Yandex

SCHOOL OF DATA ANALYSIS

Skoltech
Skolkovo Institute of Science and Technology

Decision Trees and Ensembling algorithms

Fifth Machine Learning in High Energy Physics Summer School,
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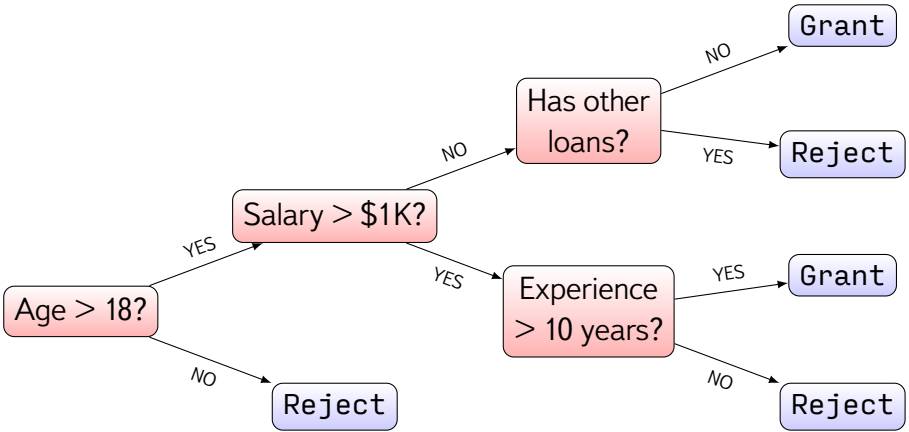
Lecture overview

- Decision Trees
- Bootstrap, Bagging, and Random Forests
- Naive boosting for regression
- Adaptive boosting
- Gradient boosting machine
- XGBoost
- Stacked generalization

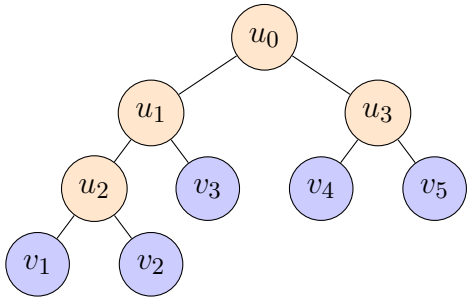
Decision trees

Decision making at a bank



Decision tree formalism

- Decision tree is a binary tree V
- Internal nodes $u \in V$: predicates $\beta_u : \mathbb{X} \to \{0, 1\}$
- Leafs $v \in V$: predictions x
- Algorithm $h(\mathbf{x})$ starts at $u = u_0$
  - Compute $b = \beta_u(\mathbf{x})$
  - If $b = 0$, $u \leftarrow \mathrm{LeftChild}(u)$
  - If $b = 1$, $u \leftarrow \mathrm{RightChild}(u)$
  - If u is a leaf, return b
- In practice: $\beta_u(\mathbf{x}; j, t) = [\mathbf{x}_j < t]$



Greedy tree learning for binary classification

› Input: training set $X^\ell = \left\{(\mathbf{x}_i, y_i)\right\}_{i=1}^{\ell}$

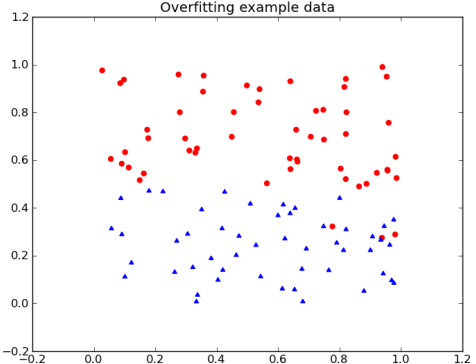
1. Greedily split X^ℓ into R_1 and R_2:

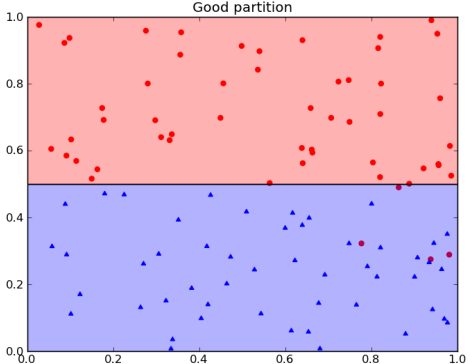
$$R_1(j,t) = \{\mathbf{x} \in X^\ell | \mathbf{x}_j < t\}, \qquad R_2(j,t) = \{\mathbf{x} \in X^\ell | \mathbf{x}_j > t\}$$

   optimizing a given loss: $Q(X^\ell, j, t) \to \min\limits_{(j,t)}$
2. Create internal node u corresponding to the predicate $[\mathbf{x}_j < t]$
3. If a stopping criterion is satisfied for u,
   declare it a leaf, setting some $c_u \in \mathbb{Y}$ as leaf prediction
4. If not, repeat 1–2 for $R_1(j,t)$ and $R_2(j,t)$

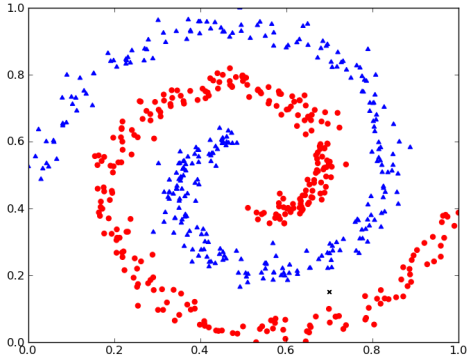
› Output: a decision tree V

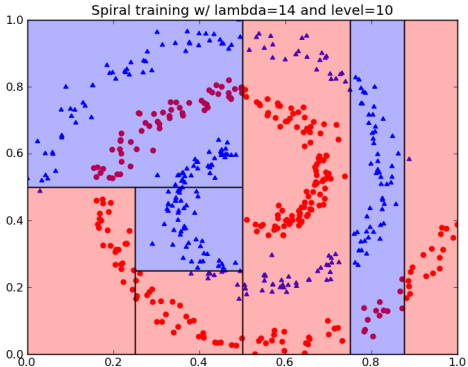
Greedy tree learning for binary classification



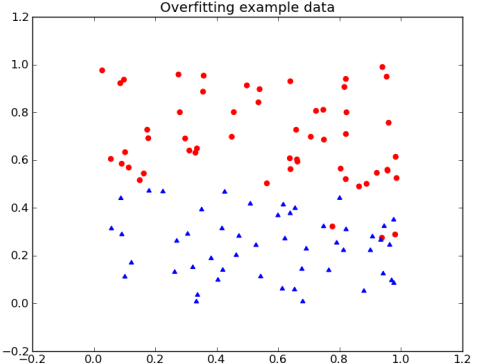


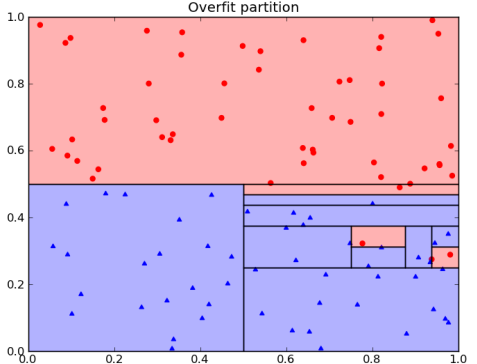
Greedy tree learning for binary classification





With decision trees, overfitting is extra-easy!





Design choices for learning a decision tree classifier

- Type of predicate in internal nodes
- The loss function $Q(X^\ell, j, t)$
- The stopping criterion
- Hacks: missing values, pruning, etc.

- CART, C4.5, ID3

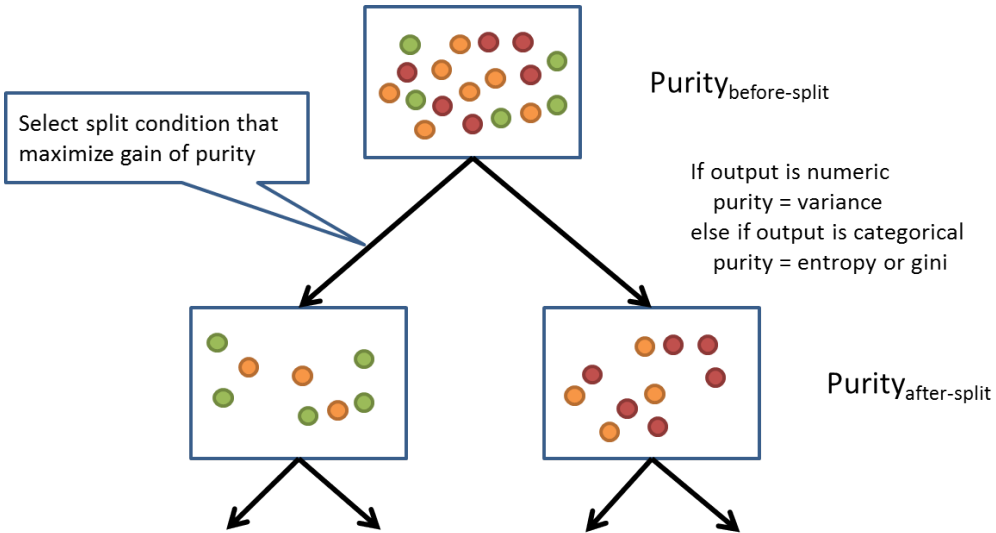
The loss function $Q(X^\ell, j, t)$

- R_m: the subset of X^ℓ at step m
- With the current split, let $R_l \subseteq R_m$ go left and $R_l \subseteq R_m$ go right
- Choose predicate to optimize

$$Q(R_m, j, t) = H(R_m) - \frac{|R_l|}{|R_m|} H(R_l) - \frac{|R_r|}{|R_m|} H(R_r) \to \max$$

- $H(R)$: impurity criterion
- Generally $H(R) = \min\limits_{c \in \mathbb{Y}} \frac{1}{|R|} \sum\limits_{(\mathbf{x}_i, y_i) \in R} L(y_i, c)$

The idea: maximize purity



Picture credit: https://dzone.com/refcardz/machine-learning-predictive

Examples of information criteria

- Regression:
  - $H(R) = \min\limits_{c \in \mathbb{Y}} |R|^{-1} \sum_{(\mathbf{x}_i, y_i) \in R} (y_i - c)^2$
  - Sum of squared residuals minimized by $c = |R|^{-1} \sum_{(\mathbf{x}_j, y_j) \in R} y_j$
  - Impurity $\equiv$ variance of the target
- Classification:
  - Let $p_k = |R|^{-1} \sum_{(\mathbf{x}_i, y_i) \in R} [y_i = k]$ (share of y_i's equal to k)
  - Miss rate: $H(R) = \min\limits_{c \in \mathbb{Y}} |R|^{-1} \sum_{(\mathbf{x}_i, y_i) \in R} [y_i \neq c]$

    Minimizing miss rate $1 - p_{k_*}$,

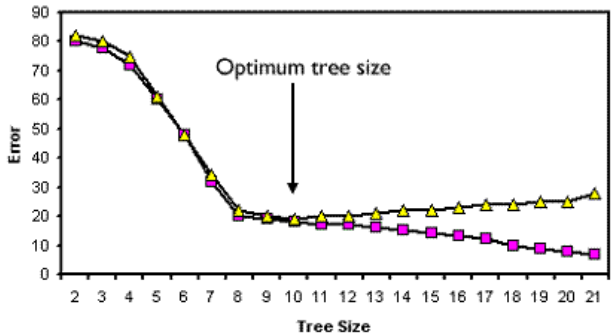
    Gini index $\sum_{k=1}^{K} p_k (1 - p_k)$,

    Cross-entropy $- \sum_{k=1}^{K} p_k \log p_k$

Stopping rules for decision tree learning

- Significantly impacts learning performance
- Multiple choices available:
  - Maximum tree depth
  - Minimum number of objects in leaf
  - Maximum number of leafs in tree
  - Stop if all objects fall into same leaf
  - Constrain quality improvement
    (stop when improvement gains drop below s%)
- Typically selected via exhaustive search and cross-validation

Decision tree pruning



- Learn a large tree (effectively overfit the training set)
- Detect overfitting via K-fold cross-validation
- Optimize structure by removing least important nodes

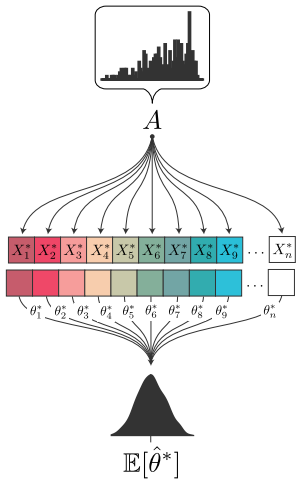
Semi-Conclusion

› Decision trees: intuitive and interpretable, yet prone to overfitting

Bagging and Random Forests

The bootstrapping procedure

- Input: a sample $X^\ell = \{(x_i, y_i)\}_{i=1}^\ell$
- Bootstrapping: generate new samples X_1^m of (x_i, y_i) drawn from X^ℓ uniformly at random with replacement (replicated (x_i, y_i) possible!)
- Ensemble learning idea:
  1. Generate N bootstrapped samples $X_1^m, \ldots, X_N^m$
  2. Learn N hypotheses $h_1, \ldots, h_N$
  3. Average predictions to obtain $h(x) = \frac{1}{N} \sum_{i=1}^N h_i(x)$
  4. Profit!



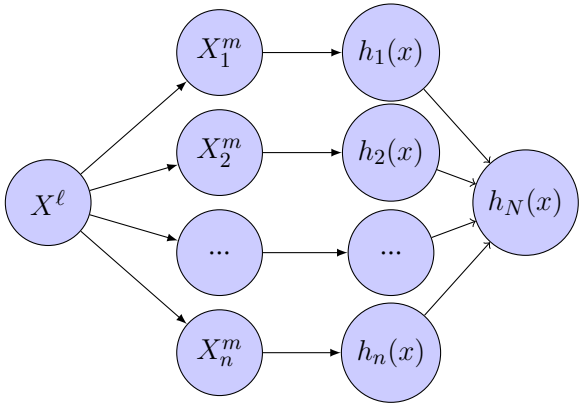
Picture credit: http://www.drbunsen.org/bootstrap-in-picture

Bagging: bootstrap aggregation (+ demo)

- Input: a sample $X^\ell = \{(x_i, y_i)\}_{i=1}^{\ell}$
- Weak learners via bootstrapping $\tilde{\mu}(X^\ell) = \mu(\tilde{X}^\ell)$
- Ensemble average

$$h_N(x) = \frac{1}{N}\sum_{i=1}^{N} h_i(x) =$$

$$= \frac{1}{N}\sum_{i=1}^{N} \tilde{\mu}(X^\ell)(x)$$



The Random Forest algorithm

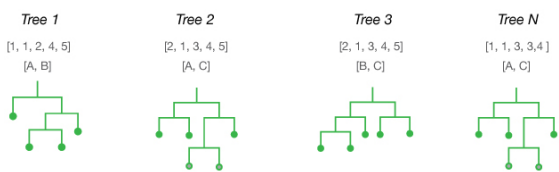
- Bagging over (weak) decision trees
- Reduce error via averaging over instances and features
- Input: a sample $X^\ell = \{(\mathbf{x}_i, y_i)\}_{i=1}^\ell$, where $\mathbf{x}_i \in \mathbb{R}^d, y_i \in \mathbb{Y}$
- The algorithm iterates for $i = 1, \ldots, N$:
  1. Pick p random features out of d
  2. Bootstrap a sample $X_i^m = \{(\mathbf{x}_i, y_i)\}_{i=1}^\ell$ where $\mathbf{x}_i \in \mathbb{R}^p, y_i \in \mathbb{Y}$
  3. Learn a decision tree $h_i(\mathbf{x})$ using bootstrapped X_i^m
  4. Stop when leafs in h_i contain less that n_{min} instances

$\mathbf{x}_i \in \{\text{A}, \text{B}, \text{C}\}$

$X^\ell = \{(\mathbf{x}_i, y_i)\}_{i=1}^5$

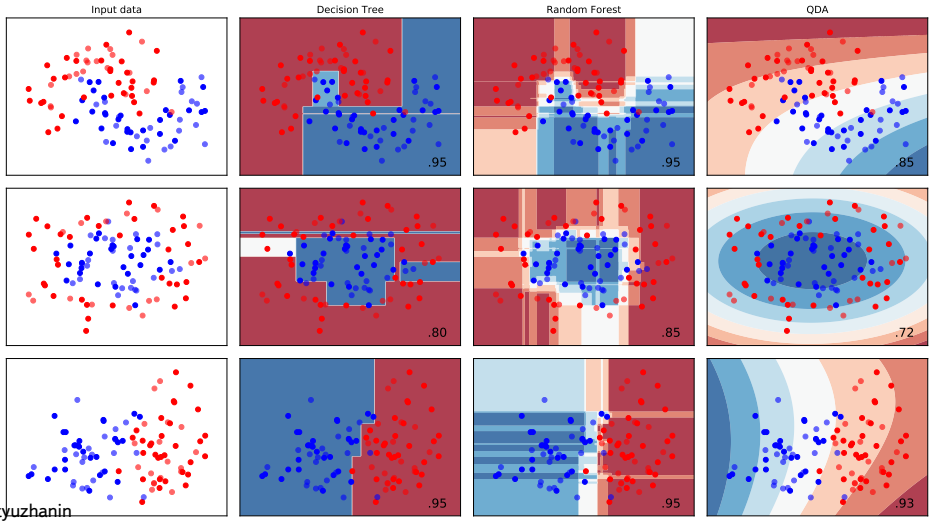
Bootstrap $X_i^m, i \in \{1, 2, 3, 4\}$

Learn Tree$_i(\mathbf{x})$ using X_i^m



Picture credit: http://www.thefactmachine.com/random-forests

Random Forest: synthetic examples



Learning Theory (continued)

Expected risk formalism

- Input: the training set $X^\ell = \{(x_i, y_i)\}_{i=1}^\ell$
- Suppose $(x_i, y_i) \in \mathbb{X} \times \mathbb{Y}$ are generated from a distribution $p(x, y)$
- Consider the MSE loss $Q(y, h) = \big(y - h(x)\big)^2$
- Expected risk: average (over $p(x, y)$) squared loss when using h

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

- A statement: the expected risk is minimized by

$$h_*(x) = \mathbb{E}[y \,|\, x] = \int_{\mathbb{Y}} y p(y \,|\, x) dy = \arg\min_h R(h)$$

Bias-variance decomposition

- Input: the training set $X^\ell = \{(x_i, y_i)\}_{i=1}^\ell$
- Learning method $\mu : (\mathbb{X} \times \mathbb{Y})^\ell \to \mathbb{H}$
- Can evaluate quality using average (over possible samples X^ℓ)

$$Q(\mu) = \mathbb{E}_{X^\ell}\left[\mathbb{E}_{x,y}\left[\left(y - \mu(X^\ell)(x)\right)^2\right]\right] =$$

$$= \int_{(\mathbb{X}\times\mathbb{Y})^\ell} \int_{\mathbb{X}\times\mathbb{Y}} \left(y - \mu(X^\ell)(x)\right)^2 p(x,y) \prod_{i=1}^{\ell} p(x_i, y_i) dx dy dx_i dy_i$$

Bias-variance decomposition

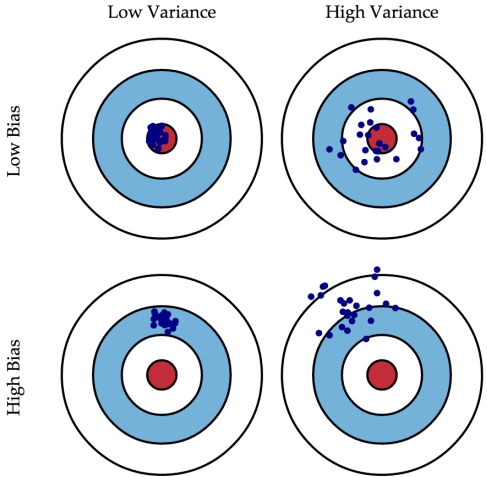
- We arrive at the famous **bias-variance**(-noise) **decomposition**

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

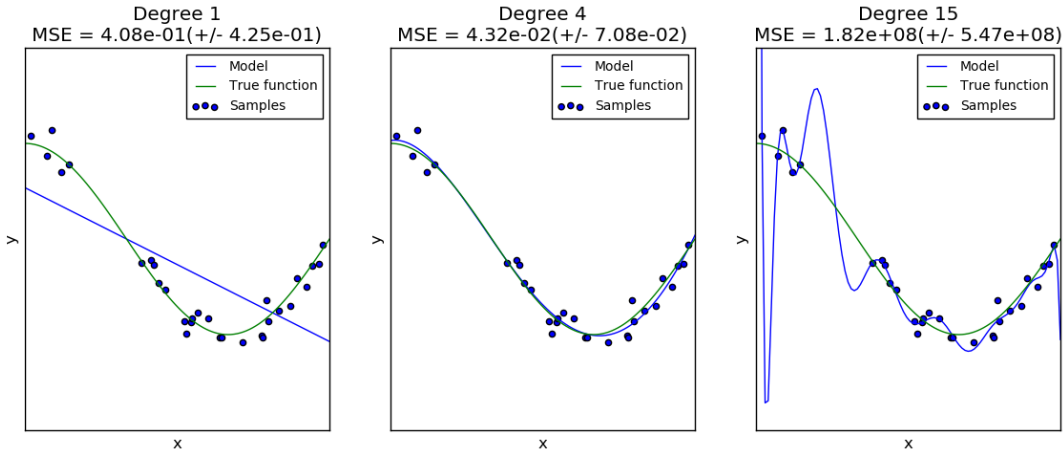
$$+ \underbrace{\mathbb{E}_x\Big[\big(\mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big] - \mathbb{E}[y \mid x]\big)^2\Big]}_{\text{bias}} + \underbrace{\mathbb{E}_x\Big[\mathbb{E}_{X^\ell}\Big[\big(\mu(X^\ell) - \mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big]\big)^2\Big]\Big]}_{\text{variance}}$$

- Noise term: an error of an ideal learner (nobody can do better!)
- Bias term: learner's approximation of the ideal algorithm
  - The more complex the learning algorithm, the lower the bias
- Variance term: sensitivity to sample replacement
  - Simple algorithms have lower variance

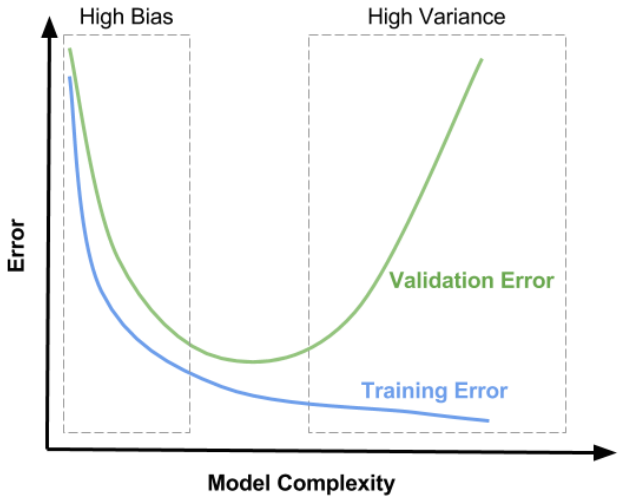
Bias-variance decomposition



Polynomial fits of different degrees



Bias-variance tradeoff



Picture credit: http://www.learnopencv.com/bias-variance-tradeoff-in-machine-learning

An application: statistical analysis of Bagging

› Bias: not made any worse by bagging multiple hypotheses

$$\mathbb{E}_{x,y}\left[\left(\mathbb{E}_{X^\ell}\left[\frac{1}{N}\sum_{n=1}^{N}\tilde{\mu}(X^\ell)(x)\right] - \mathbb{E}[y \mid x]\right)^2\right] =$$

$$= \mathbb{E}_{x,y}\left[\left(\frac{1}{N}\sum_{n=1}^{N}\mathbb{E}_X^\ell[\tilde{\mu}(X^\ell)(x)] - \mathbb{E}[y \mid x]\right)^2\right] =$$

$$= \mathbb{E}_{x,y}\left[\left(\mathbb{E}_{X^\ell}\left[\tilde{\mu}(X^\ell)(x)\right] - \mathbb{E}[y \mid x]\right)^2\right]$$

An application: statistical analysis of Bagging

› Variance: N times lower for uncorrelated hypotheses,
yet not as much an improvement for highly correlated

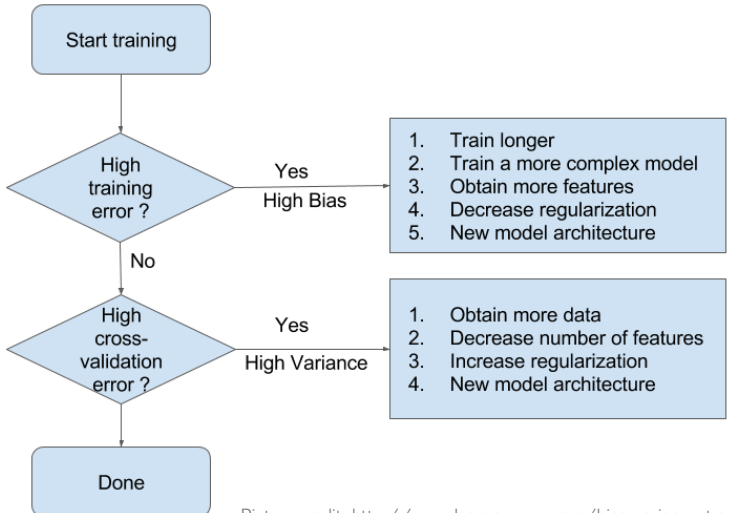
$$\mathbb{E}_{x,y}\left[\mathbb{E}_{X^\ell}\left[\left(\frac{1}{N}\sum_{n=1}^{N}\tilde{\mu}(X^\ell)(x) - \mathbb{E}_{X^\ell}\left[\frac{1}{N}\sum_{n=1}^{N}\tilde{\mu}(X^\ell)(x)\right]\right)^2\right]\right] =$$

$$= \frac{1}{N}\mathbb{E}_{x,y}\left[\mathbb{E}_{X^\ell}\left[\left(\tilde{\mu}(X^\ell)(x) - \mathbb{E}_{X^\ell}\left[\tilde{\mu}(X)(x)\right]\right)^2\right]\right] +$$

$$+ \frac{N(N-1)}{N^2}\mathbb{E}_{x,y}\left[\mathbb{E}_{X^\ell}\left[\left(\tilde{\mu}(X^\ell)(x) - \mathbb{E}_{X^\ell}\left[\tilde{\mu}(X^\ell)(x)\right]\right)\times\right.\right.$$

$$\left.\left.\times\left(\tilde{\mu}(X^\ell)(x) - \mathbb{E}_{X^\ell}\left[\tilde{\mu}(X^\ell)(x)\right]\right)\right]\right]$$

Bias-variance fix strategy



Picture credit: http://www.learnopencv.com/bias-variance-tradeoff-in-machine-learning

An intermediate conclusion

- Bootstrapping: a general statistical technique for computing sample functionals (and their variance)
- Bagging: meta-learner over arbitrary weak algorithms via **b**ootstrap **agg**regation
- The Random Forest algorithm: bagging over decision trees
- Bias/Variance trade-off - important concept that allows to understand and improve model performance

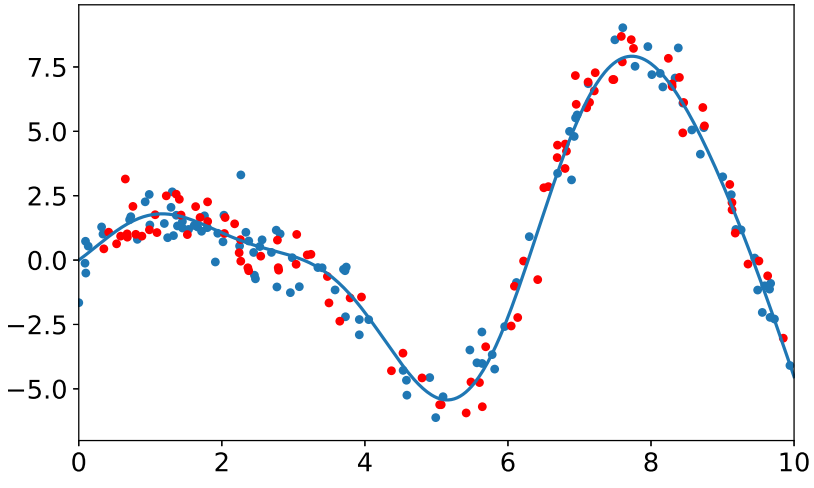
Naive boosting for regression

Boosting for regression

- Consider a regression problem $\frac{1}{2}\sum_{i=1}^{\ell}(h(x_i) - y_i)^2 \to \min_h$
- Search for solution in the form of weak learner composition $a_N(x) = \sum_{n=1}^{N} h_n(x)$ with weak learners $h_n \in \mathbb{H}$
- 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
  $$s_i^{(N)} = y_i - \sum_{n=1}^{N-1} h_n(x_i) = y_i - a_{N-1}(x_i), \qquad i = 1, \ldots, \ell$$
  3. Learn the next weak algorithm using
  $$a_N(x) := \arg\min_{h \in \mathbb{H}} \frac{1}{2}\sum_{i=1}^{\ell}(h(x_i) - s_i^{(N)})^2$$

(this implementation may be found in, e.g., `scikit-learn`)

Boosting: an example regression problem



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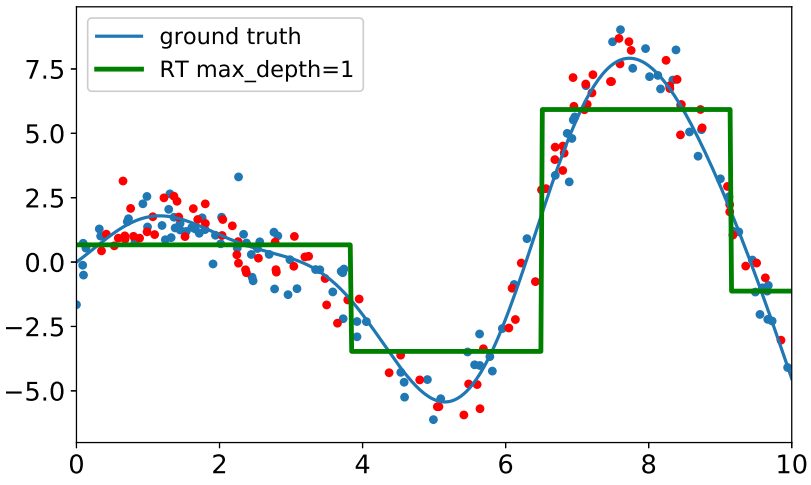

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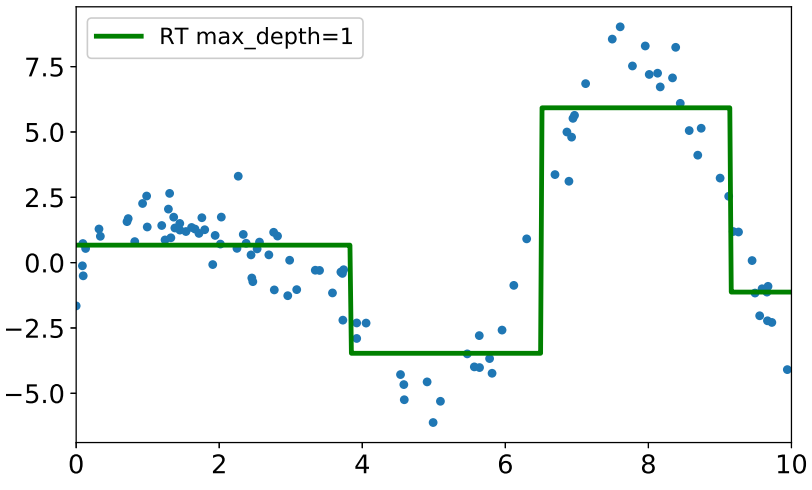
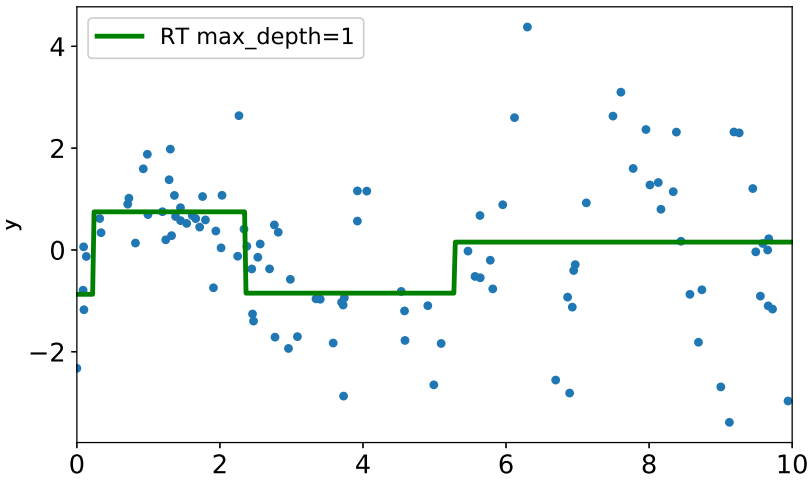


Boosting: an example regression problem



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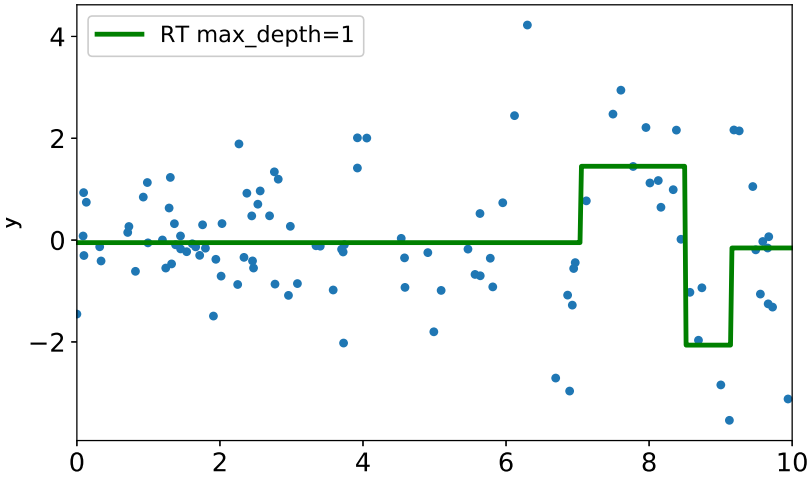
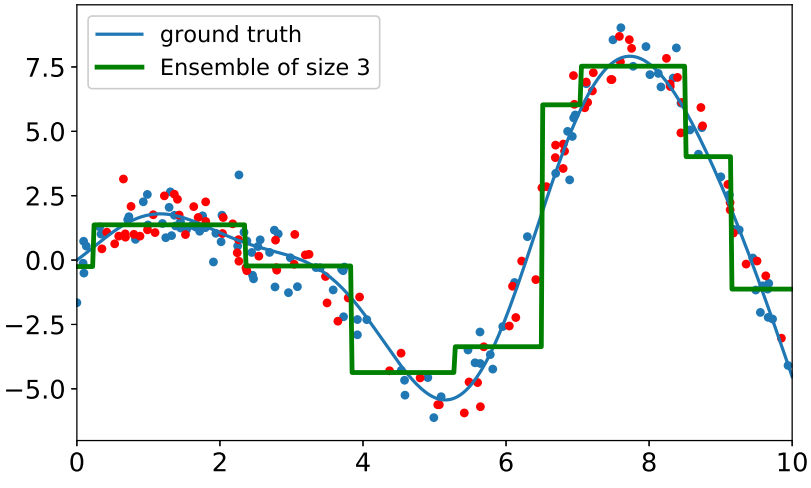


Boosting: an example regression problem

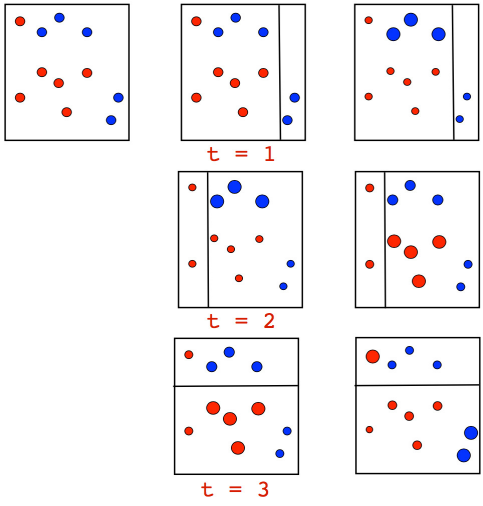


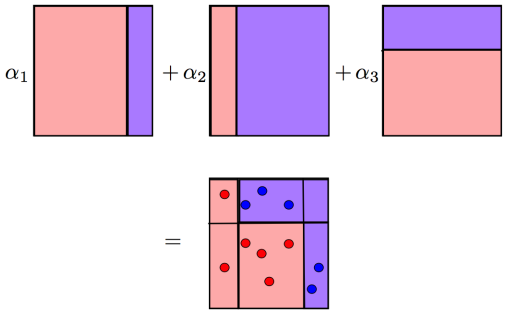
Reweighting and AdaBoost

Adaptive boosting for classification

- Training set $X^\ell = \{(\mathbf{x}_i, y_i)\}_{i=1}^\ell$, $y_i \in \{-1, +1\}$
- Search for solution in the form of a weighted sum $a_N(\mathbf{x}) = \sum_{n=1}^N \gamma_n h_n(\mathbf{x})$ with weak learners $h_n \in \mathbb{H}$
- At step N, extend a with h_N: $a_N(\mathbf{x}_i) = a_{N-1}(\mathbf{x}_i) + \gamma_N h_N(\mathbf{x}_i)$.
  How do we choose h_N and its weight γ_N?
- Measure fit quality using exponential loss $Q(a_N, X^\ell) = \sum_{i=1}^\ell \exp\{-y_i a_N(\mathbf{x}_i)\}$
- Derivation yields $h_N = \arg\min_h \sum_{i=1}^\ell (h(\mathbf{x}_i) - w_i y_i)^2$
  with weights $w_i = \exp\{-y_i a_{N-1}(\mathbf{x}_i)\}$
- Weak learner weight: minimize $\gamma_N = \arg\min_\gamma Q(a_{N-1}(\mathbf{x}_i) + \gamma h_N(\mathbf{x}_i), X^\ell)$

Adaptive boosting for classification





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

Adaptive boosting for classification

[Video: AdaBoost in Action]
https://www.youtube.com/watch?v=k4G2VCuOMMg

Gradient boosting

Gradient boosting: motivation

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

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

- Recall: functions decrease in the direction of negative gradient
- View $L(y, z)$ as a function of z ($= a_N(\mathbf{x}_i)$), execute gradient descent on z
- Search for such $s_1, \ldots, s_\ell$ that

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

- 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 [Friedman, 2001]

- Input:
  - Training set $X^\ell = \{(\mathbf{x}_i, y_i)\}_{i=1}^\ell$
  - Number of boosting iterations N
  - Loss function $Q(y, z)$ with its gradient $\frac{\partial Q}{\partial z}$
  - 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 [Friedman, 2001]

At every iteration:

1. Compute pseudo-residuals: $s_i = -\left.\frac{\partial Q(y_i, z)}{\partial z}\right|_{z=a_{N-1}(\mathbf{x}_i)}, i = 1, \ldots, \ell$
2. Learn $h_N(\mathbf{x}_i)$ by regressing onto $s_1, \ldots, s_\ell$:

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

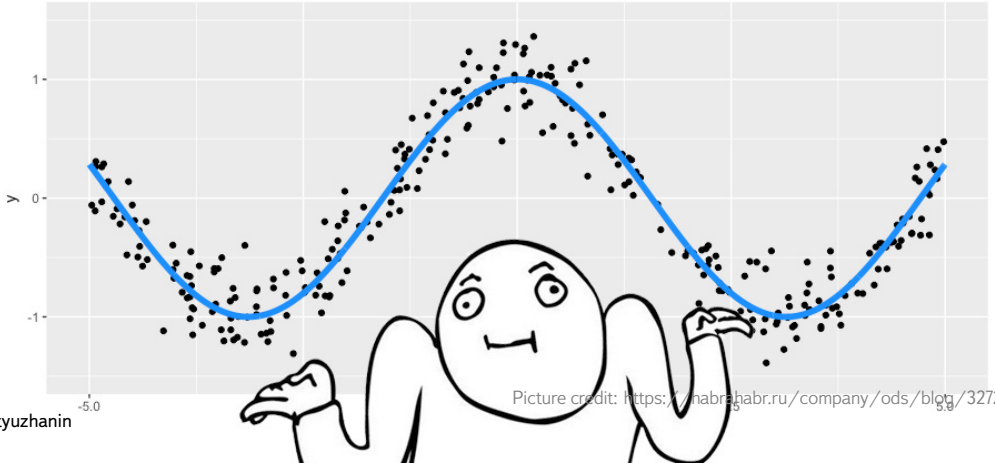
3. Find the optimal γ_N using plain gradient descent:

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

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 $x_i \in [-5, 5]$, $y_i = \cos(x_i) + \varepsilon_i$, $\varepsilon_i \sim \mathcal{N}(0, 1/5)$



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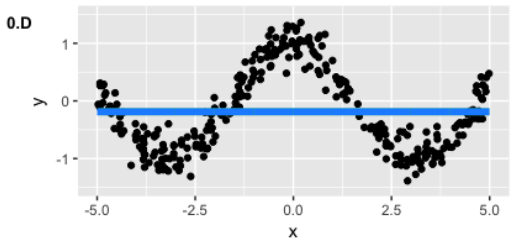
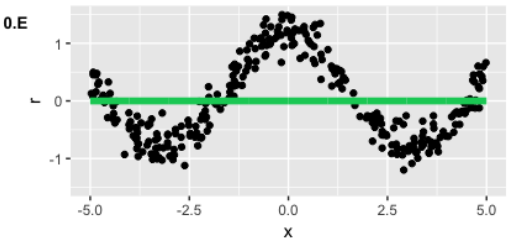
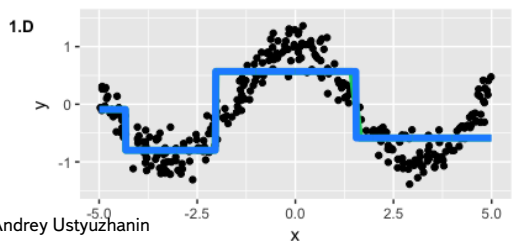
GBM: an example regression problem

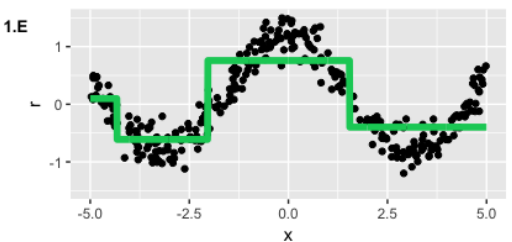
- Pick $N = 3$ boosting iterations
- Quadratic loss $Q(y, z) = (y - z)^2$
- Gradient of the quadratic loss $\frac{\partial Q(y_i, z)}{\partial z} = (y - z)$ is just redisuals
- Pick decision trees as weak learners $h_i(\mathbf{x})$
- Set 2 as the maximum depth for decision trees

GBM: an example regression problem

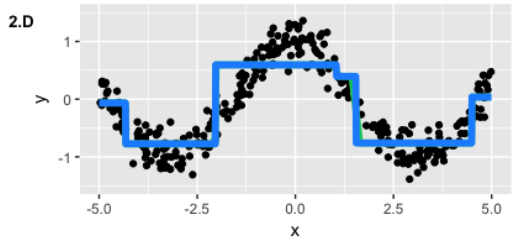


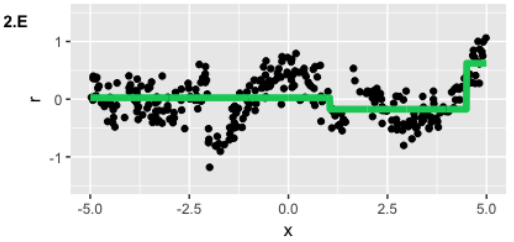


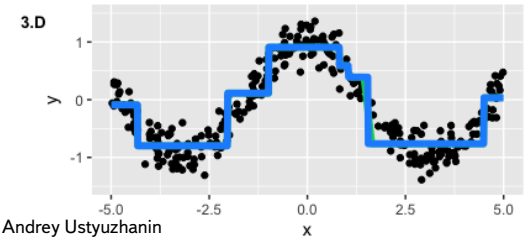


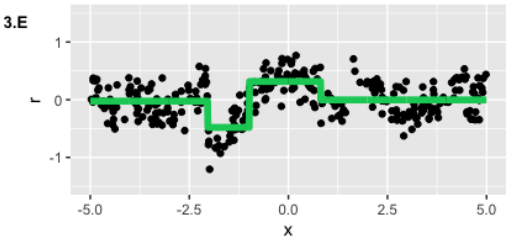


GBM: an example regression problem



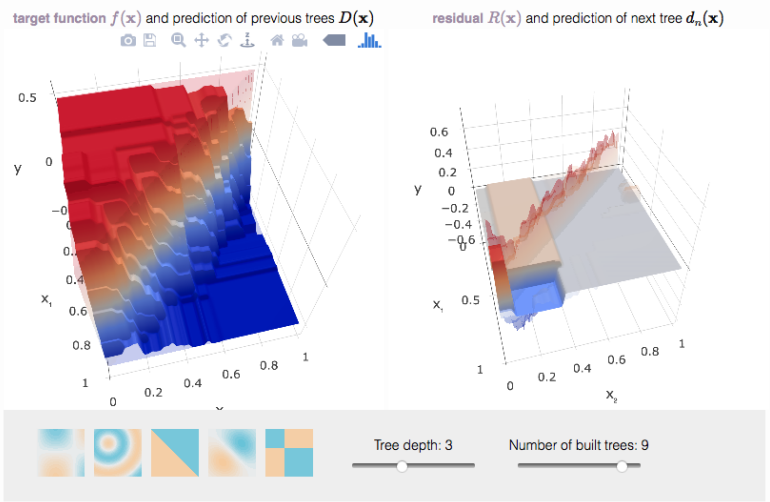






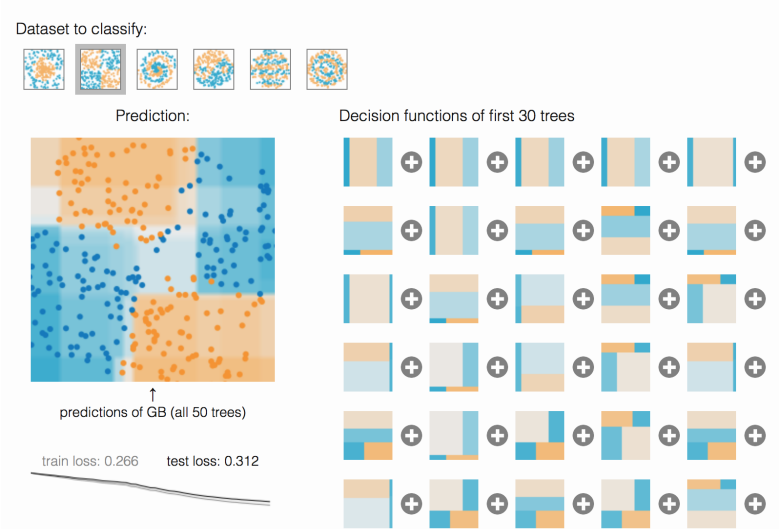
GBM: an interactive demo

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



GBM: an interactive demo

http://arogozhnikov.github.io/2016/07/05/gradient_boosting_playground.html



GBM: regulization via shrinkage

- For too simple weak learners, the negative gradient is approximated badly $\Longrightarrow$ 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 $\eta \in (0, 1]$

$$a_N(\mathbf{x}_i) \leftarrow a_{N-1}(\mathbf{x}) + \eta\gamma_N h_N(\mathbf{x})$$

(effectively distrust gradient direction estimated via weak learners)

GBM: shrinkage animated

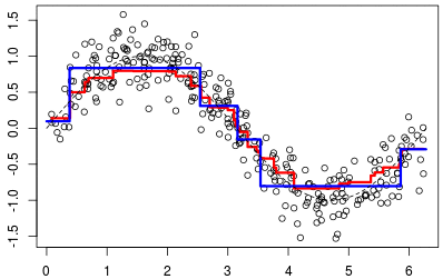


Figure: High shrinkage

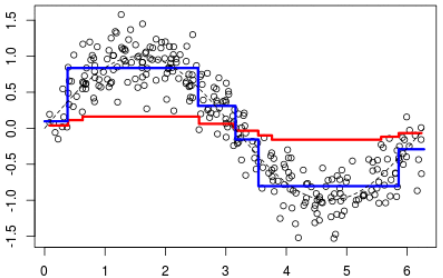
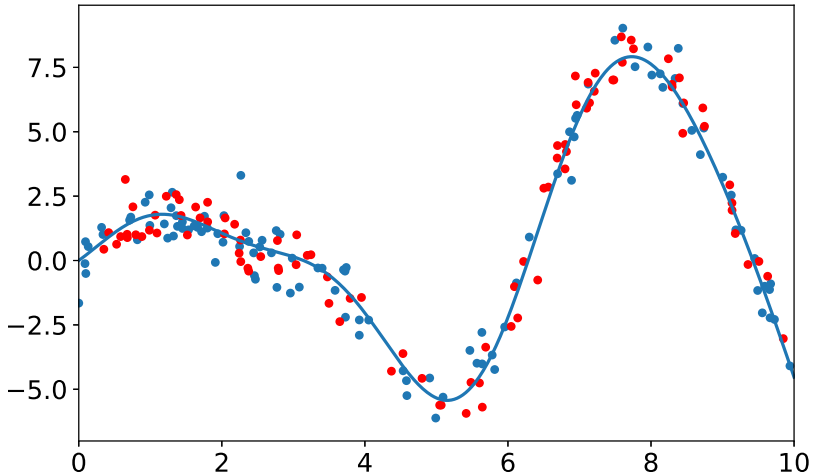
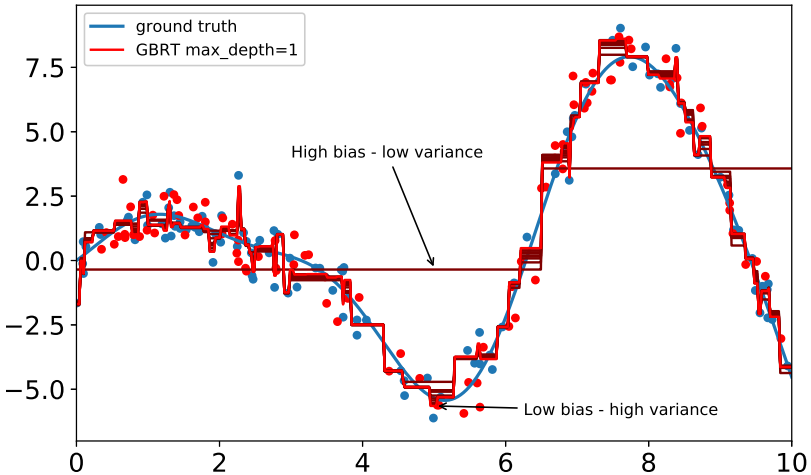


Figure: Low shrinkage

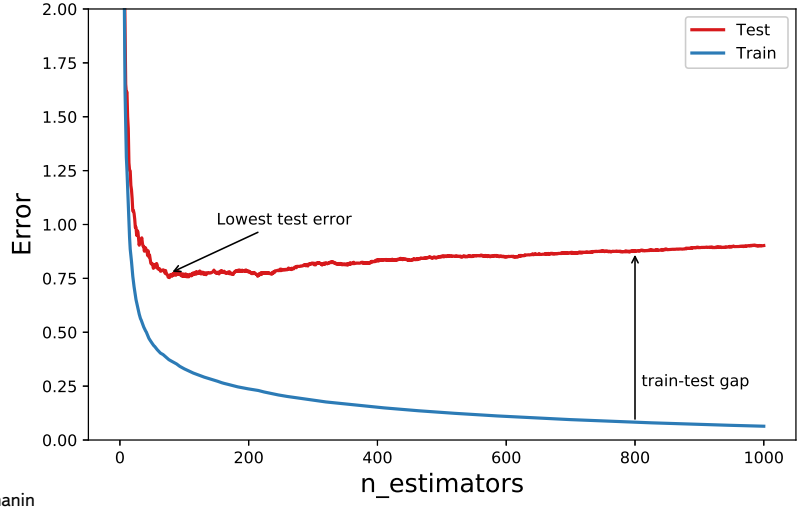
GBM: regularization approaches



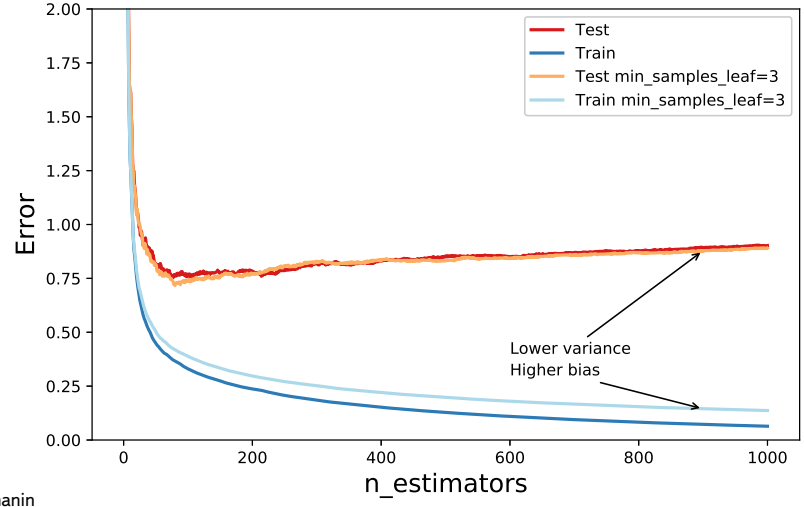
GBM: regularization approaches



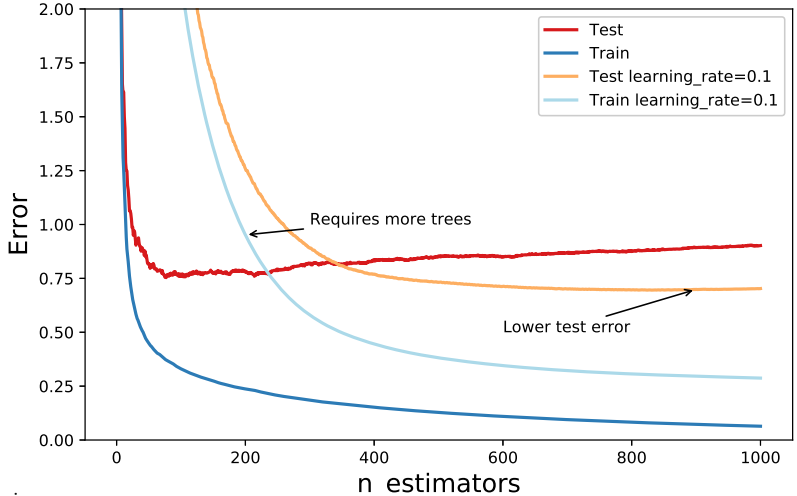
GBM: regularization approaches



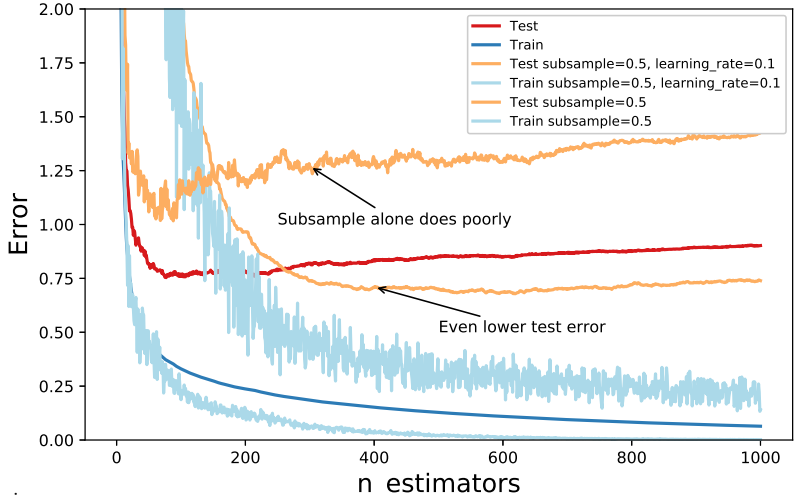
GBM: regularization approaches



GBM: regularization approaches



GBM: regularization approaches



XGBoost algorithm

Extreme Gradient Boosting

1. Approximate the descent direction constructed using second order derivatives

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

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

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

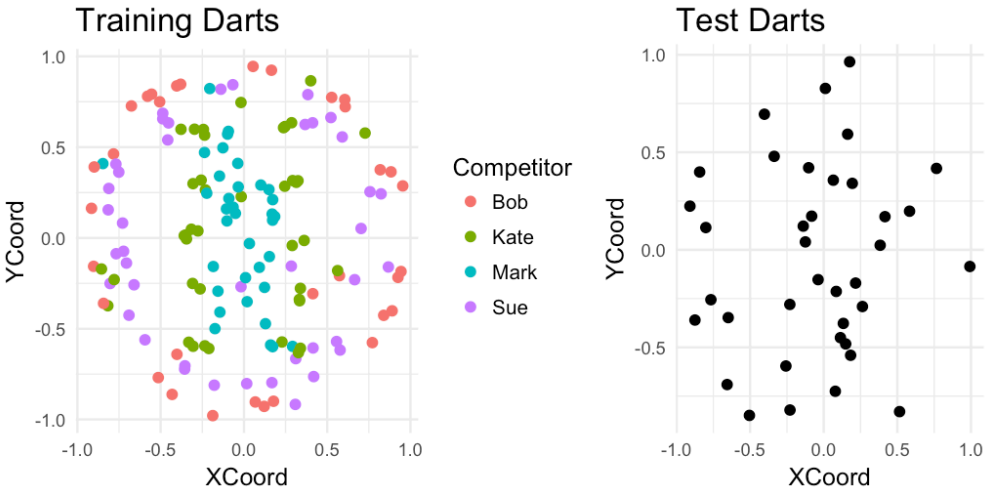
4. The stopping rule: declare the node a leaf if even the best split gives negative Q

An intermediate conclusion

- Boosting: a general meta-algorithm aimed at composing a strong hypothesis from multiple weak hypotheses
- Boosting can be applied for arbitrary losses, arbitrary problems (regression, 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
- AdaBoost: gradient boosting with an exponential loss function resulting in reweighting training instances when adding weak learners
- XGBoost: gradient boosting with second order optimization, penalized loss and particular choice of impurity criterion

Stacked generalization

Stacking motivation: the game of Darts



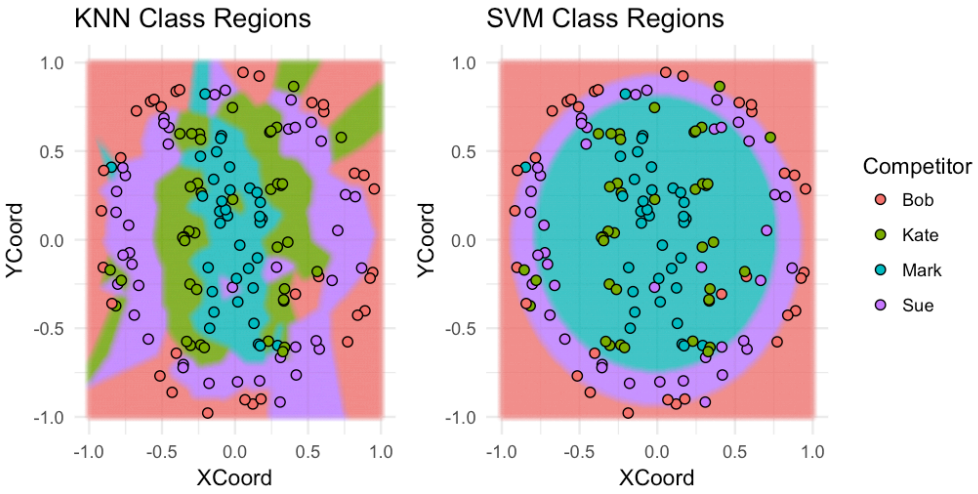
Picture credit: http://blog.kaggle.com/2016/12/27/a-kagglers-guide-to-model-stacking-in-practice/

Base model training

- Select k nearest neighbours as base model 1
- Fit base model 1 in the most fancy way possible
  (grid search for optimal k using K-fold cross-validation, etc.)
- k-NN accuracy on Test Darts: 70%

- Select Support Vector Machine as base model 2
- Fit base model 2 in the most fancy way possible
  (different penalizations, grid search for optimal kernel width using K-fold cross-validation, etc.)
- SVM accuracy on Test Darts: 78%

Results for base models



Picture credit: http://blog.kaggle.com/2016/12/27/a-kagglers-guide-to-model-stacking-in-practice/

Stacking base models

1. Partition `train` into 5 folds
2. Create `train_meta/test_meta`: same `row/fold Ids` as in `train/test`, empty `M1/M2`
3. For each $\mathrm{Fold}_i \in \{\mathrm{Fold}_1, \ldots, \mathrm{Fold}_5\}$
   - 3.1 Combine the other 4 folds for training $\to \mathrm{Fold}_{-i}$
   - 3.2 Fit each base model to Fold_{-i}, predict on Fold_i, save prdections to `M1/M2` in `train_meta`
4. Fit each base model to `train`, predict on `test`, save predictions to `M1/M2` in `test_meta`
5. Fit stacking model `S` to `train_meta`, using `M1/M2` as features
6. Use the stacked model `S` to make final predictions on `test_meta`

Results for base models

Picture credit: http://blog.kaggle.com/2016/12/27/a-kagglers-guide-to-model-stacking-in-practice

Conclusion

- Decision tree - a generic building block easy to interpret, prone to overfitting.
- Ensembling techniques - powerful mechanism for constructing complex decision machines.
- Gradient boosting - technique for effectively building model ensembles.
- Stacked generalization aka stacking: blend output of weak learners (weak signals) with raw features.

Bonus track

Minimum of the expected risk: the proof

› Transform the loss

$$\begin{aligned} Q(y, h(x)) &= (y - h(x))^2 = (y - \mathbb{E}(y \mid x) + \mathbb{E}(y \mid x) - h(x))^2 = \\ &= (y - \mathbb{E}(y \mid x))^2 + 2(y - \mathbb{E}(y \mid x))(\mathbb{E}(y \mid x) - h(x)) + \\ &+ (\mathbb{E}(y \mid x) - h(x))^2. \end{aligned}$$

› Write the expected risk

$$\begin{aligned} R(h) &= \mathbb{E}_{x,y} Q(y, h(x)) = \\ &= \mathbb{E}_{x,y}(y - \mathbb{E}(y \mid x))^2 + \mathbb{E}_{x,y}(\mathbb{E}(y \mid x) - h(x))^2 + \\ &+ 2\mathbb{E}_{x,y}(y - \mathbb{E}(y \mid x))(\mathbb{E}(y \mid x) - h(x)). \end{aligned}$$

Minimum of the expected risk: the proof

› Consider $\mathbb{E}_{x,y}(y - \mathbb{E}(y \mid x))(\mathbb{E}(y \mid x) - h(x))$ which is essentially some

$$\mathbb{E}_x \mathbb{E}_y[f(x,y) \mid x] = \int_{\mathbb{X}} \left(\int_{\mathbb{Y}} f(x,y) p(y \mid x) dy \right) p(x) dx$$

meaning that (as $\big(\mathbb{E}(y \mid x) - h(x)\big)$ is independent of y):

$$\begin{aligned}
&\mathbb{E}_x \mathbb{E}_y \Big[\big(y - \mathbb{E}(y \mid x)\big) \big(\mathbb{E}(y \mid x) - h(x)\big) \mid x \Big] = \\
&= \mathbb{E}_x \Big(\big(\mathbb{E}(y \mid x) - h(x)\big) \mathbb{E}_y \Big[\big(y - \mathbb{E}(y \mid x)\big) \mid x \Big] \Big) = \\
&= \mathbb{E}_x \Big(\big(\mathbb{E}(y \mid x) - h(x)\big) \big(\mathbb{E}(y \mid x) - \mathbb{E}(y \mid x)\big) \Big) = \\
&= 0
\end{aligned}$$

Minimum of the expected risk: the proof

› We obtain that the expected risk has the form

$$R(h) = \mathbb{E}_{x,y}(y - \mathbb{E}(y \,|\, x))^2 + \mathbb{E}_{x,y}(\mathbb{E}(y \,|\, x) - h(x))^2.$$

› Both summands are nonnegative meaning that the sum is minimized when

$$h_*(x) = \mathbb{E}(y \,|\, x) = \int_{\mathbb{Y}} y p(y \,|\, x) dy.$$

Bias-variance decomposition

- Input: the training set $X^\ell = \{(x_i, y_i)\}_{i=1}^\ell$
- Learning method $\mu : (\mathbb{X} \times \mathbb{Y})^\ell \to \mathbb{H}$
- Can evaluate quality using average (over possible samples X^ℓ)

$$Q(\mu) = \mathbb{E}_{X^\ell}\left[\mathbb{E}_{x,y}\left[\left(y - \mu(X^\ell)(x)\right)^2\right]\right] =$$

$$= \int_{(\mathbb{X}\times\mathbb{Y})^\ell} \int_{\mathbb{X}\times\mathbb{Y}} \left(y - \mu(X^\ell)(x)\right)^2 p(x,y) \prod_{i=1}^{\ell} p(x_i, y_i) dx dy dx_i dy_i$$

- For a fixed sample X^ℓ, we know the expected risk

$$\mathbb{E}_{x,y}\left[\left(y - \mu(X^\ell)\right)^2\right] = \mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \mid x]\right)^2\right] + \mathbb{E}_{x,y}\left[\left(\mathbb{E}[y \mid x] - \mu(X^\ell)\right)^2\right]$$

Bias-variance decomposition

› Plugging the expression for fixed X^ℓ into $Q(\mu)$, we obtain

$$Q(\mu) = \mathbb{E}_{X^\ell}\Big[\underbrace{\mathbb{E}_{x,y}\Big[\big(y - \mathbb{E}[y \mid x]\big)^2\Big]}_{\text{independent of } X^\ell} + \mathbb{E}_{x,y}\Big[\big(\mathbb{E}[y \mid x] - \mu(X^\ell)\big)^2\Big]\Big]$$

› Transforming the second summand

$$\mathbb{E}_{x,y}\Big[\mathbb{E}_{X^\ell}\Big[\big(\mathbb{E}[y \mid x] - \mu(X^\ell)\big)^2\Big]\Big] =$$

$$= \mathbb{E}_{x,y}\Big[\mathbb{E}_{X^\ell}\Big[\big(\mathbb{E}[y \mid x] - \mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big] + \mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big] - \mu(X^\ell)\big)^2\Big]\Big] =$$

$$= \mathbb{E}_{x,y}\Big[\mathbb{E}_{X^\ell}\Big[\underbrace{\big(\mathbb{E}[y \mid x] - \mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big]\big)^2}_{\text{independent of } X^\ell}\Big]\Big] + \mathbb{E}_{x,y}\Big[\mathbb{E}_{X^\ell}\Big[\big(\mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big] - \mu(X^\ell)\big)$$

$$+ 2\mathbb{E}_{x,y}\Big[\mathbb{E}_{X^\ell}\Big[\big(\mathbb{E}[y \mid x] - \mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big]\big)\big(\mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big] - \mu(X^\ell)\big)\Big]\Big]$$

Bias-variance decomposition

› We prove that the last term is zero:

$$\begin{aligned}
&\mathbb{E}_{X^\ell}\Big[\big(\mathbb{E}[y\,|\,x] - \mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big]\big)\big(\mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big] - \mu(X^\ell)\big)\Big] = \\
&\quad = \big(\mathbb{E}[y\,|\,x] - \mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big]\big)\mathbb{E}_X\Big[\mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big] - \mu(X^\ell)\Big] = \\
&\quad = \big(\mathbb{E}[y\,|\,x] - \mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big]\big)\Big[\mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big] - \mathbb{E}_{X^\ell}\big[\mu(X^\ell)\big]\Big] = \\
&\quad = 0.
\end{aligned}$$