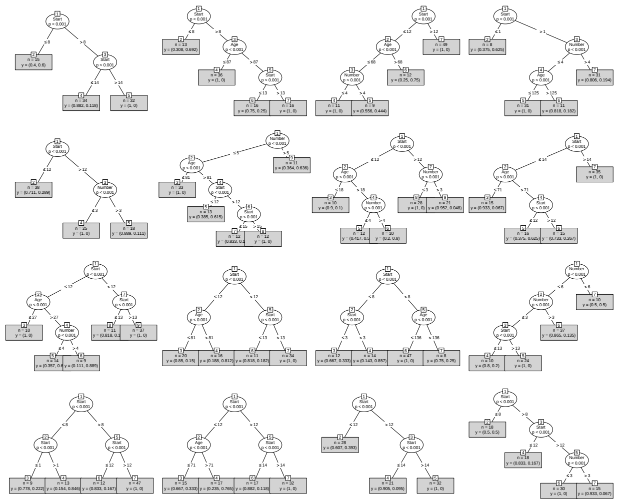
A Comparison of Different Variable Importance Measures

Carolin Strobl (LMU München)

Wien, Jänner 2009

Measuring variable importance in random forests



Measuring variable importance in random forests

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- Gini importance
  mean Gini gain produced by X_j over all trees
  (can be severely biased due to estimation bias and mutiple testing; Strobl et al., 2007)

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- Gini importance
  mean Gini gain produced by X_j over all trees
  (can be severely biased due to estimation bias and mutiple testing; Strobl et al., 2007)
- permutation importance
  mean decrease in classification accuracy after permuting X_j over all trees
  (unbiased when subsampling is used; Strobl et al., 2007)

The permutation importance

within each tree t

$$VI^{(t)}(\mathbf{x}_j) = \frac{\sum_{i \in \overline{\mathfrak{B}}^{(t)}} I\left(y_i = \hat{y}_i^{(t)}\right)}{\left|\overline{\mathfrak{B}}^{(t)}\right|} - \frac{\sum_{i \in \overline{\mathfrak{B}}^{(t)}} I\left(y_i = \hat{y}_{i,\pi_j}^{(t)}\right)}{\left|\overline{\mathfrak{B}}^{(t)}\right|}$$

$\hat{y}_i^{(t)} = f^{(t)}(\mathbf{x}_i)$ = predicted class before permuting

$\hat{y}_{i,\pi_j}^{(t)} = f^{(t)}(\mathbf{x}_{i,\pi_j})$ = predicted class after permuting X_j

$$\mathbf{x}_{i,\pi_j} = \left(x_{i,1}, \ldots, x_{i,j-1}, \; x_{\pi_j(i),j}, x_{i,j+1}, \ldots, x_{i,p}\right)$$

Note: $VI^{(t)}(\mathbf{x}_j) = 0$ by definition, if X_j is not in tree t

Variable importance in RF
Conditional variable importance in RF
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The permutation importance

over all trees:

$$VI(\mathbf{x}_j) = \frac{\sum_{t=1}^{ntree} VI^{(t)}(\mathbf{x}_j)}{ntree}$$

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What kind of independence corresponds to this kind of permutation?

obs	Y	X_j	Z
1	y_1	$x_{\pi_j(1),j}$	z_1
$\vdots$	$\vdots$	$\vdots$	$\vdots$
i	y_i	$x_{\pi_j(i),j}$	z_i
$\vdots$	$\vdots$	$\vdots$	$\vdots$
n	y_n	$x_{\pi_j(n),j}$	z_n

$$H_0 : X_j \perp Y, Z \text{ or } X_j \perp Y \wedge X_j \perp Z$$

$$P(Y, X_j, Z) \stackrel{H_0}{=} P(Y, Z) \cdot P(X_j)$$

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$\Rightarrow$ a high variable importance can result from violation of

either one!

Suggestion: Conditional permutation scheme

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obs	Y	X_j	Z
1	y_1	$x_{\pi_{j\|Z=a}(1),j}$	$z_1 = a$
3	y_3	$x_{\pi_{j\|Z=a}(3),j}$	$z_3 = a$
27	y_{27}	$x_{\pi_{j\|Z=a}(27),j}$	$z_{27} = a$
6	y_6	$x_{\pi_{j\|Z=b}(6),j}$	$z_6 = b$
14	y_{14}	$x_{\pi_{j\|Z=b}(14),j}$	$z_{14} = b$
33	y_{33}	$x_{\pi_{j\|Z=b}(33),j}$	$z_{33} = b$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

$$H_0 : X_j \perp Y | Z$$

$$\begin{aligned} & P(Y, X_j | Z) \stackrel{H_0}{=} P(Y|Z) \cdot P(X_j|Z) \\ \text{or} \quad & P(Y|X_j, Z) \stackrel{H_0}{=} P(Y|Z) \end{aligned}$$

Technically

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- use any partition of the feature space for conditioning

Technically

- use any partition of the feature space for conditioning
- here: use binary partition already learned by tree for each tree
  - determine variables to condition on (via `threshold`)
  - extract their cutpoints
  - generate partition using cutpoints as bisectors

Strobl et al. (2008)

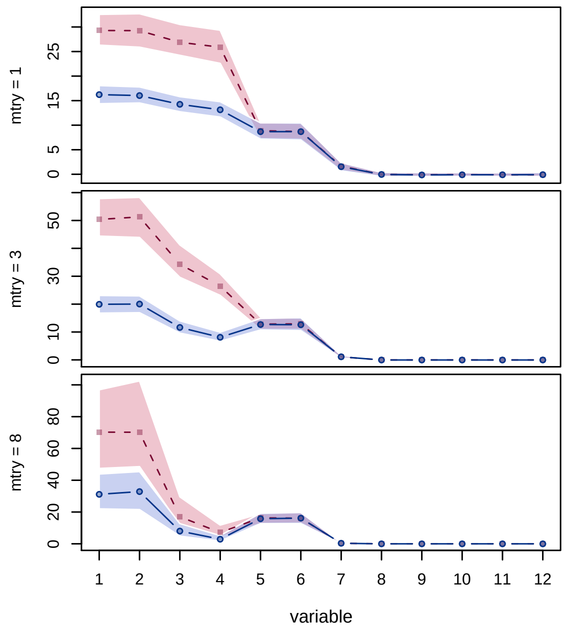
Toy example

spurious correlation between shoe size and reading skills in school-children

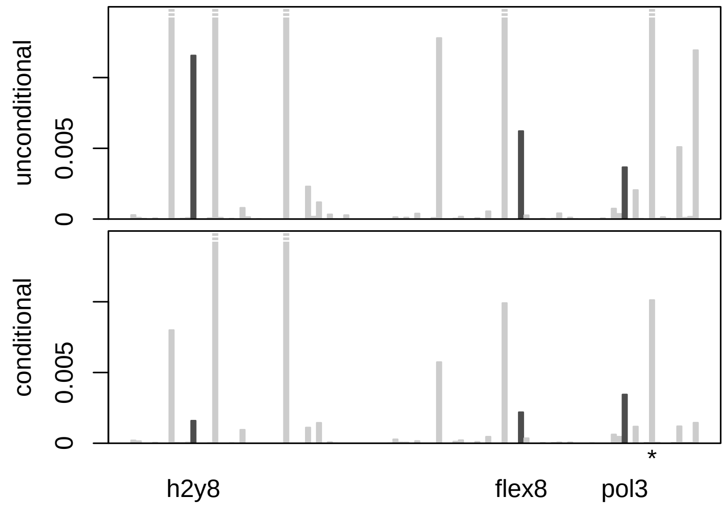
```
> mycf <- cforest(score ~ ., data = readingSkills,
+                 control = cforest_unbiased(mtry = 2))
> varimp(mycf)
nativeSpeaker          age      shoeSize
     12.62926     74.89542      20.01108
> varimp(mycf, conditional = TRUE)
nativeSpeaker          age      shoeSize
    11.808192    46.995336      2.092454
```

from `party 0.9-991`

Simulation results



Peptide-binding data



Other variable importance measures

- partial correlation, standardized beta
  conditional effect of X_j given all other variables
  in the model
- "averaging over orderings"
  - for linear models (`relaimpo`, Grömping, 2006)
    LMG Lindeman, Merenda, and Gold (1980),
    $\approx$ "dominance analysis" Azen and Budescu (2003)
    PMVD Feldman (2005)
  - for GLMs (`hier.part`, Walsh and Nally, 2008)
    "hierarchical partitioning" Chevan and Sutherland (1991)

  R^2 decomposition

Other variable importance measures

- random forest permutation importance
  $\approx$ "averaging over trees"
  unconditional varimp (`randomForest`, `party`, Breiman et al., 2006; Hothorn et al., 2008)
  conditional varimp (`party`, Hothorn et al., 0089)
- elastic net (`elasticnet`, `caret`, Zou and Hastie, 2008; Kuhn, 2008)
  grouping property: correlated predictors get similar (largest) score

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Desirable (?) properties

- *proper decomposition*: scores sum up to model R^2
- *non-negativity*
- *exclusion*: $\beta_j = 0 \Rightarrow \text{score} = 0$
- *inclusion*: $\beta_j \neq 0 \Rightarrow \text{score} \neq 0$

Grömping (2007)

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  all

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Simulation study

dgp: $y_i = \beta_1 \cdot x_{i,1} + \cdots + \beta_{12} \cdot x_{i,12} + \varepsilon_i,\ \varepsilon_i \overset{i.i.d.}{\sim} N(0,1)$
$X_1, \ldots, X_{12} \sim N(0, \Sigma)$

$$\Sigma = \begin{pmatrix} 1 & \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & 0 & \cdots & 0 \\ \mathbf{0.9} & 1 & \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & 0 & \cdots & 0 \\ \mathbf{0.9} & \mathbf{0.9} & 1 & \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & 0 & \cdots & 0 \\ \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & 1 & \mathbf{0.9} & \mathbf{0.9} & 0 & \cdots & 0 \\ \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & 1 & \mathbf{0.9} & 0 & \cdots & 0 \\ \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & \mathbf{0.9} & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & & \ddots & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

X_j	$\mathbf{X_1}$	$\mathbf{X_2}$	$\mathbf{X_3}$	$\mathbf{X_4}$	$\mathbf{X_5}$	$\mathbf{X_6}$	X_7	X_8	X_9	X_{10}	X_{11}	X_{12}
β_j	**10**	**10**	**7**	**7**	**0**	**0**	10	10	7	7	0	0

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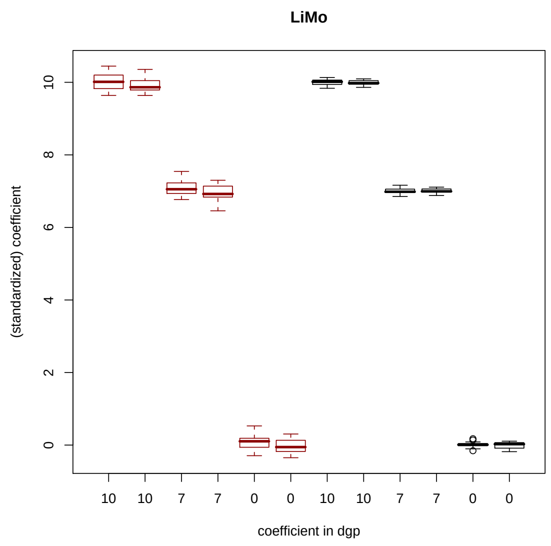
Linear model



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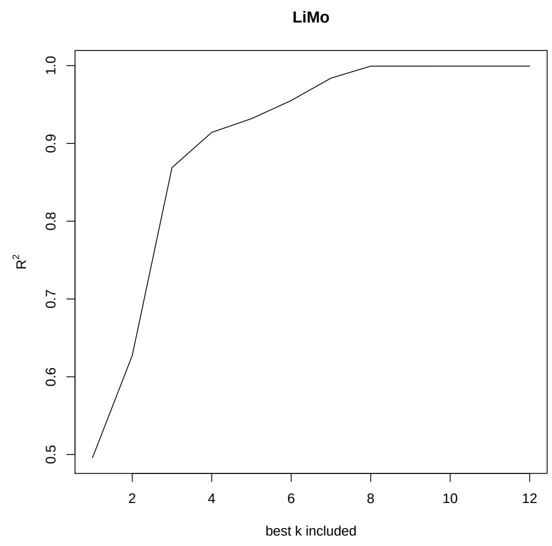

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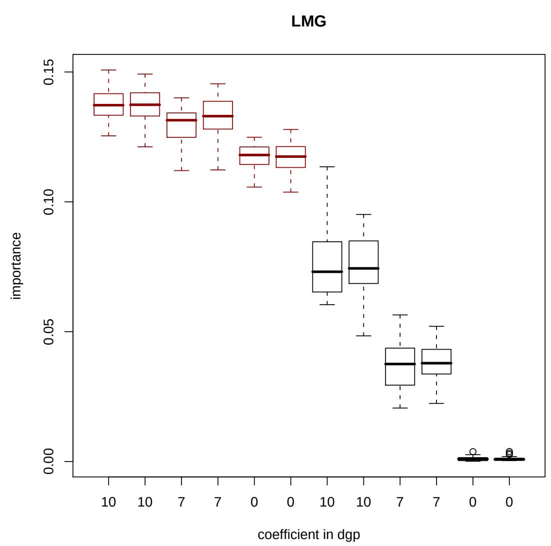
LMG



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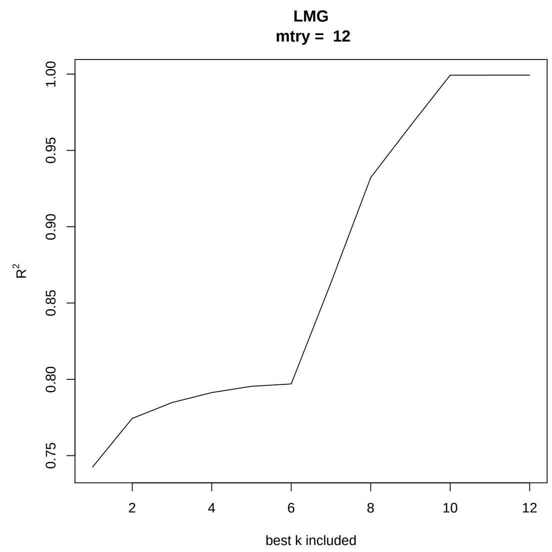

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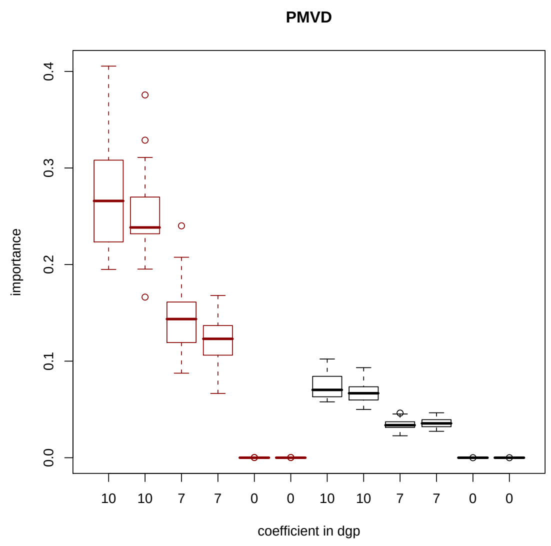
PMVD



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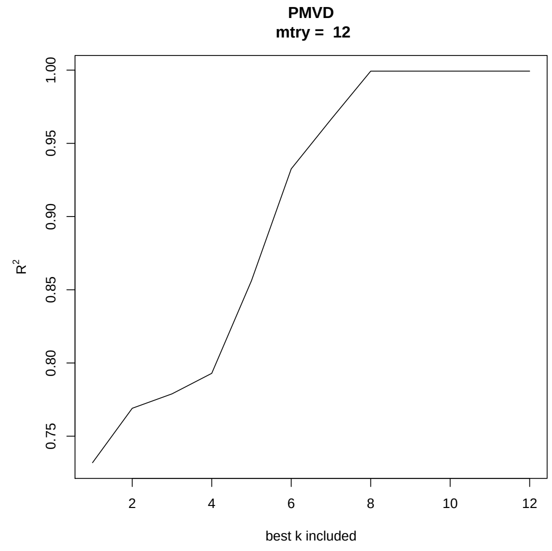

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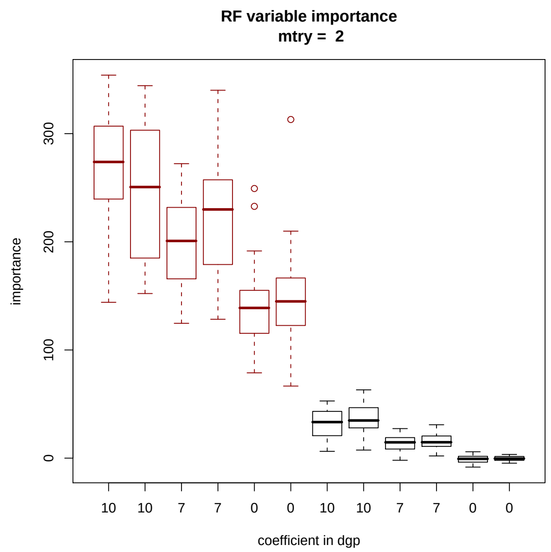
RF unconditional importance



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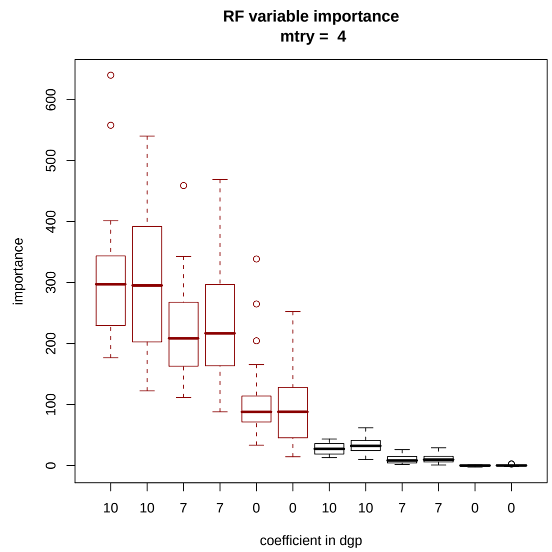

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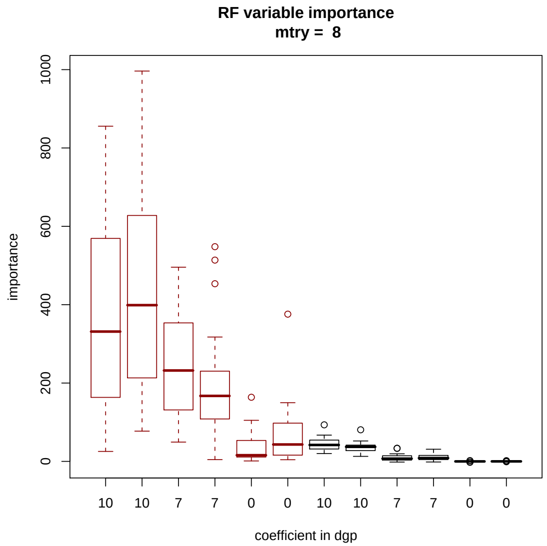

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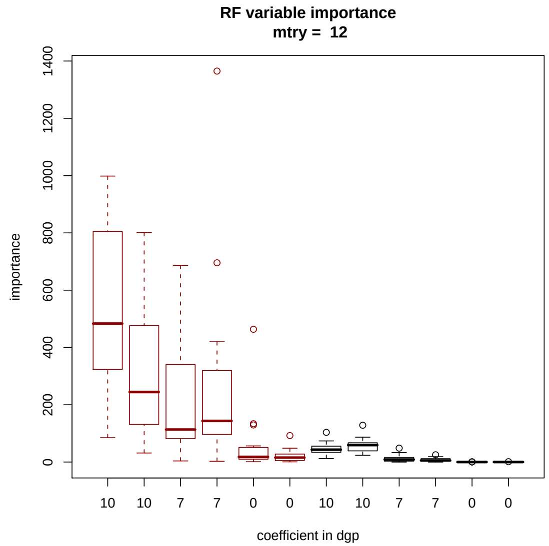

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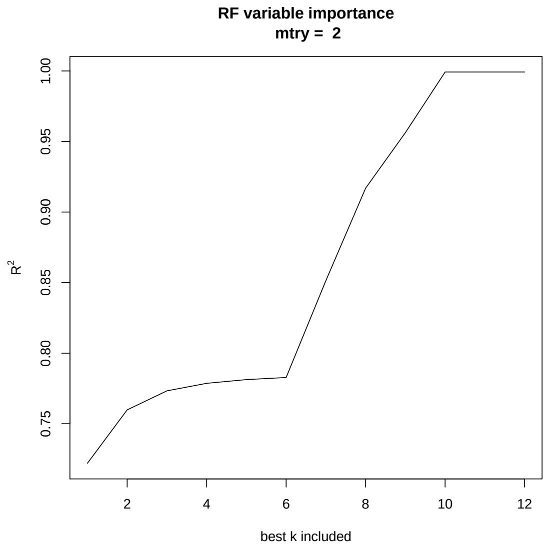

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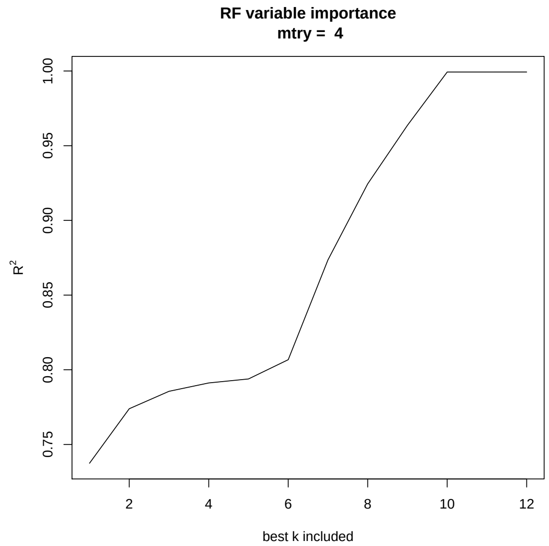

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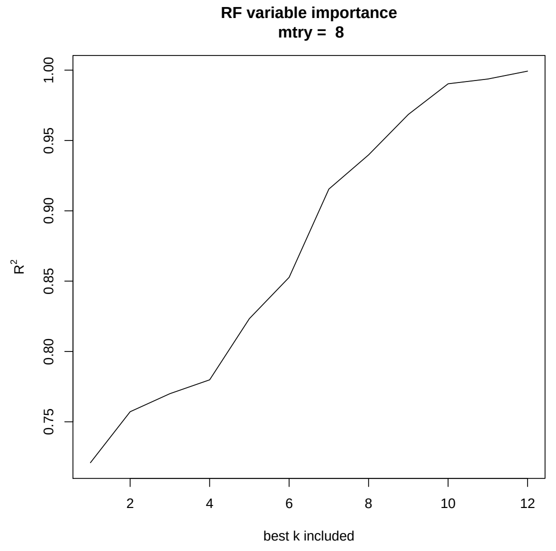

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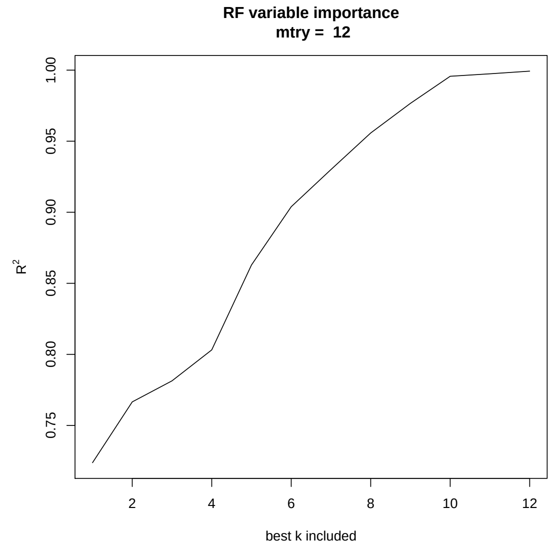

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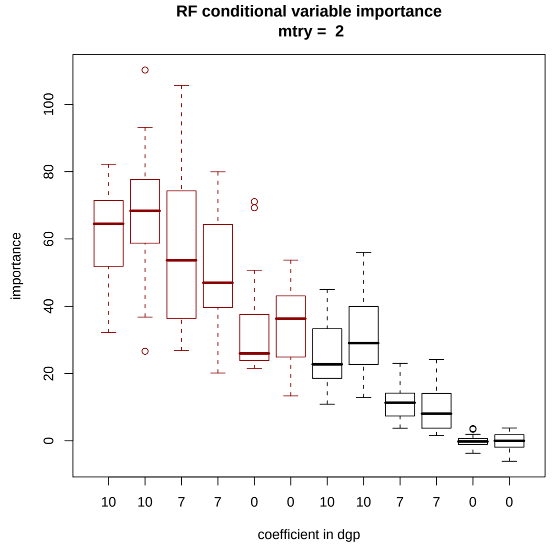

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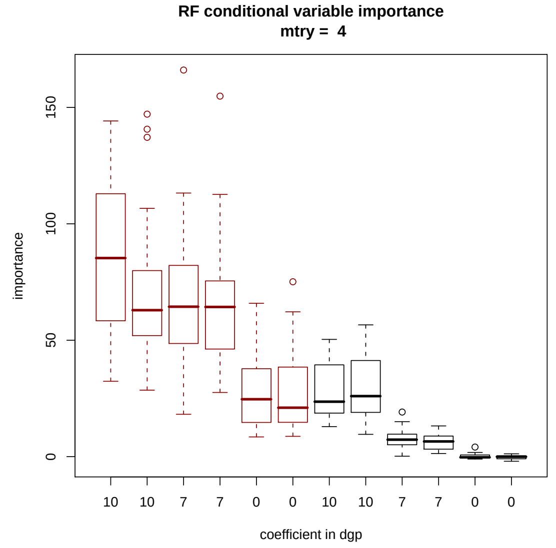

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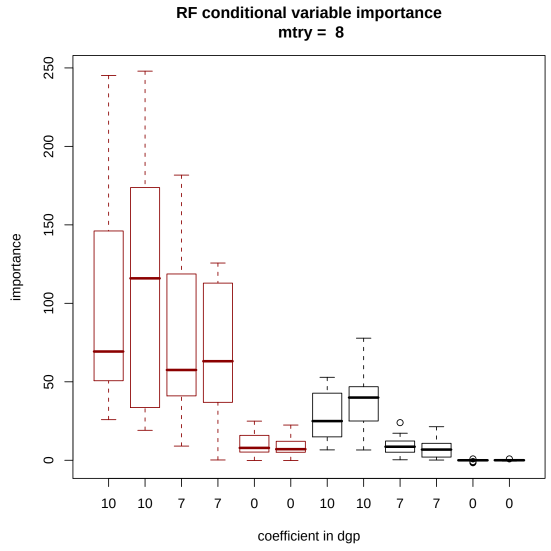

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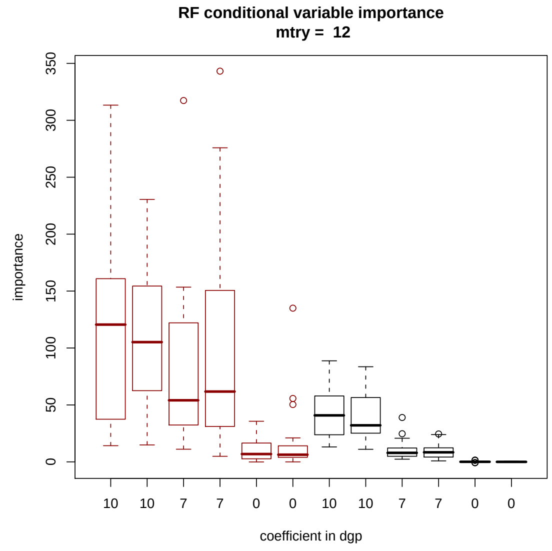

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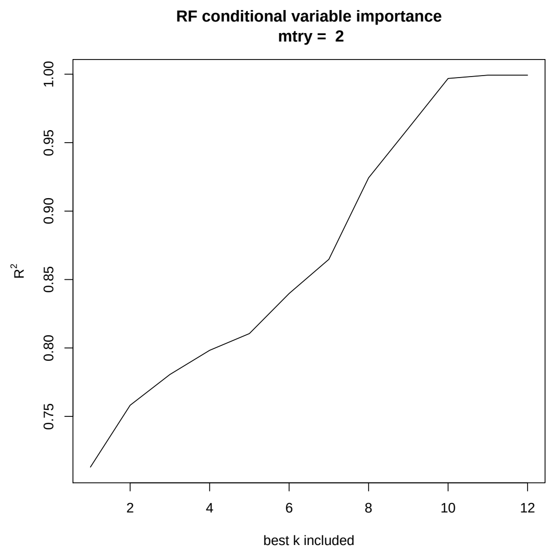

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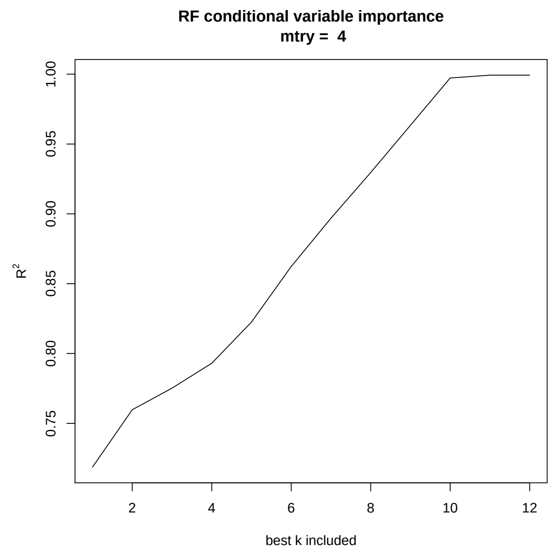

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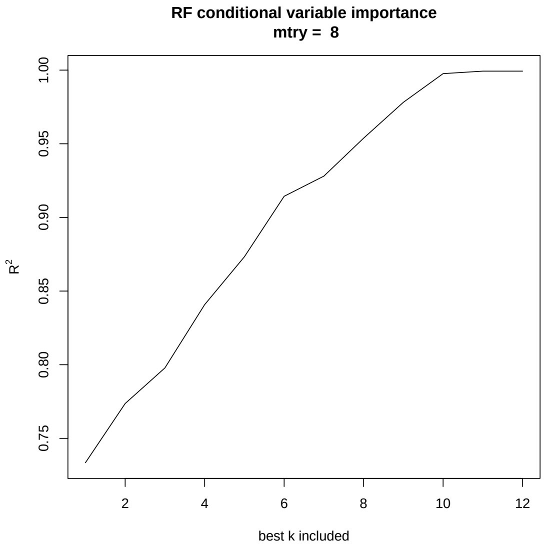

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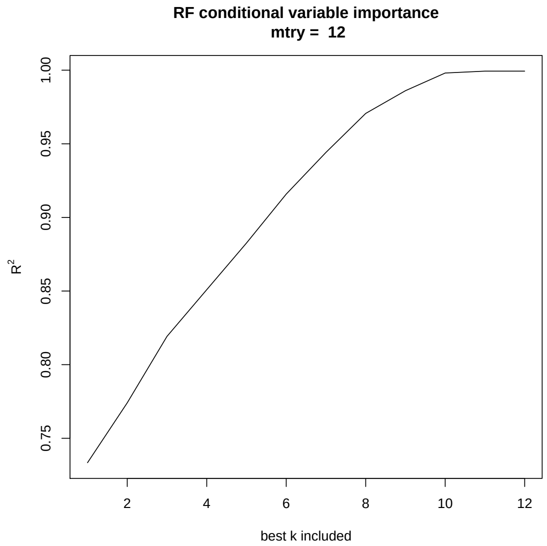

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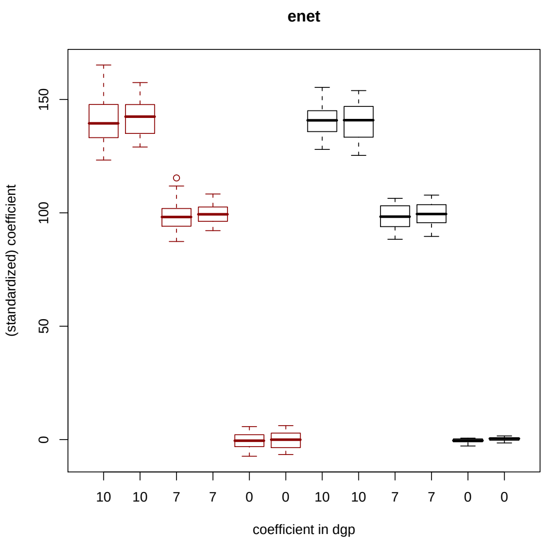
Elastic net



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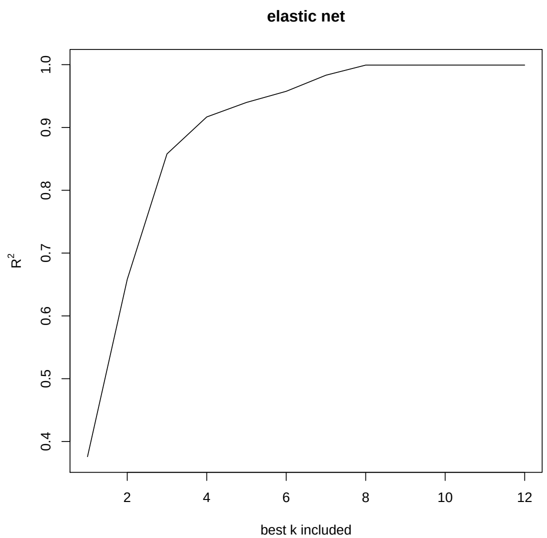

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Now wait a second...

what about elastic net's grouping property?

Elastic net

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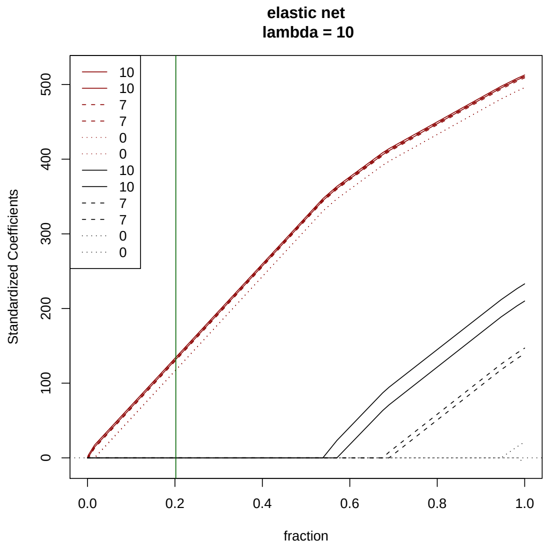

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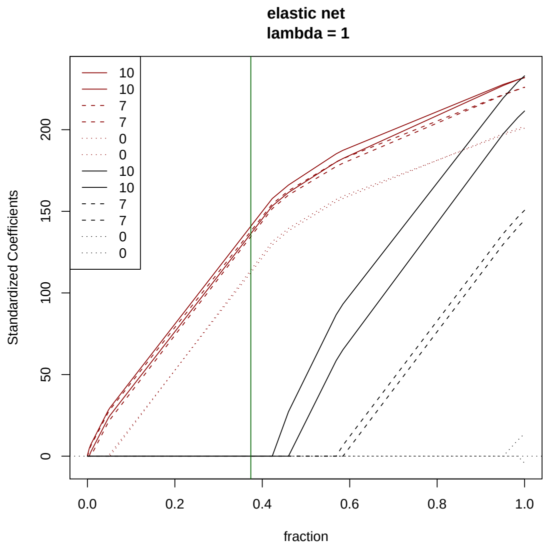

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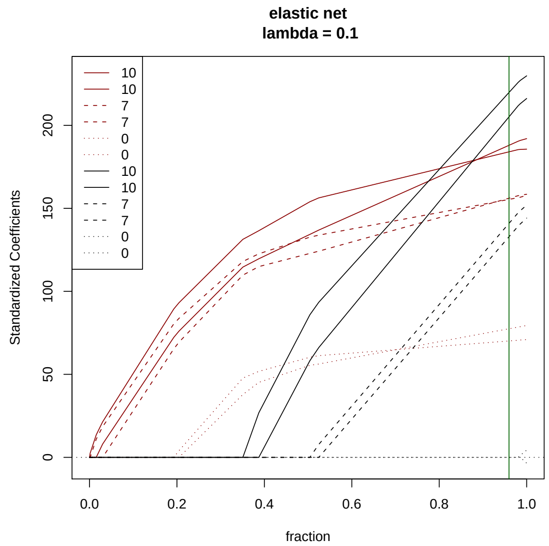

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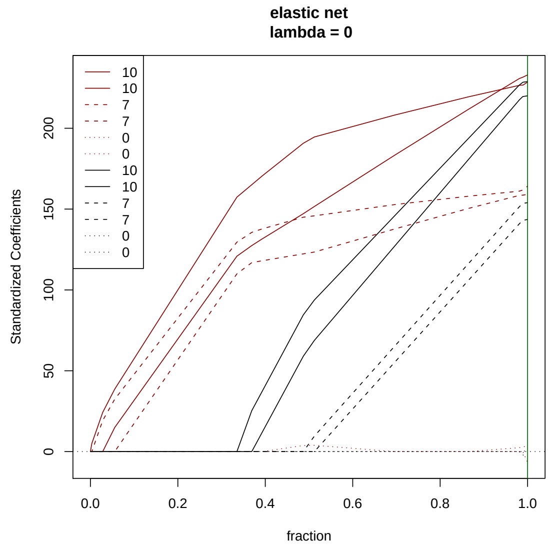

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- w.r.t. prediction accuracy: importance measures following the *exclusion* principle rule

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- w.r.t. prediction accuracy: importance measures following the *exclusion* principle rule standardized betas, PMVD (not quite), RF conditional importance (especially with large `mtry`) and elastic net (tuned!)

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- if you want elastic net to group: don't tune!?

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Azen, R. and D. V. Budescu (2003). The dominance analysis approach for comparing predictors in multiple regression. *Psychological Methods 8*(2), 129–48.

Breiman, L., A. Cutler, A. Liaw, and M. Wiener (2006). *Breiman and Cutler's Random Forests for Classification and Regression*. R package version 4.5-16.

Chevan, A. and M. Sutherland (1991). Hierarchical partitioning. *The American Statistician 45*(2), 90–96.

Feldman, B. (2005). Relative importance and value. Technical report.

Grömping, U. (2006). *relaimpo: Relative Importance of Regressors in Linear Models*. R package version 2.1.

Grömping, U. (2007). Estimators of relative importance for linear regression based on variance decomposition. *The American Statistician 61*(2), 139–147.

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Kuhn, M. (2008). *caret: Classification and Regression Training*. R package version 3.51.

Lindeman, R., P. Merenda, and R. Gold (1980). *Introduction to Bivariate and Multivariate Analysis*. Glenview: Scott Foresman & Co.

Strobl, C., A.-L. Boulesteix, T. Kneib, T. Augustin, and A. Zeileis (2008). Conditional variable importance for random forests. *BMC Bioinformatics 9:307*.

Strobl, C., A.-L. Boulesteix, A. Zeileis, and T. Hothorn (2007). Bias in random forest variable importance measures: Illustrations, sources and a solution. *BMC Bioinformatics 8:25*.

Walsh, C. and R. M. Nally (2008). *hier.part: Hierarchical Partitioning*. R package version 1.0-3.

Zou, H. and T. Hastie (2008). *elasticnet: Elastic-Net for Sparse Estimation and Sparse PCA*. R package version 1.0-5.