Three Algorithms: go-to tools in the tooboox

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GR5069
Topics in Applied Data Science
for Social Scientists

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Three Algorithms

- On a day-to-day basis, you'll commonly use just a few algorithms that help with 80% of your needs:

  1. **OLS**
  2. **logistic regression**
  3. **random forest**

- useful for both **inferential** and **predictive** purposes

Algorithm I: OLS

Three Algorithms

Algorithm 1: OLS (inferential)

- what is a regression?

$$E[Y|\mathbf{X}] = f(\mathbf{X})$$

- where $f(\mathbf{X})$ is a conditional mean function, such that

$$Y = E[Y|\mathbf{X}] + \epsilon$$

- empirically: what do we get from a regression?

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Algorithm 1: OLS (inferential)

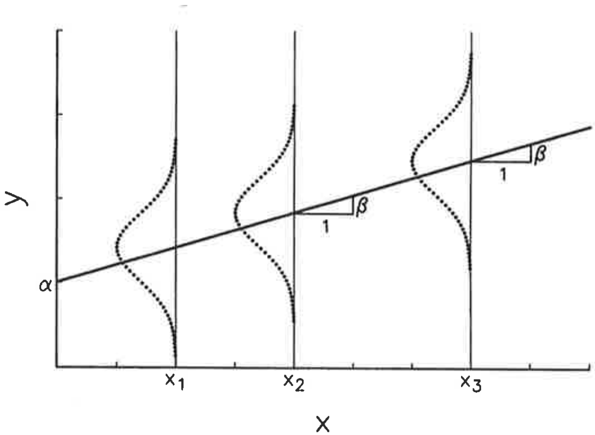

Figure 2.1. Simple Linear Regression Model With the Distribution of y Given x

Figure: Long (1997)

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Algorithm 1: OLS (inferential) - Gauss-Markov refresher

1. **linear relationship between parameters**

$$E[Y|\mathbf{X}] = \beta_1 f_1(\dots) + \beta_2 f_2(\dots) + \dots \beta_k f_k(\dots) + \epsilon$$

   - problem?

2. **No <u>linear</u> dependencies in $\mathbf{X}$**

   - problem?

3. **Zero conditional mean of ϵ**

$$E(\epsilon|\mathbf{X}) = 0, \quad Cov(\mathbf{X}, \epsilon) = 0$$

   - problem?

4. **Spherical errors: conditional homoscedasticity & no autocorrelation**

$$Var(\epsilon|\mathbf{X}) = \sigma_\epsilon^2 \mathbf{I}$$

   - problem?

Three Algorithms

Algorithm 1: OLS (inferential)

- suppose we need to better understand dynamics in `organized_crime_dead` and use available data
  - could we extract some causal insights from this data?
  - what could we learn from an OLS algorithm?
- remember: OLS works through a conditional mean function...
  - what does this mean in practice?
  - how generalizable is what we find?

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Algorithm 1: OLS (inferential)

```
Call:
lm(formula = organized_crime_dead ~ organized_crime_wounded +
    afi + army + navy + federal_police + long_guns_seized + small_arms_seized +
    clips_seized + cartridge_seized, data = AllData)

Residuals:
     Min       1Q   Median       3Q      Max
-11.6058  -0.7274  -0.4506   0.2192  27.3262

Coefficients:
                          Estimate Std. Error t value Pr(>|t|)
(Intercept)              0.4505553  0.0332307  13.558  < 2e-16 ***
organized_crime_wounded  0.3736900  0.0239171  15.624  < 2e-16 ***
afi                     -0.2261752  0.4210396  -0.537   0.5912
army                     0.3066898  0.0532594   5.758 8.96e-09 ***
navy                     0.7150402  0.1389449   5.146 2.75e-07 ***
federal_police          -0.1271515  0.0773309  -1.644   0.1002
long_guns_seized         0.1478424  0.0085972  17.197  < 2e-16 ***
small_arms_seized       -0.0437447  0.0184592  -2.370   0.0178 *
clips_seized             0.0004374  0.0003152   1.388   0.1653
cartridge_seized        -0.0001690  0.0000193  -8.760  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1  ' ' 1

Residual standard error: 1.731 on 5386 degrees of freedom
Multiple R-squared:  0.1413,Adjusted R-squared:  0.1398
F-statistic: 98.44 on 9 and 5386 DF,  p-value: < 2.2e-16
```

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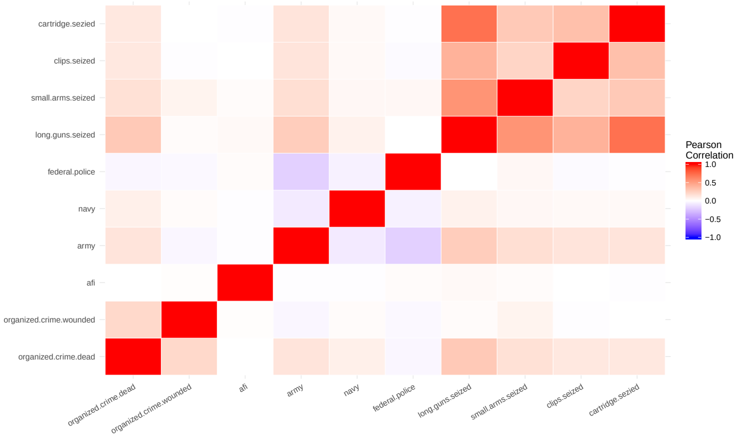
Algorithm 1: OLS (inferential)

- are these "real" results, or just a mirage from reiterated information in our variables?



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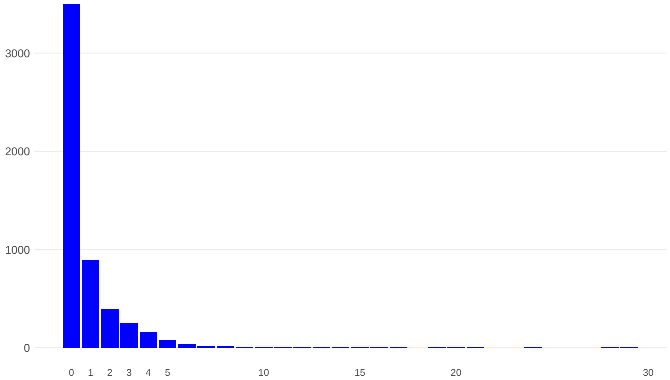
Algorithm 1: OLS (inferential)

- but wait... what does my DV look like?



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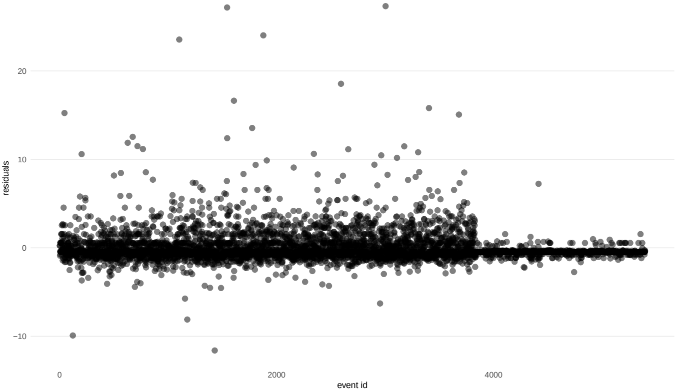
Algorithm 1: OLS (inferential)

- what's the problem with this?



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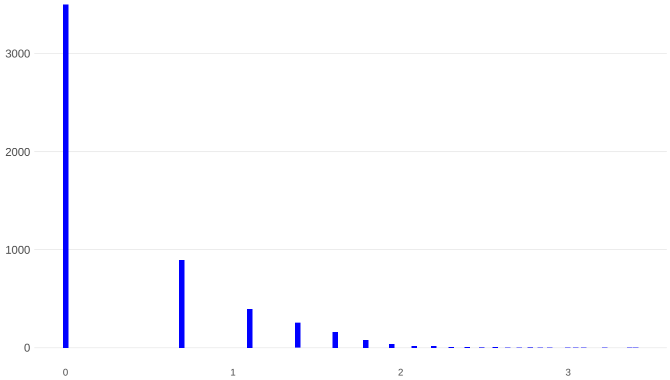
Algorithm 1: OLS (inferential)

- we can always log it, right?... think again



Three Algorithms

Algorithm 1: OLS (predictive)

- if Gauss-Markov assumptions are fulfilled, OLS produces the **B**est **L**inear **U**nbiased **E**stimator...
  - which is great for inference... but...
- remember the Hastie et al. (2009) equation?

$$EPE = Var(Y) + Bias^2 + Var(\hat{f}(x))$$

- OLS has little bias ($Bias^2$) but high variance ($Var(\hat{f}(x))$)
  - typically high variance is bad for prediction
  - we may need a tradeoff that increases bias - and reduces variance - to improve prediction

Three Algorithms

Algorithm 1: OLS (predictive)

- most important characteristic of a predictive model: **generalization**
- **objective**: optimize bias-variance **tradeoff** to **improve predictons**
- **model selection methods**: constrain [number/estimates] of parameters $k \in \{0, 1, 2, \ldots, p\}$ to minimize expected prediction error
  1. **best subset** (analytical solution criteria))
  2. **(forward-backward) stepwise selection** (analytical solution criteria))
  3. **cross-validation** (cross-validation prediction error)
  4. **shrinkage** (analytical solution criteria)
- we'll review examples of 1 and 3

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Algorithm 1: OLS (predictive)

- **best subset** methods search for the minimal optimal combination of variables that minimize expected prediction error
- rely on analytical solution criteria to select the “best” subset

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Algorithm 1: OLS (predictive)

Best Subset selection using AIC

```
##
## Call:
## lm(formula = y ~ ., data = data.frame(Xy[, c(bestset[-1], FALSE),
##     drop = FALSE], y = y))
##
## Coefficients:
##             (Intercept)  organized_crime_wounded          long_guns_seized
##               0.4498740                0.3730898                 0.1500302
##       small_arms_seized         cartridge_sezied                      army
##              -0.0434190               -0.0001668                 0.3097144
##          federal_police                     navy
##              -0.1296465                0.7166220
```

Best Subset selection using BIC

```
##
## Call:
## lm(formula = y ~ ., data = data.frame(Xy[, c(bestset[-1], FALSE),
##     drop = FALSE], y = y))
##
## Coefficients:
##             (Intercept)  organized_crime_wounded          long_guns_seized
##               0.4237166                0.3713140                 0.1389487
##        cartridge_sezied                     army                      navy
##              -0.0001567                0.3263833                 0.7347481
```

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Algorithm 1: OLS (predictive)

- **cross validation methods** split the training data into K folds, training on all but the kth fold and validating on the kth part

1	2	3	4	5
Train	Train	Validation	Train	Train

- the process iterates over $k = 1, \ldots, K$
- an additional algorithm is used to evaluate models with parameter p combinations
- the optimal number of parameters p is selected with the one-std deviation rule

Three Algorithms

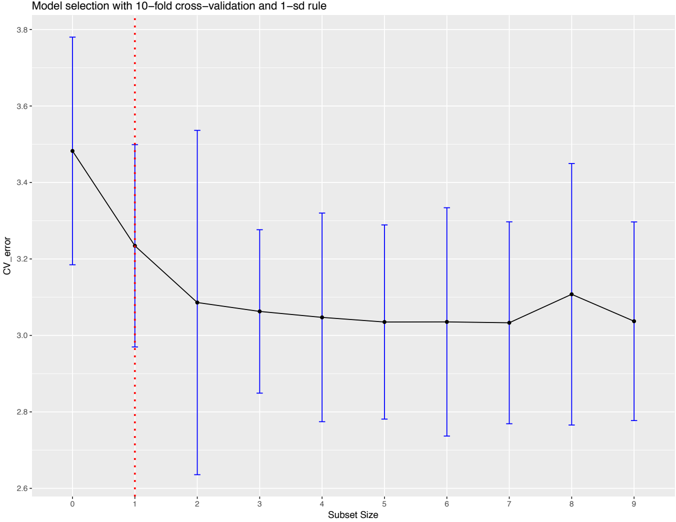
Algorithm 1: OLS (predictive)

A model with 10-fold cross-validation

```
##
## Call:
## lm(formula = y ~ ., data = data.frame(Xy[, c(bestset[-1], FALSE),
##     drop = FALSE], y = y))
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -15.4137  -0.6698  -0.6698   0.3302  27.6742
##
## Coefficients:
##                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)      0.669800   0.025822   25.94   <2e-16 ***
## long_guns_seized 0.109332   0.005091   21.47   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.791 on 5394 degrees of freedom
## Multiple R-squared:  0.07876,    Adjusted R-squared:  0.07859
## F-statistic: 461.2 on 1 and 5394 DF,  p-value: < 2.2e-16
```

Three Algorithms

Algorithm 1: OLS (predictive)



Algorithm II: Logistic Regression

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Algorithm 2: logistic regression (inferential)

- different question: **did something happen or not?**
  - essentially, binary outcome classification
  - why not just use OLS?
- one way to think about this: let y^* be a continuous (latent) variable

$$y^* = x\beta + \epsilon$$

- for which we only observe two outcomes

$$y_i = \begin{cases} 1 & \mathit{if} \quad y_i^* > \tau \\ 0 & \mathit{if} \quad y_i^* \leq \tau \end{cases}$$

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Algorithm 2: logistic regression (inferential)

- we're interested in the probability that $y = 1$

$$\pi_i = Pr(y = 1) = F(\beta x)$$

- in the case of a logit, we estimate

$$\pi_i = \Lambda(\beta x) = \frac{e^{\beta x}}{1 + e^{\beta x}}$$

- but there's also additional "flavors" (i.e. probit)

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Algorithm 2: logistic regression (inferential) - Assumptions

1. **linear relationship between parameters**

$$\pi_i = F(\beta_1 f_1(\dots) + \beta_2 f_2(\dots) + \dots \beta_k f_k(\dots) + \epsilon_i)$$

   - problem?

2. **no linear dependencies in $\mathbf{X}$**
   - problem?

3. **no autocorrelation**

$$Cov(\epsilon_i, \epsilon_j) = 0; \;\; \forall\, i \neq j$$

   - problem?

4. **a balanced sample in Y**
   - problem?

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Algorithm 2: logistic regression (inferential)

- going back to our example:
  - we have a natural dual category: **events with deaths / no deaths**
  - **could we learn something about correlates to events with organized crime deaths?**
    - we have information on federal forces involved
    - also on materiel seizures
  - **can this relationship ever be causal?**

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Algorithm 2: logistic regression (inferential)

```
Call:
glm(formula = organized_crime_death ~ organized_crime_wounded +
    afi + army + navy + federal_police + long_guns_seized + small_arms_seized +
    clips_seized + cartridge_sezied, family = binomial(link = "logit"),
    data = AllData)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-4.5396  -0.6657  -0.4731  -0.4592   2.7612

Coefficients:
                          Estimate Std. Error z value Pr(>|z|)
(Intercept)             -2.1337831  0.0599578 -35.588  < 2e-16 ***
organized_crime_wounded  0.2839835  0.0376519   7.542 4.62e-14 ***
afi                     -0.6960636  0.7234004  -0.962    0.336
army                     0.7395036  0.0812191   9.105  < 2e-16 ***
navy                     0.9292565  0.1827726   5.084 3.69e-07 ***
federal_police          -0.0628413  0.1331772  -0.472    0.637
long_guns_seized         0.1544432  0.0141145  10.942  < 2e-16 ***
small_arms_seized       -0.0137429  0.0271923  -0.505    0.613
clips_seized            -0.0004430  0.0004284  -1.034    0.301
cartridge_sezied        -0.0002413  0.0000510  -4.730 2.25e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 5185.2  on 5395  degrees of freedom
Residual deviance: 4721.3  on 5386  degrees of freedom
AIC: 4741.3
```

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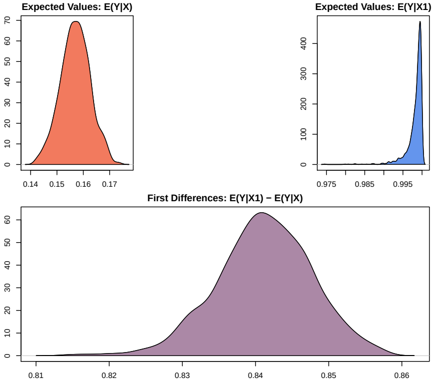
Algorithm 2: logistic regression (inferential)

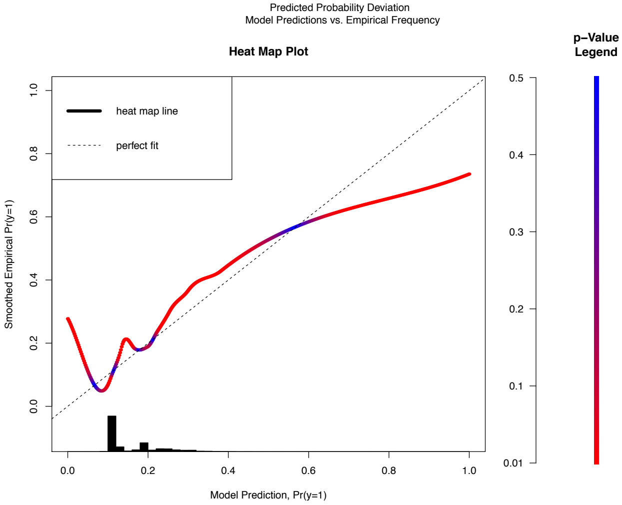
- change in probablity between `organized_crime_wounded == 0` (X) and `organized_crime_wounded == 30` (X1)



Three Algorithms

Algorithm 2: logistic regression (inferential)

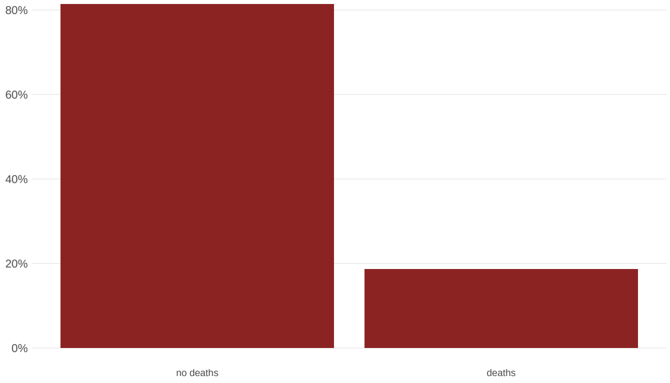
- but this model has a terrible fit!



Three Algorithms

Algorithm 2: logistic regression (inferential)

- but wait again, what does my DV look like?



- what does your "plain vanilla" logistic regression assume?

Three Algorithms

Algorithm 2: logistic regression (predictive)

Best Subset Selection (AIC)

```
##
## Call:  glm(formula = y ~ ., family = family, data = Xi, weights = weights)
##
## Coefficients:
##             (Intercept)  organized_crime_wounded          long_guns_seized
##              -2.1465619                0.2831332                 0.1479253
##       cartridge_sezied                     army                      navy
##              -0.0002407                0.7477216                 0.9415283
##
## Degrees of Freedom: 5395 Total (i.e. Null);  5390 Residual
## Null Deviance:       5185
## Residual Deviance: 4724  AIC: 4736
```

Best Subset Selection (BIC)

```
##
## Call:  glm(formula = y ~ ., family = family, data = Xi, weights = weights)
##
## Coefficients:
##             (Intercept)  organized_crime_wounded         long_guns_seized
##              -2.1465619                0.2831332                0.1479253
##        cartridge_sezied                     army                     navy
##              -0.0002407                0.7477216                0.9415283
##
## Degrees of Freedom: 5395 Total (i.e. Null);  5390 Residual
## Null Deviance:       5185
## Residual Deviance: 4724  AIC: 4736
```

10-fold cross-validation

```
##
## Call:
## glm(formula = y ~ ., family = family, data = data.frame(Xy[,
##     c(bestset[-1], FALSE), drop = FALSE], y = y))
##
## Deviance Residuals:
##    Min       1Q   Median       3Q      Max
## -5.339  -0.690  -0.514  -0.514   2.044
##
## Coefficients:
##                   Estimate Std. Error z value Pr(>|z|)
## (Intercept)      -1.957360   0.050712 -38.598   <2e-16 ***
## long_guns_seized  0.108097   0.009482  11.400   <2e-16 ***
## army              0.643469   0.076039   8.462   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 5185.2  on 5395  degrees of freedom
## Residual deviance: 4859.9  on 5393  degrees of freedom
## AIC: 4865.9
##
## Number of Fisher Scoring iterations: 4
```

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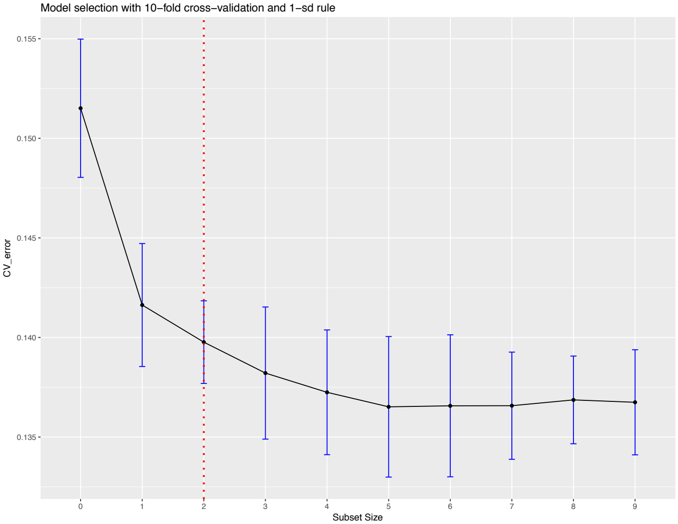
Algorithm 2: logistic regression (inferential)

10-fold cross-validation



Algorithm II:
Random Forests

Three Algorithms

Algorithm 3: random forests (predictive)

- we can also go down a different path for classification or prediction
  - gaining insight into non-linear relationships (and enhanced predictive power) at cost of interpretability
- popular choice: **random forests**
- simple but powerful algorithm: averages over trees with random selection of features

$$\hat{f}_{rf}^{B}(x) = \frac{1}{B}\sum_{b=1}^{B} T(x;\Theta_b)$$

the Random Forest algorithm (per Hastie et al. 2009, p. 588)

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 $\{T_b\}_1^B$.

Three Algorithms

Algorithm 3: random forests (predictive)

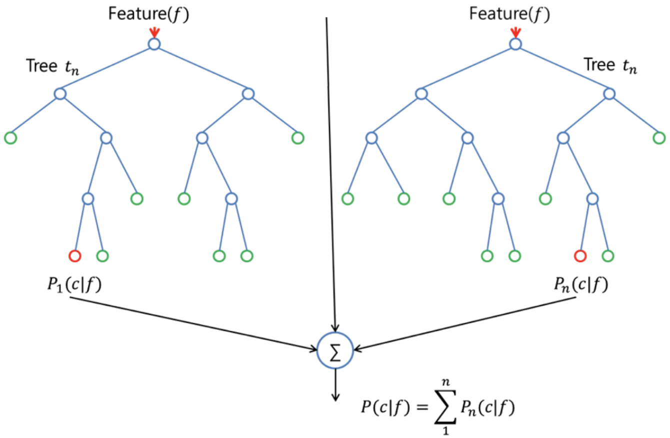


Figure: Donges (2018)

Three Algorithms

Algorithm 3: random forests (predictive)

- to generate **predictions:**
  1. **classification**
     - obtain a class “vote” from each tree
     - classifies by “majority vote”
  2. **regression**
     - predictions from each tree averaged for a point prediction
- **variable importance** measure variable contributions to split-criterion to minimize prediction error

Three Algorithms

Algorithm 3: random forests (predictive)

- **Assumptions:**
  - no distributional assumptions
  - does not assume a linear relationship in parameters
- **Advantages:**
  - work for regression and classification problems
  - use categorical features (variables)“naturally”
  - detect “important” variables and select them
  - handle non-linear interactions and boundaries
  - performs cross-validation on the fly
  - (under certain conditions) not too prone to overfitting

Three Algorithms

Algorithm 3: random forests

- going back to our example:
  - **could we learn something about predictors of organized crime deaths?**
    - we have information on a number of predictors
    - perhaps thinking of this problem as trees may help

Our estimated random forests model

```
Call:
 randomForest(formula = organized_crime_dead ~ organized_crime_wounded +
                                afi + army + navy + federal_police +
                                long_guns_seized + small_arms_seized +
                                clips_seized + cartridge_sezied,
                                data = training, method = "rf",
                                importance = TRUE,
                                prox = TRUE,
                                preProc = c("center", "scale"))
               Type of random forest: regression
                     Number of trees: 500
No. of variables tried at each split: 3

          Mean of squared residuals: 3.275263
                    % Var explained: 11.8
```

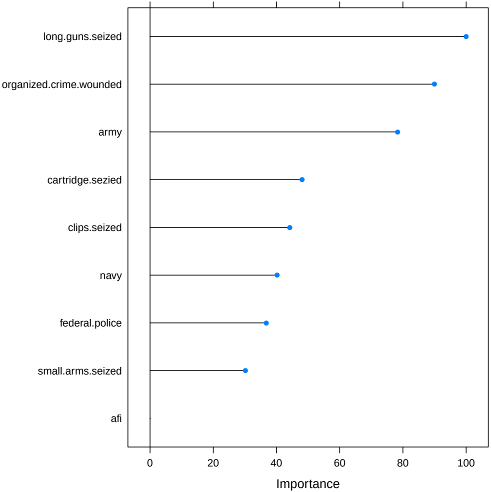
10-fold cross-validation confirms that using nearly all nine predictors produces the least error

```
       9        8        7        6        5        4        3        2        1
3.270985 3.219273 3.231779 3.244063 3.271915 3.446298 3.377251 3.483434 3.485249
```

Three Algorithms

Algorithm 3: random forests

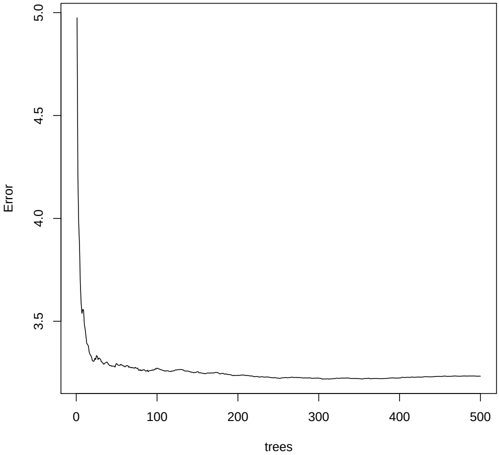
- what does variance importance tell us?



Three Algorithms

Algorithm 3: random forests

- a quick look at MSE for this model by number of trees



Three Algorithms

What did we learn from these algorithms?

- if our **inferential models** were correctly specified
- the number of organized crime deaths (**OLS**) and the likelihood of observing a death among organized crime members (**logistic regression**) tend to be higher in events where:
  - the **navy** or **army** participate
  - **organized crime wounded** exist
  - **long guns** and **catridges** are seized

Three Algorithms

What did we learn from these algorithms?

- the best **predictors** of the number of organized crime deaths (**OLS**) are:
  - the number of **organized crime wounded**, the participation of armed forces (**army**, **navy**, **federal police**), and the seizure of **long guns**, **small arms** and **cartridges** (AIC)
  - the number of **organized crime wounded**, the participation of **army** and **navy**, and the seizure of **long guns** and **cartridges** (BIC)
  - the number of **long guns seized** (cross-validation)
- the best **predictors** of the existence of at least one organized crime death (**logistic regression**) are:
  - the number of **organized crime wounded**, the participation of **army** or **navy**, and the seizure of **long guns** or **cartridges** (AIC, BIC)
  - the participation of the **army** and the seizure of **long guns** (cross-validation)

Three Algorithms

What did we learn from these algorithms?

- the best **predictors** of the number of deaths among organized crime (**random forests**) are:
  - the presence of seized **long guns**, **organized crime wounded**, and the participation of the **army**

Weekly Progress Review

Three Algorithms: go-to tools in the tooolboox

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GR5069
Topics in Applied Data Science
for Social Scientists

Spring 2018
Columbia University