Machine Learning:
Where did this Random Forest come from?

Biostats Club

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February 21, 2019

Machine Learning - da fuq?

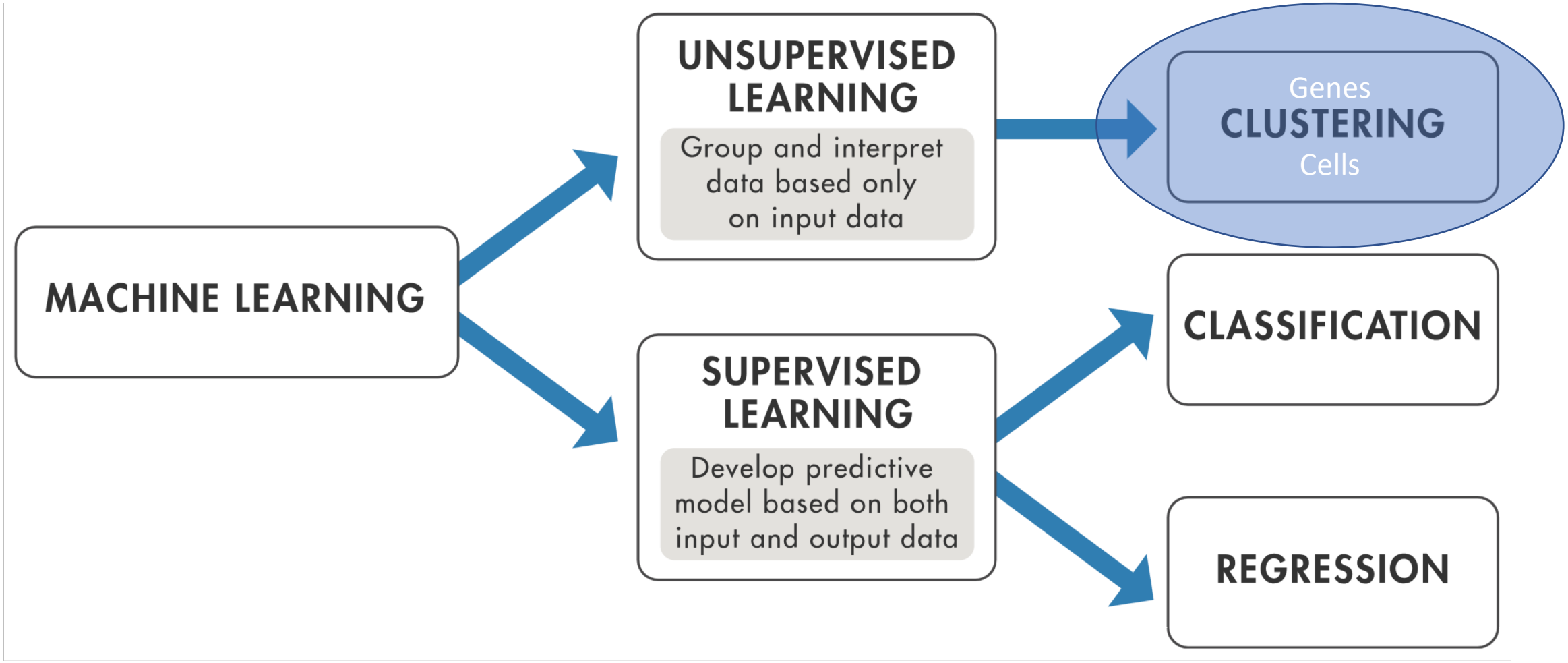
- Machine learning is any computational technique that involves “learning from experience”.
- Machine learning algorithms “learn” information directly from data, (often) without relying on a predetermined equation as a model.

- If iteration 2 involves information that came from iteration 1, that’s machine learning!

https://www.mathworks.com/discovery/machine-learning.html

We actually use machine learning all the time in analysis of big data without even thinking about it!

What can/do I do with machine learning?



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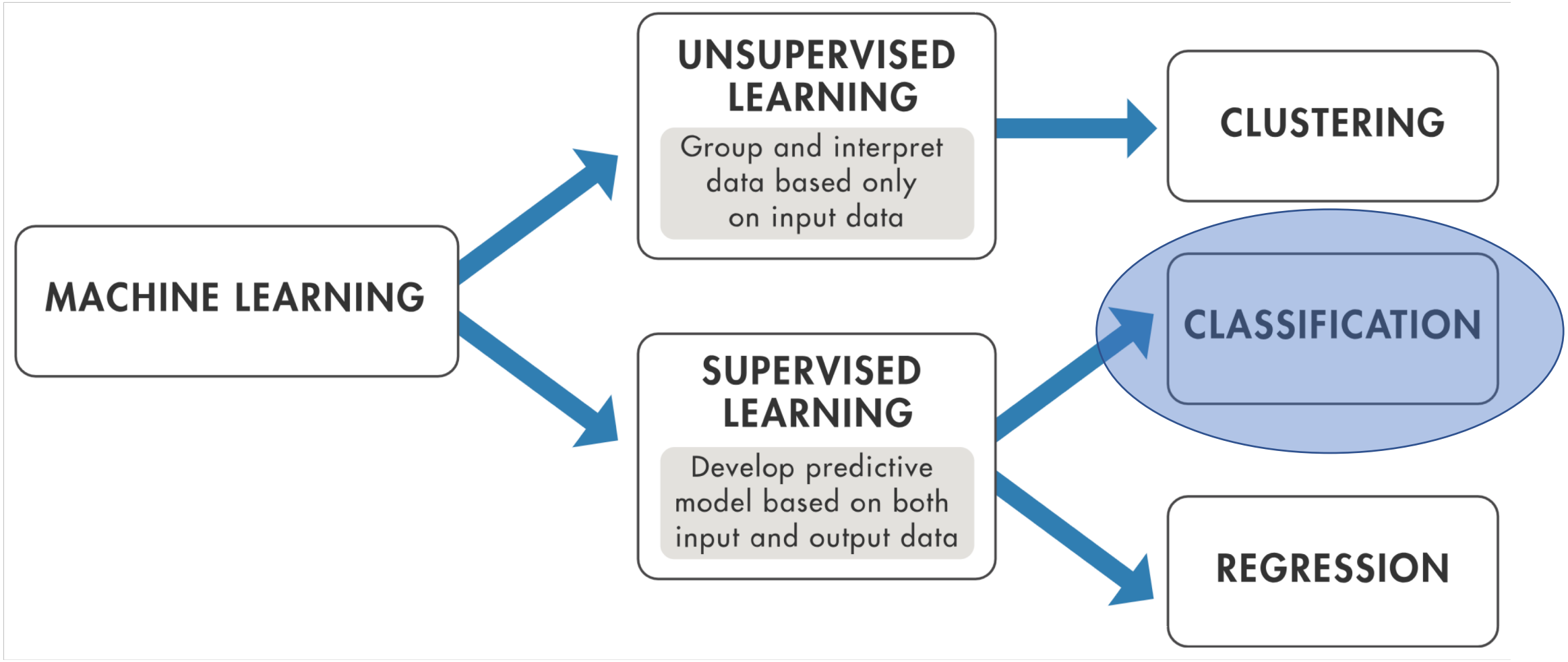

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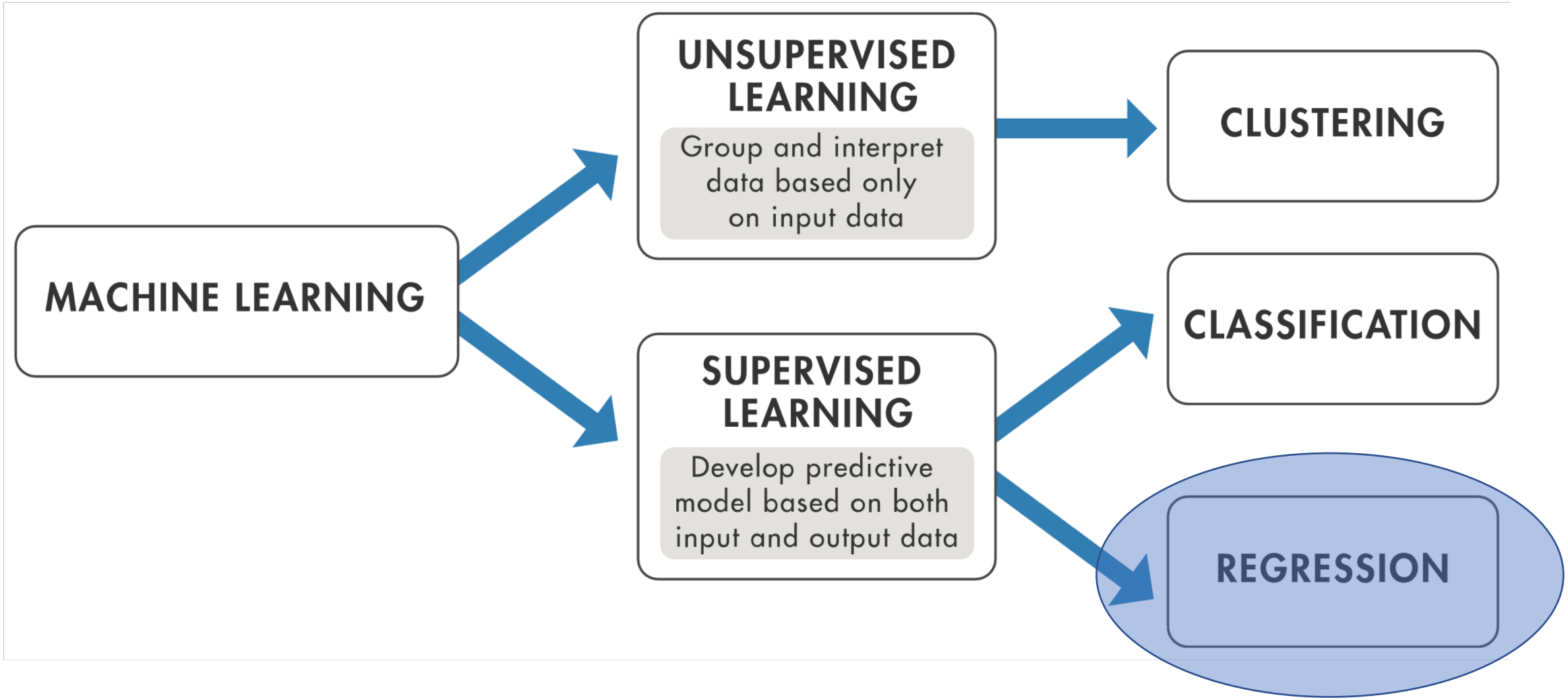

Unsupervised Learning: Group and interpret data based only on input data

- Why? To infer hidden associations or structure in the dataset

- Common Uses:
  - Hierarchical Clustering of cells / genes for a heatmap
  - Clustering of cells in single cell RNAseq data
  - Picking peaks that are above background level in ChIPseq data

Supervised Learning: Develop a predictive model based on input & output data

- Classification OR Regression
- Why? Build a model for scoring or classifying new datapoints!

- Common Uses:
  - Novel Gene Prediction (based on previous genomes, known genes/organisms)
  - Disease risk prediction (based on healthy vs diseased training sets)
  - Clustering of cells in single cell data (?)
  - Cell type classification (scRNAseq, based on pure reference datasets [Singler])

Not all highly computational analyses are machine learning

- t-SNE: YES
- PCA: NO
- Statistical significance testing: NO (most of the time)

10 tips for biological machine learning

1. **Adjust your data's structure:**
   - Start with enough data:
     - ideal = 10 samples for every feature
     - These both seem super low! (???)
   - Shuffle the order of your data
     - Removes any possibility of trends related to order
   - Clean the data
     - Remove corrupt, inaccurate, inconsistent, or outlier values
     - Normalize (= scale function) if needed (not needed for random forest)

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2. Split into Training, Validation, and Test sets

- Common breakdown:
  - 50% Training
  - 30% Validation <- not always needed
  - 20% Test
- Training & validation: for training / adjusting “hyperparameters”.
- Test set: ONLY touch once you are all done.
- “the lock box approach should be employed by every machine learning project in every field”

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3. Understand the types of machine learning

- Unsupervised / supervised
  - Classification / Regression

- Unsupervised:
  - K-means clustering, Truncated singular value decomposition, Probabilistic latent semantic analysis, and more!
- Supervised:
  - Support Vector Machines, K- Nearest Neighbors, Regression modeling, Random Forest, and more!

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4. Pick the “right” algorithm: Start with the simplest

- Suggested that you use multiple, but 🤷‍♂️
- If you start simple, you can learn & you can probably manage the debugging

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5. Take care of the imbalanced data problem

- If 90% yes, 10% no: the algorithm may not learn to pick No's well
- "Balance" your data
  - Ensure a 70%/30% split
  - (90%+50%/2 & 30%+50%/2)

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6. Optimize your hyper-parameters

- Hyper-parameter = a parameter that the algorithm uses, but does not train
  - Ex: # groups in k-means, # of “neighbors” in k-NN clustering
- Method 1: Use a grid of values, then score with validation set
- Method 2: Use an automatic selection method, like X-means

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7. Minimize overfitting

- = algorithm memorizes the training set instead of learning the concepts required for the test
- = Great classification of training set, not great performance on training/validation set

1. Cross validation

2. Be aware of the possibility, and adjust for it when you see it.

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8. **Score the model with the Matthews correlation coefficient (MCC) or the Precision-Recall curve**

- MCC: has penalization when accuracy is low for certain groups
  - Important because we often have many negatives and few positives in biology!
  - Simple accuracy: If 95% of data is truly 1, and 5% is 2. A model that always goes with 1 would be 95% accurate.

- **My advice: Google the proper test, and consider step 10.**

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10 tips

9. Use open source over proprietary algorithms

- Access to the actual code
- Enables collaboration regardless of license access

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10 tips

10. Get feedback from experts

- Statisticians think we don’t know what we are doing lol
  - It’s often true!

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10 tips: This become 5 separate steps

1. **Adjust your data's structure:**
2. **Split into Training, (Validation,) and Test sets**
3. **Understand the types of machine learning**
4. **Pick the "right" algorithm: Start with the simplest**
5. **Take care of the imbalanced data problem**
6. **Optimize your hyper-parameters**
7. **Minimize overfitting**
8. **Score the model's performance with a valid test**
9. **Use open source over proprietary algorithm**
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Step 1
Step 2
Step 3
Step 4
Step 5

Synthesized tips

1. Use the simplest model you can!
2. Mind your model:
   - train/test/validate sets
   - Randomize data order
   - Remember assumptions & try not to over-extend your conclusions
     - Ex: if you use k-means with k=4, don't say "the fact that we got 4 clusters is meaningful."
3. Over-fitting: look for it, and adjust accordingly
4. Run your method by an expert
   - Example: selecting markers based on a PCA of the entire dataset = bad practice

Why Random Forest?

- Cuz trees fight climate change!
- Incredibly Powerful yet also Flexible
  - Regression or Classification

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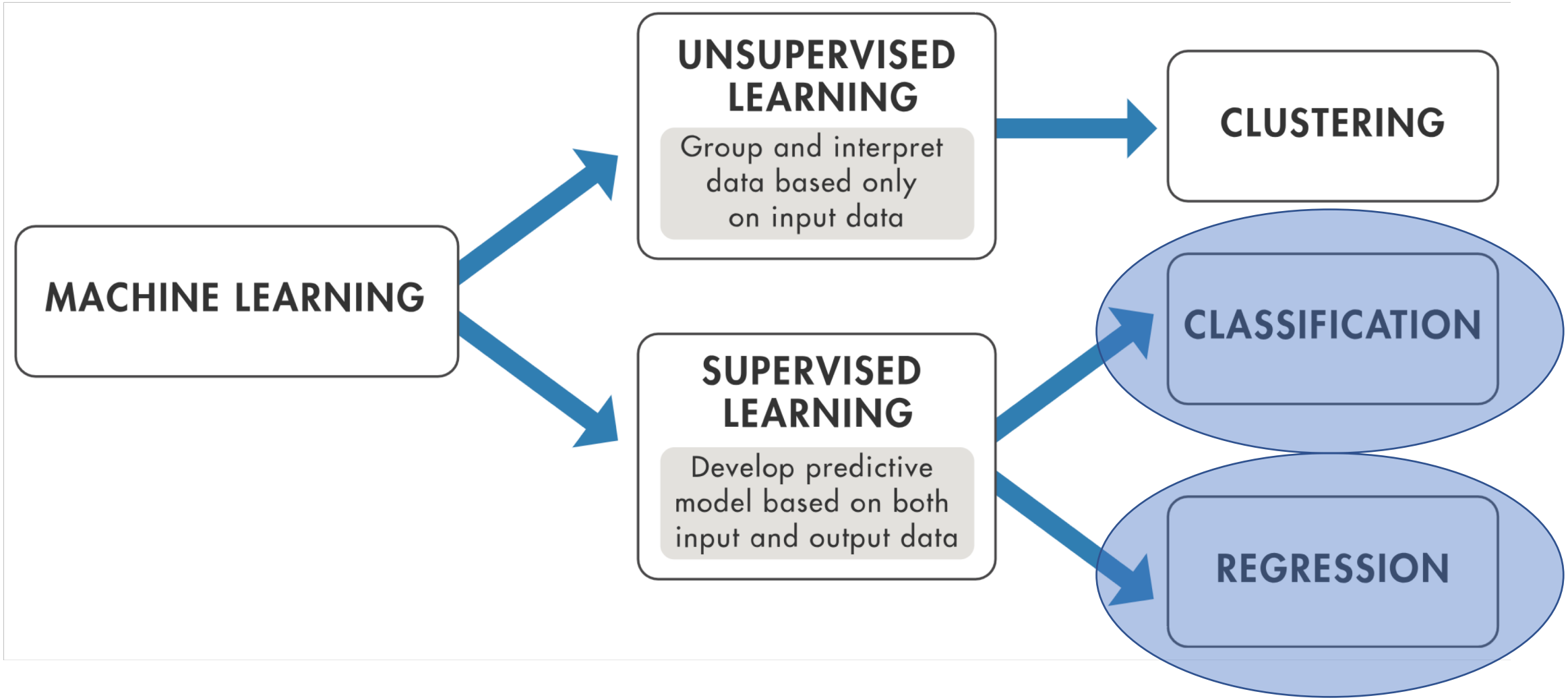
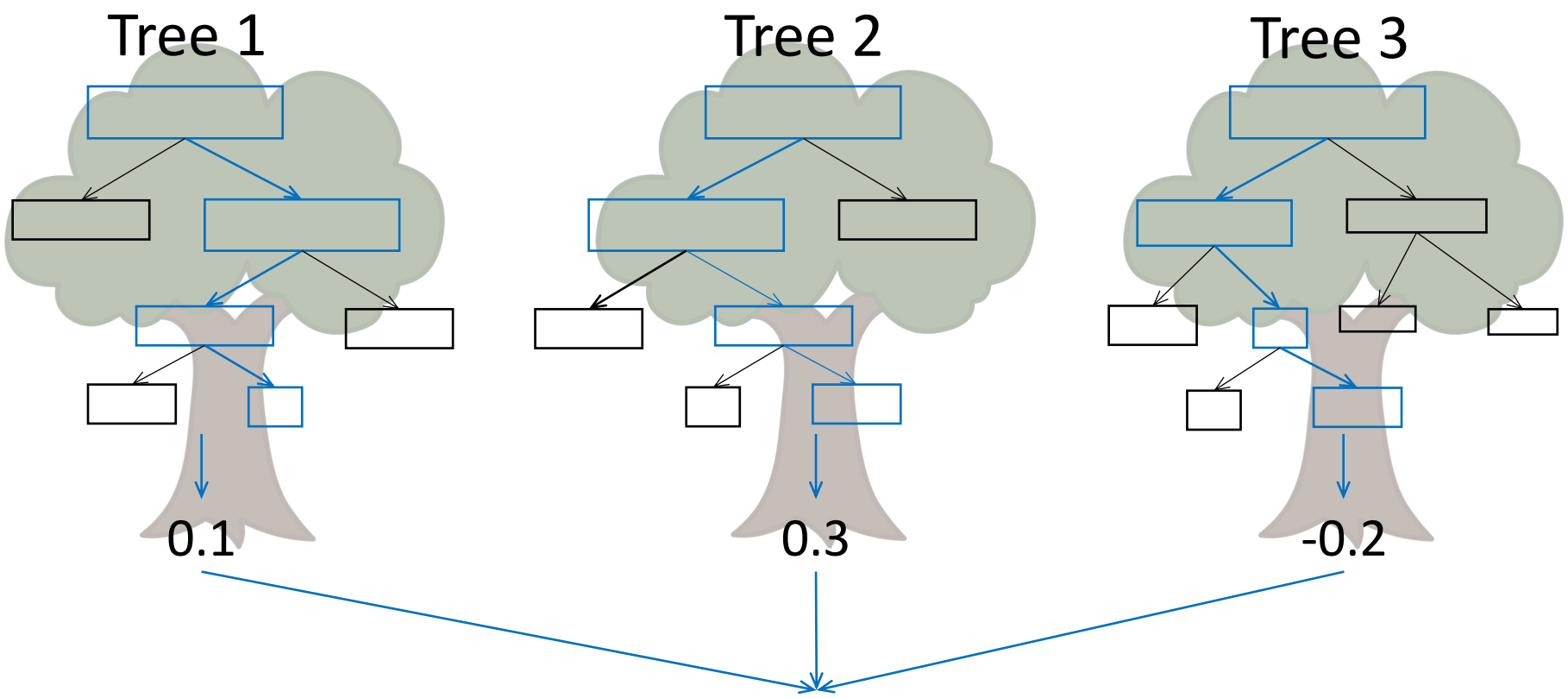


Why Random Forest?

- Cuz trees fight climate change!
- Incredibly Powerful yet also Flexible
  - Regression or Classification
- Easy to use: few hyperparameters
- Training is quick
  - seconds or minutes
- Can often reverse engineer metrics about the markers used afterwards!

Why Random “Forest”?



What is “Random” Forest?

- “Random” = bagging = a random set of samples is picked
  - Code: sample(data, size = nrow(data), replace = T) → ~2/3 of data
- Each tree is iteratively built on a different random set
- 1st marker and break point are calculated
  - Selects feature
  - Selects break point(s)
- 2nd and 3rd markers/break points …
- Repeat (500) times

Let’s use it!