Feature importance

Which features are the most predictive or have most impact?

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What does the model say about the data?

- A good model is great, but we usually want to interpret the model
- Feature importance tells us about the business or application; e.g., what matters to people renting apartments or buying used bulldozers or identifying cancer or getting a bank loan?
- Importance scores themselves don't usually mean anything, and they are often normalized 0..1 anyway
- Only relative rank/magnitude matters for feature selection to drop irrelevant features

Formal definition of feature importance?

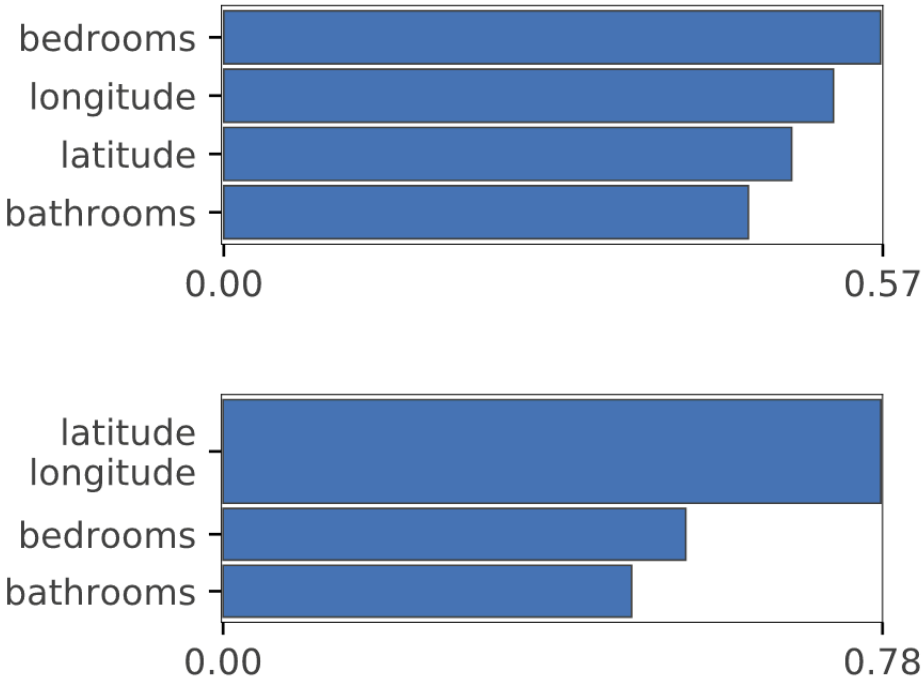
- Not sure there is an agreed-upon definition
- *Feature importance* gives (usually just) a relative ranking of the predictive strength among the features of the model; useful for simplifying models and possibly improving generality
- We'd also like a model-independent *feature impact* that identifies the effect of features on y without peering through lens of a model: "the amount of y variation attributed specifically to feature x_j" See [1]
- We want importance/impact to isolate impact of individual features
- Nonetheless, we'll focus on feature importance as proxy for impact

Coining new term to distinguish from feature importance

[1] https://arxiv.org/abs/2006.04750 for detailed discussion

Rent example

- Number of **bedrooms** appears to be the most important, meaning that it is the most predictive of rent price
- That tells us something about the market for New York City rent
- Combined, however, the location matters more by far; note: **longitude** and **latitude** are codependent features



See https://mlbook.explained.ai/first-taste.html

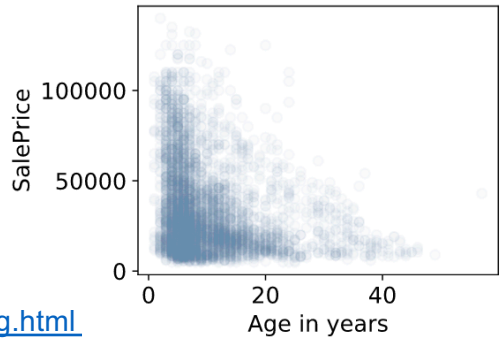
Bulldozer example

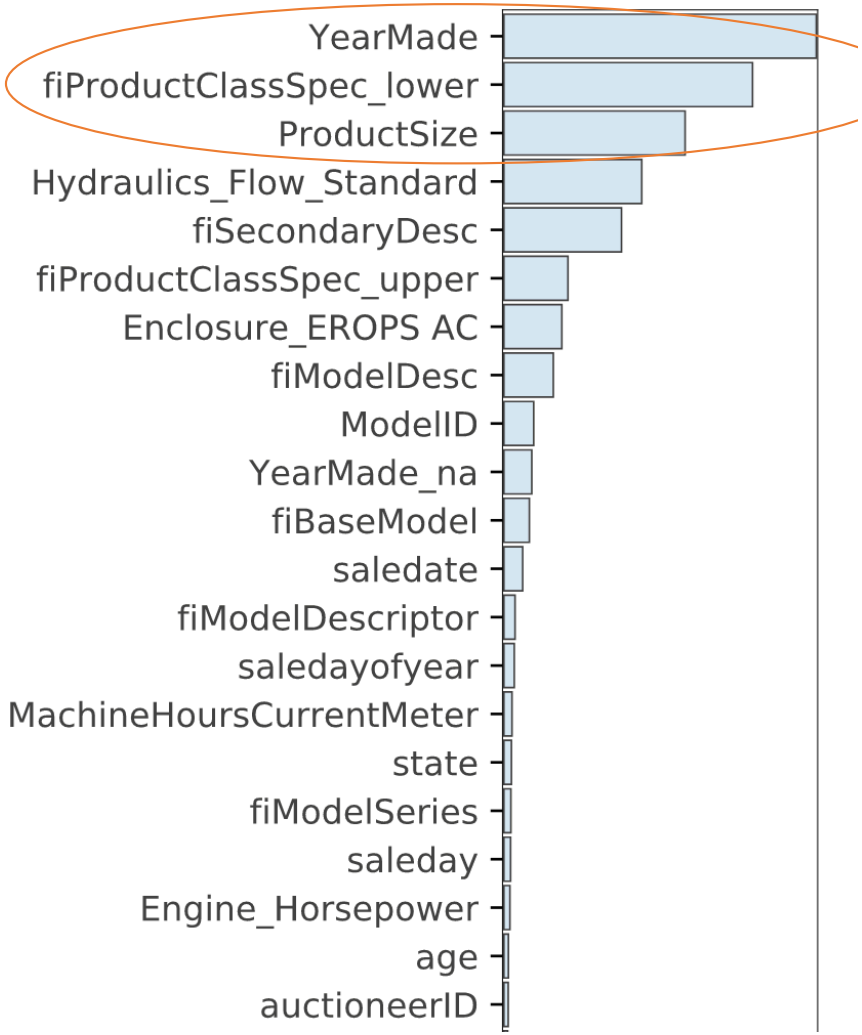
- **YearMade**, lower capacity spec, size matter most

20.0 to 75.0 Horsepower

lower *upper* *units*

- Note **age** appears unimportant but date-related features are highly correlated; other features can cover for codependent features; still looks predictive to me:

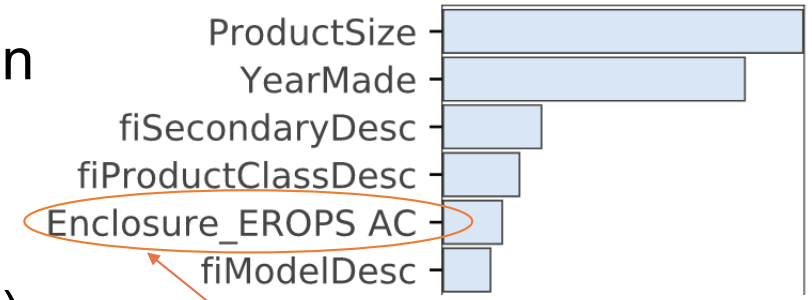




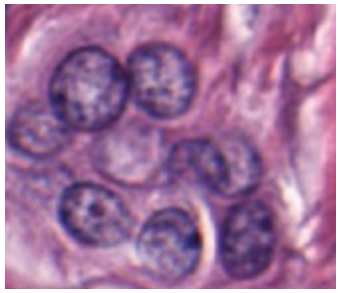
See https://mlbook.explained.ai/bulldozer-feateng.html

Bulldozer one-hot example

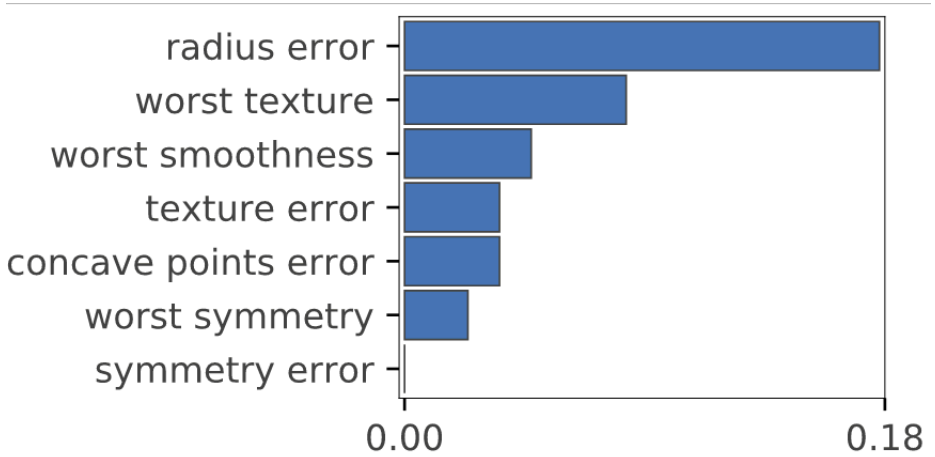
- One-hot'ing features temporarily and then examining feature importance can identify which category level is important vs just the variable
- E.g., one-hot **Enclosure** and we see that "EROPS AC" (air conditioned cab) is most important **Enclosure**, which is valuable marketing / business info (other levels are way down in the noise)
- Could be useful for improving model but definitely useful for business intelligence



Breast cancer classification example



- Distinguishing between malignant versus benign masses: **radius error** is strongly predictive
- That is "*standard error for the mean of distances from center to points on the perimeter*" which could give an indication of mass edge irregularity
- **Worst texture** is "*largest mean value for standard deviation of gray-scale values*"



See https://mlbook.explained.ai/first-taste.html

Image credit: https://pubmed.ncbi.nlm.nih.gov/27563488/

Common application: Tuning the model

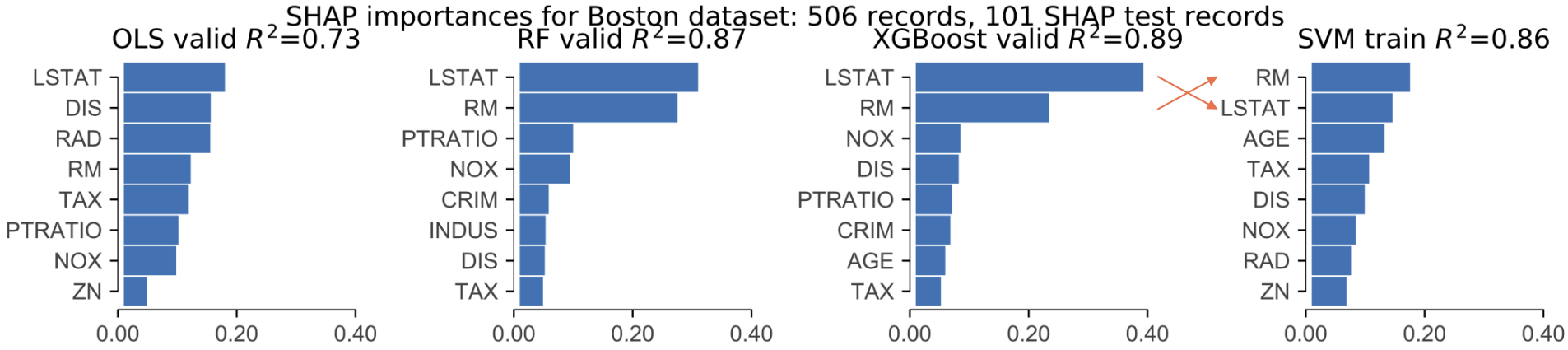
- Dropping unimportant features simplifies the model; fewer features make it easier to interpret/explain model behavior
- Often increases accuracy and generality because the model is not taking irrelevant features into consideration (e.g., noise vars)
- Simplifying models is a form of regularization
- Fewer features increases training and prediction speed
- Drop the lowest importance feature and retrain the model, redo validation metric; if validation metric worse, then we have dropped one too many features
- Codependencies between feature is why we recompute feature importances after dropping each feature; at minimum, rank of features can change dramatically after dropping a feature

Beware!

- Can't trust feature importances from *weak* models
- Can't trust feature importances from *unstable* models
- Importance says how important a feature is to a specific model
- Sum of importances not usually meaningful; doesn't tell you how much of the overall prediction your model has covered
- When possible compute importances with validation not training set; we care about features predictive for generalization
- Even with good model, importances are a clue not gospel

Importance is typically model-specific!

- Same method applied to same data can yield different importances; here's SHAP on Boston but different models



Implementation of importance

Importance directly from the data: Spearman's rank correlation

- Simplest technique for regression is to rank x_j features by their Spearman's rank correlation [1] with target y (doesn't assume linear relationship)
- The feature with largest coefficient is most important
- Measures *single-feature importance* and works well for independent features, but not good for codependent features
- Groups of features with similar relationships to the response variable receive the same or similar ranks, even though just one should be considered important
- Seems inappropriate for categorical variables

[1] https://en.wikipedia.org/wiki/Spearman%27s_rank_correlation_coefficient

Importance directly from the data: PCA

- Principle component analysis (PCA) operates on just the X explanatory matrix; limited to linear relationships and "most variance" is not always the same as "most important"
- PCA transforms data into a new space characterized by eigenvectors of X and identifies features that explain the most variance in the new space
- If the first principal component covers a large percentage of the variance, the “loads” associated with that component can indicate importance of features in the original X space
- Seems inappropriate for categorical variables

Copied from https://arxiv.org/abs/2006.04750

Importance directly from the data: mRMR

- To deal with codependencies, rank not just by *relevance* but also by *redundance*; mRMR: minimal-redundancy maximal-relevance

$$J_{\text{mRMR}}(x_k) = I(x_k, y) - \frac{1}{|S|} \sum_{x_j \in S} I(x_k, x_j)$$

- Redundance is the amount of information shared between codependent features
- $I(x_k, x_j)$ is some measure of mutual information between x_k and x_j, S is the growing set of selected features, and x_k is the candidate feature; can use Spearman's for $I(x_k, x_j)$
- Only considers single-feature relationships with y, limited to classification, what is $I(x_k, x_j)$ for categorical variables?

Importance via linear models

- For suitably prepared data without missing variables and other appropriate assumptions, linear model coefficients give the amount of y variance explained for each x_j variable
- But, linear models are often too weak in practice for modeling, which renders coefficient interpretation highly suspect
- More on difficulties of interpreting regression coefficients by Breiman https://projecteuclid.org/euclid.ss/1009213726

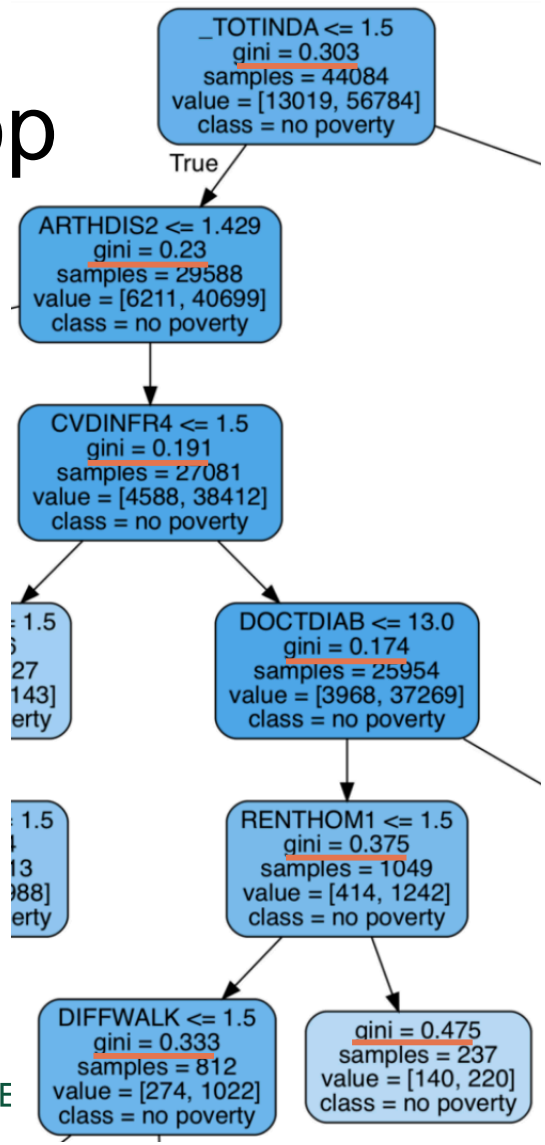
So how do we really get feature importance?

- RF specific and scikit-learn default: gini/MSE drop (I'd avoid)
- Drop-column importance
- Permutation importance
  `from sklearn.inspection import permutation_importance`
- scikit-learn added after we exposed the weakness of gini drop https://explained.ai/rf-importance/index.html and see rfpimp [1]
- SHAP (https://github.com/slundberg/shap) likely most accurate so far (w/amazing library) but I find it unbearably slow

[1] https://github.com/parrt/random-forest-importances/blob/master/README.md

Random Forest loss function drop

- Random Forests have a built-in mechanism called “gini drop” (for regression, it's “MSE drop”)
- The idea is to track how much the loss function drops from a decision node to its children (for that split variable)
- The average loss function drop for a specific x_j across decision nodes for x_j and across all trees gives the feature importance
- Unfortunately, this gives biased feature importances



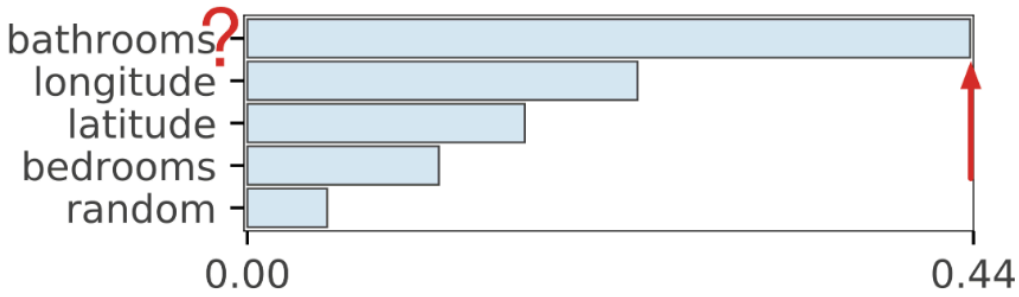
Random Forest gini/MSE drop issues

- Exhaustively testing every unique x_j value when finding decision node splits increases likelihood of finding a x_j value that, purely by chance, happens to predict y well
- That increases the likelihood that variable x_j will appear more often in the trees, which leads to inflated/biased importance
- It's likely that extremely random trees, that pick a random split value between $\min(x_j)$ and $\max(x_j)$ would not suffer from this bias; I haven't tried this theory out, but it makes sense
- Breiman: "*adding up the gini decreases for each individual variable over all trees in the forest gives a **fast** variable importance that is **often very consistent** with the permutation importance measure.*"

Read more https://explained.ai/rf-importance/index.html

Trouble in paradise (regression)

- Don't trust default ("gini drop") importances for RF in sklearn
- Here we see the unlikely idea that New Yorkers care most about bathrooms and much more than location or bedrooms
- New Yorkers can be weird, but they can't be this fixated on bathrooms
- Random noise column is last (which it should be)

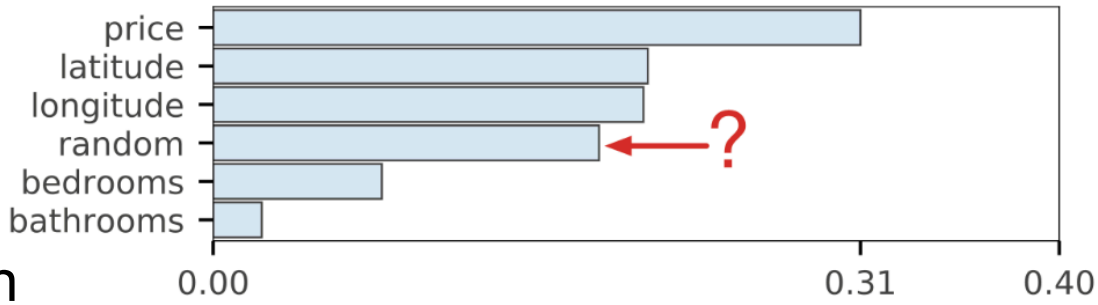


Read more https://explained.ai/rf-importance/index.html

Trouble in paradise

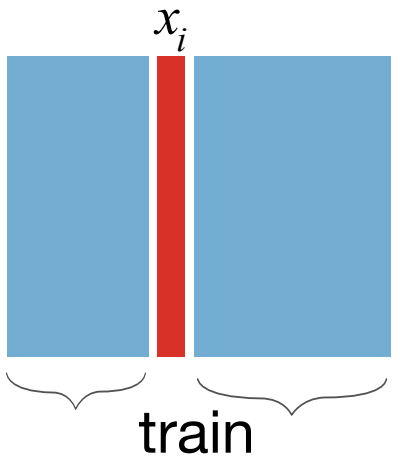
(classification: predicting interest in apt web page)

- Same data but classifying interest in apartments but price is now feature not target
- Random noise column is now somehow more important than bedrooms and bathrooms?
- Somethin ain't right
- For more on "gini drop", see: https://stackoverflow.com/questions/15810339/how-are-feature-importances-in-randomforestclassifier-determined



Hmm… what can we do instead?

Drop-column importance

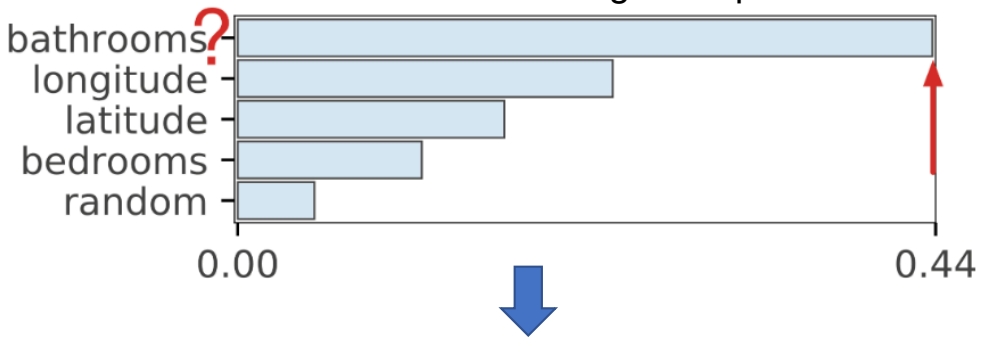


- Brute force mechanism to examine importance of any feature or combination of features
- Procedure:
  1. Compute validation metric for model trained on all features
  2. Drop column x_j
  3. Retrain model
  4. Compute validation metric set
  5. Importance score is the change in metric
- Answers the question of how loss of a feature affects overall model performance (which might not be actual importance)

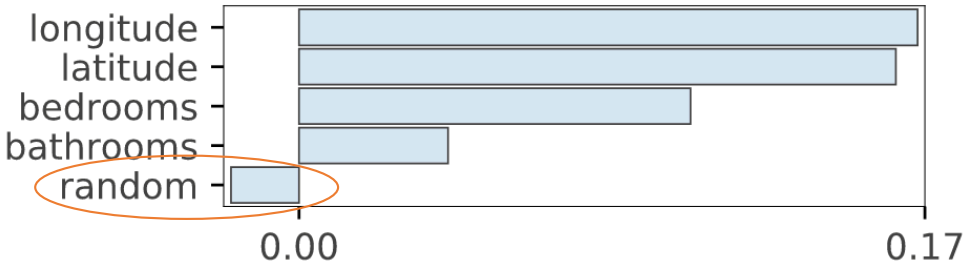
Compare drop-column to gini/MSE drop

Regressor

default sklearn ”gini drop”

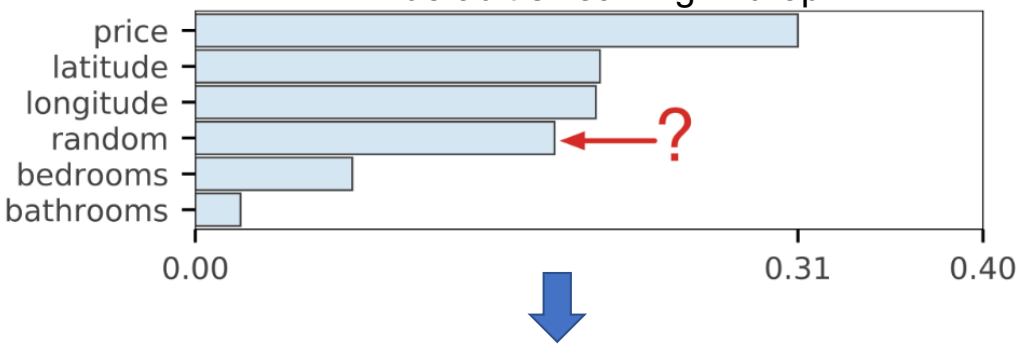


Feature importance via drop in model accuracy



Classifier

default sklearn ”gini drop”



Feature importance via drop in model accuracy

What does negative importance mean? Means dropping improves metric!

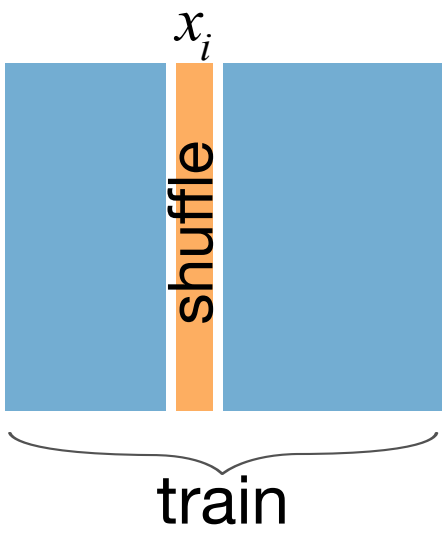
Drop-column implementation

```
def dropcol_importances(model, X_train, y_train):
    model.fit(X_train, y_train)
    baseline = metric(y_train, model.predict(X_train))
    imp = []
    for col in X_train.columns:
        X = X_train.drop(col, axis=1)
        model_ = clone(model)
        model_.fit(X, y_train)
        m = metric(y_train, model_.predict(X))
        imp.append(baseline - m)
    return imp
```

Drop-column pros/cons

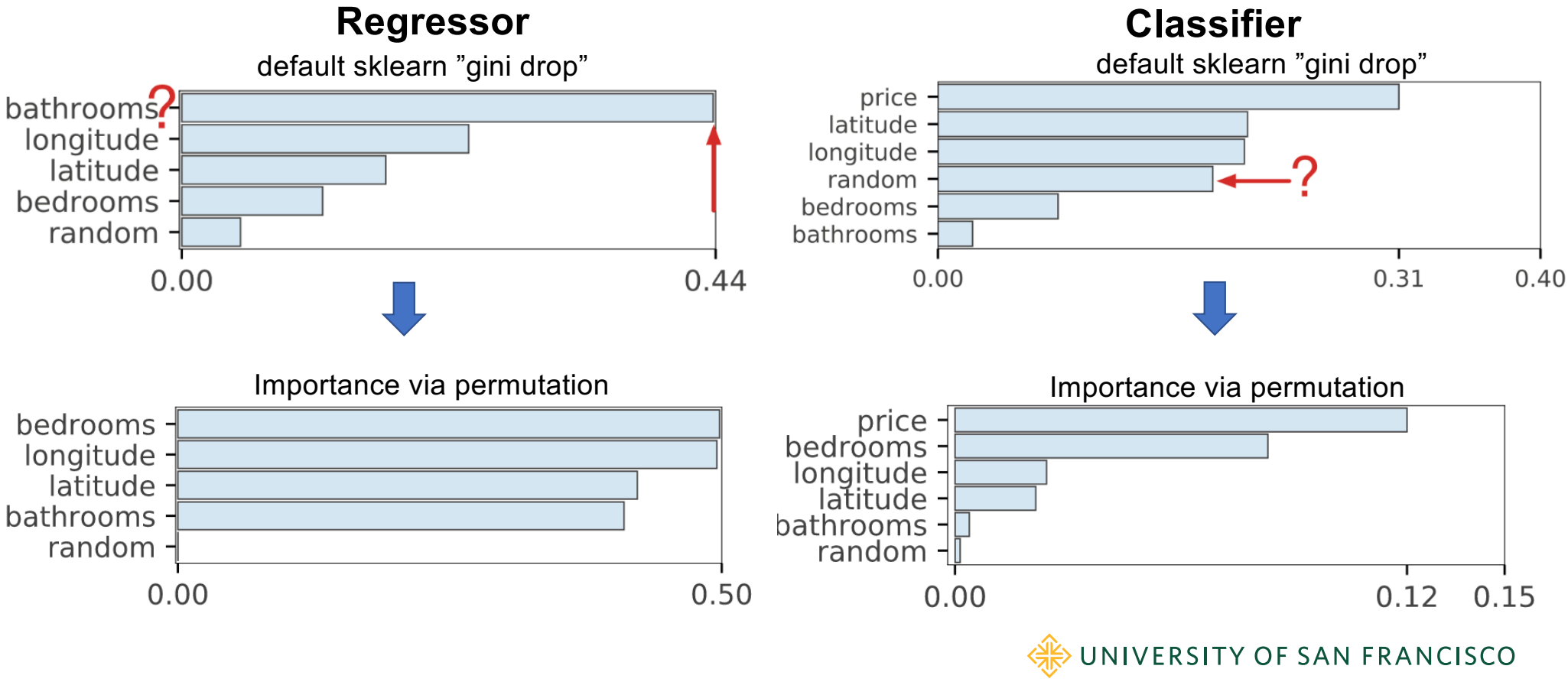
- Easy to understand
- Simple to implement
- Very direct means of measuring importance
- Works for any machine learning model
- BUT, very expensive because it means retraining the model p times for p features; try on a subset of the data for speed
- Codependent features often result in 0 or very low importance

Permutation importance



- Similar to drop column, but permute x_j instead of dropping it from the model
- Keeps same x_j distribution but breaks relationships
- Procedure:
  1. Compute validation metric for model trained on all features
  2. Permute column x_j
  3. Compute validation metric set
  4. Importance score is the change in metric

Compare permutation to gini/MSE drop



Permutation implementation

```
def permutation_importances(model, X_train, y_train):
    model.fit(X_train, y_train)
    baseline = metric(y_train, model.predict(X_train))
    imp = []
    for col in X_train.columns:
        save = X_train[col].copy()
        X_train[col] = np.random.permutation(X_train[col])
        m = metric(y_train, model_.predict(X_train))
        X_train[col] = save
        imp.append(baseline - m)
    return imp
```

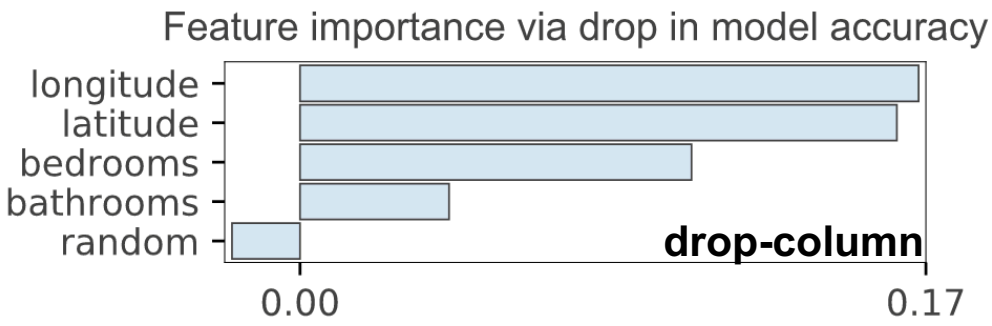
(Should really be computing metric on validation set)

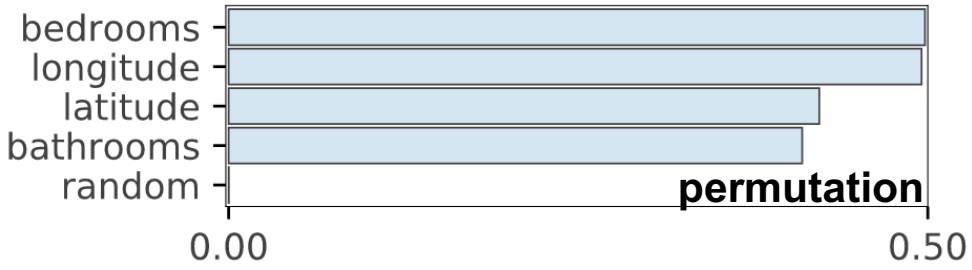
Permutation importance pros/cons

- Easy to understand
- Simple to implement
- Works for any machine learning model
- No need to retrain the model so much more efficient than drop column importance
- Can create nonsensical records through permutation, such as pregnant male, which makes the results suspect
- Codependent features often share importance, such as longitude and latitude
- Strobl et al "*permutation importance over-estimates the importance of correlated predictor variables*" https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-9-307

Compare drop column to permutation

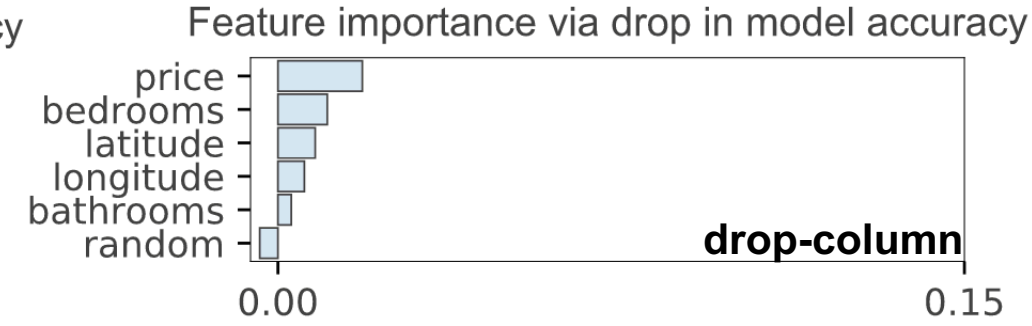
Regressor

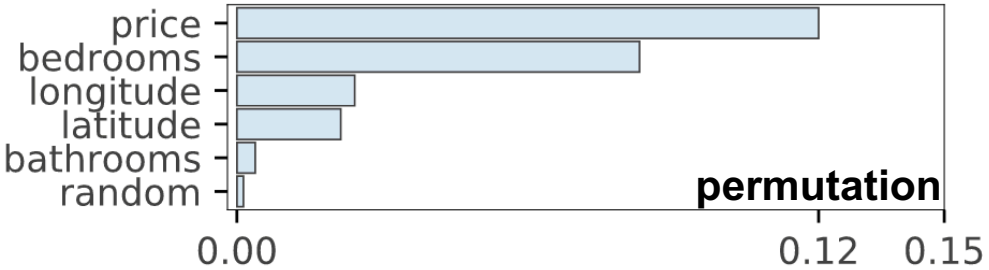




(fairly different due to codependence; permutation tends to share importance scores for codependent features)

Classifier





(very similar)

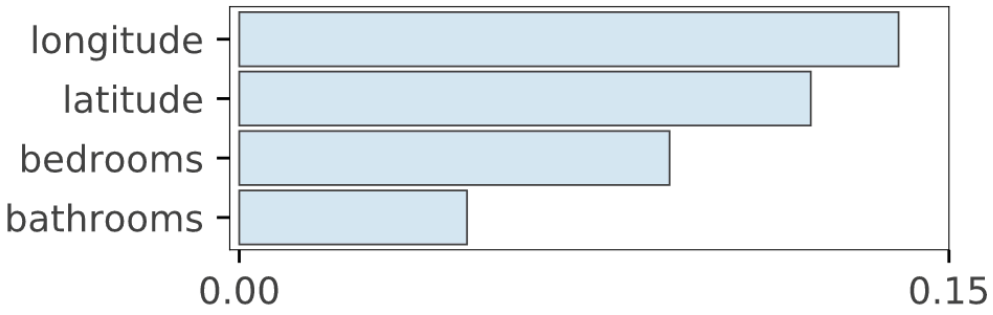
Interpreting importance results

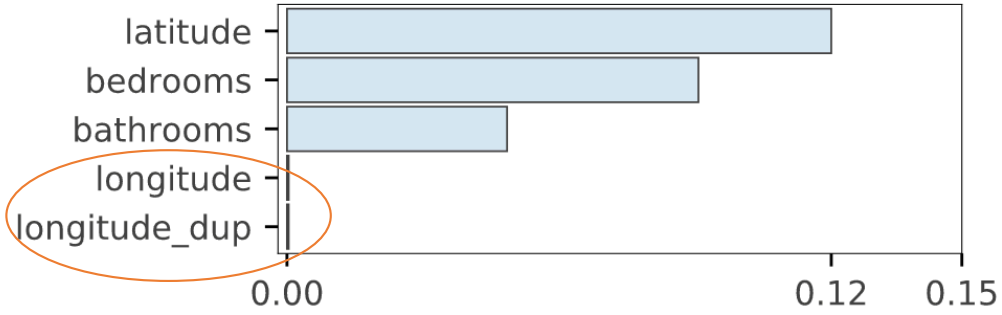
Codependent features

- Drop column and permutation importance consider each feature individually, though my **rfpimp** package lets you consider multiple features together
- If all features are totally independent, then computing feature importance individually is no problem
- If, however, two or more features are *codependent* (correlated in some way but not necessarily with a strictly linear relationship) computing feature importance individually can give unexpected results
- Drop-column tends to show low importance scores and permutation tends to share importance scores for codependent features

Effect of duplicated columns on drop column importance

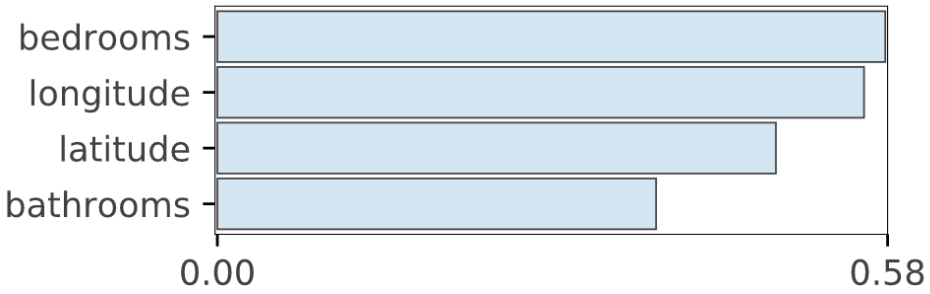
- Compare feature importances for original regressor model and another with duplicated longitude
- Shocking to see BOTH longitude and duplicated longitude both go to zero importance but we measure as drop in accuracy
- Dropping one doesn't affect accuracy; other column covers for it

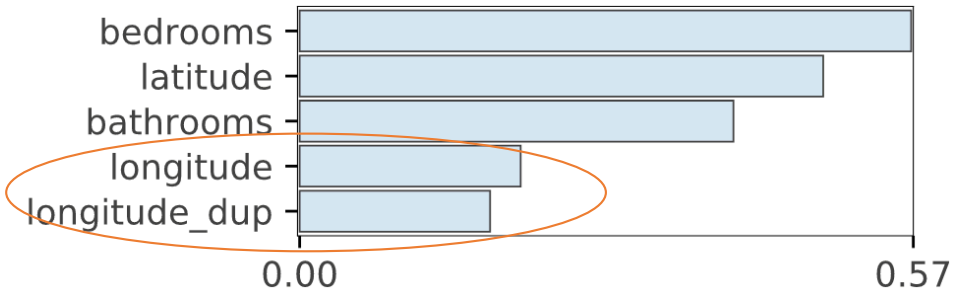




Effect of duplicated columns on permutation importance

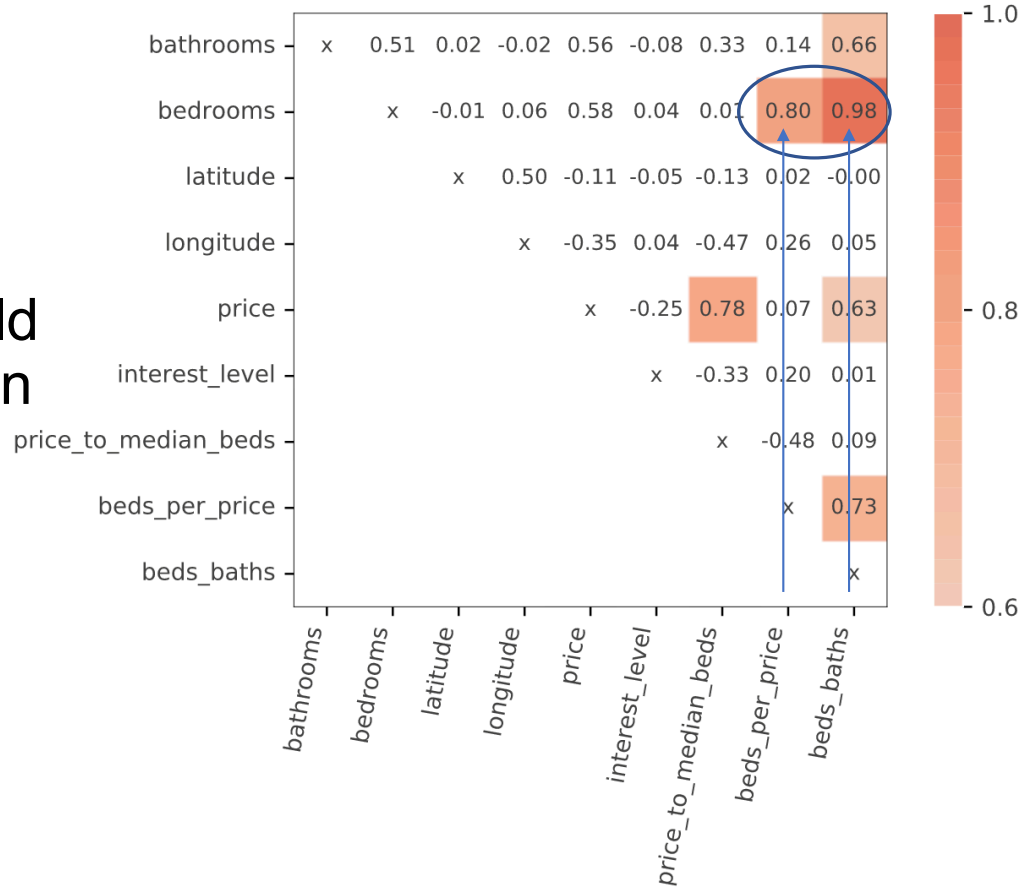
- Consider RFs; during training, node splitting should choose equally important variables roughly 50-50
- Permuting a duplicated column should still allow prediction to be half supported by the other identical column
- That's what we see in practice for duplicated columns; has the effect of pulling down the perceived importance of the original





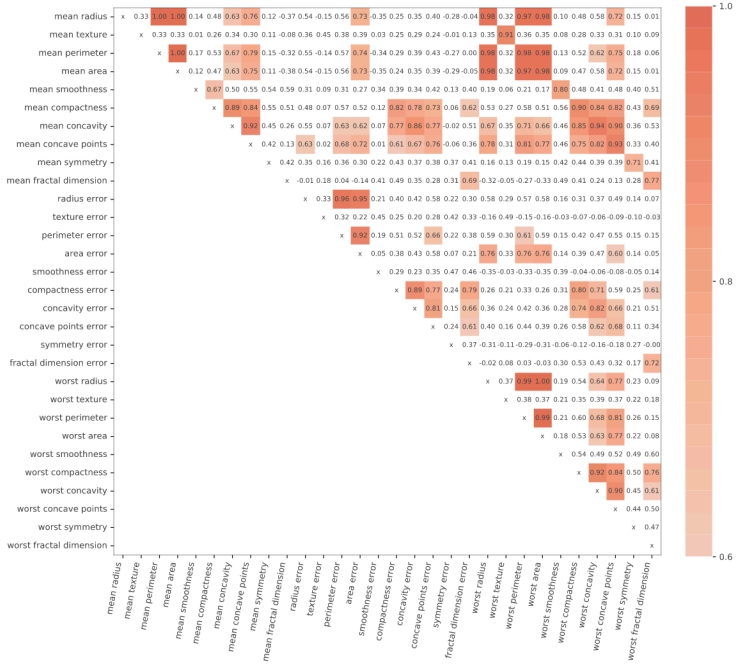
Spearman’s feature heat map

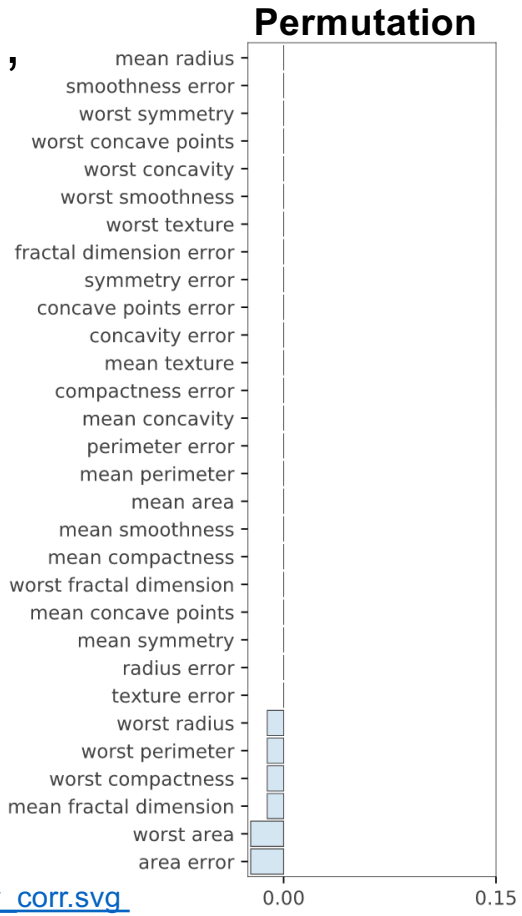
- Spearman's correlation is same as converting two variables to rank values and running standard correlation
- Highly-correlated features should be dropped/permuted together in feature importance metrics to decrease confusion; E.g., as **bedrooms**, **beds_baths**, and **beds_per_price**

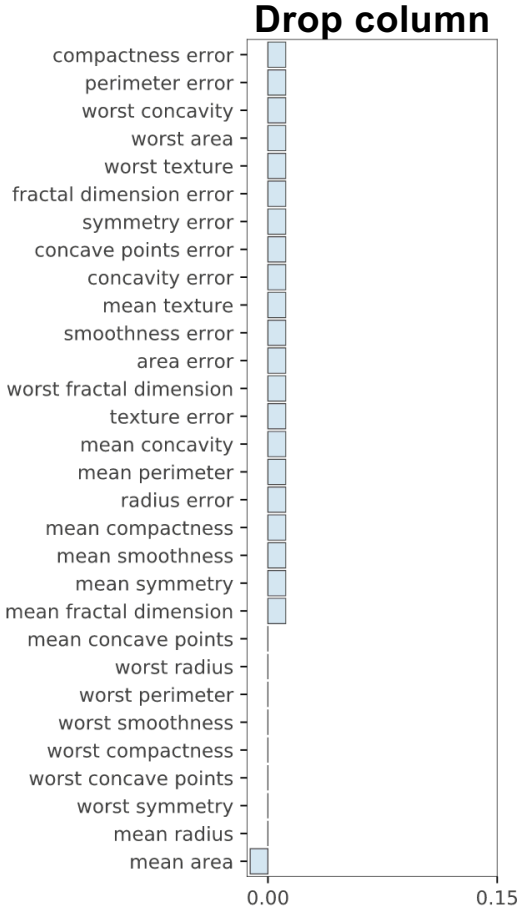


Ex: Breast cancer correlation matrix

- Features are super correlated, yielding useless feature importances





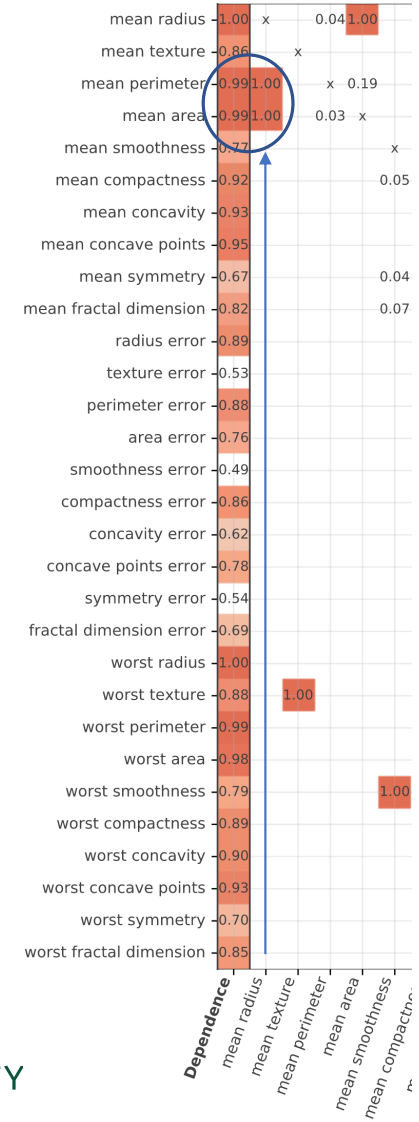


Larger correlation image https://explained.ai/rf-importance/images/cancer_corr.svg

Feature codependence

(stronger measure than spearman's)

- To identify if x_j is codependent with other features, train model using x_j as the target variable and all other features as explanatory variables (multicollinearity)
- R^2 prediction error indicates how easy it is to predict feature x_j using the other features
- Feature importances of x_j targeted model identify which features are strongly-codependents of x_j
- The higher the score, the more codependent feature x_j is with other features; can drop all but one in highly-codependent feature group to simplify model
- E.g., **mean radius** is important to predict **mean perimeter** and **mean area**; can probably drop those two
- E.g., could tell you which virus mutations develop together



Bigger image https://explained.ai/rf-importance/images/cancer_dep.svg

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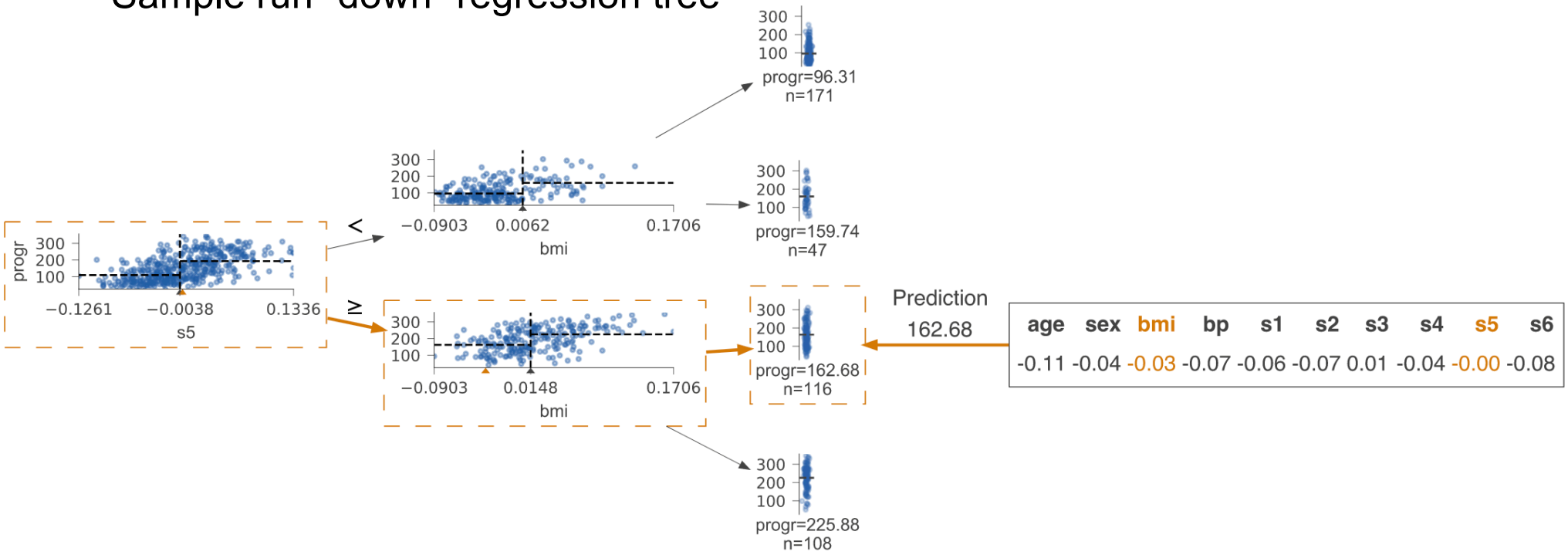
Interpreting individual record results

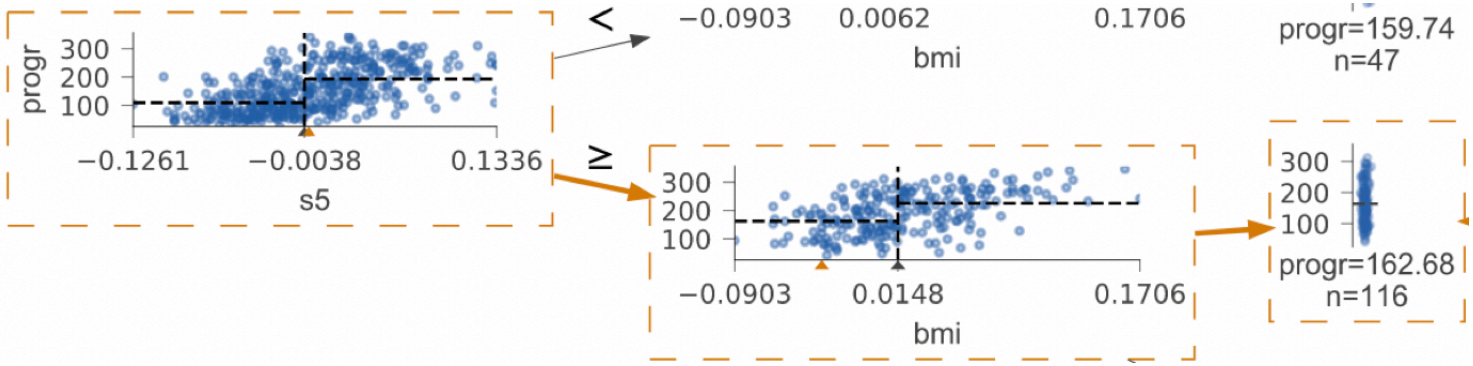
Viz how a test vector reaches leaf

Sample run ”down” regression tree



Path from root to leaf has useful info!

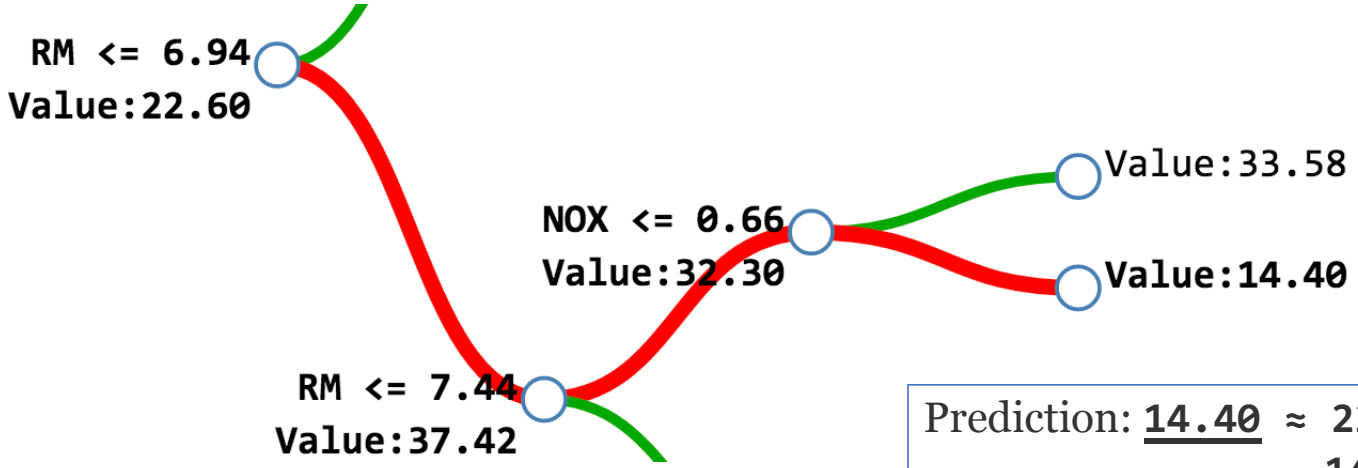
- Which features tested?
- Partitioning of feature space: *s5 > -0.0038 and bmi < 0.0148*



- Explain prediction using vars/values:
  Predict 162.68 because s5 > -0.0038 and bmi < 0.0148

Regression as sum of contributions along path

- Using change in sample mean from each node
- Start with mean(y), value of root node
- Compute sample mean deltas



Prediction: **14.40** ≈ **22.60** (trainset mean) **+**
14.82(gain from RM) **-**
5.12(loss from RM) **-**
17.9(loss from NOX)

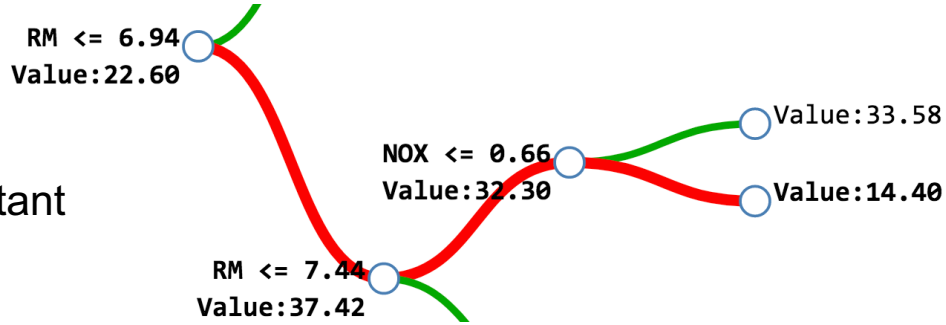
Image/example from http://blog.datadive.net/interpreting-random-forests/

Test vector feature importances (regressor example)

- Revisit earlier slide; magnitude of variable contribution acts like the importance
- Could also use MSE drop similar to gini drop in previous slide, but drop/gain in value seems more likely to be accurate

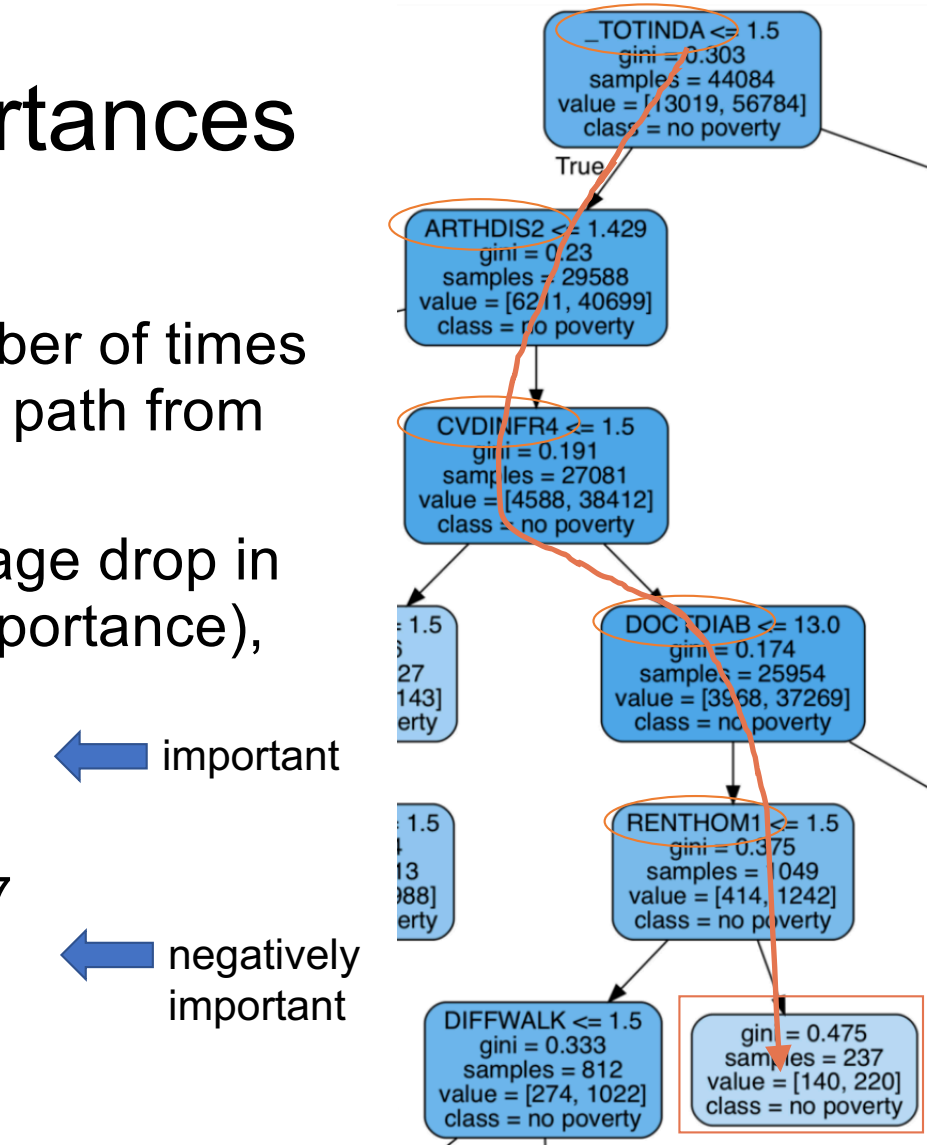
Prediction: **14.40** ≈ **22.60** (trainset mean) **+**
14.82(gain from RM) **-**
5.12(loss from RM) **-**
17.9(loss from NOX)

important



Test vector feature importances (classifier example)

- First approximation: count the number of times each variable referenced along the path from root to the leaf
- Improve by weighting vars by average drop in MSE or gini (mimicking ginidrop importance), but for a single record
  - _TOTINDA drop = .303 - .23 = 0.073
  - ARTHDIS2 drop = .23 - .191 = 0.039
  - CVDINFR4 drop = .191 - .174 = 0.017
  - DOCTDIAB gain = .174 - .375 = -.201



data set https://www.kaggle.com/cdc/behavioral-risk-factor-surveillance-system

Summary

- Use permutation importance, but check drop-column too
- Use only on stable, accurate model
- We only get relative importances, not proportion of total variance
- A 0 drop-column importance doesn't mean useless; might also be a codependent feature
- Add a noise column; can ignore any vars at or below
- RF specific: can interpret single test record as drop in value or MSE/gini on path from root to leaf
- Compute metric changes on validation not training set
- Feature importances are clues not gospel
- Useful for simplifying model
- Can tell us something about the business application / market