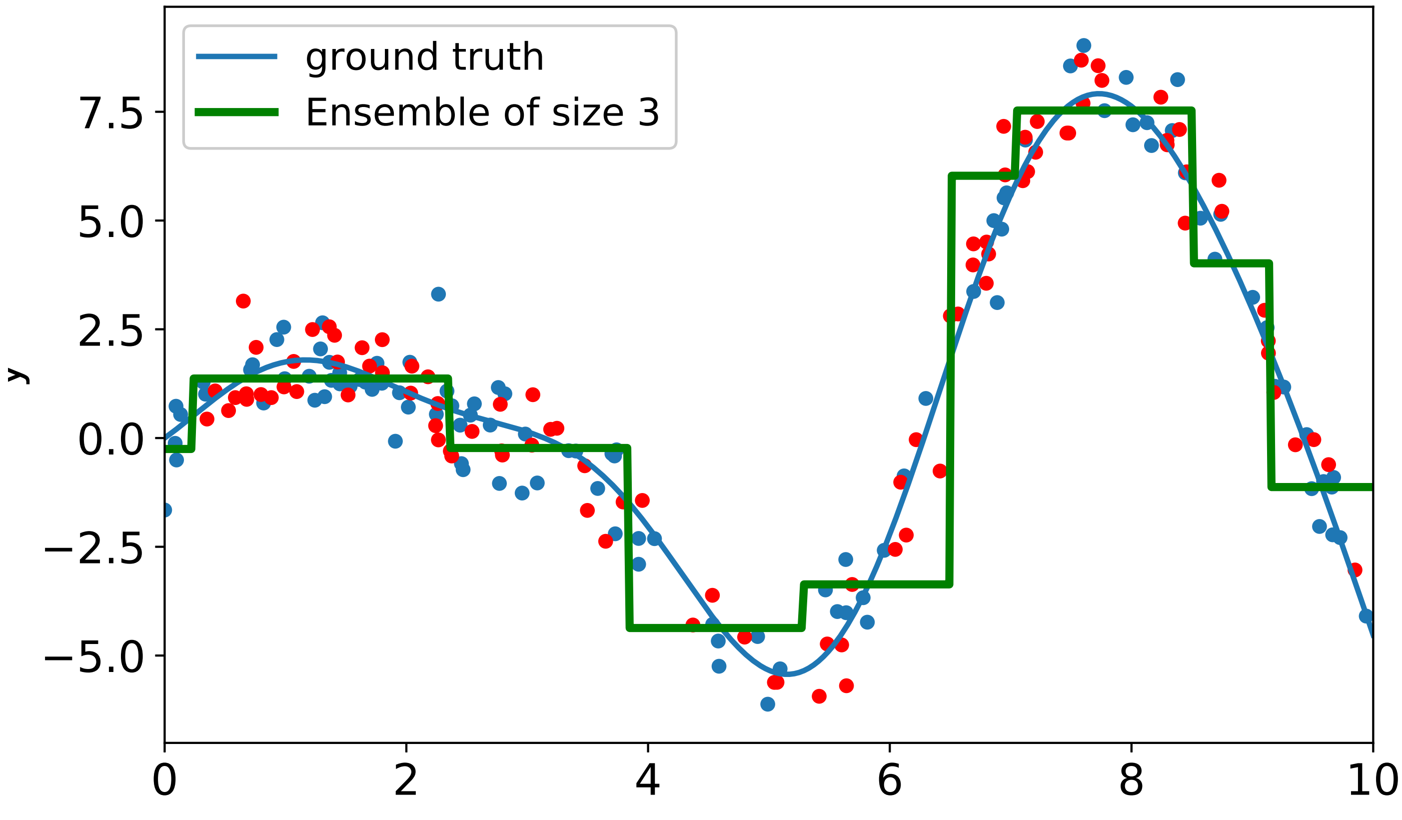

Gradient boosting

Gradient boosting: motivation

- We know how to handle the mean squared error loss
- We want to handle arbitrary losses, but how to define the residuals?
- Solution: use gradient descent!

Gradient boosting: scheme

- With $a_{N-1}(\mathbf{x})$ already built, how to find the next γ_N and h_N if

$$\sum_{i=1}^{\ell} L(y_i, a_{N-1}(\mathbf{x}_i) + \gamma h(\mathbf{x}_i)) \to \min_{\gamma, h}$$

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- Search for such $s_1, \ldots, s_\ell$ that

$$\sum_{i=1}^{\ell} L(y_i, a_{N-1}(\mathbf{x}_i) + s_i) \to \min_{s_1, \ldots, s_\ell}$$

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$$\sum_{i=1}^{\ell} L(y_i, a_{N-1}(\mathbf{x}_i) + s_i) \to \min_{s_1, \ldots, s_\ell}$$

- Choose $s_i = -\left.\frac{\partial L(y_i, z)}{\partial z}\right|_{z = a_{N-1}(\mathbf{x}_i)}$, approximate s_i's by $h_N(\mathbf{x}_i)$

The Gradient Boosting Machine

- Input:
  - Training set $D = \{(\mathbf{x}_i, y_i)\}_{i=1}^{\ell}$
  - Number of boosting iterations N
  - Loss function $L(y, z)$ with its gradient $\frac{\partial L}{\partial z}$
  - A family $\mathbb{H} = \{h(\mathbf{x})\}$ of weak learners and their associated learning procedures
  - Additional hyperparameters of weak learners (tree depth, etc.)
- Initialize GBM $h_0(\mathbf{x})$ using some simple rule (zero, most popular class, etc.)
- Execute boosting iterations $t = 1, \ldots, N$ (see next slide)
- Compose the final GBM learner: $a_N(\mathbf{x}) = \sum_{t=0}^{N} \gamma_i h_i(\mathbf{x})$

The Gradient Boosting Machine

At every iteration:

1. Compute pseudo-residuals: $s_i = -\left.\frac{\partial L(y_i, z)}{\partial z}\right|_{z=a_{N-1}(\mathbf{x}_i)}, i = 1, \ldots, \ell$

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$$h_N(x) = \arg\min_{h \in \mathbb{H}} \sum_{i=1}^{\ell} (h(\mathbf{x}_i) - s_i)^2$$

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3. Find the optimal γ_N using plain gradient descent:

$$\gamma_N = \arg\min_{\gamma \in \mathbb{R}} \sum_{i=1}^{\ell} L(y_i, a_{N-1}(\mathbf{x}_i) + \gamma h_N(\mathbf{x}_i))$$

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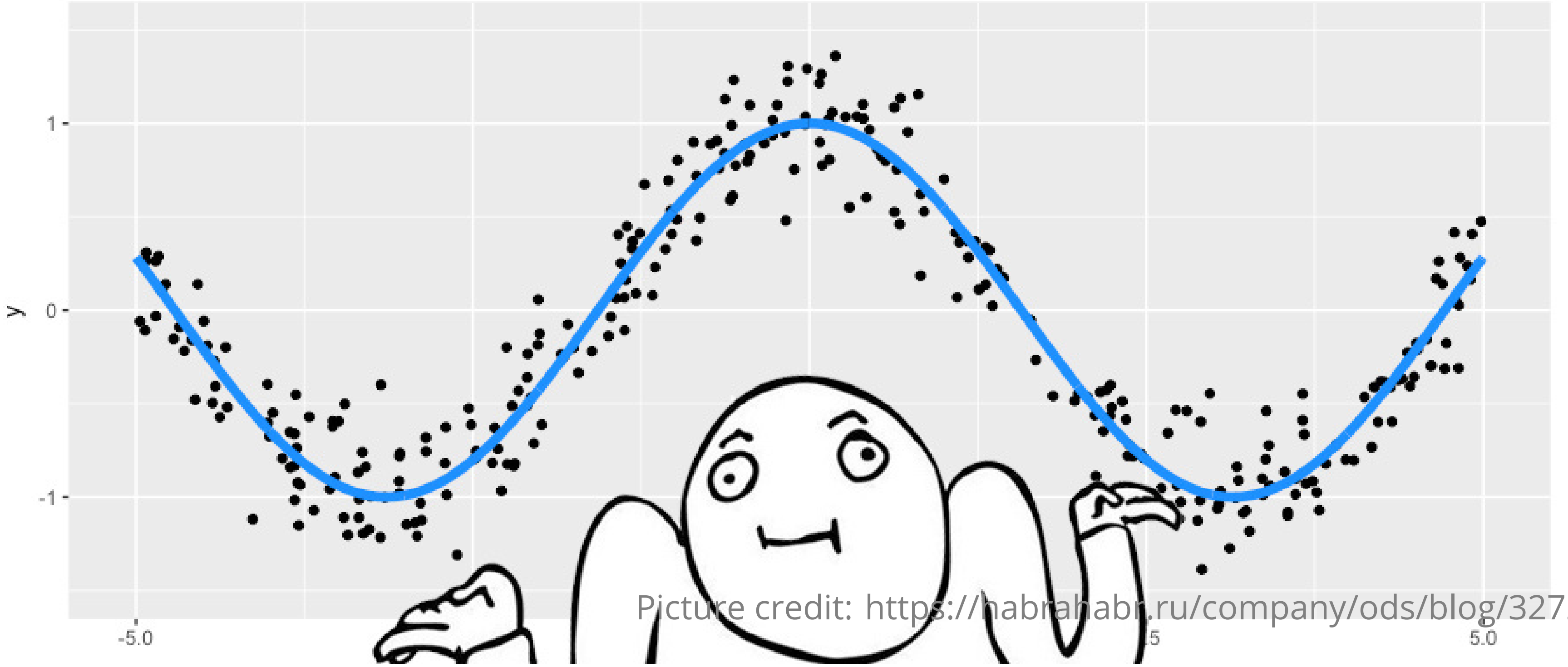
4. Update the GBM by $a_N(\mathbf{x}_i) \leftarrow a_{N-1}(\mathbf{x}) + \gamma_N h_N(\mathbf{x})$

GBM: an example regression problem

- Consider a training set for a $X^{300} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{300}$
  where $x_i \in [-5, 5]$, $y_i = \cos(x_i) + \varepsilon_i$, $\varepsilon_i \sim \mathcal{N}(0, 1/5)$

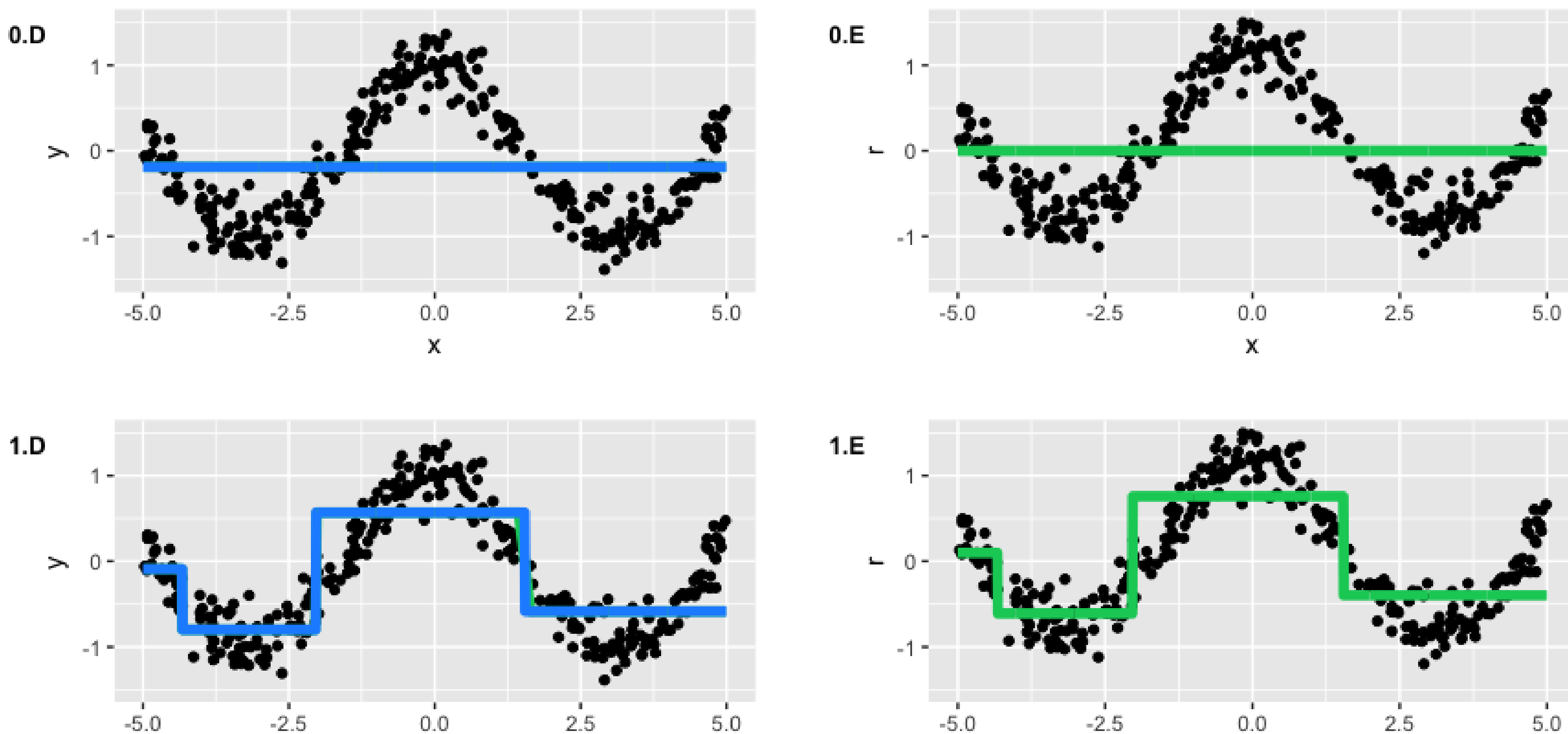


Picture credit: https://habrahabr.ru/company/ods/blog/327250

GBM: an example regression problem

- Pick $N = 3$ boosting iterations
- Quadratic loss $L(y, z) = (y - z)^2$
- Gradient of the quadratic loss $\frac{\partial L(y_i, z)}{\partial z} = (y - z)$ is just redisuals
- Pick decision trees as weak learners $h_i(\mathbf{x})$
- Set 2 as the maximum depth for decision trees

GBM: an example regression problem



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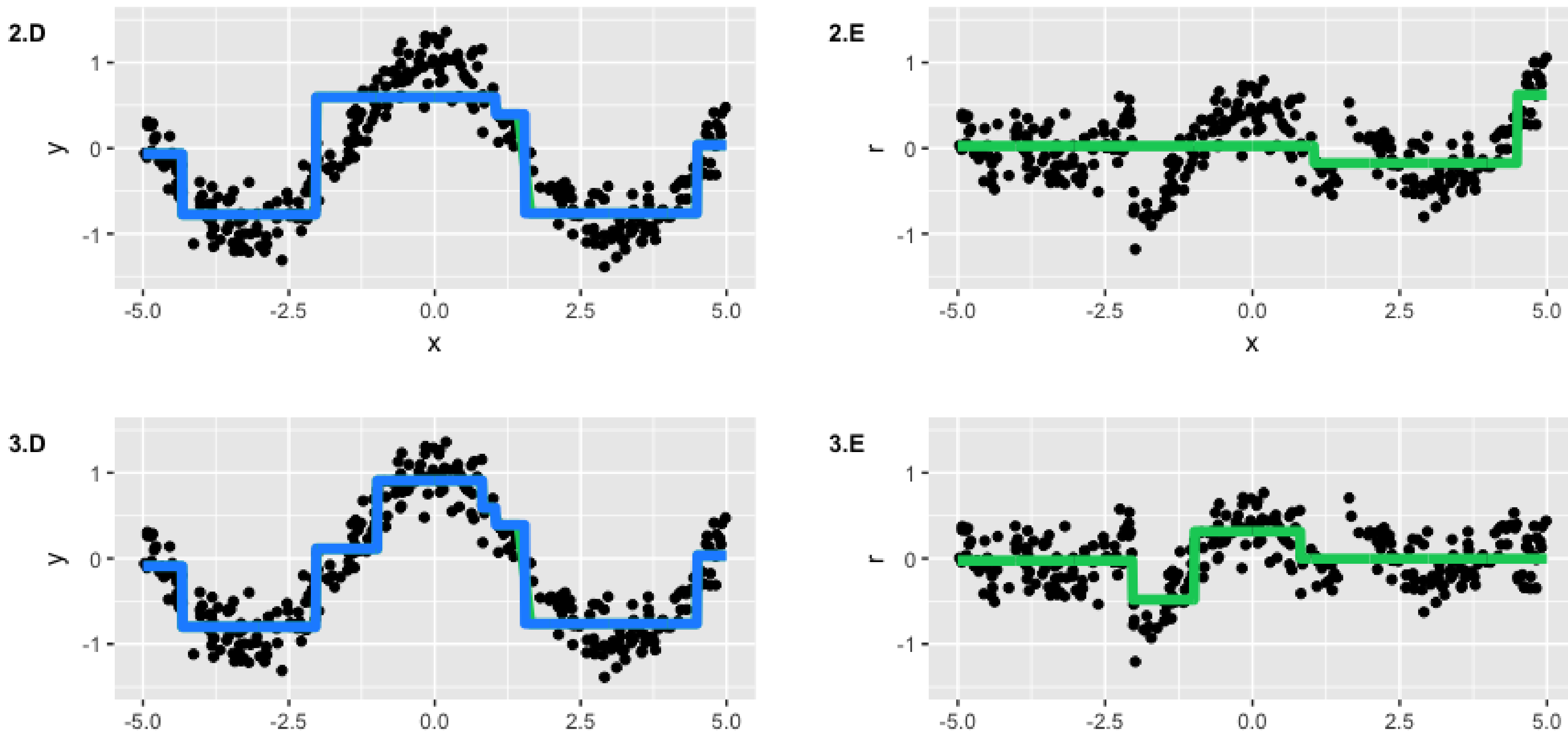
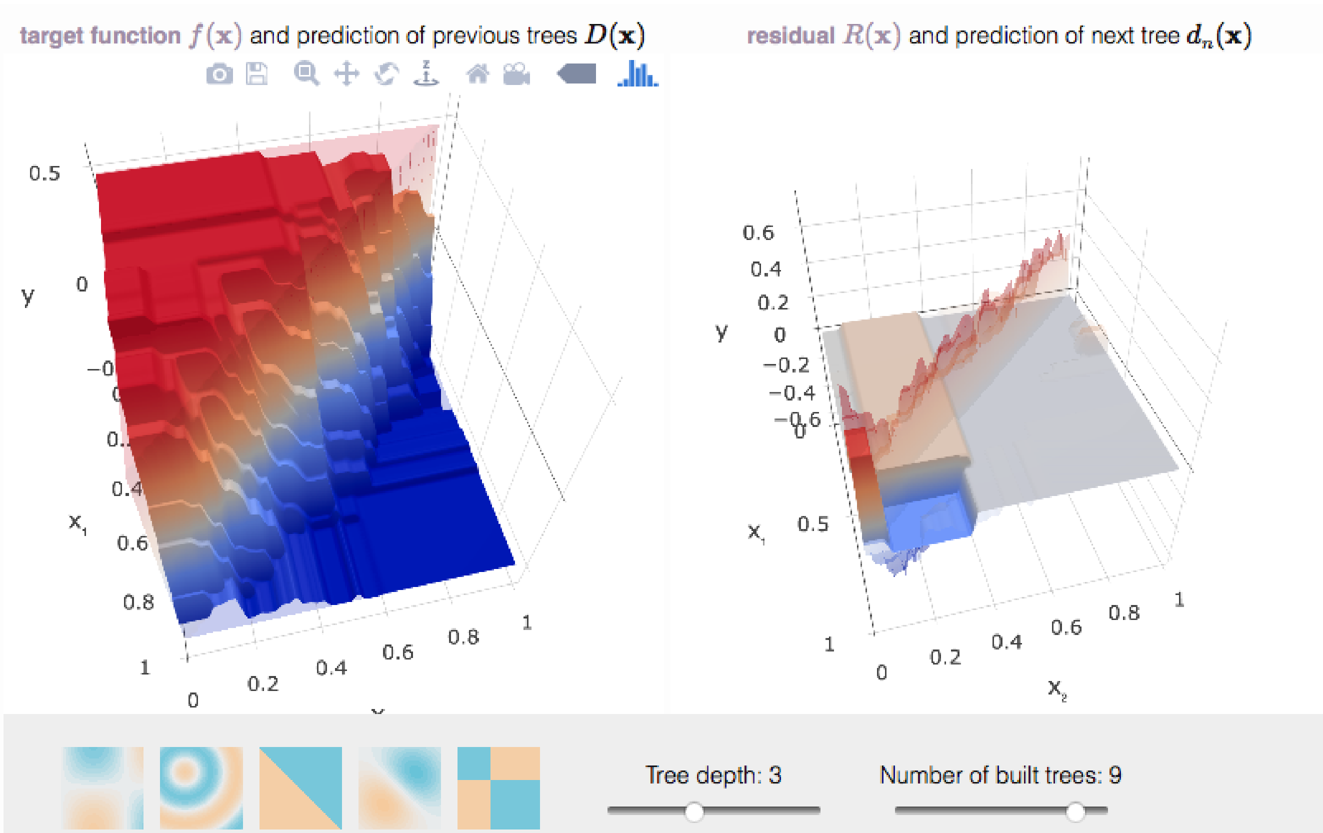


GBM: an interactive demo

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



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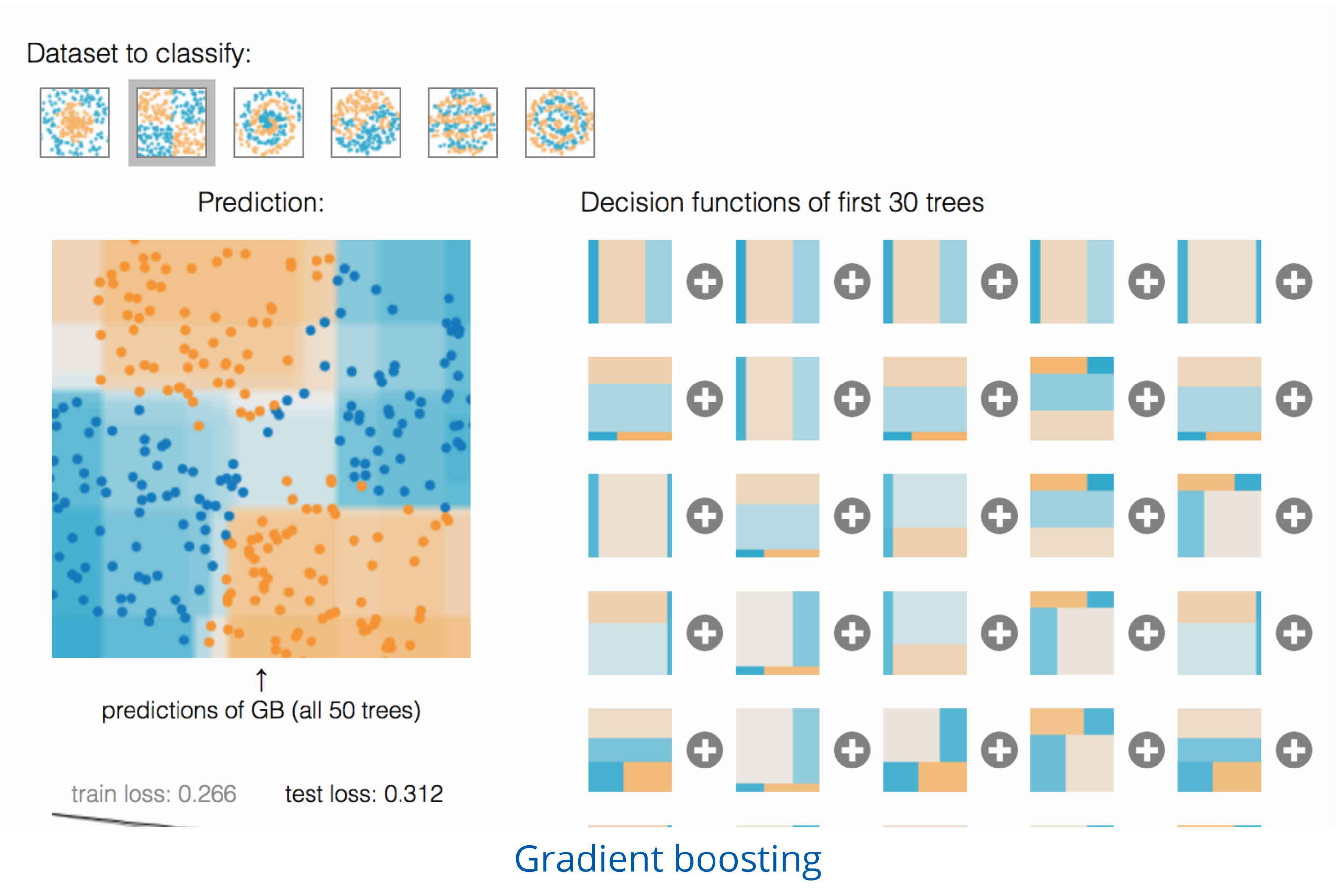


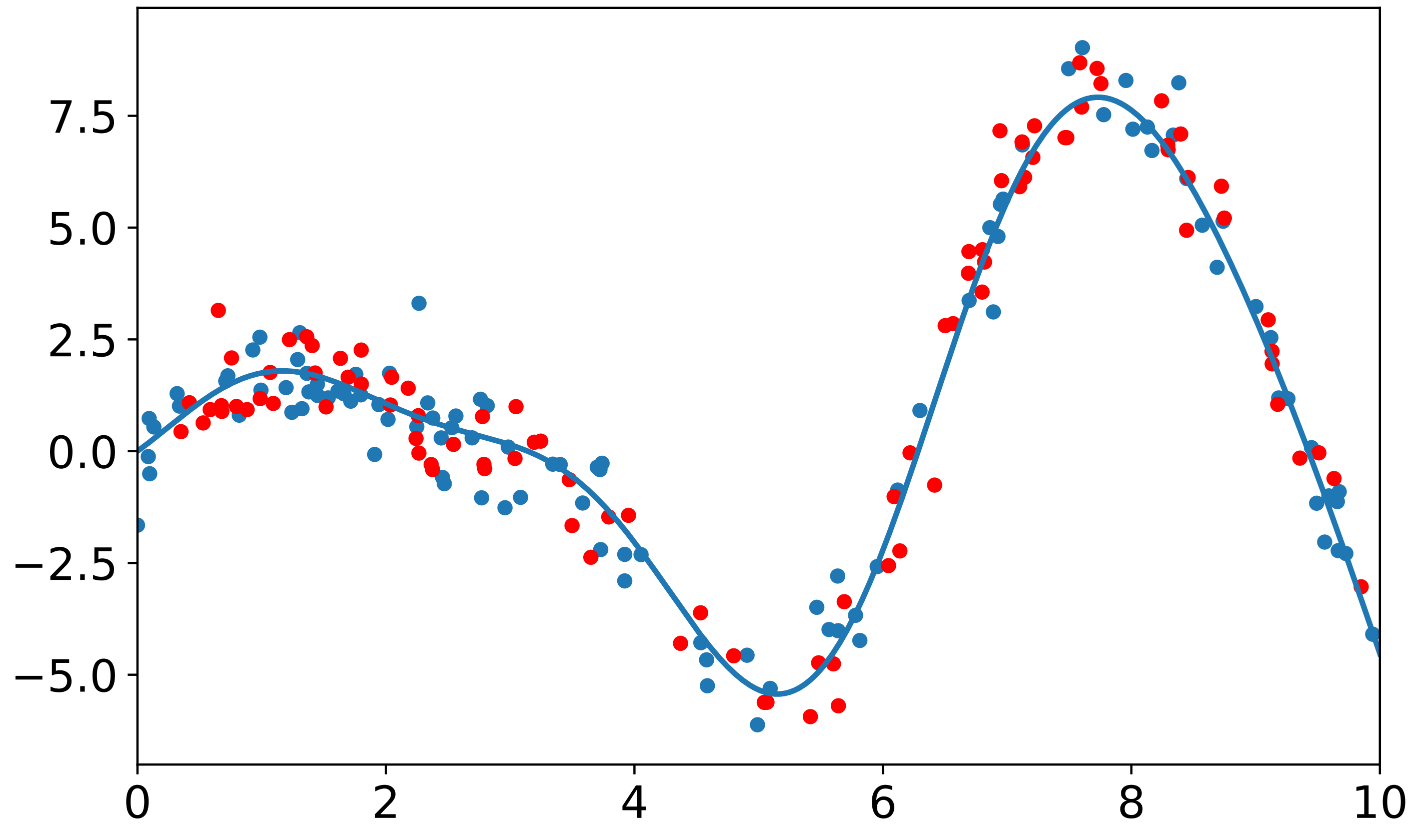
GBM: regulization via shrinkage

- For too simple weak learners, the negative gradient is approximated badly $\implies$ random walk in space of samples
- For too complex weak learners, a few boosting steps may be enough for overfitting
- **Shrinkage:** make shorter steps using a learning rate $\eta \in (0, 1]$

$$\mathrm{a}_{\mathrm{N}}(\mathbf{x}_{\mathrm{i}}) \leftarrow \mathrm{a}_{\mathrm{N}-1}(\mathbf{x}) + \eta\gamma_{\mathrm{N}}\mathrm{h}_{\mathrm{N}}(\mathbf{x})$$

(effectively distrust gradient direction estimated via weak learners)

GBM: regularization approaches



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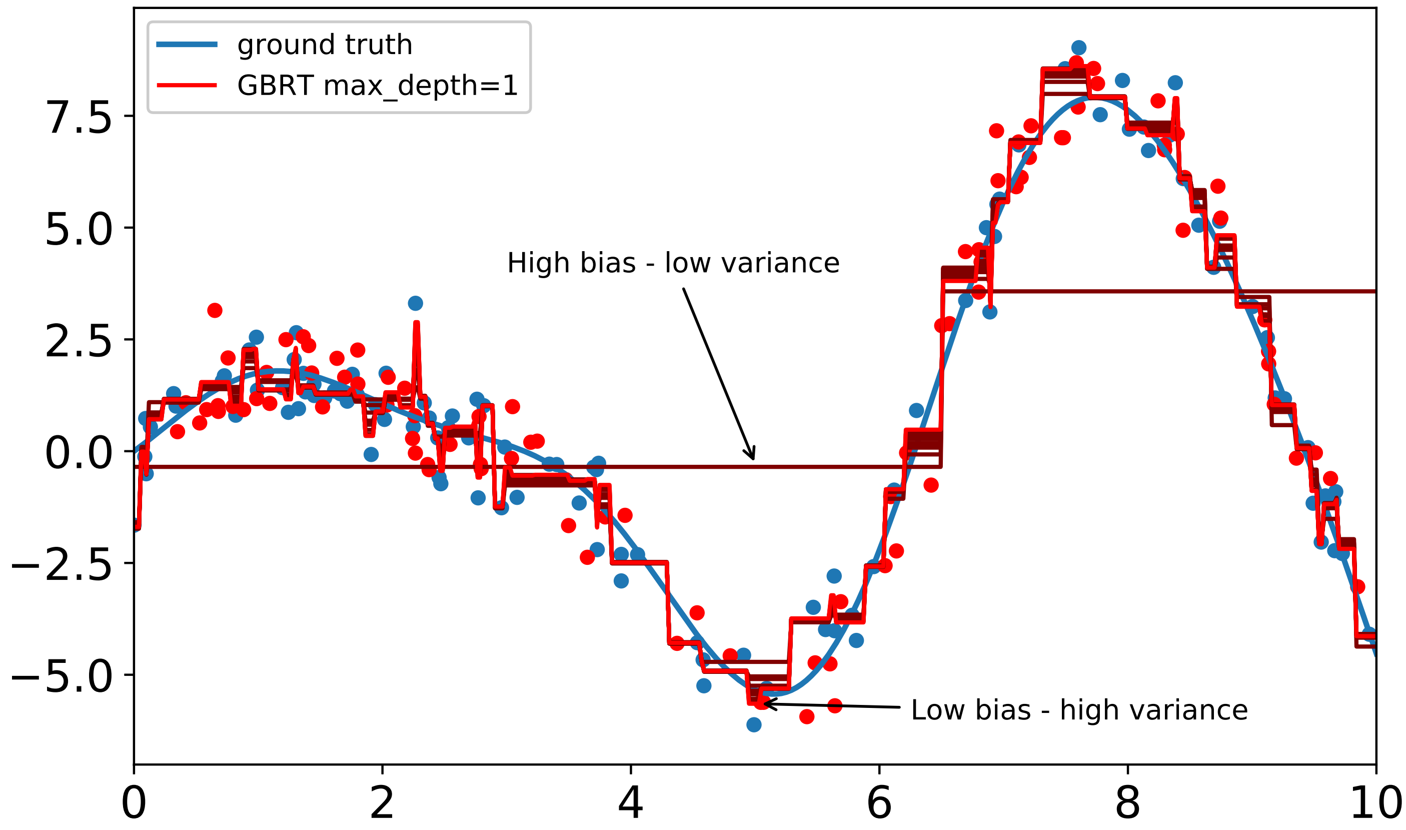

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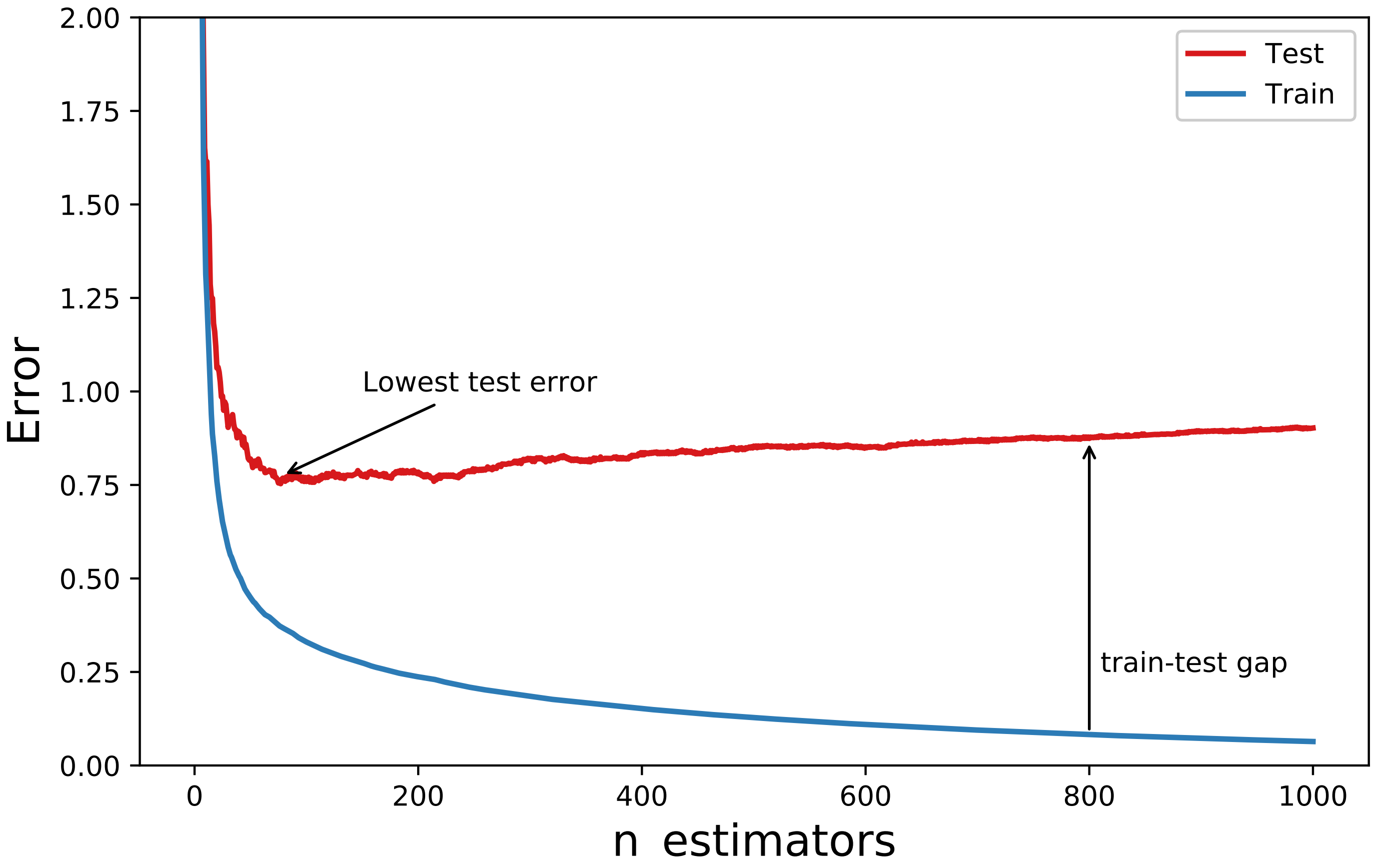

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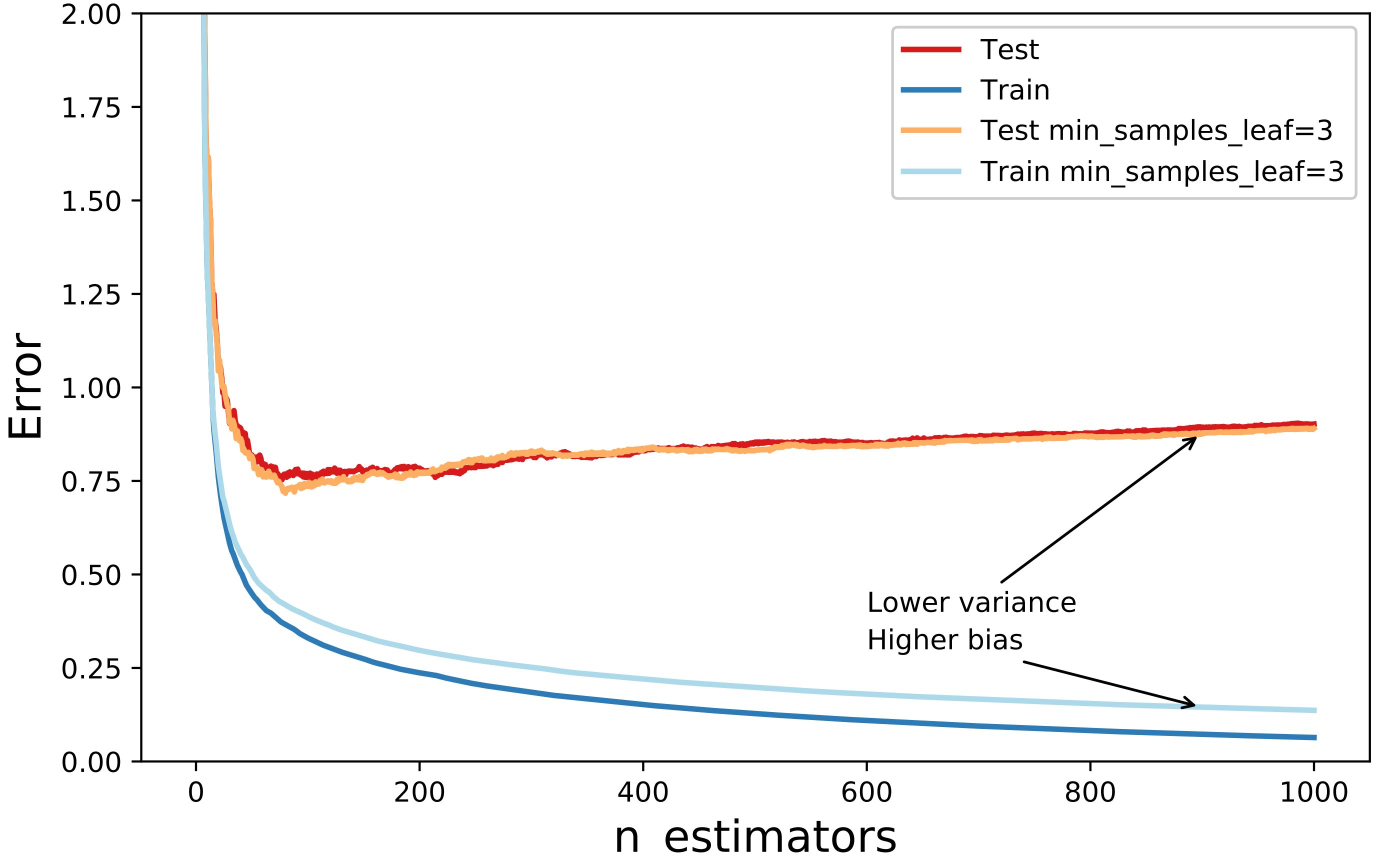

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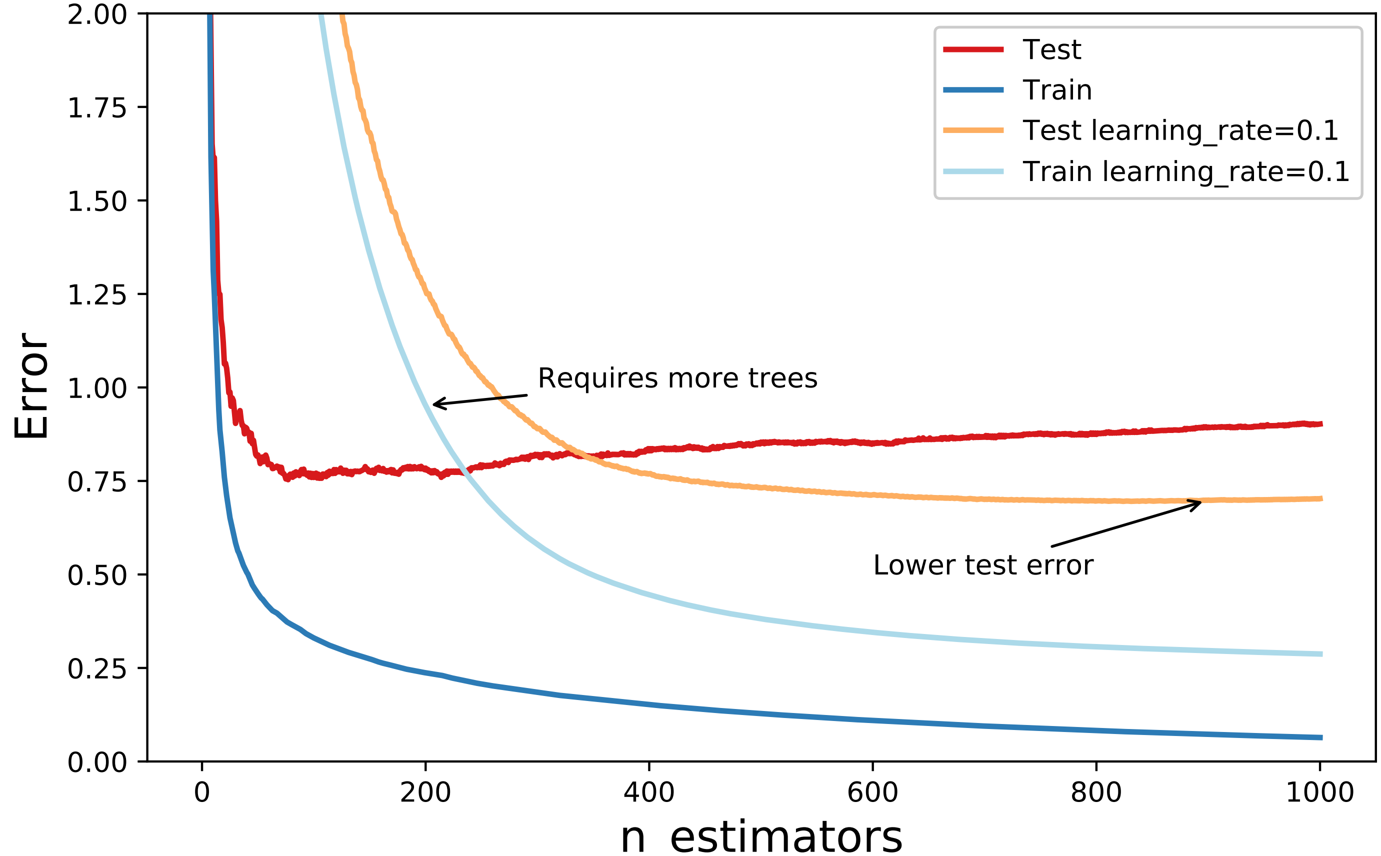

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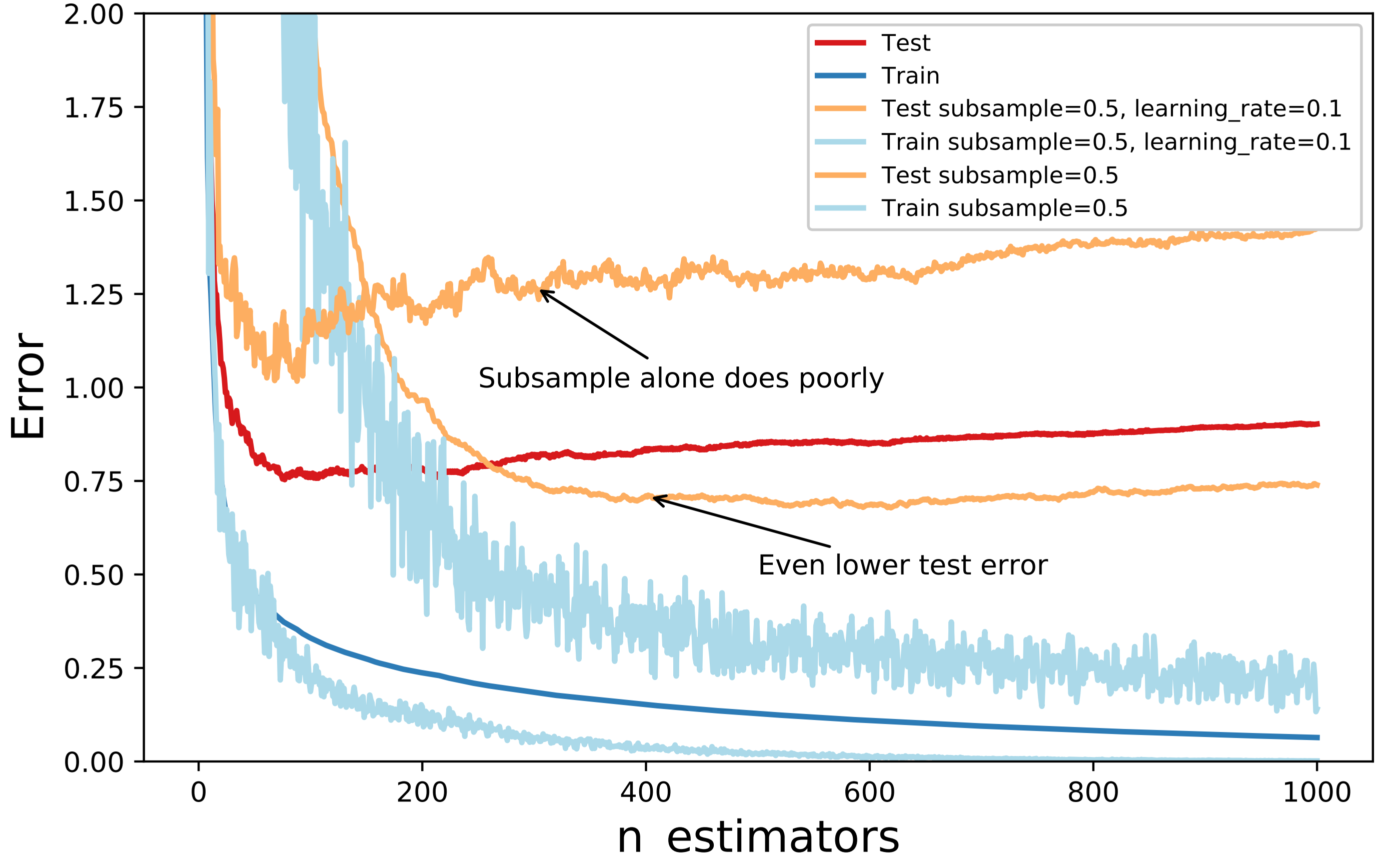

XGBoost algorithm

Extreme Gradient Boosting

1. Approximate the descent direction constructed using second order derivatives

$$\sum_{i=1}^{\ell}\left(-s_i h(\mathbf{x}_i) + \frac{1}{2} t_i h^2(\mathbf{x}_i)\right) \to \min_h, \qquad t_i = \frac{\partial^2}{\partial z^2} L(y_i, z)\Big|_{a_{N-1}(\mathbf{x}_i)}$$

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2. Penalize large leaf counts J and large leaf coefficient norm $\|b\|_2^2 = \sum_{j=1}^{J} b_j^2$

$$\sum_{i=1}^{\ell}\left(-s_i h(x_i) + \frac{1}{2} t_i h^2(x_i)\right) + \gamma J + \frac{\lambda}{2}\sum_{j=1}^{J} b_j^2 \to \min_{h}$$

where $b(\mathbf{x}) = \sum_{j=1}^{J} b_j[\mathbf{x} \in R_j]$

Extreme Gradient Boosting

3. Choose split $[\mathbf{x}_j < t]$ at node R to maximize

$$Q = H(R) - H(R_\ell) - H(R_r) \to \max,$$

where the impurity criterion

$$H(R) = -\frac{1}{2}\left(\sum_{(t_i, s_i) \in R} s_j\right)^2 \Bigg/ \left(\sum_{(t_i, s_i) \in R} t_j + \lambda\right) + \gamma$$

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4. The stopping rule: declare the node a leaf if even the best split gives negative Q

Conclusion

- Boosting: a general meta-algorithm aimed at composing a strong hypothesis from multiple weak hypotheses
- Boosting can be applied for arbitrary losses for regression and classification, and over arbitrary weak learners
- The Gradient Boosting Machine: a general approach to boosting adding weak learners that approximate gradient of the loss function
- XGBoost: gradient boosting with second order optimization, penalized loss and particular choice of impurity criterion
- You don’t have to code any of this yourself – stay tuned for the seminar, where we’ll show you how to use the state-of-the-art frameworks.

Thank you!

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Acknowledgements

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