Supervised Machine Learning I: Prediction

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Machine Learning

- The next few classes we will be studying *Machine Learning*
  - This is a vague phrase that can mean many things.
  - In fact, we have already studied versions of machine learning, ranging from OLS to penalized linear models like Lasso!
- First, we'll discuss what we usually mean when discussing "ML"
- Then, today we will focus on methods related to prediction, or forecasting
  - Subsequent classes will study how to use these methods to do heterogeneity analysis and categorization of unsupervised data

Machine learning and prediction

- What tends to delineate ML as an approach is a focus on algorithms, rather than statistical processes
  - These points are emphasized by Brieman [2001] and subseqeuntly by Athey and Imbens [2019]
- The tension argued by Brieman is a focus on “theory” vs. solving practical problems
  - E.g., are we willing to use something if we don’t already know it’s a consistent / asymptotically normal estimator?
  - What if it works well in many samples?
- A crucial distinction that has been highlighted between the ML vs. “traditional” stats settings is the difference between *prediction* and unbiased *estimation*
  - Mullinathan and Spiess (2017) refer to $\hat{y}$ vs $\hat{\beta}$

Machine learning and prediction

- Today, we're going to focus on *prediction*. What are applications when prediction is useful?

Machine learning and prediction

- Today, we’re going to focus on *prediction*. What are applications when prediction is useful?
    1. Forecasting – macro or financial.
    2. Assessing the informativeness of new data
    3. Contrasting human decision-making with algorithms
    4. Predicting valuations for unpriced goods?
    5. Others?

- The crucial concern is that prediction *is not* causal identification
    - There is no way to use more data to solve a causal inference problem
    - That’s ok though! There are circumstances where better prediction can be useful to test our models

Refresher: what have we already covered?

- Recall our lecture on *Penalized Linear Models*

- We considered linear model settings with

$$Y_i = X_i\beta + \epsilon_i,$$

  where we expanded on the traditional OLS estimation objective function with a penalty term:

$$\hat{\beta} = \arg\min_{\beta} \sum_i (Y_i - X_i\beta)^2 + \lambda(||\beta||_q)^{1/q}$$

- When $q = 1$, this was LASSO; with $q = 2$, this was ridge regression
  - There are a number of useful hybrid methods that combine different versions of this
  - These models vary in their success and in their computational tractability as K gets large
  - LASSO and ridge (and elastic net) have algorithmically had much success due to their tractability

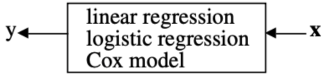
Refresher: what have we already covered?

$$\hat{\beta} = \arg\min_{\beta} \sum_i (Y_i - X_i\beta)^2 + \lambda(||\beta||_q)^{1/q}$$

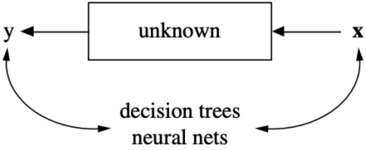
- This is already “Machine Learning”
- Conceptually, we have moved from being focused on being interested in β, and more interested in improving the MSE of $\hat{Y}$
- The models can allow for a wide range of flexible functions
  - polynomials in underlying covariates, and interactions
- Will tend to do best when underlying model is not too non-linear
  - Also has more interpretable model parameters!
  - Today we’ll work on pushing this frontier

What is the contrast being made? Breiman (2001)

- What is the focus of our analysis?



Model validation. Yes–no using goodness-of-fit tests and residual examination.



Model validation. Measured by predictive accuracy.

A primer on terminology

- One costly barrier to ML methods is a different terms for things
- Other terms worth knowing:
  - "one-hot encoding": making dummy variables
  - "validation": testing out of sample

Statistics	Machine Learning
Data Point	Instance
Covariate	Feature
Parameters	Weights
Estimation / Fitting	Learning
Regression / Classification	Supervised Learning
Clustering / Density Estimation	Unsupervised Learning
Response	Label
Test set performance	Generalization

Source: "Towards Data Science"

Distinctive Features: scalability + ensemble methods

- Many solution concepts for ML focus on the ability to
  1. Parallelize
  2. Split data up
  3. Recombine

- The parallization has obvious reasons: computational benefits

- Splitting the data up is less obvious, but pivots off of a notion of *averaging*
  - Effectively, randomly smaller samples (and random subsamples of features) will give a noisier estimate of the "truth"
  - However, averaging over many of these noisy estimates will quickly get at the right value

Distinctive Features: Testing out of sample and cross-validation

- One big difference (although perhaps should not be) in ML is the use of out of sample testing to validate models
  - This matters a ton for ML models where there is subtantial overfitting in-sample

- Conceptually, consider a fully saturated model with many categorical variables on the right hand side:

$$Y_i = X_i\beta + \epsilon_i$$

  - β is the sample mean within each X_i bin
  - as $dim(X_i)$ grows relative to n, each bin more closely approximates exactly one observation
  - This will fit *very* well in-sample
    - It will be quite bad out of sample!

Distinctive Features: Testing out of sample and cross-validation

- Useful terminology: a training dataset, and a test dataset
    - Training: estimate the model
    - Test: evaluate the fitted model

- You can easily split a sample in this way by randomizing across observations
    - A crucial assumption here is independence of the observations (instances)
    - What if they're not independent? (particularly notable in asset pricing)
        - Can consider randomizing in blocks
        - Useful to have a theory that guides these decisions

What is supervised learning / ML?

- In essence, we are interested in $f(X) = E(Y|X)$
  - This is exactly the same problem as our non-parametric regression question!
  - However, in that setting, I told you to give up as soon as $dim(X)$ got large because of data issues
    - ML folks are not so easily dissuaded!
- The solutions in ML revolve around different ways to circumvent a lack of data in higher dimensions
  - LASSO did this using penalized methods on global (linear) functions
  - Tree methods (next) do this by "widening" the comparable group
  - Deep learning-style methods "reduce" the dimensionality to improve comparability

Regression vs. Categorization

- Notably, ML methods distinguish between
  - continuous regression problems (e.g. price as an outcome)
  - classification problems (e.g. sold vs. not sold, or {red bus, blue bus, car})

- In classification problems, the object is *not* necessarily to get the probability of an event (although this is doable)
  - The canonical example is digit recognition – the USPS needs to identify handwritten addresses
  - It doesn't care about an accurate measure of probabilities for each digit!

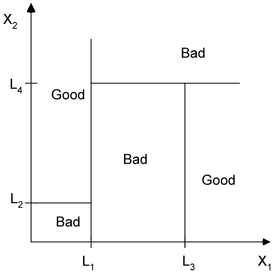
A brief tour through Trees and Forests

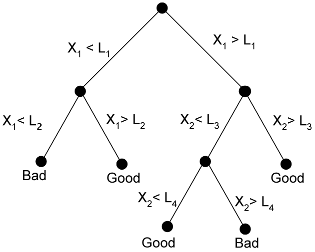
- A very popular off-the-shelf ML model that does both regression and classification is known as regression trees
    - Combinations of trees are called forests
- Given a set of parameter X_i with $dim(X) = k$, the goal is to take subsets of parameters, and split the sample based on values of individual covariates X_{ik}
- The choice of split is made to minimize within-sample error within each split sample
    - These splits are called "leaves"
- If we allowed infinite leaves, then the tree would grow until every observation was uniquely fit
    - The solution is to penalize the number of leaves allowed via "pruning"

Trees and Forests

- In essence this approach is like exhaustively dummying but:
  - The cutpoints are chosen through the data
  - the interactions and cuts are penalized to avoid full saturation

- These models MASSIVELY overfit in sample, however, and so it is important to test out of sample!





A brief tour through Trees and Forests

- These tree models are quite discrete in their cutpoints, which can have weird properties

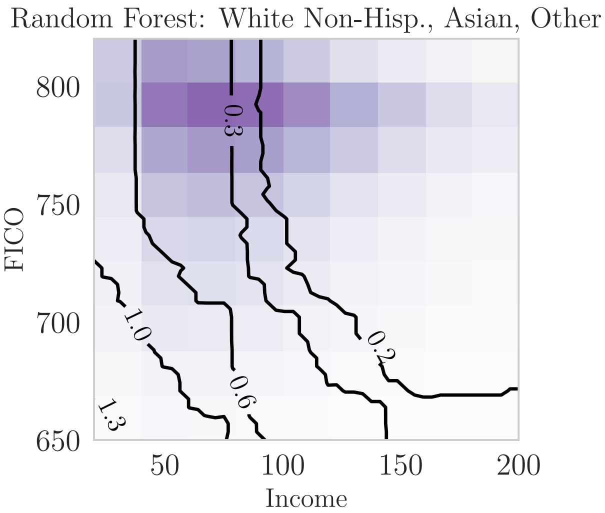
- The traditional fix to this uses *Random Forests*.

- The approach makes many different trees to construct predictions, and then "averages" them. These trees differ in two ways:
  - They use random subsamples of the data
  - They use random subsamples of the covariates

- Random sampling creates independent variation across the predictions
  - Once averaged together, the overall predictions are quite a bit smoother and also better fit out of sample

An example Forest

- These models can create much more non-linear relationships than say, Logit
- Example from Fuster et al. (2021)



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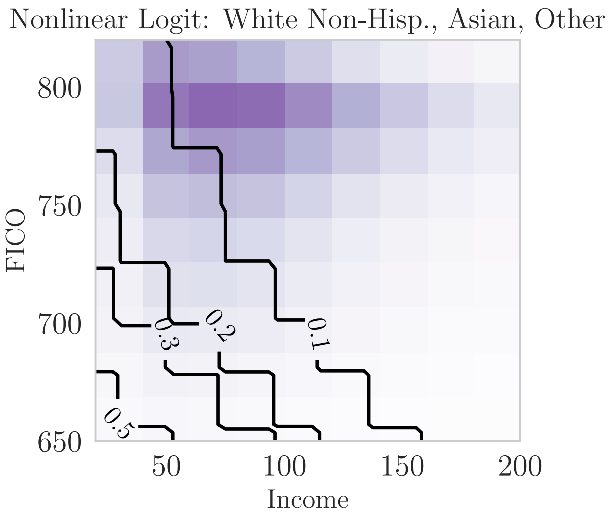

Three key insights from ML (Breiman (2001))

- Once you are fitting to predict outcome as accurately as possible, there are potentially many equally good models that will put weight on different inputs (**Rashomon**)

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- Once you are fitting to predict outcome as accurately as possible, there are potentially many equally good models that will put weight on different inputs (**Rashomon**)

- Simple and transparent models tend to be less accurate (**Occam**)

- Dimensionality is a *benefit* in ML (unlike traditional non-parametrics) (**Bellman**)

Implications of Rashomon

- Formally,

  > *What I call the Rashomon Effect is that there is often a multitude of different descriptions [equations fx] in a class of functions giving about the same minimum error rate.*

- One important implication of this is model averaging can be very successful, since the paths to getting similar error rates can be independent ("bagging")
- *significantly* cautions interpretation of weights from model inputs
- Also means that models may be highly sensitive!

Implications of Rashomon (D'amour (2021))

In recent work, 39 colleagues and I conducted a large-scale study of Rashomon effects in production-scale machine learning systems (D'Amour et al., 2020). We dubbed the problem underspecification. The systems we examined included image classifiers, medical imaging systems, natural language processing systems, and clinical risk prediction systems, based on neural networks. The general design was as follows. First, for each model, we developed a metric that probed a practically important dimension of the model's behavior that was not directly measured by predictive performance on the test set. We called these probes "stress tests", and examples included the model's accuracy on corrupted inputs (e.g., images that had been pixelated), the stability of the model's predictions across irrelevant perturbations (e.g., the gender of pronouns, or the time of day in a medical record), etc. We then trained several subtly different versions of the model (usually, the models only differed by their random weight initialization at the start of training) on the same data using the same heuristics, and checked that the final collection of models had largely the same performance on the test set. Finally, we evaluated each of these model replicates on the stress test. Across each Rashomon set of models, despite having near-identical test set performance, we observed substantially higher variability (sometimes an order of magnitude more) on stress tests. For example, we found that the sensitivity of image classifiers to pixelation, the sensitivity of language models to gender information, the sensitivity of medical imaging models to camera type, and the sensitivity of clinical risk predictors to physician behavior were all affected in substantial ways by the choice of random seed. Our conclusion was that these practically important dimensions of model performance are not well-constrainted by standard predictive criteria, and are often determined by arbitrary (even random) choices made during training. Given the sheer number of "knobs to twiddle" in modern machine learning models (a phrase Prof. Efron's comment (Efron, 2001)), we conjectured that much larger Rashomon sets are likely lurking in many successful applications of machine learning. I only realized after we completed the project that Breiman had included a small version of this experiment in Section 8!

Implications of Occam

- Many of the most effective models are hard to "explain"
  - e.g., what drives the Random Forest model?
- Is there a given input that matters? In OLS, we can look at coefficients
- This is a serious challenge in ML models (especially once combined with Rashomon)
  - Better to use ML to substitiute for "nuisance" parameters

Implications of Bellman

- Recall that for a fixed sample n, if we increase the number of features (covariates) K, we will get noisier and noisier estimates with something like OLS (or non-parametric estimation)

- This is what Richard Bellman termed "the curse of dimensionality"

- This curse is a blessing for many ML applications; why?
  - The curse shows up in estiamting underlying parameters
  - When focusing on the outcome, y, the solutions often improve as you increase the dimensionality
  - This is due, implicitly, to penalization, and avoiding a focus on unbiasedness

- Hence, key insight: rather than throw out data, use shrinkage (via penalization, or priors) to maintain an effective prediction
  - This insight goes back to Stein (1956)!

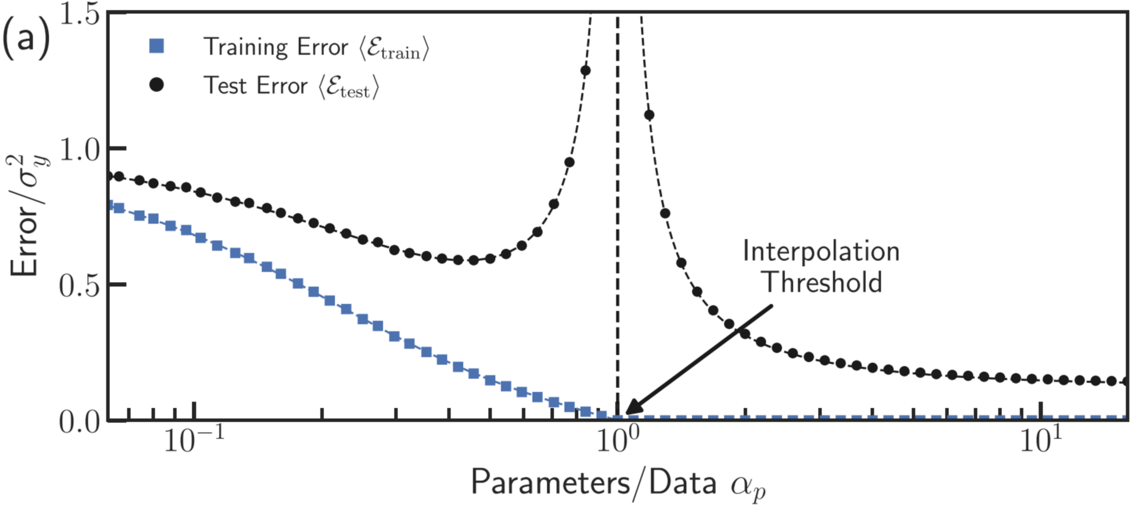
The virtue of complexity (and the double descent)

- As models grow in complexity,
  - there is a decrease in the "in-sample" error that continues until you have a fully saturated model
  - there is an initial decrease in the "out-of-sample" error initially, and then an increase due to overfitting

- This trade-off is what is often optimized using cross-validation

- However, a key new insight (see Kelly, Malamud and Zhou (2024) for an example) is that the out-of-sample error will start to improve again as the number of parameters grows (under certain models)

- This is the "double descent" curve
  - Big improvements in predicting future market returns (market timing)
  - Interesting to think of applications in other areas!


(a)
Training Error $\langle \mathcal{E}_{\mathrm{train}} \rangle$
Test Error $\langle \mathcal{E}_{\mathrm{test}} \rangle$
Interpolation Threshold
Error$/\sigma_y^2$
Parameters/Data α_p
1.5
1.0
0.5
0.0
10^{-1}
10^{0}
10^{1}

How to approach and further reading

- If you are considering ML models, the two standard programming languages with significant support are Python and R
  - It's possible that Julia and Matlab are doable, but I have seen far less here

- In Python, `scikit-learn` is a great package with many features

- In R, there is a big community of a packages that can be used as well, with `caret` as a very useful meta-engine for running diffferent estimations
  - "Hands-On Machine Learning in R" is an excellent resource for this: `https://bradleyboehmke.github.io/HOML/`

- The biggest challenge in my experience, is that the high-level concepts are very straightforward, while the nitty-gritty tuning, testing and decipering is quite hard
  - A big reason this is true is that it's very application-specific
  - Different forecasting problems have different issues

Checklist for what to look for

- What type of outcome do I have? (Classification vs. Regression)
- Do I expect highly non-linear responses, or relatively linear ones?
  - Many economics models have relatively monotonic response patterns
  - Linear models might do just fine!
- Do not use these models for data exploration – they can be computationally quite expensive, and are much less transparent
  - Identify your prediction problem carefully, and setup your estimation accordingly to cross-validate on appropriate parameters