[544] Spark MLlib

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Learning Objectives

- perform common machine learning tasks (train/test split, preprocessing, pipelining, training, prediction, and evaluation) using Spark MLLib
- describe how decision trees make predictions
- describe how the PLANET algorithm (using by Spark decision trees) efficiently trains on large, distributed data

Outline

ML Review

Training/Predicting APIs

Demos

Decision Trees

Machine Learning, Major Ideas

Categories of Machine Learning:

- **Reinforcement learning**: agent makes series of actions to maximize reword
- **Unsupervised learning**: looking for generate patterns
- **Supervised learning:** train models to predict unknowns

Models are functions that return predictions:

```
def my_model(some_info):
    ...
    return some_prediction
```

numeric (1, 2, 3) is "regression"

categorical (A, B, C) is "classification"

Example:

```
def weather_forecast(temp_today, temp_yesterday):
    ...
    return temp_tomorrow
```

Machine Learning, Major Ideas

Categories of Machine Learning:

- **Reinforcement learning**: agent makes series of actions to maximize reword
- **Unsupervised learning**: looking for generate patterns
- **Supervised learning:** train models to predict unknowns

Models are functions that return predictions:

```
def my_model(some_info):
    ...
    return some_prediction
```

computation usually involves some calculations (multiply, add) with various numbers (parameters). Training is finding parameters that result in good predictions for known training data

Example:

```
def weather_forecast(temp_today, temp_yesterday):
    ...
    return temp_tomorrow
```

Learning from Data

	x1	x2	y
0	2	8	5
1	9	2	6
2	4	1	0
3	7	9	7
4	2	2	3
5	3	4	3
6	3	5	9
7	7	1	4
8	6	6	3
9	4	3	?
10	1	2	?
11	2	9	?

- feature columns: x1 and x2
- label column: y

how can the cases where we DO know y help us predict the cases where we do not?

Learning from Data

	x1	x2	y
0	2	8	5
1	9	2	6
2	4	1	0
3	7	9	7
4	2	2	3
5	3	4	3
6	3	5	9
7	7	1	4
8	6	6	3
9	4	3	?
10	1	2	?
11	2	9	?

train

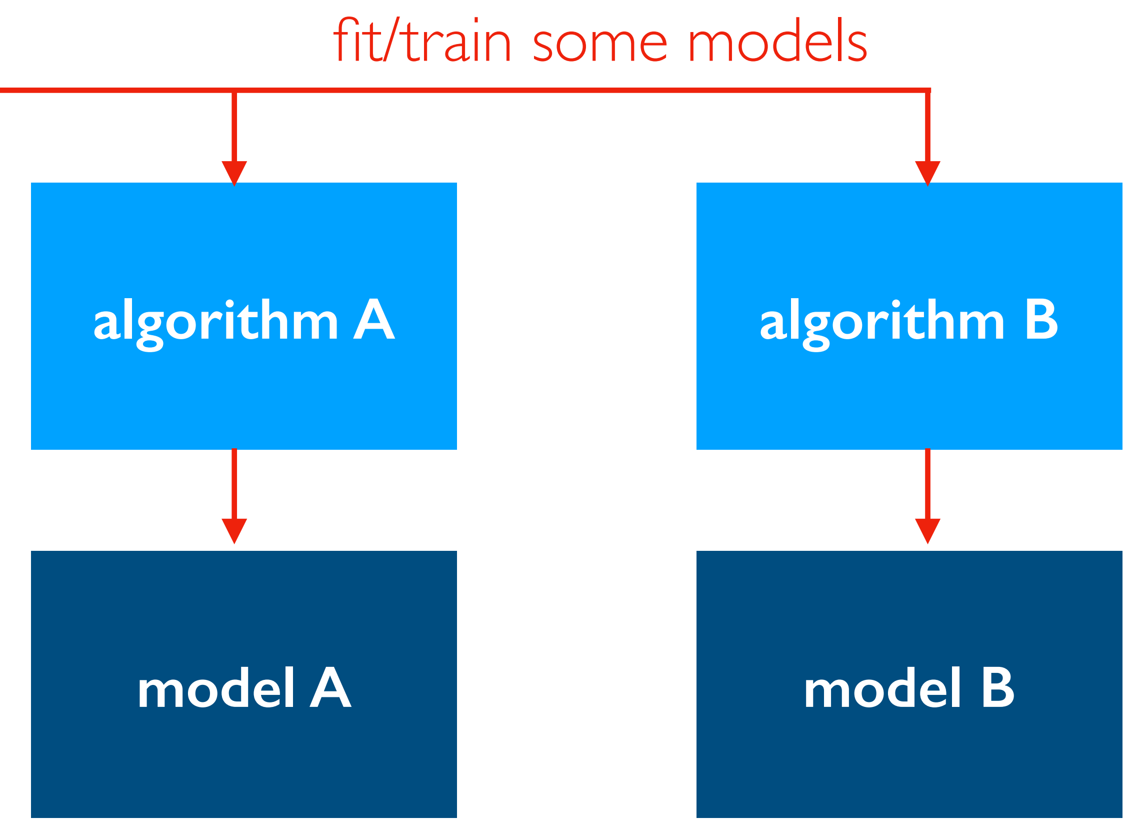
validation

test

random split

Learning from Data

		x1	x2	y
	0	2	8	5
train	1	9	2	6
	2	4	1	0
	3	7	9	7
validation	4	2	2	3
	5	3	4	3
	6	3	5	9
test	7	7	1	4
	8	6	6	3
	9	4	3	?
	10	1	2	?
	11	2	9	?



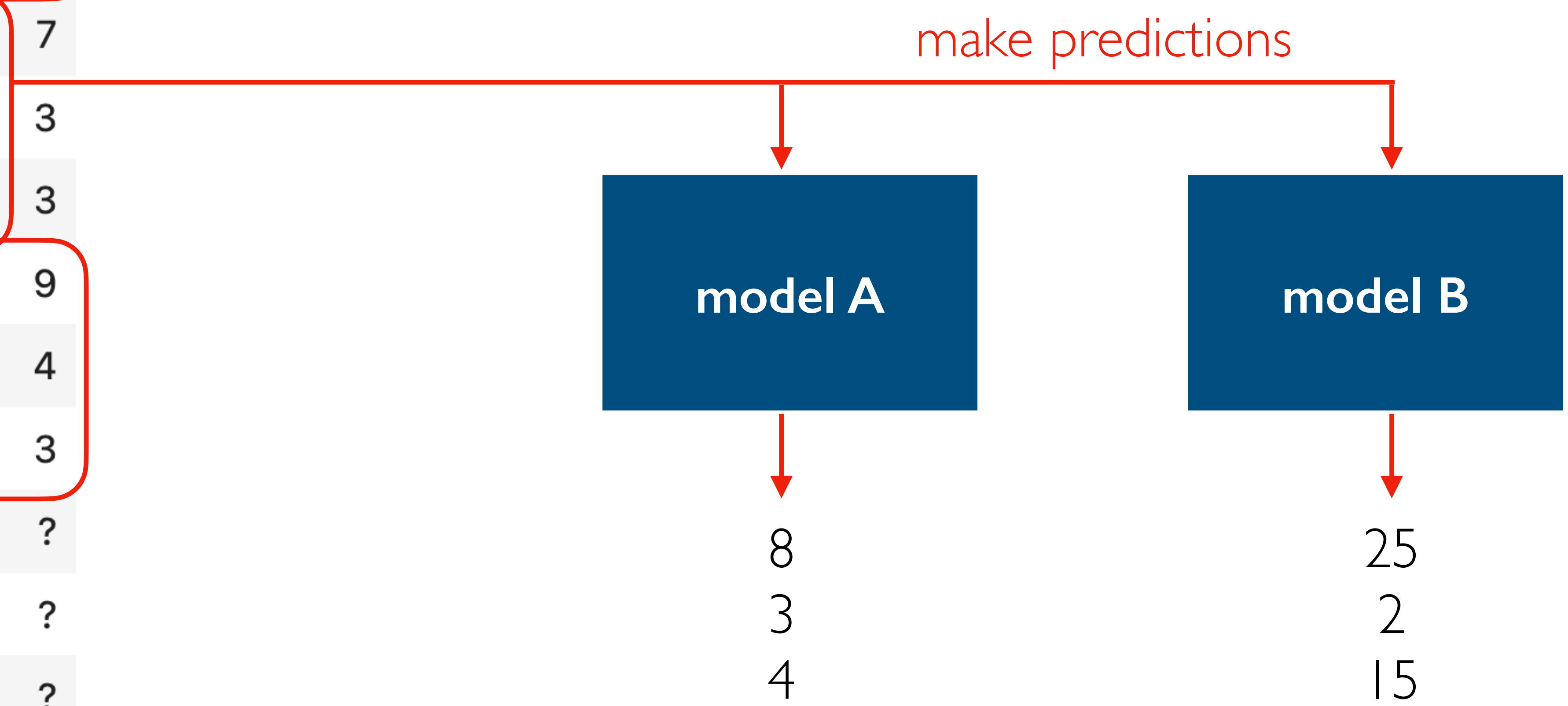
Learning from Data

	x1	x2	y
0	2	8	5
1	9	2	6
2	4	1	0
3	7	9	7
4	2	2	3
5	3	4	3
6	3	5	9
7	7	1	4
8	6	6	3
9	4	3	?
10	1	2	?
11	2	9	?

train

validation

test



Learning from Data

	x1	x2	y
0	2	8	5
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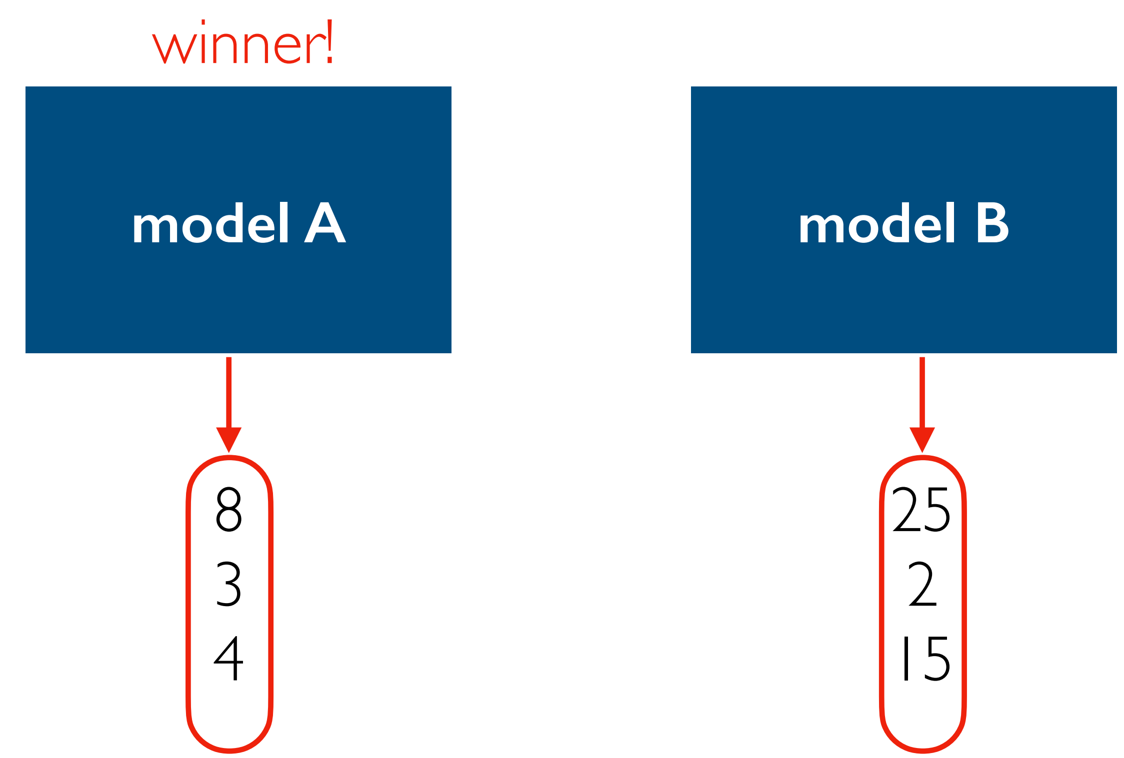
5	3	4	3
6	3	5	9
7	7	1	4
8	6	6	3
9	4	3	?
10	1	2	?
11	2	9	?

train

validation

test

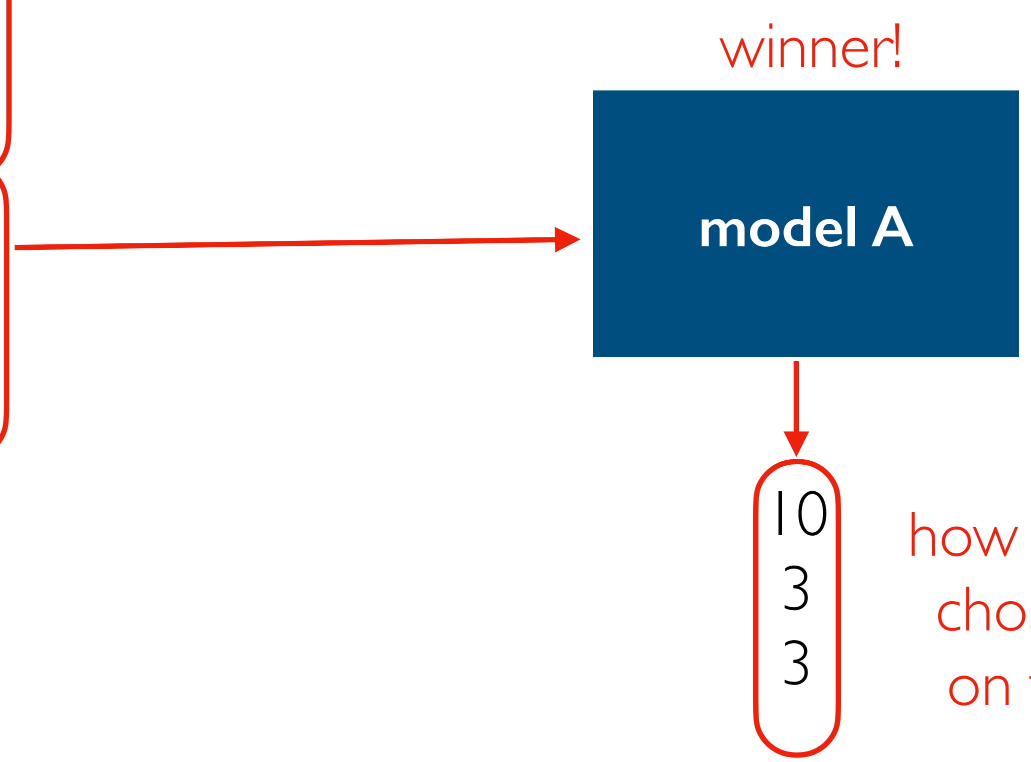
which model predicts better?



Learning from Data

		x1	x2	y
train	**0**	2	8	5
train	**1**	9	2	6
train	**2**	4	1	0
validation	**3**	7	9	7
validation	**4**	2	2	3
validation	**5**	3	4	3
test	**6**	3	5	9
test	**7**	7	1	4
test	**8**	6	6	3
	9	4	3	?
	10	1	2	?
	11	2	9	?

why might the winning model do worse on the test data than the validation data?

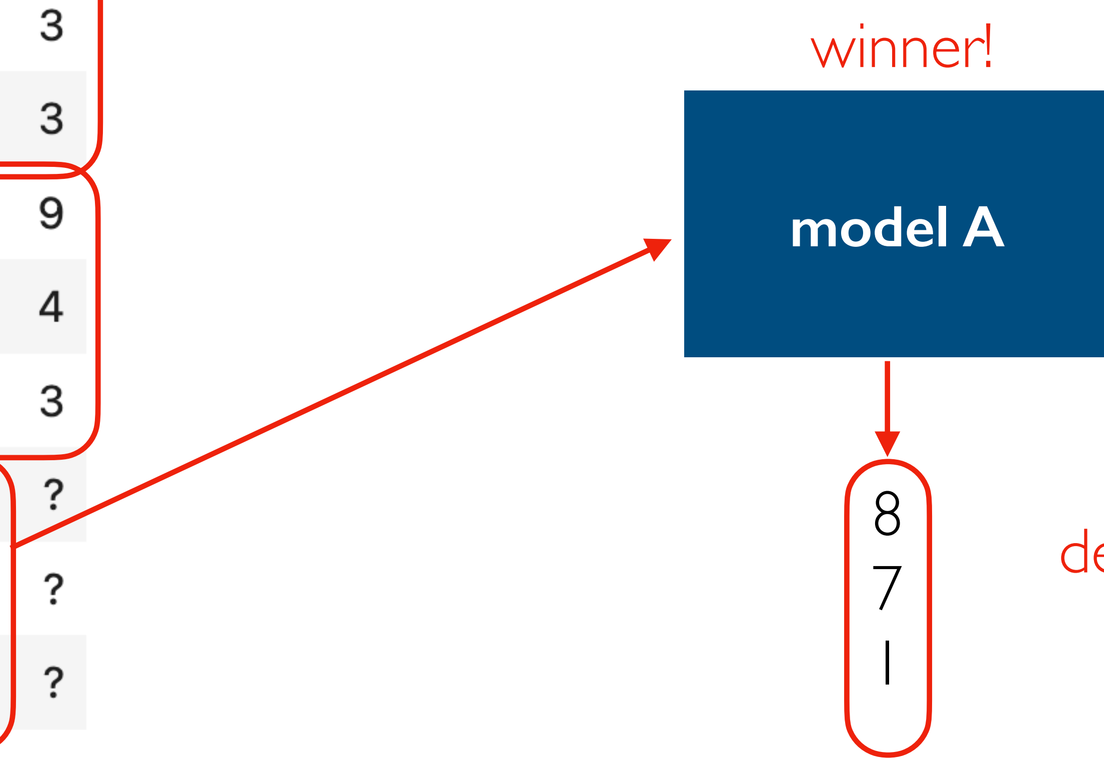


how good does the chosen model do on the test data?

models that do good on train data but bad on validation/test data have "overfitted"

Learning from Data

		x1	x2	y
train	0	2	8	5
	1	9	2	6
	2	4	1	0
validation	3	7	9	7
	4	2	2	3
	5	3	4	3
test	6	3	5	9
	7	7	1	4
	8	6	6	3
	9	4	3	?
	10	1	2	?
	11	2	9	?



deploy the model. Use it for predicting real unknowns!

Outline

ML Review

Training/Predicting APIs

- sklearn
- PyTorch
- Spark MLlib

Demos

Decision Trees

Training

scikit-learn

```
model = ????
model.fit(X, y)
# model parameters can relate X to y
```

pytorch

```
model = ????
# TODO: optimizer, loss function
# training loop
for epoch in range(????):
    for X, y in ????:
        ...
# model parameters can relate X to y
```

- models are mutable
- fitting sets/improves parameters

Spark MLlib

```
unfit_model = ????
fit_model = unfit_model.fit(df)
# fit_model params can relate x to y
```

- models are immutable
- fitting returns new model object

Predicting

scikit-learn

```
y = model.predict(X)
```

pytorch

```
y = model(X)
```

Spark MLlib

```
df2 = fit_model.transform(df)
```

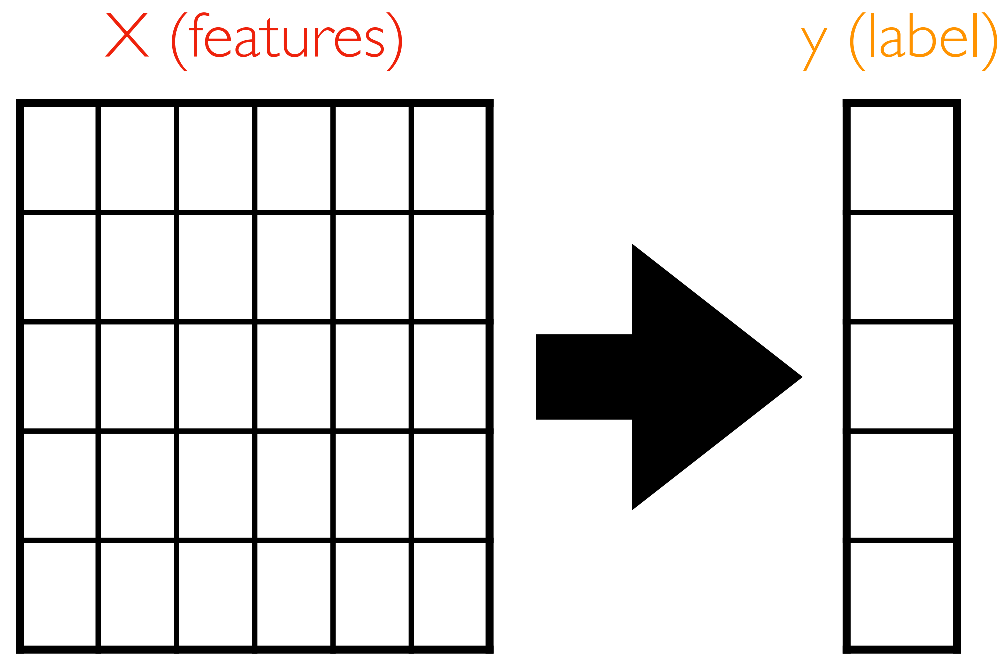
Data

scikit-learn

```
y = model.predict(X)
```

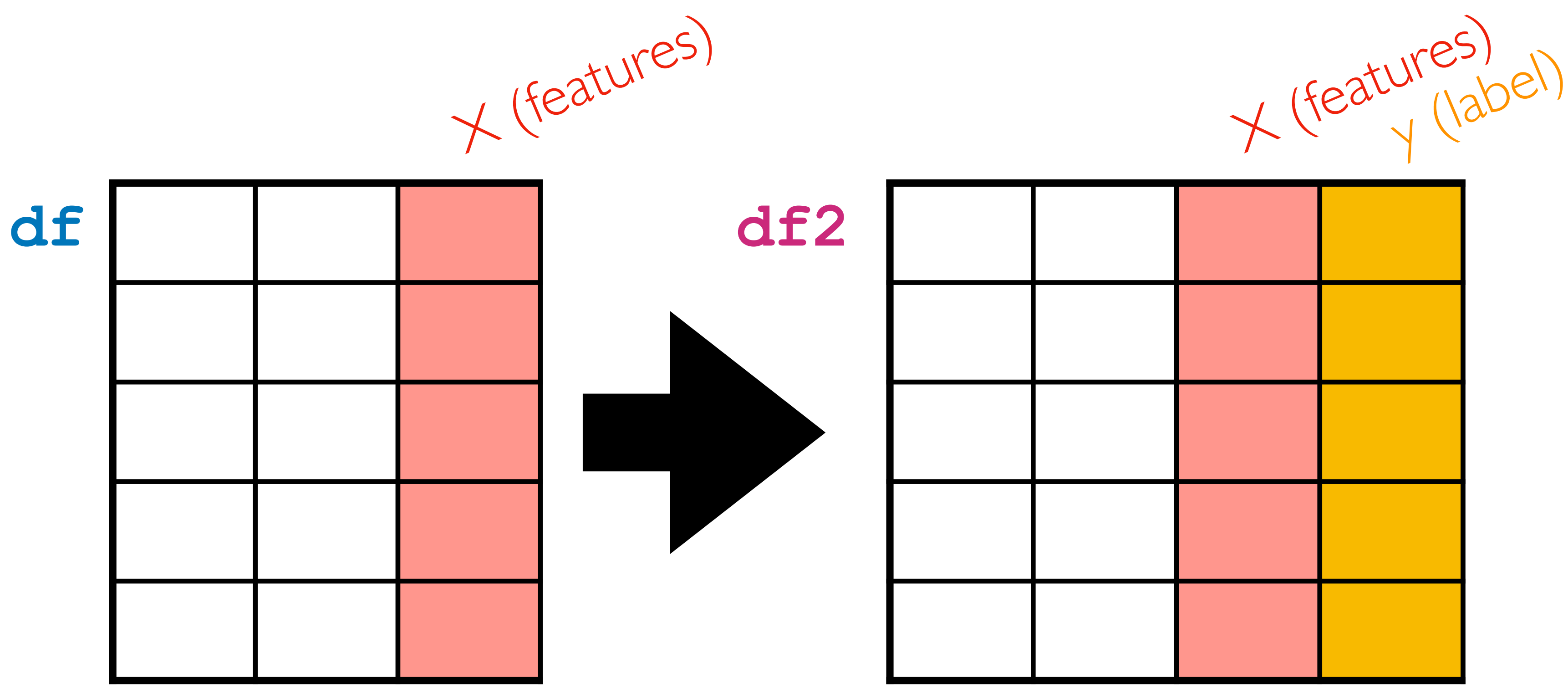
pytorch

```
y = model(X)
```



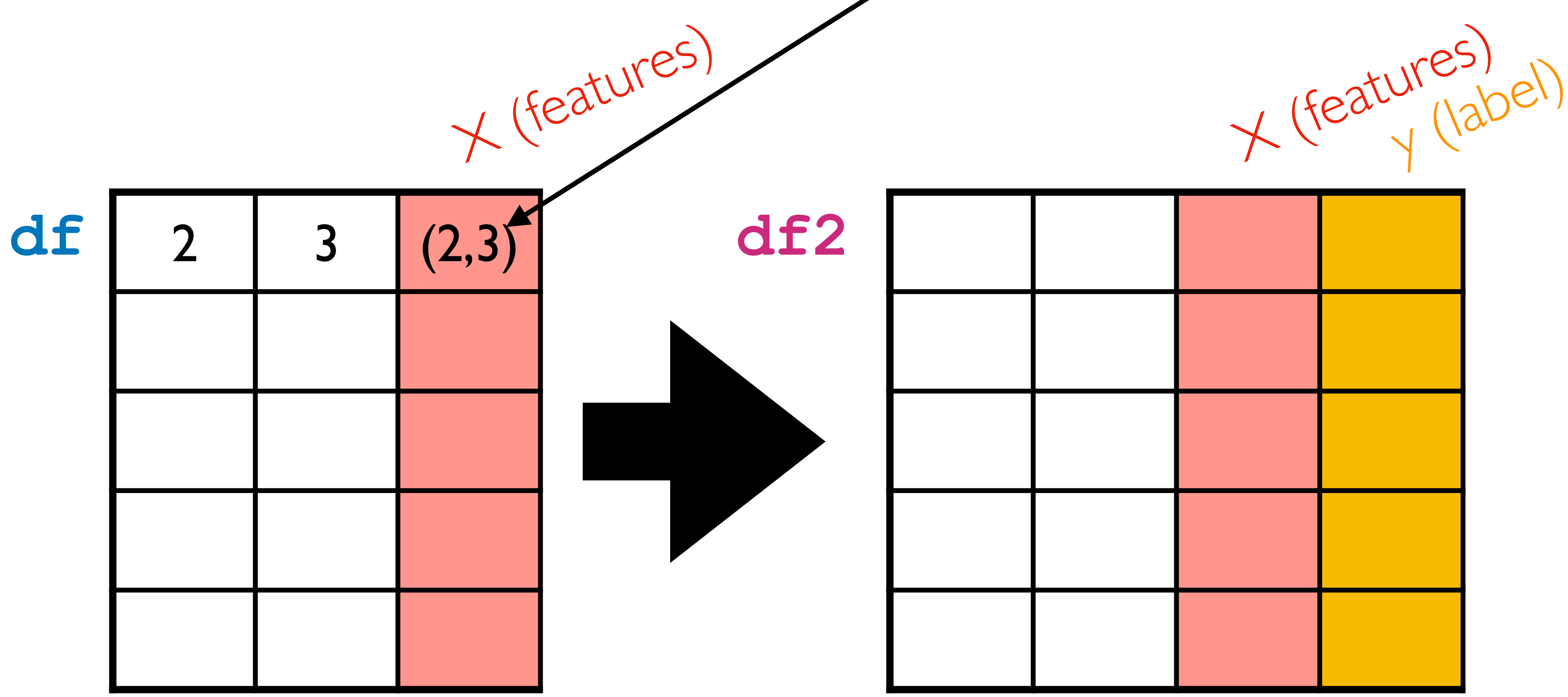
Spark MLlib

```
df2 = fit_model.transform(df)
```



Features Column

- we only get one features column
- it usually contains vectors
- those vectors typically contain values from other columns
- example:
  `(2,3)`



Terminology

Spark and scikit-learn use many of the same terms, with very different meaning.

Transformer (scikit-learn)

- object has .tranform method
- takes a DataFrame, returns a differerent DataFrame
- used as preprocessing step for a model

Transformer (Spark)

- object has .tranform method
- takes a DataFrame, returns original with 1 or more additional columns
- a fitted model is a transformer that adds a prediction column

Estimator (scikit-learn)

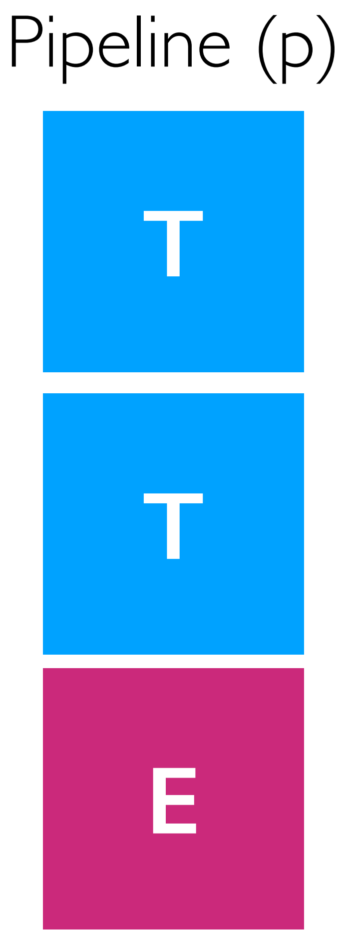
- object has .fit and .predict methods
- .fit **modifies** the object
- makes predictions after learning params

Estimator (Spark)

- object has .fit method that **returns new object**
- an unfitted model is an estimator; calling .fit returns a fitted model (a transformer)

Pipeline

Both scikit-learn and Spark: a pipeline is a series of stages (transformers/estimators). fit/transform/etc. are called as appropriate on each stage.



Pipeline (Spark Example)

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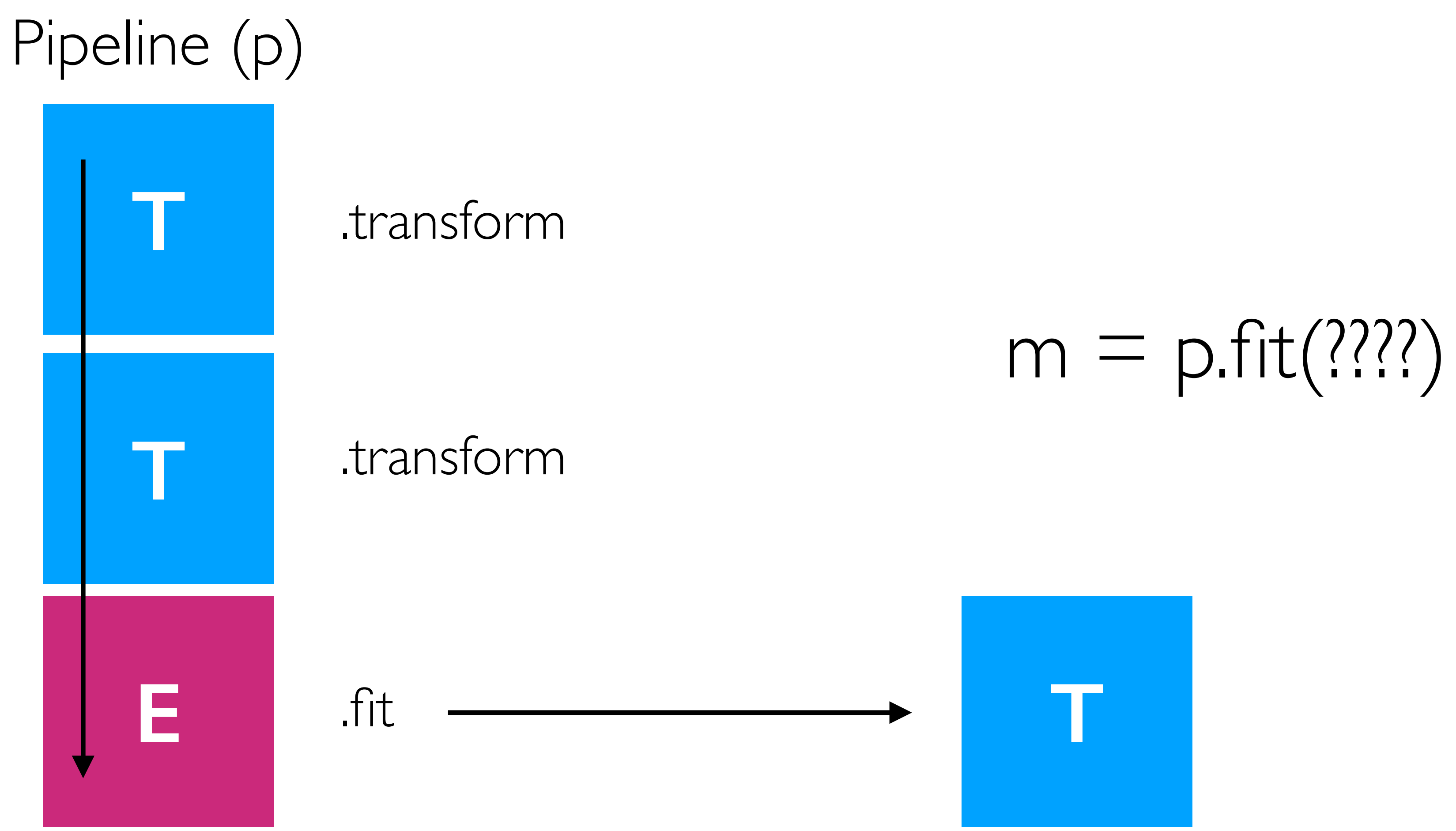

Pipeline (Spark Example)

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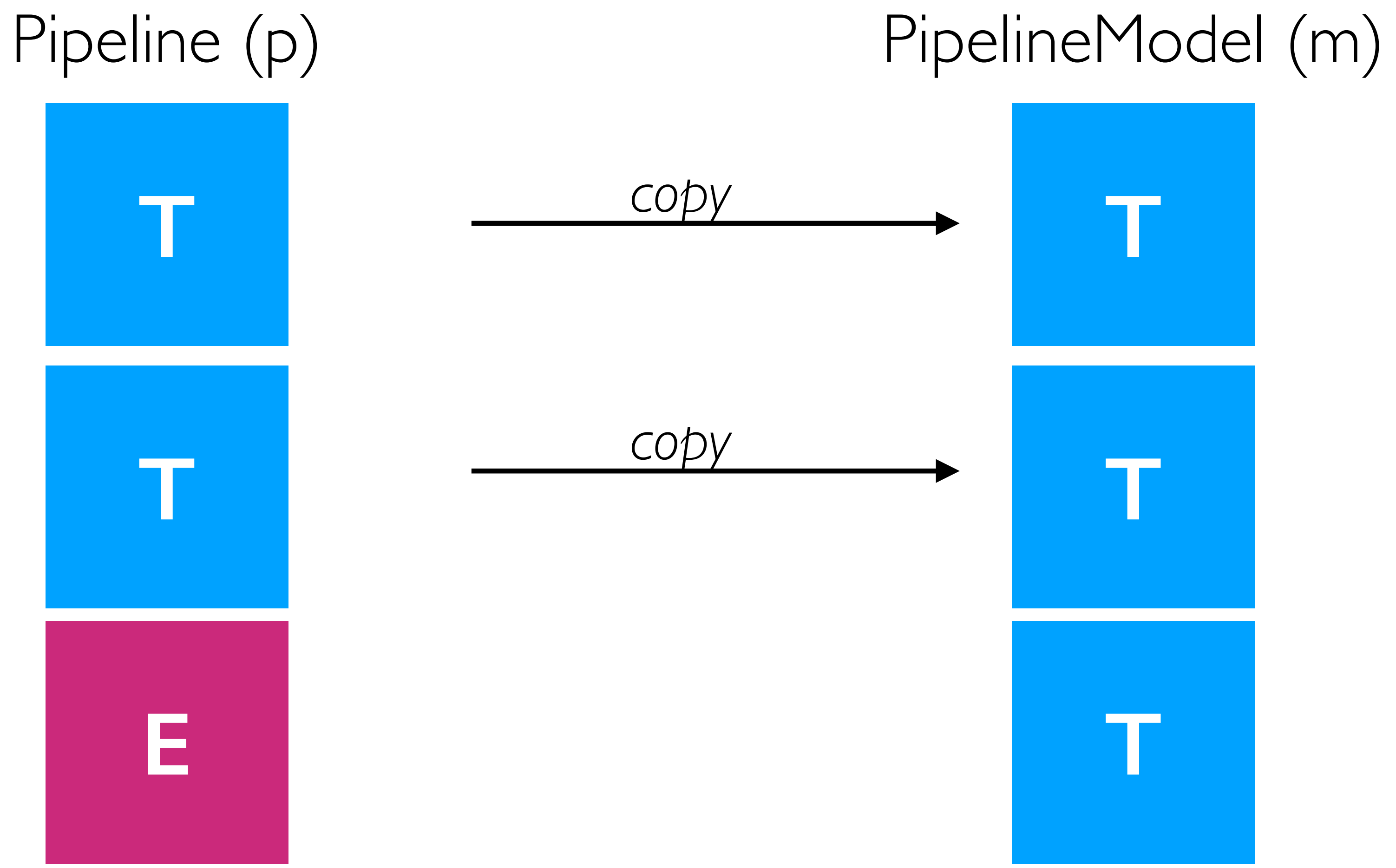

Pipeline (Spark Example)

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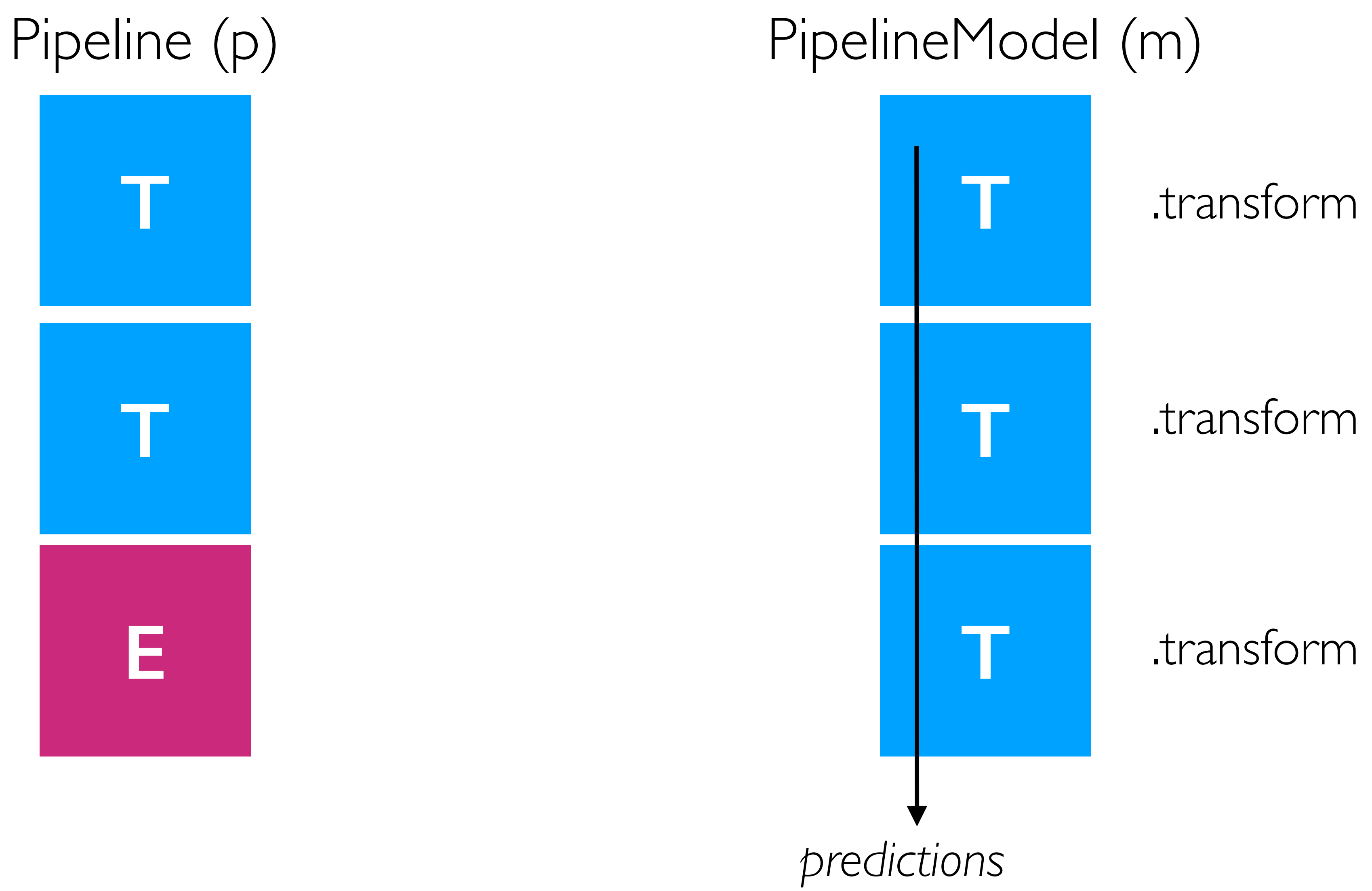

m.transform(????)

TopHat

Outline

ML Review

Training/Predicting APIs

Demos

Decision Trees

Spark mllib packages

- pyspark.mllib -- based on RDDs
- pyspark.ml -- based on DataFrames

Distribued ML Outline

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Decision Trees:

- Background
- Training in memory
- PLANET algorithm

Decision Trees

problem: if the tree is large, many subtrees might be similar

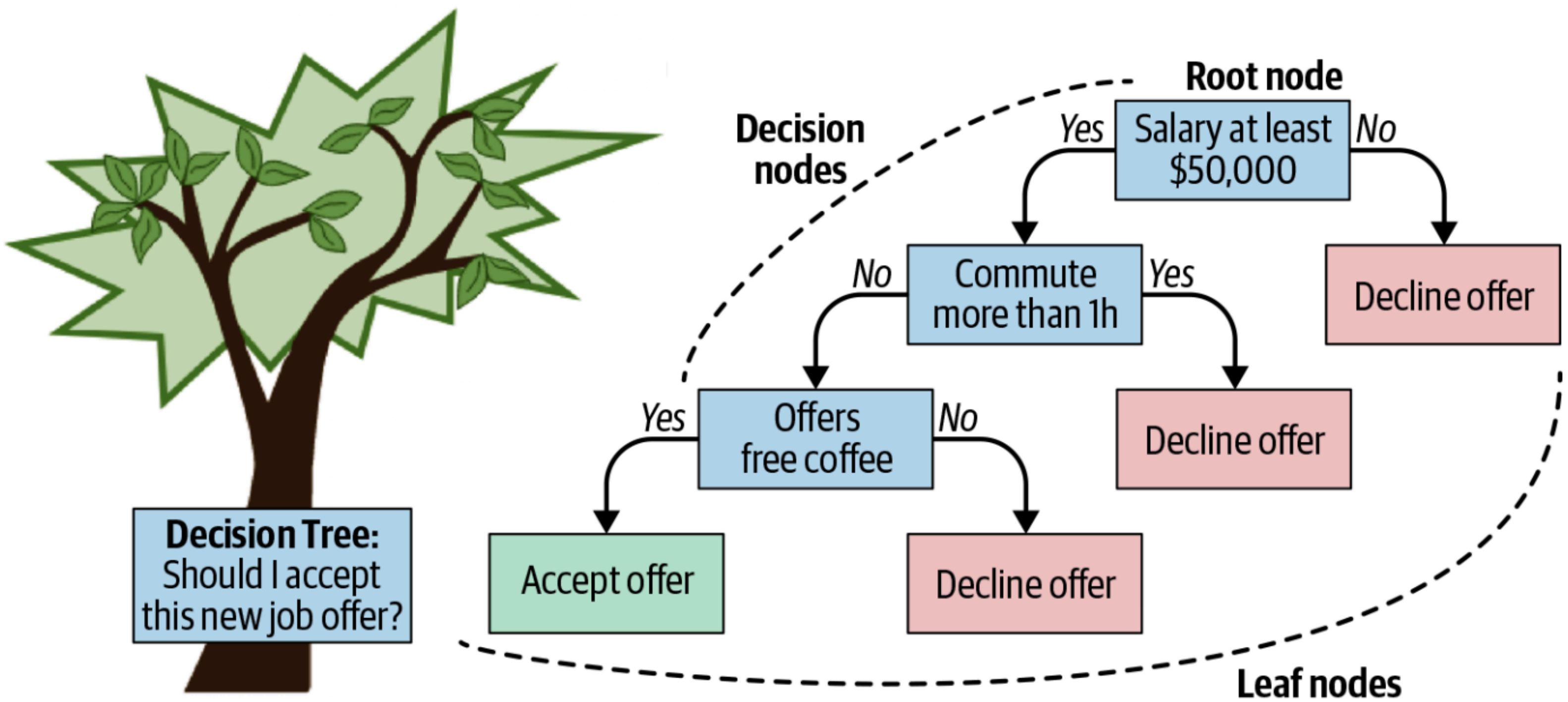
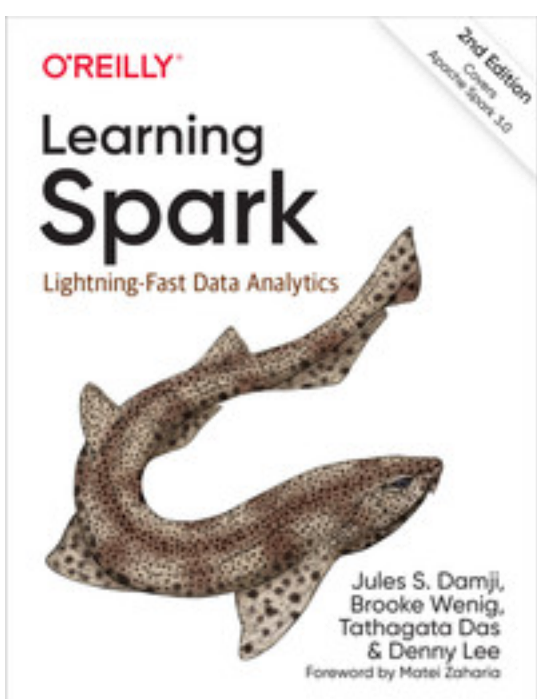


Figure 10-9. Decision tree example

decision trees are like nested if/else statements

features and labels can be numeric or categorical




```
def predict(row):
  if row.salary < 50K:
    return False
  else:
    if row.commute > 1h:
      return False
    else:
      if row.coffee == "free":
        return True
      else:
        return False
```

Ensemble Methods

Ensemble: many simple models vote. Many simple decision trees (each trained on subset of rows/columns) together are often better than one big tree. Examples:

- random forest
- gradient-boosted trees

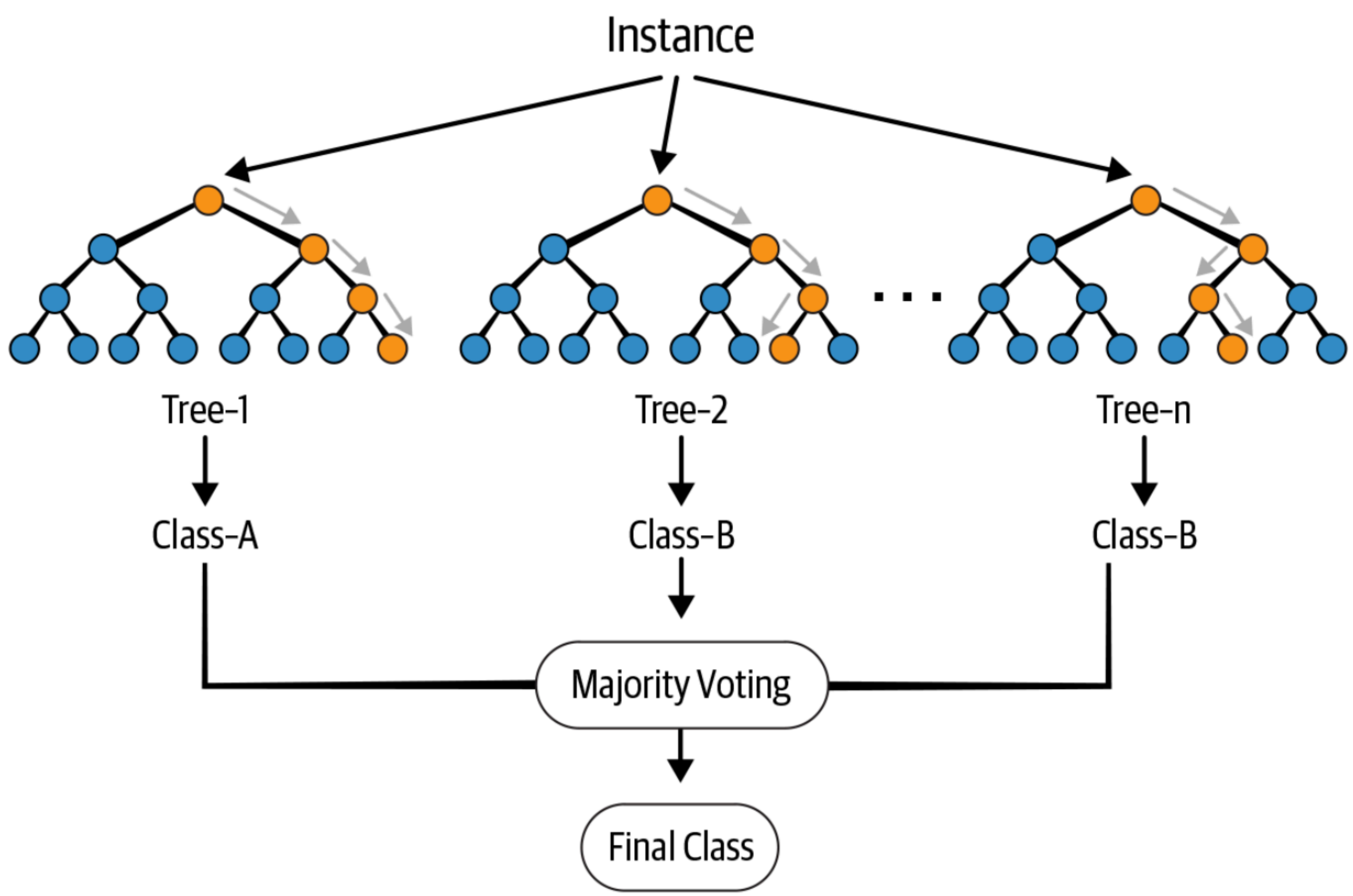
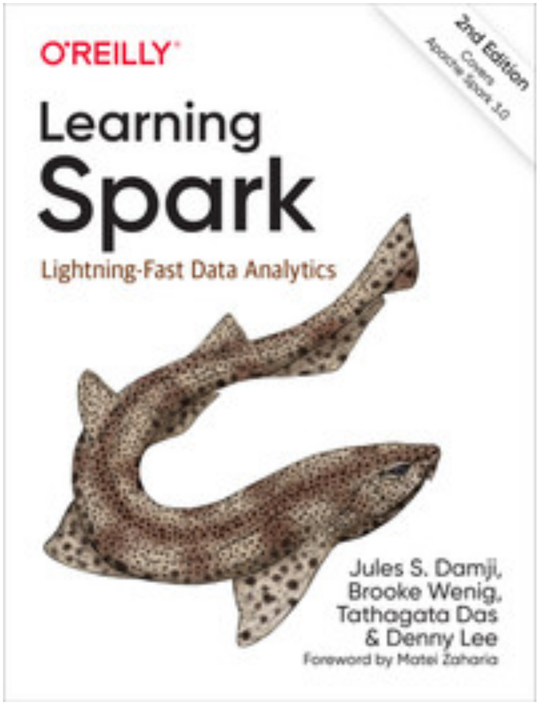
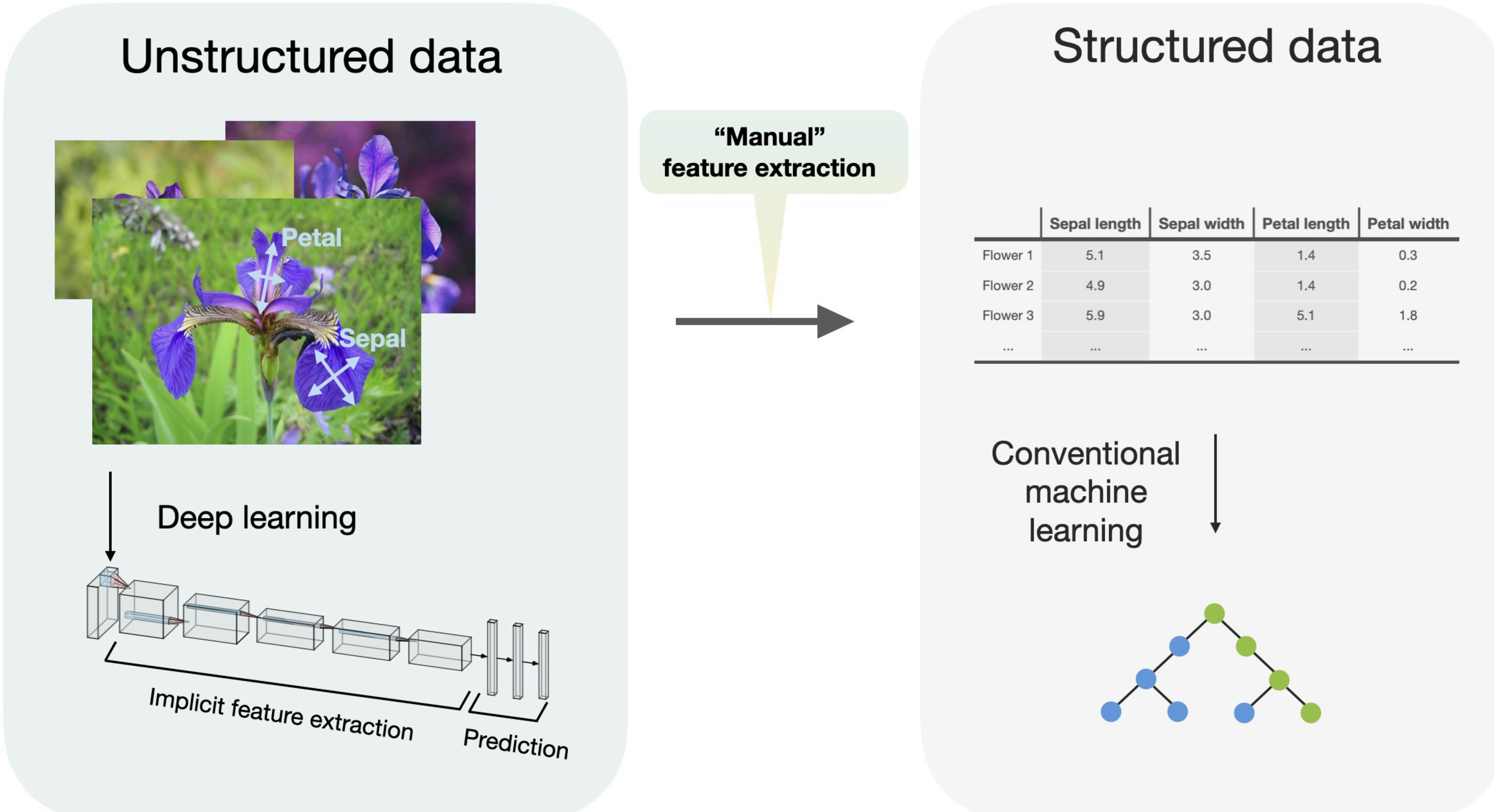


Figure 10-12. Random forest predictions



A Spark cluster can train many trees in a random forest simultaneously!

Tree methods vs. Deep Learning



	Sepal length	Sepal width	Petal length	Petal width
Flower 1	5.1	3.5	1.4	0.3
Flower 2	4.9	3.0	1.4	0.2
Flower 3	5.9	3.0	5.1	1.8
...	...	...	...	...

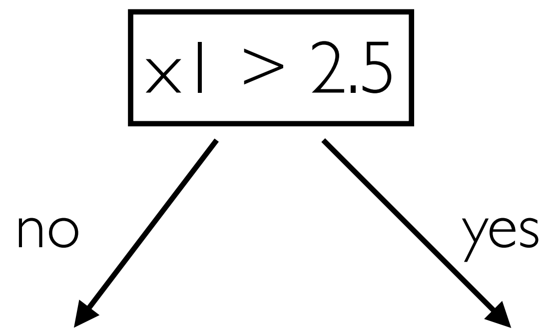
Image from Blog Post: A Short Chronology Of Deep Learning For Tabular Data, by Sebastian Raschka
https://sebastianraschka.com/blog/2022/deep-learning-for-tabular-data.html

Tree-based methods are ***still relevant*** *in the age of deep learning because there are many important tabular datasets.*

Is a Tree Good?

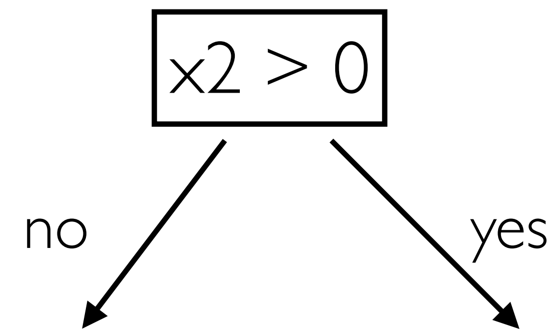
data:

x1	x2	y
1	-1	5
2	2	8.6
3	3	8.8
4	-2	5.2



x1	x2	y
1	-1	5
2	2	8.6

x1	x2	y
3	3	8.8
4	-2	5.2



x1	x2	y
1	-1	5
4	-2	5.2

x1	x2	y
2	2	8.6
3	3	8.8

which tree asks better questions about x values if we want to predict y?

Impurity

data:

x1	x2	y
1	-1	5
2	2	8.6
3	3	8.8
4	-2	5.2

x1 > 2.5

no

x1	x2	y
1	-1	5
2	2	8.6

high variance

yes

x1	x2	y
3	3	8.8
4	-2	5.2

high variance

better tree

x2 > 0

no

x1	x2	y
1	-1	5
4	-2	5.2

low variance

yes

x1	x2	y
2	2	8.6
3	3	8.8

low variance

"impurity" measures (like variance) measure how non-uniform label (y) values are in leaves

Predictions

data:

x1	x2	y
1	-1	5
2	2	8.6
3	3	8.8
4	-2	5.2
3	50	????

if a new data point lands in a leaf, assume it is similar to other rows in that leaf...

better tree

$\boxed{x2 > 0}$

no

x1	x2	y
1	-1	5
4	-2	5.2

prediction: 5.1

yes

x1	x2	y
2	2	8.6
3	3	8.8

prediction: 8.7

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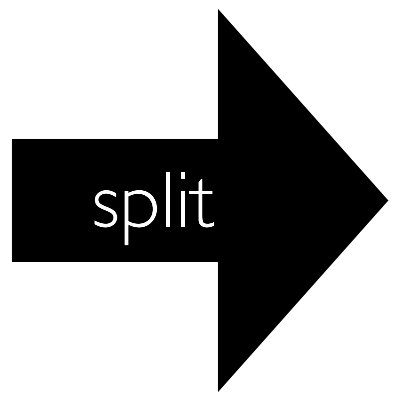
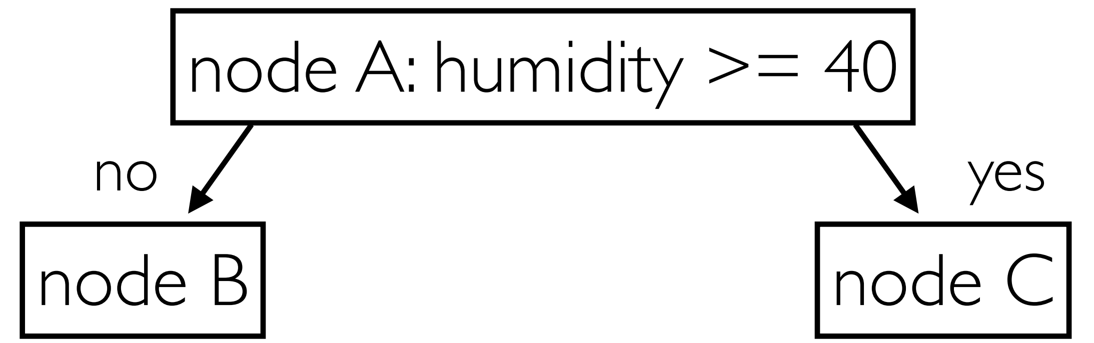
Splitting Nodes

node A

temp	humidity	rain
80	45	no
50	40	yes
45	20	no
70	25	no

probability: 25%





node B

temp	humidity	rain
45	20	no
70	25	no

probability: 0%

node C

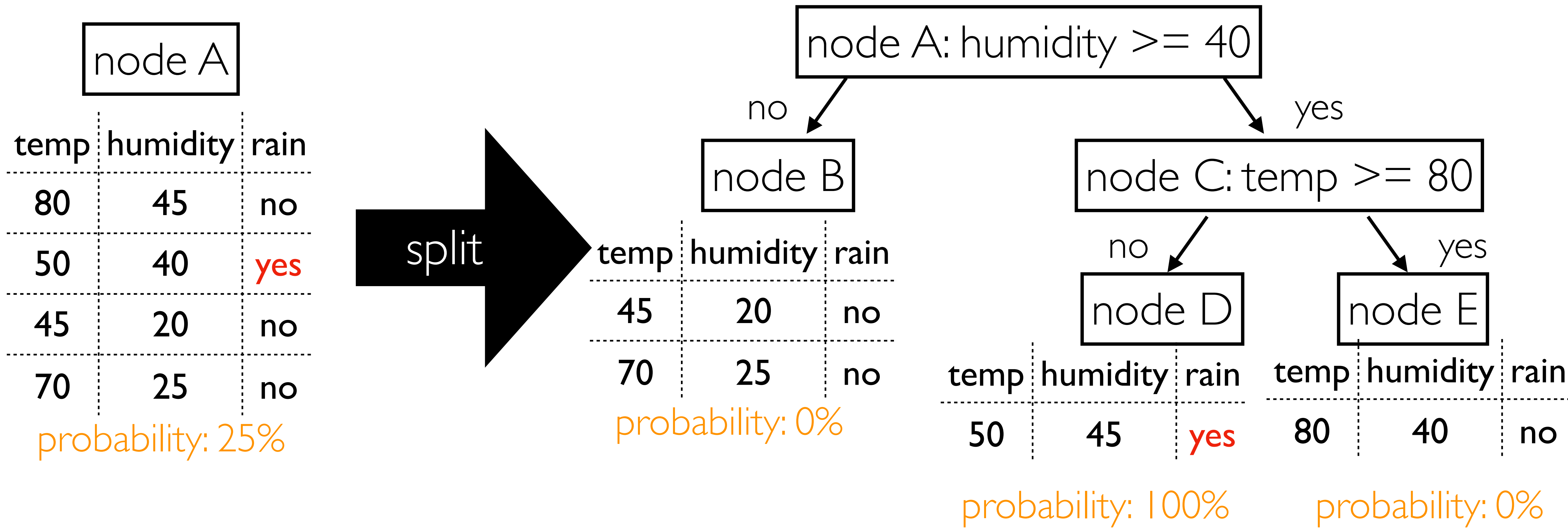
temp	humidity	rain
80	40	no
50	45	yes

probability: 50%

Algorithm

- start with one node with all data
- find split point in some column to create two children
- identify another node, recursively split
- eventually stop

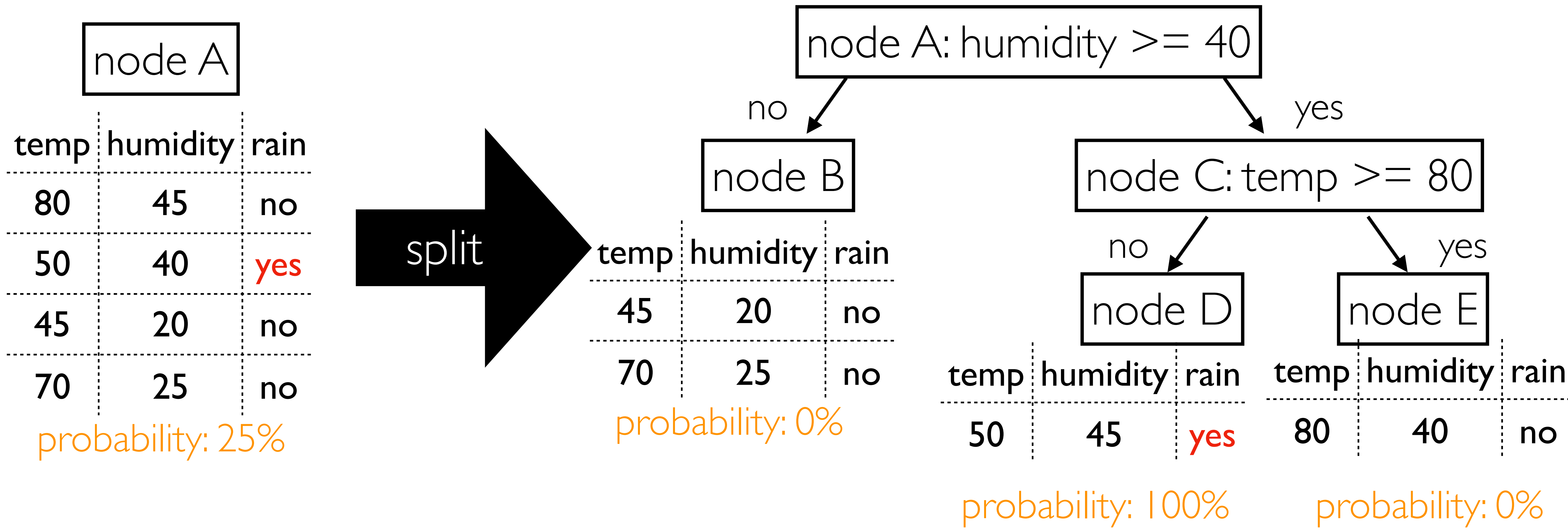
Splitting Nodes



Algorithm

- start with one node with all data
- find split point in some column to create two children
- identify another node, recursively split
- eventually stop

When to Stop Splitting?

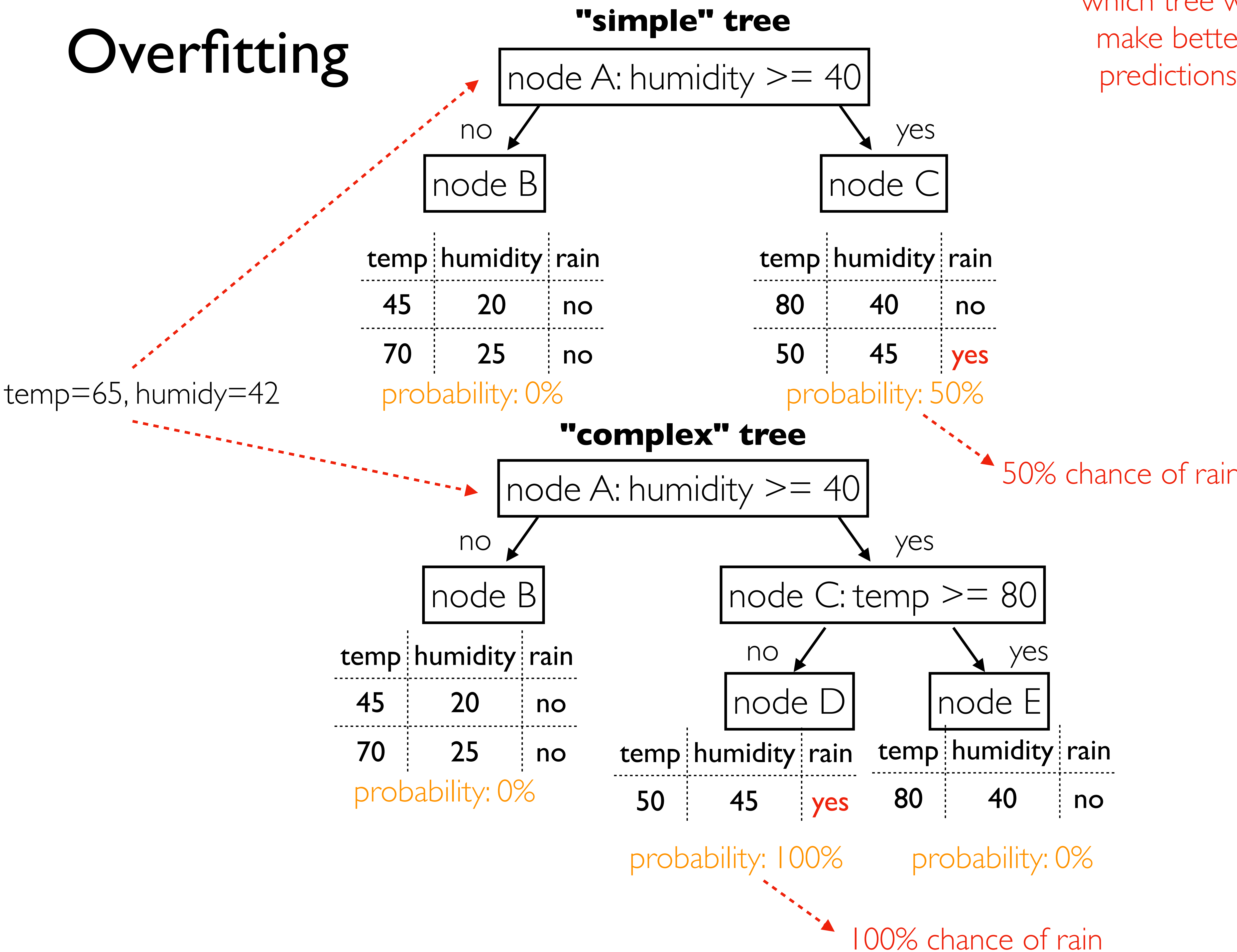


Some Approaches

- set maximum tree height
- set minimum number of rows in node required for split
- prune tree later to get rid of unhelpful/excessive splitting

Overfitting

which tree will make better predictions?



Choosing Splits

node A

temp	humidity	rain
80	45	no
50	40	yes
45	20	no
70	25	no

probability: 25%

split

Which node to split?

- 2 feature columns
- 3 ways to divide 4 rows into big small
- 2*3 = 6 choices
- try all, choose one that reduces impurity the most!
- how to do so efficiently?

Choosing Splits

node A

temp	humidity	rain
80	45	no
50	40	yes
45	20	no
70	25	no

sort by each column

temp	humidity	rain
45	20	no
50	40	yes
70	25	no
80	45	no

calculate impurity for each split (one pass)

left no	left yes	right no	right yes	impurity
1	0	2	1	...
1	1	2	0	...
2	1	1	0	...

Observation: we can incrementally compute impurity for each split point by looking at just one more row of data. Don't need to loop over all rows for every possible split point.

Choosing Splits

node A

temp	humidity	rain
80	45	no
50	40	yes
45	20	no
70	25	no

sort by each column

temp	humidity	rain
45	20	no
50	40	yes
70	25	no
80	45	no

temp	humidity	rain
45	20	no
70	25	no
50	40	yes
80	45	no

calculate impurity for each split (one pass)

left no	left yes	right no	right yes	impurity
1	0	2	1	...
1	1	2	0	...
2	1	1	0	...

left no	left yes	right no	right yes	impurity
1	0	2	1	...
2	0	1	1	...
2	1	1	0	...

choose best

Challenge: Big Data

node A

temp	humidity	rain
80	45	no
50	40	yes
45	20	no
70	25	no

sort by each column

temp	humidity	rain
45	20	no
50	40	yes
70	25	no
80	45	no

...

What if rows for a node are too big to fit in RAM on one worker?

- partitioned across many Spark workers
- maybe fits in cumulative RAM of many workers (or maybe not)
- each sort would be expensive (network shuffle/exchange)
- if looping over every possible split point, we'll be computing on one worker at any given time (the one that has data around the split point). Not parallel!

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PLANET Algorithm

PLANET: Massively Parallel Learning of Tree Ensembles with MapReduce

Biswanath Panda, Joshua S. Herbach, Sugato Basu, Roberto J. Bayardo
Google, Inc.
[bpanda, jsherbach, sugato]@google.com, bayardo@alum.mit.edu

ABSTRACT

Classification and regression tree learning on massive datasets is a common data mining task at Google, yet many state of the art tree learning algorithms require training data to plexities such as data partitioning, scheduling tasks across many machines, handling machine failures, and performing inter-machine communication. These properties have motivated many technology companies to run MapReduce

https://static.googleusercontent.com/media/research.google.com/en//pubs/archive/36296.pdf

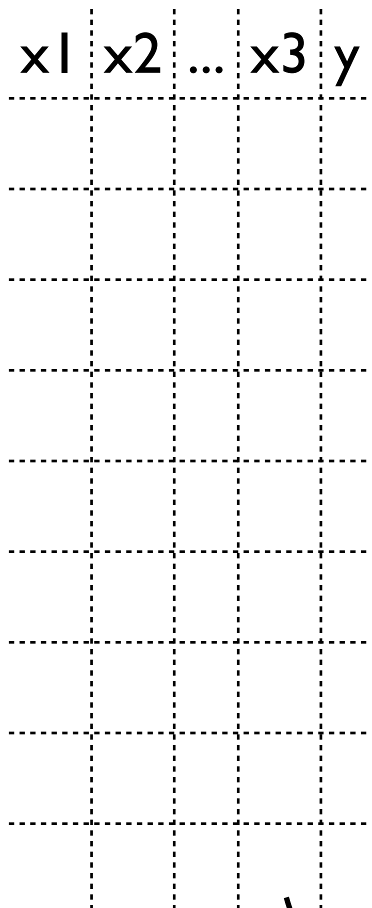
PLANET: Parallel Learner for Assembling Numerous Ensemble Trees

- originally implemented as MapReduce jobs
- Spark DecisionTreeRegressor and DecisionTreeClassifier use it too

Hybrid Approach

- in-memory splitting for nodes with few enough rows to fit in worker memory
- simplified (fewer split points) and distributed approach for nodes with lots of data

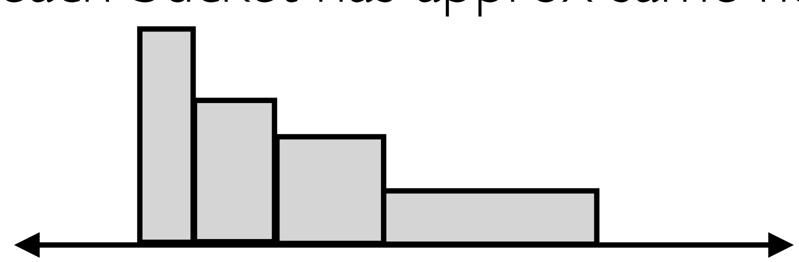
Step 1: Compute Equi-Depth Histograms



Warning: number of bins must be greater than biggest number of unique values in any categorical column

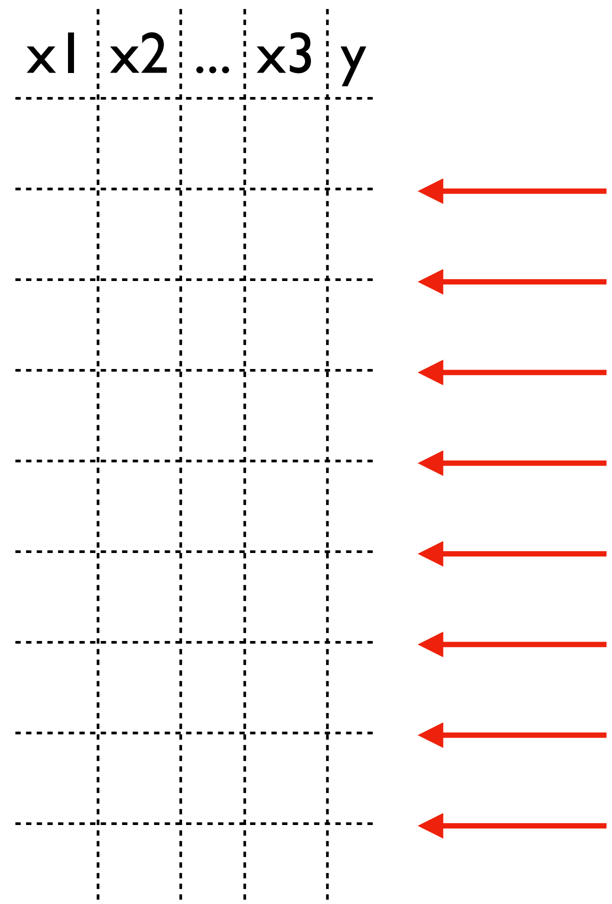
```
dt = DecisionTreeClassifier(labelCol="y")
dt.setMaxBins(4)
```

equi-depth histogram for x3 feature
(each bucket has approx same number of samples)



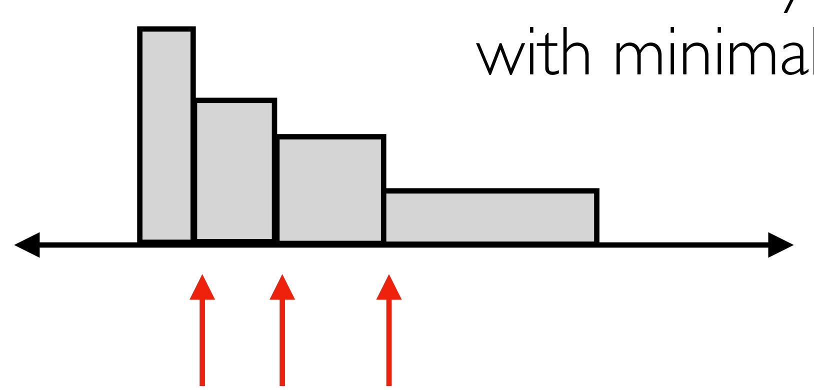
histograms for every feature...

Split Points: In-Mem vs. Distributed



split points for one-node, **in-memory** algorithm

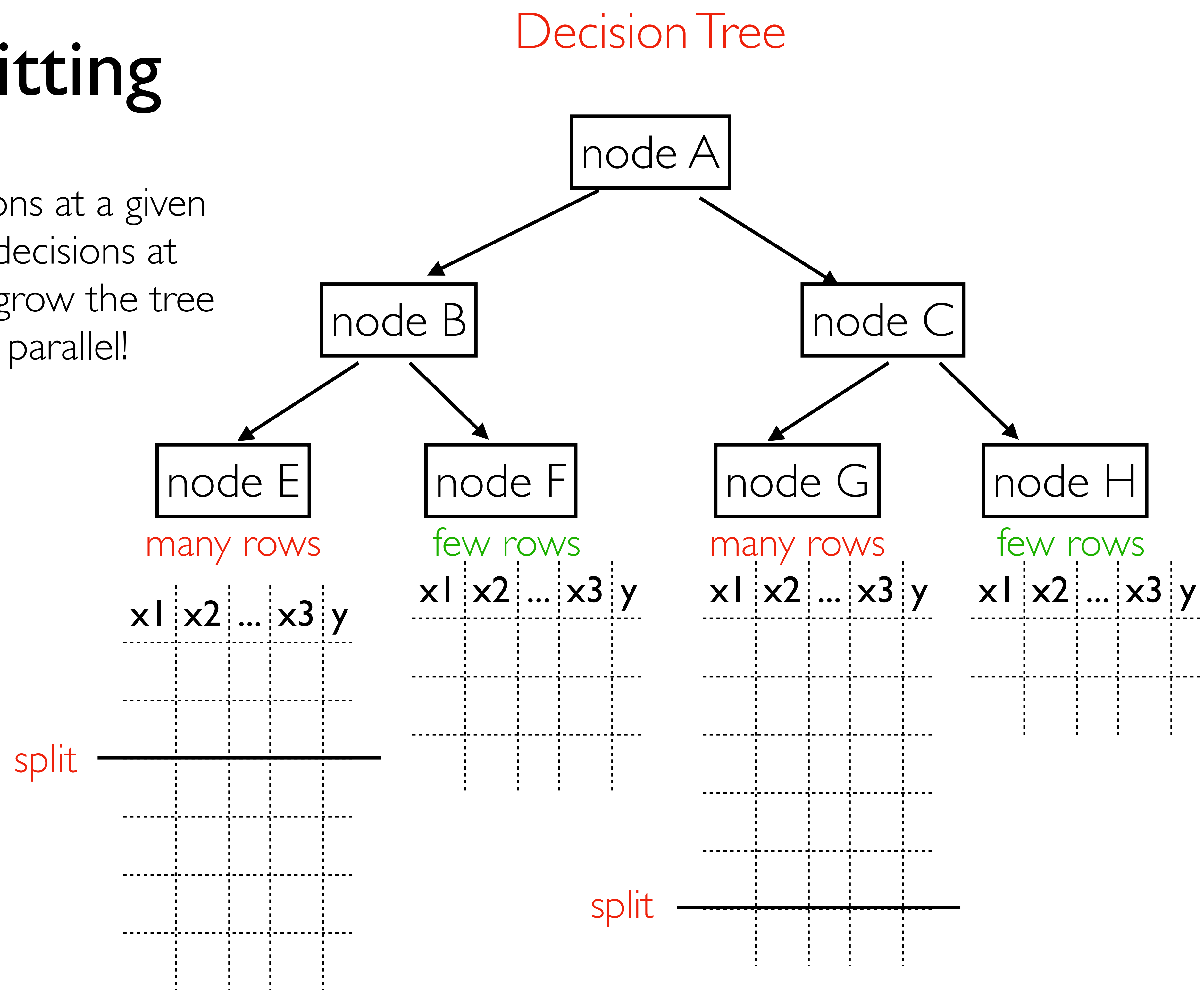
- splits based on initial data
- every task has split info for every column
- small number of pre-defined split points make it easy for executors to collaborate with minimal coordination



split points for **distributed** algorithm

Parallel Splitting

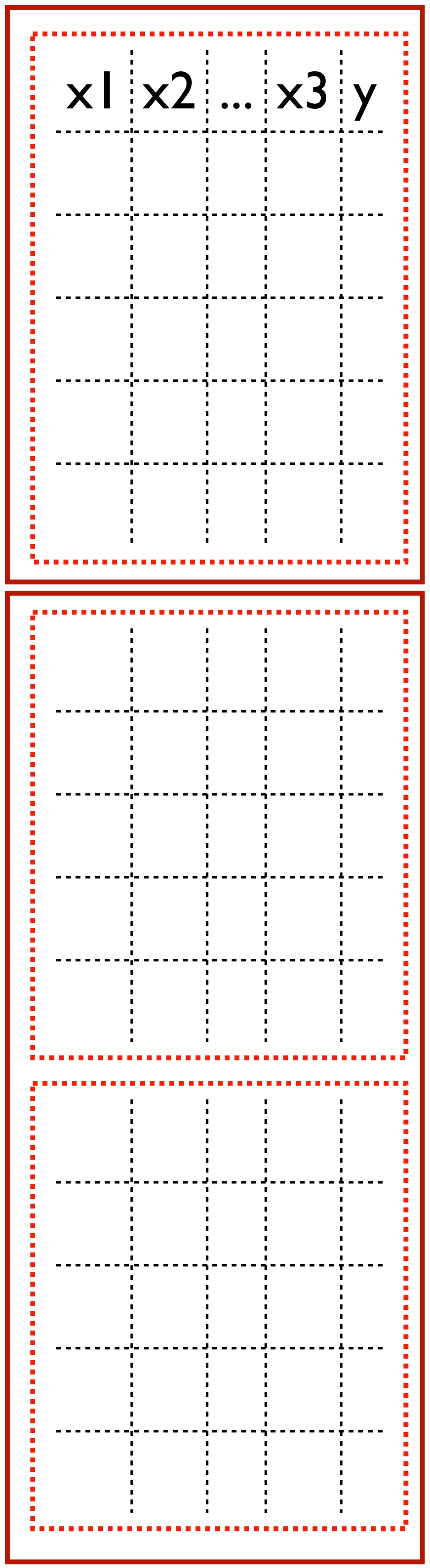
Observation: split decisions at a given node are unrelated to decisions at other nodes. It's easy to grow the tree at different places in parallel!



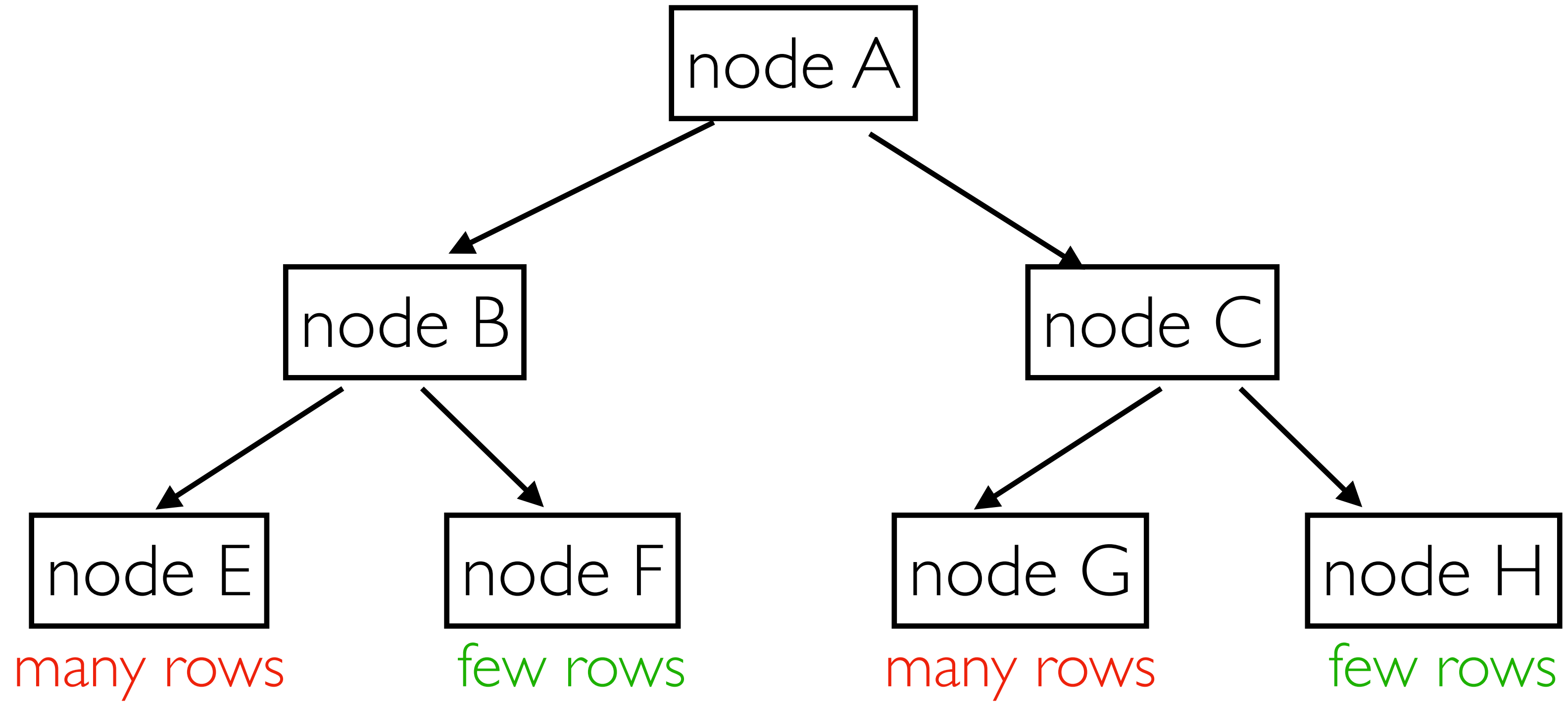
Clarification: nodes in the tree data structure DO NOT correspond to nodes in the Spark cluster.

Logical View of Rows
(rows in a DT node are NOT in the same place physically)

Physical Layout



Decision Tree

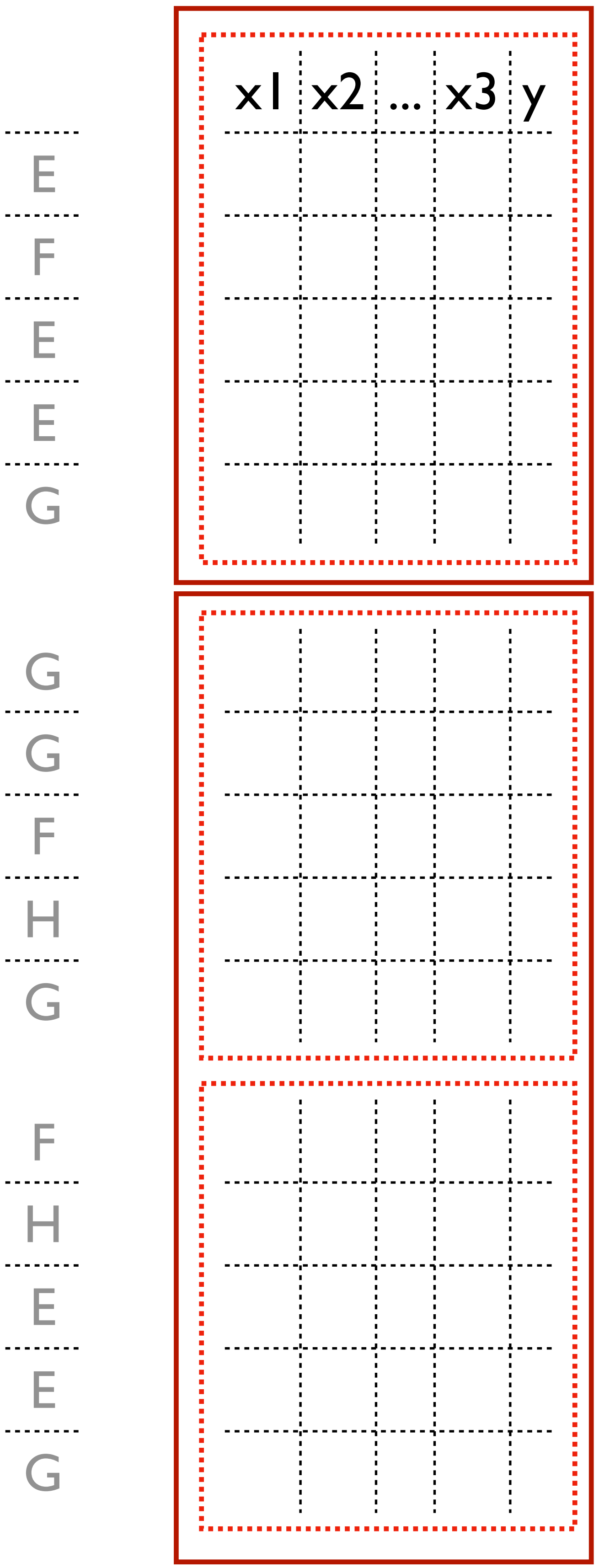


Spark executor

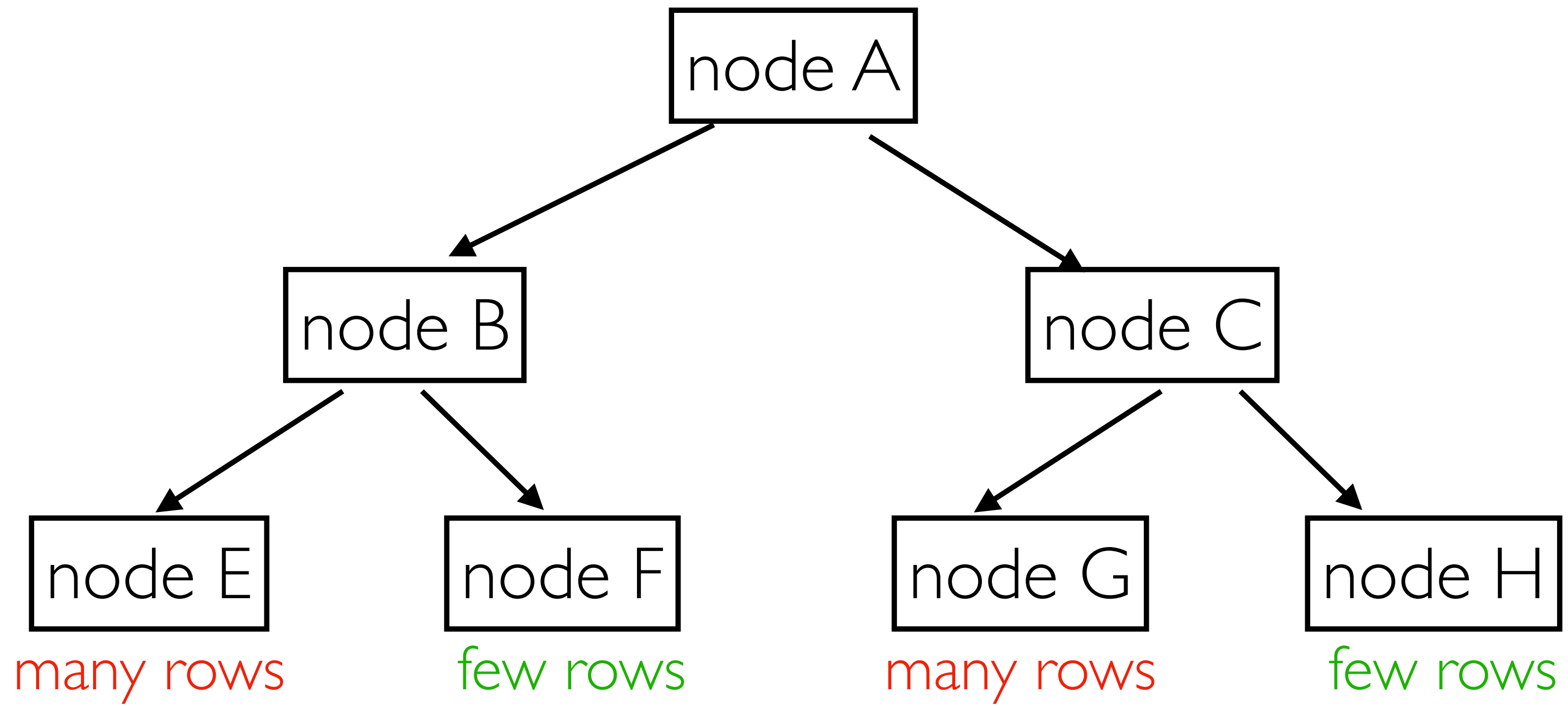
Spark partition

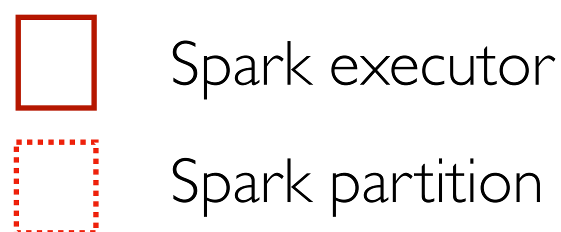
- all rows are in one big Spark DataFrame
- no particular order for rows

Physical Layout



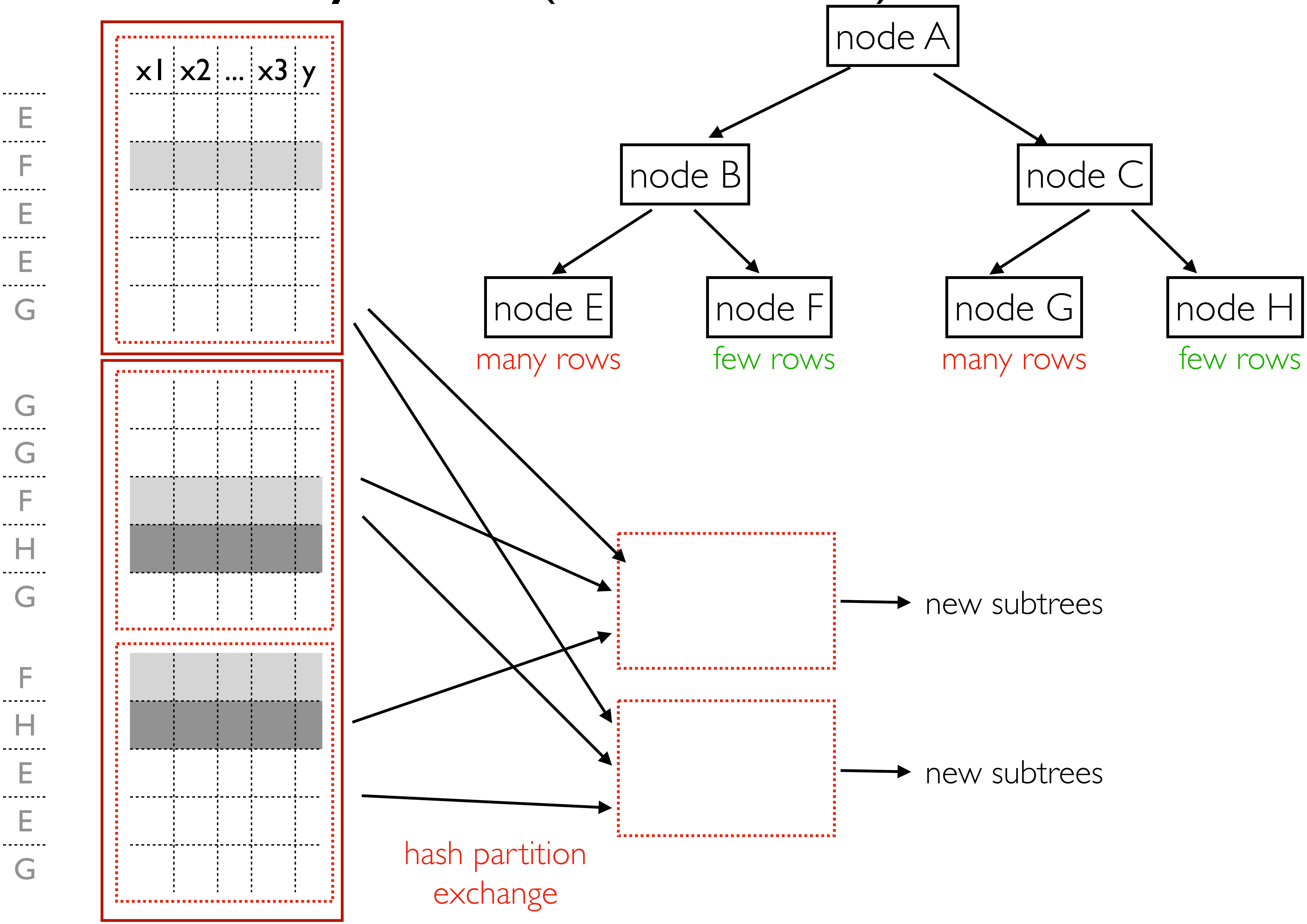
Decision Tree



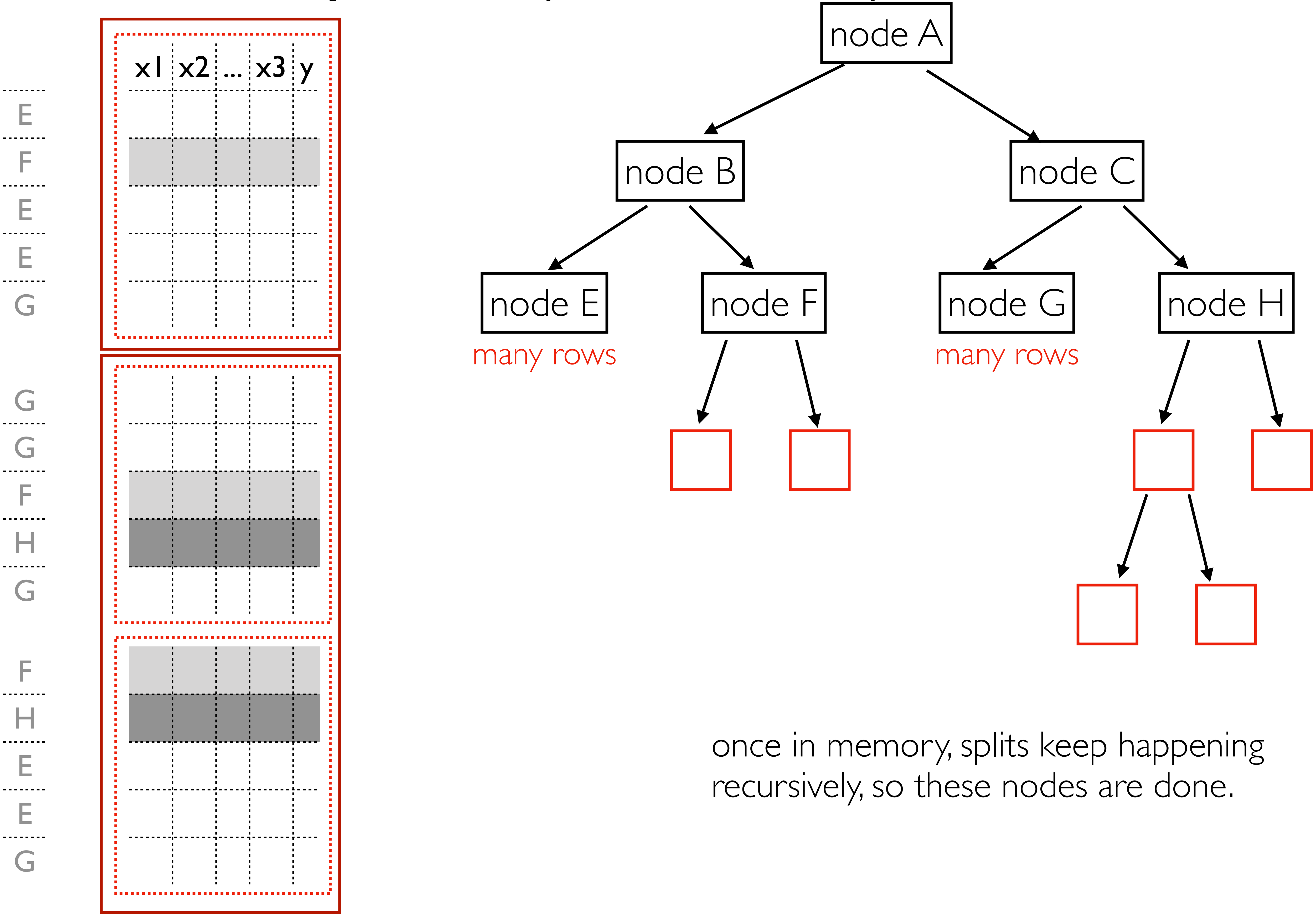


- all rows are in one big Spark DataFrame
- no particular order for rows
- given current tree and x1...xN values, we can infer what leaf node in the tree owns each row

In Memory Build (small nodes)

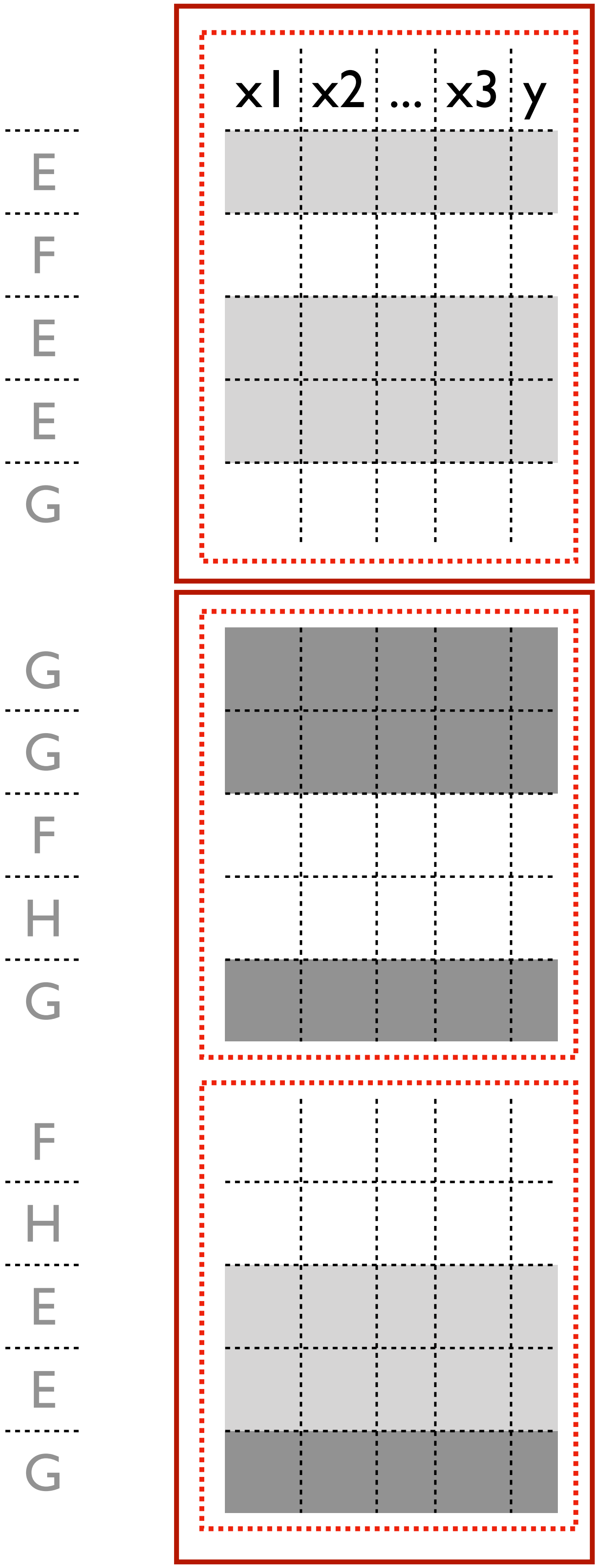


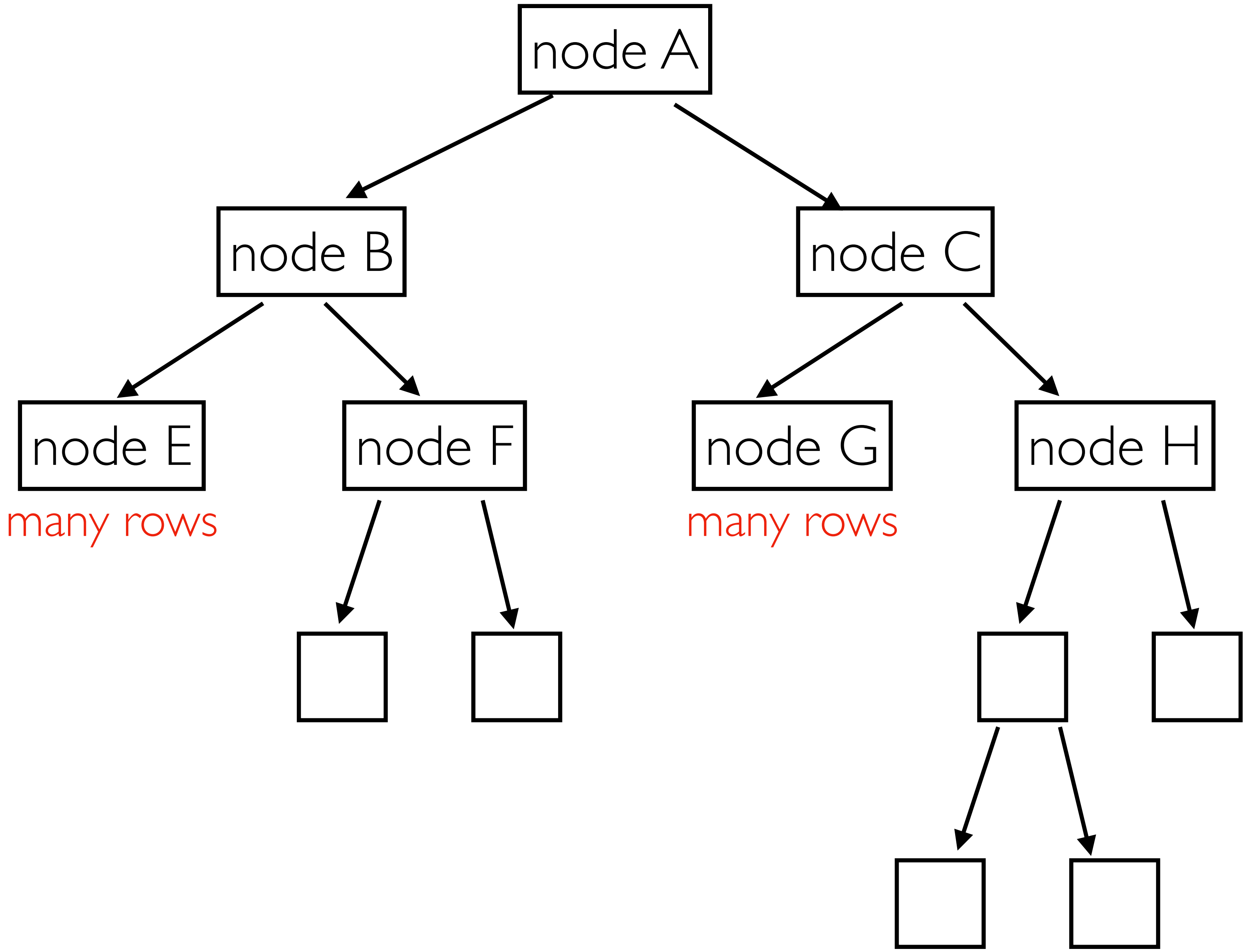
In Memory Build (small nodes)



once in memory, splits keep happening recursively, so these nodes are done.

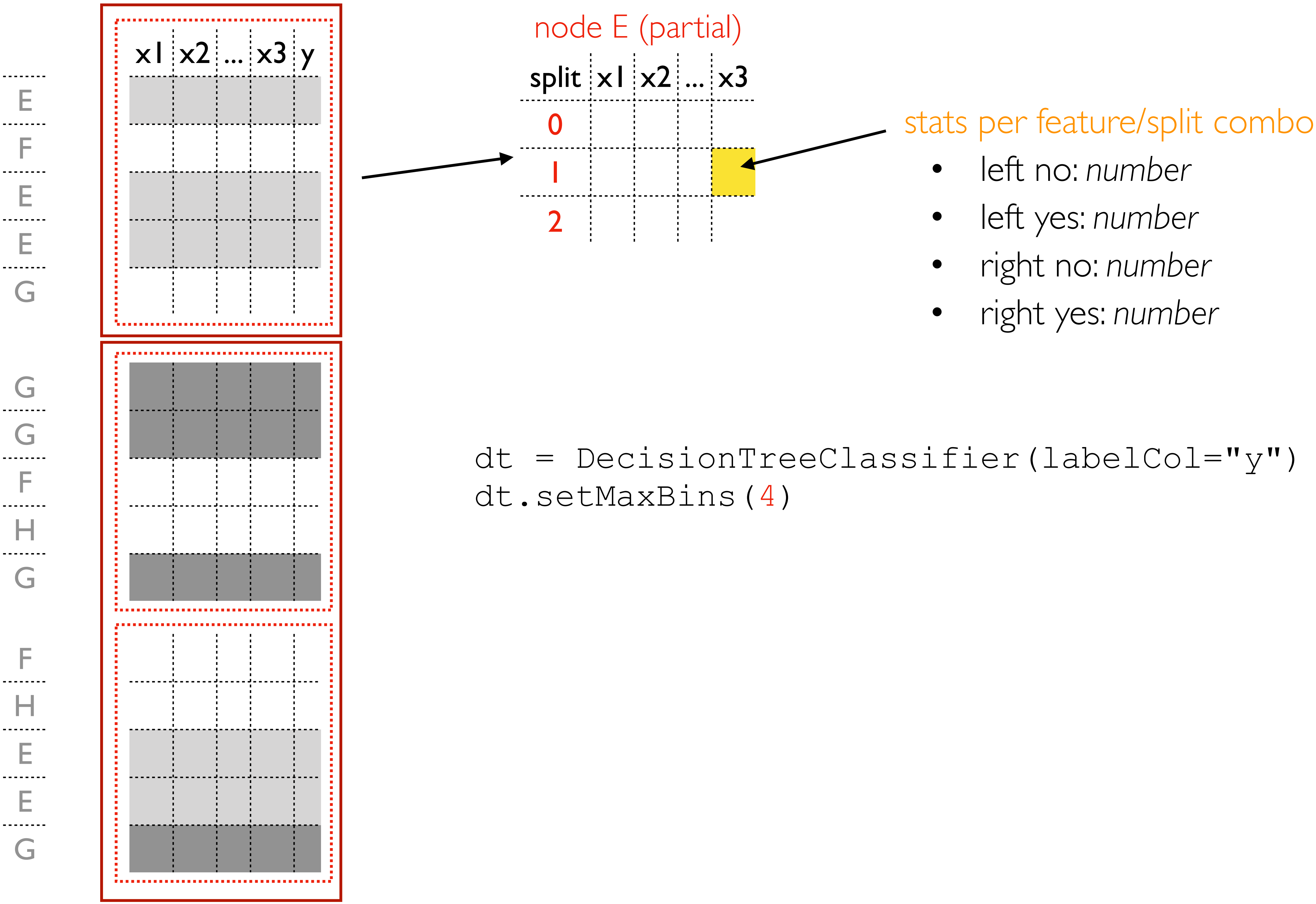
Big Nodes





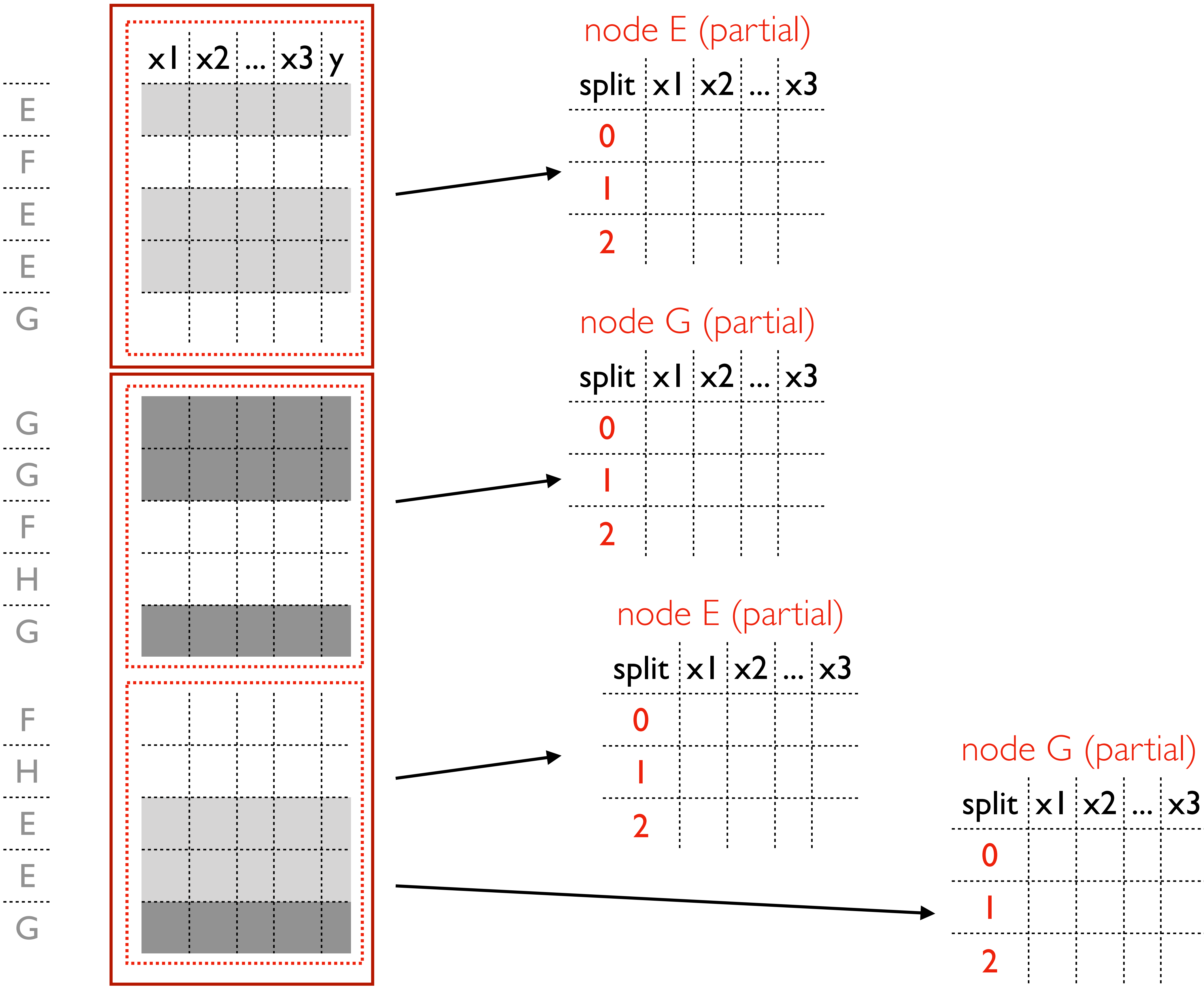
- don't move row data between machines!
- just output stats per partition for every split/feature option

Big Nodes

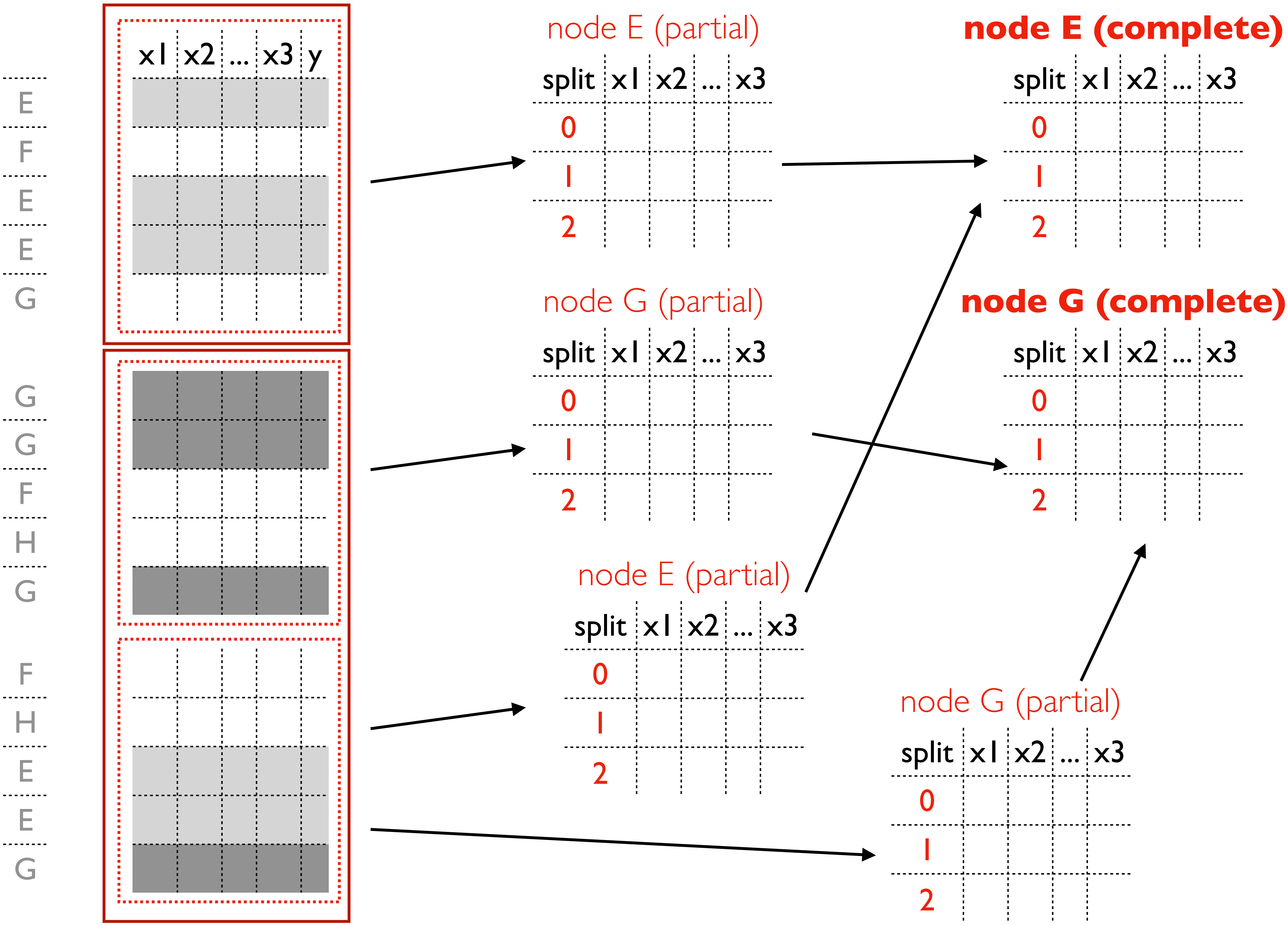



```
dt = DecisionTreeClassifier(labelCol="y")
dt.setMaxBins(4)
```

Big Nodes

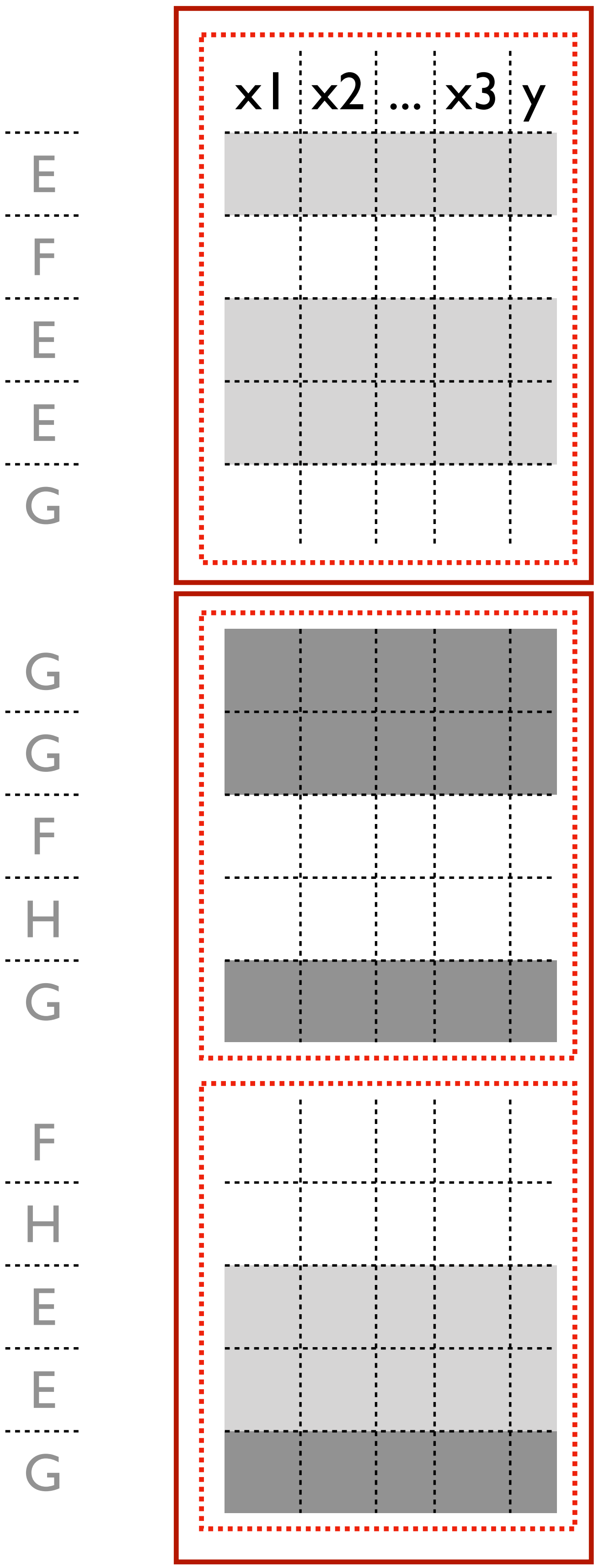

x1 x2 ... x3 y
E
F
E
E
G
G
G
F
H
G
F
H
E
E
G
node E (partial)
split x1 x2 ... x3
0
1
2
node G (partial)
split x1 x2 ... x3
0
1
2
node E (partial)
split x1 x2 ... x3
0
1
2
node G (partial)
split x1 x2 ... x3
0
1
2

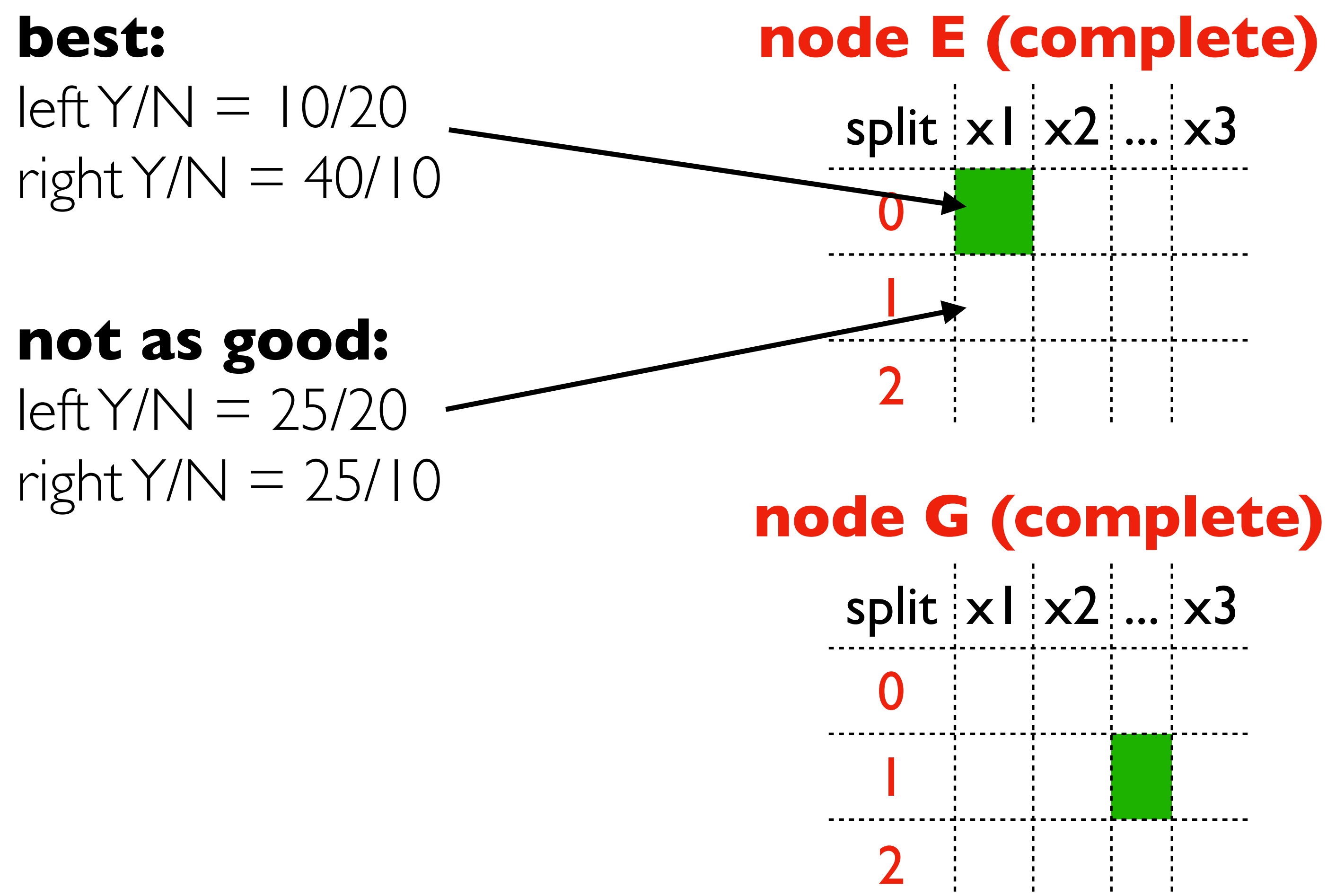
Big Nodes



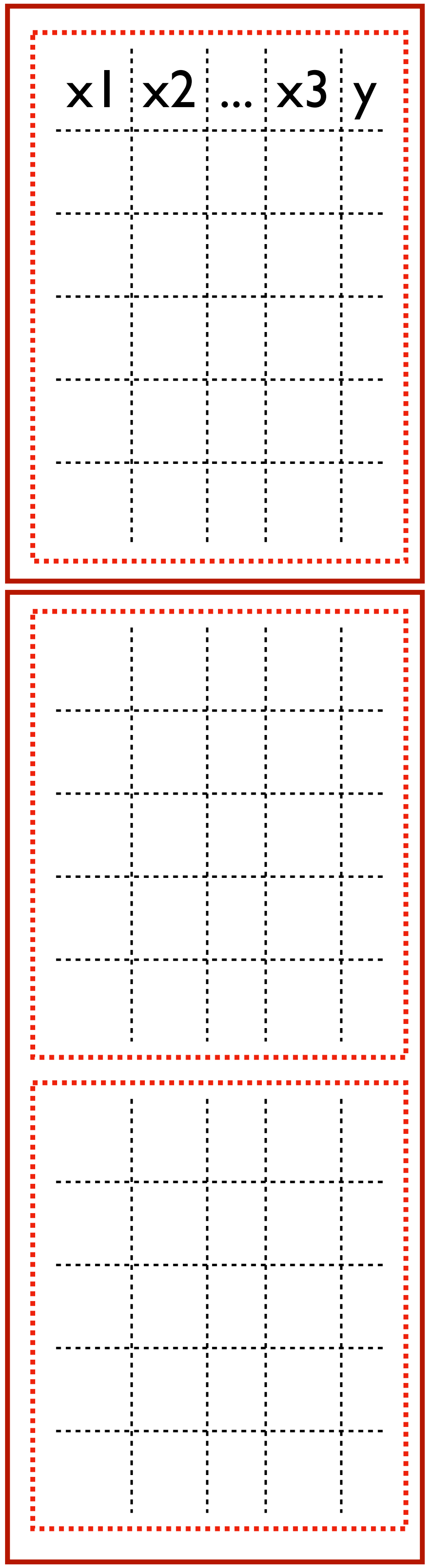
x1 x2 ... x3 y
E
F
E
E
G
G
G
F
H
G
F
H
E
E
G
node E (partial)
split x1 x2 ... x3
0
1
2
node E (complete)
split x1 x2 ... x3
0
1
2
node G (partial)
split x1 x2 ... x3
0
1
2
node G (complete)
split x1 x2 ... x3
0
1
2
node E (partial)
split x1 x2 ... x3
0
1
2
node G (partial)
split x1 x2 ... x3
0
1
2

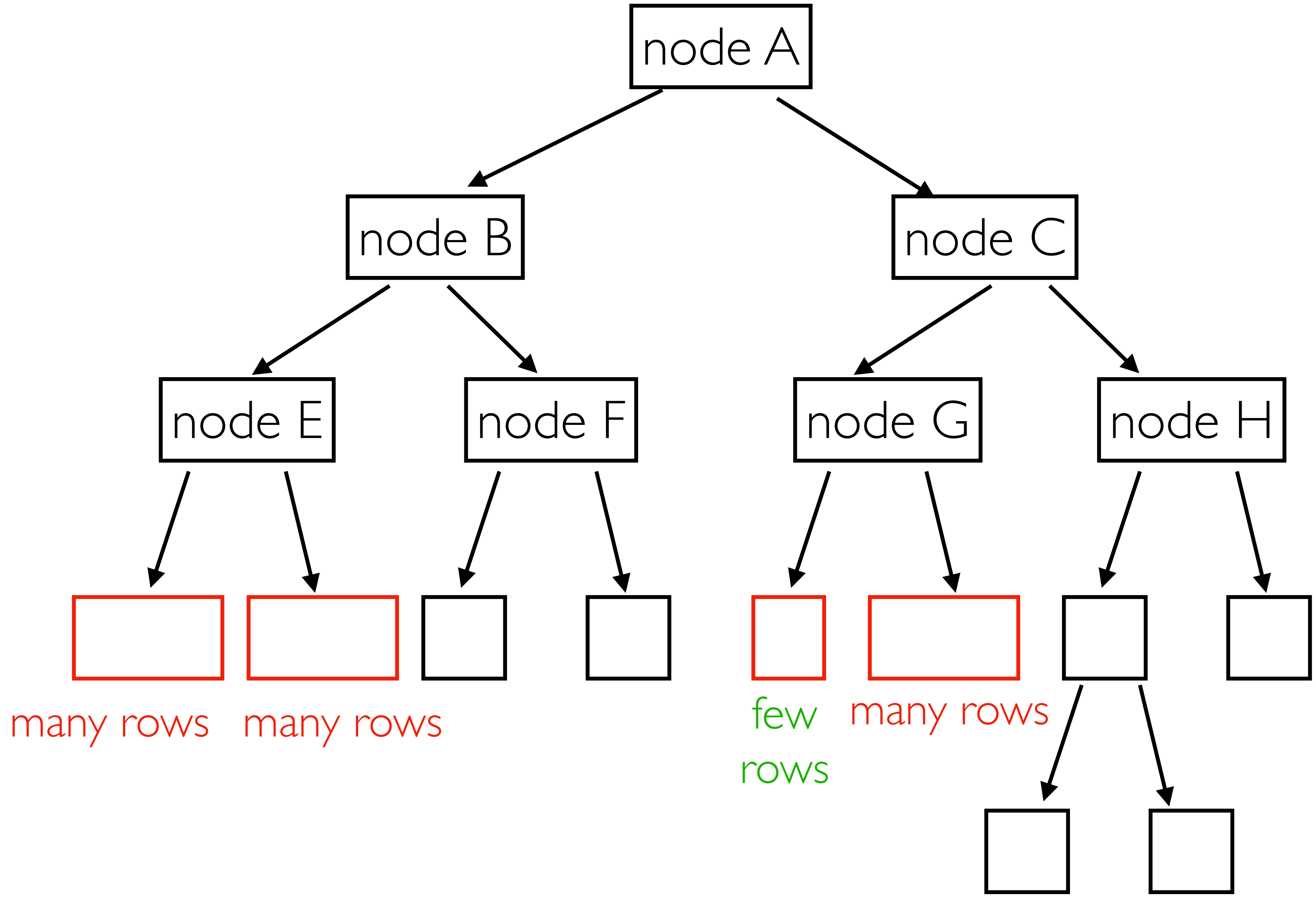
Big Nodes





- each stats table corresponds to a DT node we can split (we will choose best split for each node)
- each column represents a feature we could split on
- each row represents a threshold we could use for that split





- we split E and G, creating 4 new nodes
- we DID NOT shuffle rows of data
- we DID shuffle statistics about split choices
- recursively keep splitting (either distributed or in-memory, depending on remaining size)

TopHat