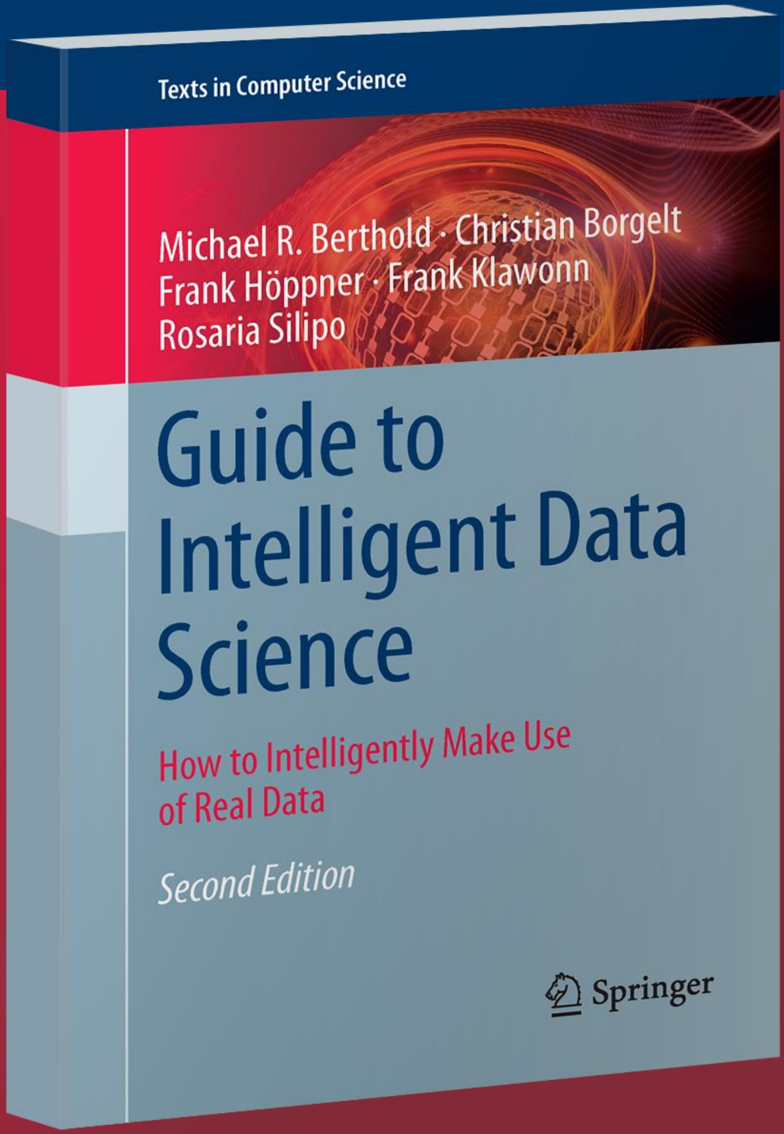
Ensemble Learning



Caption

"If I do not believe the news in todays paper, I buy 100 copies of the paper. Then I believe."
-Ludwig Wittgenstein

How can we learn from multiple models together?

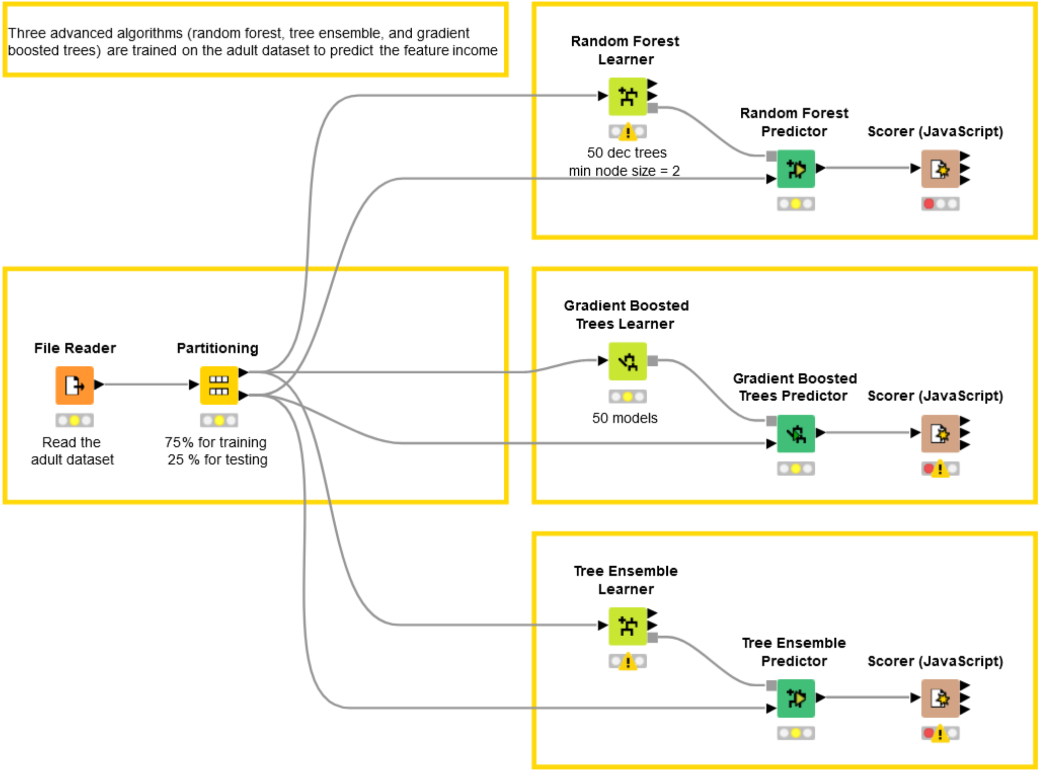
**This lesson refers to chapter 9 of the GIDS book*

What you will learn

- Ensemble Learning
  - Wisdom of the Crowd
  - Bagging & Boosting
  - Stacking and Cascade Generalization
  - Cascading and Delegating
  - Tree Ensembles and Random Forest
  - AdaBoost
  - Gradient Boosted Trees
  - Practical Examples

Datasets used : adult dataset

- „Random Forest, Gradient Boosted Trees, and Tree Ensemble“ https://kni.me/w/Ueq3QR9hty8Osh2E
  - Random forest
  - Gradient boosting
  - Tree ensemble



Ensemble Models

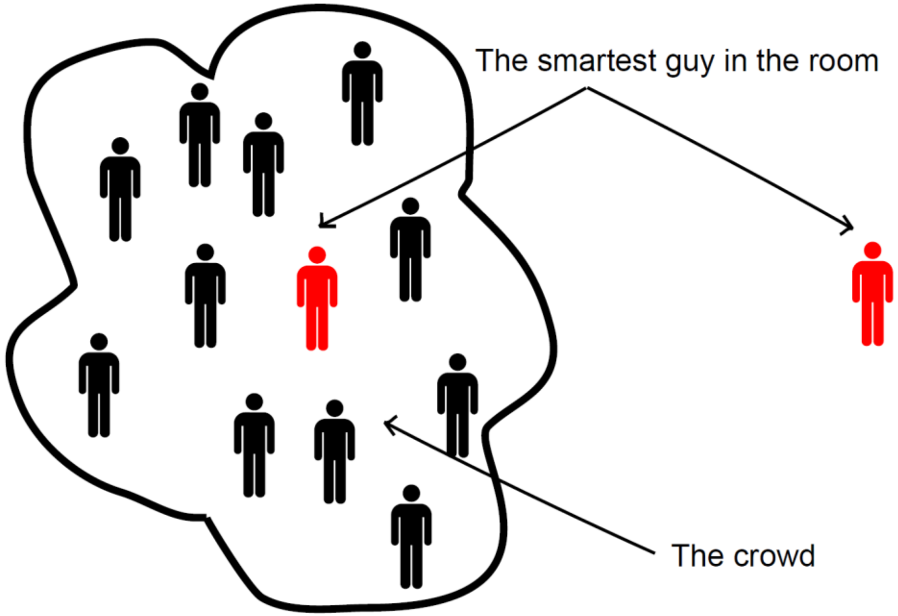
- General idea: take advantage of the “wisdom of the crowd”

- Training of many weak classifiers (or regression models)
- Combining them to construct a classifier (regression model) more accurate than any of the individual ones

- Leads to a more accurate and robust model
- Interpretation of an ensemble learning model is difficult
  - Since it consists of many models!

Wisdom of the Crowd

Wisdom of the Crowd



Crowd wiser than **any individual**

- When?
- For which questions?

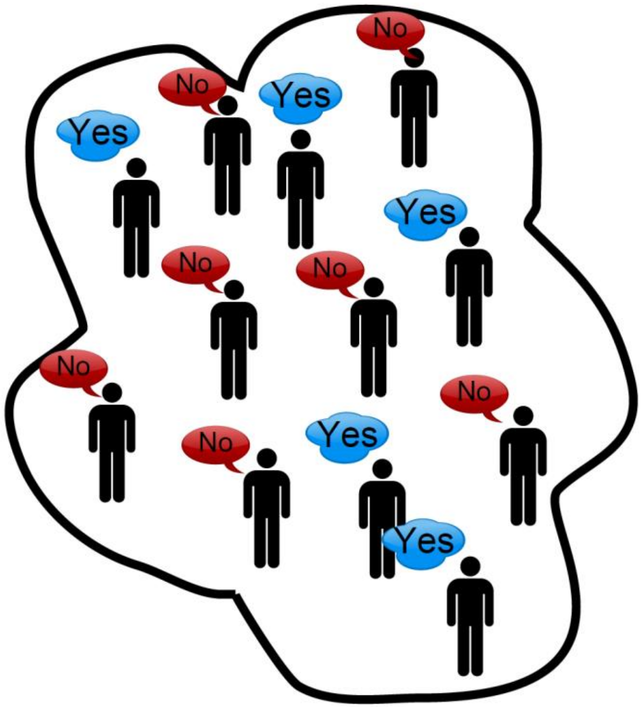
– The **collective knowledge** of a *diverse* and *independent* body of people typically **exceeds** the knowledge of **any single individual** and can be harnessed by voting.

– http://www.csc.kth.se/utbildning/kth/kurser/DD2431/ml11/schedule/07-ensamble.pdf

Wisdom of the Crowd: Scenario

– Ask each person in the crowd:
– Will Mr. X win the general election in country Y?

– **The Crowd's prediction:**
– MAJORITY answer.
– This crowd predicts **No**. (Mr. X will not win the election.)

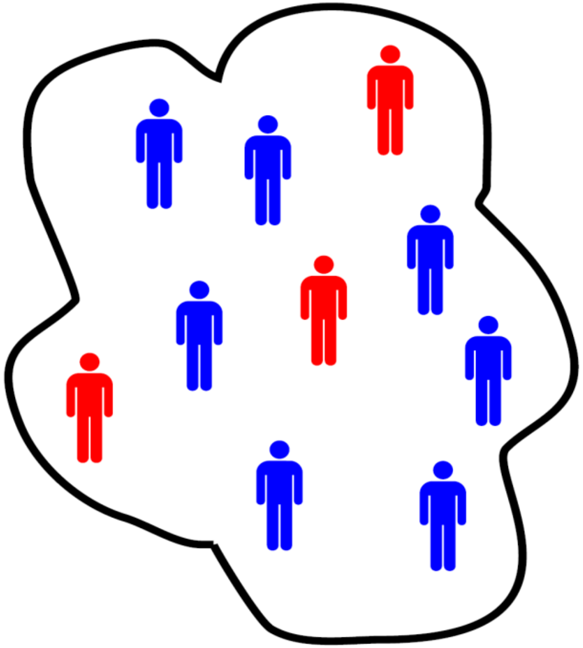


Wisdom of the Crowd: Scenario

- Has the crowd made a good prediction?

- Composition of crowd:
  - 30% EXPERTS.
  - 70% NON-EXPERTS.

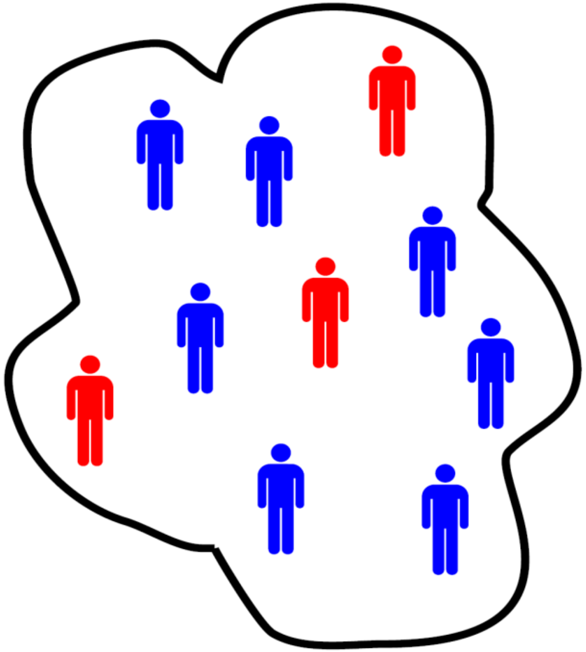
- and their level of expertise:
  - P(correct predict|expert) = p_e
  - P(correct predict|non-expert) = p_{ne}



Wisdom of the Crowd: Scenario

- Let $p_e = 0.8$ and $p_{ne} = 0.5$

- For a random person from the crowd
- P(correct predict|individual) = $0.3\, p_e + 0.7 p_{ne} = 0.59$

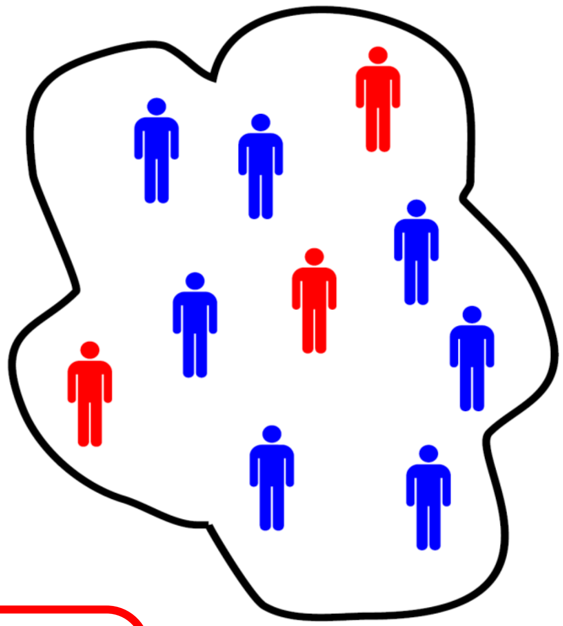


Wisdom of the Crowd: Scenario

- Let $p_e = 0.8$ and $p_{ne} = 0.5$
- For a random person from the crowd
- P(correct predict|individual) = $p_i = 0.59$

- **If crowd contains 50 *independent* people:**
- P(correct predict|crowd)

$$= \sum_{k=26}^{50} \binom{50}{k} {p_i}^k \cdot (1 - p_i)^{50-k} = 0.8745$$



- This crowd has made a prediction with probability .875 of being correct which is $> p_i$.
- **It is wiser than each of the experts!**

- Ensemble of predictors often outperform individual predictors
- Consider a majority voting of 5 independent classifiers in a binary classification problem.
- Each predictor, the error probability is 0.3
- Probability of three or more predictors yielding a wrong result (i.e., the majority misclassifies) is very low:

$$\sum_{i=3}^{5} \binom{5}{i} 0.3^{i} \cdot 0.7^{5-i} = 0.08748$$

- Substantial reduction in error rate!
- In reality, classifiers are rarely independent of each other

But ...

- **Why didn't I just asked a bunch of experts??**

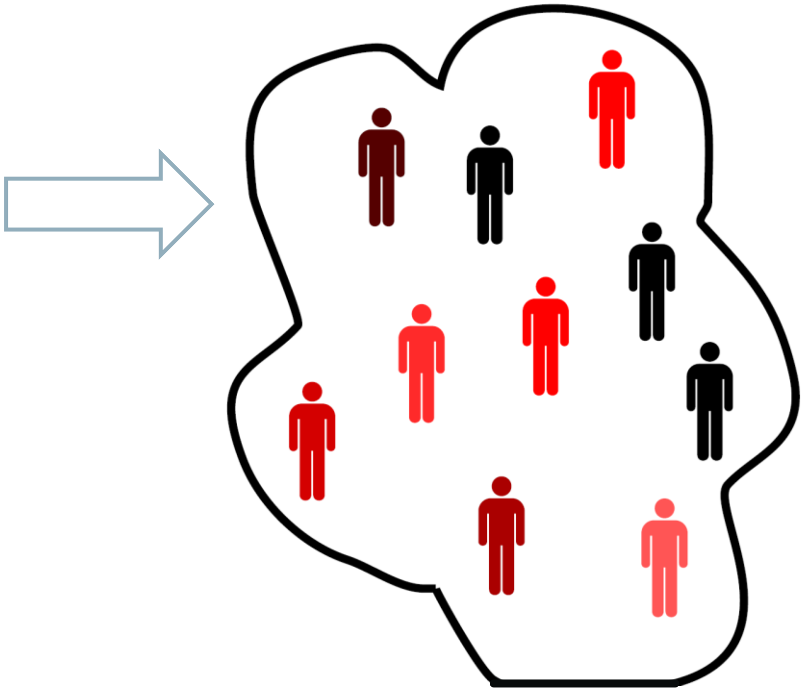
- Large enough crowd
  - => high probability that a sufficient number of experts will be in crowd (for any question).

- Random selection
  - => don't make a biased choice in experts.

- For some questions it may be hard to identify a diverse set of experts

- Given a **random question** expect each **person** to have a **different level** of **expertise**.

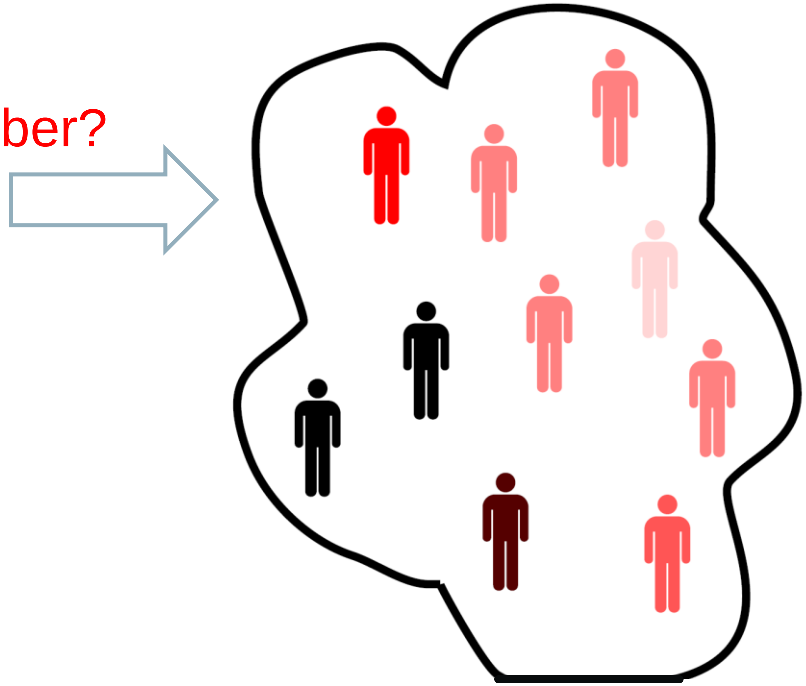
- Will it rain tomorrow?
  - redness proportional to expertise



For a random crowd

- Given a **random question** expect each **person** to have a **different level** of **expertise**.

- Will the world go down in December?
  - redness proportional to expertise



What makes a crowd wise?

According to *James Surowiecki* there are four elements required to form a wise crowd:

- **Diversity of opinion.** People in crowd should have a range of experiences, education and opinions. (Encourages independent predictions)
- **Independence.** Prediction by person in crowd is not influenced by other people in the crowd.
- **Decentralization.** People have specializations and local knowledge.
- **Aggregation.** There is a mechanism for aggregating all predictions into one single prediction.

The crowd must be careful

In the analysis of the crowd it is implicitly assumed:

- each person is not concerned with the opinions of others, no-one is copying anyone else in the crowd.

In the analysis of the crowd we implicitly assumed:

- The non-experts will predict a **completely random wrong answer** - these will cancel each other out (to some degree).

However, there may be a systematic and consistent bias in the non-experts' predictions.

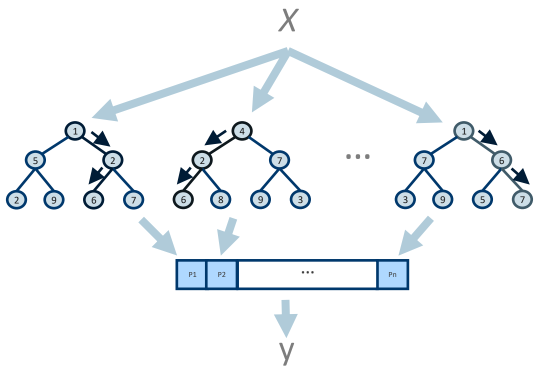
... Back to Ensemble Models

We will exploit **Wisdom of crowd** ideas for specific tasks by:

- combining (classifier) predictions
- aim to combine independent and diverse predictors (classifiers).

We can also use labeled training data

- to identify the expert classifiers in the pool;
- to identify complementary classifiers;
- to indicate how to best combine them.



Why Do Ensemble Methods Work?

Statistical reason:

- Able to average many good models
- Reduces the influence of bad models

Computational reason:

- Able to explore the model space efficiently

Representational reason:

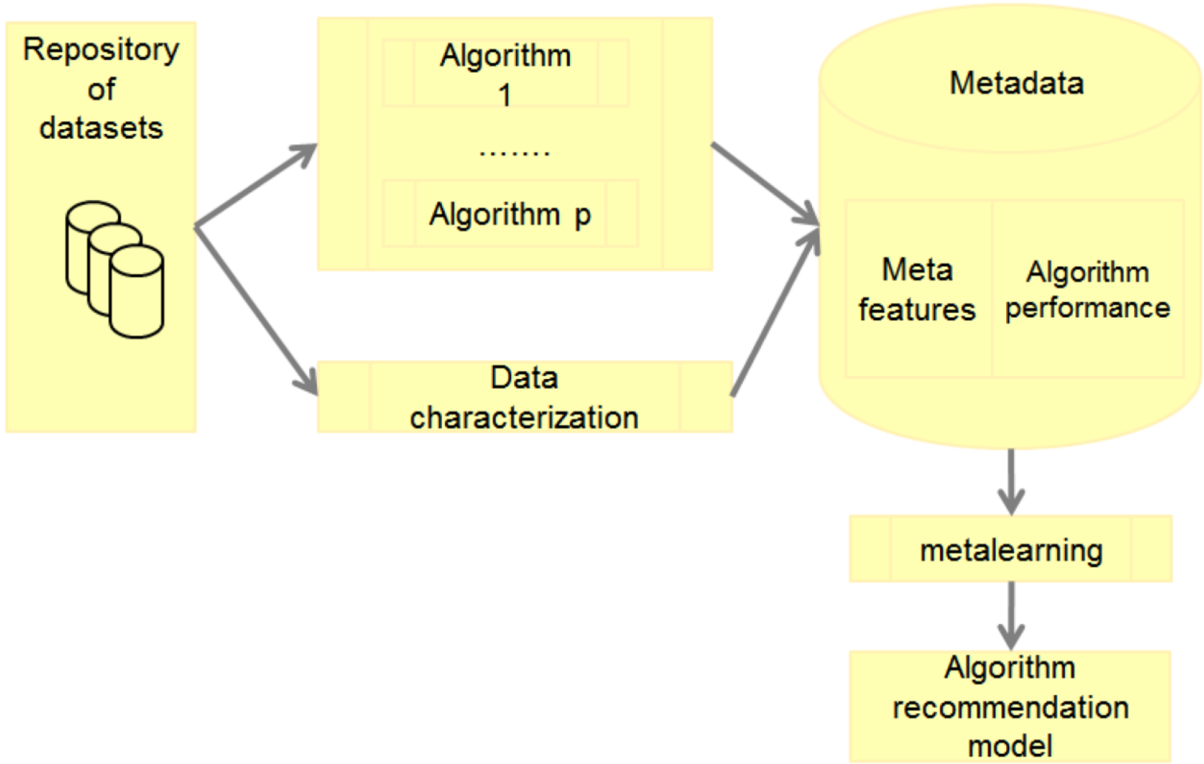
- Reduce the bias of a learning algorithm by extending its model space

Remember?

- Bias = model error + algorithmic error
  - **Model error**: the error we get by selecting a model
  - **Algorithmic error**: by selecting the algorithm itself and the parameters of the algorithm

- Base-Learning: Fixed Bias / User parameterized
- Meta-Learning: Dynamic bias selection using meta-knowledge
- Meta-Knowledge: Knowledge achieved during the learning process

Ensemble Learning for Algorithm Recommendation



Combining base-learners: Categories

Philosophy	Technique
Bagging, Boosting	Variation in data
Stacking	Variation among learners (multi-expert)
Cascading, Delegating	Variation among learners (multi-stage)
Arbitrating	Variation among learners (refereed)
Meta decision trees	Variation in data and among learners

Bagging and Boosting

- Best-known techniques
- Based on selection of multiple data sub sets
- Meta model is created by combining the base models

- Advantages:
  - Reduces overfitting
  - Most effective when the base learner is highly sensitive to data
  - Typically increases accuracy

- Disadvantages:
- Interpretability of interpretable base learners is lost

Bagging :

- Select N independent samples of the Training Data
- Learn one model on each of the samples => $h_1, \ldots, h_N$

- Classification: Use the class most predicted by all classifiers
- Regression: Use the mean of all predictions

Boosting:

- Tries to learn a weighting for the models
- Later base learners focus more on the examples that previous base learners misclassified
- There is no single “best” boosting method

One boosting method after Schapire

Training :

- Create $c1$: base learner on a sample $t1$ of the data
- Create $t2$: sample which is 50% misclassified by $c1$
- Create $c2$: base learner on the sample $t2$
- Create $t3$: subset of the data where $c1$ predicts differently than $c2$
- Create $c3$: base learner on the sample $t3$

Classification :

- Classify with $c1$ and $c2$
- If unequal, use $c3$ as final classification

Stacking and Cascade Generalization

Stacking

- In Bagging and Boosting: we used always the same base learner
- Stacking exploits differences among base learners

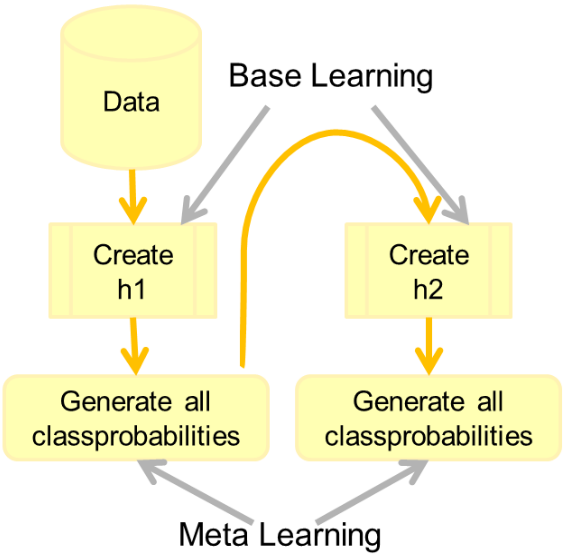
- Two levels of learning
  1. Base learners are trained, each on the whole data set
  2. Meta learners are created on meta data (e.g. predicted class) obtained in level 1

- Two levels of classifying
  1. Base learner are used on data point
  2. Meta learners are applied on base learner predictions

Stacking: Base learners are used in parallel

Cascade Generalization

- Base learners are used in a sequence with ”partial” meta-learners
- Knowledge from previous classifiers can be used in later ones
- After each base learner has been trained, the data set is adjusted using the new information



For classification :

- Only the last model is used, which incorporates the knowledge from previous models (all base methods are used)

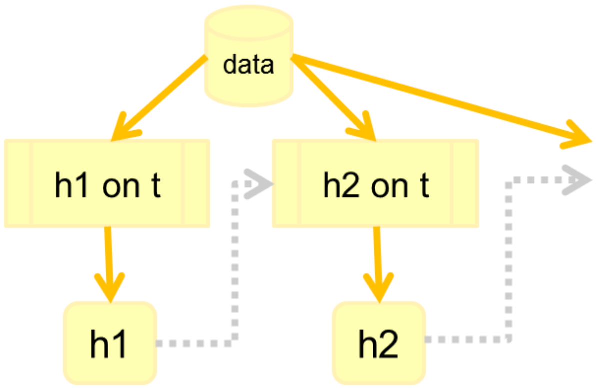
Cascading and Delegating

Cascading and Delegating

- Until now: all base classifiers are used for classification
- Here: Multistage classifiers, not all are required for classification
- Main advantage: faster classification

Cascading

- Multilearner version of boosting
- Uses learned confidence of previous models
- Train base learner h_i using knowledge from previous base learner...
- ...on data, which was most probably misclassified by previous learners



- **Classification:** go through all base models, stop and use as classification if the model has confidence greater than epsilon

- Cascading: all instances are used in each step

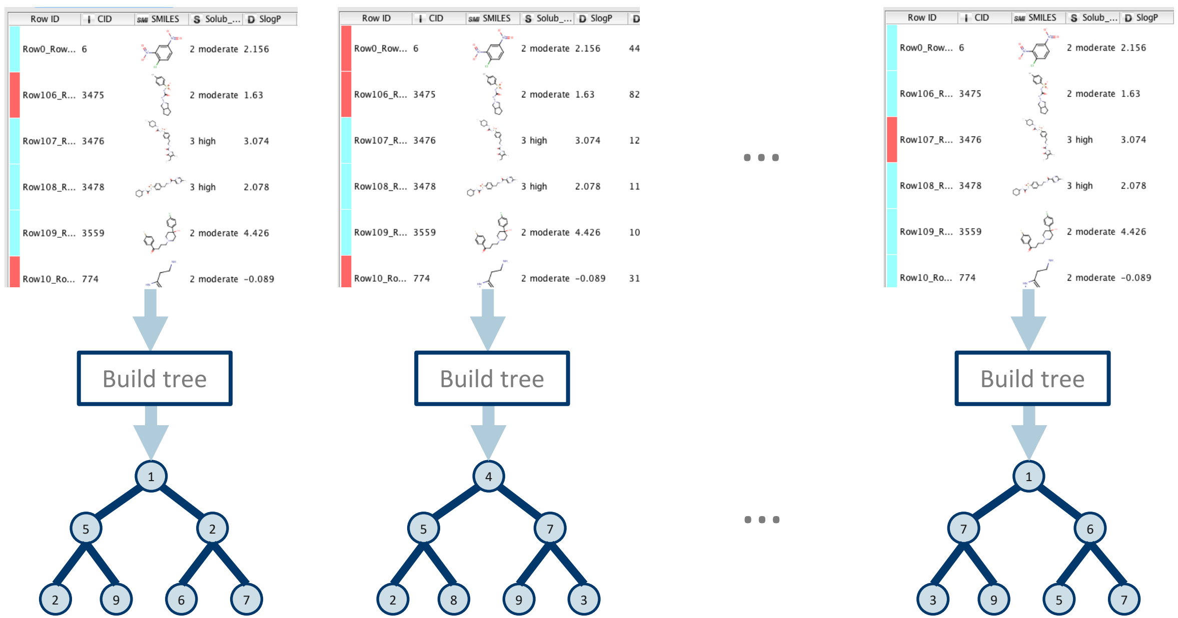
- **Delegating**: only instances below confidence threshold are processed in the next step

- Idea:
  - Use everything and test for which data points you are good enough
  - Pass the remaining work to someone else.
  - If there is no someone else, ... guess
- Advantages:
  - Still understandable (no model combination)
  - Improved efficiency, due to the decreasing number of examples.

Tree Ensembles and Random Forest

Bagging - Idea

- Bagging ≡ Bootstrap AGGregatING
- For each tree / model a training set is generated by sampling uniformly with replacement from the standard training set



Example for Bagging

Full training set

RowID	x_1	x_2	y
Row_1	2	6	Class 1
Row_2	4	1	Class 2
Row_3	9	3	Class 2
Row_4	2	7	Class 1
Row_5	8	1	Class 2
Row_6	2	6	Class 1
Row_7	5	2	Class 2

Sampled training set

RowID	x_1	x_2	y
Row_3	9	3	Class 2
Row_6	2	6	Class 1
Row_1	2	6	Class 1
Row_3	9	3	Class 2
Row_5	8	1	Class 2
Row_6	2	6	Class 1
Row_1	2	6	Class 1

Bagging - Idea

Why sampling with replacement?

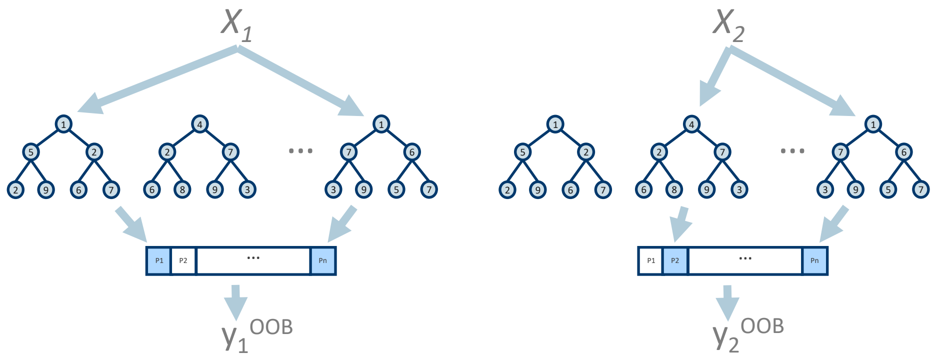
→ So that a sample approximates the distribution of the population

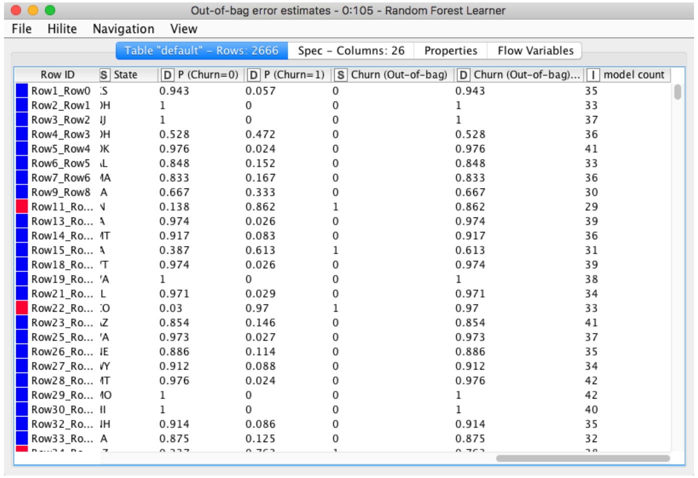
- Frequent values are represented more
- Less frequent values are represented less

Ultimately leads to the model with smaller variance and smaller bias

An Extra Benefit of Bagging: Out of Bag Estimation

- Able to evaluate the model using the training data
- Apply trees to samples that haven’t been used for training





Out-of-bag error estimates - 0:105 - Random Forest Learner

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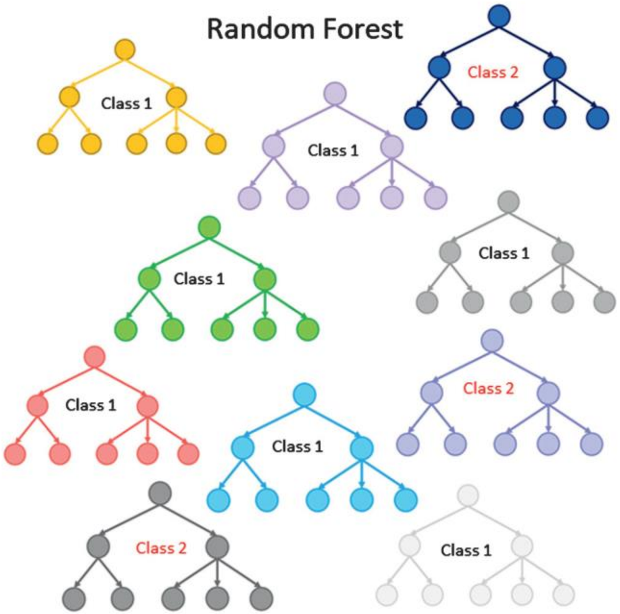
Table "default" – Rows: 2666 | Spec – Columns: 26 | Properties | Flow Variables

Row ID	S State	D P (Churn=0)	D P (Churn=1)	S Churn (Out-of-bag)	D Churn (Out-of-bag)...	I model count
Row1_Row0	:S	0.943	0.057	0	0.943	35
Row2_Row1	)H	1	0	0	1	33
Row3_Row2	IJ	1	0	0	1	37
Row4_Row3	)H	0.528	0.472	0	0.528	36
Row5_Row4	)K	0.976	0.024	0	0.976	41
Row6_Row5	\L	0.848	0.152	0	0.848	33
Row7_Row6	ΜA	0.833	0.167	0	0.833	36
Row9_Row8	A	0.667	0.333	0	0.667	30
Row11_Ro...	|	0.138	0.862	1	0.862	29
Row13_Ro...	\	0.974	0.026	0	0.974	39
Row14_Ro...	IT	0.917	0.083	0	0.917	36
Row15_Ro...	\	0.387	0.613	1	0.613	31
Row18_Ro...	'T	0.974	0.026	0	0.974	39
Row19_Ro...	'A	1	0	0	1	38
Row21_Ro...	L	0.971	0.029	0	0.971	34
Row22_Ro...	:O	0.03	0.97	1	0.97	33
Row23_Ro...	\Z	0.854	0.146	0	0.854	41
Row25_Ro...	'A	0.973	0.027	0	0.973	37
Row26_Ro...	IE	0.886	0.114	0	0.886	35
Row27_Ro...	VY	0.912	0.088	0	0.912	34
Row28_Ro...	IT	0.976	0.024	0	0.976	42
Row29_Ro...	IO	1	0	0	1	42
Row30_Ro...	II	1	0	0	1	40
Row32_Ro...	IH	0.914	0.086	0	0.914	35
Row33_Ro...	A	0.875	0.125	0	0.875	32

- Bag of decision trees, with an extra element of randomization
- Each node in the decision tree only "sees" a subset of the input features → ***Random Subspace Selection***
- typically $\sqrt{n}$ to pick from
- Random forests tend to be very robust w.r.t. overfitting



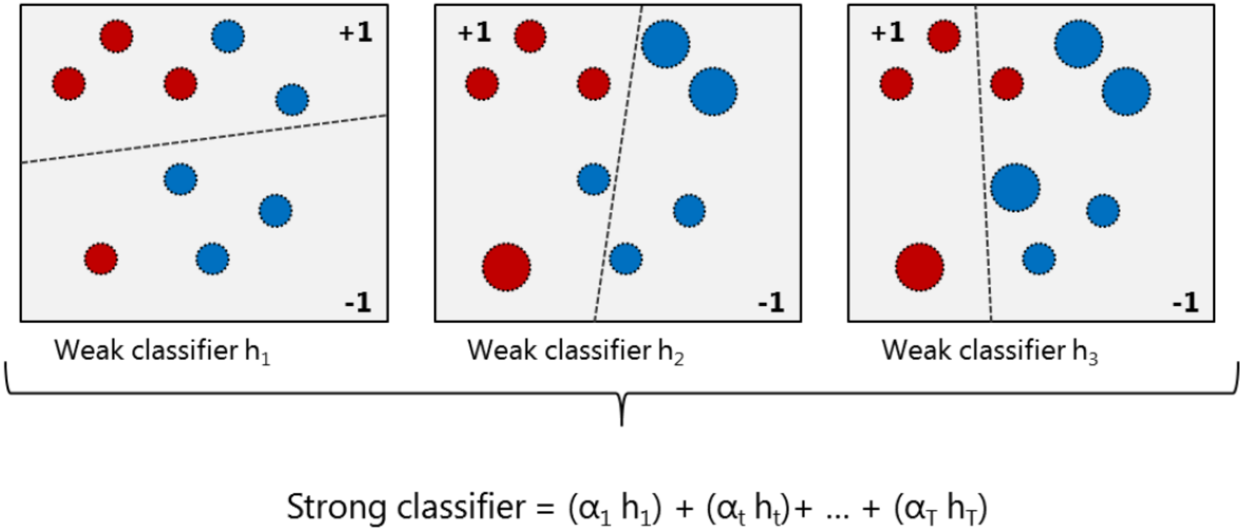
AdaBoost

AdaBoost

- Freund & Schapire (1995)

- AB is a linear classification algorithm
- AB has good generalization properties (Avoids overfitting as long as the training data is not too noisy)
- AB is a feature selector

AdaBoost



- AdaBoost classifier: $\sum_{t=1}^{T}(\alpha_t h_t(\boldsymbol{x}))$
- Where a weak classifier $h_t(\boldsymbol{x})$ is weighted by α_t for steps up to T
- Misclassified data points are weighted more in subsequent steps
- Classification result: $H(\boldsymbol{x}) = sign(\sum_{t=1}^{T} \alpha_t h_t(\boldsymbol{x}))$

AdaBoost: Terminology

- Strong Classifier: $\sum_{t=1}^{T}(\alpha_t h_t(\boldsymbol{x}))$
- Where $h_t(\boldsymbol{x})$ is a base classifier weighted by α_t
- Classification result: $\mathrm{H}(\boldsymbol{x}) = sgn(\sum_{t=1}^{T}(\alpha_t h_t(\boldsymbol{x})))$

AdaBoost

- Initially, all data points are given the same weight $w_{i,1} = 1/n$.
- At step t, the classifier weight α_t is calculated as

$$\alpha_t = \frac{1}{2}\ln\left(\frac{1-e_t}{1+e_t}\right)$$

- Where e_t is given by

$$e_t = \frac{\sum_{i=1}^{n} w_{i,t} y_i h_t(\boldsymbol{x}_i)}{\sum_{i=1}^{n} w_{i,t}}$$

- Weights w's are updated as

$$w_{i,t+1} = \frac{w_{i,t}\exp(-\alpha_t y_i h_t(\boldsymbol{x}_i))}{\sum_{j=1}^{n} w_{j,t}\exp(-\alpha_t y_j h_t(\boldsymbol{x}_j))}$$

Adaboost pseudo-code Overview

Algorithm Ada Boost

Initialize weight of x_i with $D_0(i) = \frac{1}{m}$

for $t = 1, \ldots, T$: **do**

1. h_t = "Base-Learner"

   Calculate error $\epsilon_t = \sum_{i=1}^{m} D_t(i)\delta_{(y_i, h_t(x_i))}$

3. Calculate weight of learner $\alpha_t = \log \frac{1-\epsilon_t}{\epsilon_t}$
4. Update the weights $D_t(i)$ of all x_i

end for

Resulting classificator

$H(x) = sgn\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$

Adaboost pseudo-code Overview

Algorithm Base learner

Train a set H of many many base learners h on the data

Return the one h with the lowest weighted classification error

$h = \arg\min_{h_j \in H} \epsilon = \arg\min_{h_j \in H} \left(\sum_{i=1}^{m} D(i) \delta_{(y_i, h_t(x_i))} \right)$

Make sure $\epsilon < 0.5$

Algorithm Ada Boost

Initialize weight of x_i with $D_0(i) = \frac{1}{m}$

for $t = 1, ..., T$: **do**

1. h_t = "Base-Learner"
   Calculate error $\epsilon_t = \sum_{i=1}^{m} D_t(i)\delta_{(y_i, h_t(x_i))}$
3. Calculate weight of learner $\alpha_t = \log \frac{1-\epsilon_t}{\epsilon_t}$
4. Update the weights $D_t(i)$ of all x_i

end for

Resulting classificator

$H(x) = sgn\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$

Update of weights of Training Samples

- Update weights and normalize them:

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \exp(-\alpha_t \, y_i \, h_t(x_i))$$

$$Z_t(i) = \sum_{i=0}^{m} D_t(i) \exp(-\alpha_t \, y_i \, h_t(x_i))$$

- Weight of correct classified examples is decreased
- Weight of incorrect classified examples is increased

AdaBoost: Why does it work?

- Weighting the base learners "Upper-Bound Theorem"
- Primary goal is to minimize

$$\epsilon_{tr}(H) = \frac{1}{m}\,|\{i\colon H(x_i \neq y_i)\}|$$

- Global error is bounded by

$$\epsilon_{tr}(H) \leq Z_t \qquad t = 1, \ldots, T$$

$$Z_t = \sum_{i=0}^{m} D_t(i)\exp(-\alpha_t\ y_i\, h_t(x_i))$$

AdaBoost: Why does it work?

- Weighting the base learners

- That's why

- Minimizing $Z_t = \sum_{i=0}^{m} D_t(i) \exp(-\alpha_t \; y_i \; h_t(x_i))$ results in a minimization of the global error

- Upper-Bound can be minimized by ...
  1. Choosing the optimal hypothesis h_t ...
  2. ... with an optimal weight α_t

- Minimizing Z_t results in $\alpha_t = \log \frac{1 - \epsilon_t}{\epsilon_t}$

Advantages

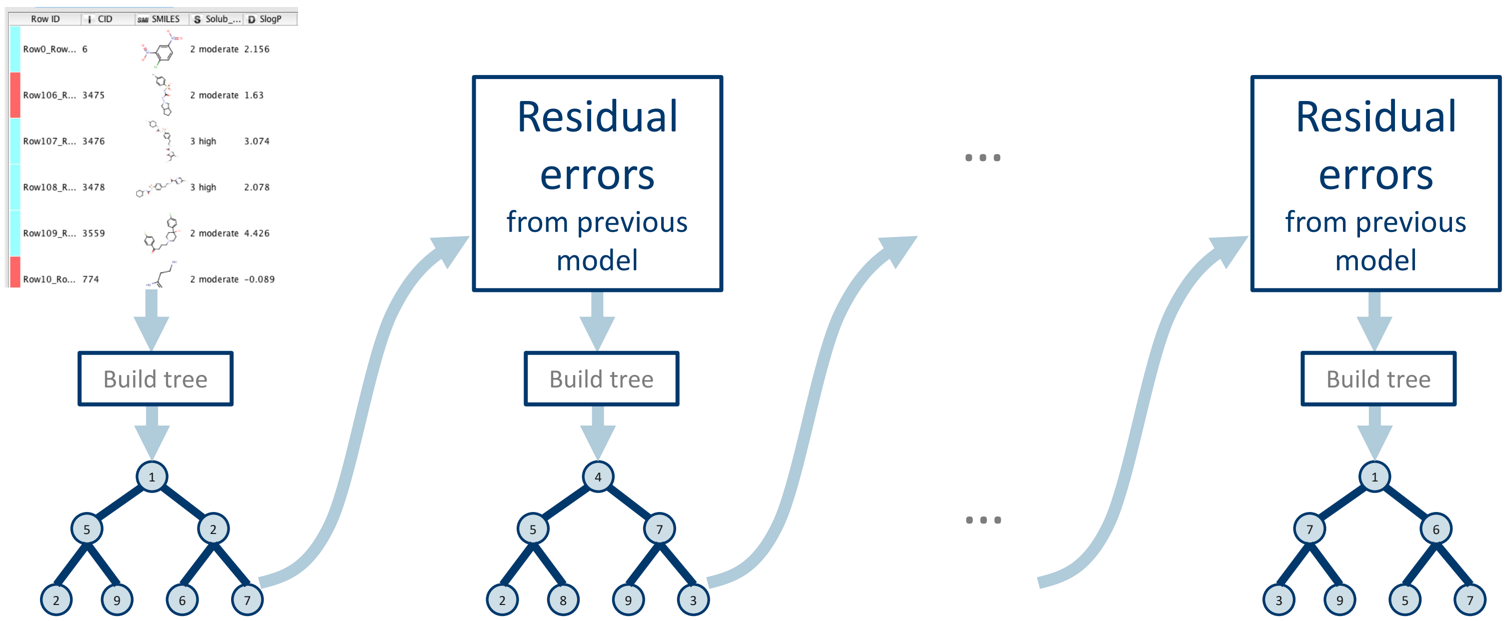
- Very simple to implement
- Feature selection on very large features spaces
- Fairly good generalization

Disadvantages

- Can overfit in presence of noise
- Unclear which weak-learning algorithm fits best for a given problem

Gradient Boosted Trees

– Starts with a single tree built from the data
– Fits a tree to residual errors from the previous model to refine the model sequentially



A shallow tree (depth 4 or less) is built at each step

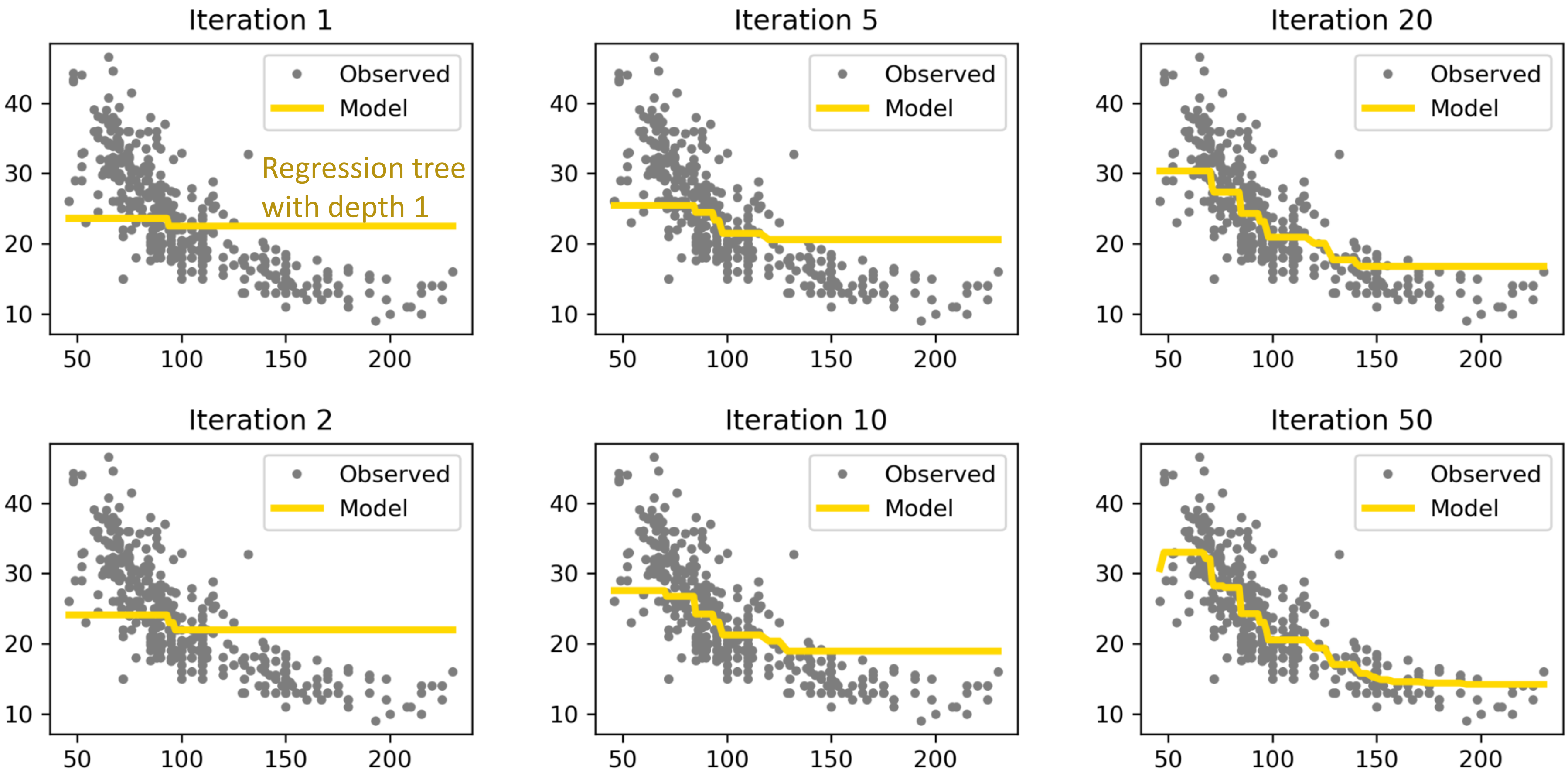
- To fit residual errors from the previous step
- Resulting in a tree $h_m(x)$

The resulting tree is added to the latest model to update

$$F_m(x) = F_{m-1}(x) + \gamma_m h_m(x)$$

- Where $F_{m-1}(x)$ is the model from the previous step
- The weight γ_m is chosen to minimize the loss function
  - Loss function: quantifies the difference between model predictions and data

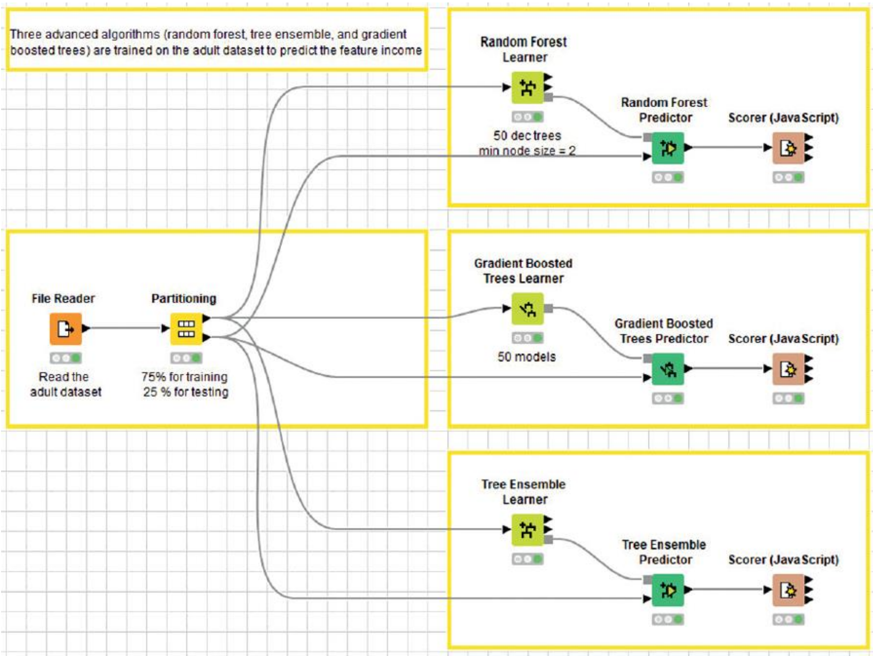
Gradient Boosted Trees Example – Regression



- Can be used for classification and regression
- Large number of iterations – prone to overfitting
  - ~100 iterations are sufficient
- Can introduce randomness in choice of data subsets (“stochastic gradient boosting”) and choice of input features

Practical Examples with KNIME Analytics Platform

Tree Ensemble, Random Forest, and Gradient Boosted Tree



– Tree Ensemble, Random Forest, and Gradient Boosted Tree applied to the adult dataset

For any questions please contact: email@email.com