Kinds of Ensemble

Tested on apple quality dataset

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Apple quality dataset

Variables

- `Size`
- `Weight`
- `Sweetness`
- `Crunchiness`
- `Juiciness`
- `Ripeness`
- `Acidity`

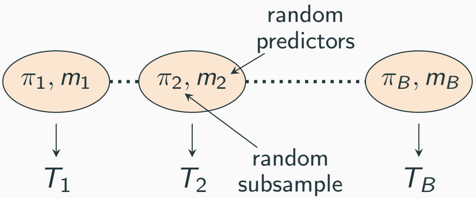
Binary classification task

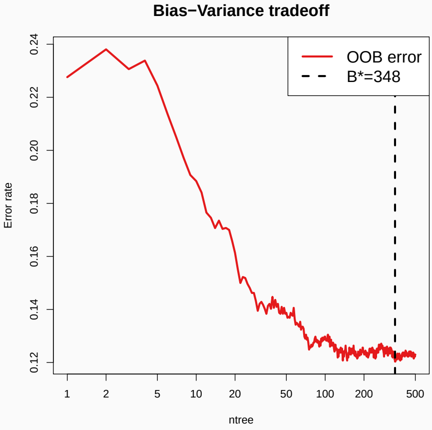
Class distribution: 0.49 – 0.51

Methods

- kNN, Decision tree
- Random forest
- AdaBoost
- Super Learner

Random forest

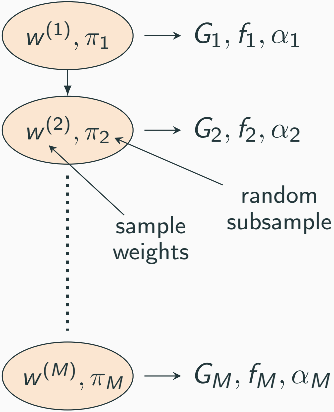




$$G(x) = \arg\max_k \sum_{b=1}^{B} \mathbb{I}(T_b(x) = k)$$

$$\texttt{mtry} = \lfloor \sqrt{p} \rfloor$$

AdaBoost algorithm



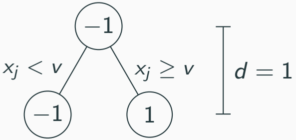
$$f_m(x) = f_{m-1}(x) + \lambda \alpha_m G_m(x)$$

$$G(x) = \text{sign}(f_M(x))$$

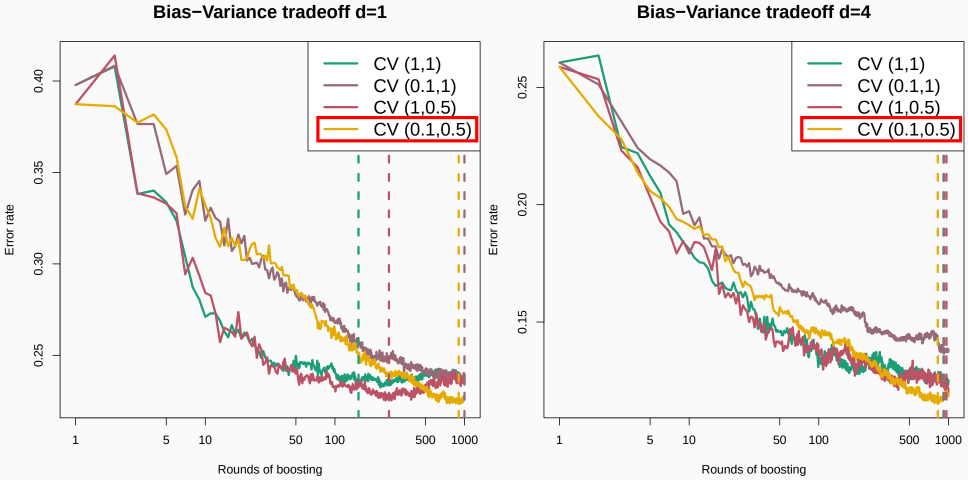
$$L(y, f(x)) = \exp(-yf(x))$$

Encoding $\mathcal{Y} \in \{-1, 1\}$

```
ada::ada(x, y,
  loss="exponential",
  type="discrete",
  iter ← M*, nu ← λ*,
  bag.frac ← π*,
  control=base.learner)
```

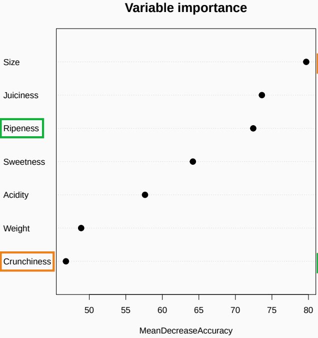


AdaBoost tuning

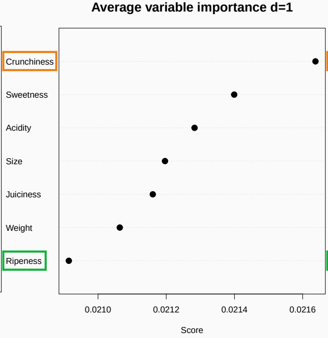


Variable importance comparison

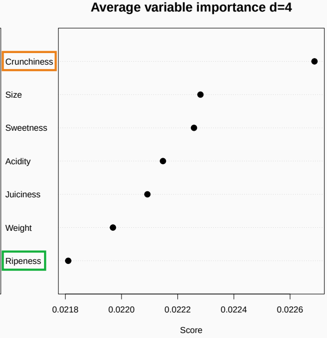
Random Forest



AdaBoost$_{d=1}$



AdaBoost$_{d=4}$



Super Learner flow diagram

$$\hat{\alpha} = \arg\min_\alpha \sum_{i=1}^N L(Y_i, m(z_i|\alpha))$$

$$m(z|\alpha) = \sum_{k=1}^K \alpha_k \hat{\varphi}_{k,T(\nu)}(\boldsymbol{X}_{V(\nu)})$$

strong learners
on full $\mathcal{D}$, $\hat{\varphi}_k(\boldsymbol{X})$

$\boxed{\hat{\varphi}_1, \hat{\varphi}_2, \ldots, \hat{\varphi}_K}$

learners
prediction

$$\mathcal{D} = \{(x_i, y_i)\}_1^N$$

$$\hat{\varphi}_{\text{SL}} = \sum_{k=1}^K \hat{\alpha}_k \hat{\varphi}_k$$

prediction
weights

cross-validation
$\hat{\varphi}_{k,T(\nu)}(\boldsymbol{X}_{V(\nu)})$

$\hat{\varphi}_1$	$\hat{\varphi}_2$	$\ldots$	$\hat{\varphi}_K$	Y
1	1	$\ldots$	1	1
2	2	$\ldots$	2	2
$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
V	V	$\ldots$	V	V

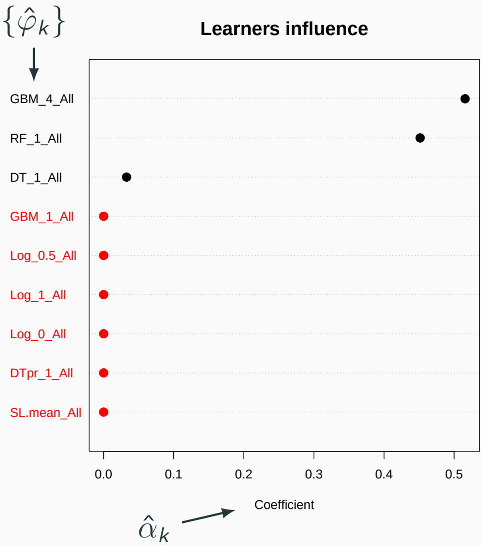
Super Learner in practice

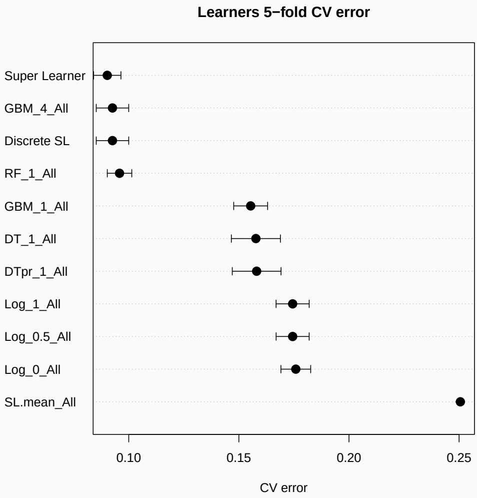
```
SuperLearner(Y, X,
  family=binomial(),
  cluster,
  SL.library ← {φ_k},
  cvControl=list(
    V=10,shuffle=FALSE))

CV.SuperLearner(...)
```

What's in the ensemble?

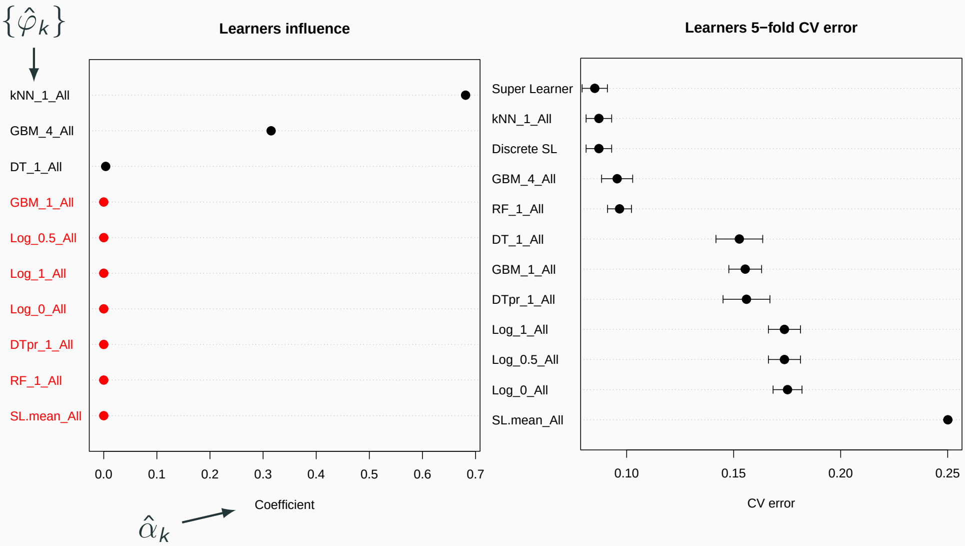
- Response variable mean $\bar{y}$
- Logistic Regression with $\alpha = 0,\ 1$ and 0.5
- Grown and pruned Decision Tree
- Random Forest
- Gradient Boosting Machine with $d = 1$ and $d = 4$
- kNN

Super Learner CV error (reduced, w/out kNN)





Super Learner CV error (full)



Performance

Model	Train score	Test score
kNN	0.9029	0.8950
CART	0.8841	0.8290
Random Forest	0.8808	0.8890
AdaBoost$_{d=1}$	0.7983	0.7922
AdaBoost$_{d=4}$	0.9996	0.8845
Super Learner$_{\text{red}}$	0.9899	0.8785
Super Learner$_{\text{full}}$	0.9303	0.8897

Questions?

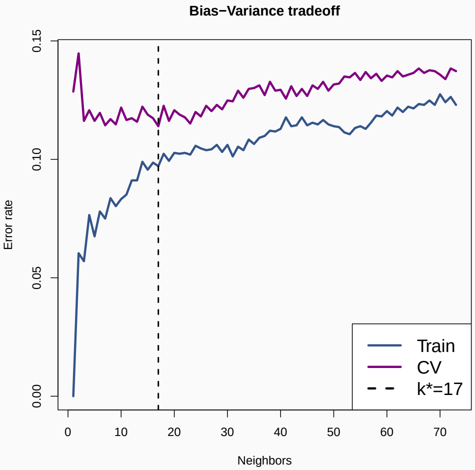
References i

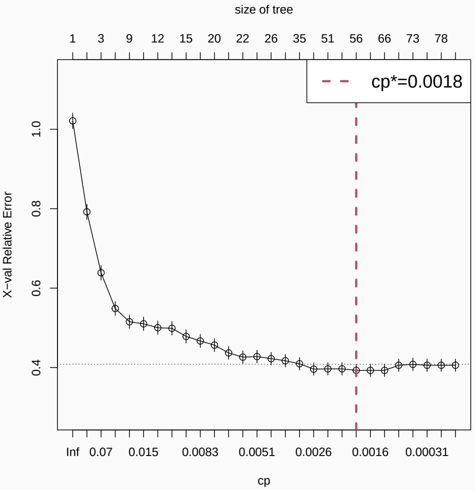
T. Hastie, R. Tibshirani, and J. H. Friedman
The Elements of Statistical Learning
Springer, 2009.

E. C. Polley, and M. J. van der Laan
Super Learner in Prediction
U.C. Berkeley Division of Biostatistics Working Paper Series. Working Paper 266, 2010

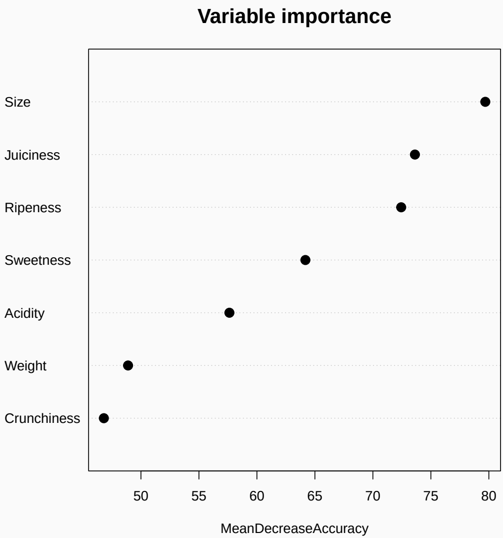
M. Culp, K. Johnson and G. Michailidis
`ada`: **The R Package Ada for Stochastic Boosting**
Journal of Statistical Software, 17(2), 1–27, 2006

*k*NN and CART tuning

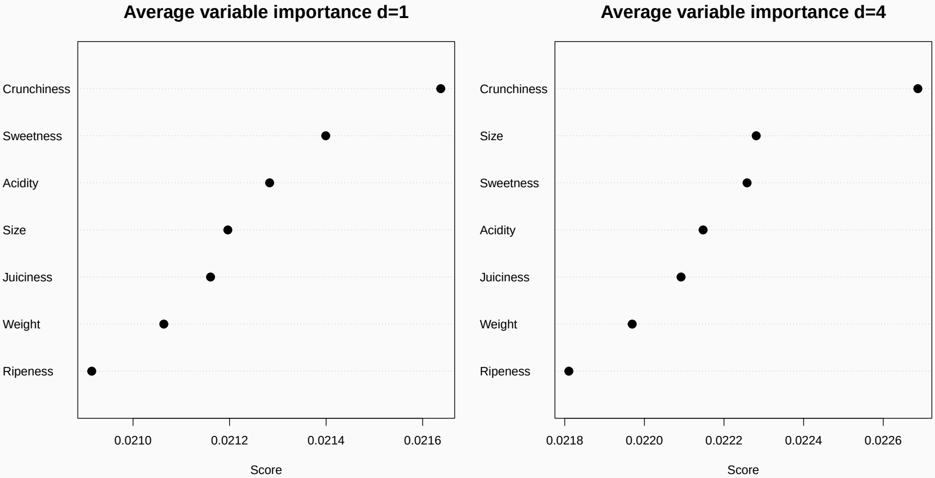




Random forest variable importance



AdaBoost variable importance



Discrete AdaBoost algorithm

Discrete AdaBoost with shrinkage and out-of-bag, as an additive model with prediction function $f_m(x)$

Input: M, $\{(x_i, y_i)\}_1^N$, $x_i \in \mathbb{R}^p$

Initialize $f_0(x) = 0$;

for $m = 1$ **to** M **do**

  Set $w_i^{(m)} = -\frac{\partial L(y,g)}{\partial g}\Big|_{g=f_m(x)}$ s.t. $\sum_{i=1}^N w_i^{(m)} = 1$;

  Fit classifier $G_m(x)$ using $w_i^{(m)}$ with samples from π_m;

  Weighted error rate $\mathrm{err}_m = \sum_{i=1}^N w_i^{(m)} \mathbb{I}(y_i \neq G(x_i))$;

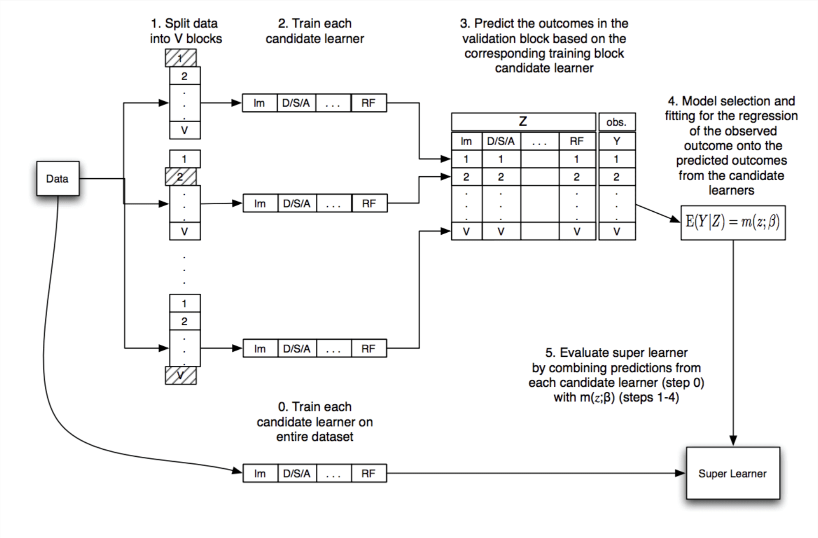
  Set $\alpha_m = \frac{1}{2} \log\left(\frac{1-\mathrm{err}_m}{\mathrm{err}_m}\right)$;

  Update $f_m(x) \leftarrow f_{m-1}(x) + \lambda \alpha_m G_m(x)$;

end

Output: $G(x) = \mathrm{sign}(f_M(x))$

Super Learner algorithm flow diagram



Input: $\mathcal{D} = \{(x_i, y_i)\}_1^N$, $\mathcal{L} = \{\varphi_k(X)\}_{k=1}^K$

foreach *strong learner in* $\mathcal{L}$ **do**

  Fit φ_k on $\mathcal{D} \Rightarrow \hat{\varphi}_k(\boldsymbol{X}) \rightarrow \hat{\mathcal{L}} = \{\hat{\varphi}_k\}_{k=1}^K$;

end

for $\nu = 1, 2, \ldots, V$ **do**

  foreach *strong learner in* $\mathcal{L}$ **do**

    Fit φ_k on $T(\nu)$, predict $\hat{\varphi}_{k,T(\nu)}(X_i \in V(\nu))$;

  end

end

Stack output in an $N \times K$ matrix $Z = \left\{\hat{\varphi}_{k,T(\nu)}\left(X_{V(\nu)}\right)\right\}$;

Propose a family of weighted combinations

$$m(z|\alpha) = \sum_{k=1}^{K} \alpha_k \hat{\varphi}_{k,T(\nu)}\left(\boldsymbol{X}_{V(\nu)}\right) \rightarrow \hat{\alpha} = \arg\min_{\alpha} \sum_{i=1}^{N} L(Y_i, m(z_i|\alpha))$$

of size N s.t. $\alpha_k \geq 0$, $\sum_k \alpha_k = 1$ and minimizes $\sum_k \alpha_k \hat{\varphi}_k$;

Combine $\hat{\alpha}$ with the library $\hat{\mathcal{L}} \rightarrow \hat{\varphi}_{\mathrm{SL}}(\boldsymbol{X}) = \sum_{k=1}^K \hat{\alpha}_k \hat{\varphi}_k(\boldsymbol{X})$;

Output: $\hat{\varphi}_{\mathrm{SL}}$