

Frontier Topics in Empirical Economics: Week 3

Machine Learning and Model Selection

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Machine Learning and Model Selection: Introduction

- In the last lecture, we learn some non-parametric and semi-parametric methods
- We now have many tools in our box beyond linear regression
 - Kernel regression, local polynomial regression
 - Spline regression, partial linear regression
 - ...
- Which method should we choose?

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Machine Learning and Model Selection: Introduction

- Even for a given method, such as simple regression
- The functional form is still flexible
 - Why linear? Simple? Why not $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$?
 - What variables to include?
 - In linear regression, we regress on x_1, x_2, \dots, x_p . Why not $\sin(x_1)$?

Machine Learning and Model Selection: Introduction

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In Mincer equation, we regression *wage* on *edu*, *exp*, and *exp*². Why not *edu*³?

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- More due to data availability issue
- Nowadays, more and more datasets are available with huge sizes
- **BIG DATA! More chances!**
- We should seriously consider model selection issue
- Let's first introduce a major statistical concept: Bias-variance tradeoff

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Machine Learning and Model Selection: Bias-variance Tradeoff

- A traditional linear model

$$y = x\beta + \epsilon \quad (1)$$

- A model with quadratic term

$$y = x\beta + x^2\alpha + \epsilon \quad (2)$$

- A non-parametric model

$$y = g(x) + \epsilon \quad (3)$$

- Why not always the second or the third one?

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- Model A

$$y = x_1' \beta + \epsilon \quad (4)$$

- Model B

$$y = x_1' \beta_1 + x_2' \beta_2 + \epsilon \quad (5)$$

- Why not always the second one?
- Always better to have a more complicated model?

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Machine Learning and Model Selection: Bias-variance Tradeoff

■ Model Selection: Bias vs. Variance

Assume that:

$$Y = f(X) + \epsilon$$

- $\hat{f}(x)$ is a model trained by some data
- It will be changed when sample is changed: $\hat{f}^1(x), \hat{f}^2(x), \dots$
- Expectation $E[\hat{f}(x)]$ is taken over different samples
- How good is the model?

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Machine Learning and Model Selection: Bias-variance Tradeoff

- The prediction error at some point x_0 :

$$\begin{aligned} E[(Y - \hat{f}(x_0))^2 | X = x_0] &= \sigma_e^2 + [E\hat{f}(x_0) - f(x_0)]^2 + E[\hat{f}(x_0) - E\hat{f}(x_0)]^2 \\ &= \text{irreducible error} + \text{Bias}^2 + \text{Variance} \end{aligned}$$

- Model complexity \Rightarrow Bias \downarrow , Variance \uparrow
- Super complicated model \Rightarrow Variance $\uparrow\uparrow\uparrow$ (very sensitive when data change)
- Overfit current data \Rightarrow Poor out-of-sample prediction

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Machine Learning and Model Selection: An Example of Overfitting

- Consider a data generating process

$$Y = 1 + 1.5X + \epsilon$$

$$\epsilon \sim N(0, 100)$$

It is a noisy process.

- Simulate 30 observations from this process
- Let's start to fit it with different polynomials
- Green line is the true DGP
- Red line is the fitting function

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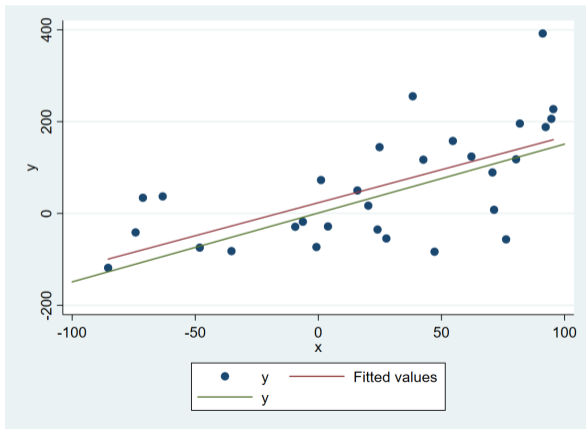
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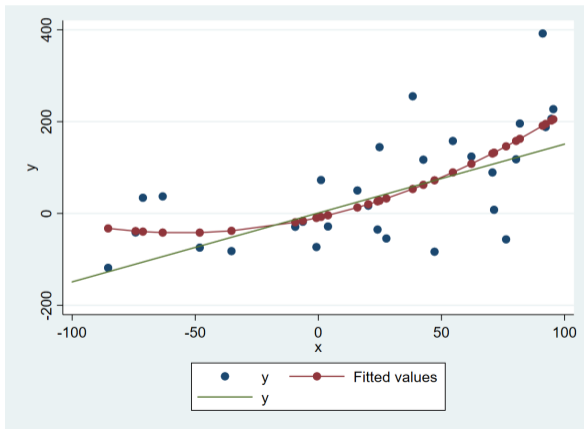
Machine Learning and Model Selection: An Example of Overfitting

Figure: First Order (Linear) Fitting



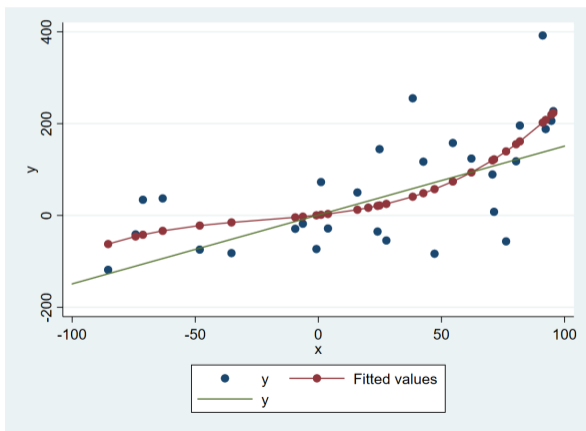
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Figure: Second Order (Quadratic) Fitting



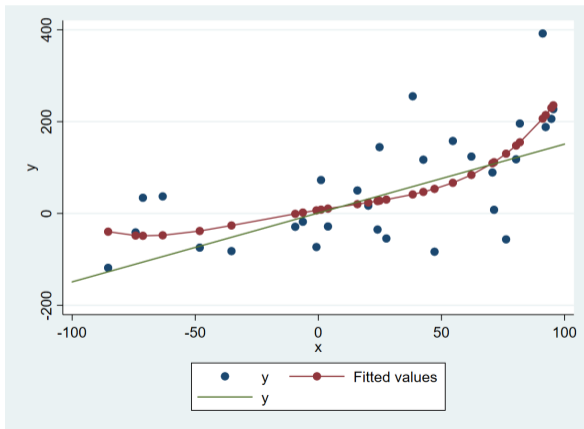
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Figure: Third Order (Cubic) Fitting



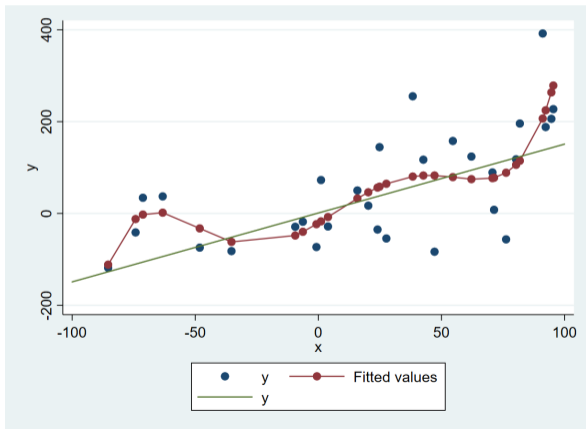
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Figure: Fourth Order Fitting



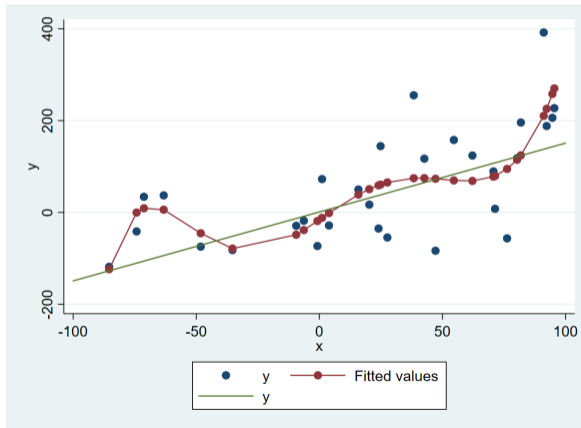
Machine Learning and Model Selection: An Example of Overfitting

Figure: Fifth Order Fitting



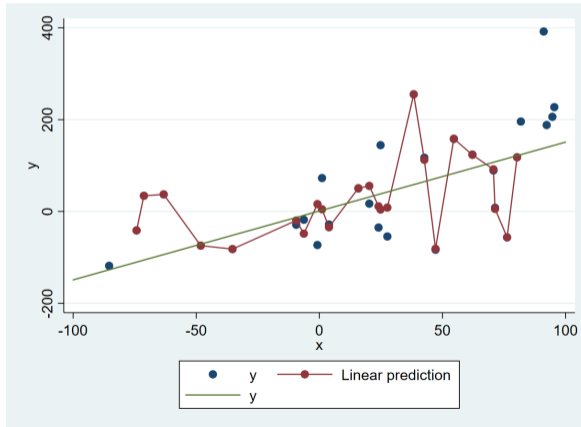
Machine Learning and Model Selection: An Example of Overfitting

Figure: Sixth Order Fitting



Machine Learning and Model Selection: An Example of Overfitting

Figure: Twentieth Order Fitting



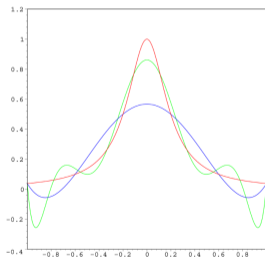
Machine Learning and Model Selection: An Example of Overfitting



High order polynomials: Picking up noises, not signals!!!
Bad out-of-sample prediction!!!

Machine Learning and Model Selection: An Example of Overfitting

- We have actually learned two kinds of overfitting
- Runge phenomenon and Gibbs phenomenon



Machine Learning and Model Selection: Goodness of Fit

There are many ways to measure the goodness of fit, considering overfitting

- Adjusted R-squared: the proportion of explained variations in y
Still remember why we need to adjust for the number of regressors?
- AIC: Akaike Information Criterion
 $AIC = 2k + n \ln(RSS/n)$, k is the number of regressors
- BIC: Bayesian Information Criterion
This is motivated by the Bayesian approach to model selection

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Another important measure is Cross-Validation (CV)

- The basic idea is to separate all samples into training sample and validation sample
- Training sample is used to train (estimate) the model
- Validation sample is then used to check the "out-of-sample" prediction
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Here is the process of CV



- First, we separate all samples into K parts
- Each time, we choose $K-1$ parts to train (estimate) the model
- We then use the remaining one part k to calculate the mean squared predicted error MSE_k
- We rotate the samples K times so that each part is used as the validation sample once, and have K pieces of MSE_k
- We take the average of them to have: $CV = \frac{1}{K} \sum_{k=1}^K MSE_k$
- This is called "K-fold Cross-Validation"

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Here is the process of CV



- First, we separate all samples into K parts
- Each time, we choose $K-1$ parts to train (estimate) the model
- We then use the remaining one part k to calculate the mean squared predicted error MSE_k
- We rotate the samples K times so that each part is used as the validation sample once, and have K pieces of MSE_k
- We take the average of them to have: $CV = \frac{1}{k} \sum_{k=1}^K MSE_k$
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- CV measures the goodness of the out-of-sample prediction
- It mimics a situation when you have some data that is not used in the estimation to check your estimation validity
- It helps you to determine which model fits better to the data, in terms of out-of-sample prediction
- Smaller CV means better fitting

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- That is, the "standard" of what is a "good" model
- Would that be possible to have an automatic algorithm to find a good model for us?
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- What is machine learning?

"Machine learning (ML) is an umbrella term for solving problems for which development of algorithms by human programmers would be cost-prohibitive, and instead the problems are solved by helping machines 'discover' their 'own' algorithms, without needing to be explicitly told what to do by any human-developed algorithms." from Wikipedia

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Machine learning usage in Economics

- Main target: How complicated the model should be? How to *predict* Y given X ?
- When Y is discrete: Classification
- When Y is continuous: Prediction
- There are so many machine learning algorithms
- We briefly introduce three of them: Penalized regression, Tree-based method, Neural network

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Machine Learning and Model Selection: Penalized Regressions

- Let's consider a linear regression
- What if I have so many potential regressors?
- For instance, you have a household survey with 1000 questions
- Is there an automatic way to select the best predictors?

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- Linear function: $y_i = x_i' \beta + \epsilon_i$
- OLS: $\hat{\beta}^{OLS} = \operatorname{argmin} \sum_i (y_i - x_i' \beta)^2$
All regressors x play roles.
- We estimate β by minimizing SSR \Rightarrow More β means smaller SSR
- We need a mechanism to penalize the usage of β

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 - p=1: Lasso regression, drop some x with small prediction power
 - p=2: Ridge regression, shrink some x with small prediction power
- λ : tuning parameter, how strong we penalize additional "x"
- How to choose λ ? Cross-validation
- Combination: Elastic Net
$$\hat{\beta}^{Pen} = \operatorname{argmin} \sum_i (y_i - x_i' \beta)^2 + \lambda (\alpha \|\beta\|_1 + (1 - \alpha) (\|\beta\|_2)^2)$$

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Machine Learning and Model Selection: Tree-based Method

- Tree-based methods partition the feature (X) space into a set of rectangles, and then fit a simple model (constant) in each one.
- Classification and Regression Tree (CART)
- Partition into regions $R_1, R_2 \dots R_M$, assign average value in a region as the predicted value
$$\hat{f}(x_i) = \sum_{m=1}^M c_m I(x \in R_m)$$
- How to partition (Grow the tree)?

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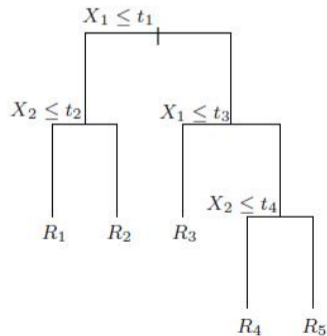
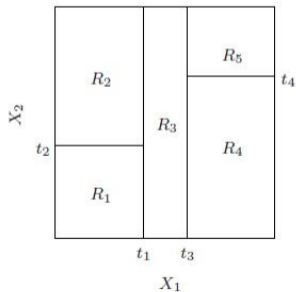
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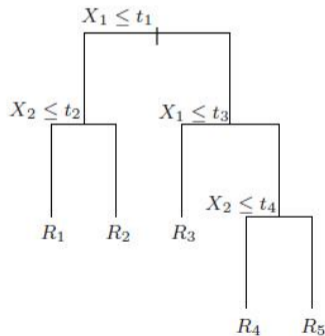
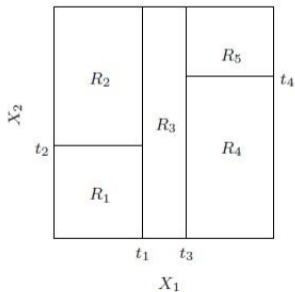
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- $(X_1, t_1) \rightarrow ((X_2, t_2), (X_1, t_3)) \rightarrow (X_2, t_4)$



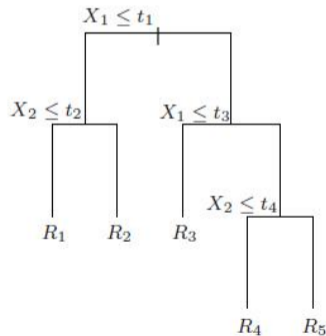
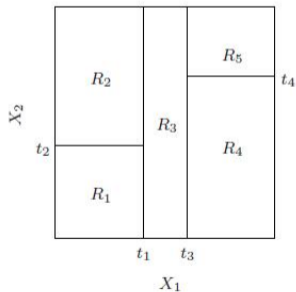
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Machine Learning and Model Selection: Tree-based Method

- Two choices: continue partitioning or stop + where to partition
- Greedy algorithm
- For each region R_m (leaf), we define:

Size (# of obs): $N_m = \#\{x_i \in R_m\}$

Fitted value (mean as fit): $\hat{c}_m = \frac{1}{N_m} \sum_{x \in R_m} y_i$

SSE (error in leaf): $Q_m(T) = \frac{1}{N_m} \sum_{x \in R_m} (y_i - \hat{c}_m)^2$

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Machine Learning and Model Selection: Tree-based Method

- First, conditional on continuing grow, how to determine partition?
- For j -th predictor, cut position s
- Define half plane $R_1(j, s) = \{X | X_j \leq s\}$, $R_2(j, s) = \{X | X_j > s\}$
- How to find (j, s) in each branch? Minimize SSE (Easy)

$$\min_{j, s} \left[\min_{c_1} \sum_{x_i \in R_1(j, s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j, s)} (y_i - c_2)^2 \right]$$

- Here c_1 and c_2 are conditional means (in leaf 1 and 2)

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- Second, how to choose to continue growing the tree or stop?
- Too large \rightarrow Overfitting; Too small \rightarrow Losing information
- Grow a big tree T_0 , then prune it!
 - Step 1: Grow T_0 when some minimum node size is reached (say M_0)
 - Step 2: Pruning: Choose the tree $T \in \mathcal{T}_0$ with the lowest cost function $C_{\text{test}}(T)$
 - $\mathcal{T} \in \mathcal{T}_0$ means any tree T that can be obtained by collapsing any number of internal nodes in T_0

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$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha |T|$$

α as the tuning parameter; $|T|$ as number of terminal nodes

- Total SSE (bias) + Size penalty
- α determines how hard to penalize tree size

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$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha |T|$$

α as the tuning parameter; $|T|$ as number of terminal nodes

- Total SSE (bias) + Size penalty
- α determines how hard to penalize tree size

Machine Learning and Model Selection: Random Forests

- Using sub-sampling or bagging to reduce variance of a single tree
- Draw a lot of different samples $(1, 2, \dots, B)$ with sub-sampling ($n < N$) (Jackknife) or bagging ($n = N$) (Bootstrap)
- De-correlation: In each split, randomly select m variables to do the partition

$$\hat{f}^B(x) = \frac{1}{B} \sum_{b=1}^B T_b(x)$$
$$V(\hat{f}) \approx \rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$$

- Random Forests = Tree Method + Sampling average (Many De-correlated Trees)
- To reduce $V(\hat{f})$: $B \uparrow$ (more sampling), $\rho \downarrow$ (smaller correlation)

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Machine Learning and Model Selection: Random Forests

Algorithm 15.1 *Random Forest for Regression or Classification.*

1. For $b = 1$ to B :
 - (a) Draw a bootstrap sample \mathbf{Z}^* of size N from the training data.
 - (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.
 - i. Select m variables at random from the p variables.
 - ii. Pick the best variable/split-point among the m .
 - iii. Split the node into two daughter nodes.
2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point x :

Regression: $\hat{f}_{\text{rf}}^B(x) = \frac{1}{B} \sum_{b=1}^B T_b(x)$.

Classification: Let $\hat{C}_b(x)$ be the class prediction of the b th random-forest tree. Then $\hat{C}_{\text{rf}}^B(x) = \text{majority vote } \{\hat{C}_b(x)\}_1^B$.

Machine Learning and Model Selection: Random Forests

- We reduce the variance by bagging (B) and de-correlation (ρ)
- This is a method similar to kernels and nearest-neighbor method
 - Making predictions using weighted averages of "nearby" observations
- Difference: Weighting scheme
 - Nearest Neighbor: Not adaptive; Random Forests: Adaptive
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Machine Learning and Model Selection: Causal Forests

- Main topic in causal inference: Treatment effect
Mostly ATE, LATE etc.
- Heterogeneous Treatment Effect
Cherry picking? \Rightarrow Institutional restrictions on trials
- Unexpected heterogeneity
- Wager and Athey develop a machine learning tool, Causal Forests (An extension of Random Forests)
- To reveal the true underlying heterogeneous treatment effects

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- It tells us how to divide groups to get the "real" heterogeneous TE
- Data of (X_i, Y_i, W_i) , W_i is treatment assignment. L as a leaf (region).
- Treatment effect: $\tau(x) = E[Y_i^{(1)} - Y_i^{(0)} | X_i = x]$
- Unconfoundness: $\{Y_i^{(0)}, Y_i^{(1)}\} \perp W_i | X_i$

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Machine Learning and Model Selection: Causal Forests

- Estimation of TE: Given x in leaf $L(x)$, the difference of the average outcome Y for treated/non-treated group

$$\hat{\tau}(x) = \frac{1}{|\{i: W_i=1, X_i \in L\}|} \sum_{\{i: W_i=1, X_i \in L\}} Y_i - \frac{1}{|\{i: W_i=0, X_i \in L\}|} \sum_{\{i: W_i=0, X_i \in L\}} Y_i$$

- Implement the Random Forests using a criterion: maximizing variance of $\hat{\tau}(X_i)$

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- A tree is honest, if for each training example i , it is either used to estimate τ or used to decide splits
- Double-Sample Trees: Averagely divide samples into two parts I and J . Grow the tree using I and then estimate τ in each leaf using J .
- Honest Causal Forests is consistent and asymptotically normal

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Machine Learning and Model Selection: Application of Causal Forests

- Paper report
Levy (2021) Social Media, News Consumption, and Polarization: Evidence from a Field Experiment
- Please also read Online Appendix C.5

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- It attracts people's attention during these days in media
- AI, AlphaGo...Sky Net (kidding)

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- Consider a single layer classification model, where Y_k refers to each choice/class

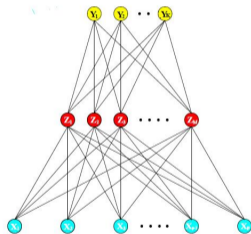


FIGURE 11.2. Schematic of a single hidden layer, feed-forward neural network.

- X - Input; Z - Hidden layer/unit; Y - Output

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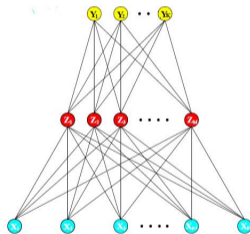


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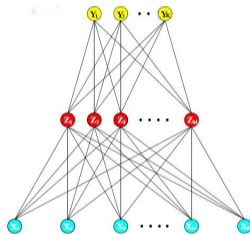


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- Step 1: from input X to hidden unit Z

$$Z_m = \sigma(\alpha_{0m} + \alpha_m^T X), m = 1, \dots, M$$

- σ is a nonlinear function (Step or Logit)
- Step 2: from hidden unit Z to output Y

$$T_k = \beta_{0k} + \beta_k^T Z, k = 1, \dots, K$$
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- Because it was first developed as models for the human brain
- Each unit represents a neuron
- Connections are synapses
- There can be multiple layers
- When step function is used for σ and g , neurons fire when signal passed to the unit ($\alpha_{0m} + \alpha_m^T X$) exceeds some threshold

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- How to estimate this model?
- Simply nonlinear Least Square
- How to avoid overfitting?
- Regularize the optimization problem $\min R(\theta)$ with a penalty term:

$$\min R(\theta) + \lambda J(\theta)$$
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- λ is a tuning parameter

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- In general, there are many standards to evaluate model's goodness-of-fit
CV, AIC, BIC
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