# 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 $-\mathbf{g}_m$:

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

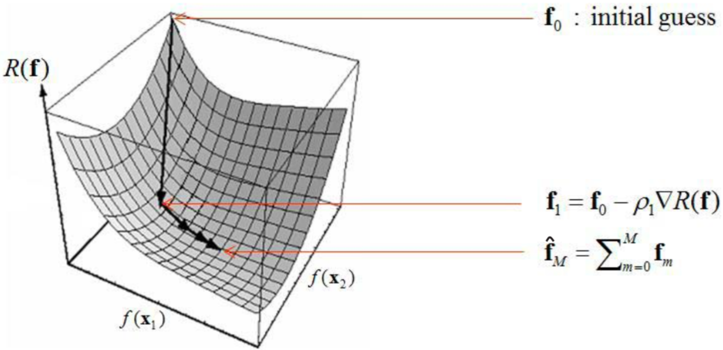
    3. Choose fixed step size $\nu_m = \nu \in (0, 1]$ [$v = 0.1$ is typical], or take

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

    4. Take the step:

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

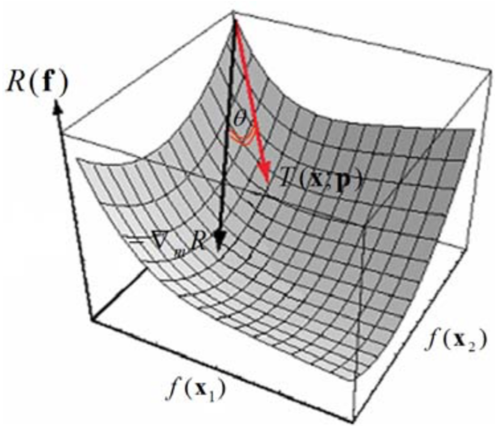
# Unconstrained Functional Gradient Stepping




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 -$\mathbf{g}$=-$\nabla R$ 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!

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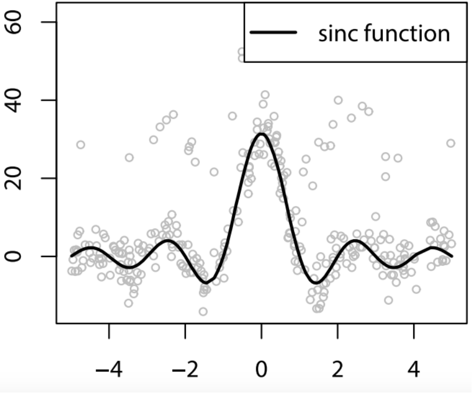
- For trees, there are other tweaks on the algorithm one can do
  - See HTF 10.9-10.12

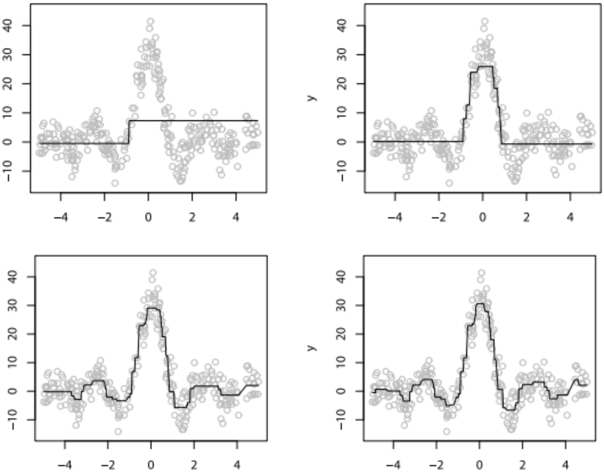
# GBM Regression with Stumps

# Sinc Function: Our Dataset




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

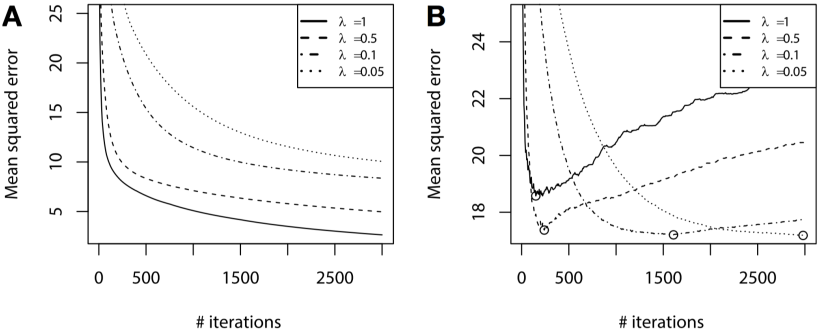
# Fitting with Ensemble of Decision Stumps




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

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- How small a fraction can we take?

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- XGBoost paper says: "According to use feedback, using column sub-sampling prevents overfitting even more so than the traditional row sub-sampling."

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- 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)