Machine Learning: short introduction (trees and ANN), part 2

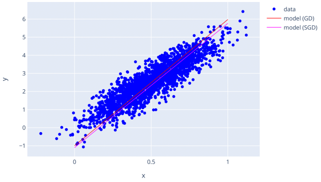
Sergey Korpachev on behalf of Dépôt

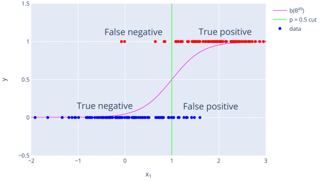
Outline

- Machine learning (ML)
- Data
- Features in ML
- ML pipeline
- Linear model
- Decision tree
- Neural network
- Summary

Decision tree

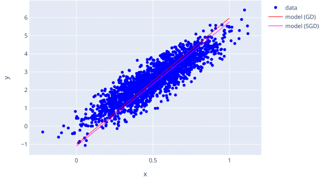
Decision tree — motivation

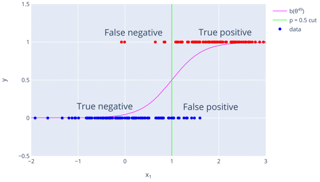


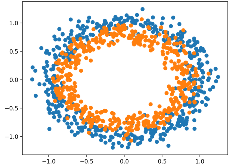


- In the previous part we explored linear models:
  - nicely describe linear correlations
  - fast and easy to train

Decision tree → motivation







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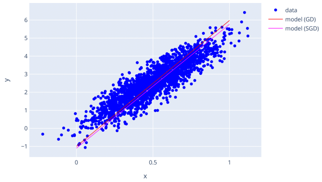
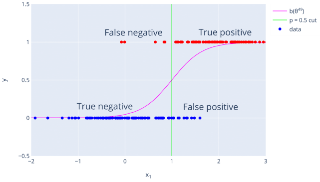
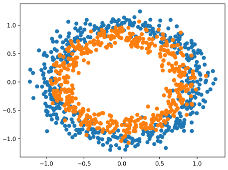
- However, they are poor in modelling non-linearities
- Additional heuristics might be applied (e.g. polynomial features) but are ad-hoc







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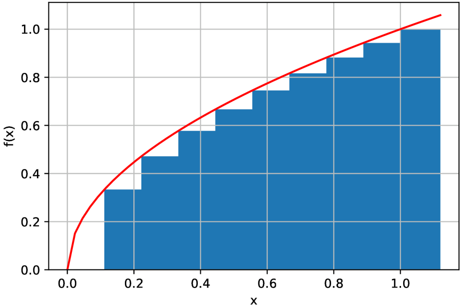
Is there a more general way to describe non-linearities?

Decision tree — motivation

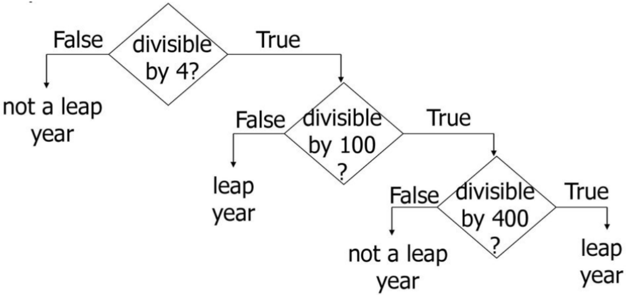
- What is the simplest way to approximate a function?
- Using **piecewise linear function**



$$f(x) = \begin{cases} 0, & x < 0.12 \\ 0.35, & 0.12 \leq x < 0.22 \\ 0.47, & 0.22 \leq x < 0.36 \\ \ldots \end{cases}$$

Decision tree — intuition

- What is the simplest way to categorize things?
- Ask **yes/no questions**



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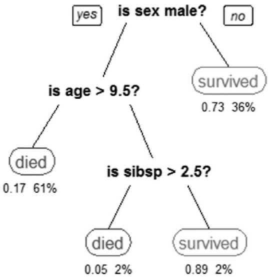

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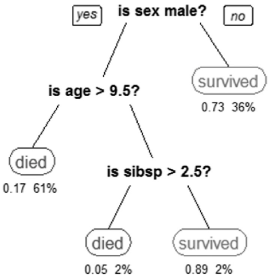


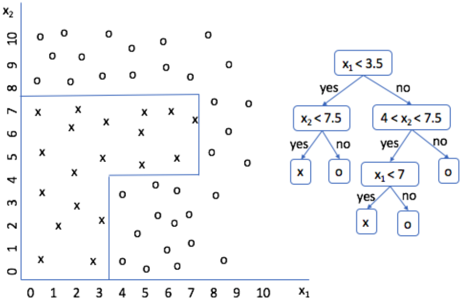
Can we mathematically formulate this?

Decision tree — algorithm

Algorithm 1: Decision tree

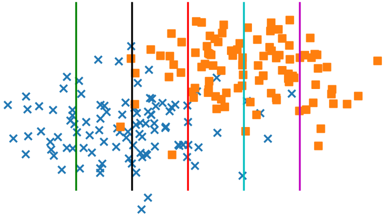
1: Initialize: hyperparameters, leaf set = $\{X_{\text{train}}\}$

2: **while** not stopping criteria **do**
3: leaf to split = Choose(leaf set)
4: left leaf, right leaf = Split(leaf to split)
5: Add left leaf, right leaf to leaf set
6: Remove leaf to split from leaf set
7: **end while**



Decision tree — split criteria

- Suppose there is a classification problem
- So we want to separate one class from the other by constructing **decision boundary**
- And using decision tree algorithm described earlier
- To do that we need to start splitting on features
- Which **split** is the best?



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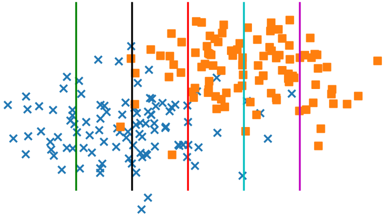
→ We need some criteria



Decision tree — split criteria

more about IG

- Suppose we have n features $x^{(1)}, x^{(2)}, ..., x^{(n)}$ in our dataset X
- If we want to split on some feature $x^{(j)}$ at threshold t then we propose to maximize **Information Gain** (IG):

$$\mathrm{IG}(\mathrm{X}, \mathrm{a}) = \mathrm{H}(\mathrm{X}) - \mathrm{H}(\mathrm{X} \mid \mathrm{a}) \to \max_{\mathrm{a}}$$

$$\mathrm{H}(\mathrm{X} \mid \mathrm{a}) = \sum_{v \in vals(\mathrm{a})} \frac{|S_{\mathrm{a}}(v)|}{|\mathrm{X}|} \cdot \mathrm{H}\left(S_{\mathrm{a}}(v)\right)$$

- In case of a binary tree with L(R) elements in the left (right) split we've got:

$$\mathrm{H}(X, j, t) = \frac{|\mathrm{L}|}{|\mathrm{X}|}\mathrm{H}(\mathrm{L}) + \frac{|\mathrm{R}|}{|\mathrm{X}|}\mathrm{H}(\mathrm{R}) \to \min_{j,t}$$

more about IG

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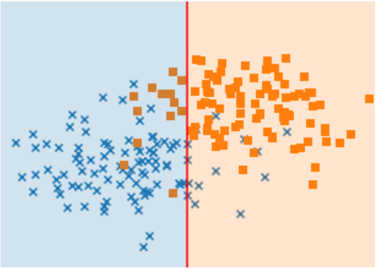
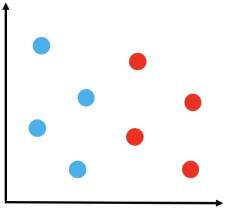
How to choose H(X)?

Decision tree — split criteria



The "best" split is a central one because it introduces **purity** in the best way. And we have some functions to measure the purity!

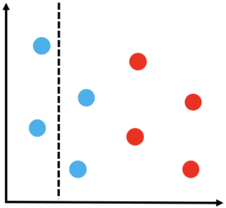
Decision tree → split criteria



$p = \frac{4}{8}, p = \frac{4}{8}$

$I = \frac{4}{8}\left(1 - \frac{4}{8}\right) + \frac{4}{8}\left(1 - \frac{4}{8}\right) = \frac{1}{2}$

Bad split



$p = \frac{2}{2}, p = \frac{0}{2}$

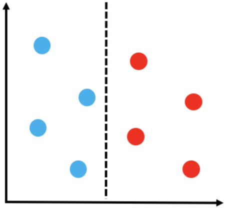
$I_{left} = \frac{2}{2}\left(1 - \frac{2}{2}\right) + \frac{0}{2}\left(1 - \frac{0}{2}\right) = 0$

$p = \frac{2}{6}, p = \frac{4}{6}$

$I_{right} = \frac{2}{6}\left(1 - \frac{2}{6}\right) + \frac{4}{6}\left(1 - \frac{4}{6}\right) = \frac{4}{9}$

$\Delta I = \frac{1}{2} - 0\frac{2}{8} - \frac{4}{9}\frac{6}{8} = \frac{1}{6}$

Best split



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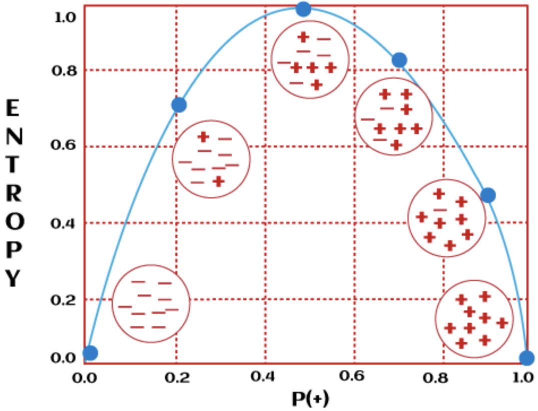
Михаил Гущин, НИУ ВШЭ

Decision tree — split criteria



Источник: https://www.javatpoint.com/entropy-in-machine-learning

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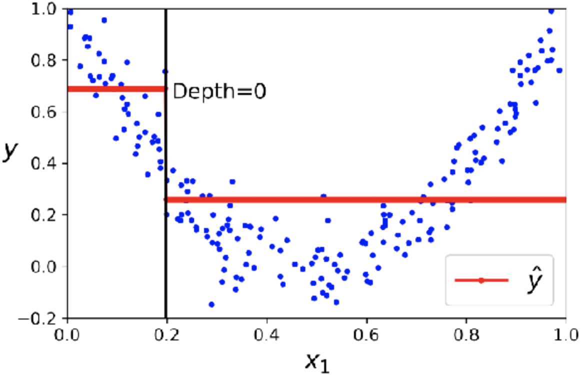
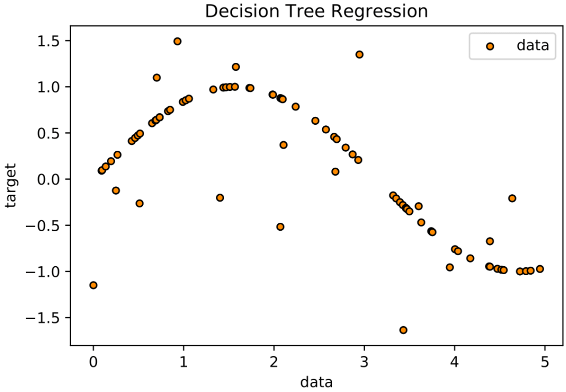
Decision tree → split criteria

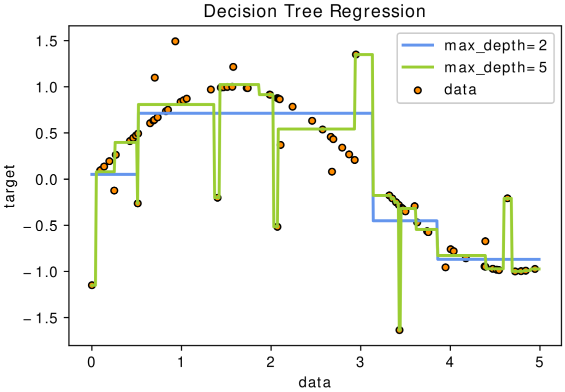


Decision tree → regression



Can we use decision tree approach for regression problem?

Decision tree — regression



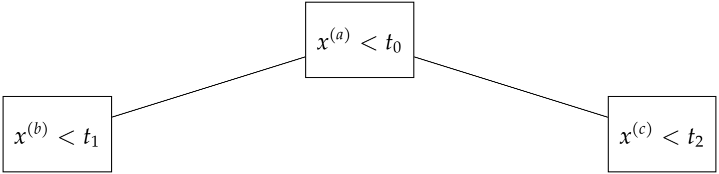
Can we use decision tree approach for regression problem? Yes

What about tree construction?

$$\boxed{x^{(a)} < t_0}$$

Decision tree — growing

What about tree construction? Do it recursively by **greedy** algorithm



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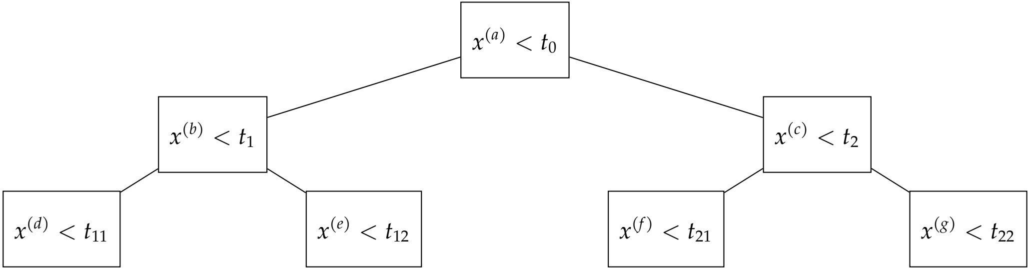

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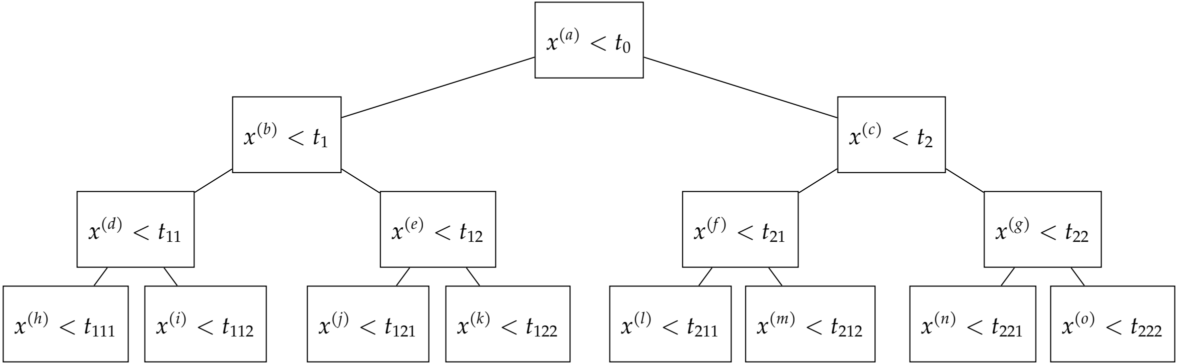
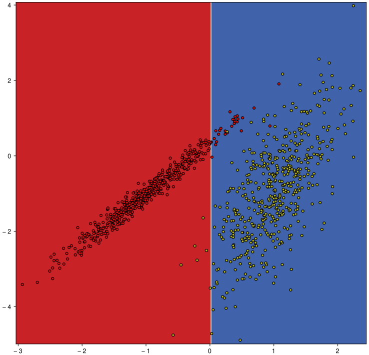
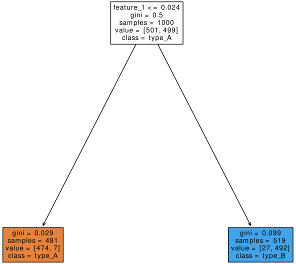


Decision tree —○ growing

check out also these visuals





Decision tree → growing

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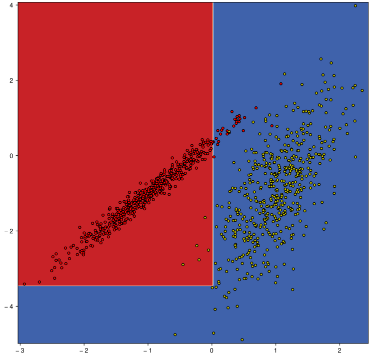

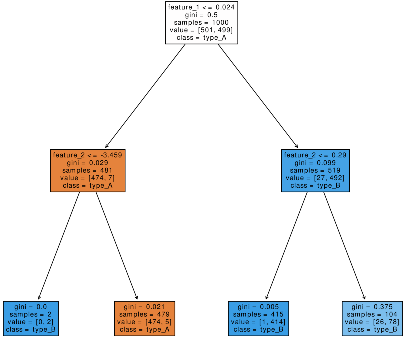

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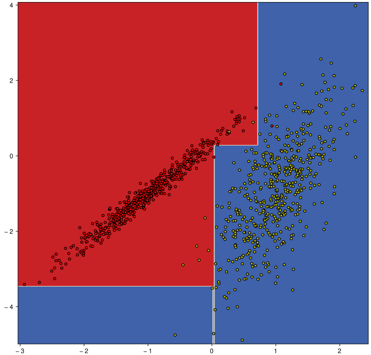

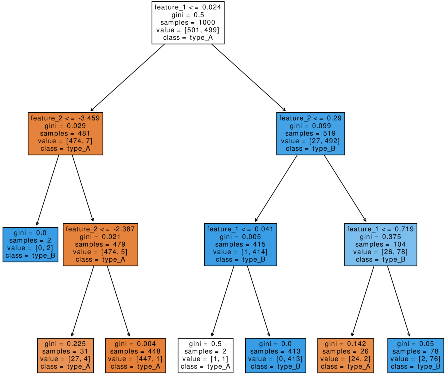

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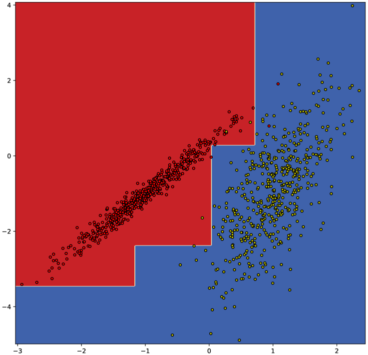

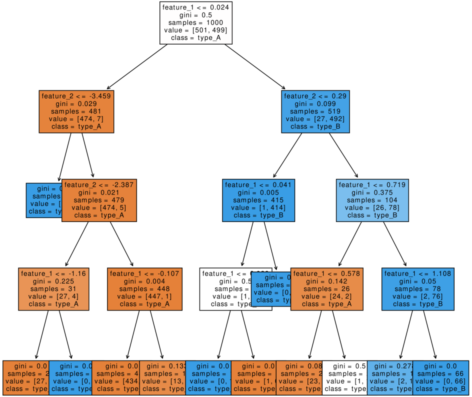

Random forest and gradient boosting

Random forest and gradient boosting

what's next after decision trees?