Ensembling methods

Stacking, bagging, boosting

Machine Learning and Data Mining, 2024

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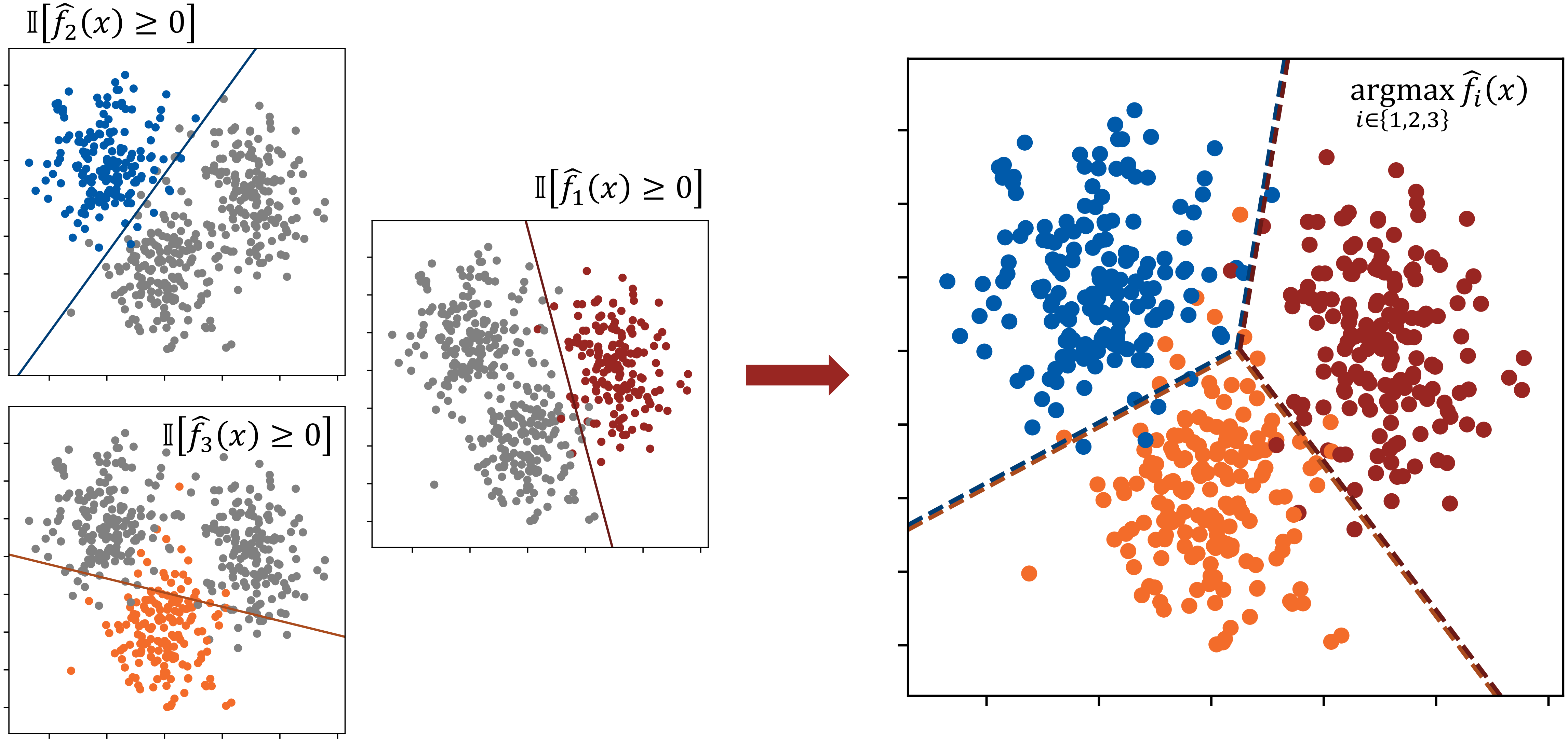
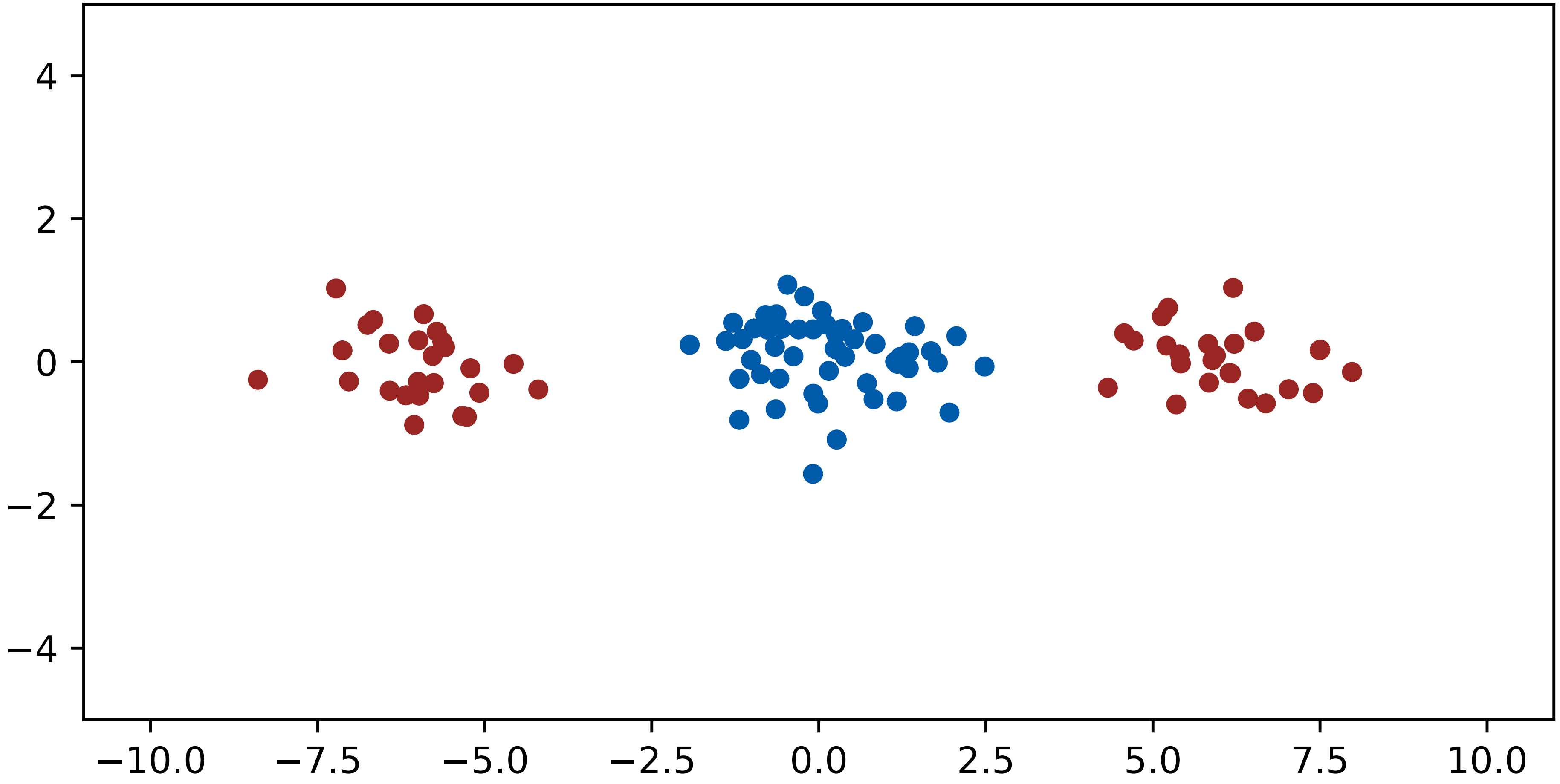
Why ensembles?

One-vs-rest classification scheme



Increasing complexity of simple underfitting models



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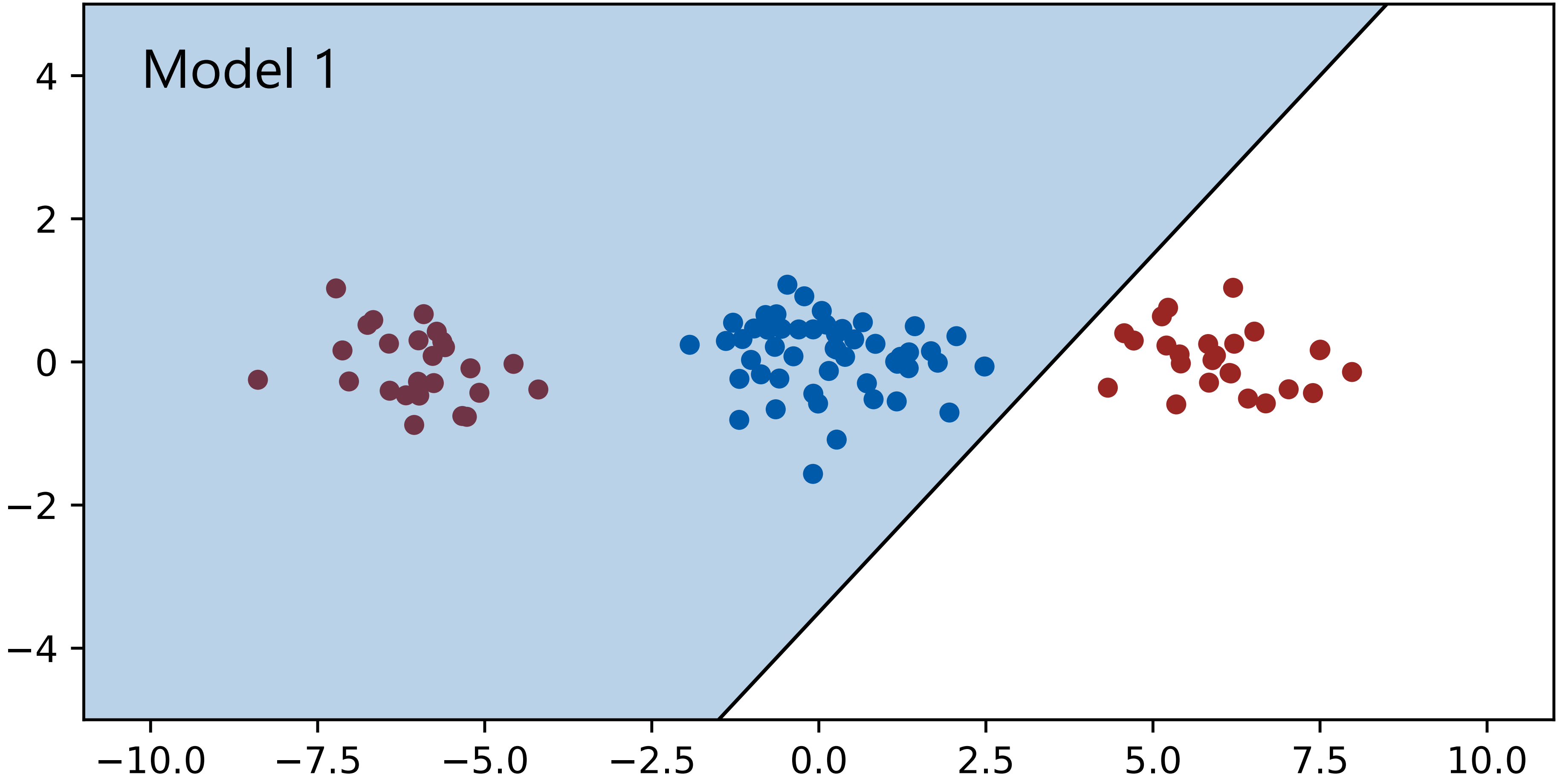

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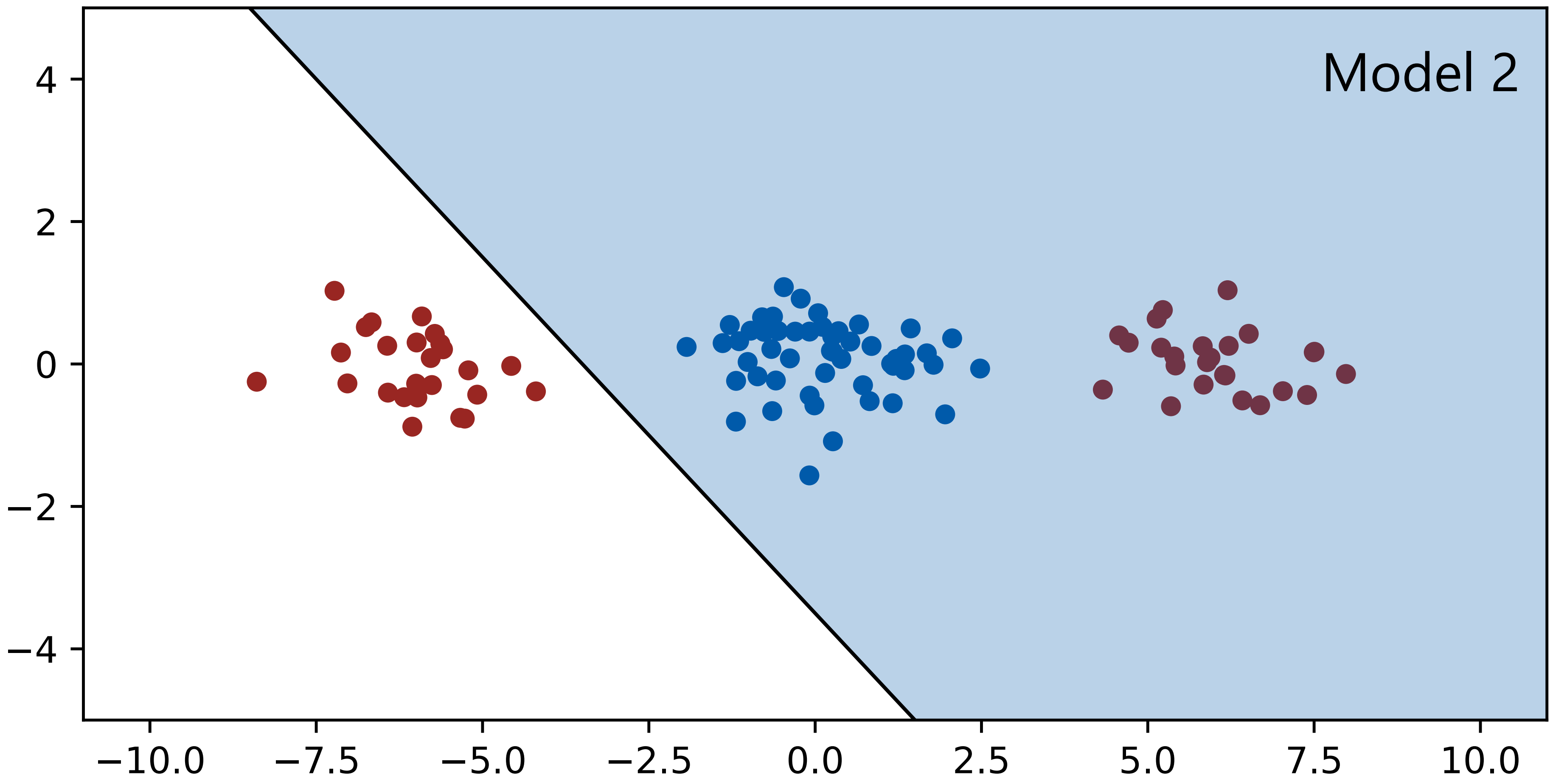

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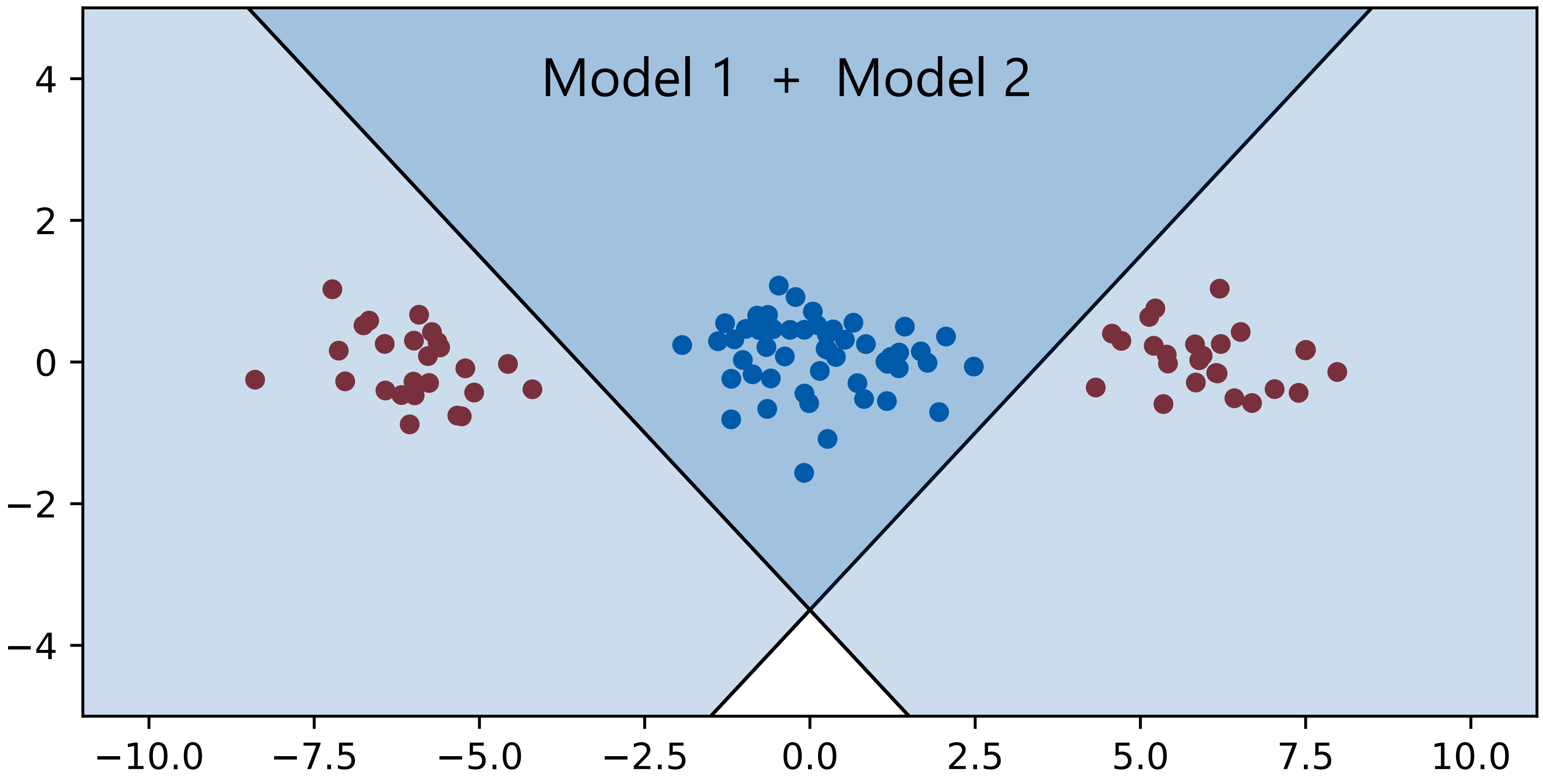
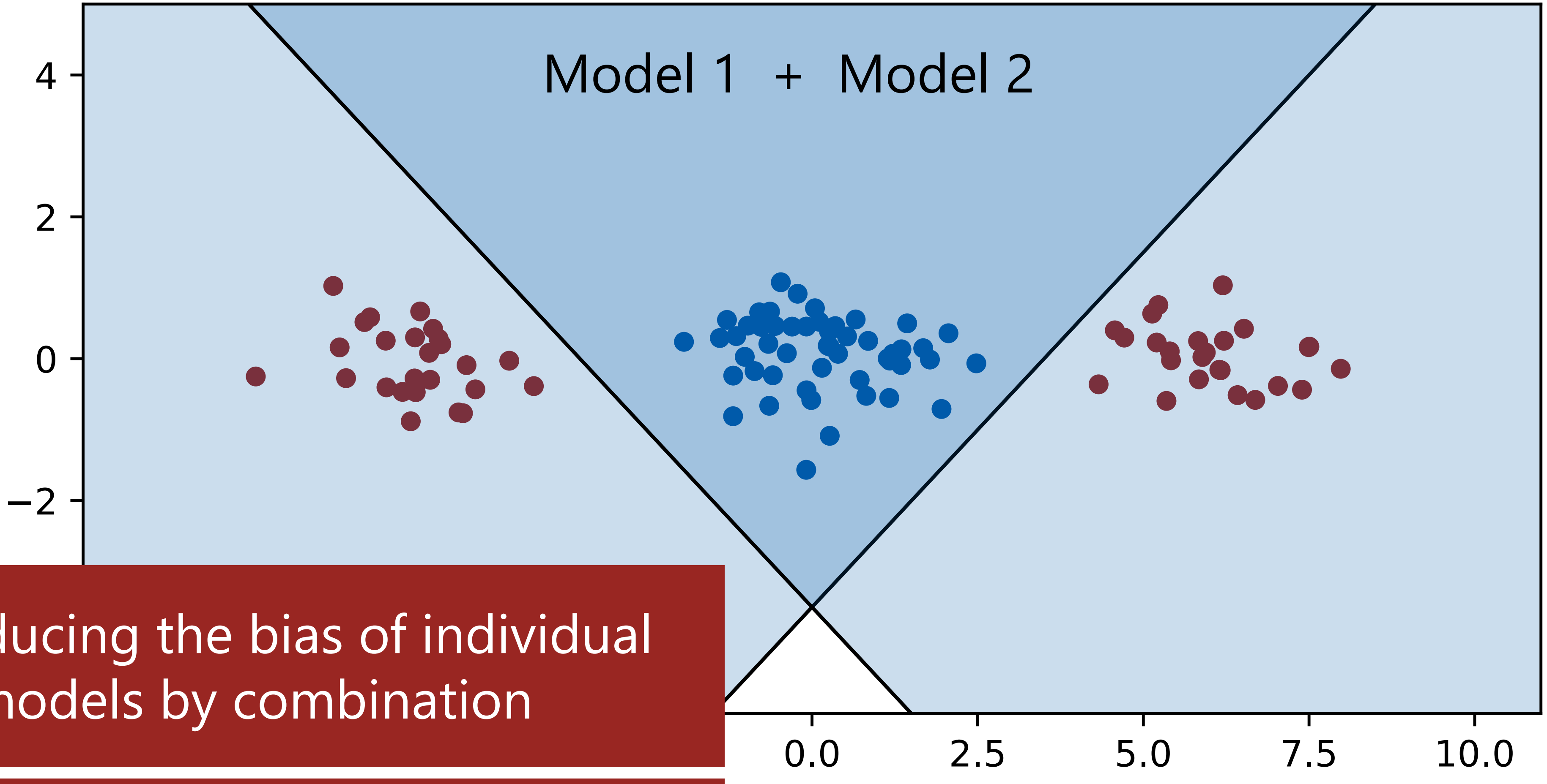


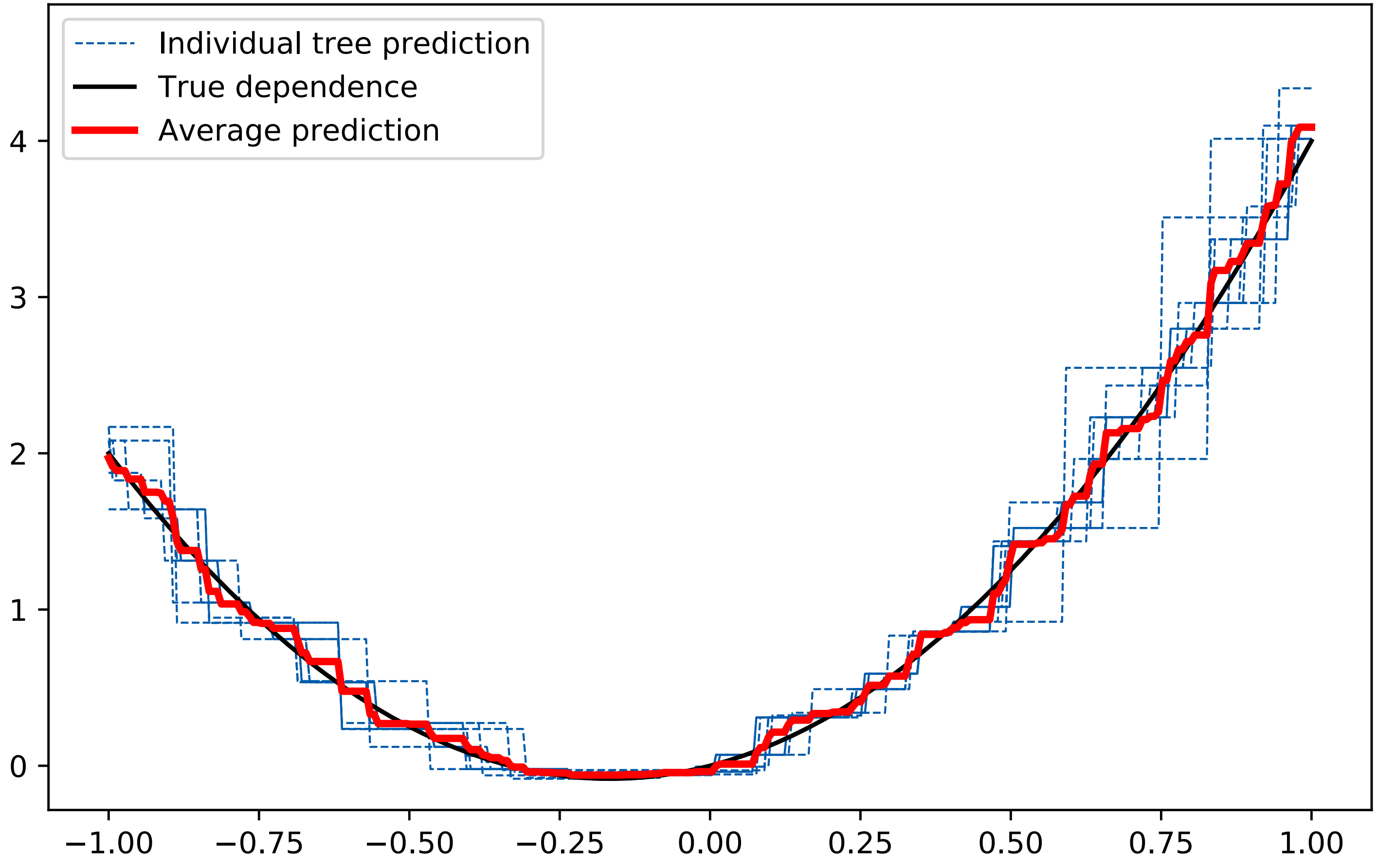
Increasing complexity of simple underfitting models



I.e. reducing the bias of individual models by combination

May increase variance

Reducing variance by averaging



Take a set of overfitting (high-variance) models $\widehat{f_1}(x), \dots, \widehat{f_M}(x)$

- E.g. decision trees trained on different training sets

For regression – average their predictions:

$$F(x) = \frac{1}{M}\sum_{i=1}^{M} \widehat{f_i}(x)$$

For classification – majority voting

Ambiguity decomposition

Consider the following ensemble:

$$F(x) = \sum_i w_i f_i(x), \qquad w_i \geq 0, \qquad \sum_i w_i = 1$$

Then it's easy to show that:

$$\underbrace{(F(x) - y)^2}_{\textbf{Ensemble error}} = \underbrace{\sum_i w_i (f_i(x) - y)^2}_{\textbf{Base learner error}} - \underbrace{\sum_i w_i \big(f_i(x) - F(x)\big)^2}_{\textbf{Ambiguity}}$$

Disagreement reduces the error!

[Ambiguity decomposition proof]

$$F(x) = \sum_i w_i f_i(x), \qquad w_i \geq 0, \qquad \sum_i w_i = 1$$

$$(F(x) - y)^2 = \left(\sum_i w_i f_i(x) - y\right)^2 = \sum_i w_i f_i(x) \cdot F(x) - 2\sum_i w_i f_i(x) \cdot y + \sum_i w_i y^2$$

$$= \sum_i w_i [f_i(x) \cdot F(x) - 2 f_i(x) \cdot y + y^2]$$

$$= \sum_i w_i \left[f_i^2(x) - 2 f_i(x) \cdot y + y^2 - f_i^2(x) + 2 f_i(x) \cdot F(x) - F^2(x) + F^2(x) - f_i(x) \cdot F(x)\right]$$

$$= \sum_i w_i \left[(f_i(x) - y)^2 - \left(f_i(x) - F(x)\right)^2 + F^2(x) - f_i(x) \cdot F(x)\right]$$

$$= \sum_i w_i (f_i(x) - y)^2 - \sum_i w_i \left(f_i(x) - F(x)\right)^2$$

Majority voting classifier error

Assume we have M classifiers with prediction error probability $p < \frac{1}{2}$ each

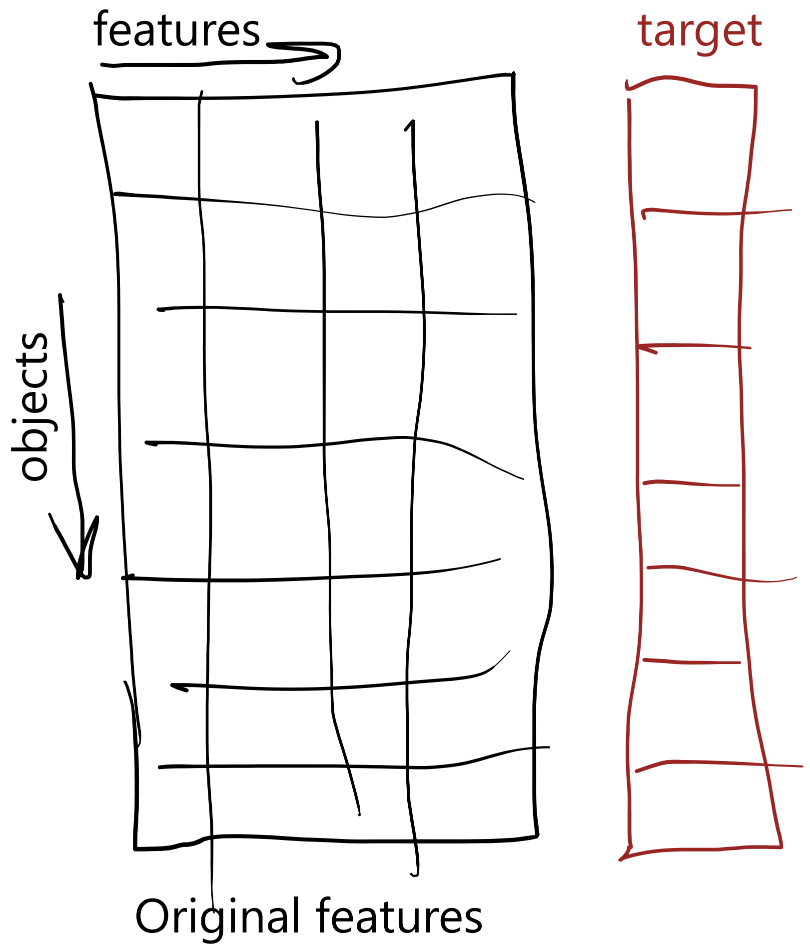
Suppose the guesses are wrong or correct independently of each other

Then major vote error probability $\rightarrow 0$ as $\mathrm{M} \rightarrow +\infty$.

Stacking

Stacking

Using output of initial models as features for the aggregation model



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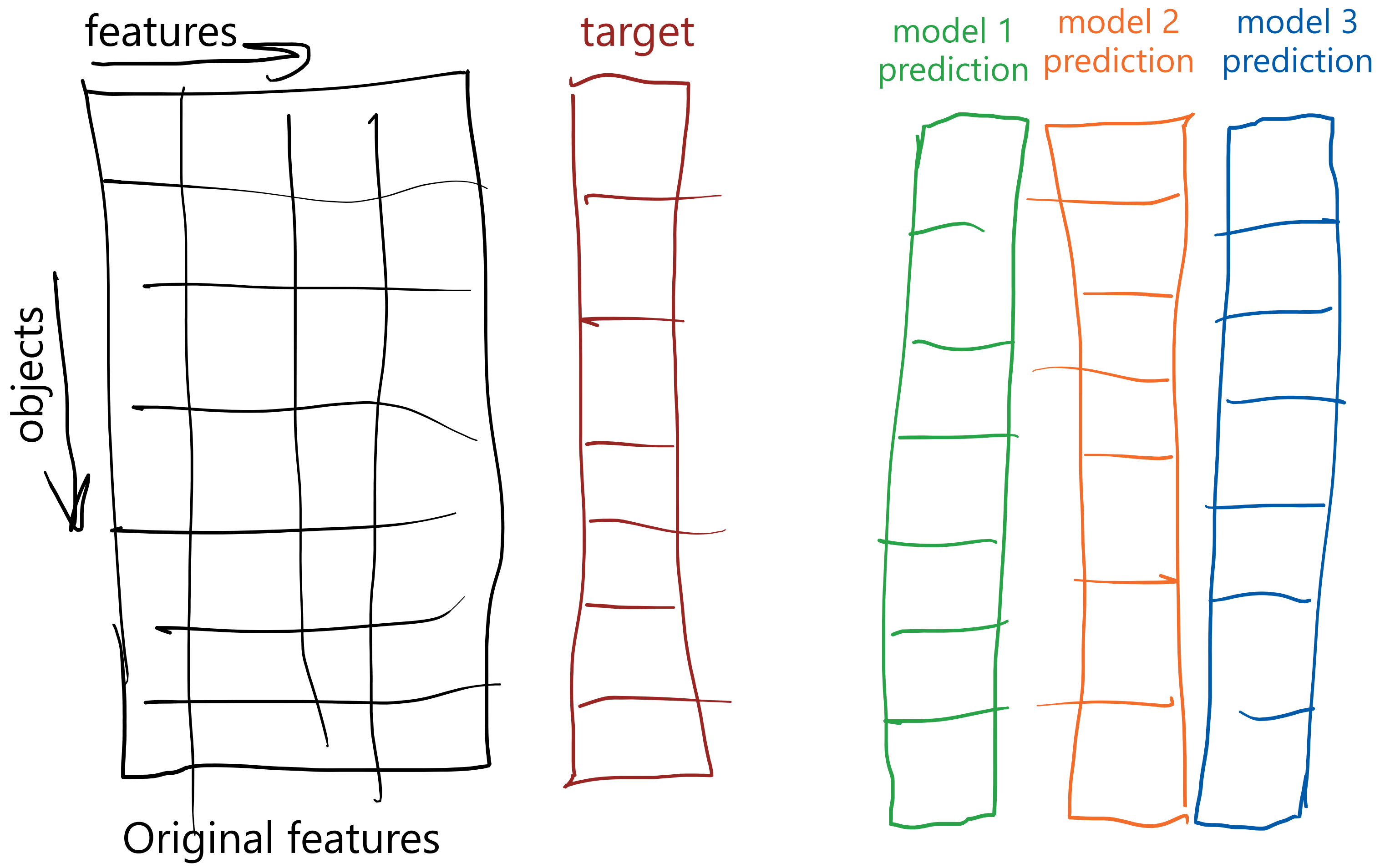

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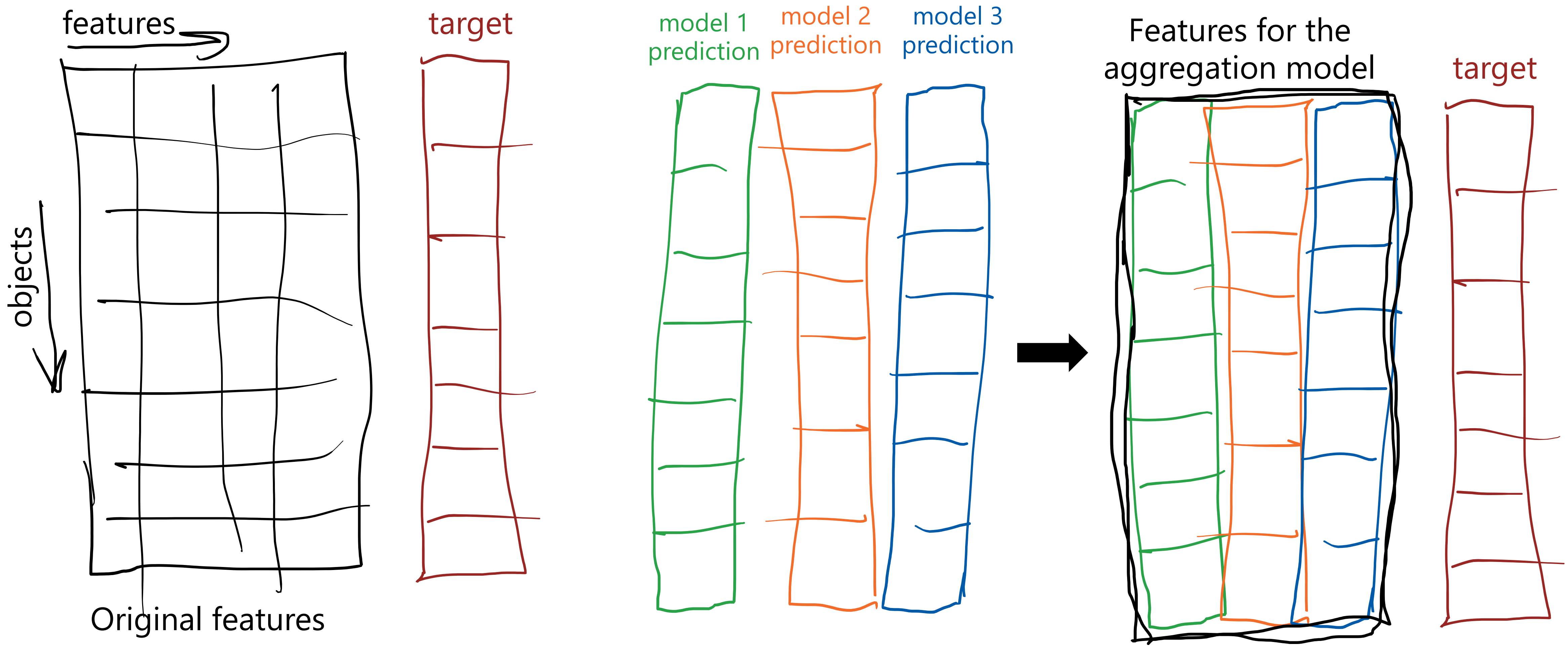

Stacking

Using output of initial models as features for the aggregation model

Easy to overfit if using the base models’ predictions from the train data

Solution: use cross-validated estimates

Bagging

Bagging

Bagging = bootstrap aggregating

Generate bootstrap samples (re-sample your data with replacement)

Train independent base models on those samples

Combine their predictions

Example

- Bagged decision trees
- Random Forest (= bagged trees + feature subsampling)
- Extra random trees (= Random Forest + randomized splits)

Boosting

Forward stagewise additive modeling (FSAM)

Loss function: $L(f(x), y)$

Base learners $\widehat{f_{\mathrm{m}}}$

Approximate the output as:

$$F_M(x) = \widehat{f_0}(x) + \sum_{m=1}^{M} \widehat{c_m} \cdot \widehat{f_m}(x)$$

Do so in steps:

- Start from 0, constant or just fit $\widehat{f_0}$ to data
- At each step solve:

$$\left(\widehat{c_m}, \widehat{f_m}\right) = \underset{c,f}{\operatorname{argmin}} \left[\sum_{n=1}^{N} L(F_{m-1}(x_n) + c \cdot f(x_n), y_n) \right]$$

AdaBoost

AdaBoost = FSAM with exponential loss

$$L(f(x), y) = \exp[-y \cdot f(x)]$$

$$y \in \{-1, +1\},$$

– and base learners being binary classifiers: $\widehat{f_m}(x) \in \{-1, +1\}$

Minimization can be done analytically

– if individual learners allow for weighted samples

AdaBoost

Loss at step m:

$$\sum_{n=1}^{N} \exp\left[-y_n\left(F_{m-1}(x_n) + c \cdot f(x_n)\right)\right]$$

AdaBoost

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$$\sum_{n=1}^{N} \exp\left[-y_n\left(F_{m-1}(x_n) + c \cdot f(x_n)\right)\right]$$

$$= \sum_{n=1}^{N} \exp[-y_n \cdot F_{m-1}(x_n)] \cdot \exp[-y_n \cdot c \cdot f(x_n)] = \sum_{n=1}^{N} w_n \cdot \exp[-y_n \cdot c \cdot f(x_n)]$$

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$$= \sum_{y_n = f(x_n)} w_n \cdot e^{-c} + \sum_{y_n \neq f(x_n)} w_n \cdot e^{c}$$

AdaBoost

Loss at step m:

$$\sum_{n=1}^{N} \exp\left[-y_n\left(F_{m-1}(x_n) + c \cdot f(x_n)\right)\right]$$

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$$= \sum_{n=1}^{N} w_n \cdot e^{-c} + \sum_{y_n \neq f(x_n)} w_n \cdot (e^{c} - e^{-c})$$

AdaBoost

So at step m we optimize:

$$\left(\widehat{c_m}, \widehat{f_m}\right) = \underset{c,f}{\operatorname{argmin}} \left[\sum_{n=1}^{N} w_n \cdot e^{-c} + \sum_{y_n \neq f(x_n)} w_n \cdot \left(e^{c} - e^{-c}\right) \right]$$

$$w_n = \exp[-y_n \cdot F_{m-1}(x_n)]$$

In other words, find $\widehat{f_m}$, s.t. $\sum_{\widehat{f_m}(x_n) \neq y_n} w_n$ is minimized

Easy to show that for c:

$$c_m = \frac{1}{2} \ln \frac{\sum_{\widehat{f_m}(x_n) = y_i} w_n}{\sum_{\widehat{f_m}(x_n) \neq y_i} w_n}$$

AdaBoost

So at step m we optimize:

$$(\widehat{c_m}, \widehat{f_m}) = \underset{c,f}{\operatorname{argmin}} \left[\sum_{n=1}^{N} w_n \cdot e^{-c} + \sum_{y_n \neq f(x_n)} w_n \cdot (e^c - e^{-c}) \right]$$

$$w_n = \exp[-y_n \cdot F_{m-1}(x_n)]$$

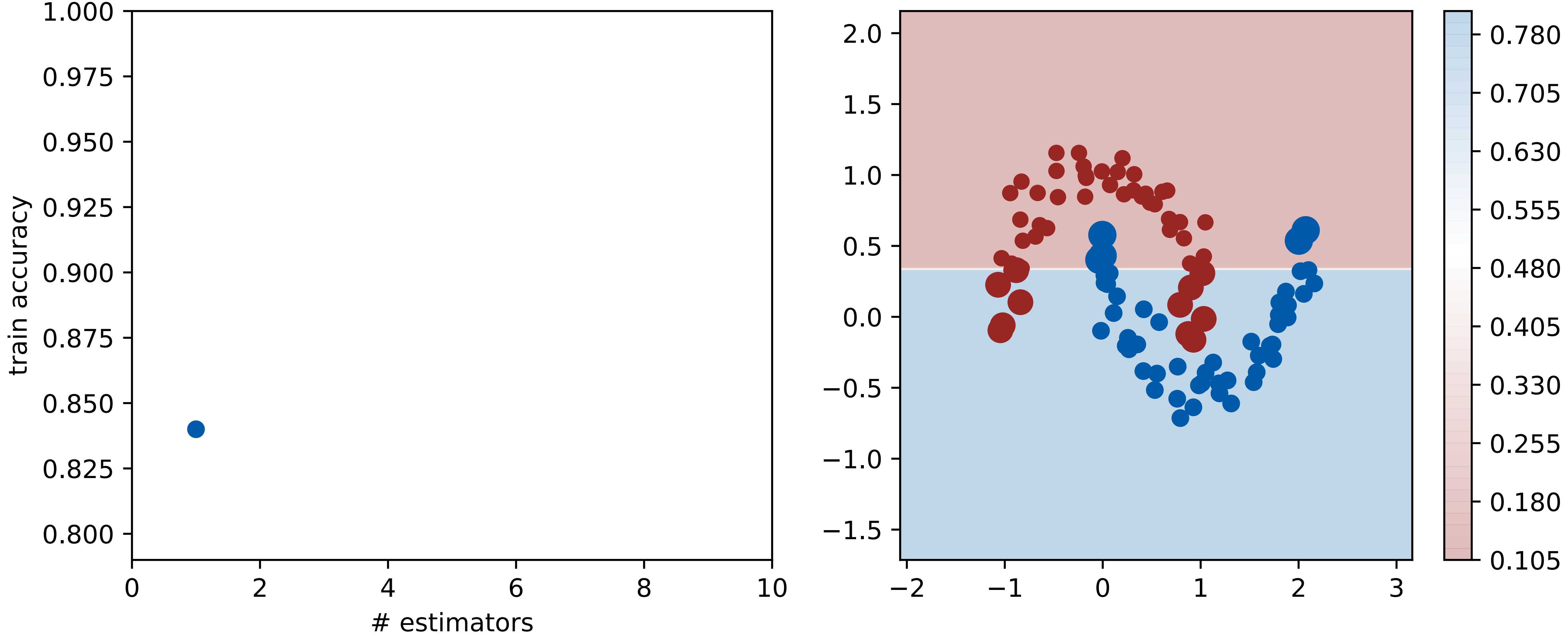
pay more attention to objects predicted wrongly

In other words, find $\widehat{f_m}$, s.t. $\sum_{\widehat{f_m}(x_n) \neq y_n} w_n$ is minimized

Easy to show that for c:

$$c_m = \frac{1}{2} \ln \frac{\sum_{\widehat{f_m}(x_n) = y_i} w_n}{\sum_{\widehat{f_m}(x_n) \neq y_i} w_n}$$

Example


train accuracy
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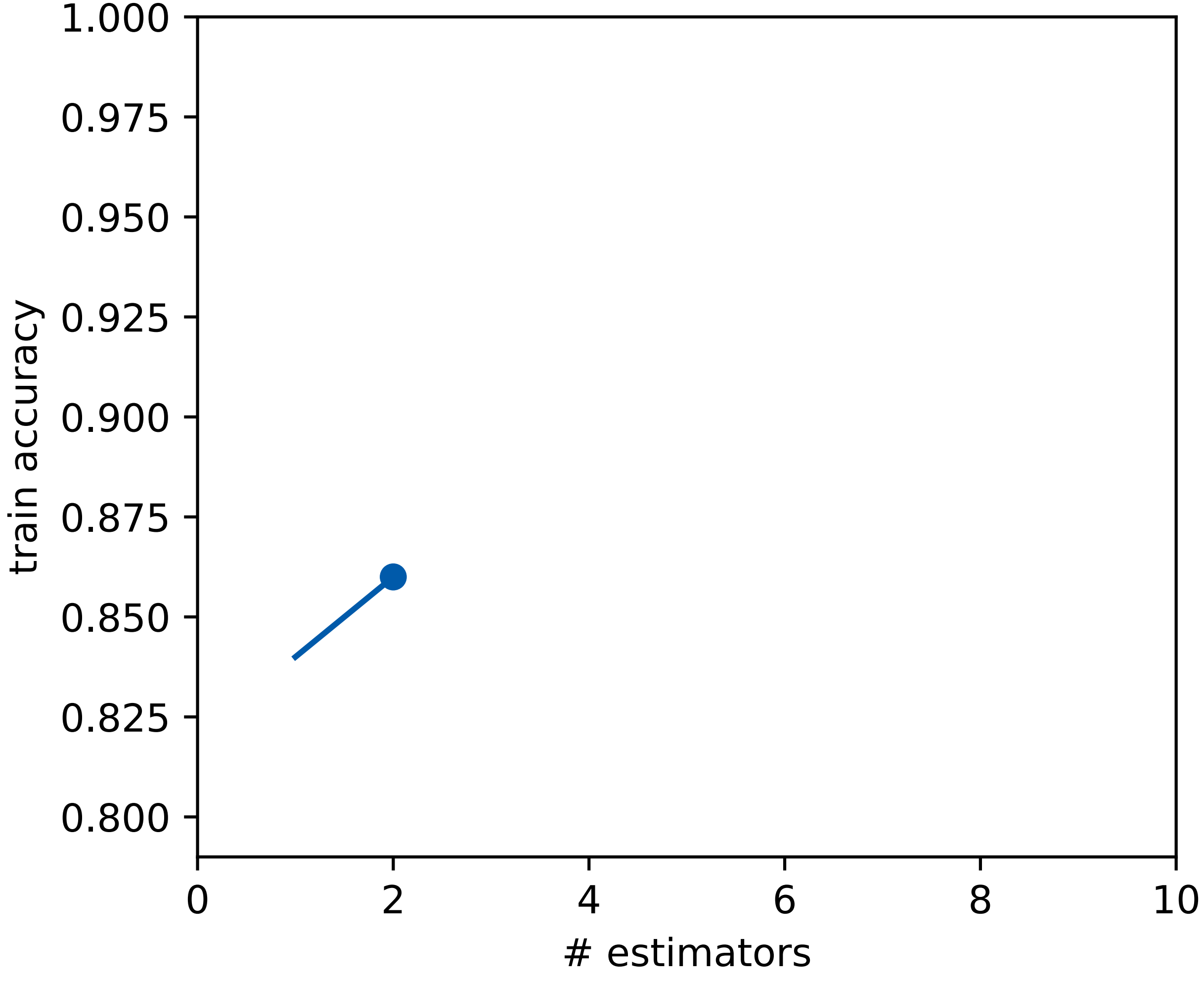
Example



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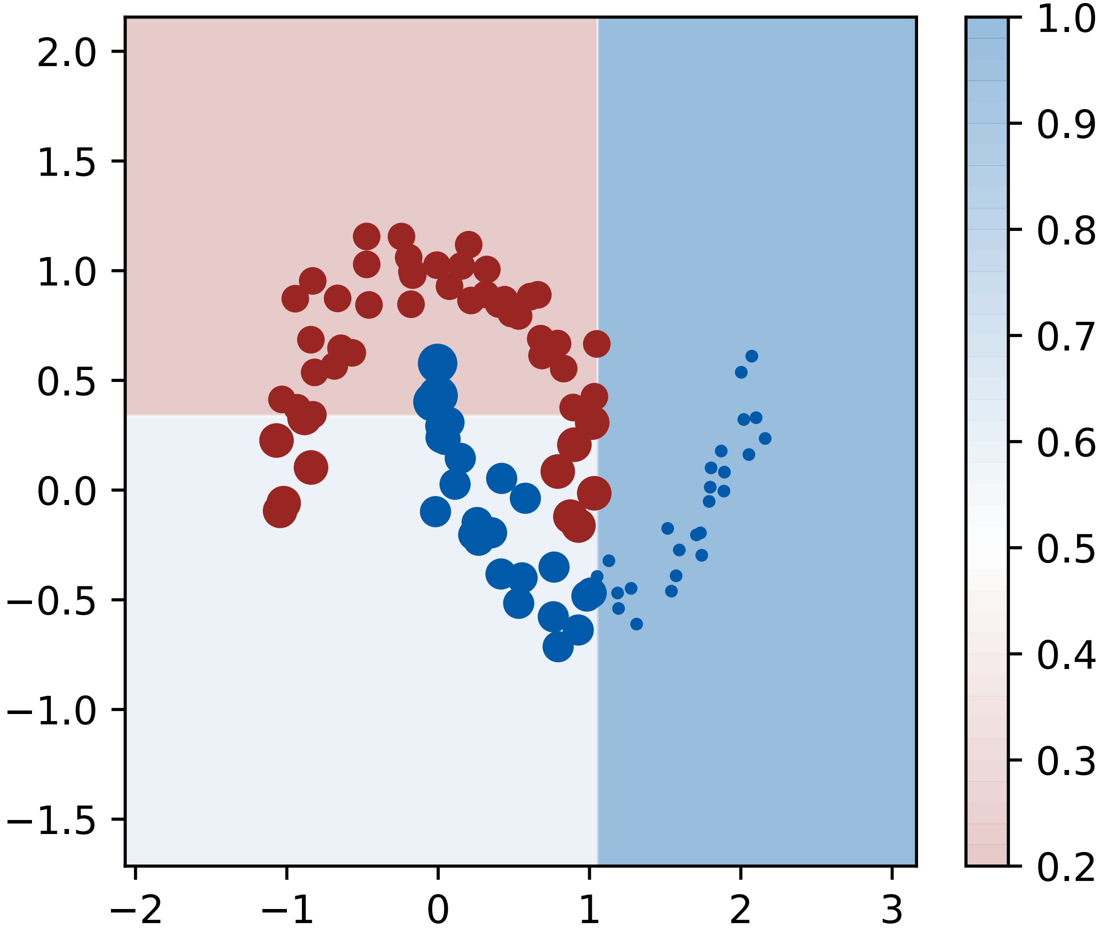

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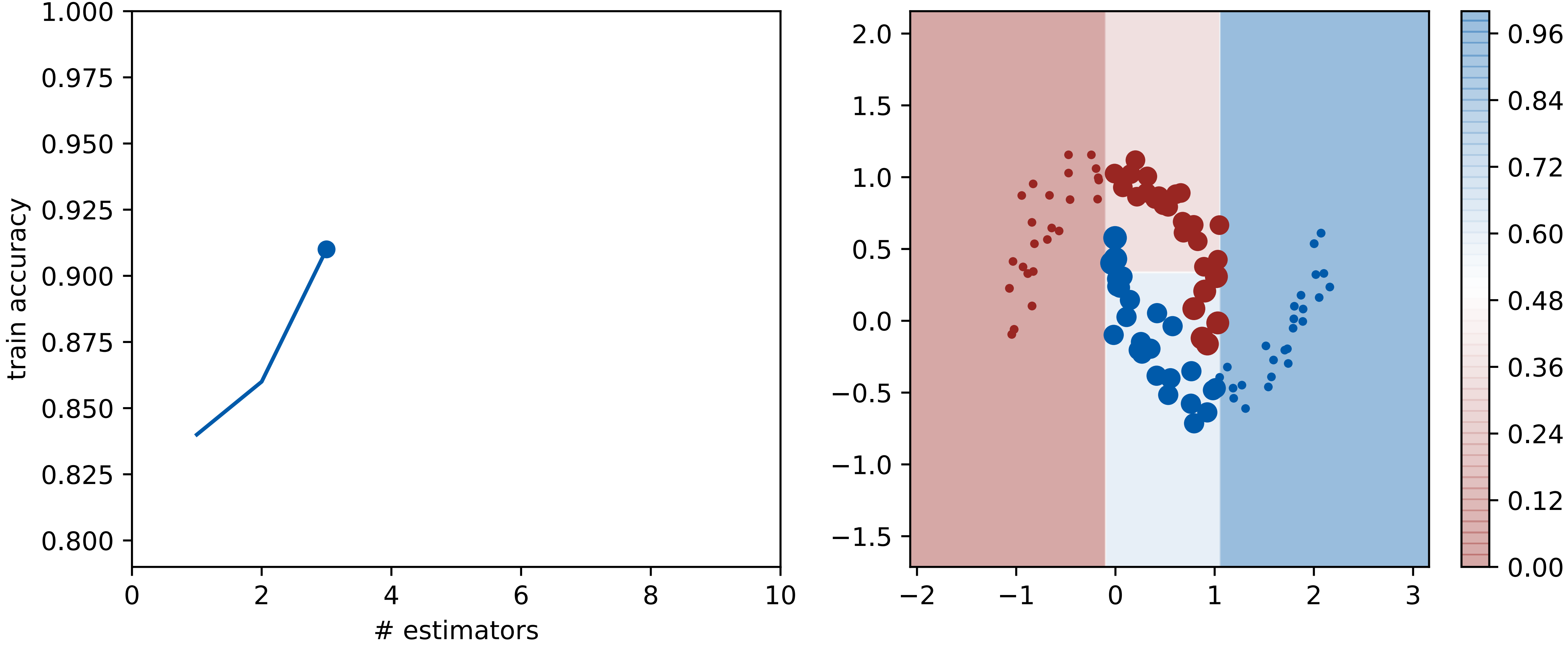
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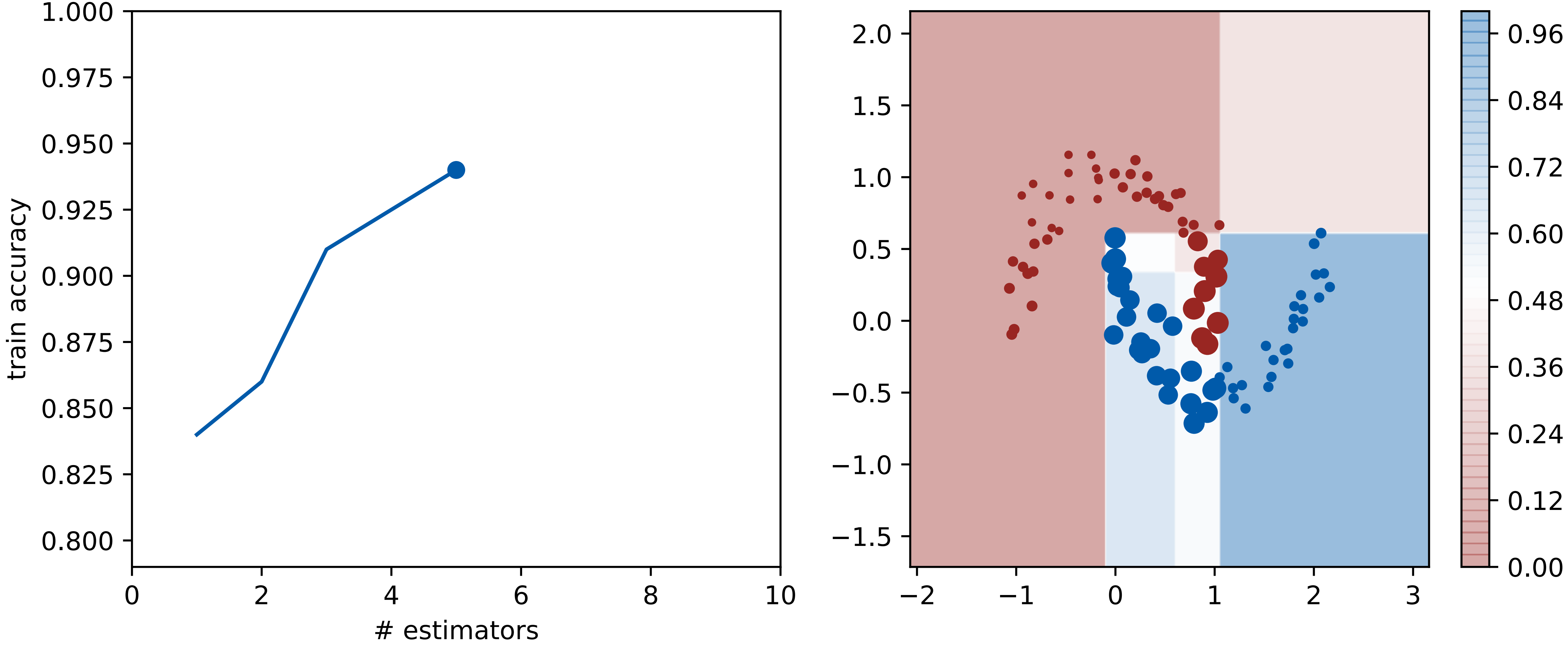
Example



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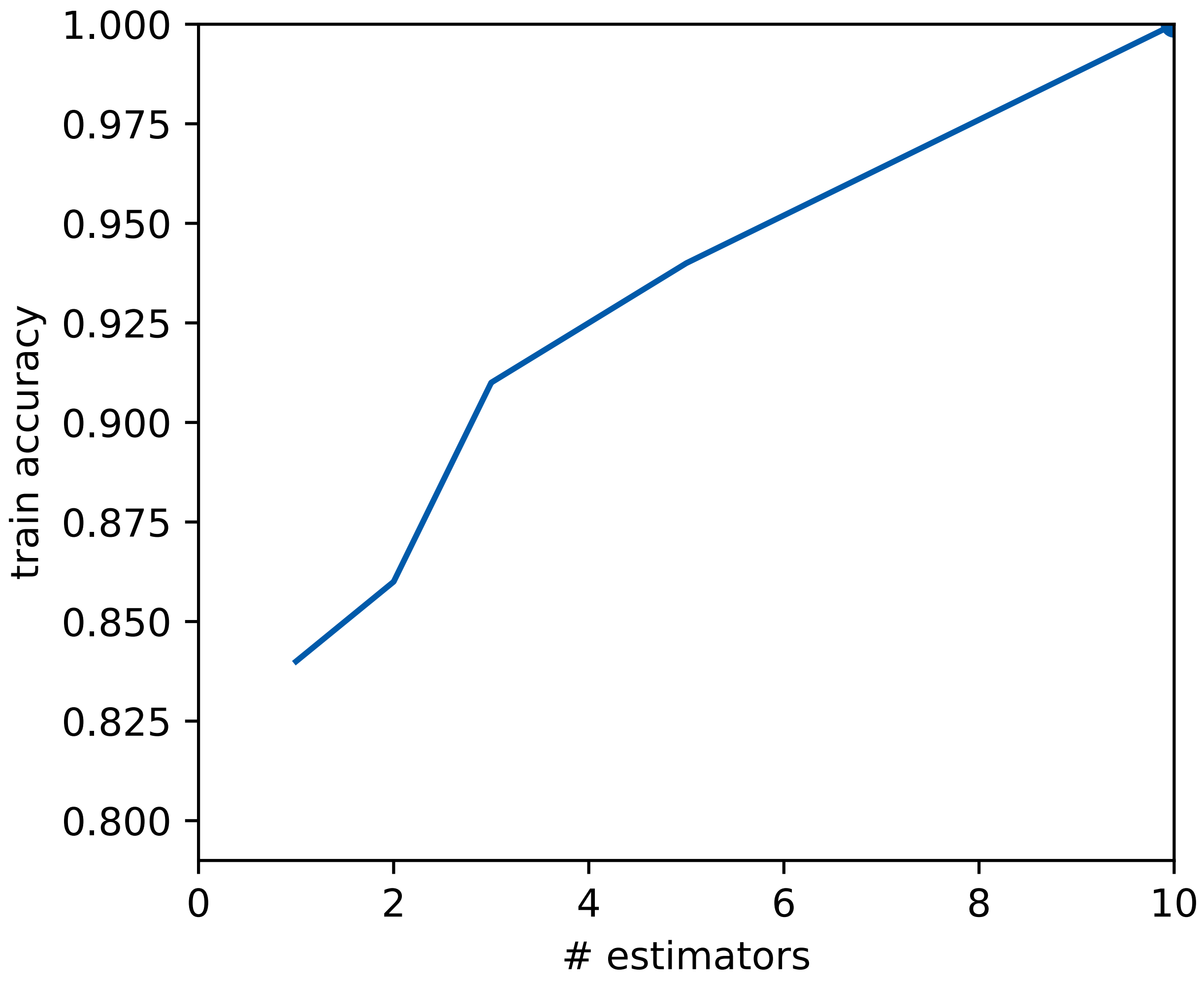

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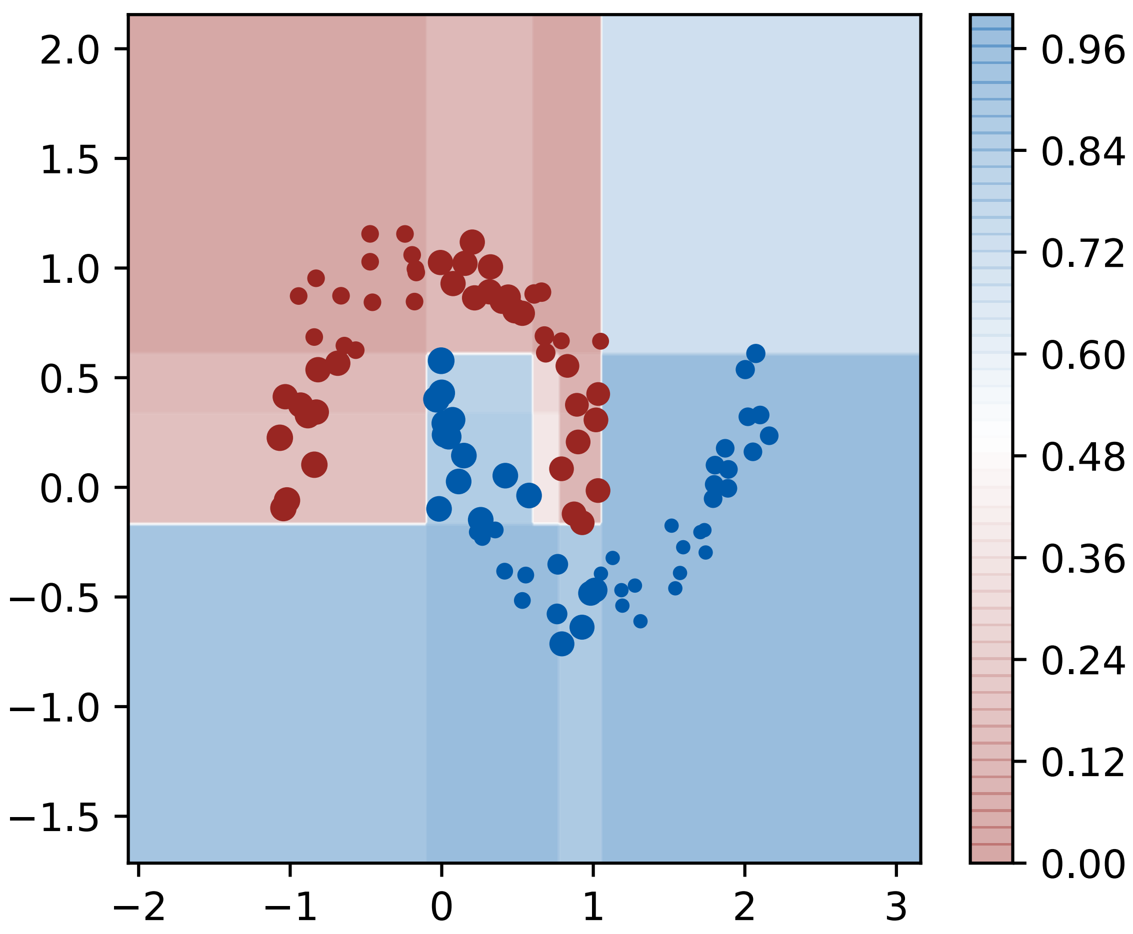

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Gradient Boosting

FSAM minimization cannot be solved analytically for a general loss function

Find approximation (linear):

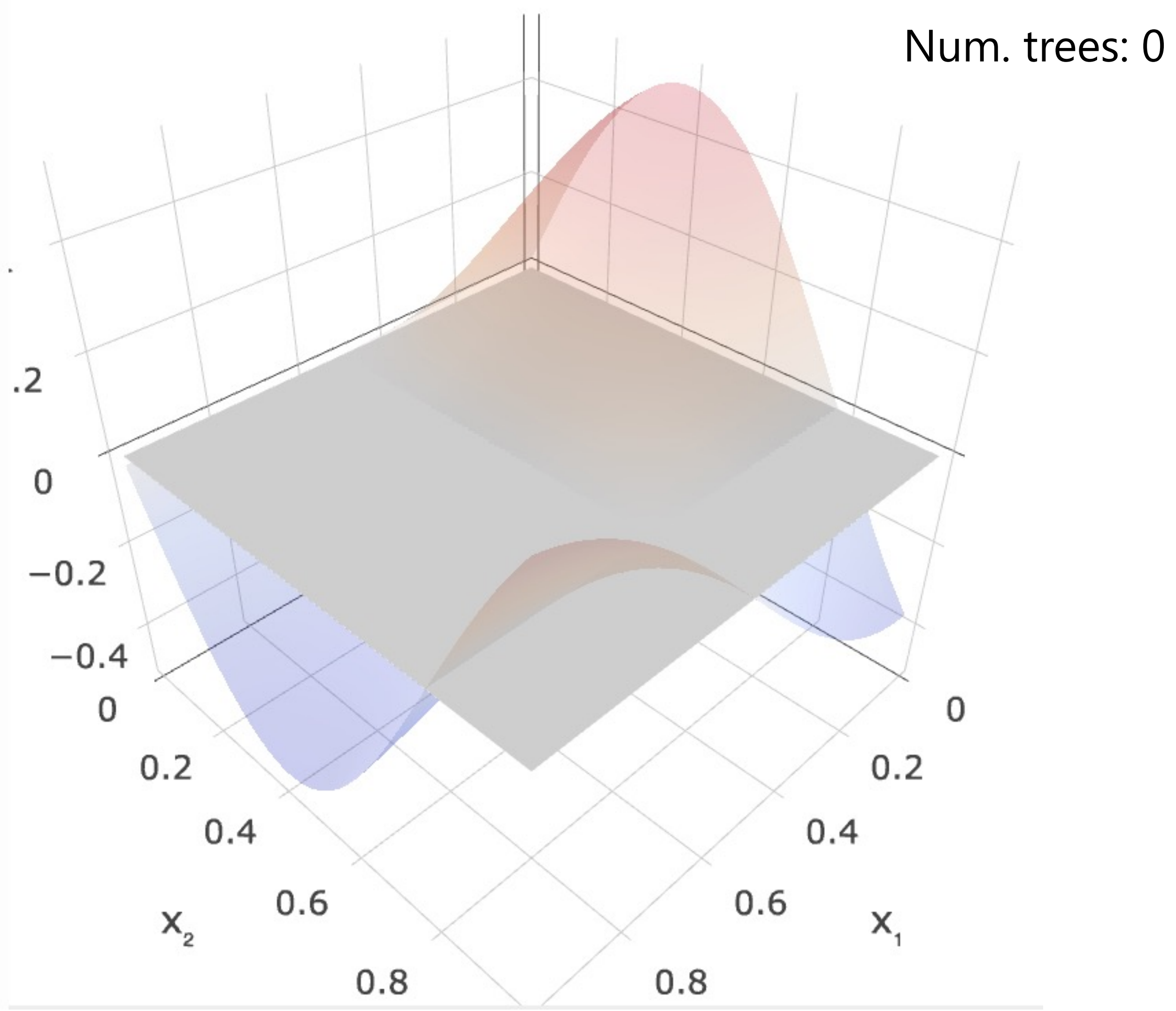
$$L(F(x) + f(x), y) \approx L(F(x), y) + \frac{\partial L(F, y)}{\partial F} f(x)$$

Gradient shows the direction of maximal increase $\Rightarrow$ fit $f(x)$ to the negative of the gradient

Then solve for c:

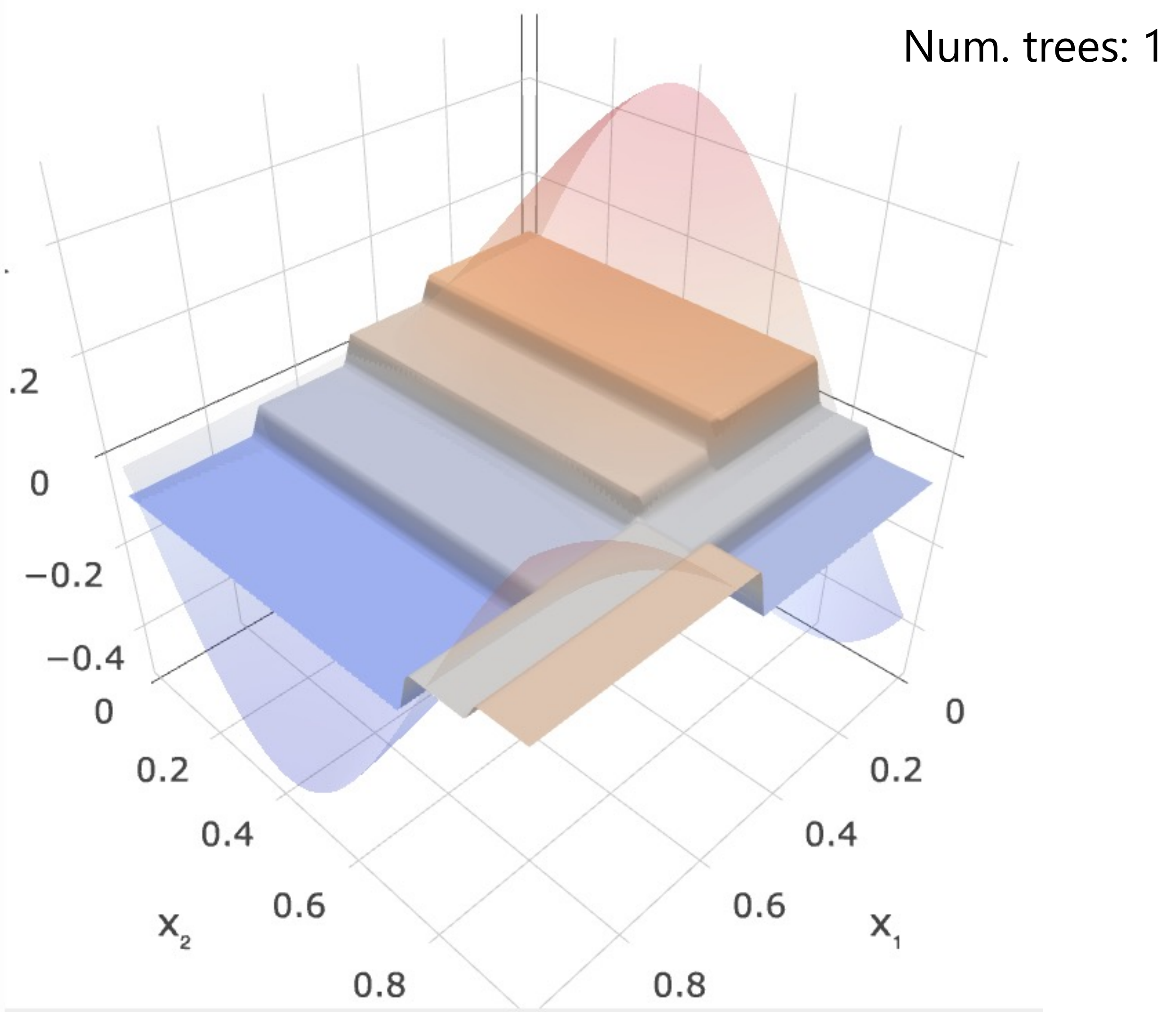
$$L(F(x) + c \cdot f(x), y) \rightarrow \min_c$$

Example



Nice demo: http://arogozhnikov.github.io/2016/06/24/gradient_boosting_explained.htm

Example



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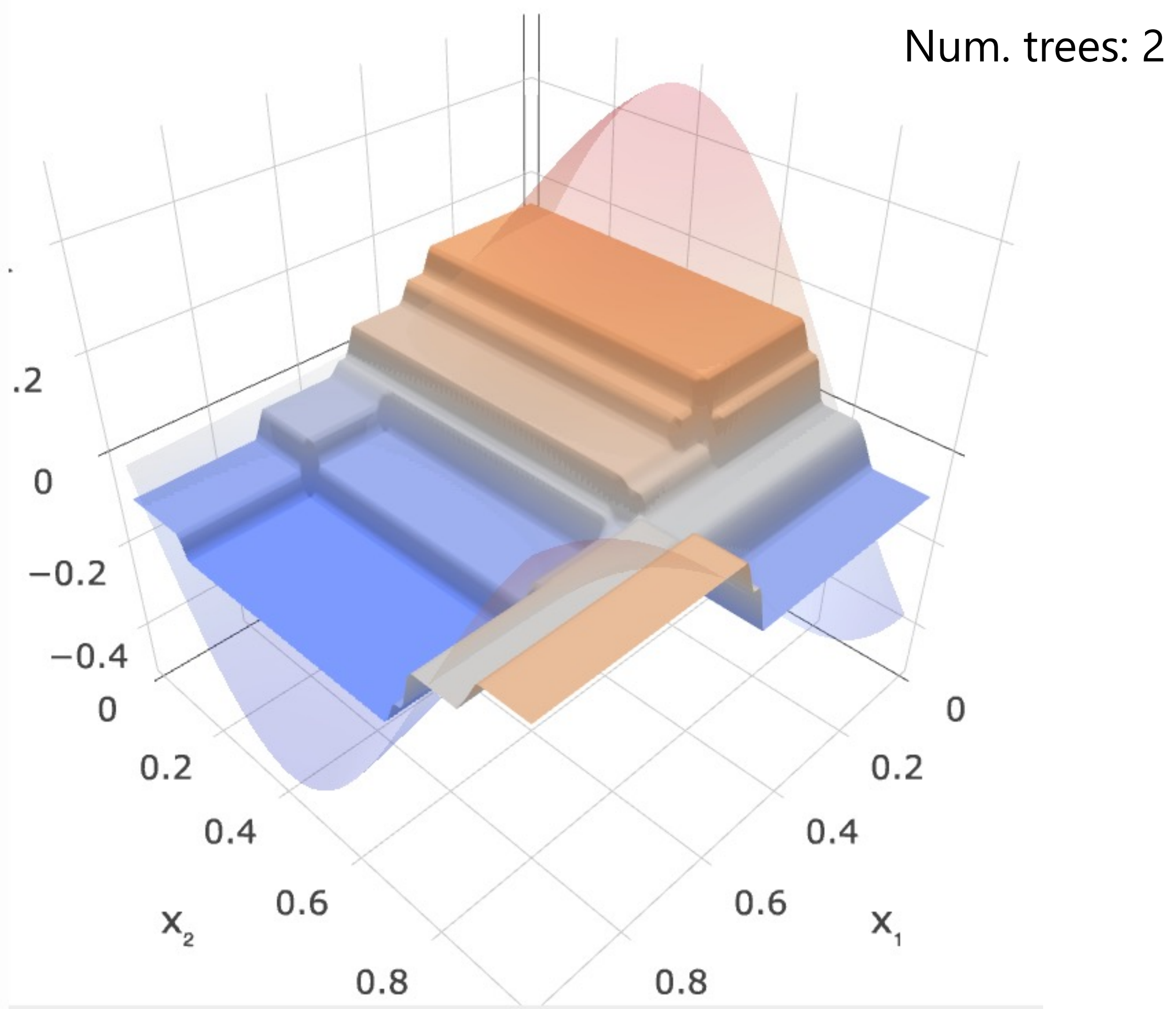

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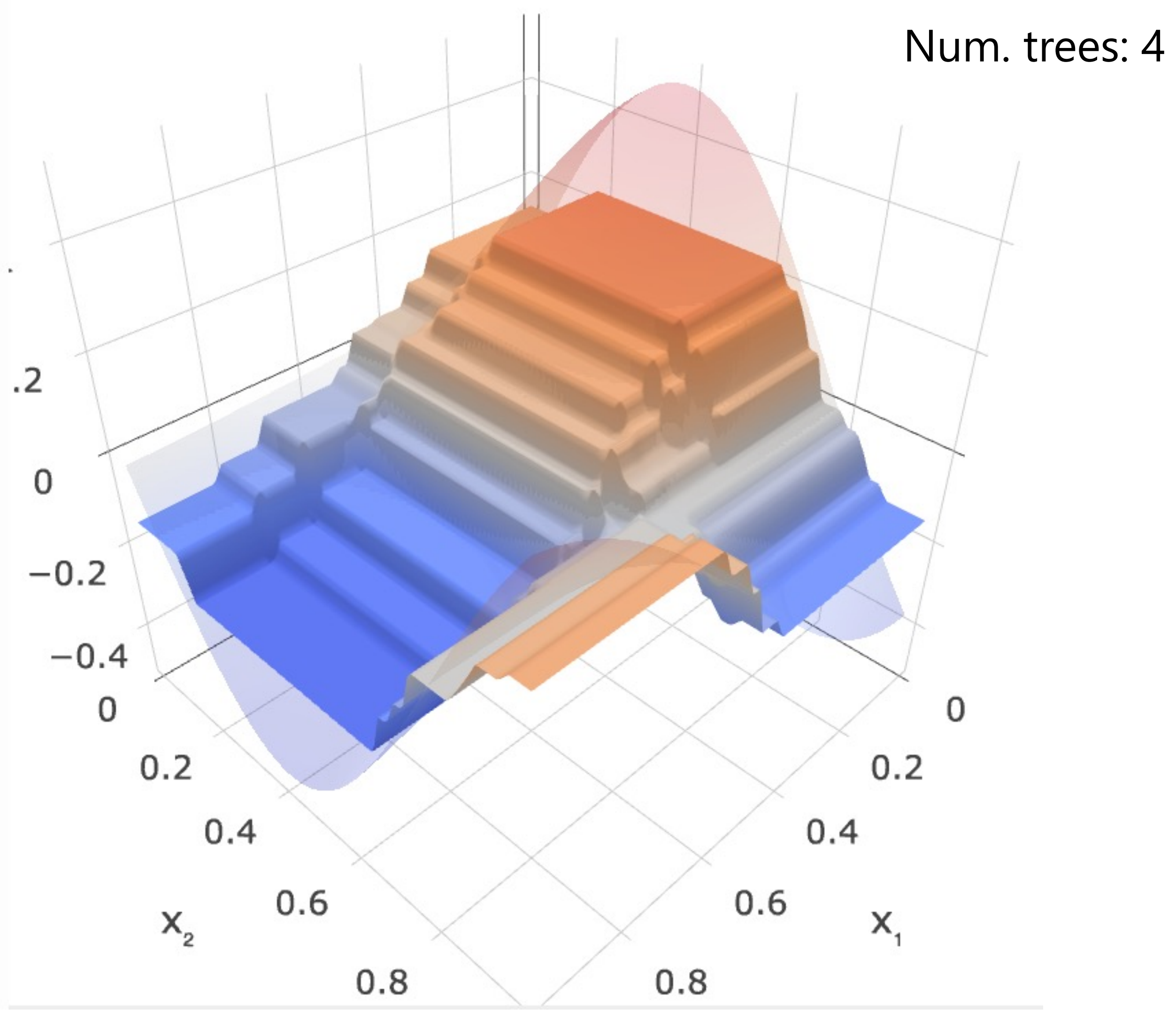

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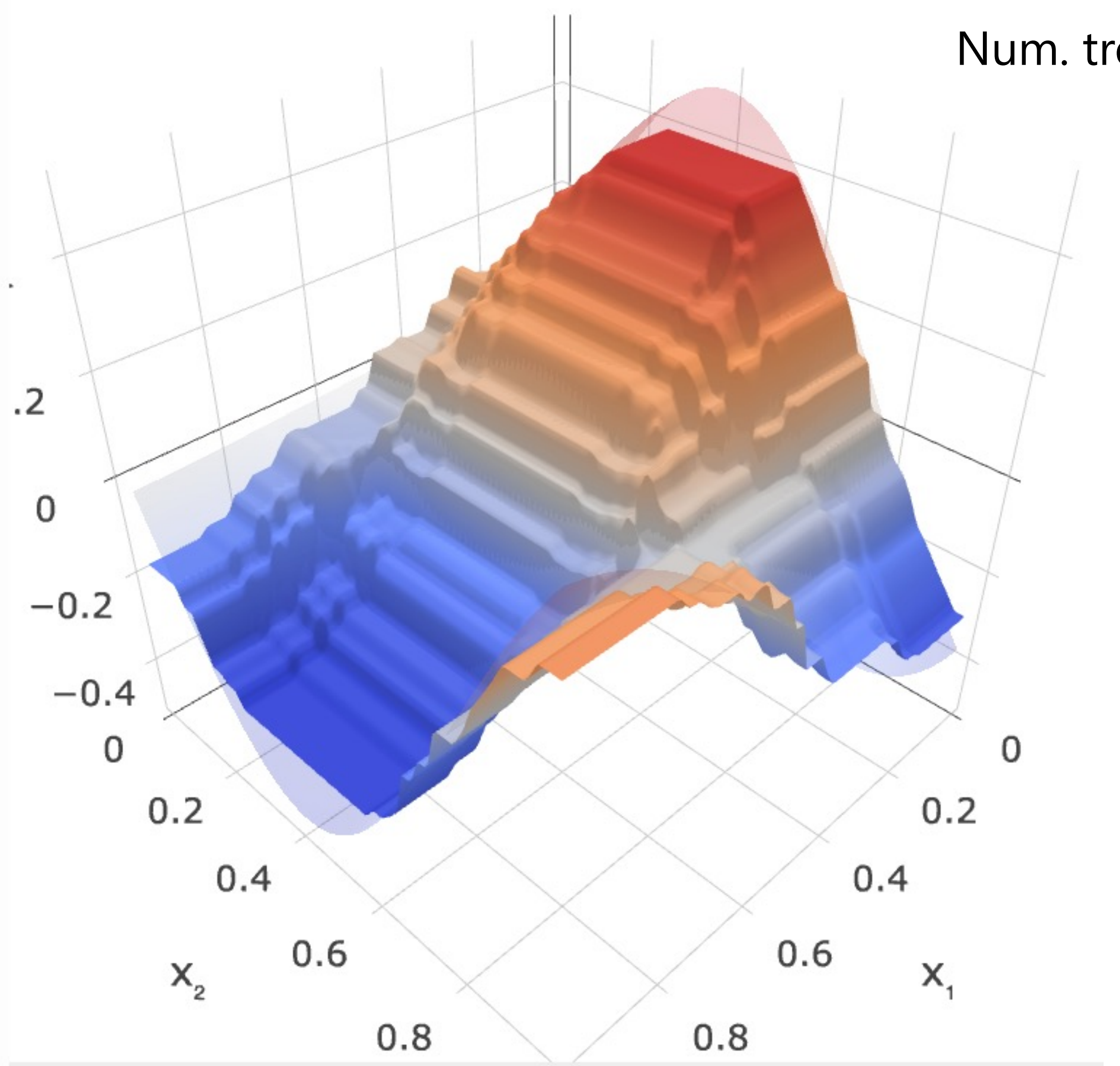

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Quadratic approximation

$$L(F(x)+f(x),y) \approx L(F(x),y) + \frac{\partial L(F,y)}{\partial F} f(x) + \frac{1}{2}\frac{\partial^2 L(F,y)}{\partial F^2}\left(f(x)\right)^2$$

$$= \underbrace{\frac{1}{2}\frac{\partial^2 L(F,y)}{\partial F^2}}_{\textbf{sample weights}} \left(f(x) + \underbrace{\frac{\frac{\partial L(F,y)}{\partial F}}{\frac{\partial^2 L(F,y)}{\partial F^2}}}_{\textbf{negative of the fitting targets}} \right)^2 + const\left(f(x)\right)$$

See also: very nice explanation in the xgboost documentation:

- https://xgboost.readthedocs.io/en/latest/tutorials/model.html

Summary

Ensembling may allow to reduce variance and/or bias of the base learners

Averaging the prediction of **independent** high-variance models reduces the variance

With bagging, the base learners are made (quasi-) independent using bootstrapping

- Can be done in parallel

With boosting, the base learners are built in sequence, each next one trying to improve upon the mistakes of the previous steps

- One of the most powerful classes of models

Question to you: does it make sense to boost linear regression?

Thank you!

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