Gradient Boosting, Continued

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Review: Gradient Boosting

The Gradient Boosting Machine

1. Initialize $f_0(x) = 0$.
2. For $m = 1, 2, \ldots$ (until stopping condition met)
    1. Compute **unconstrained gradient**:

    $$\mathbf{g}_m = \left(\frac{\partial}{\partial f(x_i)} \left(\sum_{i=1}^{n} \ell(y_i, f(x_i)) \right) \Bigg|_{f(x_i) = f_{m-1}(x_i)} \right)_{i=1}^{n}$$

    2. Fit regression model to $-\mathbf{g}_m$:

    $$h_m = \operatorname*{arg\,min}_{h \in \mathcal{F}} \sum_{i=1}^{n} \left((-\mathbf{g}_m)_i - h(x_i) \right)^2.$$

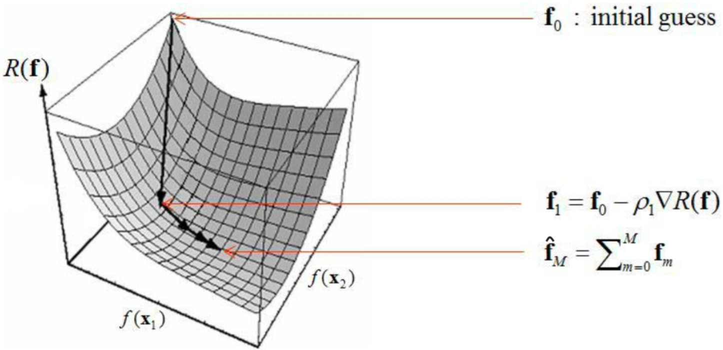
    3. Choose fixed step size $\nu_m = \nu \in (0, 1]$ [$v = 0.1$ is typical], or take

    $$\nu_m = \operatorname*{arg\,min}_{\nu > 0} \sum_{i=1}^{n} \ell\{y_i, f_{m-1}(x_i) + \nu h_m(x_i)\}.$$

    4. Take the step:

    $$f_m(x) = f_{m-1}(x) + \nu_m h_m(x)$$

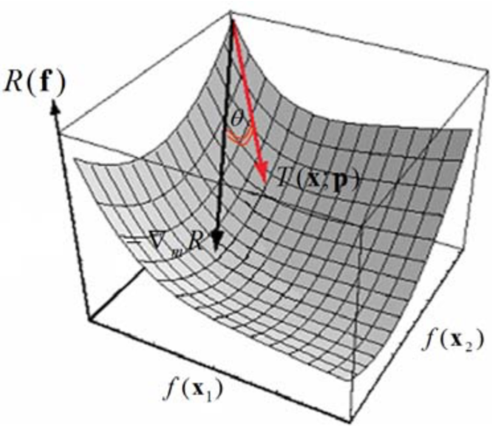
Unconstrained Functional Gradient Stepping



Where $R(\mathbf{f})$ is the empirical risk.
Issue: $\hat{\mathbf{f}}_M$ only defined at training points.

From Seni and Elder's *Ensemble Methods in Data Mining*, Fig B.1.

Projected Functional Gradient Stepping



$T(x;p) \in \mathcal{F}$ is our actual step direction (projection of -**g**=-∇R onto $\mathcal{F}$)

From Seni and Elder's *Ensemble Methods in Data Mining*, Fig B.2.

The Gradient Boosting Machine: Recap

- Take any [sub]differentiable loss function.
- Choose a base hypothesis space for regression.
- Choose number of steps (or a stopping criterion).
- Choose step size methodology.
- Then you're good to go!

Gradient Tree Boosting

Gradient Tree Boosting

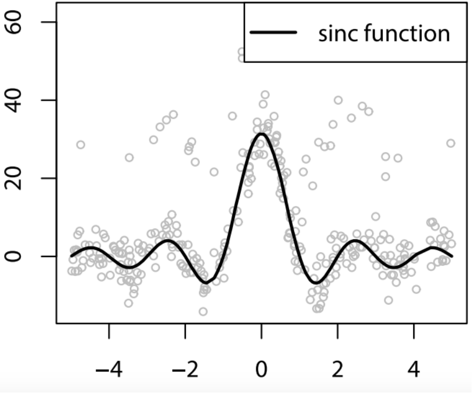
- Common form of gradient boosting machine takes

$$\mathcal{F} = \{\text{regression trees of size } J\},$$

  where J is the number of terminal nodes.
- $J = 2$ gives decision stumps
- HTF recommends $4 \leqslant J \leqslant 8$.
- Software packages:
  - Gradient tree boosting is implemented by the **gbm package** for R
  - as `GradientBoostingClassifier` and `GradientBoostingRegressor` in **sklearn**
- For trees, there are other tweaks on the algorithm one can do
  - See HTF 10.9-10.12

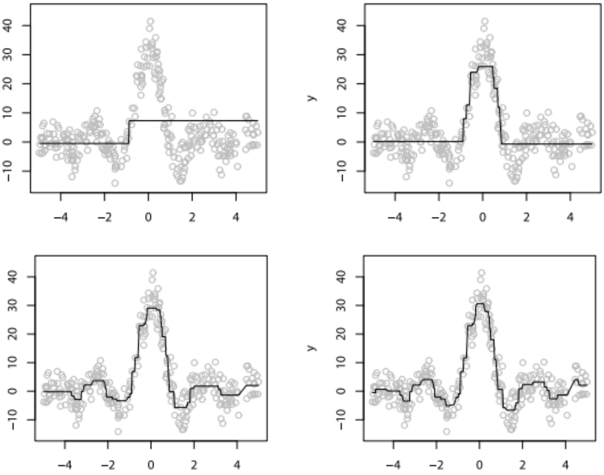
GBM Regression with Stumps

Sinc Function: Our Dataset



From Natekin and Knoll's "Gradient boosting machines, a tutorial"

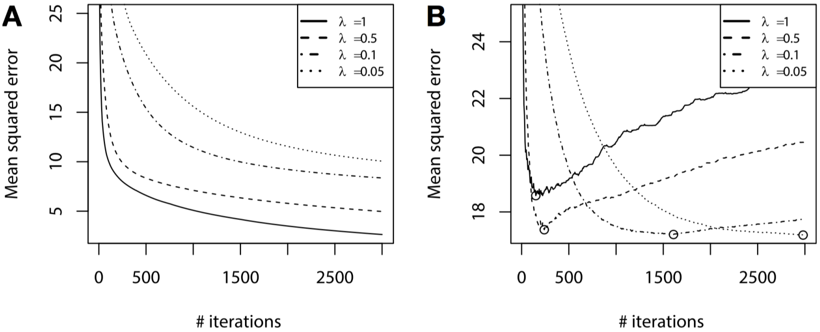
Fitting with Ensemble of Decision Stumps



Decision stumps with 1, 10, 50, and 100 steps, step size $\lambda = 1$.

From Natekin and Knoll's "Gradient boosting machines, a tutorial"

Step Size as Regularization



Performance vs rounds of boosting and step size.

From Natekin and Knoll's "Gradient boosting machines, a tutorial"

Variations on Gradient Boosting

Stochastic Gradient Boosting

- For each stage,
  - choose random subset of data for computing projected gradient step.
  - Typically, about 50% of the dataset size.
  - Fraction is often called the **bag fraction**.
- Why?
  - Faster.
  - Subsample percentage is additional regularization parameter.
- How small a fraction can we take?

Column / Feature Subsampling for Regularization

- Similar to random forest, randomly choose a subset of features for each round.
- XGBoost paper says: "According to use feedback, using column sub-sampling prevents overfitting even more so than the traditional row sub-sampling."

Newton Step Direction

- For GBM, we find the closest $h \in \mathcal{F}$ to the negative gradient
$$-\mathbf{g} = -\nabla_{\boldsymbol{f}} J(\mathbf{f}).$$
- This is a "first order" method.
- Newton's method is a "second order method":
  - Find 2nd order (quadratic) approximation to J at $\boldsymbol{f}$.
    - Requires computing gradient and Hessian of J.
  - Newton step direction points towards minimizer of the quadratic.
  - Minimizer of quadratic is easy to find in closed form
- Boosting methods with projected Newton step direction:
  - LogitBoost (logistic loss function)
  - XGBoost (any loss – uses regression trees for base classifier)