Deep Dive into scikit-learn's HistGradientBoosting Classifier and Regressor

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Scikit-learn API 🛠️

```python
from sklearn.experimental import enable_hist_gradient_boosting
from sklearn.ensemble import HistGradientBoostingClassifier

clf = HistGradientBoostingClassifier()

clf.fit(X, y)

clf.predict(X)
```

Supervised learning 📖

$$y = f(X)$$

- X of shape `(n_samples, n_features)`
- y of shape `(n_samples,)`

HistGradientBoosting

Boosting 🏂

$$f(X) = h_0(X) + h_1(X) + h_2(X) + \dots$$

$$f(X) = \sum_i h_i(X)$$

HistGradientBoosting

Gradient ⛰️ (Loss Function)

- **Regression**
  1. `least_squares`
  2. `least_absolute_deviation`
- **Classificaiton**
  1. `binary_crossentropy`
  2. `categorical_crossentropy`

Gradient ⛰️ (Regression Loss Function)

- `least_squares`

$$L(y, f(X)) = \frac{1}{2}||y - f(X)||^2$$

Gradient ⛰️ - `least_squares`

- **Gradient**

$$\nabla L(y, f(X)) = -(y - f(X))$$

- **Hessian**

$$\nabla^2 L(y, f(X)) = 1$$

Gradient Boosting 🏂

- Initial Condition

$$f_0(X) = C$$

- Recursive Condition

$$f_{m+1}(X) = f_m(X) - \eta \nabla L(y, f_m(X))$$

where η is the learning rate

Gradient Boosting 🏂 - `least_squares`

$$f_{m+1}(X) = f_m(X) + \eta(y - f_m(X))$$

- Let $h_m(X) = (y - f_m(X))$

$$f_{m+1}(X) = f_m(X) + \eta h_m(X)$$

- We need to learn $h_m(X)$!
- For the next example, let $\eta = 1$

Gradient Boosting 🏂 (Example, part 1)

$$f_0(X) = C$$

X	y	$f_0(X)$	$y - f_0(X)$	$h_0(X)$
35	70	78	-8	-7
45	90	78	12	10
25	80	78	2	5
15	50	78	-28	-20
55	100	78	22	25

Gradient Boosting 🏂 (Example, part 2)

$$f_{m+1}(X) = f_m(X) + h_m(X)$$

$f_0(X)$	$h_0(X)$	$f_1(X)$	$y - f_1(X)$	$h_1(X)$	$f_2(X)$
78	-7	71	-1	-1	70
78	10	88	2	1	89
78	5	83	-3	-4	79
78	-20	58	-8	-6	52
78	25	103	-3	-2	101

Gradient Boosting 🏂 (Example, part 3)

With two iterations in boosting:

$$f(X) = C + h_0(X) + h_1(X)$$

- **predict**: With X = 40

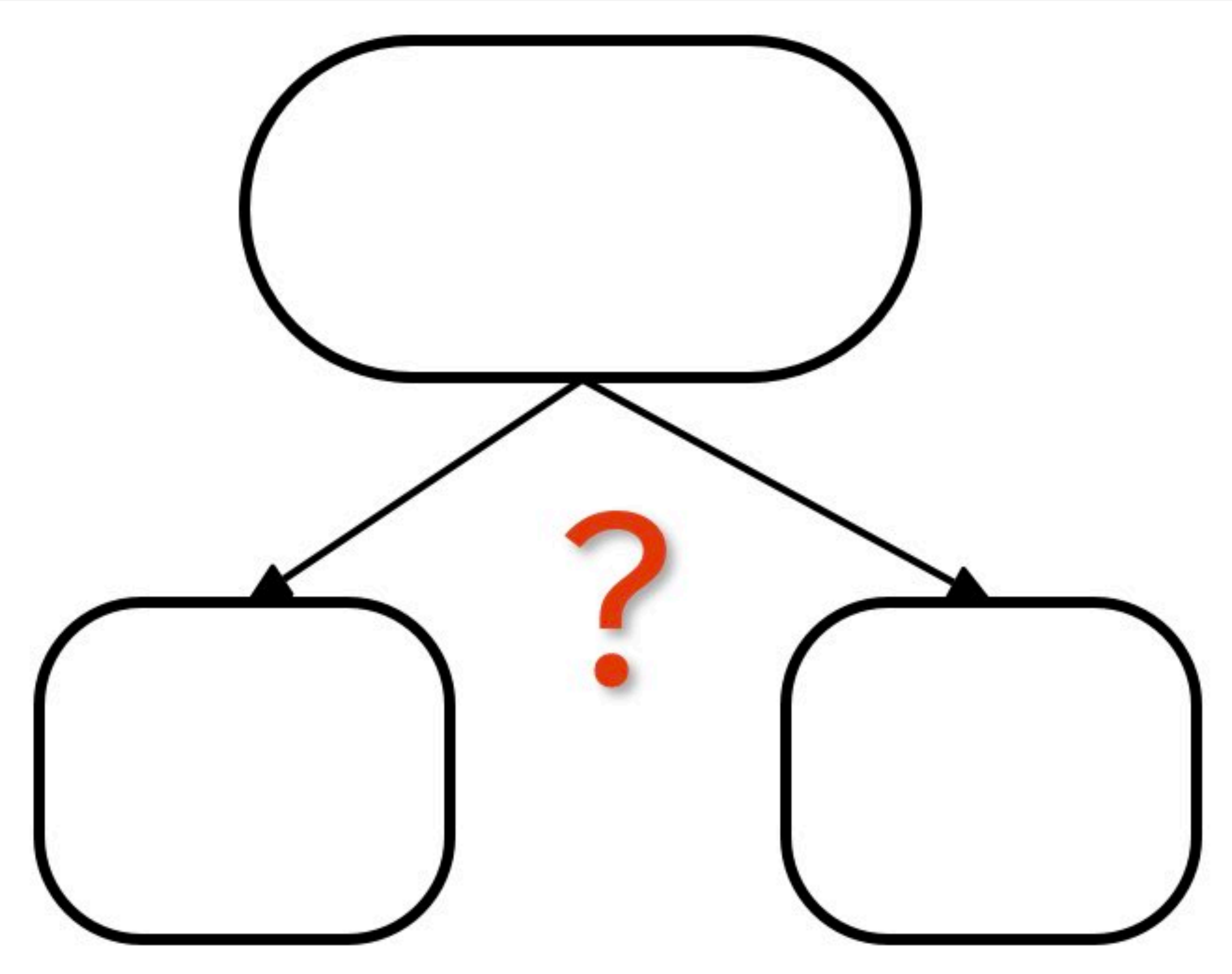
$$f(40) = 78 + h_0(40) + h_1(40)$$

How to learn $h_m(X)$?

🌲!

Tree Growing 🌲 (part 1)

1. For every feature
    1. Sort feature
    2. For every split point
        1. Evaluate split
2. Pick **best** split



Tree Growing 🌲 (part 2)

- Recall Loss, Gradient, Hessian

$$L(y, f(X)) = \frac{1}{2}||y - f(X)||^2$$

$$G = \nabla L(y, f(X)) = -(y - f(X))$$

$$H = \nabla^2 L(y, f(X)) = 1$$

Tree Growing 🌲 (part 3)

- How to evaluate split?

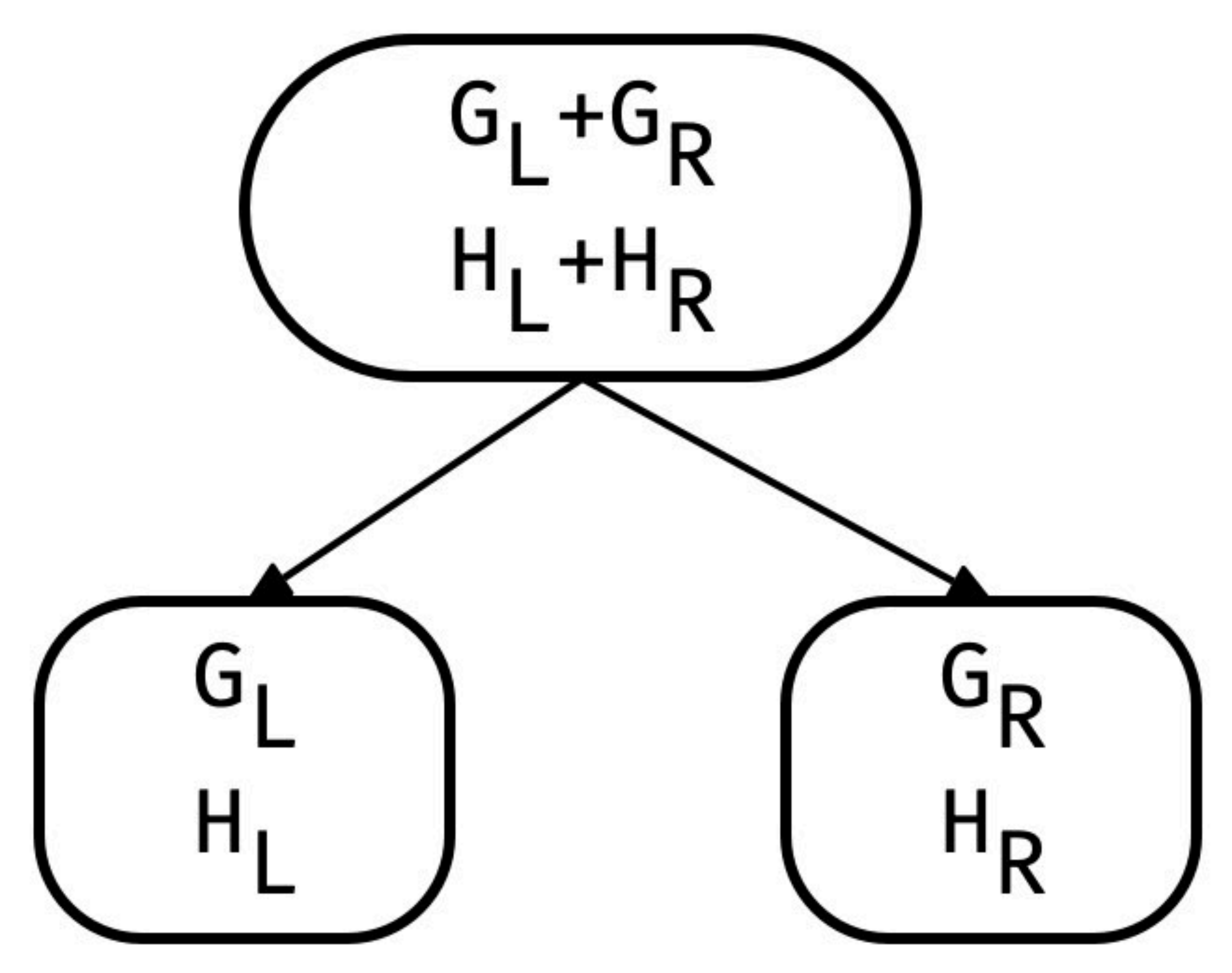
$$Gain = \frac{1}{2}\left[\frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{(G_L + G_R)^2}{H_L + H_R + \lambda}\right]$$

- λ: `l2_regularization=0`

Tree Growing 🌲 (part 4)

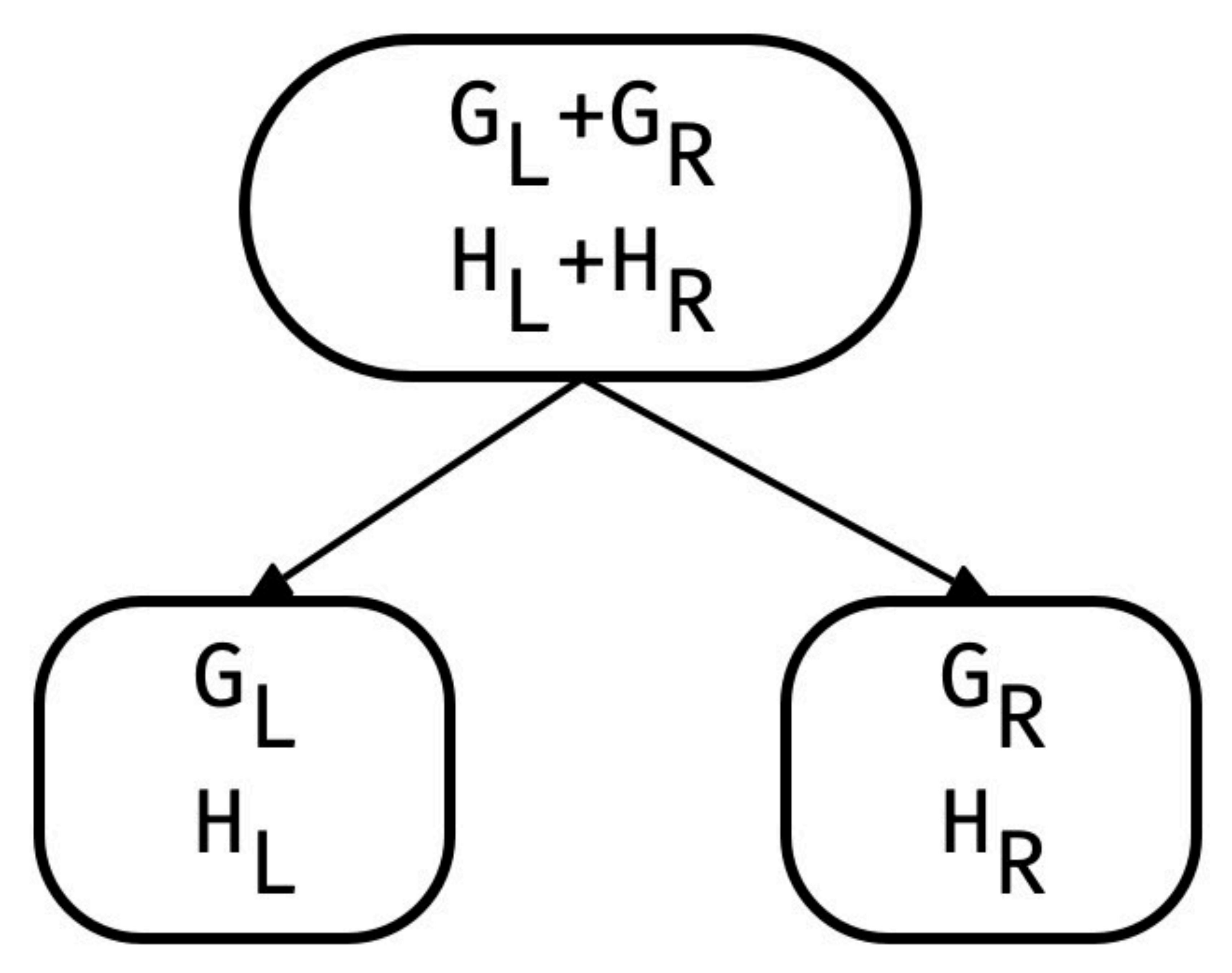
1. For every feature
    1. Sort feature
    2. For every split point
        1. Evaluate split
2. Pick **best** split

- Done?



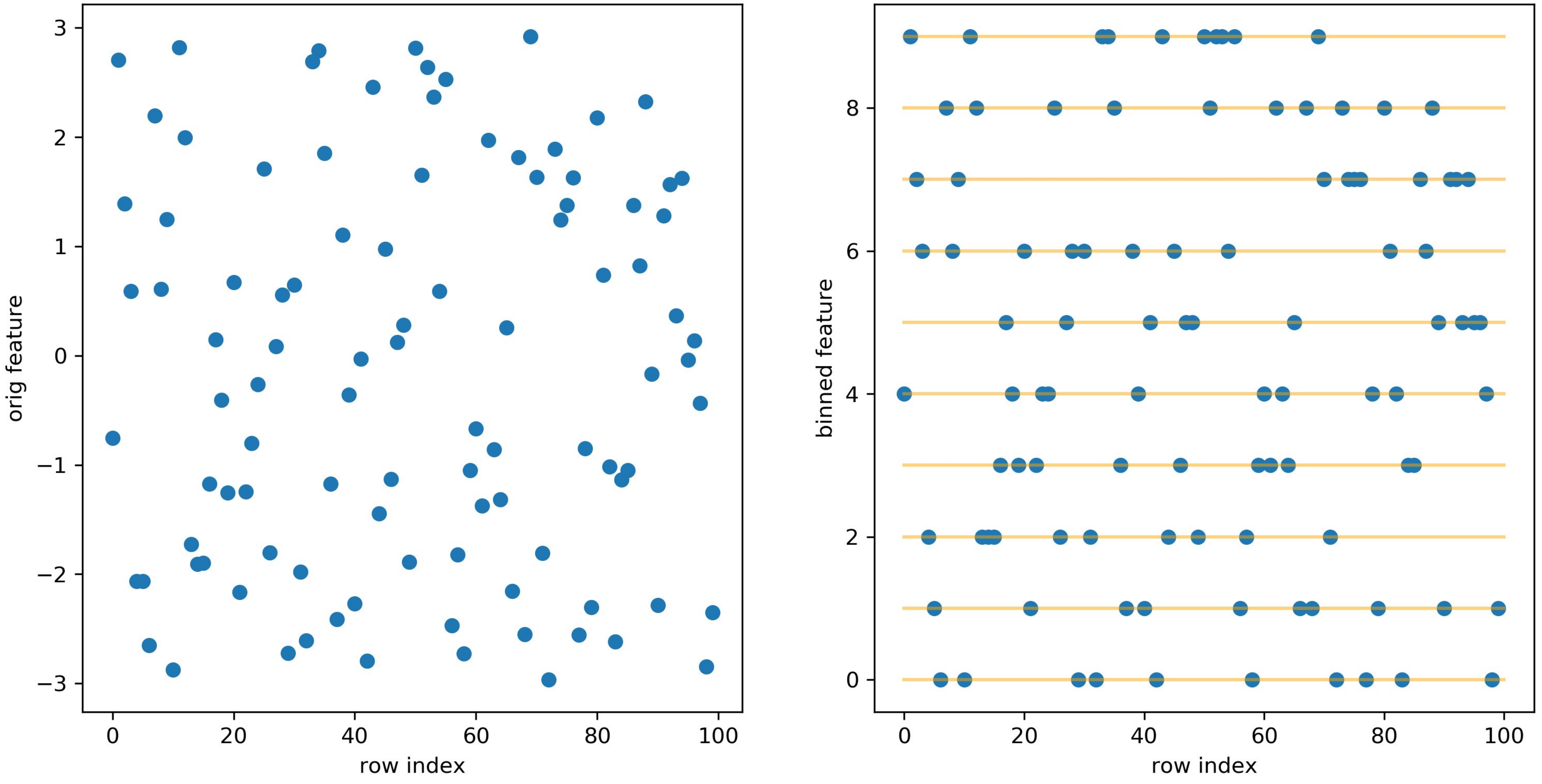
Tree Growing 🌲 (part 5)

1. For every feature
    1. Sort feature - **O(nlog(n))**
    2. For every split point - **O(n)**
        1. Evaluate split
2. Pick **best** split



HistGradientBoosting

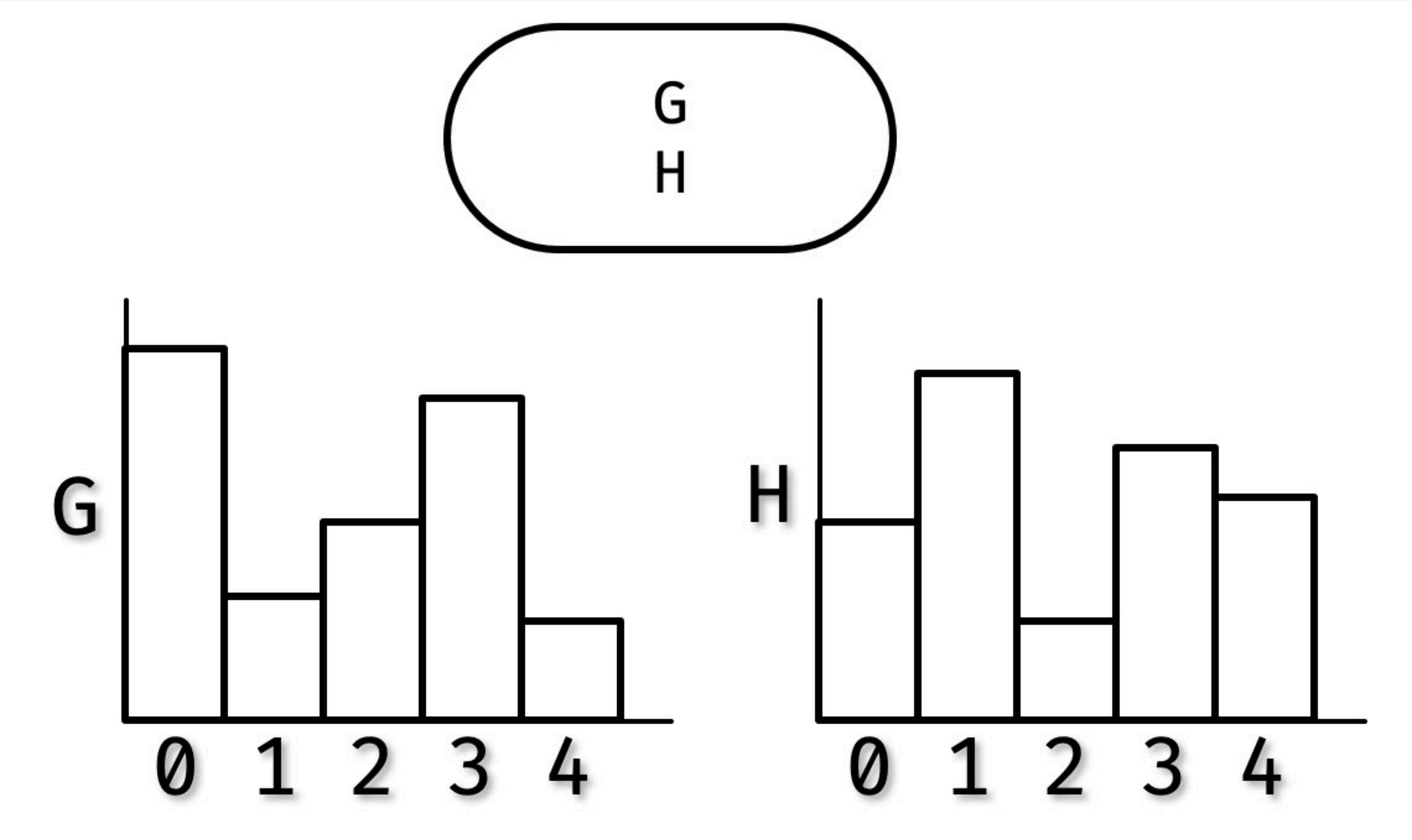
Binning! 🗑️ (part 1)



Binning! 🗑️ (part 2)

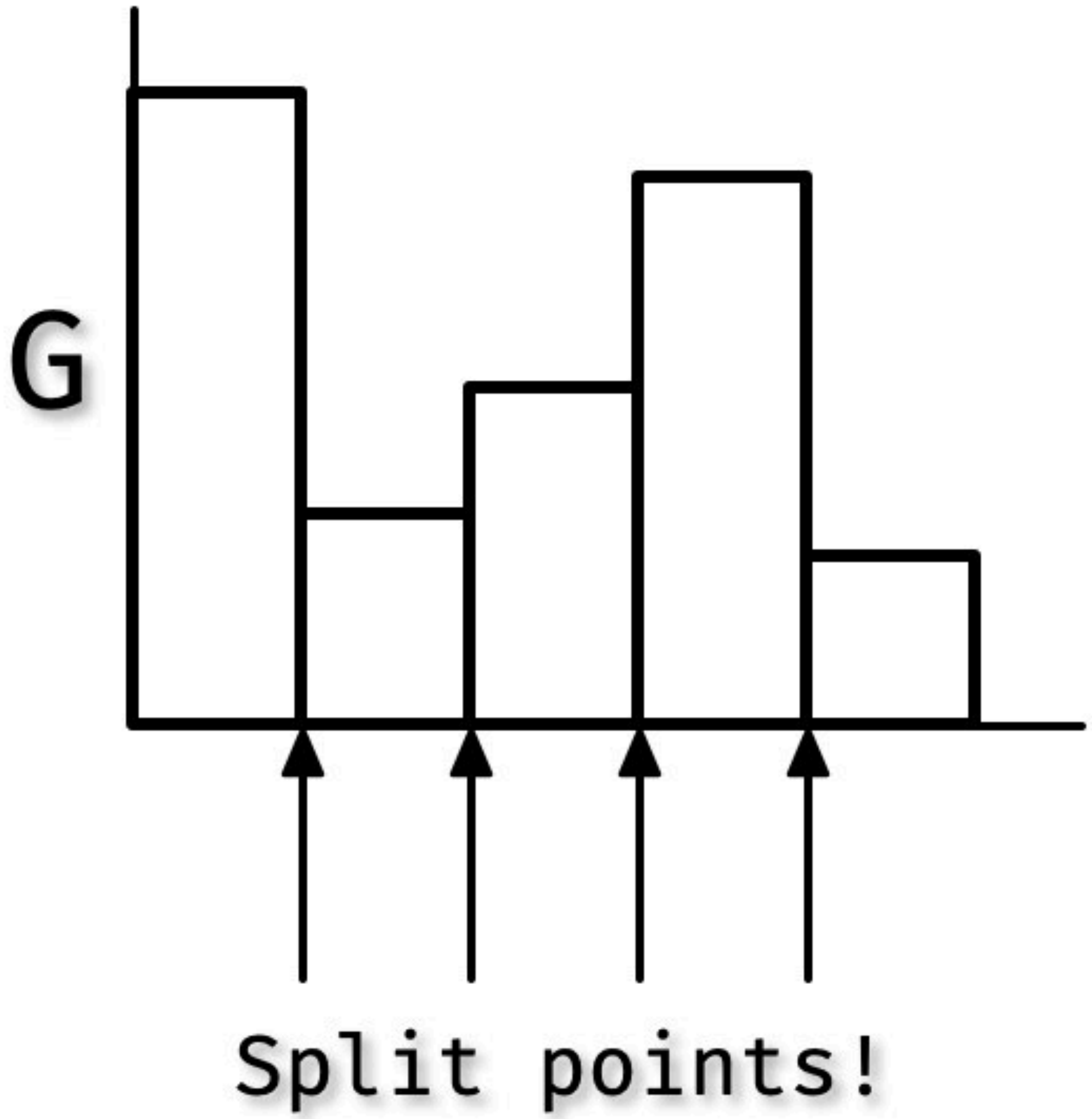
```
# Original data
[-0.752,  2.7042,  1.3919,  0.5091, -2.0636,
 -2.064, -2.6514,  2.1977,  0.6007,  1.2487, ...]

# Binned data
[4, 9, 7, 6, 2, 1, 0, 8, 6, 7, ...]
```

Histograms! 📊 (part 1)

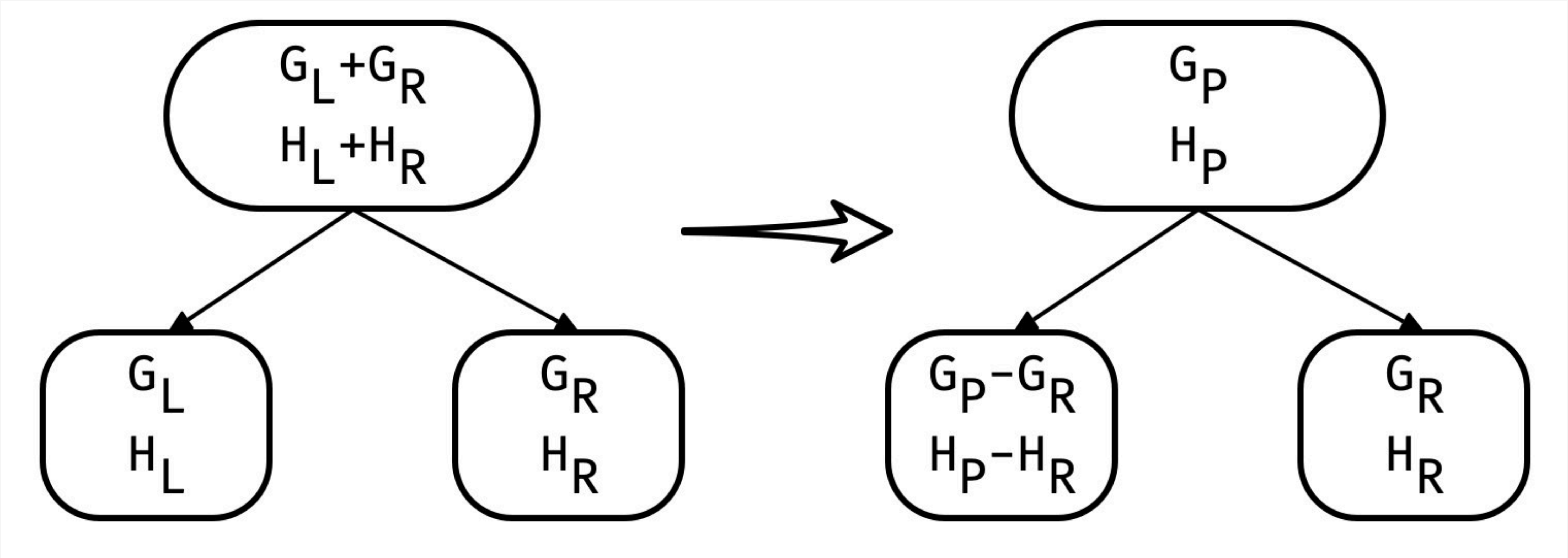


Histograms! 📊 (part 2)

1. For every feature
    1. Build histogram **O(n)**
    2. For every split point - **O(n_bins)**
        1. Evaluate split
2. Pick **best** split



Histograms! 📊 (part 3)



Trees = $h_m(X)$ 🌲

$$f(X) = C + \eta \sum h_m(X)$$

Overview of Algorithm 👀

1. Bin data
2. Make initial predictions (constant)
3. Calculate gradients and hessians
4. Grow Trees For Boosting
    1. Find best splits
    2. Add tree to predictors
    3. Update gradients and hessians

Implementation? 🤔

- Pure Python?
- Numpy?
- Cython?
- Cython + OpenMP!

OpenMP! (Bin data 🗑️, part 1)

1. **Bin data**
2. Make initial predictions (constant)
3. Calculate gradients and hessians
4. Grow Trees For Boosting
    1. Find best splits by building histograms
    2. Add tree to predictors
    3. Update gradients and hessians

OpenMP! (Bin data 🗑️, part 2)

```
for i in range(data.shape[0]):
    left, right = 0, binning_thresholds.shape[0]
    while left < right:
        middle = (right + left - 1) // 2
        if data[i] <= binning_thresholds[middle]:
            right = middle
        else:
            left = middle + 1
    binned[i] = left
```

OpenMP! (Bin data 🗑️, part 3)

```
# sklearn/ensemble/_hist_gradient_boosting/_binning.pyx
for i in prange(data.shape[0],
                schedule='static',
                nogil=True):
    left, right = 0, binning_thresholds.shape[0]
    while left < right:
        middle = (right + left - 1) // 2
        if data[i] <= binning_thresholds[middle]:
            right = middle
        else:
            left = middle + 1
    binned[i] = left
```

OpenMP! (building histograms 🌋, part 1)

1. Bin data
2. Make initial predictions (constant)
3. Calculate gradients and hessians
4. Grow Trees For Boosting
    1. Find best splits by **building histograms**
    2. Add tree to predictors
    3. Update gradients and hessians

OpenMP! (building histograms 🌋, part 2)

```
# sklearn/ensemble/_hist_gradient_boosting/histogram.pyx
with nogil:
    for feature_idx in prange(n_features, schedule='static'):
        self._compute_histogram_brute_single_feature( ... )

for feature_idx in prange(n_features, schedule='static',
                          nogil=True):
    _subtract_histograms(feature_idx, ... )
```

OpenMP! (Find best splits ✂️, part 1)

1. Bin data
2. Make initial predictions (constant)
3. Calculate gradients and hessians
4. Grow Trees For Boosting
    1. **Find best splits** by building histograms
    2. Add tree to predictors
    3. Update gradients and hessians

OpenMP! (Find best splits ✂️, part 2)

```
# sklearn/ensemble/_hist_gradient_boosting/splitting.pyx
for feature_idx in prange(n_features, schedule='static'):
    # For each feature, find best bin to split on
```

OpenMP! (Splitting ✂️, part 3)

```
# sklearn/ensemble/_hist_gradient_boosting/splitting.pyx
for thread_idx in prange(n_threads, schedule='static',
                         chunksize=1):
    # splits a partition of node
```

OpenMP! (Update gradients and hessians 🏔️, part 1)

1. Bin data
2. Make initial predictions (constant)
3. Calculate gradients and hessians
4. Grow Trees For Boosting
    1. Find best splits by building histograms
    2. Add tree to predictors
    3. **Update gradients and hessians**

OpenMP! (Update gradients and hessians 🏔️, part 2)

- `least_squares`

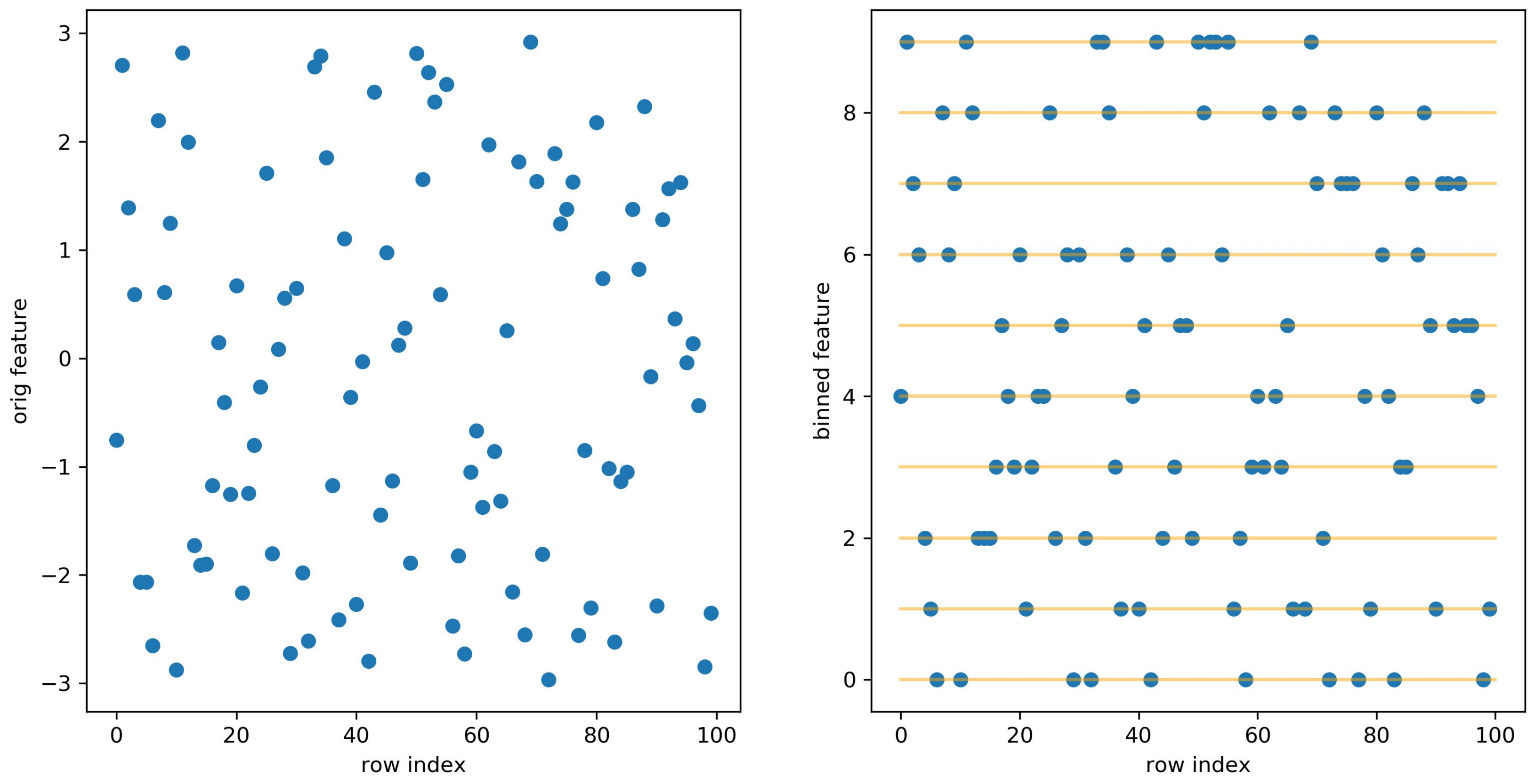
```
# sklearn/ensemble/_hist_gradient_boosting/_loss.pyx
for i in prange(n_samples, schedule='static', nogil=True):
    gradients[i] = raw_predictions[i] - y_true[i]
```

Hyperparameters (Bin data 🗑️, part 1)

1. **Bin data**
2. Make initial predictions (constant)
3. Calculate gradients and hessians
4. Grow Trees For Boosting
    1. Find best splits by building **histograms**
    2. Add tree to predictors
    3. Update gradients and hessians

Hyperparameters (Bin data 🗑️, part 2)

- `max_bins=255`



Hyperparameters (Loss 📉, part 1)

1. Bin data
2. **Make initial predictions (constant)**
3. Calculate **gradients and hessians**
4. Grow Trees For Boosting
    1. Find best splits by building histograms
    2. Add tree to predictors
    3. **Update gradients and hessians**

Hyperparameters (Loss 📉, part 2)

- `HistGradientBoostingRegressor`
  1. `loss=least_squares` (default)
  2. `least_absolute_deviation`
- `HistGradientBoostingClassifier`
  1. `loss=auto` (default)
  2. `binary_crossentropy`
  3. `categorical_crossentropy`
- `l2_regularization=0`

Hyperparameters (Boosting 🏂, part 1)

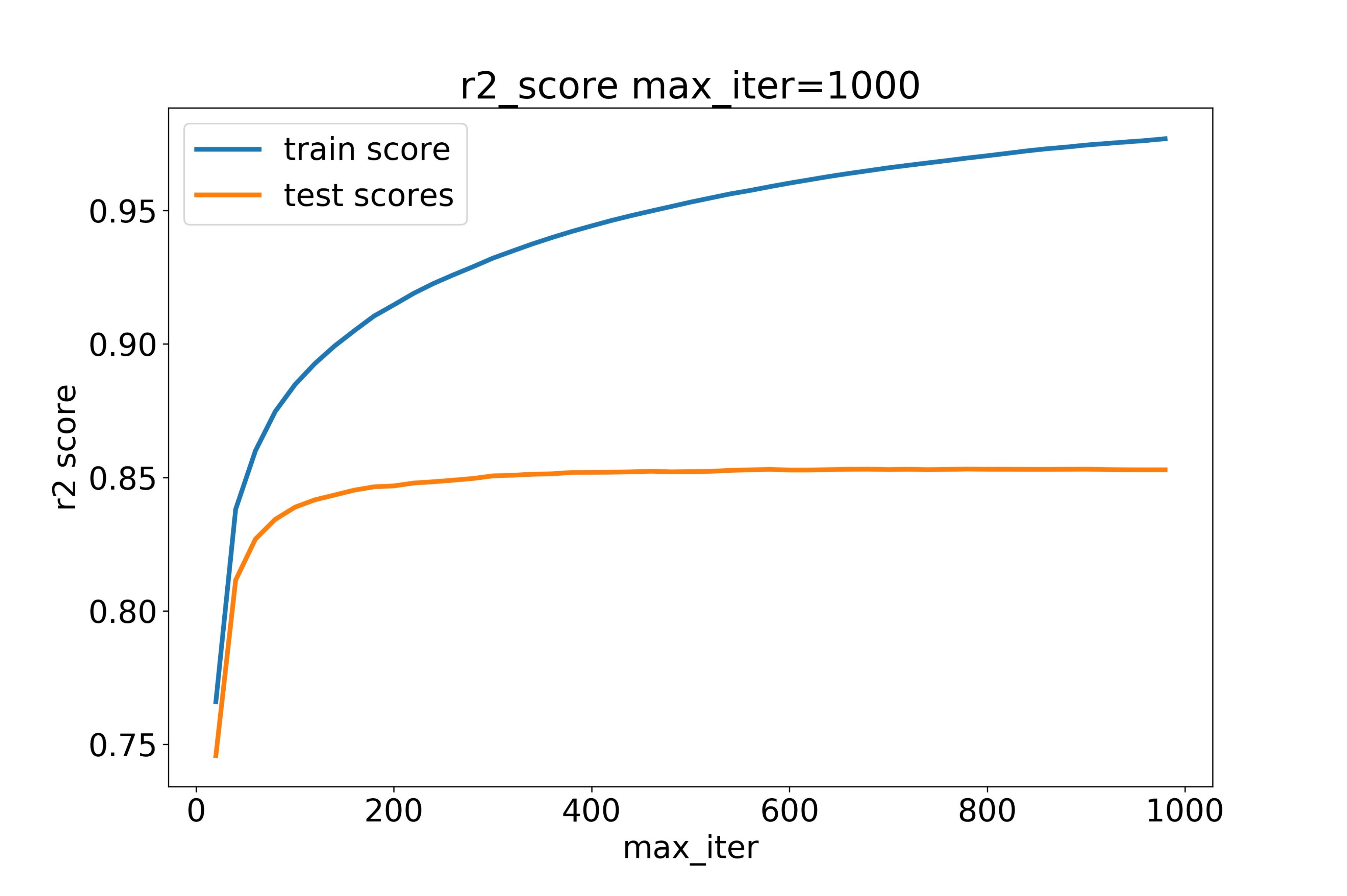
1. Bin data
2. Make initial predictions (constant)
3. Calculate gradients and hessians
4. Grow Trees For **Boosting**
    1. Find best splits by building histograms
    2. Add tree to predictors
    3. Update gradients and hessians

Hyperparameters (Boosting 🏂, part 2)

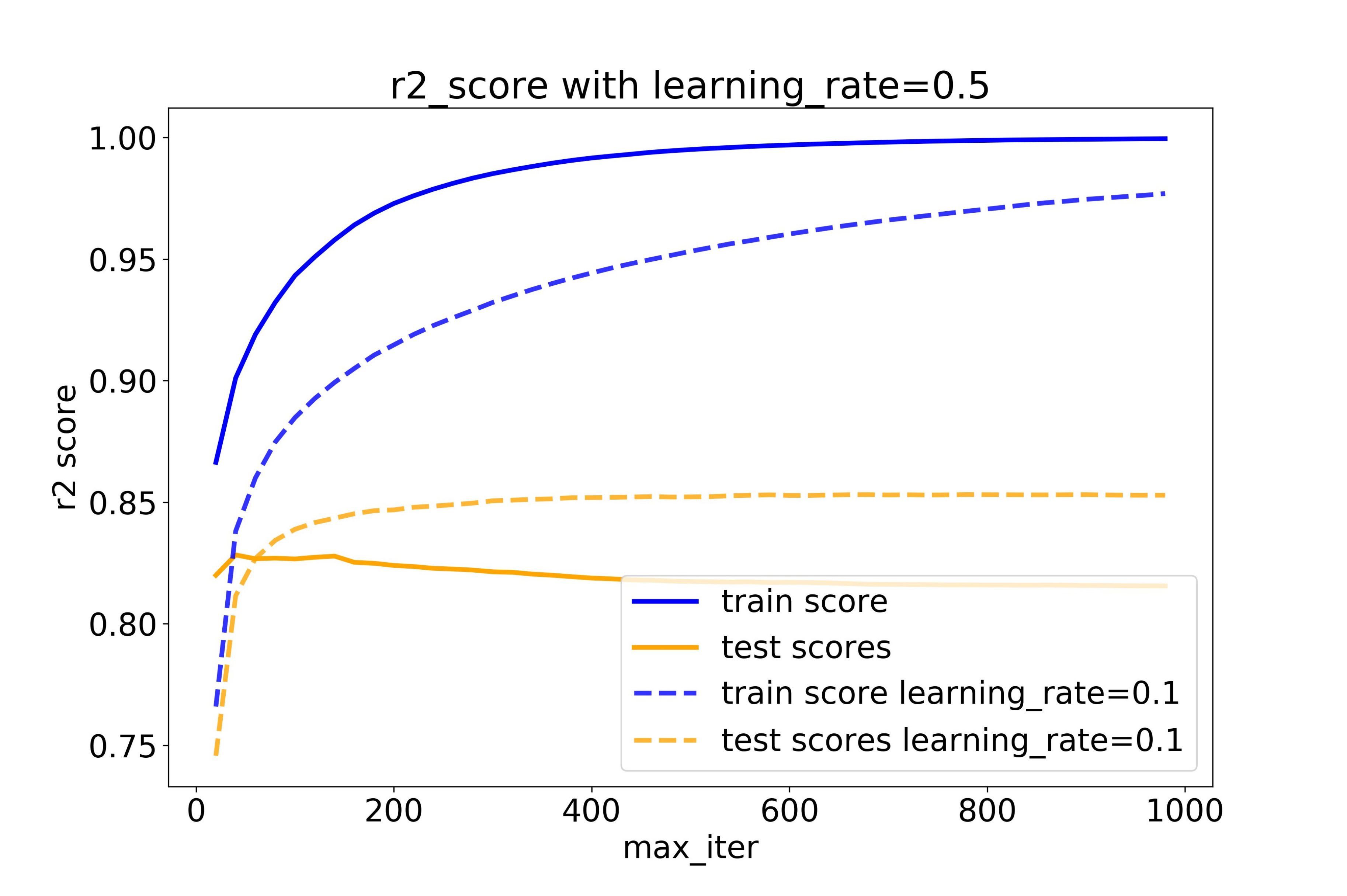
- `learning_rate=0.1` (η)
- `max_iter=100`

$$f(X) = C + \eta \sum_{m}^{max\_iter} h_m(X)$$

Hyperparameters (Boosting 🏂, part 3)



Hyperparameters (Boosting 🏂, part 4)



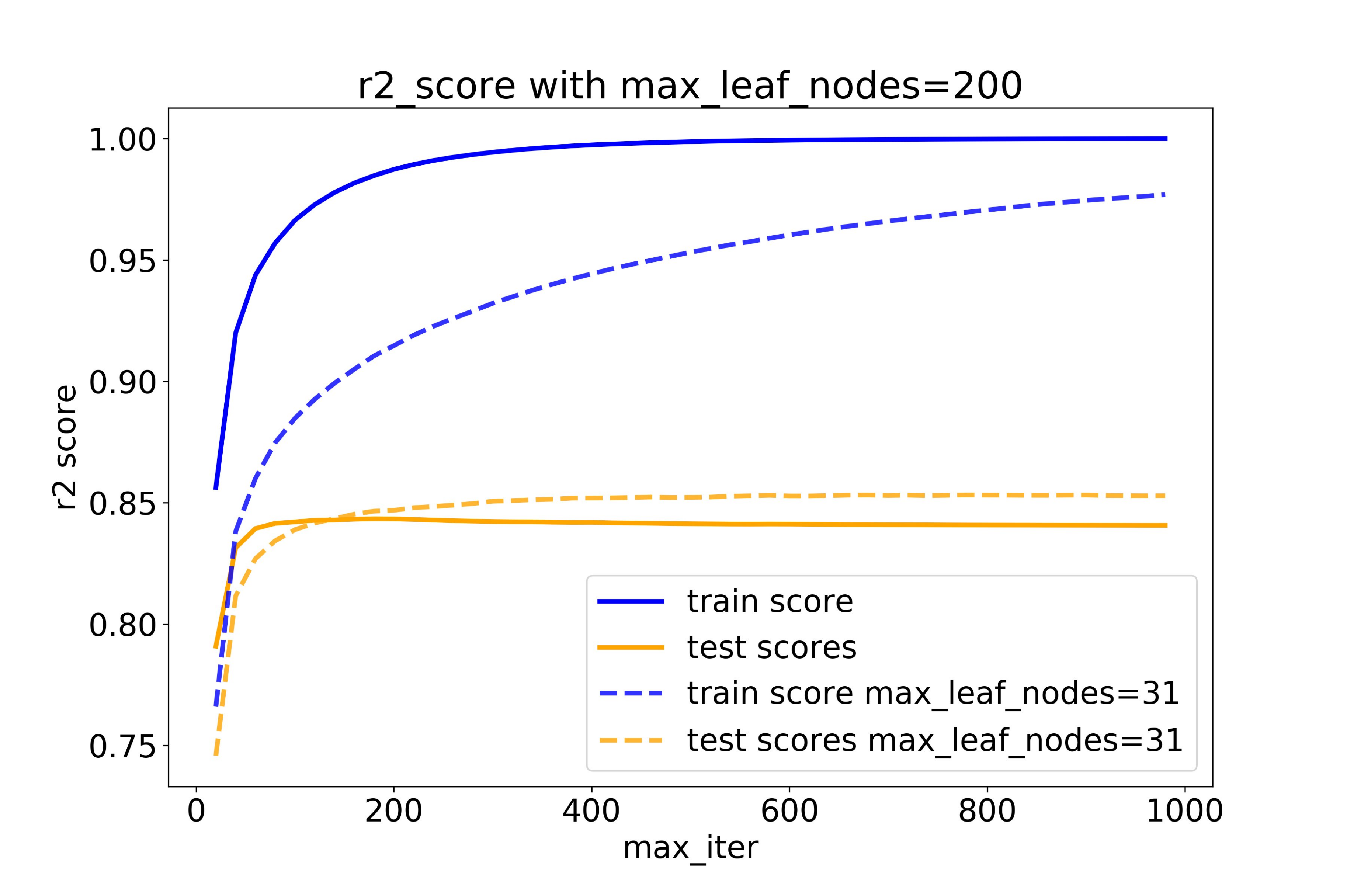
Hyperparameters (Grow Trees 🎄, part 1)

1. Bin data
2. Make initial predictions (constant)
3. Calculate gradients and hessians
4. **Grow Trees** For Boosting
    1. Find best splits by building histograms
    2. Add tree to predictors
    3. Update gradients and hessians

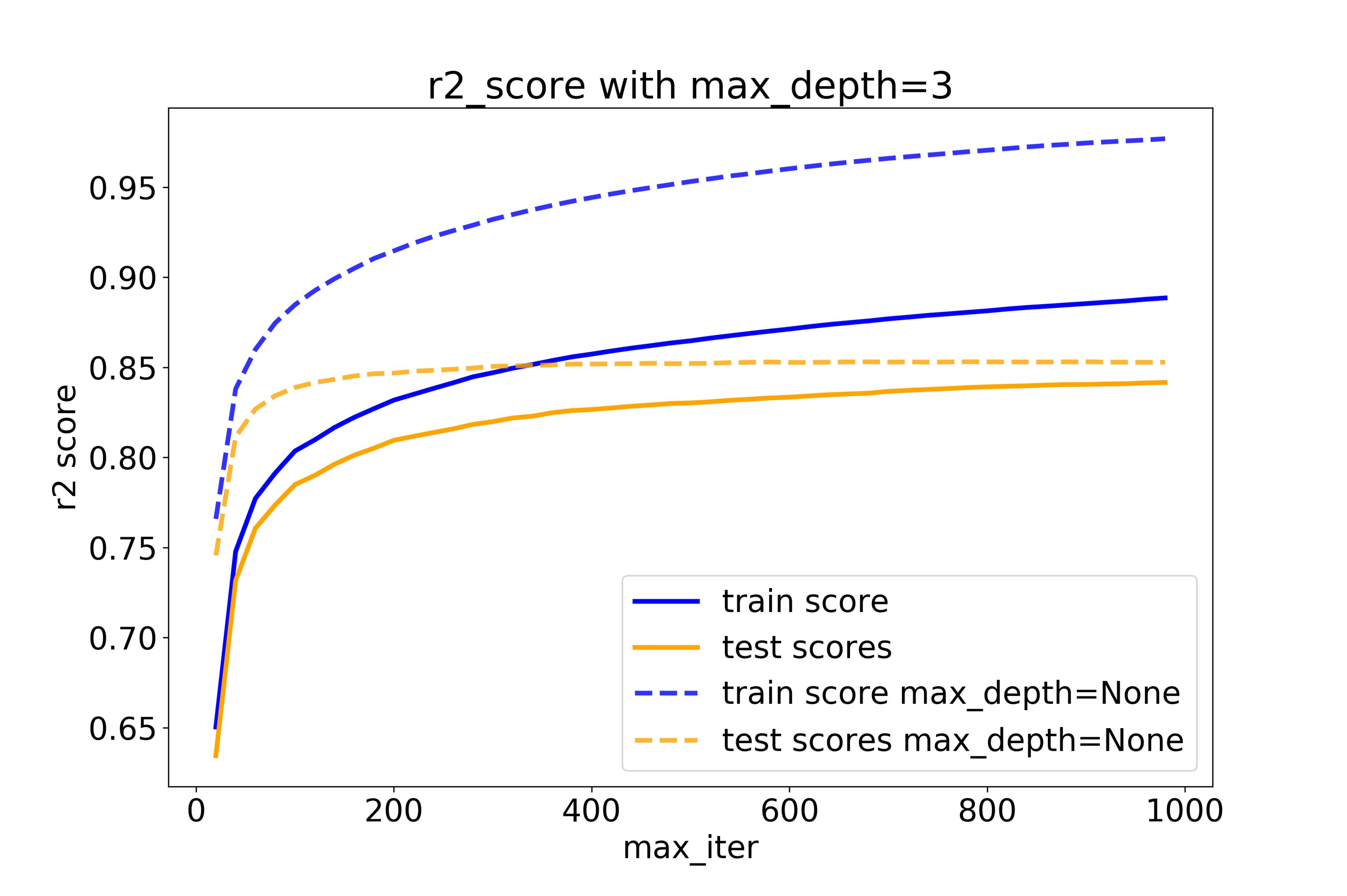
Hyperparameters (Grow Trees 🎄, part 2)

- `max_leaf_nodes=31`
- `max_depth=None`
- `min_samples_leaf=20`

Hyperparameters (Grow Trees 🎄, part 3)



Hyperparameters (Grow Trees 🎄, part 4)



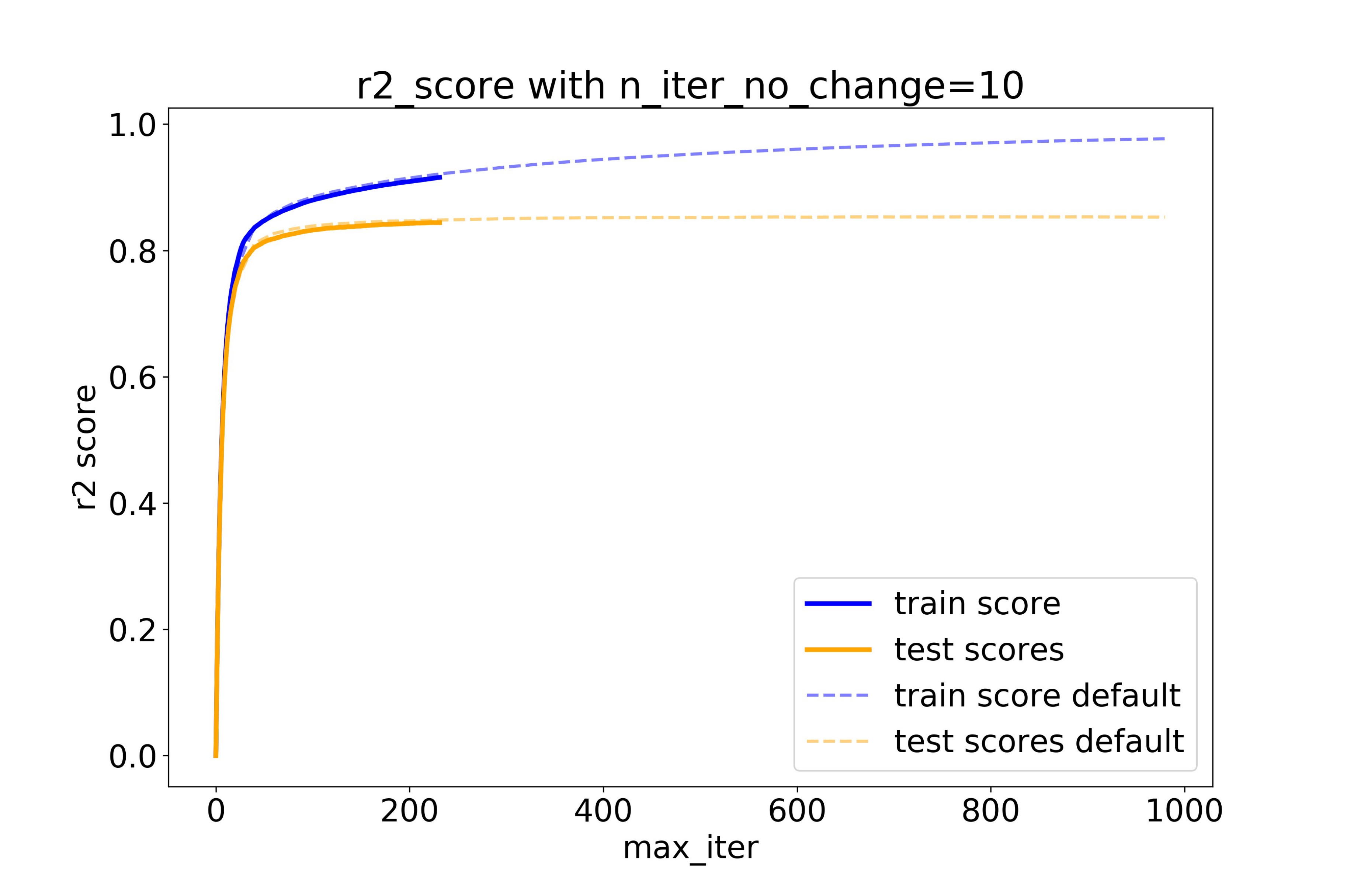
Hyperparameters (Early Stopping 🛑, part 1)

1. Bin data
2. **Split into a validation dataset**
3. Make initial predictions (constant)
4. Calculate gradients and hessians
5. Grow Trees For Boosting
    1. ...
    2. **Stop if early stop condition is true**

Hyperparameters (Early Stopping 🛑, part 2)

- `scoring=None` (could be 'loss')
- `validation_fraction=0.1`
- `n_iter_no_change=None`
- `tol=1e-7`

Hyperparameters (Early Stopping 🛑, part 3)



Hyperparameters (Misc 🎁)

- `verbose=0`
- `random_state=None`
- `export OMP_NUM_THREADS=12`

Benchmarks 🚀 (HIGGS Part 1)

- 8800000 records
- 28 features
- binary classification (1 for signal, 0 for background)

Benchmarks 🚀 (HIGGS Part 2)

- `max_iter=100`, `learning_rate=0.1`, `export OMP_NUM_THREADS=12`

library	time	roc auc	accuracy
sklearn	38s	0.8125	0.7324
lightgbm	39s	0.8124	0.7322
xgboost	48s	0.8126	0.7326
catboost	100s	0.8004	0.7222

Benchmarks 🚀 (HIGGS Part 3)

- `max_iter=500`

library	time	roc auc	accuracy
sklearn	129s	0.8281	0.7461
lightgbm	125s	0.8283	0.7462
xgboost	149s	0.8285	0.7465
catboost	427s	0.8225	0.7412

Benchmarks 🚀 (HIGGS Part 4)

`export OMP_NUM_THREADS=4` `max_iter=100` (on my laptop)

library	**time (12 cores)**	**time (4 cores)**
sklearn	38s	85s
lightgbm	39s	86s
xgboost	48s	115s
catboost	100s	164s

Benchmarks 🚀 (HIGGS Part 5)

DEMO!

Roadmap 🛣️ (In upcoming 0.22)

- ~~Missing Values~~

```
from sklearn.experimental import enable_hist_gradient_boosting
from sklearn.ensemble import HistGradientBoostingClassifier
from sklearn.datasets import make_classification

X, y = make_classification(random_state=42)
X[:10, 0] = np.nan

gbdt = HistGradientBoostingClassifier().fit(X, y)
print(gbdt.predict(X[:20]))
# [0 0 1 1 0 0 0 1 0 1 1 0 0 0 1 1 1 0 0 1]
```

Roadmap 🛣️ (After 0.22)

- Discrete (Categorical) Feature support
- Sparse Data
- Sample Weights

Thank you Working on This 🎉

- @hug_nicolas - Associate Research Scientist @ Columbia University
- All the core developers for reviewing!

Conclusion 🎉

```python
from sklearn.experimental import enable_hist_gradient_boosting
from sklearn.ensemble import HistGradientBoostingClassifier
from sklearn.ensemble import HistGradientBoostingRegressor
```

- Try out the dev build (for missing values):

```
pip install --pre -f https://sklearn-nightly.scdn8.secure.raxcdn.com scikit-learn
```

- github.com/thomasjpfan/pydata-2019-histgradientboosting
- Twitter: @thomasjpfan

Appendix

- Loss function with l2 regularization

$$L(y, f(X)) = \frac{1}{2}||y - f(X)||^2 + \lambda \sum_i w_i^2$$

where w_i score of the leaves.