Trees, forests and boosting

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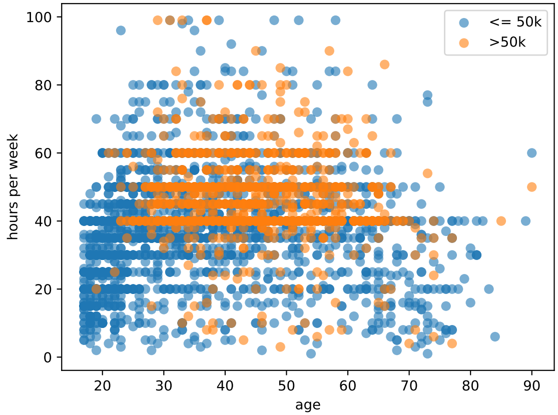
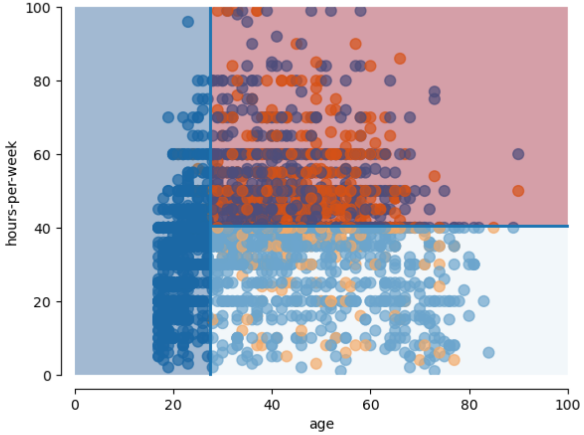
Motivation: nonlinear data



How would logistic regression perform on this dataset?

A potential classifier?



Outline

Trees

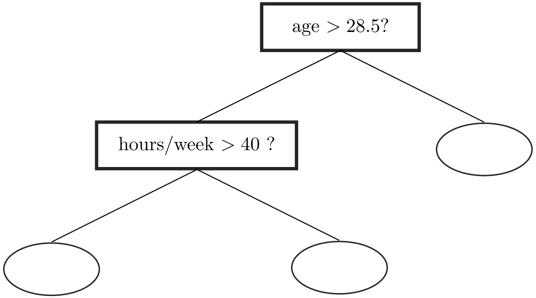
Ensemble methods: bagging and random forests

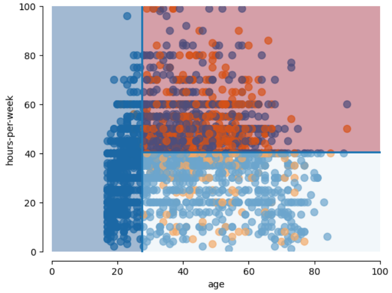
Adaboost

What is a tree?

Trees partition the whole space into rectangular cells:

- A node has exactly either zero or two children
- Each split (= question) defines two child nodes, the left and right child nodes
- A node with zero children is called a leaf
- We pass from a node to the left or right children by answering a question of type “Is $x_j \geq \alpha$?” for some coordinate j and threshold α





CART: Classification and Regression Trees

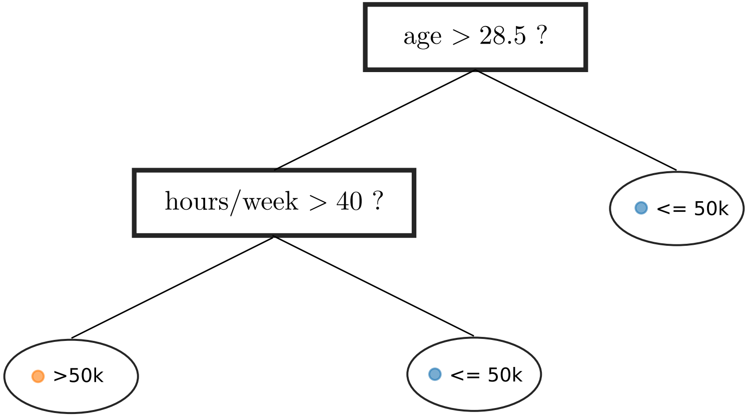
CART = an algorithm to build a tree out of a training set $\{(\mathbf{x}_1, y_1)\}_{i=1}^n$

- Partition the space, use **constant prediction** over leaves
- Objective : split the space to fit training data well
- Adapted to two settings:
  - y_i qualitative with K modalities ($y_i \in \{1, \dots, K\}$): classification tree (`DecisionTreeClassifier`)
  - y_i quantitative, $y_i \in \mathbb{R}$: regression tree (`DecisionTreeRegressor`)

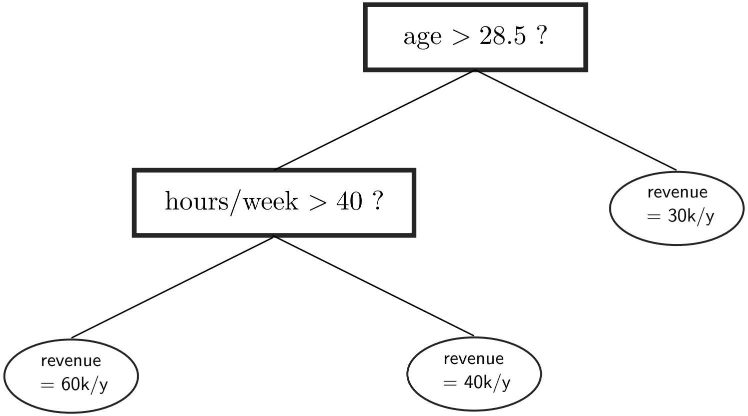
Pros of trees:

Easy to interpret
Nonparametric model: no assumption on the data distribution.

Example of classification tree

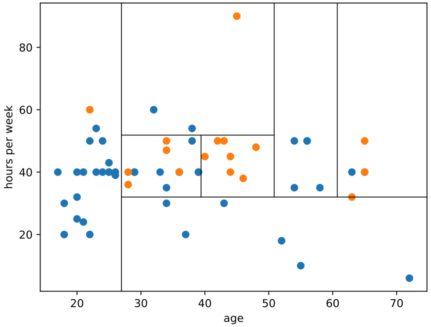


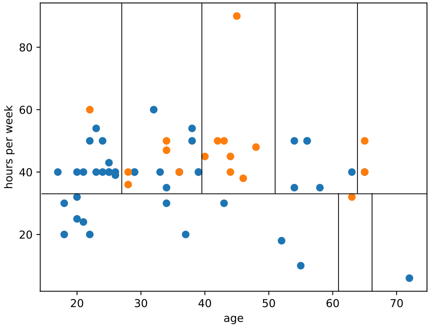
Example of regression tree



Building a tree = partitioning the space

Building a tree aims at finding a partition of the input space into a set of rectangles that separates blue points from orange points





How to classify new samples?

Classification $\rightarrow$ A simple majority vote to predict class probabilities

- select $C(\mathbf{x})$ the cell containing $\mathbf{x}$
- predict majority class inside $C(\mathbf{x})$:

$$\hat{y}(\mathbf{x}) = \begin{cases} +1 \text{ if } \sum_{i:\mathbf{x}_i \in C(\mathbf{x})} \mathbb{1}_{y_i=1} > \sum_{\mathbf{x}_i \in C(\mathbf{x})} \mathbb{1}_{y_i=-1} \\ -1 \text{ otherwise.} \end{cases}$$

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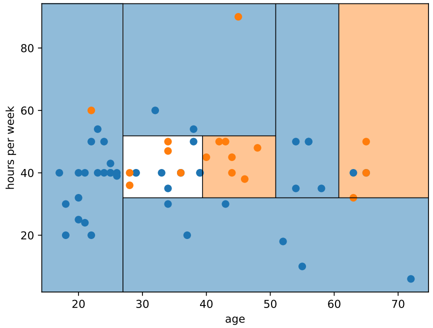

How to classify new samples?

Regression $\rightarrow$ A simple average in each leaf to predict a value (in each region the predicted value is constant)

- select $C(\mathbf{x})$ the cell containing $\mathbf{x}$
- predict mean of target of training points inside $C(\mathbf{x})$:

$$\hat{y}(\mathbf{x}) = \frac{\sum_{i:\mathbf{x}_i \in C(\mathbf{x})} y_i}{|C(\mathbf{x})|}$$

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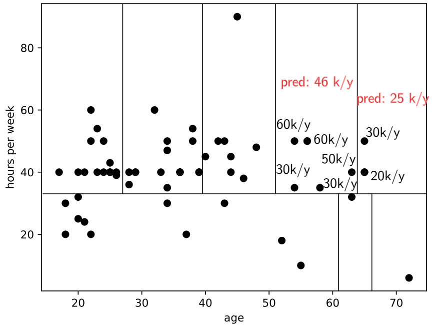
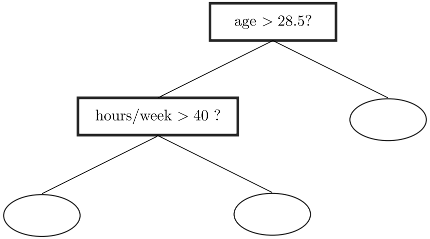
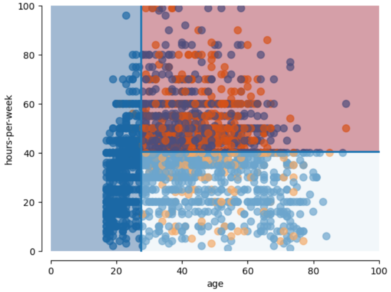


An algorithm to build a tree: CART

- The CART algorithm builds the partition recursively (split after split)
- At each step, the method splits an existing cell into two regions according to a split variable (j in x_j) and a threshold point (t): the question is: "$x_j > t$?"





This is the best tree found by `scikit-learn`. How were the splits found?

Penguin time

`01-grow_a_tree.ipynb`

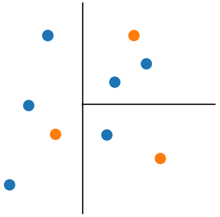
How to build the optimal tree? Recap after notebook

Iteratively (split after split)

- We want to split a node N into a left child node N_L and a right child node N_R
- The children depend on the cut = the (feature, threshold) pair denoted by (j, t)

$$N_L(j,t) = \{x \in N : x_j < t\} \quad N_R(j,t) = \{x \in N : x_j \geq t\}.$$

- a measure of cell "purity" is used; take split that maximizes gain in purity
- for all current leaves N, all possible feature/threshold pairs, compute purity gain if we used this split. Pick split with maximal gain.



How many splits to try?

How to split?

Heuristic: greedy algorithm

At each new cut, choose a split so that the two new regions are as homogeneous as possible

Homogeneous nodes

For classification: class proportions should be as close as possible to $(0, 1)$ or $(1, 0)$
For regression: labels should be very concentrated around their mean in a node/cell

How to quantify homogeneity?

Gini index, Entropy (classification)
Variance (regression)

Regression: split measure

- Impurity is the variance of the target y inside the node N:

$$V(N) = \sum_{i:\mathbf{x}_i \in N} (y_i - \bar{y}_N)^2 \quad \bar{y}_N = \frac{1}{|N|} \sum_{i:\mathbf{x}_i \in N} y_i \quad |N| = |\{i : \mathbf{x}_i \in N\}|$$

- Information gain is given by

$$IG(j,t) = V(N) - \frac{|N_L(j,t)|}{|N|} V(N_L(j,t)) - \frac{|N_R(j,t)|}{|N|} V(N_R(j,t))$$

Regression: Finding the best split

Maximize the information gain:

$$\max_{j,t}\left[\min_{\bar{y}_L}\sum_{i:\mathbf{x}_i\in N_L(j,t)}(y_i-\bar{y}_L)^2+\min_{\bar{y}_R}\sum_{i:\mathbf{x}_i\in N_R(j,t)}(y_i-\bar{y}_R)^2\right]$$

For any (j,t) the inner minimization is solved by

$$\bar{y}_L=\frac{\sum_{i:\mathbf{x}_i\in N_L(j,t)}y_i}{|N_L(j,t)|};\quad \bar{y}_R=\frac{\sum_{i:\mathbf{x}_i\in N_R(j,t)}y_i}{|N_R(j,t)|}$$

For each j, finding t can be done quickly $\rightarrow$ determination of the best (j,t) is feasible!

Classification: split measure

Given the classes distribution inside cell N, $p_N = (p_{N,1}, \dots, p_{N,K})$, with $p_{N,k} = \frac{|\{i: \mathbf{x}_i \in N,\ y_i = k|\}}{|N|}$
(if two classes only: $p_N = (p, 1-p)$)

- Two possible impurity measures:

$$G(N) = G(p_N) = \sum_{k=1}^{K} p_{N,k}(1 - p_{N,k}) \quad \text{Gini index}$$

$$H(N) = H(p_N) = -\sum_{k=1}^{K} p_{N,k} \log_2(p_{N,k}) \quad \text{Entropy}$$

  basically: maximal when $P_N = (1/K, \dots, 1/K)$ (cell is not pure!)

- Information gain is given by ($I = G$ or $I = H$):

$$IG(j,t) = I(N) - \frac{|N_L(j,t)|}{|N|} I(N_L(j,t)) - \frac{|N_R(j,t)|}{|N|} I(N_R(j,t))$$

- best split: enumerate all possible splits...

CART algorithm

CART builds the partition iteratively. At each iteration:

- Find the best (node, feature, threshold) triplet (N, j, t) that maximizes $IG(N, j, t)$
- Create the two new children of the leaf
- Stop if some stopping criterion is met
- Otherwise continue

Stopping criterion?

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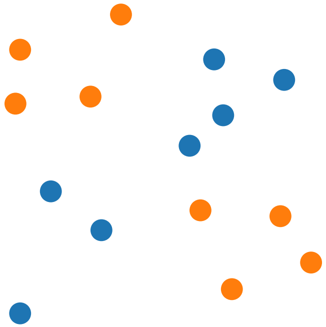
Stopping criterion?

- Maximum depth of the tree
- All leaves have less then a chosen number of samples
- Impurity in all leafs is small enough
- Testing error is increasing
- see parameters in `sklearn.tree.DecisionTreeClassifier`

Post processing: pruning

What should we do here?



Final remarks on trees

- ☺ leads to nice interpretable results
- ☺ insensitive to datascaling (no preprocessing needed!)
- ☹ usually overfit
- ☹ usually not the best for prediction
- ☺ but the basis of more powerful techniques: random forests, boosting (ensemble methods)

Outline

Trees

Ensemble methods: bagging and random forests

Adaboost

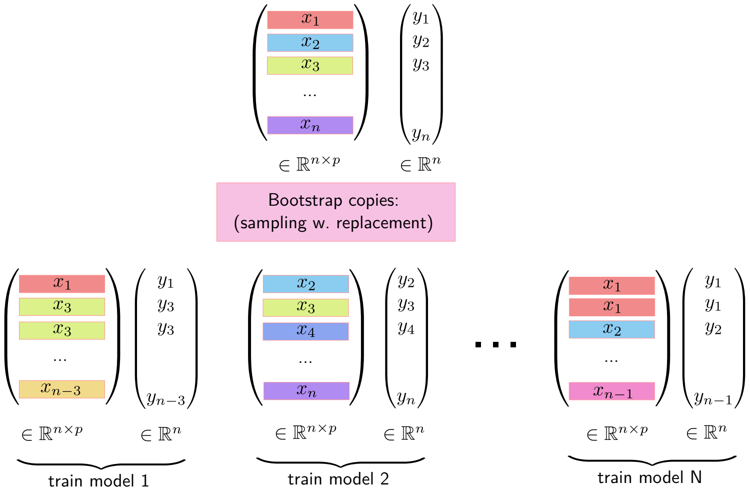
Ensemble methods

Basic idea

Aggregate multiple models or “weak learners” trained for the same problem. Weak models combined rightly give accurate model

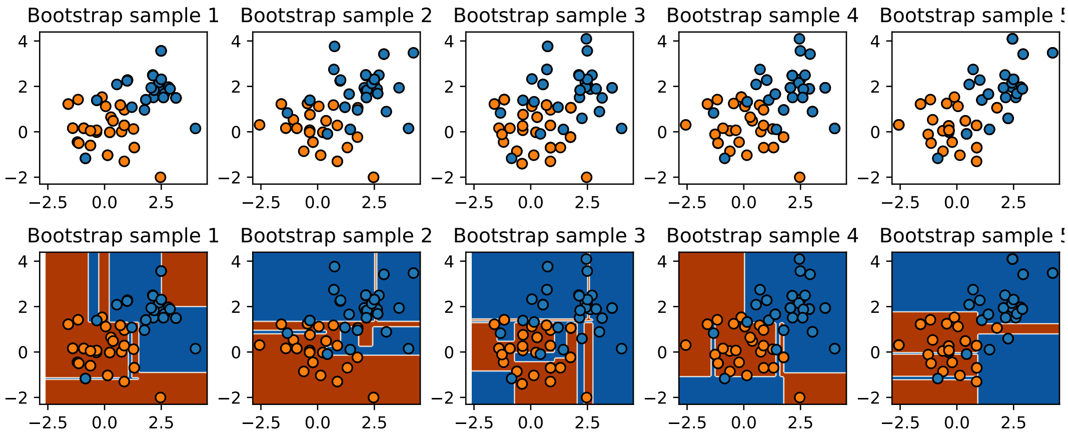
- Bagging: multiple weak models of the same type that learn from different data sets in parallel and are combined to decrease the variance on the prediction
- Boosting: weak models learn sequentially and adaptively to improve model predictions of a learning algorithm.

Bagging: training models on bootstrap samples

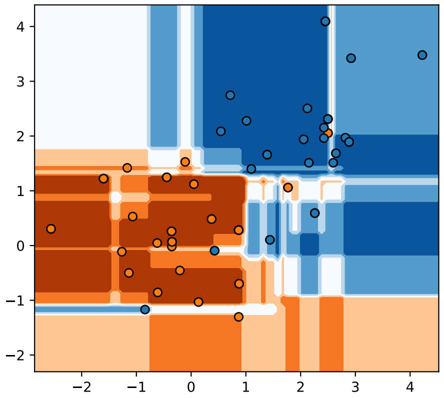

$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \dots \\ x_n \end{pmatrix} \in \mathbb{R}^{n \times p}$
$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \\ y_n \end{pmatrix} \in \mathbb{R}^{n}$
Bootstrap copies:
(sampling w. replacement)
$\begin{pmatrix} x_1 \\ x_3 \\ x_3 \\ \dots \\ x_{n-3} \end{pmatrix} \in \mathbb{R}^{n \times p}$
$\begin{pmatrix} y_1 \\ y_3 \\ y_3 \\ \\ y_{n-3} \end{pmatrix} \in \mathbb{R}^{n}$
train model 1
$\begin{pmatrix} x_2 \\ x_3 \\ x_4 \\ \dots \\ x_n \end{pmatrix} \in \mathbb{R}^{n \times p}$
$\begin{pmatrix} y_2 \\ y_3 \\ y_4 \\ \\ y_n \end{pmatrix} \in \mathbb{R}^{n}$
train model 2
$\dots$
$\begin{pmatrix} x_1 \\ x_1 \\ x_2 \\ \dots \\ x_{n-1} \end{pmatrix} \in \mathbb{R}^{n \times p}$
$\begin{pmatrix} y_1 \\ y_1 \\ y_2 \\ \\ y_{n-1} \end{pmatrix} \in \mathbb{R}^{n}$
train model N

Final model = aggregation of N models (majority vote or averaging)

Bagging


Bootstrap sample 1
Bootstrap sample 2
Bootstrap sample 3
Bootstrap sample 4
Bootstrap sample 5
Bootstrap sample 1
Bootstrap sample 2
Bootstrap sample 3
Bootstrap sample 4
Bootstrap sample 5
−2.5
0.0
2.5
−2
0
2
4

Bagging: averaging the 5 models



overfits way less than individual models!

A refinement of bagging: Random Forests

- fore more robustness, in bagging we can also subsample **features** for each bootstrap copy
- see `sklearn.ensemble.BaggingClassifier`
- Random forest can subsample features **at each split** (no need for absolute best split) $\hookrightarrow$ weak learners are not treated as black boxes!
- see `sklearn.ensemble.RandomForestClassifier`
- check more ensemble classifiers in the `sklearn.ensemble` submodule

Pros and cons of bagging and RFs?

Pros and cons of RFs

- many models to train
- many models to evaluate for prediction
- model can be trained in parallel (`n_jobs` parameter)
- base models are usually simple/small
- aggregating models gives more expressivity (vs linear models)
- RF is the go to estimator to try on real data: fast to train, easy to tune

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Adaboost

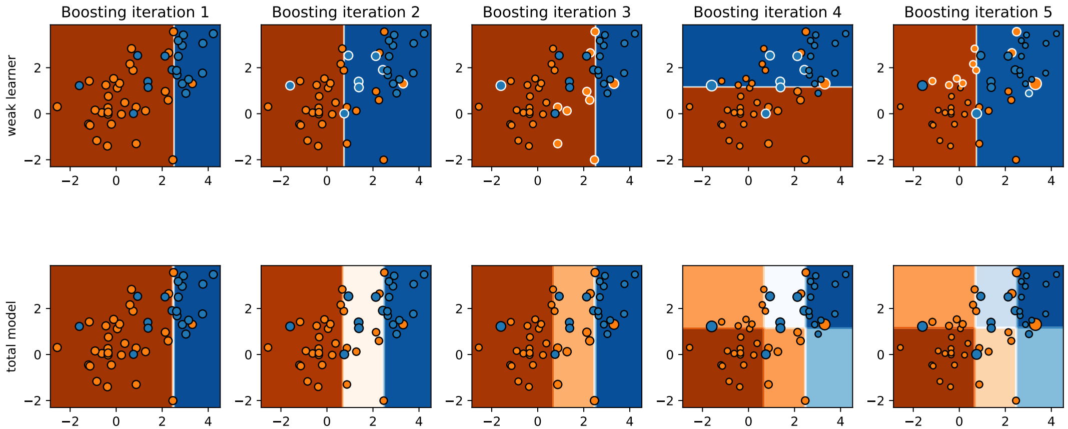
- Freund & Schapire 1995 (Gödel prize 2003)
- setup: binary classification, $y_i \in \{-1, 1\}$
- (very) weak learners $h^{(t)}$ learnt on **weighted** training points
- iteratively give more weight to misclassified points
- Final classifier: $H(\mathbf{x}) = \mathrm{sign}(\sum_{t=1}^{T} \alpha^{(t)} h^{(t)}(\mathbf{x}))$

Adaboost

Algorithm 1 Adaboost

```
Data: $D_n = (\mathbf{x}_i, y_i)_1^n \in (\mathbb{R}^d \times \{-1, 1\})^n$
1  $\mathbf{w}^{(1)} = (1/n, \dots, 1/n) \in \mathbb{R}^n$ // uniform weight initialization
2  for $t = 1, \dots, T$ do
3      $h^{(t)} = \texttt{weak\_learner}(D_n, \mathbf{w}^{(t)})$ // base learner with weighted loss
4      $\gamma^{(t)} = \sum_1^n w_i h^{(t)}(\mathbf{x}_i) y_i$ // edge: 1 - 2 $\times$ error
5      $\alpha^{(t)} = \frac{1}{2} \log\left(\frac{1+\gamma^{(t)}}{1-\gamma^{(t)}}\right)$ // coefficient of $h^{(t)}$
6      for $i = 1, \dots, n$ do
7          if $h^{(t)}(\mathbf{x}_i) \neq y_i$ then
8              $w_i^{(t+1)} = w_i^{(t)} \frac{1}{1-\gamma^{(t)}}$
9          else
10             $w_i^{(t+1)} = w_i^{(t)} \frac{1}{1+\gamma^{(t)}}$
11 Return $f^{(T)} = \sum_{t=1}^T \alpha^{(t)} h^{(t)}$
```

Adaboost



- point size is proportional to weights
- white points are points which were misclassified by the weak learner at previous iteration

Adaboost generalization: gradient boosting

- Handles any loss, beyond binary
- many implementations: Xgboost (apple), lightGBM (MS), CatBoost (yandex)
- supports feature binning (sklearn `HistGradientBoostingClassifier`), robust to preprocessing
- tree-based models outperform deep learning on tabular data: “*Why do tree-based models still outperform deep learning on tabular data?*”
- almost always involved in winning submission on Kaggle