Gradient Boosted Regression Trees

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DataRobot

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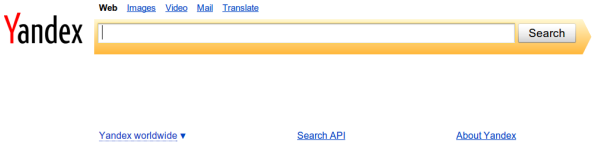
Motivation


NETFLIX
Browse
Recommendations
Friends
Queue
Buy DVDs
Movies For You
You really liked it...


Heritage Health Prize
Better Health Through Analytics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March - May 2010
CHALLENGE


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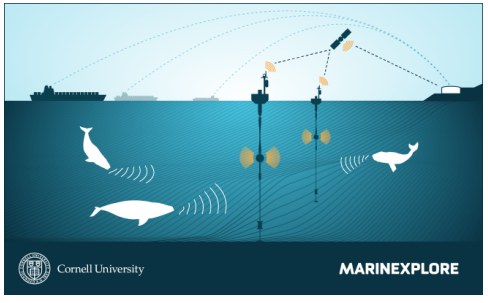
Wind Forecasting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CARVANA
SELL NO EVIL.

Motivation


NETFLIX
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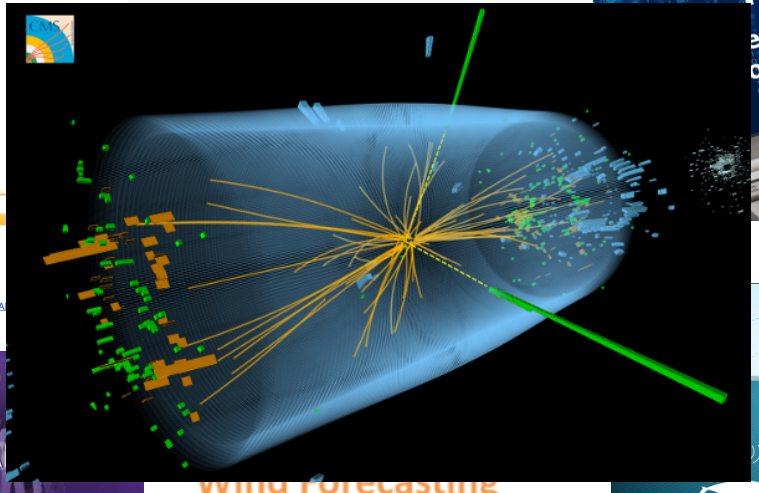
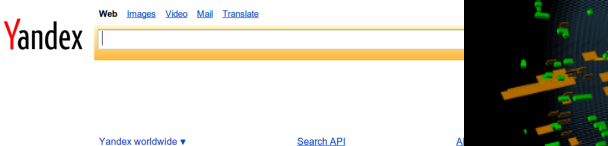
You really liked it...
The Big One


Heritage Health Prize

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LEARNING TO RANK
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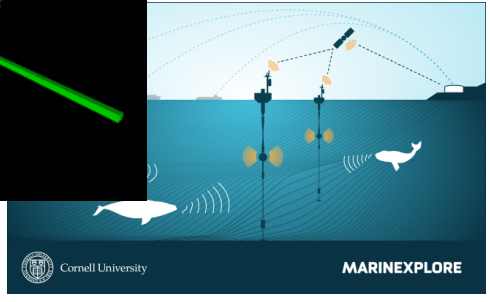
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Outline

About us

Peter

- @pprett
- Python & ML $\sim$ 6 years
- sklearn dev since 2010

Gilles

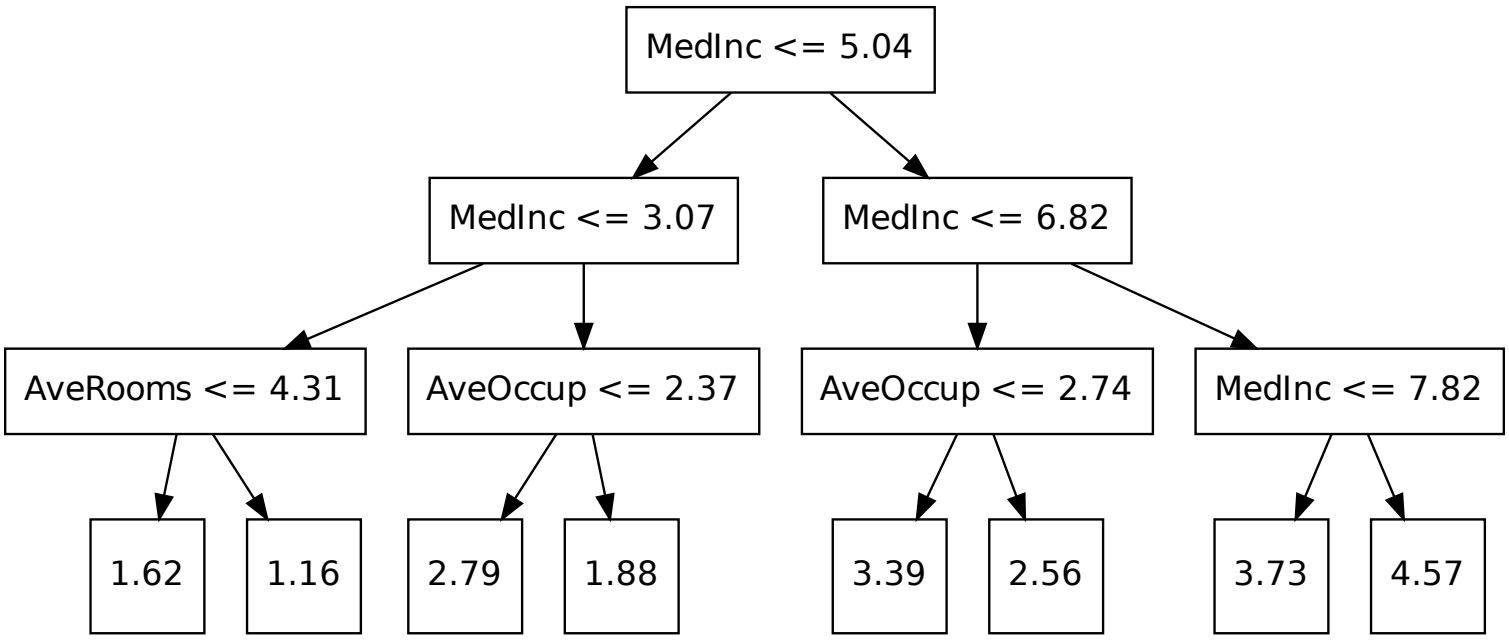
- @glouppe
- PhD student (Liège, Belgium)
- sklearn dev since 2011
  Chief tree hugger

Outline

Machine Learning 101

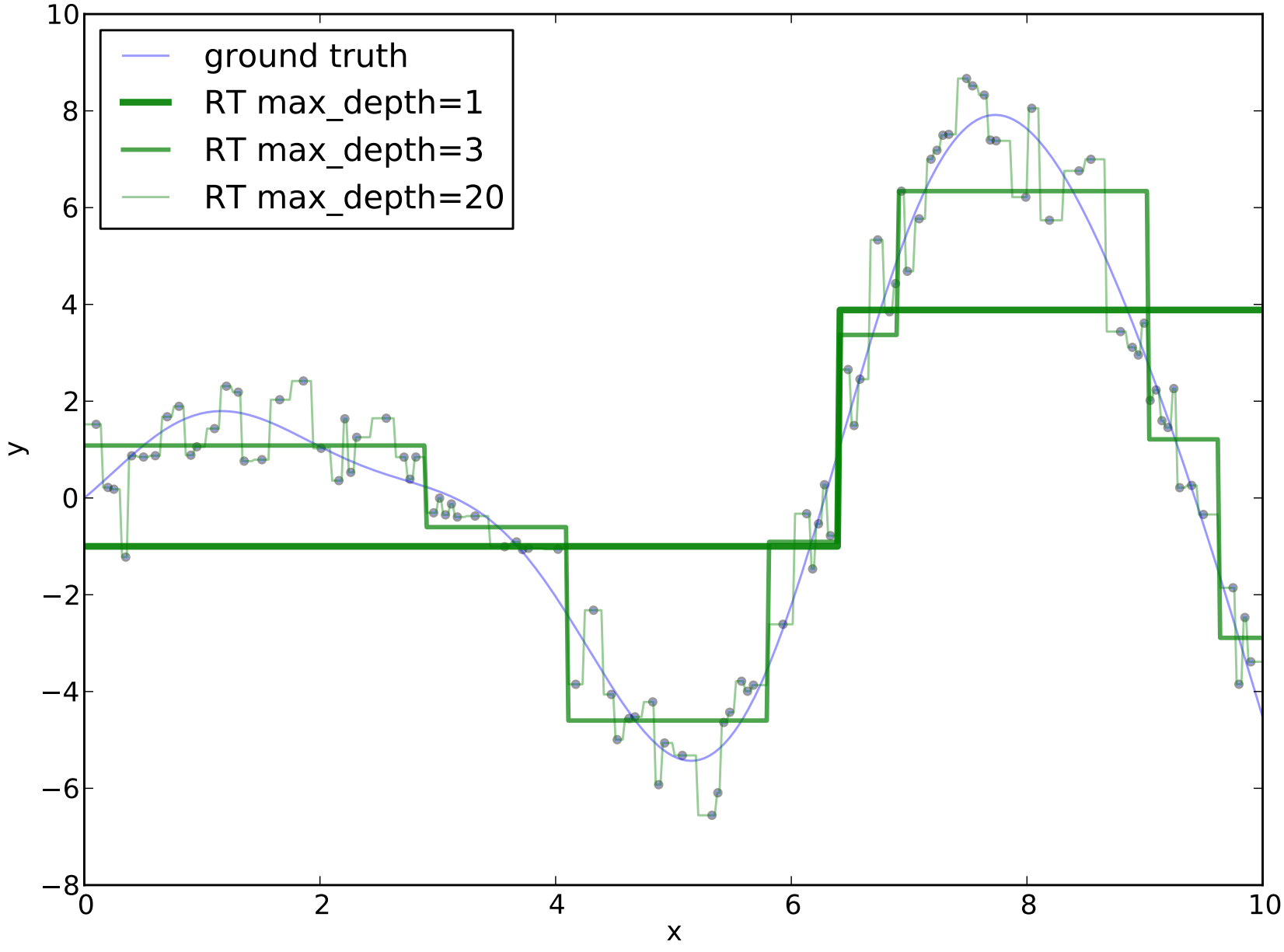
- Data comes as...
  - A set of examples $\{(\mathbf{x}_i, y_i) | 0 \leq i < \text{n\_samples}\}$, with
  - Feature vector $\mathbf{x} \in \mathbb{R}^{\text{n\_features}}$, and
  - Response $y \in \mathbb{R}$ (regression) or $y \in \{-1, 1\}$ (classification)
- Goal is to...
  - Find a function $\hat{y} = f(\mathbf{x})$
  - Such that error $L(y, \hat{y})$ on new (unseen) $\mathbf{x}$ is minimal

Classification and Regression Trees [Breiman et al, 1984]

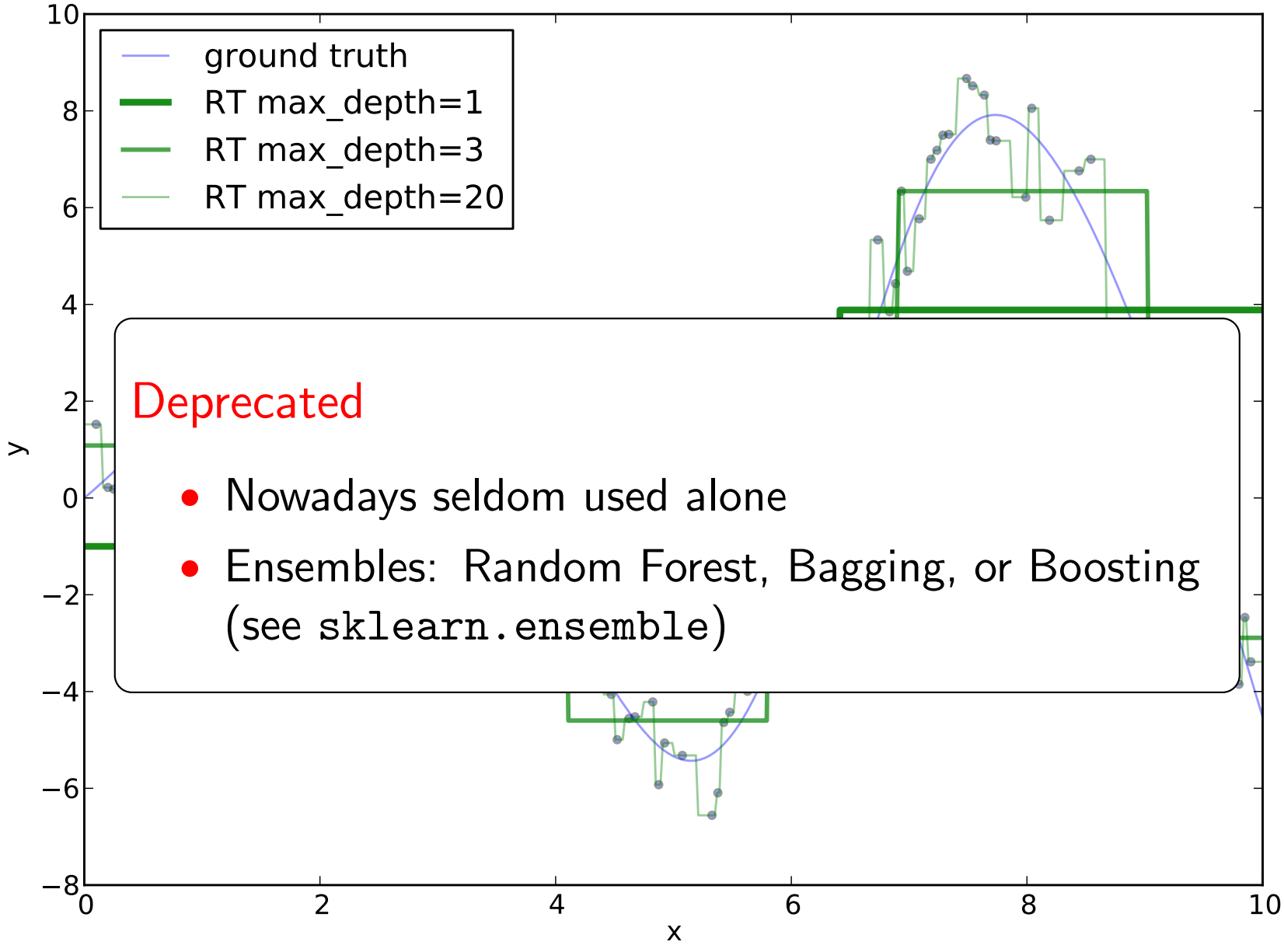


`sklearn.tree.DecisionTreeClassifier|Regressor`

Function approximation with Regression Trees



Function approximation with Regression Trees



Deprecated

- Nowadays seldom used alone
- Ensembles: Random Forest, Bagging, or Boosting (see `sklearn.ensemble`)

Outline

Gradient Boosted Regression Trees

Advantages

- Heterogeneous data (features measured on different scale)
- Supports different loss functions (e.g. huber)
- Automatically detects (non-linear) feature interactions

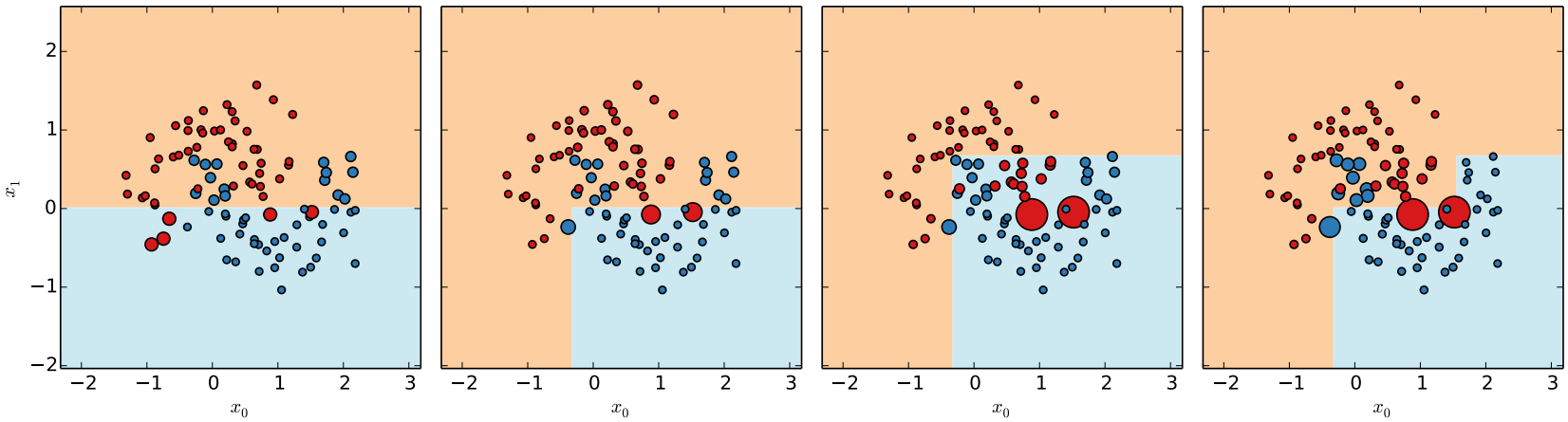
Disadvantages

- Requires careful tuning
- Slow to train (but fast to predict)
- Cannot extrapolate

Boosting

AdaBoost [Y. Freund & R. Schapire, 1995]

- Ensemble: each member is an expert on the errors of its predecessor
- Iteratively re-weights training examples based on errors

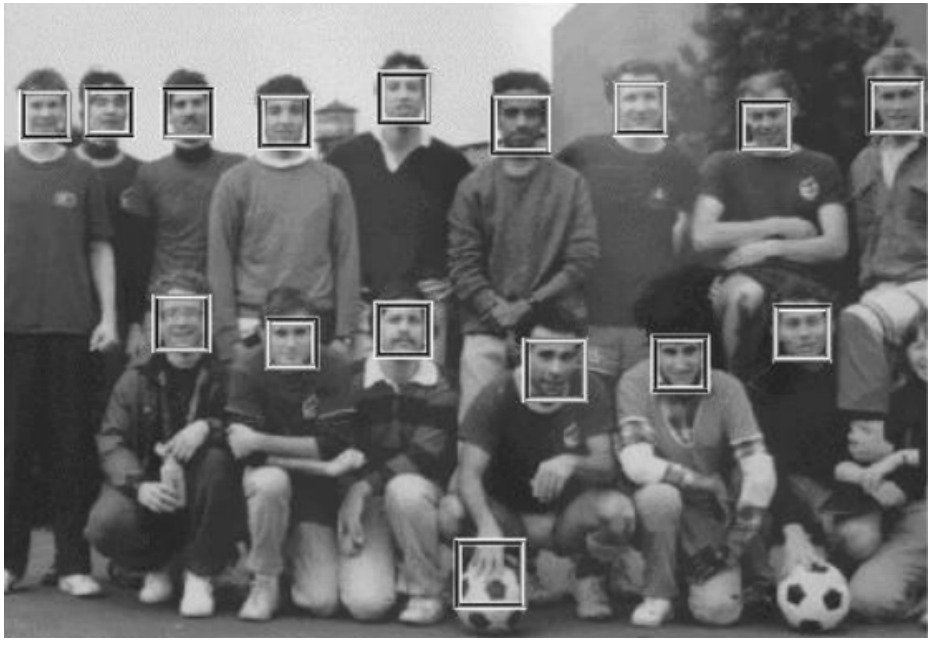


`sklearn.ensemble.AdaBoostClassifier|Regressor`

Boosting

Huge success

- Viola-Jones Face Detector (2001)



- Freund & Schapire won the Gödel prize 2003

`sklearn.ensemble.AdaBoostClassifier|Regressor`

Gradient Boosting [J. Friedman, 1999]

Statistical view on boosting

- $\Rightarrow$ Generalization of boosting to arbitrary loss functions

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Statistical view on boosting

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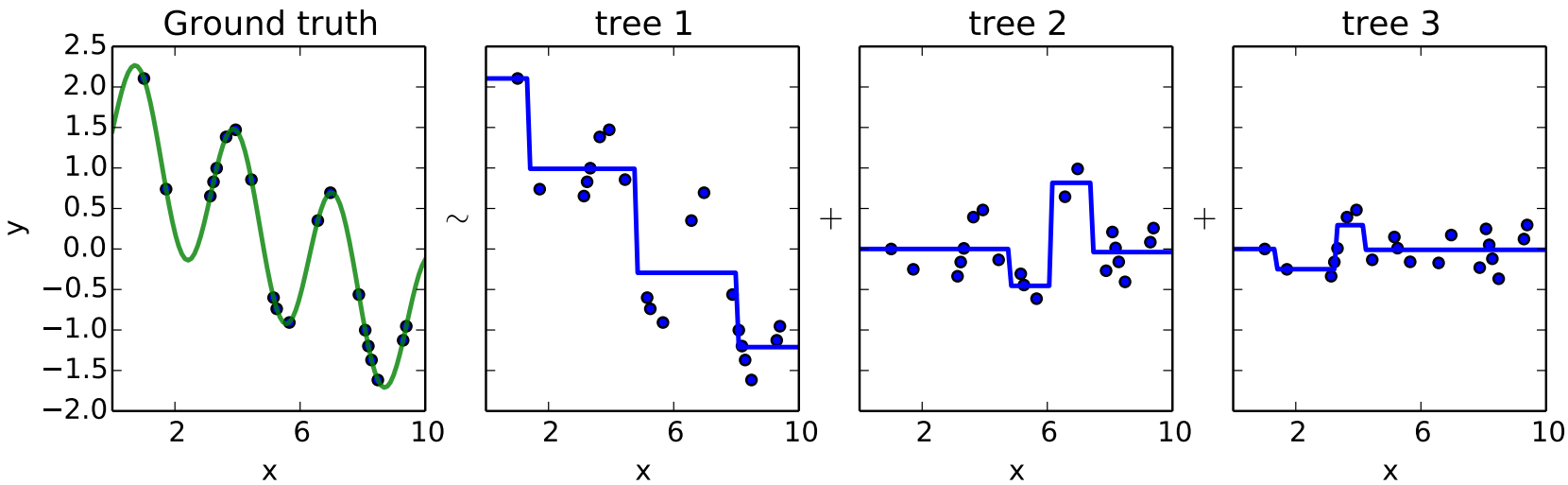
Residual fitting



Functional Gradient Descent

Least Squares Regression

- Squared loss: $L(y_i,\ f(\mathbf{x}_i)) = (y_i - f(\mathbf{x}_i))^2$
- The residual $\sim$ the (negative) gradient $\frac{\partial L(y_i,\, f(\mathbf{x}_i))}{\partial f(\mathbf{x}_i)}$

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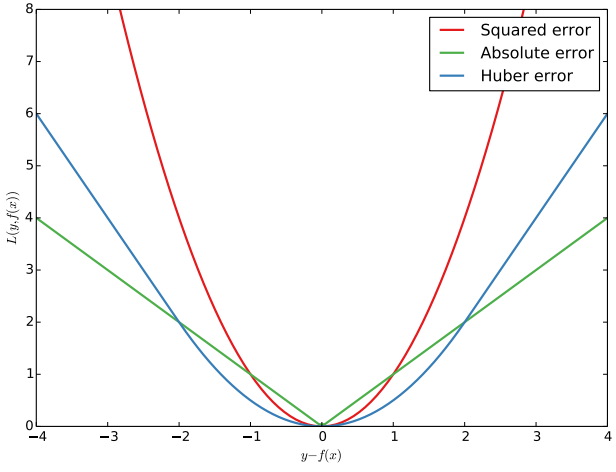
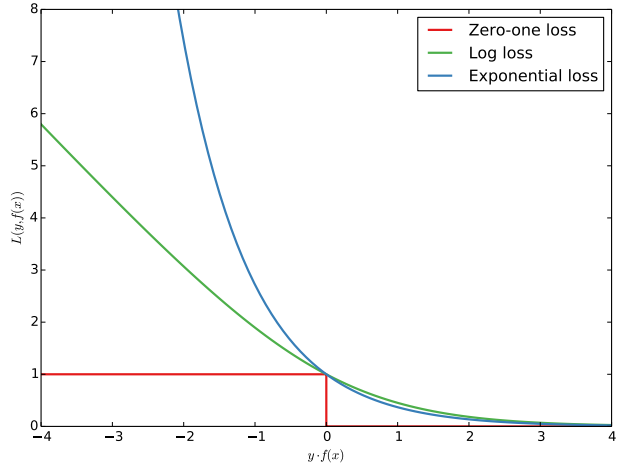
Steepest Descent

- Regression trees approximate the (negative) gradient
- Each tree is a successive gradient descent step





Outline

Notebook

http://github.com/pprett/pydata-gbm-tutorial

Tipps & Tricks 1

Input layout

Use dtype=np.float32 to avoid memory copies and fortan layout for slight runtime benefit.

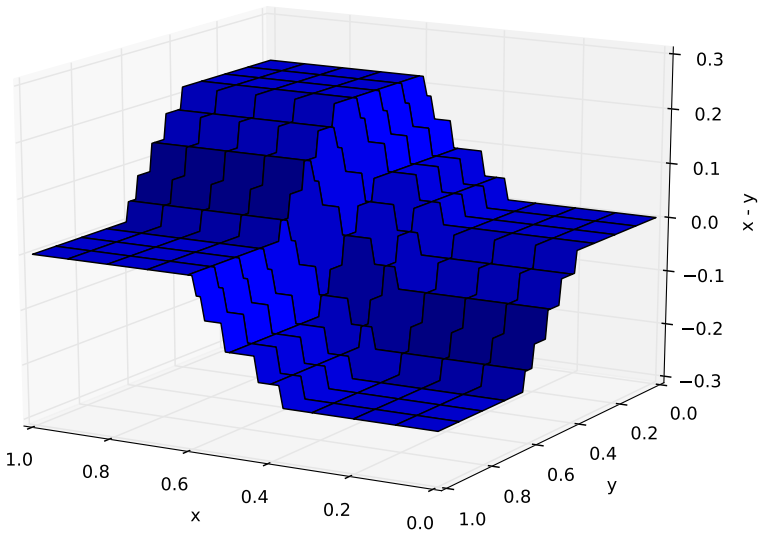
```
X = np.asfortranarray(X, dtype=np.float32)
```

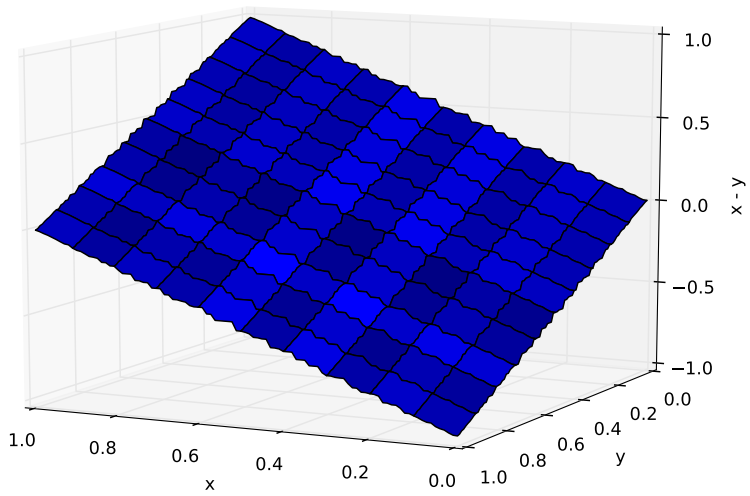
Tipps & Tricks 2

Feature interactions

GBRT automatically detects feature interactions but often explicit interactions help.

Trees required to approximate $X_1 - X_2$: 10 (left), 1000 (right).





Tipps & Tricks 3

Categorical variables

Sklearn requires that categorical variables are encoded as numerics. Tree-based methods work well with ordinal encoding:

```
df = pd.DataFrame(data={'icao': ['CRJ2', 'A380', 'B737', 'B737']})
# ordinal encoding
df_enc = pd.DataFrame(data={'icao': np.unique(df.icao,
                return_inverse=True)[1]})
X = np.asfortranarray(df_enc.values, dtype=np.float32)
```