Data Mining as Exploratory Data Analysis

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The Problem(s)

- presumptions
  - social systems are complex
  - causal identification is difficult/impossible with many data sources
  - theory not generally predictively reliable (may be exceptions to this)

- conclusions
  - confidence in assumptions is low
  - analysis is exploratory/descriptive and/or predictive
  - ability to discover unexpected patterns is desirable
Not a bad thing!

- estimation of \( f : X \rightarrow Y \) under minimal assumptions
- adapt to data (within a representation class)
- control overadaptation (by minimizing excess risk)

Expected risk (generalization error):

\[
R(f) = \mathbb{E} [L(Y, f(X))] 
\]

Learning \( f \) does not result in directly interpretable output
Data Mining (II)

- statistical theory is hard to come by
- estimation/learning is often heuristic (i.e., not globally optimal)
- Some examples...
Decision Trees (I)

Idea: approximate $f$ by recursively splitting $y$ into bins until $y$ is sufficiently homogenous in said bins: predict by using a constant function of $y$ in each bin

- Pros: interpretability, fitting/evaluation speed
- Cons: overadaptation, variance (sharp boundaries), greedy
  (some work on global optimality though, see evtree)
Figure 1: Predicting partisanship from age and ideology (simulated).
Decision Trees (III)

Figure 2: \( \hat{f} \) learned from \( \sin(x), x \sim U(-4, 4) \) with a decision tree.
Ensembles of Decision Trees

aggregation (bagging)

meta-learning (boosting)

randomization (random forests)
Random Forests (I)

Nice for description/EDA for:

- computational reasons
- usability for many tasks
- some (studied) methods for interpretation
- low number of tuning/hyperparameters
- good empirical performance
- some theory
Random Forests (II)

Figure 3: $\hat{f}$ learned from $\sin(x)$, $x \sim U(-4, 4)$ with a randomized, bagged, ensemble of decision trees.
Since most machine learning methods are designed for prediction, their generalization error is low (because they are attempting to make the optimal bias/variance tradeoff.

Predicting a complex phenomena reliably gives us some basis on which to interpret $\hat{f}$ (though obviously this is not a causal inference).

But what did $\hat{f}$ learn about $f$ by using $X$?
Interpreting Black Box Functions (I)

The Marginal Distribution (A)

\[ X = X_S \cup X_C \]

S we care about and C we do not

The marginal distribution summarizes how \( \hat{f} \) depends on \( X_s \).

\[ \hat{f}_S(X_S) = \mathbb{E}_{X_C} \hat{f}(X_S, X_C) \]

The expectation, variance, multiple moments, or the full marginal distribution can then be used.
Interpreting Black Box Functions (I)

The Marginal Distribution (B)

Ideas from Friedman (2001), ESL, and Goldstein et al. (2015)

We have a function which we can evaluate, so functions of the learned joint distribution are easy!

\[
\hat{f}_S(x_S) = \hat{E}_{X_C}(\hat{f}(x)) = \frac{1}{N} \sum_{i=1}^{N} \hat{f}(x_S, x_C^{(i)})
\]

\[
\hat{f}_S(x_S^{(i)}) = \hat{E}_{X_C}^{(i)}(x^{(i)}) = \hat{f}(x_s, x_c^{(i)})
\]
Interpreting Black Box Functions (II)

Derivatives

If $\hat{f}$ is additive in $(X_S, X_C)$ then:

$$\frac{\partial \hat{f}}{\partial X_S} = g(X_S)$$

If not then:

$$\frac{\partial \hat{f}}{\partial X_S} = g(X_S)h(X_C)$$

Numerical differentiation can be applied if $\hat{f}$ continuous and in estimating the derivative of the individual conditional expectation function we can get an idea of whether or not $\hat{f}$ is additive in $(X_S, X_C)$.
Interpretation of Black Box Functions (III)

Feature/Variable Importance

How important is $X_S$ in achieving $R(\hat{f})$?

If the theoretical joint distribution $P(Y, X_S, X_C) = P(Y, X_C)P(X_S)$ then permuting $X_S$ won’t increase the prediction error.

$$I_{X_S} = \frac{1}{N} \sum_{i=1}^{N} C(x^{(i)}_{S\pi}, x^{(i)}_C)$$

$$I_{X^{(i)}_S} = C(x^{(i)}_{S\pi}, x^{(i)}_C)$$

By using the individual ($i$) importance rather than the expectation combined with a density estimator, we can estimate the density of the cost function under $x_{S\pi}$ for different points in the distribution of $Y$ (as estimated from $y$).
Implementations

- **mlr**: Machine Learning with R (contributor, first via GSoC)
- **edarf**: Exploratory Data Analysis using Random Forests (my package)
- **ICEbox**: Individual Conditional Expectation plot toolbox (Goldstein et. al. 2015)

On to the demonstration! (mlr.R and edarf.R)

On my website under “Talks.” and at github.com/zmjones/imc
Future Work on Interpretation

All of this will be in MLR!

- extrapolation detection
- more variance estimation
- functional ANOVA decomposition (e.g., best additive decomposition of \( \hat{f} \), c.f., Giles Hooker’s work)
- local feature importance and density estimation
Future Work on Learning/Estimation

- dependent data! (coming to MLR)
- conditional independence not generally different (i.e., include structure as features)
- estimation of latent variables
- resampling methods
- preprocessing/filtering
Relevant Papers/Writing on Interpretation

- ESL (10.13.2)
- Freidman (2001)
- Roosen (1995)
- Goldstein et. al. (2015)