Model estimation

The GBDT approach was originally proposed by Friedman (2001) and developed into a R package by Ridgeway (2007). Following the notations by Ridgeway (2020), $(\boldsymbol{X}_i, y_i)$ is the ith observation in the sample space S, which has N observations. $\boldsymbol{X}_i$ indicates the vector of independent variables and y_i is the dependent variable. $\boldsymbol{X}$ is the matrix of independent variables of all observations.

Before model estimation, the GBDT approach requires to set three parameters: tree depth K, learning rate λ, and the number of iterations T. The approach first uses a constant to initialize $\hat{f}(\boldsymbol{X}) = argmin_\rho \sum_{i=1}^{N} \Psi(y_i, \rho)$, where Ψ denotes the loss function of squared errors and ρ is the optimal value. Then the following steps will be iterated for T times. For the tth iteration,

Step 1. use Equation (A1) to calculate the negative gradient z_i of the ith observation:

$$z_i = -\frac{\partial}{\partial f(\boldsymbol{X}_i)} \Psi(y_i, f(\boldsymbol{x}_i))|_{f(\boldsymbol{X}_i)=\hat{f}(\boldsymbol{X}_i)}. \quad \text{(A1)}$$

Step 2. fit a decision tree with K terminal nodes using a subsample. Friedman (2002) found that fitting decision trees with a subsample randomly selected from the original sample produces better performance. He suggested that the subsample should include $0.5 \times N$ observations.

Step 3. calculate the optimal prediction ρ_k for the kth terminal node of the fitted decision tree in Step 3 using Equation (A2):

$$\rho_k = argmin_\rho \sum_{\boldsymbol{x}_i \in S_k} \Psi(y_i, \hat{f}(\boldsymbol{X}_i) + \rho), \quad \text{(A2)}$$

where S_k is the set of observations categorized into the kth terminal node of the fitted decision tree.

Step 4. update $\hat{f}(\boldsymbol{X})$ using Equation (A3):

$$\hat{f}(\boldsymbol{X}) \leftarrow \hat{f}(\boldsymbol{X}) + \lambda \rho_{k(\boldsymbol{X})}, \quad \text{(A3)}$$

where $k(\boldsymbol{X})$ indicates the index of the terminal node of the fitted decision tree where the observations are located.

Relative importance

Equation (A4) is used to calculate the total variance reduction $\hat{J}_j^2$ by the independent variable x_j (Ridgeway 2020):

$$\hat{J}_j^2 = \sum_{splits\ on\ x_j} I_t^2 \tag{A4}$$

where I_t^2 is the variance reduction by splitting on x_j.

Relative importance (RI) of x_j is calculated with Equation (A5):

$$RI_j = \frac{\hat{J}_j^2}{\sum_1^N \hat{J}_j^2} \times 100\% \tag{A5}$$

Accumulated Local Effect (ALE) estimation

Following the notations by Molnar (2020), x_j is split into $k_j(\boldsymbol{x})$ intervals. The uncentered ALE for x_j can be estimated by Equation (A6):

$$\hat{\tilde{f}}_{j,ALE}(\boldsymbol{X}) = \sum_{k=1}^{k_j(\boldsymbol{X})} \frac{1}{n_j(k)} \sum_{i:x_j^{(i)} \in N_j(k)} [f\left(z_{k,j}, \boldsymbol{x}_{\setminus j}^{(i)}\right) - f\left(z_{k-1,j}, \boldsymbol{x}_{\setminus j}^{(i)}\right)], \tag{A6}$$

where $N_j(k)$ is the space of the kth interval, $n_j(k)$ is the number of observations in the kth interval, $z_{k,j}$ is the maximum value of x_j in $N_j(k)$, $z_{k-1,j}$ is the minimum value of x_j in $N_j(k)$, $\boldsymbol{x}_{\setminus j}^{(i)}$ is the ith observation without x_j in $N_j(k)$, and $f(.,.)$ is the estimated GBDT model.

The centered ALE for x_j can be computed using Equation (A7):

$$\hat{f}_{j,ALE}(\boldsymbol{x}) = \hat{\tilde{f}}_{j,ALE}(\boldsymbol{x}) - \frac{1}{n}\sum_{i=1}^{n} \hat{\tilde{f}}_{j,ALE}\left(\boldsymbol{x}_j^{(i)}\right), \tag{A7}$$

where n is the number of observations in the sample.

Reference

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