A Very Brief Introduction to Machine Learning for Regression

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Abstract: These slides attempt to demystify machine learning. The slides cover standard machine learning methods such as k-fold cross-validation, lasso, regression trees and random forests.

The slides conclude with some recent econometrics research that incorporates machine learning methods in causal models estimated using observational data.

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More at http://cameron.econ.ucdavis.edu/e240f/machinelearning.html.

October 27, 2017

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Introduction

- The goal is **prediction**.
- Machine learning means that no stuctural model is given.
 - Instead the machine is given an algorithm and existing data.
 - > These train the machine to come up with a prediction model.
 - This model is then used to make predictions given new data.
- Various methods guard against **overfitting** the existing data.
- There are many, many algorithms
 - a given algorithm may work well for one type of data and poorly for other types.
- Forming data to input can be an art in itself (data carpentry)
 - e.g. what **features** to use for facial recognition.
- What could go wrong?
 - correlation does not imply causation
 - social science models can help here.

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Overview

- Terminology
- Oross-validation
- Regression (Supervised learning for continuous y)
 - Subset selection of regressors
 - Ø Shrinkage methods: ridge, lasso, LAR
 - Oimension reduction: PCA and partial LS
 - High-dimensional data
- Nonlinear models in including neural networks
- Segression trees, bagging, random forests and boosting
- Olassification (categorical y)
- O Unsupervised learning (no y)
- Oausal inference with machine learning
- 9 References

1. Terminology

- Topic is called machine learning or statistical learning or data learning or data analytics where data may be big or small.
- Supervised learning = Regression
 - We have both outcome y and regressors x
 - ▶ 1. **Regression**: y is continuous
 - 2. Classification: y is categorical

• Unsupervised learning

- We have no outcome y only several **x**
- ▶ 3. Cluster Analysis: e.g. determine five types of individuals given many psychometric measures.
- These slides
 - focus on 1

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Terminology (continued)

- Machine learning methods guard against overfitting the data.
- Consider two types of data sets
 - 1. training data set (or estimation sample)
 - \star used to fit a model
 - 2. test data set (or hold-out sample or validation set)
 - * additional data used to determine model goodness-of-fit
 - ***** a test observation (\mathbf{x}_0, y_0) is a previously unseen observation.
- Models are created on 1. and we use the model that does best on 2.

2. Cross Validation

- **Goal:** Predict *y* given *p* regressors *x*₁, ..., *x*_{*p*}.
- Criterion: use squared error loss $(y \hat{y})^2$
 - some methods adapt to other loss functions.
- **Training data set:** yields the prediction rule $\hat{f}(x_1, ..., x_p)$
 - e.g. OLS yields $\widehat{y} = \widehat{\beta}_0 + \widehat{\beta}_1 x_1 + \cdots + \widehat{\beta}_p x_p$.
- Test data set: yields an estimate of the true prediction error
 - This is $E[(y_0 \hat{y}_0)^2]$ for $(y_0, x_{10}, ..., x_{p0})$ not in the training data set.
- Note that we do not use the training data set mean squared error

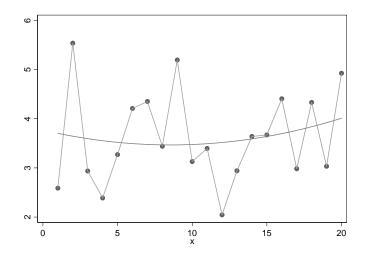
• MSE =
$$\frac{1}{n} \sum_{i=1}^{n} (y_i - \widehat{y}_i)^2$$

• because models overfit in sample (they target y not $E[y|x_1, ..., x_p]$)

* e.g. if
$$p = n - 1$$
 then $R^2 = 1$ and $\sum_{i=1}^{n} (y_i - \widehat{y}_i)^2 = 0$.

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Bias-variance tradeoff



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Stata Example

• D.g.p. is quadratic with n = 40. Fit OLS polynomial of degree 4.

```
. * Generate data: quadratic with n=40 (total) and n=20 (train) and n=20 (test)
. qui set obs 40
. set seed 10101
. gen x1 = _n - mod(_n+1,2) // x1 = 1 1 3 3 5 5 .... 39 39
. gen x2 = x1^2
. gen x3 = x1^3
. gen x4 = x1^4
. gen dtrain = mod(_n,2)==1 // dtrain = 1 0 1 0 .... 1 0
```

```
. gen y = 2 + 0.1*(x1-20)^2 + rnormal(0,10)
```

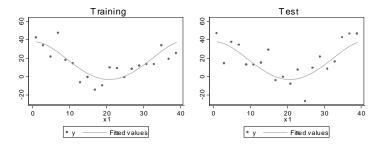
. reg y x1-x4, noheader

У	Coef.	Std. Err.	t	P> t	[95% Conf.	Interval]
x1	.4540487	3.347179	0.14	0.893	-6.341085	7.249183
x2	437711	.3399652	-1.29	0.206	-1.127877	.2524551
x3	.020571	.0127659	1.61	0.116	0053452	.0464871
x4	0002477	.0001584	-1.56	0.127	0005692	.0000738
_cons	37.91263	9.619719	3.94	0.000	18.38357	57.4417

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Predictions in training and test data sets

- Now fit to only training data $(n_{Train} = 20)$ and plot predictions.
- Quartic model predicts worse in test dataset (right panel)
 - Training data (left): scatterplot and fitted curve $(n_{Test} = 20)$:.
 - Test data (right): scatter plot (different y) and predictions (n = 20).



Single split-sample validation

- Fit polynomial of degree k on training data for k = 1, ..., 4
 - compute MSE $\sum_{i} (y_i \hat{y}_i)^2$ for training data and test data
- Test MSE is lowest for quadratic
 - Training MSE is lowest for quartic due to overfitting.

```
* Split sample validation - training and test MSE for polynomials up to deg 4
 forvalues k = 1/4 {
  2.
       gui reg y x1-x`k' if dtrain==1
  3.
       qui predict y`k'hat

 qui gen y`k'errorsq = (y`k'hat - y)^2

    gui sum v`k'errorsg if dtrain == 1

  qui scalar mse`k'train = r(mean)
  7.
       qui sum v`k'errorsq if dtrain == 0
       qui scalar mse`k'test = r(mean)
  8.
  9. }
. di _n "MSE linear Train = " mseltrain " Test = " mseltest _n ///
     "MSE quadratic Train = " mse2train " Test = " mse2test _n ///
>
                     Train = " mse3train " Test = " mse3test n ///
     "MSE cubic
>
     "MSE quartic
                     Train = " mse4train " Test = " mse4test n
>
MSE linear
               Train = 252.32258 Test = 412.98285
MSE guadratic Train = 92.781786 Test = 184.43114
MSE cubic Train = 87.577254 Test = 208.24569
MSE quartic Train = 72.864095 Test = 207.78885
```

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k-fold Cross Validation

- Problem: with single-split validation
 - ▶ 1. Lose precision due to smaller training set, so may actually overestimate the test error rate (MSE) of the model.
 - ▶ 2. Results depend a lot on the particular single split.
- Solution: Randomly divide data into K groups or folds of approximately equal size
 - First fold is the validation set
 - Method is fit in the remaining K 1 folds
 - Compute MSE for the first fold
 - Repeat K times (drop second fold, third fold, ...) yields

$$\mathsf{CV}_{(\mathcal{K})} = rac{1}{\mathcal{K}} \sum_{j=1}^{\mathcal{K}} \mathit{MSE}_{(j)};$$
 typically $\mathcal{K} = 5$ or $\mathcal{K} = 10.$

• Aside: Leave-one-out cross-validation used in bandwidth selection for nonparametric regression (local fit) is the case K = n.

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k-fold cross validation for full sample

- Begin with all 40 observations
 - Randomly form five folds
 - Five times estimate on four $(n_{Train} = 32)$, predict on fifth $(n_{Test} = 8)$.
- Following does this for the quadratic model.

•
$$CV_{(5)} = \frac{1}{5}(15.27994 + \dots + 8.444316) = 12.39305.$$

. * Five-fold cross validation example for quadratic

. set seed 10101

. crossfold regress y x1 x2

	RMSE
est1	15.27994
est2	16.77849
est3	11.15653
est4	10.30595
est5	8.444316

. * Compute five-fold cross validation measure - average of the above . matrix RMSEs = r(est)

```
. macri x km3E3 = 1(e3c)
```

```
. svmat RMSEs, names(rmses)
```

. sum rmses

Variable	Obs	Mean	Std. Dev.	Min	Мах		
rmses1	5	12.39305	3.501561	8.444316	16.77849	э	৶৻ড়

Five-fold cross validation for all models

- Do this for polynomials of degree 1, 2, 3 and 4
 - CV measure is lowest for the quadratic.

```
. * Five-fold cross validation measure for polynomials up to degree 4
. forvalues k = 1/4 {
2. qui set seed 10101
3. qui crossfold regress y x1-x`k'
4. qui matrix RMSEs`k' = r(est)
5. qui symat RMSEs`k', names(rmses`k')
6. qui sum rmses`k'
7. qui scalar cv`k' = r(mean)
8. }
. di _n "CV(5) for k = 1,..,4 = " cv1 ", " cv2 ", "cv3 ", "cv4
CV(5) for k = 1,..,4 = 12.393046, 12.393046, 12.629339, 12.475117
```

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Penalty measures

- Alternative to cross-validation that uses all the data and is quicker.
 - though is more model specific and less universal.
- Focused on loss function squared error or log-likelihood
 - whereas cross-validation approach quite universal.
- Leading examples
 - Akaike's information criterion: AIC = $-2 \ln L + 2p$
 - Bayesian information criterion: $BIC = -2 \ln L + p \ln N$
 - Mallows CP
 - Adjusted R^2 (\overline{R}^2)

AIC and BIC penalty measures for full sample

- Compute AIC and BIC for polynomials of degree 1, 2, 3 and 4 (n = 40)
- Both AIC and BIC are minimized by the quadratic model.

```
. * Full sample estimates with AIC, BIC penalty - polynomials up to deg 4
. forvalues k = 1/4 {
2. qui reg y x1-x`k'
3. qui scalar aic`k' = -2*e(11) + 2*e(rank)
4. qui scalar bic`k' = -2*e(11) + e(rank)*ln(e(N))
5. }
. di _n "AIC for k = 1,...,4 = " aic1 ", " aic2 ", "aic3 ", "aic4, ///
> _n "BIC for k = 1,...,4 = " bic1 ", " bic2 ", "bic3 ", "bic4
AIC for k = 1,...,4 = 348.99841, 314.26217, 316.01317, 315.3112
BIC for k = 1,...,4 = 352.37617, 319.32881, 322.76869, 323.7556
```

3. Regression Methods

- A flexible linear (in parameters) regression model with many regressors may fit well.
- Consider linear regression model with *p* potential regressors where *p* is too large.
- Methods that reduce the model complexity are
 - choose a subset of regressors
 - shrink regression coefficients towards zero
 - ★ ridge, lasso, LAR
 - reduce the dimension of the regressors
 - ★ principal components analysis.
- Linear regression may predict well if include interactions and powers as potential regressors.

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Subset Selection of Regressors

- General idea is for each model size choose best model and then chose between the different model sizes.
- So
 - ▶ 1. For k = 1, 2, ..., p choose a "best" model with k regressors
 - 2. Choose among these p models based on model fit with penalty (e.g. CV or AIC) for larger models.
- Methods include
 - best subset
 - forwards stepwise
 - backwards stepwise
 - hybrid.

Variance-bias trade-off

• Consider regression model

 $y = f(\mathbf{x}) + \varepsilon$ $E[\varepsilon] = 0$ and ε independent of \mathbf{x}

• For out-of-estimation-sample point (y_0, \mathbf{x}_0) the MSE

$$\begin{array}{lll} E[(y_0 - \widehat{f}(\mathbf{x}_0))^2] &= & Var[\widehat{f}(\mathbf{x}_0)] + \{Bias(\widehat{f}(\mathbf{x}_0))\}^2 + Var(\varepsilon) \\ & \mathsf{MSE} &= & \mathsf{Variance} + \mathsf{Bias-squared} + \mathsf{Error variance} \end{array}$$

- Lesson 1: more flexible models have less bias but more variance
- Lesson 2: bias can be good if minimizing MSE is our goal.
 - shrinkage estimators exploit this.

Shrinkage Methods

- There is a mean-variance trade-off.
- Shrinkage estimators minimize RSS (residual sum of squares) with a penalty for model size
 - this shrinks parameter estimates towards zero.
- The extent of shrinkage is determined by a tuning parameter
 - this is determined by cross-validation or e.g. AIC.
- Ridge and lasso are not invariant to rescaling of regressors, so first standardize the data
 - so x_{ij} below is actually $(x_{ij} \bar{x}_j)/s_j$.
- Ridge penalty is a multiple of $\sum_{j=1}^{p} \beta_{j}^{2}$.
- Lasso penalty is a multiple of $\sum_{j=1}^{p} |\beta_j|$.

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Ridge Regression

- Penalty for large models is $\sum_{j=1}^{p} \beta_{j}^{2}$.
- The ridge estimator $\widehat{oldsymbol{eta}}_\lambda$ of $oldsymbol{eta}$ minimizes

$$\sum_{i=1}^{n} (y_i - \mathbf{x}'_i \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

- where $\lambda \ge 0$ is a tuning parameter.
- Equivalently, ridge minimizes RSS subject to $\sum_{i=1}^{p} \beta_i^2 \leq s$.
- The ridge estimator is

$$\widehat{oldsymbol{eta}}_\lambda = (\mathbf{X}'\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}'\mathbf{y}.$$

Features

- clearly biased
- shrinks all coefficients towards zero
- algorithms exist to quickly compute $\widehat{oldsymbol{eta}}_{\lambda}$ for many values of λ
- then choose λ by cross validation.

Lasso (Least Absolute Shrinkage And Selection)

- Penalty for large models is $\sum_{j=1}^{p} |\beta_j|$.
- The lasso estimator $\widehat{oldsymbol{eta}}_\lambda$ of $oldsymbol{eta}$ minimizes

$$\sum_{i=1}^{n} (y_i - \mathbf{x}'_i \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

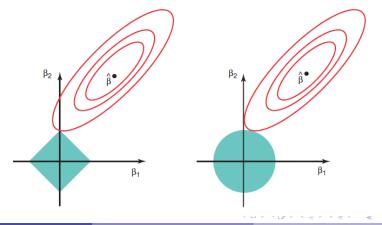
- where $\lambda \ge 0$ is a tuning parameter.
- Equivalently lasso minimizes RSS subject to $\sum_{i=1}^{p} |\beta_i| \leq s$.
- Features
 - drops regressors
 - ▶ best when a few regressors have $\beta_i \neq 0$ and most $\beta_i = 0$
 - leads to a more interpretable model than ridge.

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Lasso

Lasso versus Ridge

- $\widehat{\boldsymbol{\beta}} = (\widehat{\beta}_1, \widehat{\beta}_2)$ minimizes residual sum of squares
 - bigger ellipses have larger RSS
 - choose the first ellipse to touch the shaded (constrained) area.
- Lasso (left) gives a corner solution with $\hat{\beta}_1 = 0$.



Dimension Reduction

- **Reduce** from p regressors to M < p linear combinations of regressors
 - Form $\mathbf{X}^* = \mathbf{X}\mathbf{A}$ where \mathbf{A} is $p \times M$ and M < p
 - $\mathbf{Y} = \beta_0 + \mathbf{X} \boldsymbol{\beta} + \mathbf{u}$ reduced to
 - $\mathbf{Y} = \boldsymbol{\beta}_0 + \mathbf{X}^* \boldsymbol{\beta} + \mathbf{v}$ = $\boldsymbol{\beta}_0 + \mathbf{X} \boldsymbol{\beta}^* + \mathbf{v}$ where $\boldsymbol{\beta}^* = \mathbf{A} \boldsymbol{\beta}$.
- Two methods
 - ▶ 1. Principal components
 - use only X to form A (unsupervised)
 - 2. Partial least squares
 - * also use relationship between **y** and **X** to form **A** (supervised).

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High-Dimensional Models

• High dimensional simply means p is large relative to n

- in particular p > n
- n could be large or small.
- Problems with p > n:
 - C_p , AIC, BIC and \overline{R}^2 cannot be used.
 - due to multicollinearity cannot identify best model, just one of many good models.
 - cannot use regular statistical inference on training set
- Solutions
 - ► Forward stepwise, ridge, lasso, PCA are useful in training
 - Evaluate models using cross-validation or independent test data
 - * using e.g. MSE or R^2 .

4. Nonlinear Models

Basis function models

- 1. polynomial regression
- 2. step functions
- ► 3. regression splines
- 4. smoothing splines, B-splines, …
- ▶ 5. wavelets
- polynomial is global while the others break range of x into pieces.

Other methods

- local polynomial regression
- generalized additive models
- neural networks.

Neural Networks

- Neural network is a very rich parametric model for $f(\mathbf{x})$
 - only parameters need to be estimated
 - as usual guard against overfitting.
- Consider a neural network with two layers
 - Y depends on $m \mathbf{Z}'s$ (a hidden layer) that depend on $p \mathbf{X}'s$.

$$Z_{1} = g(\alpha_{01} + \mathbf{X}'\alpha_{1}) \qquad \text{e.g. } g(v) = 1/(1 + e^{-v})$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$Z_{m} = g(\alpha_{0m} + \mathbf{X}'\alpha_{m})$$

$$T = \beta_{0} + \sum_{m=1}^{M} \beta_{m}Z_{m}$$

$$f(\mathbf{X}) = h(T) \qquad \text{usually } h(T) = T$$

 \bullet So with above $g(\cdot)$ and $h(\cdot)$

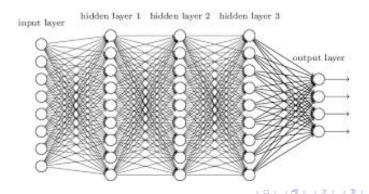
$$f(\mathbf{x}_i) = \beta_0 + \sum_{m=1}^M \beta_m \times \frac{1}{1 + \exp(-\alpha_{0m} - \mathbf{x}_i' \alpha_m)}$$

• We need to find the number M of hidden units and estimate the $\alpha's$.

Neural Networks (continued)

- Minimize the sum of squared residuals but need a penalty on α's to avoid overfitting.
 - Since penalty is introduced standardize x's to (0,1).
 - Best to have too many hidden units and then avoid overfit using penalty.
- Neural nets are good for prediction
 - especially in speech recognition, image recognition, ...
 - but very difficult (impossible) to interpret.
- Deep learning uses nonlinear transformations such as neural networks
 - deep nets are an improvement on original neural networks
 - e.g. led to great improvement of Google Translate.

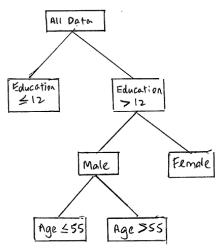
- Off-the-shelf software
 - 1. converts e.g. image or text to y and x to data input
 - 2. runs the deep net using stochastic gradient descent
 - ▶ e.g. CNTK (Microsoft), or Tensorflow (Google) or mxnet
- Inference: neural net gives in-sample $\widehat{y}_i = \psi_i(\mathbf{x}_i)'\widehat{oldsymbol{eta}}$
 - so out-of-sample OLS regress y_i on $\psi_i(\mathbf{x})$ gives $\widetilde{\boldsymbol{\beta}}$ and se $(\widetilde{\boldsymbol{\beta}})$.



5. Regression Trees

- Regression Trees sequentially split regressors x into regions that best predict y
 - e.g., first split is education < or > 12and second split is on gender for education > 12and third split is on age ≤ 55 or > 55 for male with education > 12and could then re-split on education
- Then $\hat{y}_i = \bar{y}_{R_i}$ is the average of y's in the region that \mathbf{x}_i falls in
 - with J blocks RSS $= \sum_{j=1}^{J} \sum_{i \in R_j} (y_i \bar{y}_{R_j})^2$.
- Need to determine both the regressor *j* to split and the split point *s*.
 - Each split is the one that reduces RSS the most.
 - Stop when e.g. less than five observations in each region.

• Example: annual earnings y depend on education, gender, age,



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Bagging, Random Forests and Boosting

- Trees do not predict well due to high variance
 - e.g. split data in two then can get quite different trees
 - e.g. first split determines future splits.
 - called a greedy algorithm as does not consider future splits.
- Bagging (bootstrap averaging) computes regression trees
 - for many different samples obtained by bootstrap
 - then average predictions across the trees.
- **Random forests** use only a subset of the predictors in each bootstrap sample
- Boosting grows tree using information from previously grown trees
 - and is fit on a modified version of the original data set
- Bagging and boosting are general methods (not just for trees).

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6. Classification Methods

- y's are now categorical (e.g. binary if two categories).
- Use (0,1) loss function
 - 0 if correct classification and 1 if missclassified.
- Methods
 - Iogistic regression, multinomial regression, k nearest neighbors
 - linear and quadratic discriminant analysis
 - support vector classifiers and support vector machines

7. Unsupervised Learning

- Challenging area: no y, only X.
- Principal components analysis.
- Clustering Methods
 - k means clustering.
 - hierarchical clustering.

8. Causal Inference with Machine Learning

- Focus on **causal estimation** of a key parameter, such as an average marginal effect, after controlling for confounding factors.
- For models with selection on observables (unconfoundedness)
 - e.g. regression with controls or propensity score matches
 - good controls makes this assumption more reasonable
 - so use only use machine learning methods (notably lasso) to select best controls.
- And for instrumental variables estimation with many possible instruments
 - using a few instruments avoids many instruments problem
 - use machine learning methods (notably lasso) to select best instruments
- But valid statistical inference needs to control for this data mining
 - currently active area of econometrics research.

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 Commercial example is online website predicting quantity demand change from price change.

•
$$q(p) = f(p) + e(p)$$
 where $e(p)$ is error

- naive machine learners will fit f(p) well
- but dq(p)/dp = df(p)/dp + de(p)/dp
- Suppose $y = g(x) + \varepsilon$ where x is endogenous
 - there are instruments $E[\varepsilon|z] = 0$.
 - then $\pi(z) = E[y|z] = E[g(x)|z] = \int_{\mathcal{A}} g(x) dF(x|z)$
 - use machine learner to get $\widehat{\pi}(z)$ and $\widehat{F}(x|z)$
 - then solve the above integral equation
- Easier for economists to use off-the-shelf machine learners
 - than for machine learners to learn methods for endogeneity.

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9. Big Data

- Hal Varian (2014), "Big Data: New Tricks for Econometrics", JEP, Spring, 3-28.
- Tools for handling big data
 - file system for files split into large blocks across computers
 - ★ Google file system (Google), Hadoop file system
 - database management system to handle large amounts of data across many computers
 - ★ Bigtable (Google), Cassandra
 - accessing and manipulating big data sets across many computers
 - ★ MapReduce (Google), Hadoop.
 - Ianguage for Mapreduce / Hadoop
 - ★ Sawzall (Google), Pig
 - Computer language for parallel processing
 - ★ Go (Google open source)
 - simplified structured query language (SQL) for data enquiries
 - ★ Dremel, Big Query (Google), Hive, Drill, Impala.

10. Conclusion

- Machine learning focuses on prediction
 - guarding for overfitting using validation or AIC/BIC.
- Supervised learning predicts y given x
 - ▶ usual regression minimizes MSE = bias² + variance
 - classification minimizes (0,1) loss function.
- Most popular machine learning method
 - deep neural nets.
- Economists / econometricians adapt to causal inference using
 - LASSO
 - Random forests.

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11. Book References

- http://cameron.econ.ucdavis.edu/e240f/machinelearning.html
- Next two books I used have free pdf and \$25 softback.
- Undergraduate / Masters level book
 - Gareth James, Daniela Witten, Trevor Hastie and Robert Tibsharani (2013), An Introduction to Statistical Learning: with Applications in R, Springer.
- Masters / PhD level book
 - Trevor Hastie, Robert Tibsharani and Jerome Friedman (2009), The Elements of Statistical Learning: Data Mining, Inference and Prediction, Springer.
- A recent book
 - Bradley Efron and Trevor Hastie (2016), Computer Age Statistical Inference: Algorithms, Evidence and Data Science, Cambridge University Press.
- Interesting general audience book is Cathy O'Neil, Weapons of Math Destruction: *How Big Data Increases Inequality and Threatens*

Democracy. A. Colin Cameron Univ. of California- Davis

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Simpler Articles

- Hal Varian (2014), "Big Data: New Tricks for Econometrics", *Journal* of *Economic Perspectives*, Spring, 3-28.
- Sendhil Mullainathan and J. Spiess (2017), "Machine Learning: An Applied Econometric Approach", *Journal of Economic Perspectives*, Spring, pp. 87-106.
- A. Belloni, V. Chernozhukov and C. Hansen (2014), "High-Dimensional Methods and Inference on Treatment and Structural Effects in Economics," *Journal of Economic Perspectives* Spring, pp.29-50.
- Following are leaders in causal econometrics and machine learning
 - ► Victor Chernozhukov, Alex Belloni, Christian Hansen + coauthors
 - ★ use Lasso a lot.
 - SusanAthey and Guido Imbens
 - ★ use random forests a lot.

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