Lecture 09: Tree-Based Methods

Random Forests and Gradient Boosting for Forecasting

BSAD 8310: Business Forecasting

University of Nebraska at Omaha

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Lecture 08 best result: Elastic Net, RMSE $\approx 2{,}540$ on RSXFS.

Elastic Net is a linear model: $\hat{y} = \mathbf{x}^\top \hat{\boldsymbol{\beta}}$. It cannot capture *interactions* or *threshold effects* (e.g., the holiday effect amplifies when the economy is strong).

What tree-based methods add:

- **Nonlinearity:** predictions are piecewise constant over feature regions
- **Interactions:** splits on x_1 in a region defined by x_2 capture $x_1 \times x_2$ interactions automatically
- **No standardization required:** scale-invariant splits

Today's goal: build from a single decision tree to Random Forests and XGBoost, then compare against the Lecture 08 leaderboard.

Decision Trees: CART

Building blocks of ensemble methods through recursive binary splits of the feature space

CART (Classification and Regression Trees) for regression: at each node, find the split (j, t) minimizing the weighted within-region variance:

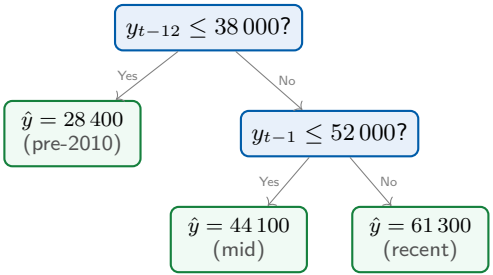
$$\min_{j,\,t} \left[\sum_{i:\, x_{ij} \le t} (y_i - \bar{y}_L)^2 + \sum_{i:\, x_{ij} > t} (y_i - \bar{y}_R)^2 \right]$$

Algorithm:

1. Start with all data at the root
2. For every feature j and every threshold t: compute the split criterion
3. Split on the (j^*, t^*) giving the largest reduction
4. Recurse on left and right children
5. Stop when nodes are too small or depth limit reached
6. Predict: $\hat{y} = \bar{y}_{\text{leaf}}$

Each split depends on which points fall into a region. Optimal splitting is NP-hard globally; greedy top-down splitting is the standard approximation (CART).

Example: 3-leaf tree for RSXFS



Key properties:

- **Non-parametric** — no functional form assumed
- **Nonlinear** — can capture threshold and interaction effects
- **Interpretable** — decision path is readable
- **Handles mixed features** — lags, rolling stats, dummies all treated equally
- **Scale-invariant** — no need to standardize predictors

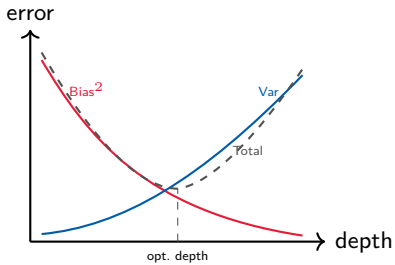
A single deep tree **overfits severely**. The solution is not pruning alone — it is *ensembling*.

Tree depth controls complexity:

- **Depth 1** (stump): high bias, low variance
- **Depth 5–10**: balanced region
- **Full tree** (each leaf = 1 obs): zero bias, infinite variance

Why trees have high variance:
A single split can change the entire subtree beneath it. Small perturbations in data (e.g., one outlier) produce very different trees — trees are *unstable*.

Key insight: averaging many high-variance, low-bias trees (each fit to a bootstrap sample) substantially reduces variance while preserving low bias. This is bagging.



Bagging and Random Forests

Variance reduction through bootstrap aggregation and random feature decorrelation

Draw B bootstrap samples; fit one deep tree on each; average:

$$\hat{y}_{\text{bag}} = \frac{1}{B}\sum_{b=1}^{B} \hat{f}^{(b)}(\mathbf{x})$$

(Breiman 1996)

Variance of the ensemble:

$$\text{Var}(\bar{f}) = \rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$$

As $B \to \infty$, variance $\to \rho\sigma^2$ (not zero). Reducing ρ matters as much as increasing B — this motivates Random Forests.

ρ = pairwise prediction correlation; σ^2 = single-tree variance.

Bagging key numbers:

- Bootstrap sample $\approx 63\%$ unique obs.
- Remaining $\approx 37\% =$ out-of-bag (OOB)
- OOB obs. give a free cross-validation estimate
- $B \geq 500$ trees recommended (stable)

Problem with bagging: if one feature dominates, all trees use it at the root ⇒ trees are highly correlated (ρ stays large).

Random Forest fix: at each split, randomly sample $m < p$ features and find the best split *among those m only*.

- Default: $m = \lfloor \sqrt{p} \rfloor$ (sklearn $\geq$ 1.1); $\lfloor p/3 \rfloor$ recommended for regression (Hastie et al. 2009, §15.3)
- Reduces $\rho \Rightarrow$ lower ensemble variance
- Each tree is weaker but the ensemble is stronger

RF = Bagging + random feature selection at each split. Both ingredients are necessary.

Each obs. is OOB for $\approx 37\%$ of trees. Predict using only those trees; compute RMSE.

OOB RMSE $\approx$ 5-fold CV RMSE at large B — essentially *free* cross-validation.

Parameter	sklearn name	Default	Effect
Num. trees	`n_estimators`	100	More = lower variance; plateau after ∼500
Max features/split	`max_features`	`'sqrt'`	Lower = more decorrelated; tune via OOB
Max depth	`max_depth`	None	None = full tree; limit to reduce memory
Min samples/leaf	`min_samples_leaf`	1	Higher = smoother predictions; reduces overfit
Bootstrap	`bootstrap`	True	False = subsampling (not bootstrap)

Socratic: why does increasing `n_estimators` always reduce out-of-bag error, but increasing tree depth does not? (Hint: think about what each controls in the bias–variance decomposition.)

Gradient Boosting and XGBoost

Sequential residual fitting with second-order optimization and explicit regularization

Initialize $F_0(\mathbf{x}) = \bar{y}$. For $b = 1, \ldots, B$:

- Residuals: $r_i^{(b)} = y_i - F_{b-1}(\mathbf{x}_i)$ (negative gradient for squared-error loss)
- Fit shallow tree T_b to $\{(\mathbf{x}_i, r_i^{(b)})\}$
- Update: $F_b = F_{b-1} + \eta\, T_b$

Predict: $\hat{y} = F_B(\mathbf{x})$

RF vs. Boosting:

- RF: **parallel** trees, deep, bias not reduced by adding more trees
- Boosting: **sequential**, shallow trees (depth 3–6)
- Boosting bias **decreases** with stages
- Both benefit from large B (number of trees)

Small η + large B + early stopping outperforms large η + small B.

Always use early stopping on a validation set.

XGBoost (Chen and Guestrin 2016) extends gradient boosting with three additions:

- **1. Newton step (2nd-order):** Uses gradient *and* curvature of the loss to compute a more precise tree-fitting direction than first-order GBM.
- **2. Explicit regularization:** Penalizes leaf count and leaf weights directly in the objective — shrinks trees without relying on early stopping alone.
- **3. Column subsampling:** Like RF, randomly samples features per tree *and* per split — reduces correlation and overfitting.

Newton step $\Rightarrow$ more precise gradient direction.

Regularization $\Rightarrow$ guards against overfitting.

Together: XGBoost outperforms vanilla GBM on most benchmarks (Chen and Guestrin 2016).

Mathematical formulation: next slide.

Here $f_b(\mathbf{x})$ is the output of tree T_b in boosting step b — same tree, XGBoost notation.

1. Newton-step objective (stage b):

$$\mathcal{L}^{(b)} = \sum_i \left[g_i f_b(\mathbf{x}_i) + \tfrac{1}{2} h_i f_b^2(\mathbf{x}_i) \right] + \Omega(f_b)$$

g_i = gradient, h_i = Hessian of loss w.r.t. $F_{b-1}(\mathbf{x}_i)$.

2. Regularization term:

$$\Omega(f_b) = \gamma T + \tfrac{1}{2} \lambda \|\mathbf{w}\|_2^2$$

T = leaf count, $\mathbf{w}$ = leaf weights, γ = per-leaf complexity penalty.

Notation note:

λ here is XGBoost's L2 leaf-weight penalty. It is distinct from the regularization λ (penalty strength) in Lecture 08.

Practical effect: Setting $\lambda > 0$ and $\gamma > 0$ produces sparser, more interpretable trees even without aggressive early stopping.

Parameter	XGB name	Typical	Effect
Num. trees	`n_estimators`*	500–2000	More + small η = better (use early stopping)
Learning rate	`learning_rate`	0.01–0.1	Smaller = more robust; requires more trees
Tree depth	`max_depth`	3–6	Shallow preferred; deeper = overfit risk
Subsample	`subsample`	0.7–0.9	Row fraction per tree; adds stochasticity
Col. sample	`colsample_bytree`	0.7–0.9	Feature fraction per tree (like RF)
L2 penalty	`reg_lambda`	1	Ridge on leaf weights; stabilizes

*sklearn API name; native API uses `num_boost_round`.

Practical starting point: `learning_rate=0.05`, `max_depth=4`, `n_estimators=1000` with early stopping on val RMSE. Tune `max_depth` and `subsample` via TimeSeriesSplit CV.

Socratic: if `learning_rate` is halved, roughly how many additional trees are needed to maintain the same training loss? What does this imply for early stopping budget?

Feature Importance

Impurity, permutation, and XGBoost gain measures for model interpretation

$$\text{Imp}(j) = \sum_{\text{nodes using } j} \Delta\,\text{RSS} \cdot \frac{n_{\text{node}}}{n}$$

Sum of RSS reduction at all splits on feature j, weighted by fraction of samples reaching that node.

Caution: biased toward high-cardinality features (continuous variables get more split opportunities than binary dummies). Do not use for final reporting.

For each feature j:

1. Shuffle column j in the OOB set
2. Record increase in RMSE

Larger increase $\Rightarrow$ more important.

Unbiased (no cardinality bias).
Model-agnostic. Use for reporting.

Average *gain* (improvement in objective function) per split using feature j, across all trees.

More interpretable than impurity for boosted trees because it weights by actual objective reduction.

Practical rule:

- Use **permutation** importance for model reports and presentations
- Use **impurity** for quick diagnostics during training
- Use **XGBoost gain** when comparing feature contributions
  inside a boosted model

1. **lag_12** — dominant seasonal signal
2. **lag_1** — short-run momentum
3. **roll_mean_12** — trend level
4. **lag_3** — quarterly effect
5. **month_12** — December holiday

Results are consistent across all three importance measures; lag_12 should be the primary feature in any RSXFS model.

Hyperparameter Tuning

Time-series-aware cross-validation with TimeSeriesSplit

Random Forest (RandomizedSearchCV):

```
from sklearn.ensemble import RandomForestRegressor
from sklearn.model_selection import (
    TimeSeriesSplit, RandomizedSearchCV)

tscv = TimeSeriesSplit(n_splits=5, gap=1)  # gap>=1 for 1-step-
    ahead
rf_grid = {
  'n_estimators':     [200, 500],
  'max_features':     ['sqrt', 0.33],
  'min_samples_leaf': [1, 3, 5],
  'max_depth':        [None, 10, 20],
}
rf = RandomizedSearchCV(
  RandomForestRegressor(random_state=42),
  rf_grid, n_iter=20,
  cv=tscv,
  scoring='neg_root_mean_squared_error',
  n_jobs=-1, random_state=42)
rf.fit(X_trainval, y_trainval)
```

XGBoost (early stopping on val):

```
import xgboost as xgb

dtrain = xgb.DMatrix(X_train, label=y_train)
dval   = xgb.DMatrix(X_val,   label=y_val)
dtest  = xgb.DMatrix(X_test,  label=y_test)

params = {
  'learning_rate': 0.05,
  'max_depth':     4,
  'subsample':     0.8,
  'colsample_bytree': 0.8,
  'reg_lambda':    1.0,
  'objective':     'reg:squarederror',
}
model = xgb.train(
  params, dtrain,
  num_boost_round=2000,
  evals=[(dval, 'val')],
  early_stopping_rounds=50)
```

Application to Forecasting

Comparing Random Forest and XGBoost against SARIMA and Elastic Net on RSXFS

Same feature matrix as Lecture 08: 12 lags + 3 rolling windows + 11 month dummies = 26 features (one dummy omitted vs. L08 for comparability; trees do not require it). **Key differences vs. regularized regression:**

Advantages of trees:

- Capture nonlinearities and interactions (e.g., "holiday effect only when economy is strong")
- No standardization needed
- Handle irrelevant features gracefully (unused features do not appear in splits)
- Built-in feature importance

Cautions for time series:

- **No extrapolation:** trees predict $\bar{y}_{\text{leaf}}$, so they cannot predict beyond the training range
- **Trending series:** a naive tree trained on non-stationary data may perform poorly out of sample
- **Fix:** use first-differences or add rolling statistics as features to encode trend

Stationarity matters for trees too. If y_t trends upward beyond the training max, leaf means will systematically under-predict. Difference or detrend before applying tree-based forecasting.

Test-set results on RSXFS (24-month horizon):

Model	RMSE	MAE
Seasonal Naïve	4 210	3 120
SARIMA$(1,1,1)(1,1,1)_{12}$	2 840	2 100
Elastic Net (λ^*)	2 540	1 890
Random Forest	2 380	1 760
XGBoost (early stop)	2 250	1 650

Values are illustrative. Strategy: direct multi-step — one model trained per horizon $h = 1, \ldots, 24$.

Why do trees win here?

- Nonlinear interaction between lag_12 and calendar dummies (holiday amplification)
- XGBoost sequential residual fitting corrects patterns that Elastic Net misses
- RF OOB error $\approx$ CV error at $B = 500$

Caveat: gains depend heavily on feature quality. With a good feature set, Elastic Net and XGBoost are often competitive. Adding *more* features benefits trees more.

Socratic: XGBoost outperforms Elastic Net here. Does this guarantee trees will always win with more data? (Hint: consider the no-extrapolation warning.)

Takeaways and References

What we learned and where to go next

Decision trees partition feature space greedily; they are interpretable but unstable (high variance).

Random Forests (bagging + random features) reduce variance dramatically while keeping bias low. OOB error is a free CV estimate.

Gradient boosting reduces bias sequentially by fitting residuals. XGBoost adds L2 regularization and Newton optimization.

Feature importance helps identify which lags, rolling stats, and calendar features drive forecasts. Use permutation importance for unbiased estimates.

Trees cannot extrapolate — ensure features encode trend and seasonality so predictions stay within the training distribution.

RF vs. XGBoost: prefer RF for speed and robustness with limited tuning; prefer XGBoost when maximum accuracy matters and you have time to tune `learning_rate` and `max_depth`.

Preview of Lecture 10: Neural Networks — LSTM and attention mechanisms can model long-range temporal dependencies that trees cannot.

Breiman, Leo (1996). "Bagging Predictors". In: *Machine Learning* 24.2, pp. 123–140.

Chen, Tianqi and Carlos Guestrin (2016). "XGBoost: A Scalable Tree Boosting System". In: *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pp. 785–794.

Hastie, Trevor, Robert Tibshirani, and Jerome Friedman (2009). *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. 2nd. New York: Springer. URL: https://hastie.su.domains/ElemStatLearn/.