Technology Review

Formulation group

Zichen Zhu; Chenyi Mao; Lin Zhang; Dawei Gu; Jinge Xu

1. Background

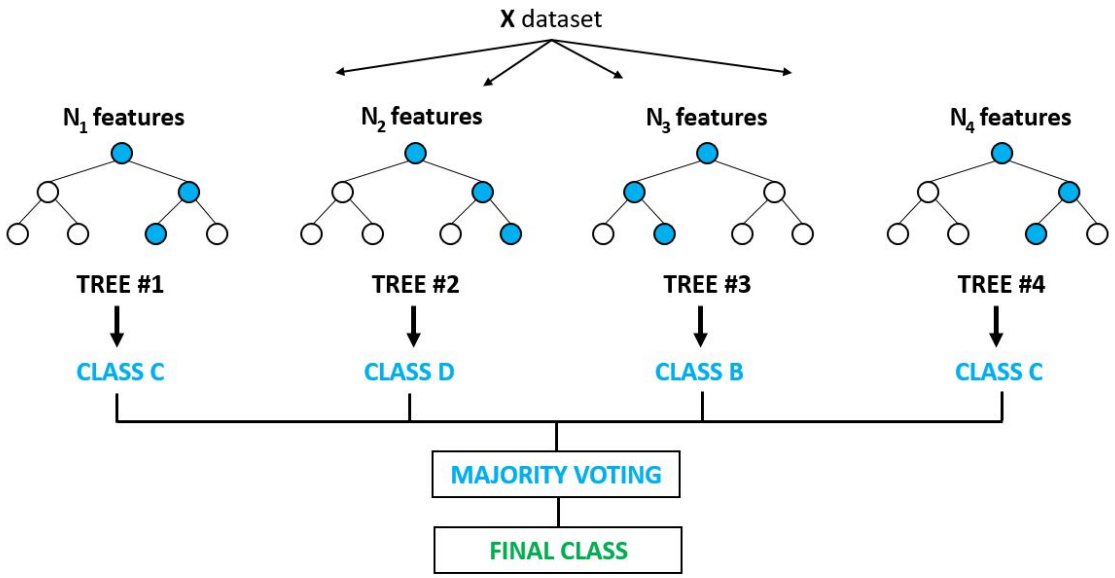
- Dataset: 927 drugs includes more than 10 properties.
- Purpose: Build a model can predict the formulation of certain active pharmaceutical indigent(API).
- Properties of Drugs: solubility at various pH, polar surface area, molecular weight, etc…
- Significance: simulate the form of API based on various medical situation.
- Also, this model could potentially predict other features and missing value

2. Lists of available technologies

1. K Nearest Neighbor (value of parameter K)
2. Support Vector Machines (two-class, sparse data)
3. Random Forest (multiclass, heterogeneous features)
4. Neural Networks (fancier but more complicated)

1	Generic Name	Formulation	Measured Solubility (mg/mL)	MW Drug (g/mol)	Measured LogP	HBA	HBD	PSA (Å^2)
2	Abacavir Sulfate	tablets	77	286.34	1.20	6	3	95.80
3	Acarbose	tablets		645.62	-8.83	19	14	351.80
4	Acebutolol Hydrochl	capsules		336.43	1.71	5	3	97.05
5	Acetaminophen; Par	tablets	23.7	151.17	0.20	2	2	55.41
6	Acetohexamide	tablets	3.43	324.40	2.44	4	2	103.22
7	Acetylsalicylic Acid;	tablets	10	180.16	1.19	3	1	68.21
8	Adenosine	solution	5	267.25	-0.98	8	4	135.44

3. Intro to Random Forest Classifier



- Aggregating a number of binary decision trees.
- Each tree is fitted to a bootstrapped training set.
- When fitting each tree, at each split, choose a sample of m predictors as split candidates.
- To aggregate the prediction results, take the majority.
- Sklearn.ensemble.

  RandomForestClassifier

4. Appeal of Random Forest Classifier (RFC)

Why do we choose RFC:

- It provides high accuracy.
- It is very simple to get started.
- It has the power to handle a large data set with higher dimensionality.

Why do we choose Scikit-learn package:

- Because that's the only package that I could find has built-in RFC module.
- Almost every other ML package is doing NN only.

Ref: Random Forest Analysis in ML and when to use it

5. Drawbacks of Random Forest Classifier

- Random forest models are not that interpretable, more like black boxes
- When dealing with large data sets, the huge size of the trees would take up a lot of memory
- Random forest models can tend to overfit