M3239.005300 Machine Learning & Deep Learning I

Spring 2024

Lab 2

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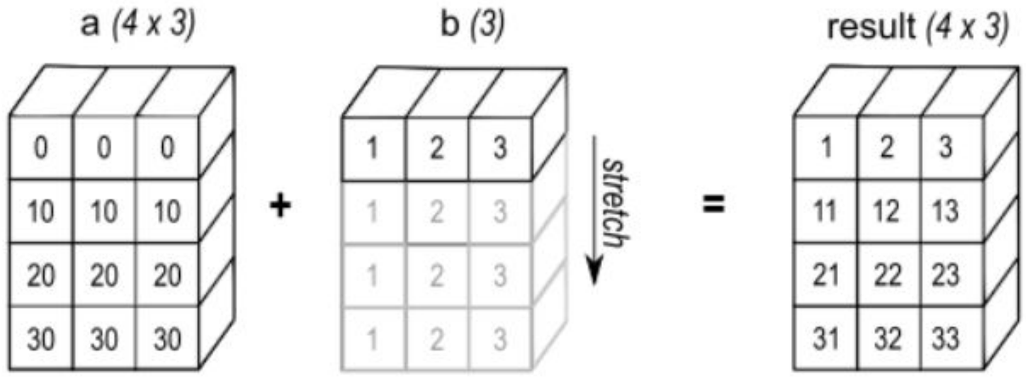
Vectorization in Numpy

Two Major Tips for Vectorization in Numpy

1. Broadcasting



2. Boolean Indexing & Fancy Indexing

```
a = np.array([1,2,3,4,5])
a[a%2==0] = 0
a
✓ 0.0s

array([1, 0, 3, 0, 5])
```

Regularization

Ridge Regression

- Estimation in Ridge Regression

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} (\mathbf{Y} - \mathbf{X}\beta)^\top (\mathbf{Y} - \mathbf{X}\beta) + \lambda \|\beta\|_2^2$$

$$\begin{aligned} \frac{\partial \mathrm{RSS}(\beta)}{\partial \beta} &= -\mathbf{X}^\top (\mathbf{Y} - \mathbf{X}\beta) - (\mathbf{Y} - \mathbf{X}\beta)^\top \mathbf{X} + 2\lambda\beta \\ &= -\mathbf{X}^\top (\mathbf{Y} - \mathbf{X}\beta) - \mathbf{X}^\top (\mathbf{Y} - \mathbf{X}\beta) + 2\lambda\beta \\ &= -2\mathbf{X}^\top (\mathbf{Y} - \mathbf{X}\beta) + 2\lambda\beta = 0 \end{aligned}$$

$$\mathbf{X}^\top \mathbf{Y} - \mathbf{X}^\top \mathbf{X}\beta - \lambda\beta = 0$$

$$\beta = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{Y}$$

$d \times 1$ $n \times d$ $d \times d$ $n \times 1$ Check dimensions!

Ridge Regression

- Implement the method `fit` in the class `RidgeRegression`

Ordinary Least Squares Estimator

- $\hat{\beta}_{OLS} = (X^T X)^{-1} X^T Y$

Ridge Estimator

- $\hat{\beta}_R = (X^T X + \lambda I)^{-1} X^T Y$

$d \times 1$ $n \times d$ $d \times d$ $n \times 1$

Hint:
`np.eye`

```python
np.eye(3)
```

✓ 0.0s

```
array([[1., 0., 0.],
       [0., 1., 0.],
       [0., 0., 1.]])
```

Lasso Regression

- Estimation in Lasso Regression

$$\hat{\beta} = \underset{\beta}{\mathrm{argmin}}(\mathbf{Y} - \mathbf{X}\beta)^\top(\mathbf{Y} - \mathbf{X}\beta) + \lambda||\beta||_1$$

- No closed form solution.
  -> Let's use gradient descent!

learning rate

$$\beta^{\text{new}} = \beta^{\text{old}} - \alpha \nabla_\beta \mathcal{L}(\beta)$$

Gradient

$$\frac{\partial}{\partial\beta}L = 2X^T(X\beta - y) + \lambda \times \mathrm{sign}(\beta)$$

Lasso Regression

- Implement the method `fit` in the class `LassoRegression`

learning rate

$$\beta^{\text{new}} = \beta^{\text{old}} - \alpha \nabla_{\beta} \mathcal{L}(\beta)$$

Gradient

$$\frac{\partial}{\partial \beta} L = 2X^T(X\beta - y) + \lambda \times \text{sign}(\beta)$$

Hint:
`np.sign`

```
np.sign([-1,2,-3,4])
```

✓ 0.0s

```
array([-1,  1, -1,  1])
```

Decision Trees

Decision Tree Classification

- Recursive Binary Splitting

```
while (!stopping condition):
  for all splittable node v, dimension j, threshold s:
    split R1(v, j, s) = v(x_j < s)
    split R2(v, j, s) = v(x_j ≥ s)

    compute y1 = argmax_k(y_i = k) for x_i in R1
    compute y2 = argmax_k(y_i = k) for x_i in R2

    err(v, j, s) = impurity(R1)/|{x: x  ∈ R1}|
               + impurity(R2)/|{x: x  ∈ R2}|

  pick (v, j, s) with minimum err(v, j, s)
  split node v at x_j = s
```

Three Nested For-loops

Decision Tree Classification

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  for all splittable node v, dimension j, threshold s:
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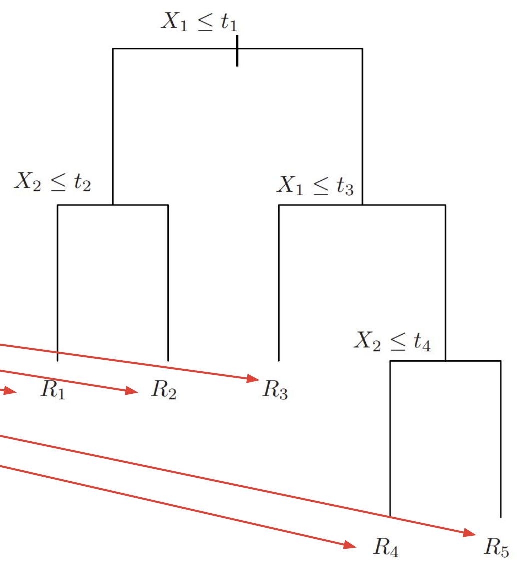

Decision Tree Classification

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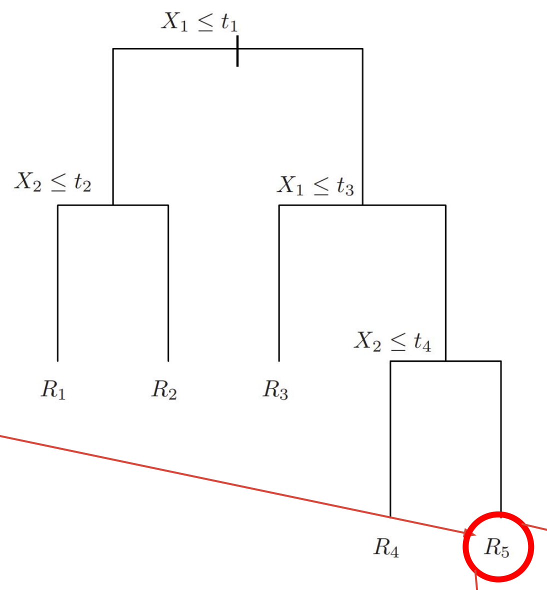

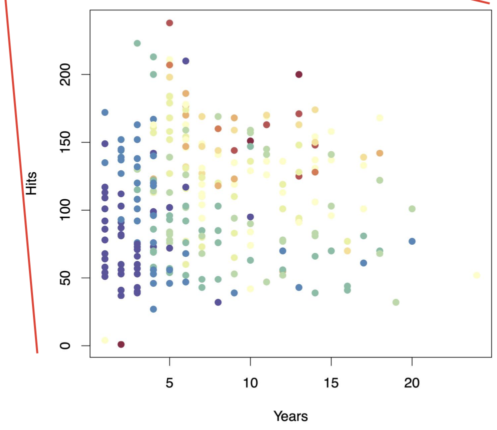

Decision Tree Classification

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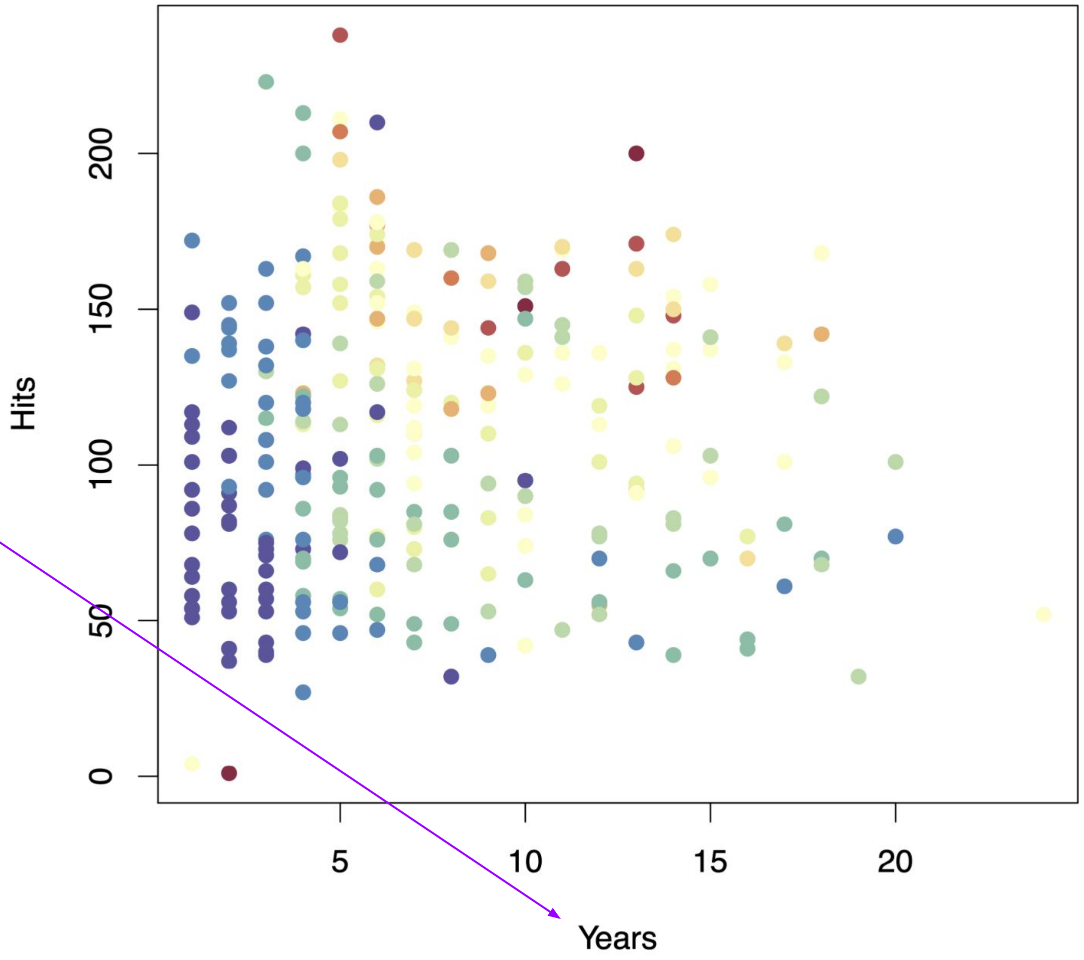

Decision Tree Classification

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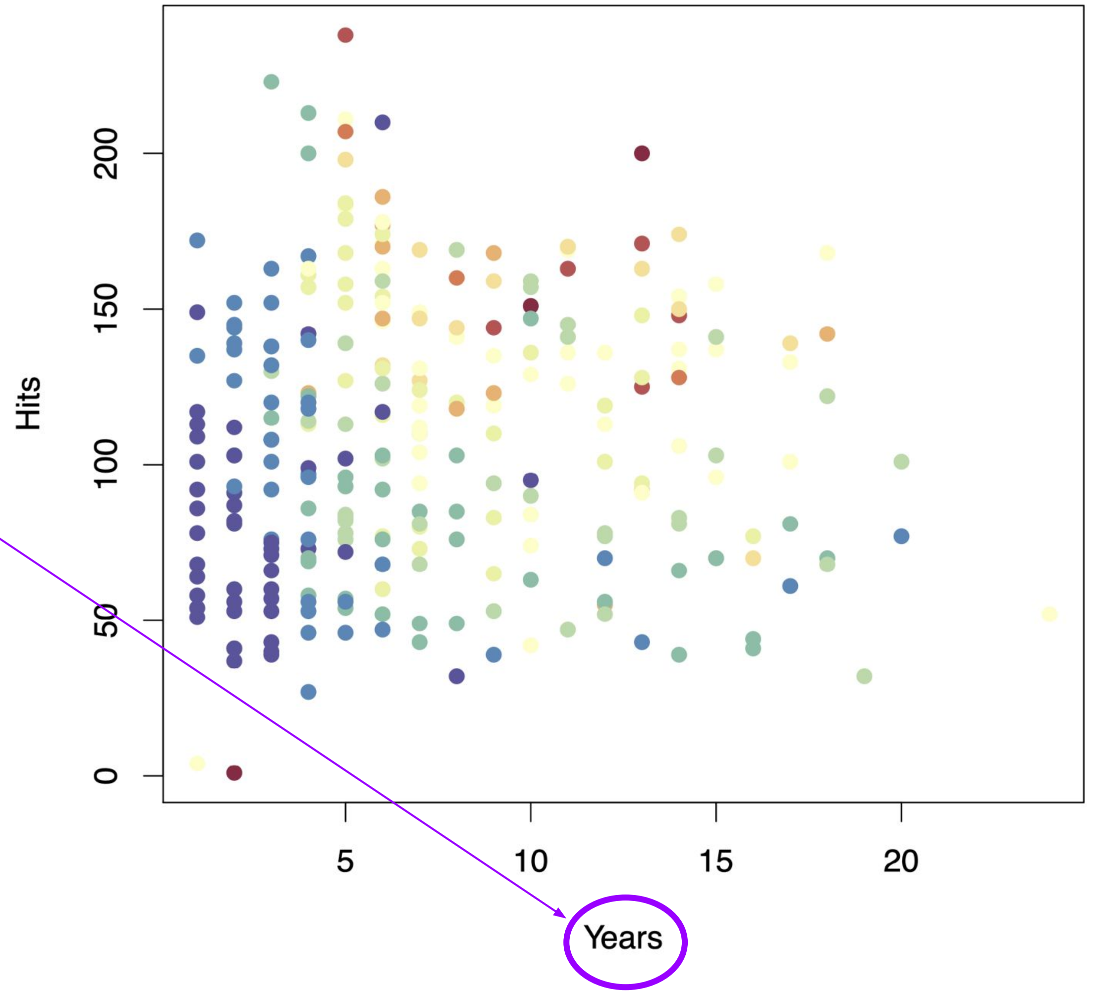

Decision Tree Classification

```
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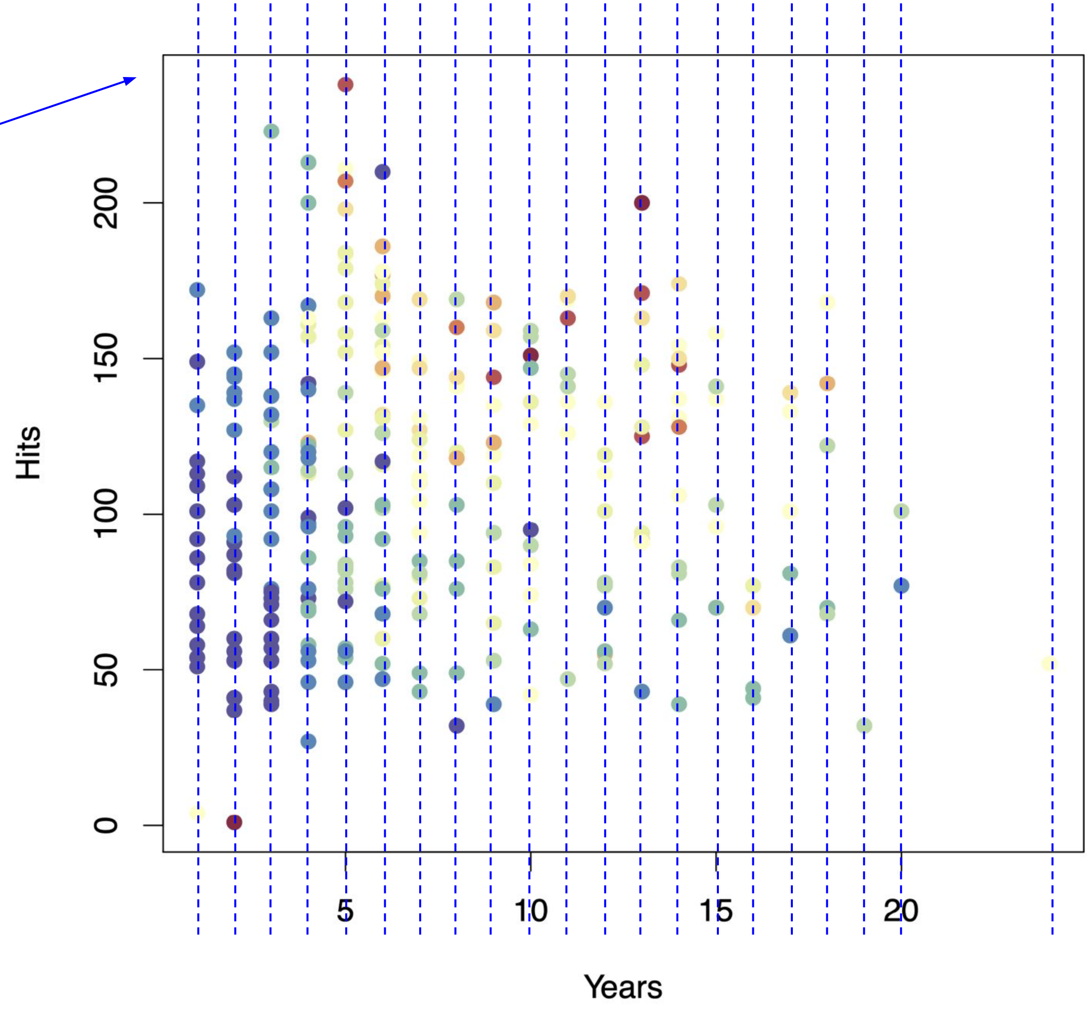

Decision Tree Classification

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  split node v at x_j = s
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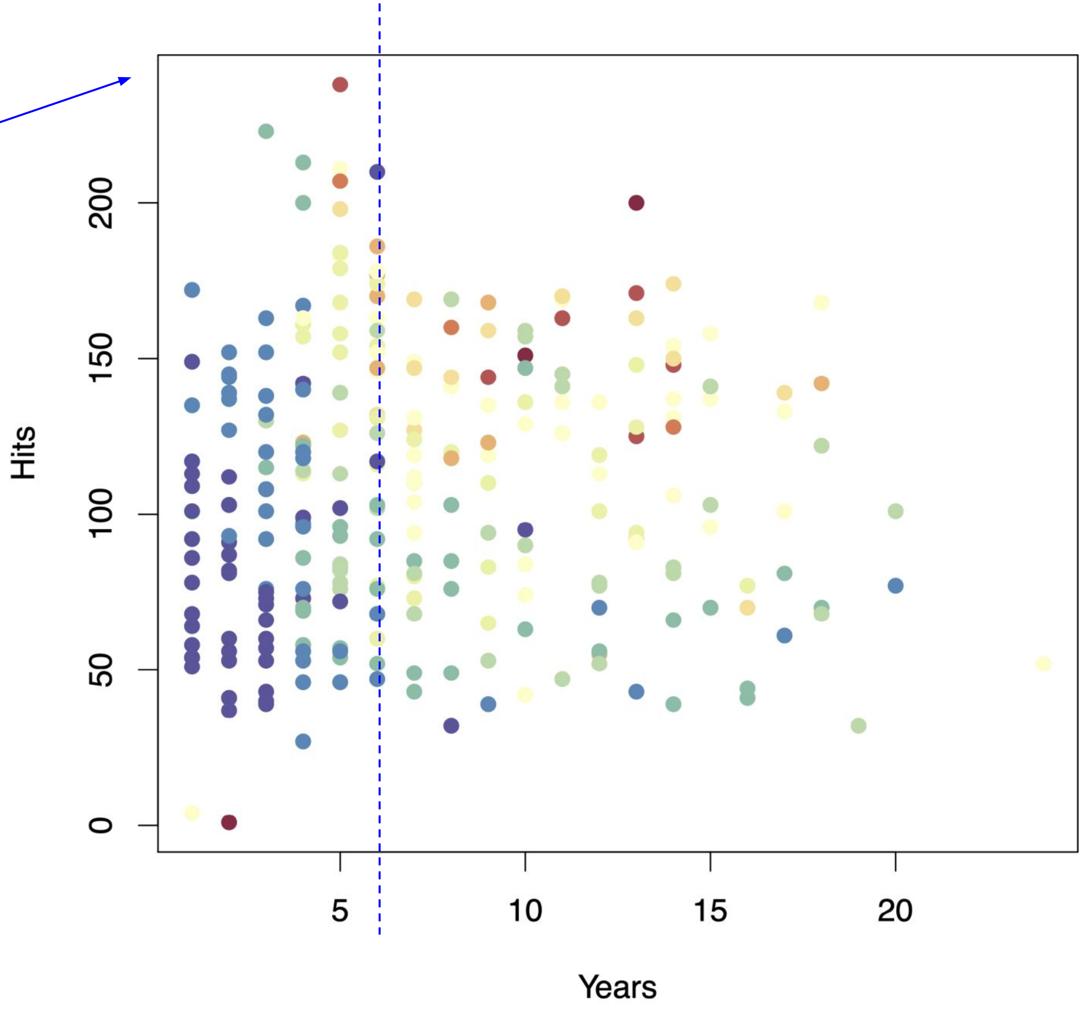


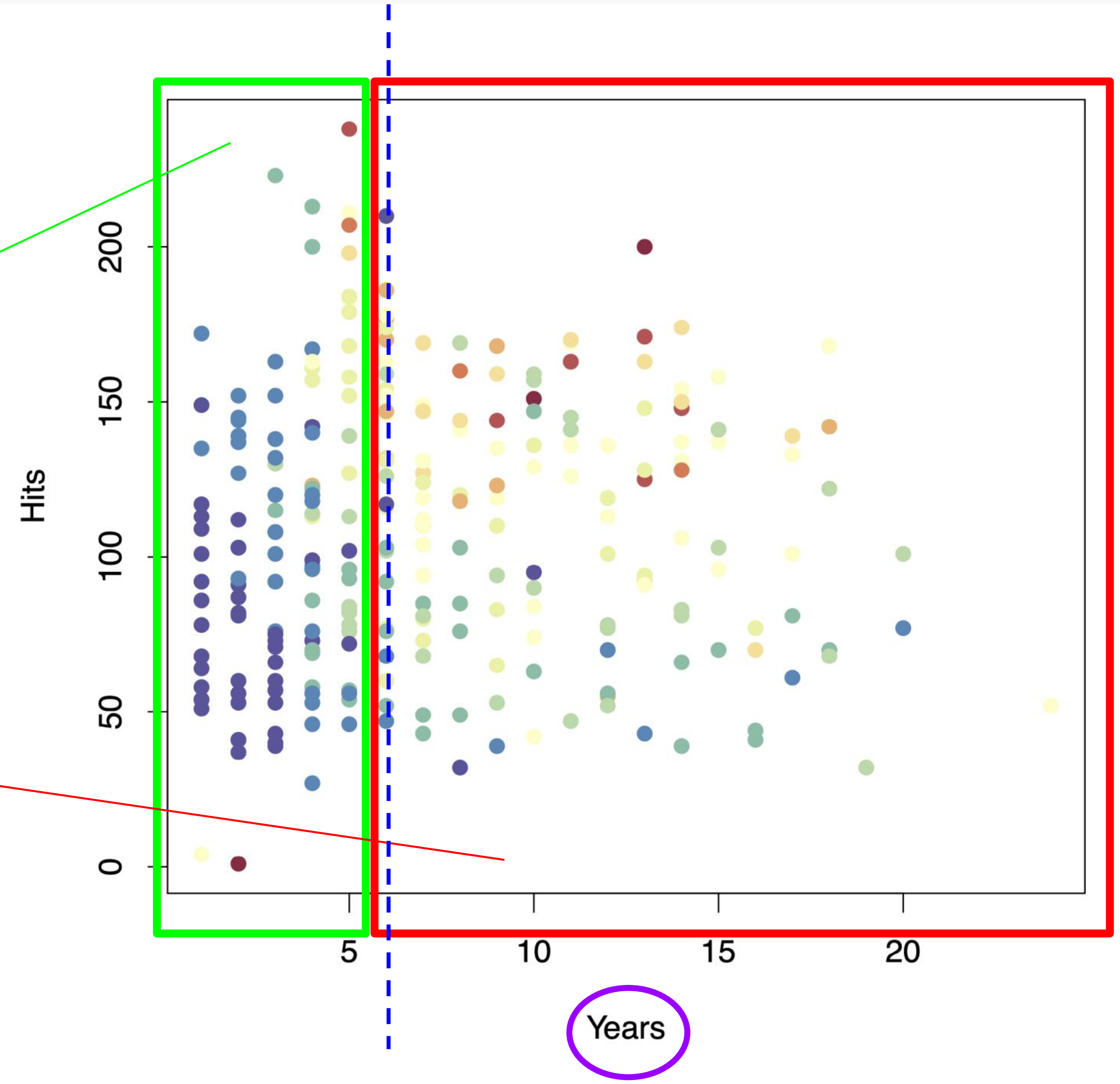
Decision Tree Classification

```
while (!stopping condition):
  for all splittable node v, dimension j,  threshold
s:
    split R1(v, j, s) = v(x_j < s)
    split R2(v, j, s) = v(x_j ≥ s)

    compute y1 = argmax_k(y_i = k) for x_i in R1
    compute y2 = argmax_k(y_i = k) for x_i in R2

    err(v, j, s) = impurity(R1)/|{x: x  ∈ R1}|
               + impurity(R2)/|{x: x  ∈ R2}|

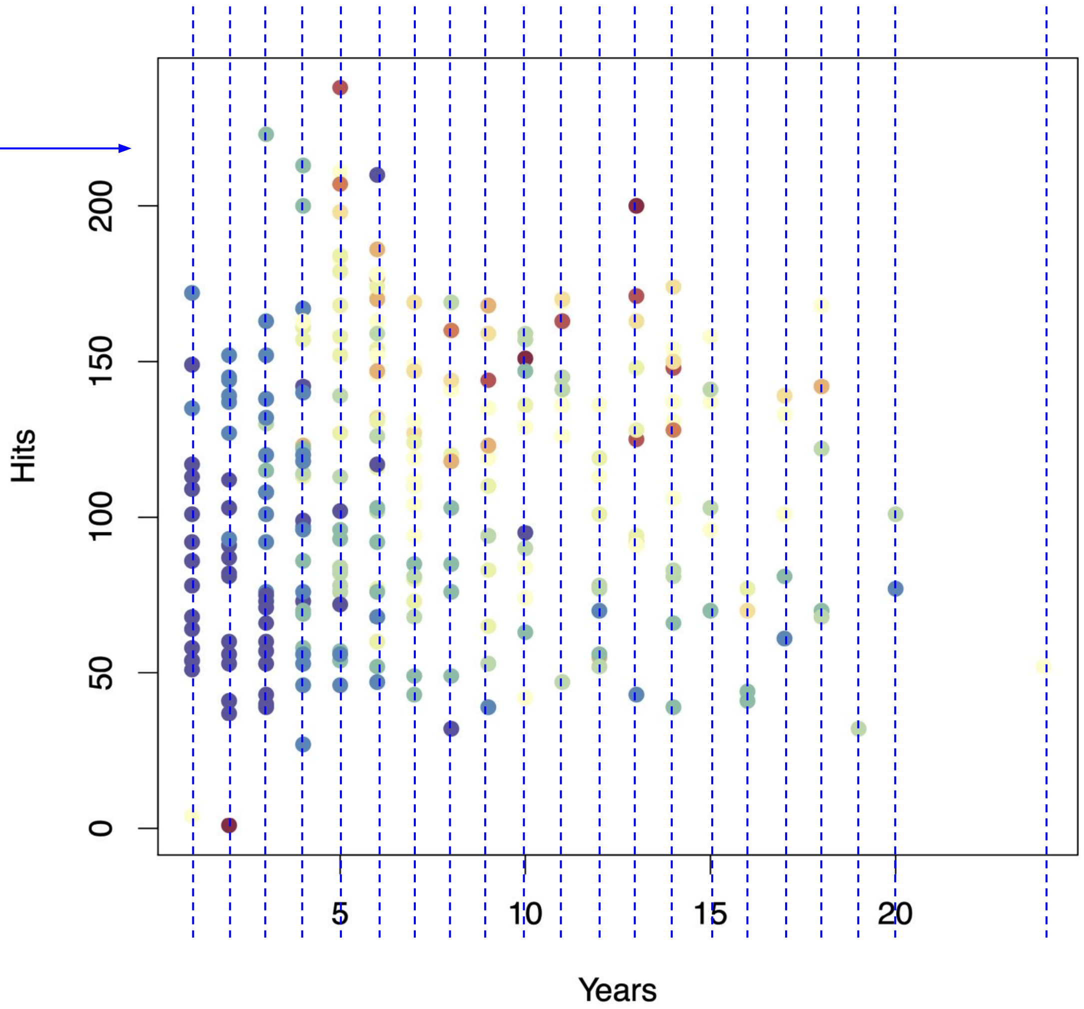
  pick (v, j, s) with minimum err(v, j, s)
  split node v at x_j = s
```



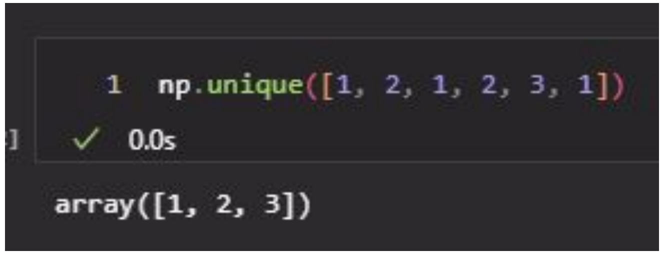
Decision Tree Classification

- Complete the method `_best_split` in the class `DecisionTree`

```
while (!stopping condition):
  for all splittable node v, dimension j,  threshold s:
    …
```



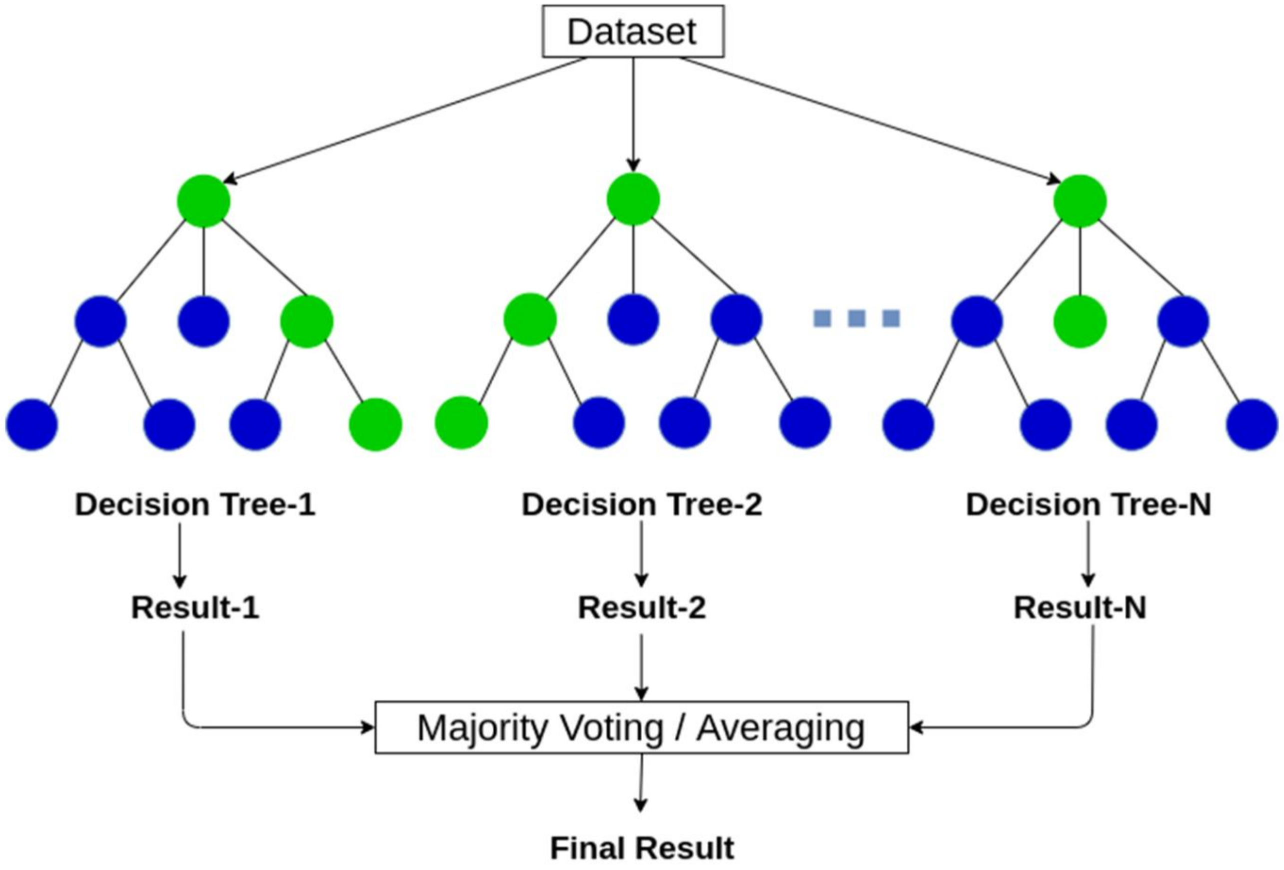
Hint:
`np.unique`



Ensemble Methods and Boosting

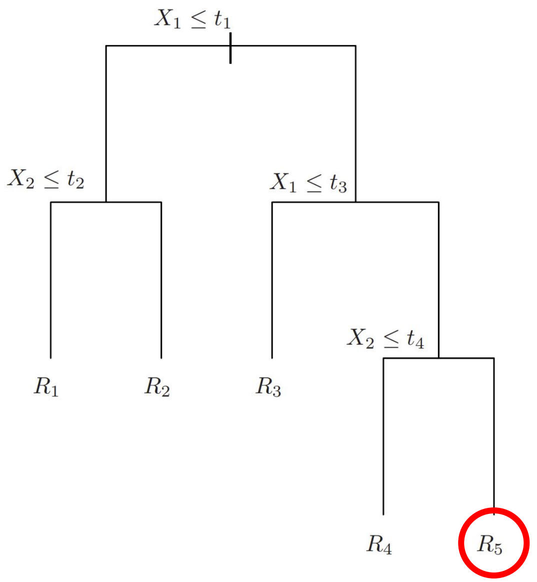
Random Forest Classification

- Bagged Trees



Random Forest Classification

- A split in a tree of Random Forest
  - **Random forests** provide an improvement over bagged trees with a small tweak that decorrelates the trees.
    - **At each time to split in training decision trees, only a subset of *m* predictors are considered as candidates, from the full set of *p* predictors.**
    - A typical value of $m \approx \sqrt{p}$



To split this node,

$$X_1, X_2, X_3, X_4, X_5, \ldots, X_p$$

Randomly choose m predictors!

$$X_2, X_5, \ldots, X_{p-3}$$

Random Forest Classification

- A split in a tree of Random Forest

```
while (!stopping condition):
  for all splittable node v, dimension j, threshold s:
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    err(v, j, s) = impurity(R1)/|{x: x  ∈ R1}|
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  pick (v, j, s) with minimum err(v, j, s)
  split node v at x_j = s
```

$$X_1, X_2, X_3, X_4, X_5, \ldots, X_p$$

$$\Big\downarrow$$

Randomly choose m predictors!

$$X_2, X_5, \ldots, X_{p-3}$$

Random Forest Classification

- Complete the method `_best_split_with_random` in the class `DecisionTreeForRF`

$$X_1, X_2, X_3, X_4, X_5, \ldots, X_p$$

To split this node,

Randomly choose $\sqrt{p}$ predictors!

$$X_2, X_5, \ldots, X_{p-3}$$

Hint:

`np.random.choice`

```python
print(np.random.choice(5, size=2, replace=False))
print(np.random.choice(5, size=2, replace=False))
print(np.random.choice(5, size=2, replace=False))
```

✓ 0.0s

```
[0 2]
[2 1]
[1 3]
```

Ensemble Methods and Boosting

AdaBoost

- Training AdaBoost

Input: training dataset $\{\mathbf{x}_i, \mathbf{y}_i\}$ for i = 1, ..., n, $\mathbf{y} \in \{-1, +1\}$

- Initialize $D_1(i) = 1/n$
- for t = 1, ..., T:
  - Train a base learner, h_t: $\mathbf{x} \rightarrow \{+1, -1\}$, with D_t
  - $\epsilon_t = p_{D_t}[h_t(\mathbf{x}_i) \neq \mathbf{y}_i]$
  - $\alpha_t = \frac{1}{2}\log\frac{1-\epsilon_t}{\epsilon_t}$
  - $\forall i D_{t+1}(i) = D_t(i)e^{-\alpha_t \mathbf{y}_i h_t(\mathbf{x}_i)}$
  - $\forall i D_{t+1}(i) = \frac{D_{t+1}(i)}{\sum_{j=1}^{n} D_{t+1}(j)}$
- Output $H(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})\right)$

D_t: Sampling weight distribution over training samples at step t.
→ We start with uniform distribution.

We train T base learners sequentially.

Each base learner is trained on a training set sampled with D_t.

ε_t is the error rate under the current sample distribution D_t.

α_t is log (success rate / error rate), going to -∞ if $\varepsilon_t \rightarrow 1$, to +∞ if $\varepsilon_t \rightarrow 0$, and being zero if success rate = 50%.

Data distribution update for the next step:
$\mathbf{y}_i h_t(\mathbf{x}_i) > 0$ if h_t is correct for $\mathbf{x}_i$, and $\mathbf{y}_i h_t(\mathbf{x}_i) < 0$ if incorrect.
For correct examples, weight D_{t+1} gets smaller than D_t.
For incorrect ones, weights D_{t+1} gets larger than D_t.

Then, normalize D_{t+1} so that it sums to 1.

Final classifier is a weighted sum of base learners, weighted by their log success rate (α_t).

AdaBoost

- Complete the method `fit` in the class `AdaBoost`

Input: training dataset {$\mathbf{x}_i$, $\mathbf{y}_i$} for i = 1, ..., n, $\mathbf{y} \in$ {-1, +1}

- Initialize $D_1(i) = 1/n$
- for t = 1, ..., T:
  - Train a base learner, h_t: $\mathbf{x} \rightarrow$ {+1, -1}, with D_t
  - $\epsilon_t = p_{D_t}[h_t(\mathbf{x}_i) \neq \mathbf{y}_i]$
  - $\alpha_t = \frac{1}{2}\log\frac{1-\epsilon_t}{\epsilon_t}$
  - $\forall i D_{t+1}(i) = D_t(i)e^{-\alpha_t \mathbf{y}_i h_t(\mathbf{x}_i)}$
  - $\forall i D_{t+1}(i) = \frac{D_{t+1}(i)}{\sum_{j=1}^{n} D_{t+1}(j)}$
- Output $H(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})\right)$

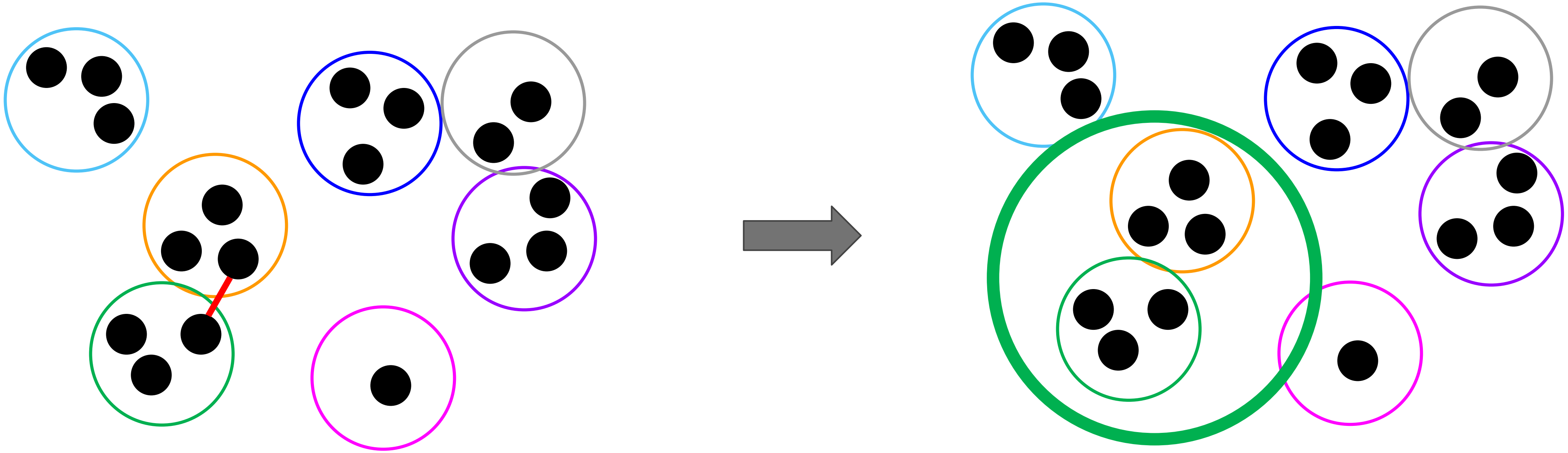
Sampling Weight Update

Hint:
`np.exp`
`np.sum`

Clustering

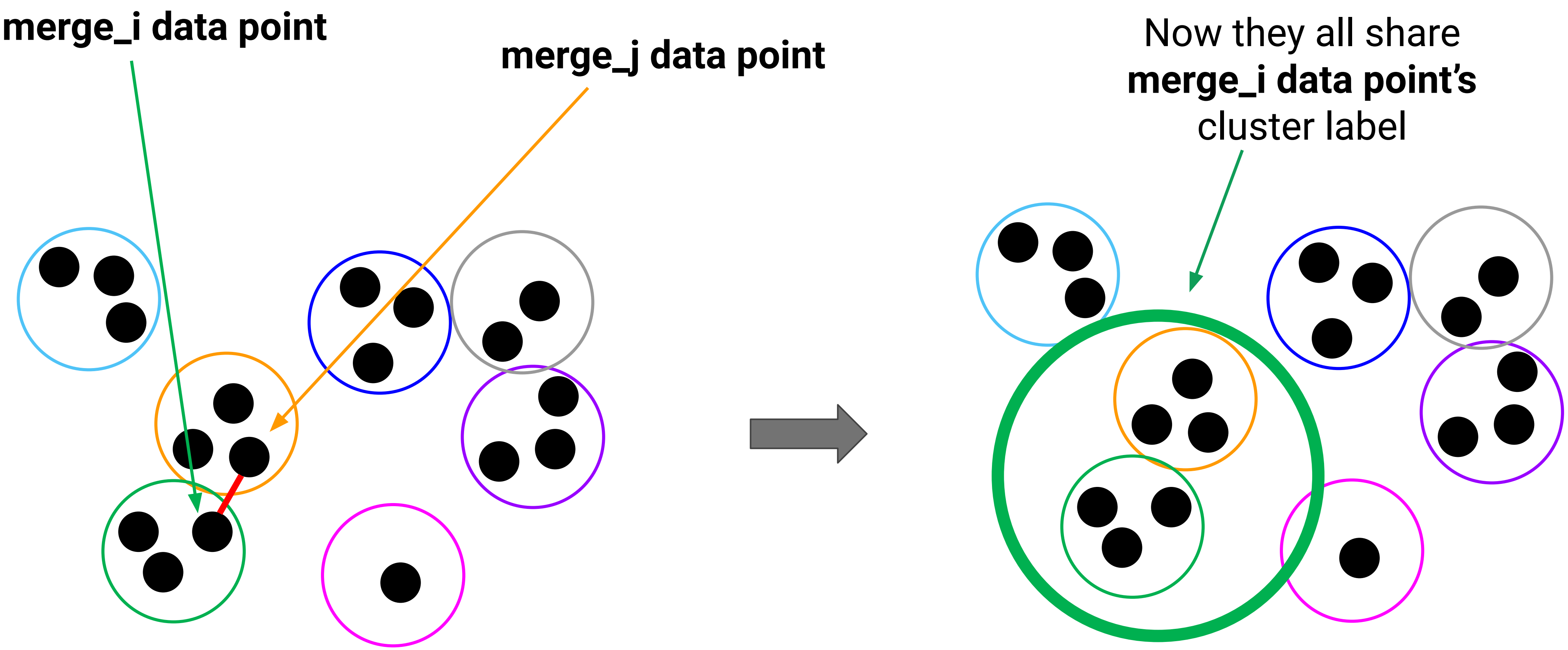
Hierarchical Clustering

- Agglomerative Clustering
  - Level 0: Start from singleton clusters (each example is a cluster).
  - while there remain only *N* clusters:
    - Calculate the distances between all the data pairs from different cluster
    - **Find the closest data pair and merge their clusters into one cluster**



Hierarchical Clustering

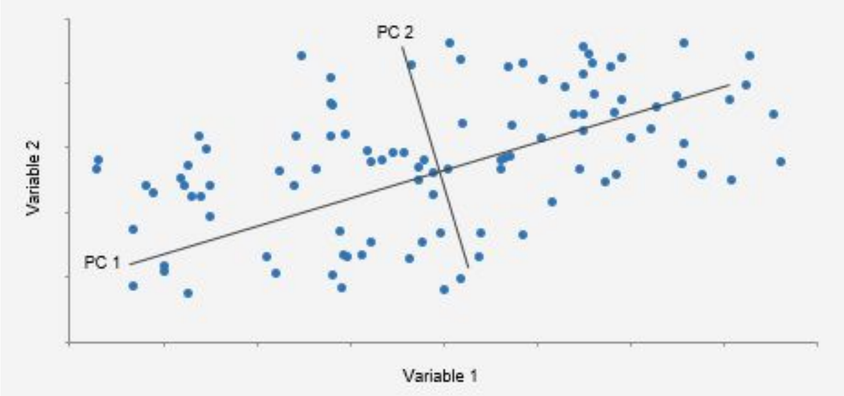
- Complete the method `fit` in the class `HierarchicalClustering`



Dimension Reduction

Principal Component Analysis

- PCA Algorithm
  <u>Step 1</u>. Zero-center (+ and normalize) the data
  <u>Step 2</u>. Estimate the covariance matrix
  <u>Step 3</u>. Perform the **eigenvalue decomposition** of $\hat{\Sigma}$. Then, order them by eigenvalues in decreasing order: $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$
  <u>Step 4</u>. If we choose the first $k << d$ eigenvectors (with largest k eigenvalues) and discard the rest, we get a k-dimensional space such that the original data loses least amount of information (in terms of variance).



Homework 2

Homework 2

- **Due:** 4/30 Tue 6pm
  - No late penalty until 6:30 pm

- **Comments from HW1**
  - **Optimize your code** as much as you can.
  - Submit the code **with your output and without unnecessary output.**
  - Double check your submission.

- We **DO NOT** guarantee to run **unreasonably inefficient codes** for grading.

K-Means Clustering

Image Compression

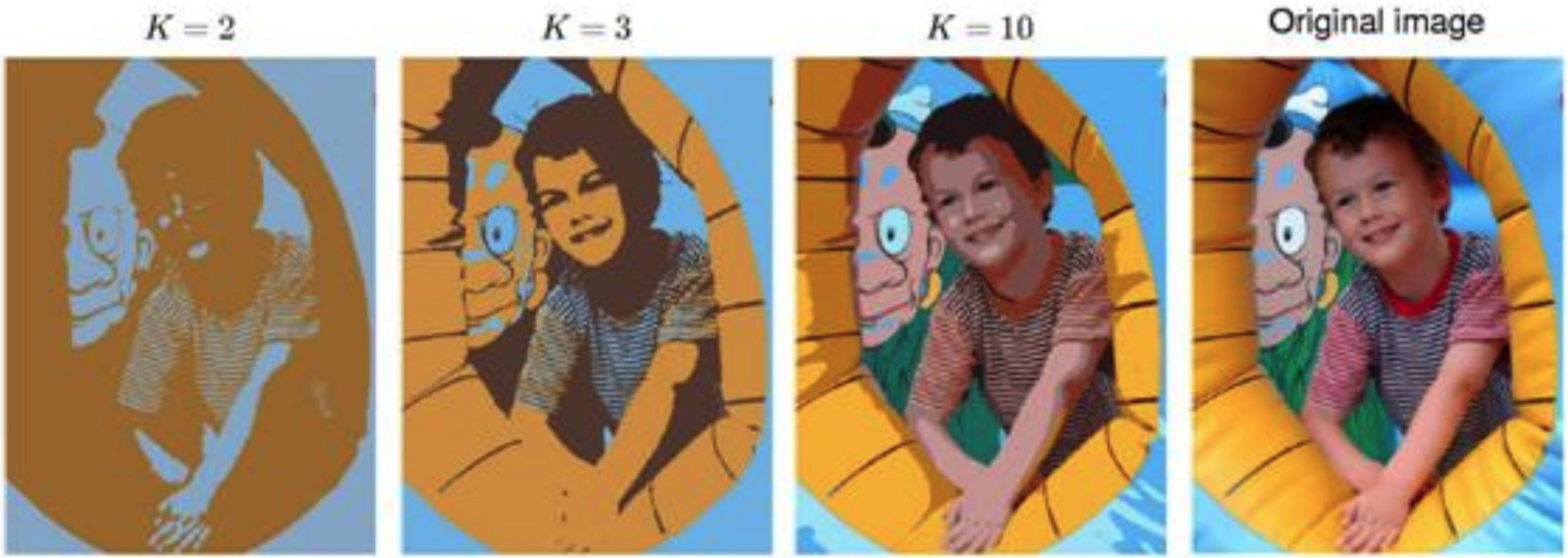


Image Compression

- **Image shape = (Height, Width, Channel)**

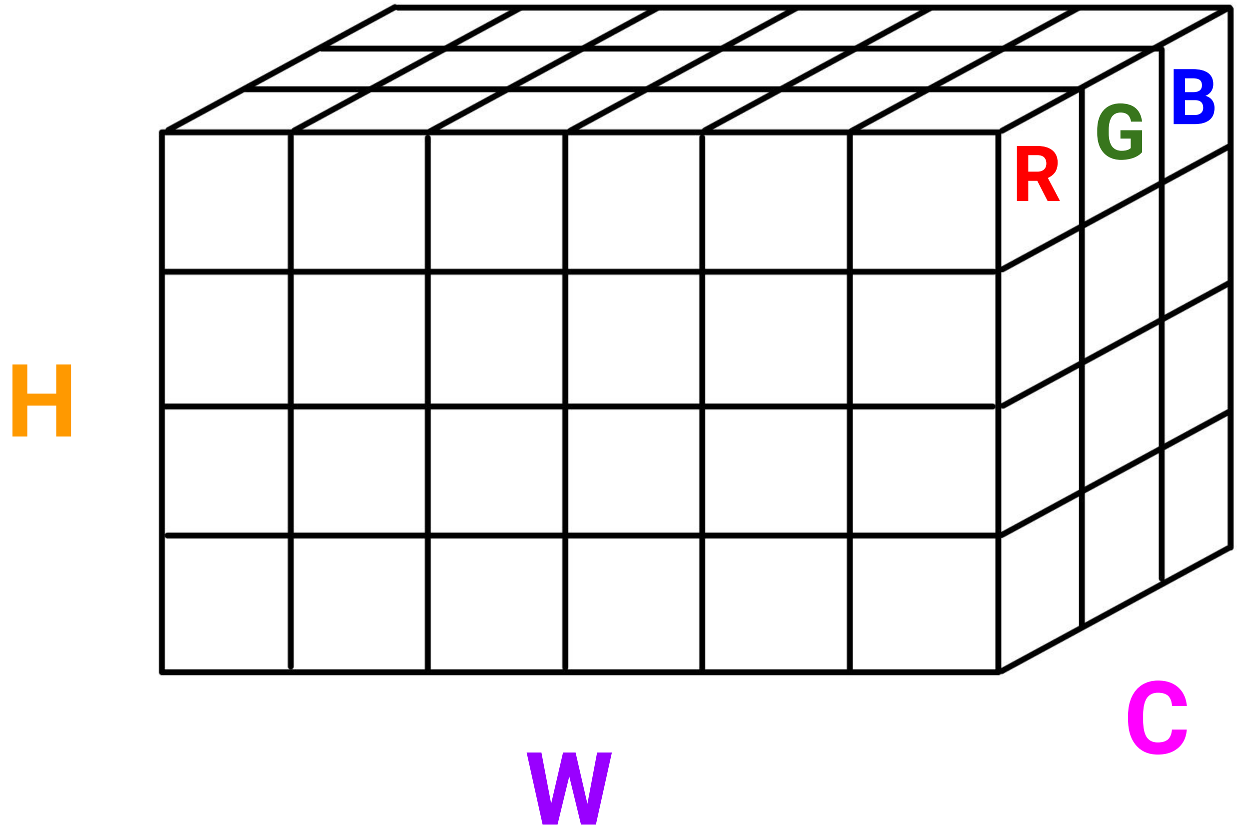
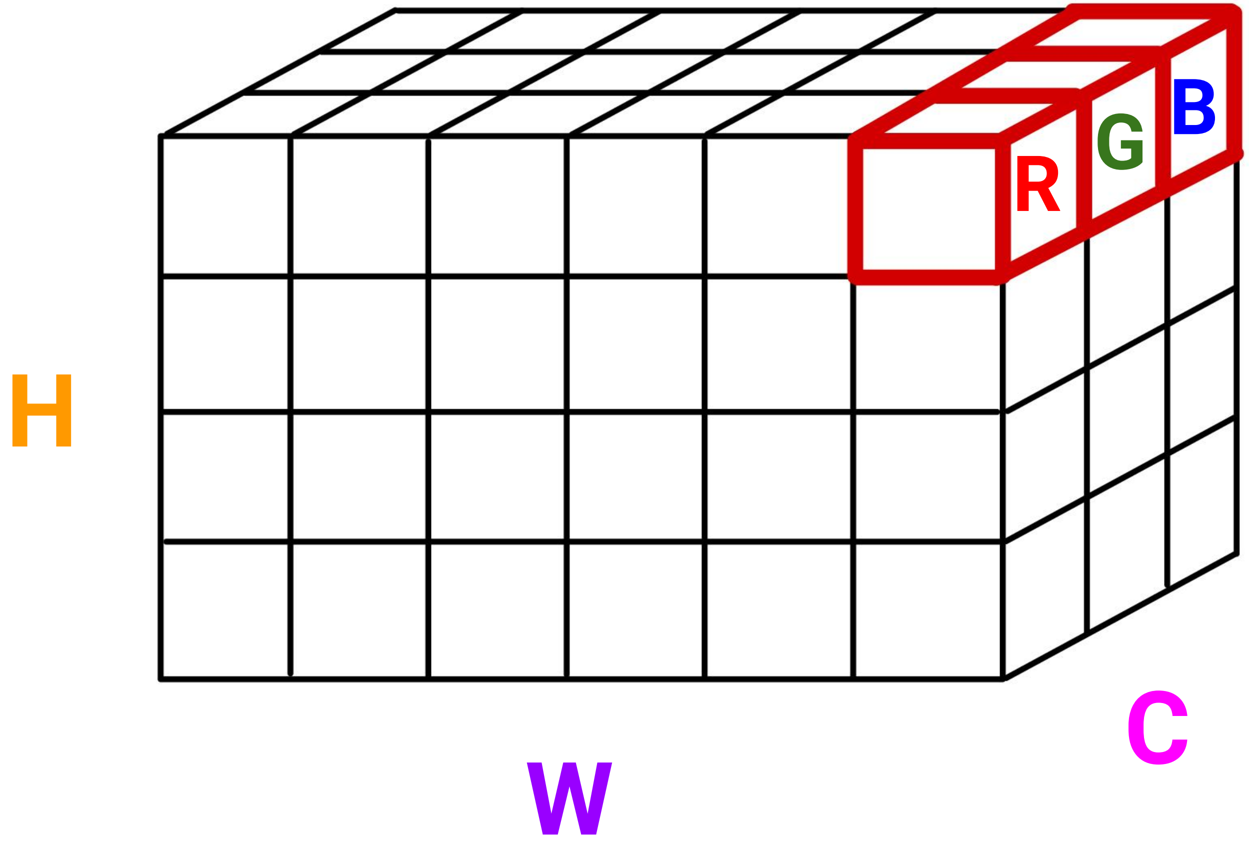


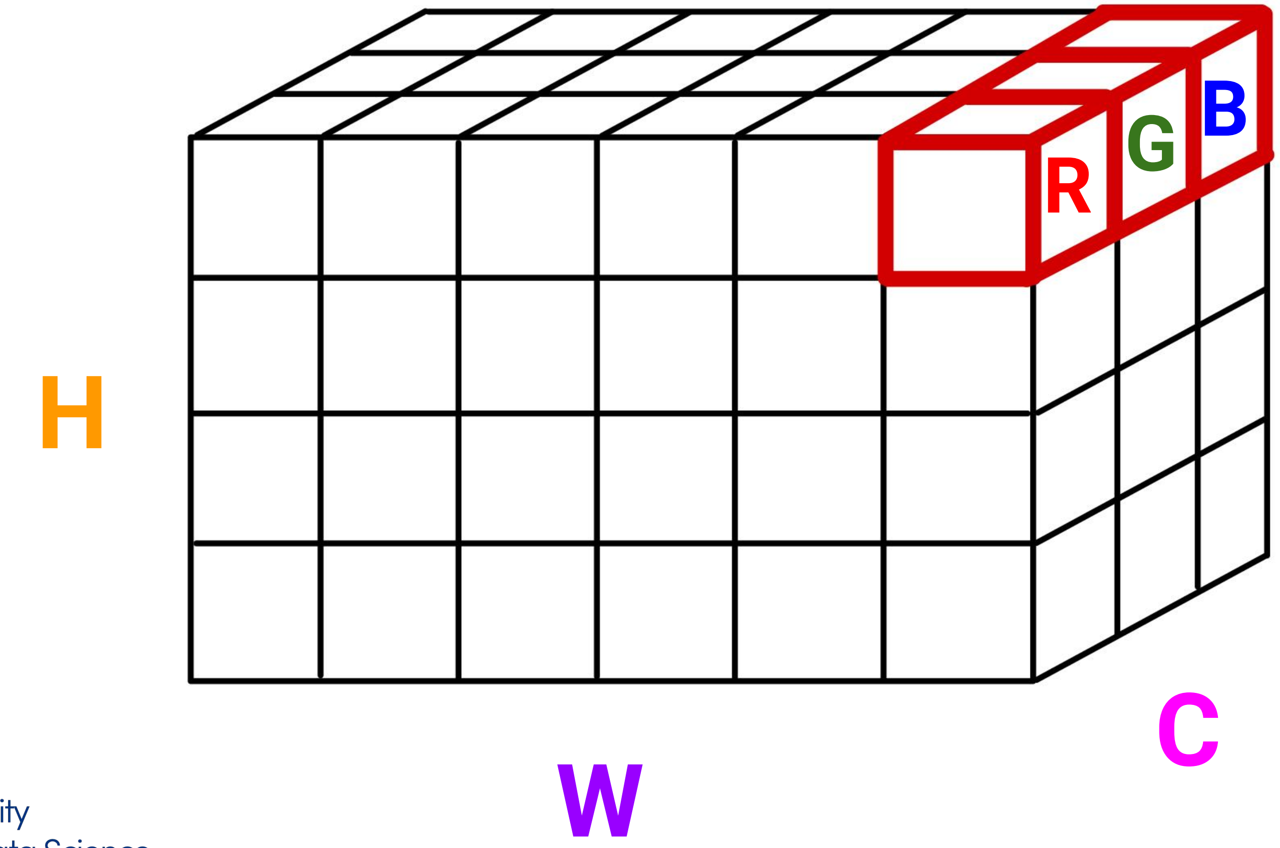
Image Compression

- One pixel value = (R, G, B)



K-Means Clustering Algorithm

1. Randomly initialize the centroids (number of centroids = *K*)
2. **Assign each pixel to the closest centroid**
3. **Calculate the mean of each pixel in the same cluster and update the centroid**
4. **Repeat updating with max_iter times**



K-Means Clustering Algorithm

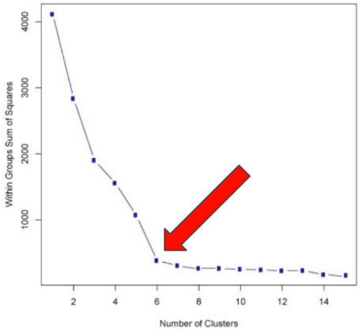
- Decide your *K* according to the value of *J*

K-Means

- How to decide *K*?
  - Usually, we do not know natural distribution of the data.
  - What about choosing the *K* resulting in minimum value of *J*?

$$J = \sum_{i=1}^{N}\sum_{k=1}^{K} r_{i,k}\|x_i - \mu_k\|^2$$

  - Unfortunately, *J* decreases always with larger *K*.



  - If there are natural clusters in the data, you may observe an **elbow point**. Choose it in that case.
  - Life is not that easy. You may not observe such a point...

Classification

Classification

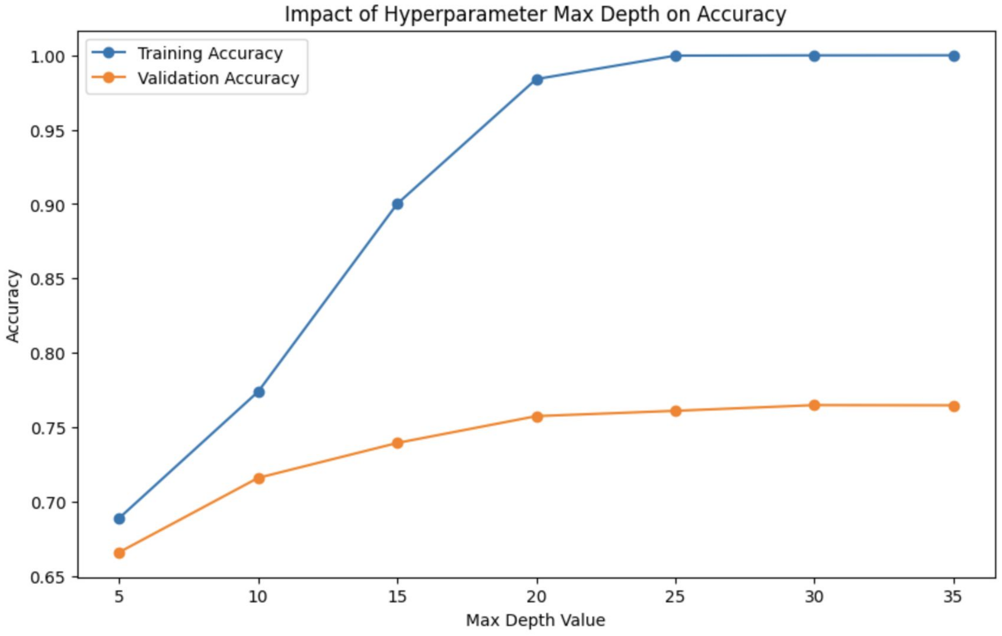
- Classifiers we have learned:
  - discriminant analysis, logistic regression, SVM, Naive Bayes, Random Forest …
- Datasets: (1)diabetes.csv, (2)credit_score.csv
  - For each dataset, implement and train classifier models among the above. (scikit-learn allowed)

Classification

- (a), (c): Train *at least 2* models for each dataset and briefly explain your choice of models. Write the code and report the performances of the models.
  *Make sure your **codes are all run** and the evaluated **model performance is printed out**!*

Classification

- (b), (d): Report the **best model** among the models you've trained.
  - What you should include:
    - **Comparison** of the models you trained in (a)/(c).
    - **Justification** on why you chose the final model.
    - Explanation on the **optimizations** you applied to your model to get the best performance.
      - e.g., regularization, hyperparameter tuning, cross validation,...
      - You will get full credit if you **plot** the process of model optimization. (example below)



Classification

- (e): Discuss the **differences or commonalities between the two datasets** with respect to *why you chose the best model for each dataset.*
    - If you chose the same model for the two datasets, why?
    - If you chose different models for the two datasets, why?