Applied modeling with BART: How, Why, and When

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Follow along!

- GitHub Repo: https://go.wisc.edu/0f5xi5
- Slides & code (as RMarkdown documents & R scripts

Nonparametric regression & classification

- Observed data: $(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)$ with $\boldsymbol{x}_n \in [0,1]^p$
- Regression: $y_n = f(\boldsymbol{x}_n) + \sigma\epsilon_n; \epsilon_n \sim \mathcal{N}(0,1)$
- Classification (w/ probit link): $\mathbb{P}(Y = 1) = \Phi(f(\boldsymbol{x}))$
- Simultaneous (and often competing) goals:
  - Prediction: value of $f(\boldsymbol{x}^\star)$ & $y^\star$
  - UQ: uncertainty intervals for $f(\boldsymbol{x}^\star)$ & $y^\star$
  - Variable importance/selection: on which X_j does f depend?

Approaches to learning f

- Assume $f(\boldsymbol{x}) = \sum_d \beta_d \phi_d(\boldsymbol{x})$
  - Basis $\{\phi_d\}$ could be linear, polynomial, splines, Fourier, etc.
  - Estimate β_d's with OLS, LASSO, Bayesian linear regression, etc.
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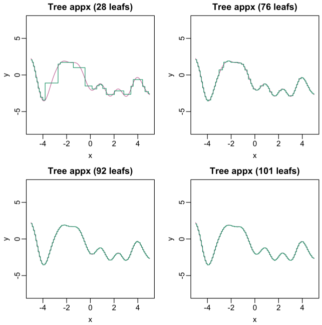
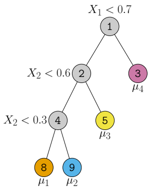
- Ensemble methods
  - Approximate f with a (weighted) average of "weak learners":

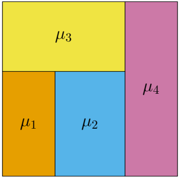
$$\hat{f}(\boldsymbol{x}) = \sum_{m=1}^{M} w_m \hat{f}_m(\boldsymbol{x})$$

  - Each $\hat{f}_m$ may not fit data well but together they do
  - ☺ Tremendous empirical success (e.g. Netflix Prize, Kaggle)

Step function approximations

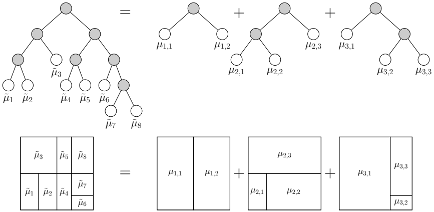






- Step functions are universal function approximators!
- Step functions can be represented as binary regression trees
- Often need very deep tree to appx complicated f well

Sums of trees



- Sum of step functions is just another step function!
- Sums of regression trees is a more complicated regression tree!

☺ Averaging/ensembling introduces certain degree of smoothness

Digression: Pointillism

A Sunday afternoon on the island of La Grande Jatte, Georges Seurat
Source

Preliminaries

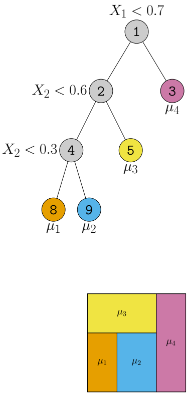
Introducing BART

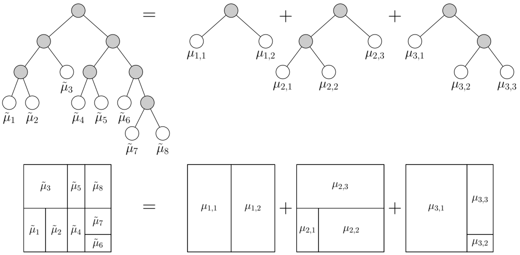
BART in practice

Parting Thoughts

Bayesian Additive Regression Trees

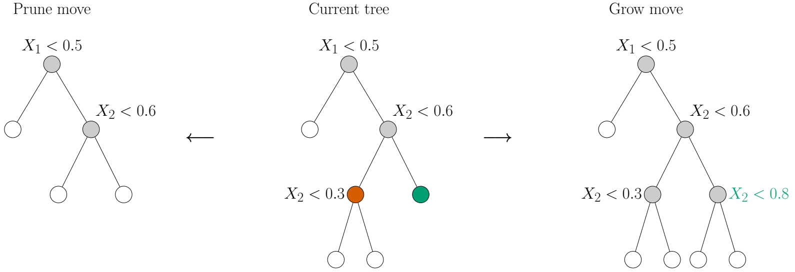
- Regression: $y_n = f(\boldsymbol{x}_n) + \sigma\varepsilon_n; \varepsilon_n \sim \mathcal{N}(0,1)$ & $\boldsymbol{x}_n \in [0,1]^p$
- Main idea: approximate $f(\boldsymbol{x})$ with sum of M regression trees
- Prior encourages trees to be "weak learners"
- Gibbs sampler: update each tree conditionally on fit of all others





Posterior computation & implementation

- Metropolis-within-Gibbs: update each tree sequentially fixing others
  - Update decision tree with MH (randomly grow or prune tree)
  - Update leaf parameters / tree outputs conditional on tree
- No optimization involved!!



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Several implementations

- **BART**: Sparapani, Spanbauer, & McCulloch (2021)
  - Support for many extensions (e.g., classification, survival)
  - Based on efficient C++ regression tree class & sampler
- **dbarts**: Dorie (2020)
  - Makes it easy to include a sum-of-trees component in a larger model
  - E.g. $y_i = \boldsymbol{x}_i^\top \beta + f(\boldsymbol{x}_i) + \sigma\epsilon_i$
- **flexBART**: available at (GitHub repo)
  - Flexibly handle categorical predictors and observations on networks
  - Much faster than **BART**
  - Still under active development
- **bartMachine**: Kapelner & Bleich (2014)
  - Core fitting written in Java
  - 😑 Non-trivial overhead in installing & setting up system
- **PyMC-BART**: From the PyMC team
  - Uses sequential Monte Carlo & is rather different than the above

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- Partial dependence plots
  - $\overline{f}_j(x) = n^{-1}\sum_i f(x_{i,1},\ldots,x_{i,j-1},x,x_{i,j+1},\ldots,x_{i,p})$
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- Linero (2018) modifies BART so that
  - Split on X_j with prob. θ_j (in prior & in MH transition)
  - $\boldsymbol{\theta}$ given a sparsity-inducing Dirichlet prior
  - Adaptation: more accepted splits on $X_j \Rightarrow$ more proposed splits on X_j
  - Select X_j if more than 50% of ensembles involve a split on X_j

BART extensions

- Classification: probit w/ Albert & Chib (1993) data augmentation
- Survival models: Sparapani et al. (2016)
- Log-linear models: Murray (2019)
- Heteroscedasticity: Pratola et al. (2020)
  - $y_n = f(\boldsymbol{x}_n) + \sigma(\boldsymbol{x}_n)\varepsilon_n$, write $\log\left(\sigma^2(\boldsymbol{x})\right)$ as a sum-of-trees!
- Monotonic BART: Chipman et al. (2019)
- Estimating smooth functions
  - Starling et al. (2020): jumps μ_ℓ are Gaussian processes
- Varying coefficient models: D. et al. (2020+)
  - $Y = \beta_0(Z) + \beta_1(Z)X_1 + \cdots + \beta_p(Z)X_p + \sigma\epsilon$
  - E.g. time & demographic varying mediation effects
- Causal inference: Hill (2011) & Hahn et al (2020)

Concluding remarks

- BART: approximate f with sum of regression trees
- Avoids pre-specification of functional form of $f(\boldsymbol{x}) = \mathbb{E}[Y \mid X = \boldsymbol{x}]$
- Excellent performance off-the-shelf
- Lots still in development ... get in touch!

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Thanks, y'all!

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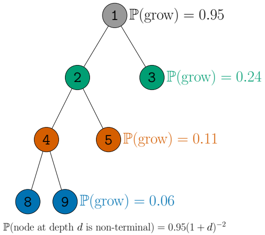
Workshop Material: https://go.wisc.edu/0f5xi5

A prior over regression trees



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- Overwhelming prior prob. that tree depth < 5

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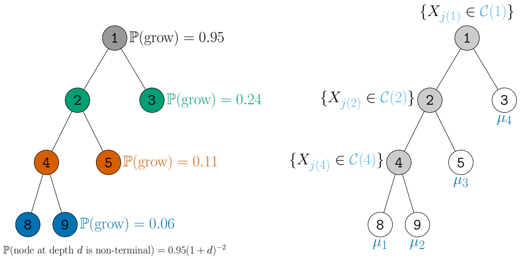

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- Decision rule $\{X_j \in \mathcal{C}\}$
  - X_j continuous: $\mathcal{C}$ is an interval $[0, c)$
  - X_j categorical: $\mathcal{C}$ is a discrete subset of X_j's levels

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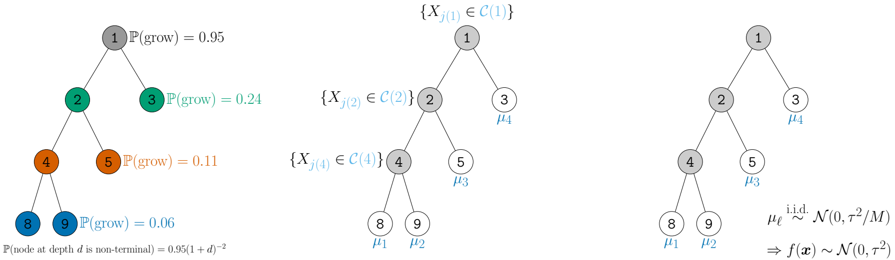

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- Leaf outputs $\mu_\ell \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \tau^2/M)$

Decision rule prior

1. Draw $j \sim \text{Multinomial}(\theta_1, \ldots, \theta_p)$ where $\theta_j = \mathbb{P}(\text{split on } X_j)$
2. Compute set of all available values $\mathcal{A}_j$
   - $\mathcal{A}_j$ determined by rules at ancestors
   - X_j continuous $\rightarrow \mathcal{A}$ is an interval
   - X_j categorical $\rightarrow \mathcal{A}$ is discrete set
3. Draw random subset $\mathcal{C}$ from $\mathcal{A}_j$
   - X_j ccontinuous: draw $c \sim \mathcal{U}(\mathcal{A}_j)$ and set $\mathcal{C} = [0, c)$
   - X_j categorical: assign elements of $\mathcal{A}_j$ to $\mathcal{C}$ with probability 0.5