Fast Gradient Boosting with Numba

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pygbm: fast gradient boosting in Python with `Numba`

Outline

1. Gradient Boosting is a gradient descent
2. Making it fast with histograms
3. `Numba`: field report (and a tiny bit of `Cython`)

slides at https://bit.ly/2YFaIPO

Gradient Boosting

$$\hat{y}_i = \sum_{m=1}^{\text{n\_iter}} h_m(\mathbf{x}_i)$$

h_m: "weak" estimator that predicts **gradients** (not the target)

This is a gradient descent!

Linear regression

$$L = \sum_i (y_i - \hat{y}_i)^2$$

$\hat{y}_i = x_i^\top \theta$

Gradient boosting

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$$\theta^{(m+1)} = \theta^{(m)} - \alpha \frac{\partial L}{\partial \theta^{(m)}}$$

Gradient boosting

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Gradient Descent

Hack # 1

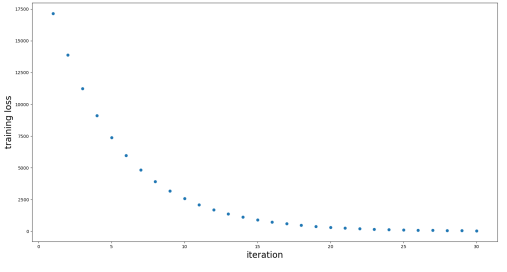
Optimize w.r.t. predictions: $\hat{\mathbf{y}}^{(m+1)} = \hat{\mathbf{y}}^{(m)} - \alpha \frac{\partial \mathcal{L}}{\partial \hat{\mathbf{y}}^{(m)}}$

```
def compute_gradient(y_true, y_pred):
    return -2 * (y_true - y_pred)  # Least squares loss gradient

y_pred = np.zeros(shape=n_samples)

for m in range(n_iterations):
    negative_gradient = -compute_gradient(y_true, y_pred)
    y_pred += alpha * negative_gradient

    # save training loss value for plotting
    loss_values.append(np.mean((y_true - y_pred)**2))
```



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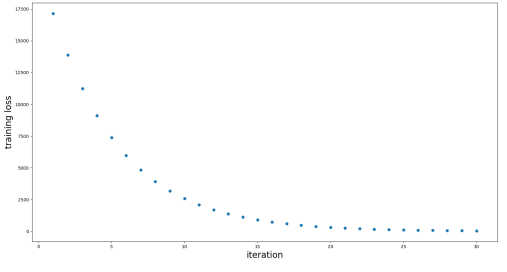

Prediction for new data???

Hack # 2

Train weak predictor h to predict the gradients!

```
for m in range(n_iterations):
    negative_gradient = -compute_gradient(y_true, y_pred)
    h = DecisionTree().fit(X, y=negative_gradient)
    y_pred += alpha * h.predict(X)
    self.predictors.append(h)  # save predictor for later
```

We can now use the h_m for new data

```
def predict(X):
    pred = np.zeros(...)
    for h in self.predictors:
        pred += alpha * h.predict(X)
    return pred
```

$$\hat{y}_i = \sum_{m=1}^{\text{n\_iter}} h_m(\mathbf{x}_i)$$

That's our gradient descent!

Recipe for Gradient Boosting

1. Choose a (differentiable) loss
2. Optimize loss w.r.t **predictions** instead of a model parameter
3. Predict the GD step with a base estimator (a regressor)
4. Use these base estimators to predict unseen data

Making it fast

Taking inspiration from LightGBM

What is slow: split finding

```
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```
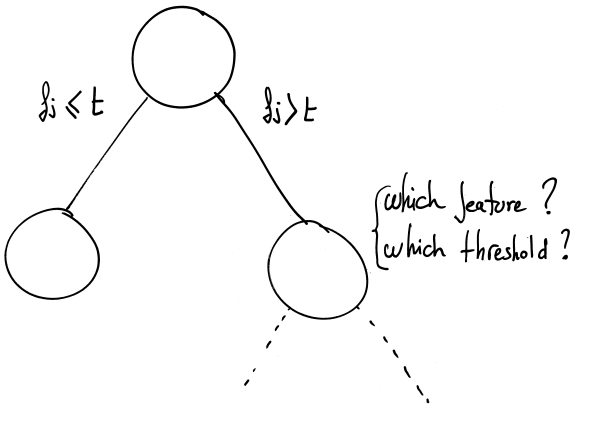



Repeated for each tree, at every node

What is slow: split finding

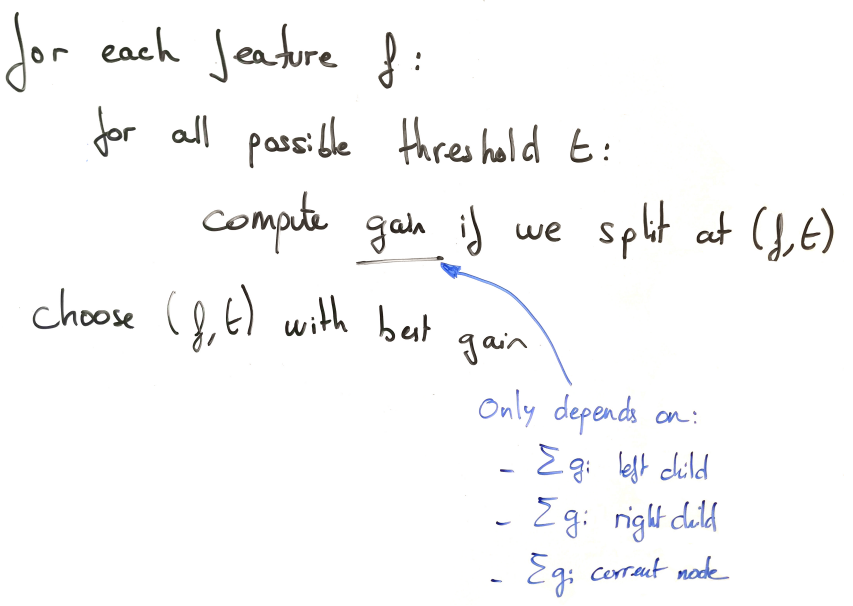
for each feature f:

  for all possible threshold t:

    compute gain if we split at (f, t)

choose (f, t) with best gain

What is slow: split finding



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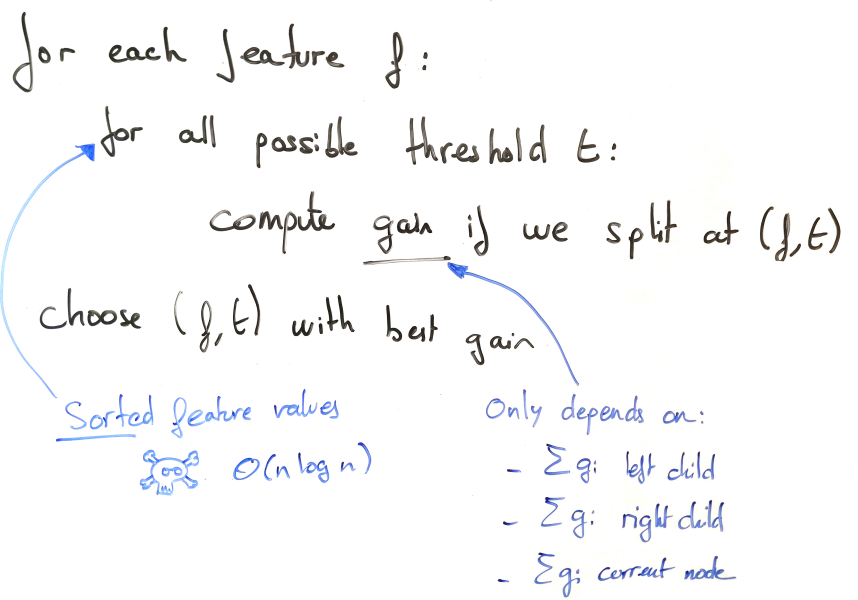

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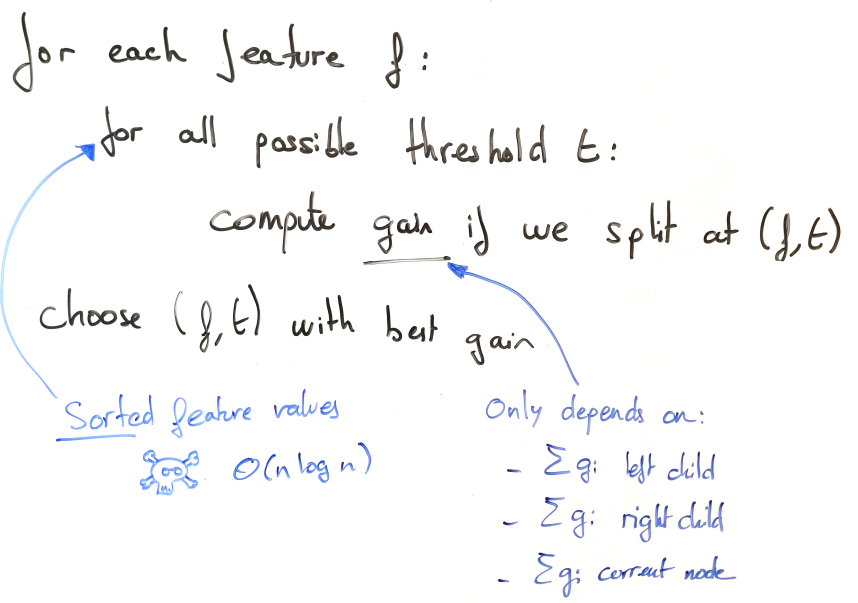
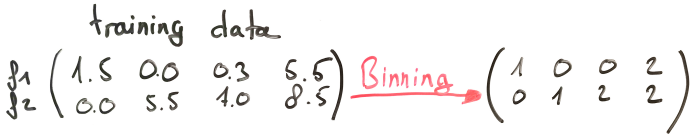


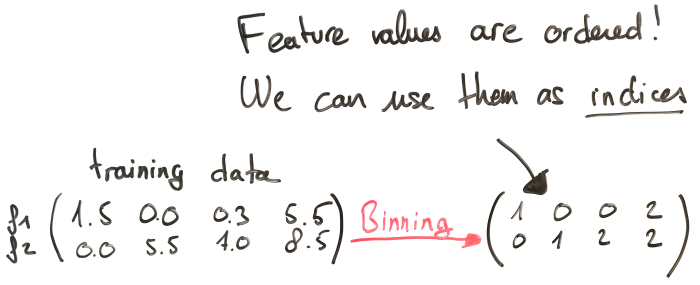
From $\mathcal{O}(n \log n)$ to $\mathcal{O}(n)$: Histograms

Bin the data!



We bin once and for all at the start of the fitting process

Bin the data!



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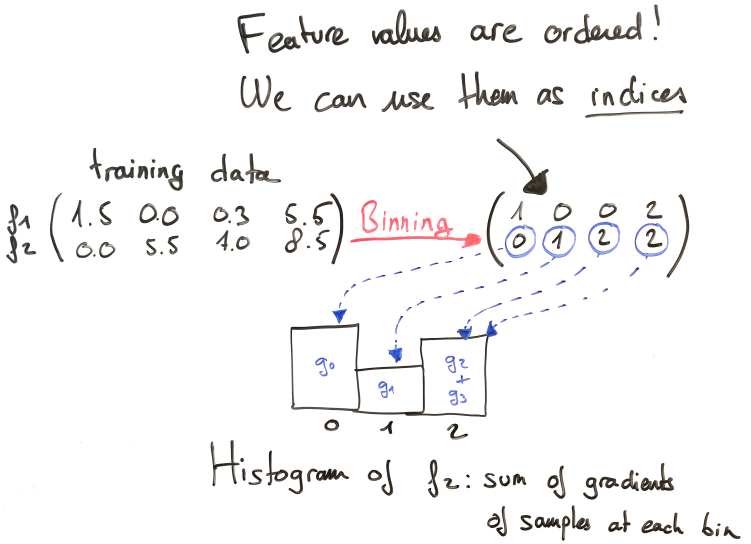

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Histograms are then computed at each node, for each feature

Split finding now

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    build histogram

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        Compute gain

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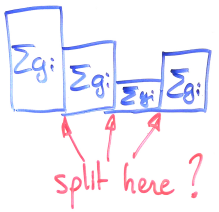


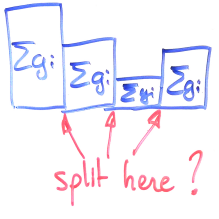
depends on Σg_i in | left / right / current

Split finding now

for each feature f:

was $\mathcal{O}(n \log n)$

- build histogram $\mathcal{O}(n)$
- for each bin with threshold t: $\mathcal{O}(n\_bins)$
  - Compute gain



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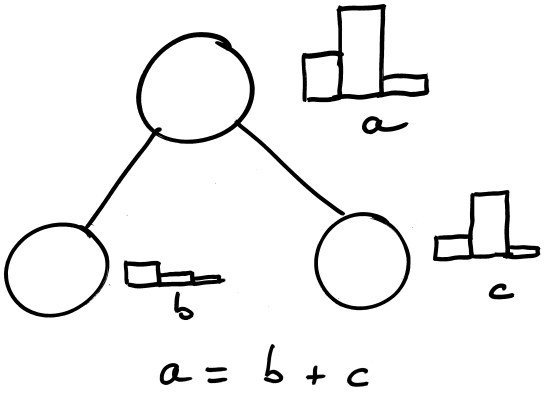
Subtraction trick



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Hist(parent) = Hist(left) + Hist(right)

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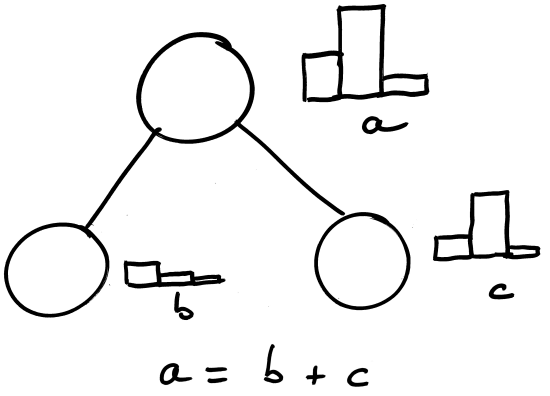

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For half of the nodes:
$\mathcal{O}(n)$ --> $\mathcal{O}$(n_bins)

Numba makes Python code fast

Numba is an open source JIT compiler that translates a subset of Python and NumPy code into fast machine code.

GBDT implementation with `Numba`:

github.com/ogrisel/pygbm

Support for custom dtypes (structured arrays)

```
HISTOGRAM_DTYPE = np.dtype([
    ('g', np.float32),  # sum gradients
    ('h', np.float32),  # sum hessians
])

@njit
def subtract_histograms(hist_a, hist_b):
    out = np.zeros(n_bins, dtype=HISTOGRAM_DTYPE)

    for i in range(n_bins):
        out[i]['g'] = hist_a[i]['g'] - hist_b[i]['g']
        out[i]['h'] = hist_a[i]['h'] - hist_b[i]['h']

    return out
```

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Support for parallelization (OpenMP or Intel TBB)

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for feature in prange(n_features):  # parallel loop
    subtract_histograms(...)
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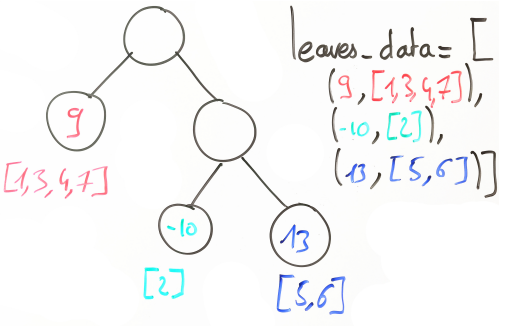
`Cython` equivalent:

- need to declare C-struct equivalent to DTYPE
- cannot allocate numpy array in function
  - parallel code needs GIL to be released
  - allocate outside and pass it as a parameter

Lists of different length? No problem

```
for m in range(n_iterations):  # main GB loop
    ...
    y_pred += h.predict(X)  # can be optimized for training data!
    ...
```




```
@njit(parallel=True)
def update_predictions(leaves_data, y_pred):
    for leaf in prange(len(leaves_data)):
        leaf_value, sample_indices = leaves_data[leaf]
        for i in sample_indices:
            y_pred[i] += leaf_value
```

It's fast

Higgs boson dataset (10E7 samples), 20 trees, 4 cores

```
pygbm (ignoring compile time!)
done in 42.851s, ROC AUC: 0.7229, ACC: 0.7245

Lightgbm
done in 42.400s, ROC AUC: 0.7232, ACC: 0.7250
```

Overall experience with Numba

- the doc is good ♥♥♥
- low barrier to entry
- from slow code to fast code: easy process
- code looks like Python (with for loops): stay Pythonic
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  - profiling?
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It's still WIP though

Use it!

Thanks!

(BTW, check out our new GBDTs in scikit-learn!)