The cutpointr package
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Improved and tidy estimation of optimal cutpoints

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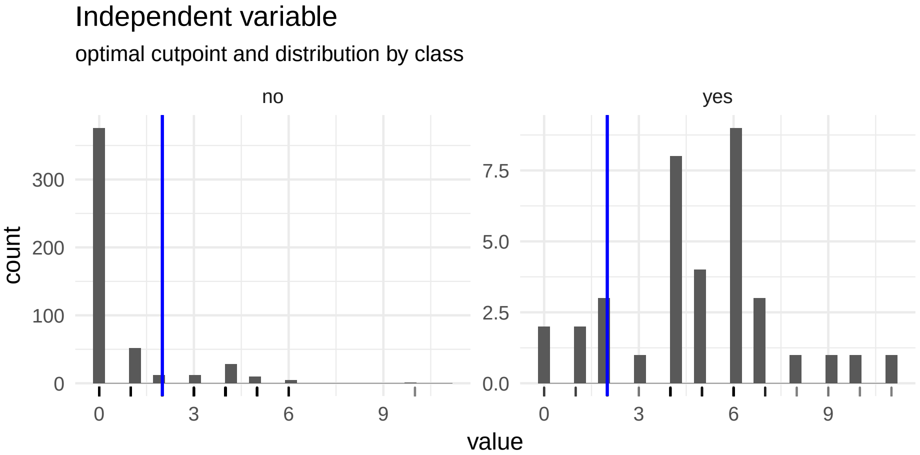
What do we want ‘optimal’ cutpoints for?

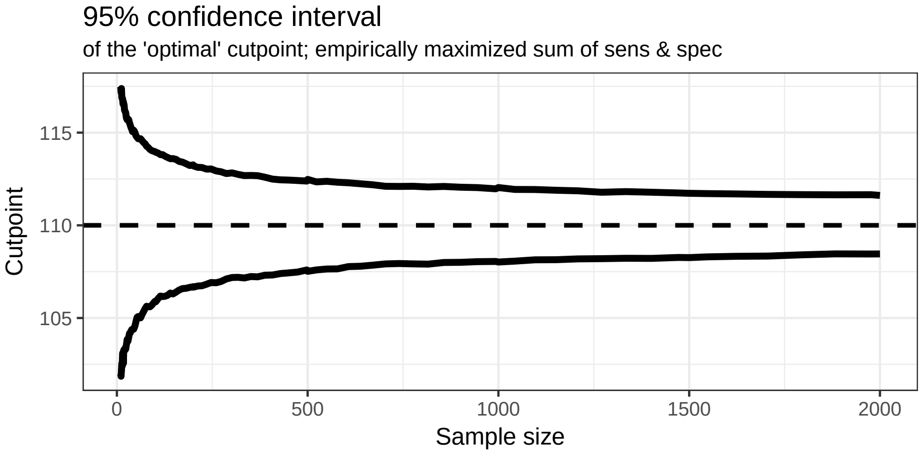
Binary classification via:

- Biological markers
- Psychological scores
- Model predictions



Problems with ‘optimal’ cutpoints

- Prone to overfitting
- Selecting the ‘optimal’ cutpoint by trying out all possible ones leads to
  - overestimation of accuracy
  - highly variable cutpoints



Some features of cutpointr

- More robust methods for lower variability of 'optimal' cutpoints
  - Max. sens + spec based on Kernel smoothed densities per class
  - Search for optimal cutpoint after LOESS smoothing the function cutpoint ~ metric
  - Max. sens + spec parametrically assuming normality
- Included bootstrapping (parallelizable)
  - Assessment of cutpoint variability
  - A way of estimating the out-of-sample performance
- Extensibility by user-defined functions
  - `method` function
  - `metric` function
- Tidy interface and output
  - Output as a tibble, not a list
  - "pipe-friendly"
  - Standard and nonstandard evaluation versions

Built-in methods

The function in `method` takes the data and the necessary parameters (predictor, class, which the positive class is, etc.). It returns the 'optimal' cutpoint.

- `maximize_metric` and `minimize_metric`
- `maximize_loess_metric` and `minimize_loess_metric`
- `oc_youden_normal`
- `oc_youden_kernel`
- `oc_OptimalCutpoints`
- `oc_manual`

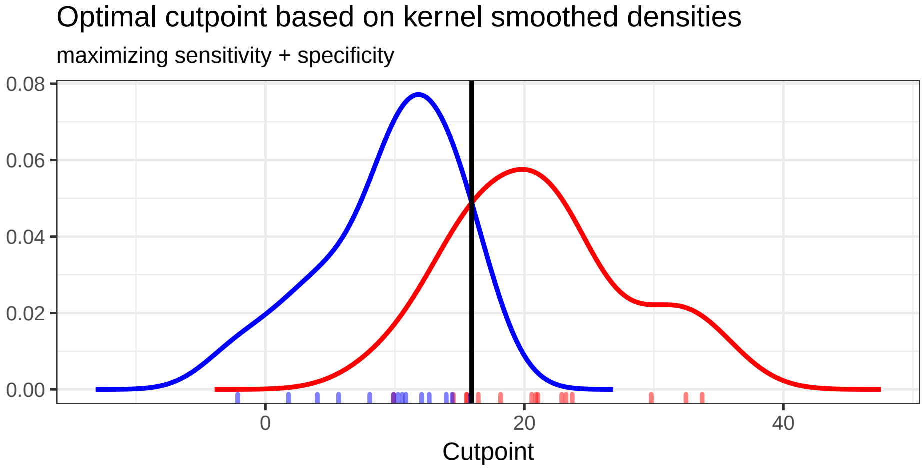
Built-in metrics

The following metrics are already built-in for use with the maximization and minimization functions:

- Accuracy
- Youden- or J-Index and sum of sensitivity and specificity
- Sum and product of PPV and NPV
- Cohen's Kappa
- Absolute difference between sensitivity and specificity (max. balance)
- Absolute difference between PPV and NPV
- F1-score
- Odds Ratio
- p-value of a Chi-squared test
- Total utility and misclassification cost

Kernel method

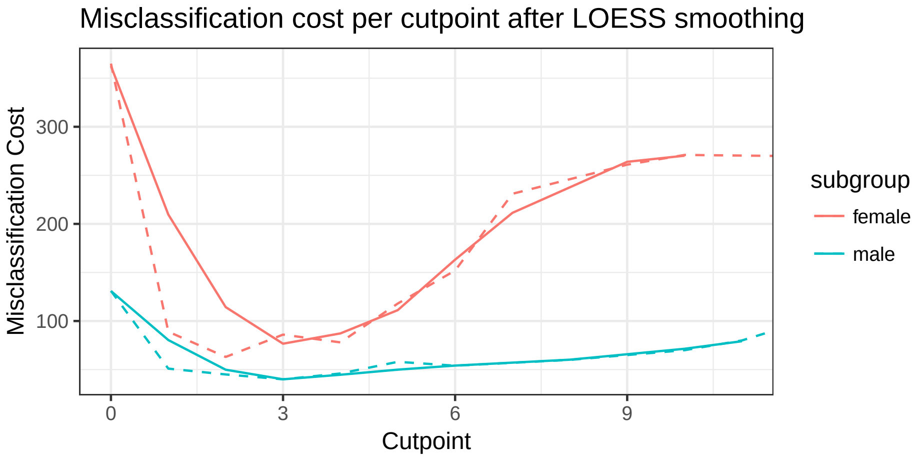
- lower variability for maximizing sensitivity + specificity



Loess method

Additional arguments of `maximize_loess_metric` and `minimize_loess_metric`:

`criterion` (`"aicc"`, `"gvc"`), `degree` (1, 2, 3), `family` (`"gaussian"`, `"symmetric"`), `user.span`

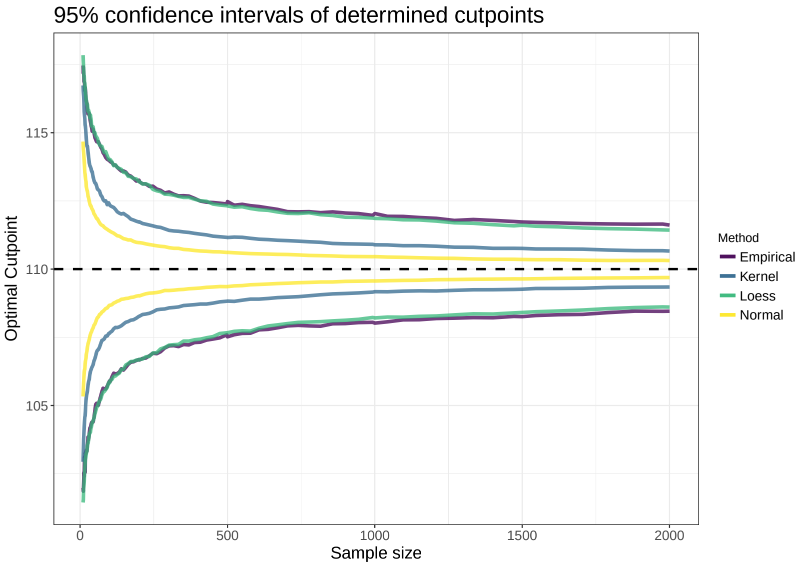


Method based on assuming normal distributions

If the predictor can be assumed to follow a normal distribution in both classes, a low variance method for calculating the ‘optimal’ cutpoint for maximizing sens + spec is

$$c^* = \frac{(\mu_D \sigma_H^2 - \mu_H \sigma_D^2) - \sigma_H \sigma_D \sqrt{(\mu_H - \mu_D)^2 + (\sigma_H^2 - \sigma_D^2) log(\sigma_H^2 / \sigma_D^2)}}{\sigma_H^2 - \sigma_D^2}$$

Variance comparison of several methods

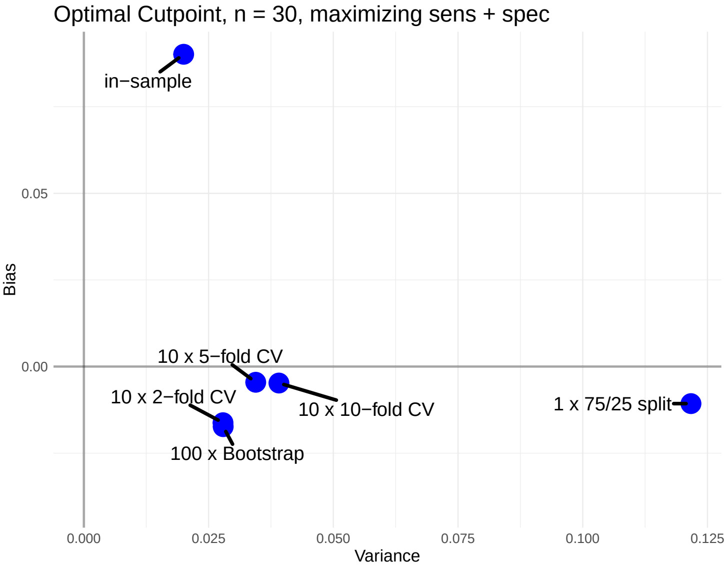


Bootstrap validation

An included bootstrapping routine can be run. This serves two purposes:

- To simulate the variability of the 'optimal' cutpoint
- As a form of cross-validation the out-of-bag metrics are calculated

Bias and variance comparison of different validation methods



Tidy interface and output

```r
suicide %>%
    cutpointr(x = dsi, class = suicide,
              subgroup = gender,
              method = maximize_metric,
              metric = accuracy,
              direction = ">=",
              pos_class = "yes",  neg_class = "no",
              boot_runs = 200)
```

Tidy interface and output

Automatic 'guessing' of the positive / negative class and whether higher or lower predictor values imply the positive class

The returned object is also a normal tibble

```
> suicide %>% cutpointr(dsi, suicide, gender, boot_runs = 200)
Assuming yes as the positive class
Assuming the positive class has higher x values
# A tibble: 2 × 18
  subgroup direction optimal_cutpoint          method Sum_Sens_Spec
     <chr>     <chr>            <dbl>           <chr>         <dbl>
1   female        >=                2 maximize_metric      1.808118
2     male        >=                3 maximize_metric      1.625106
   accuracy sensitivity specificity       AUC pos_class neg_class
      <dbl>       <dbl>       <dbl>     <dbl>    <fctr>    <fctr>
1 0.8852041   0.9259259   0.8821918 0.9446474       yes        no
2 0.8428571   0.7777778   0.8473282 0.8617472       yes        no
  prevalence outcome predictor grouping              data
       <dbl>   <chr>     <chr>    <chr>            <list>
1 0.06887755 suicide       dsi   gender <tibble [392 × 2]>
2 0.06428571 suicide       dsi   gender <tibble [140 × 2]>
           roc_curve                 boot
              <list>               <list>
1 <tibble [11 × 10]> <tibble [200 × 18]>
2 <tibble [11 × 10]> <tibble [200 × 18]>
```

Data per group as nested tibbles

ROC curve and bootstrap results as nested tibbles

Summary

```r
summary(cp)
```

```
 optimal_cutpoint Sum_Sens_Spec accuracy sensitivity specificity    AUC n_pos n_neg
                2        1.7518   0.8647      0.8889      0.8629 0.9238    36   496

          observation
prediction yes  no
       yes  32  68
       no    4 428

Predictor summary:
      Min.    1st Qu.     Median       Mean    3rd Qu.       Max.         SD
 0.0000000  0.0000000  0.0000000  0.9210526  1.0000000 11.0000000  1.8527143

Predictor summary per class:
    Min. 1st Qu. Median      Mean 3rd Qu. Max       SD
no     0       0      0 0.6330645       0  10 1.412225
yes    0       4      5 4.8888889       6  11 2.549821

Bootstrap summary:
                   Min. 1st Qu. Median   Mean 3rd Qu.    Max     SD
optimal_cutpoint 1.0000  2.0000 2.0000 2.1950  2.0000 4.0000 0.8187
Sum_Sens_Spec    1.3939  1.6442 1.7240 1.7072  1.7729 1.8778 0.0941
Accuracy_b       0.7462  0.8534 0.8703 0.8623  0.8835 0.9267 0.0375
Accuracy_oob     0.7143  0.8462 0.8639 0.8538  0.8758 0.9196 0.0417
Sensitivity_b    0.7419  0.8680 0.8974 0.8985  0.9378 1.0000 0.0522
Sensitivity_oob  0.5000  0.7857 0.8750 0.8531  0.9286 1.0000 0.1091
Specificity_b    0.7321  0.8516 0.8663 0.8596  0.8824 0.9306 0.0415
Specificity_oob  0.6979  0.8438 0.8620 0.8541  0.8780 0.9412 0.0484
Kappa_b          0.2012  0.3679 0.4155 0.4127  0.4645 0.6042 0.0737
Kappa_oob        0.1775  0.3413 0.3950 0.3878  0.4440 0.5455 0.0818
```

Optimal cutpoint and AUC for multiple variables

```
dat <- iris %>%
    dplyr::filter(Species %in% c("setosa", "virginica"))
purrr::map_df(colnames(dat)[1:4], function(coln) {
    cutpointr_(dat, x = coln, class = "Species",
               pos_class = "setosa",
               use_midpoints = TRUE) %>%
        mutate(variable = coln) %>%
        dplyr::select("variable", "direction",
                      "optimal_cutpoint", "AUC")
})
```

```
## # A tibble: 4 x 4
##       variable direction optimal_cutpoint    AUC
##          <chr>     <chr>            <dbl>  <dbl>
## 1 Sepal.Length        <=             5.55 0.9846
## 2  Sepal.Width        >=             3.35 0.8344
## 3 Petal.Length        <=             3.20 1.0000
## 4  Petal.Width        <=             1.00 1.0000
```

User defined metric functions

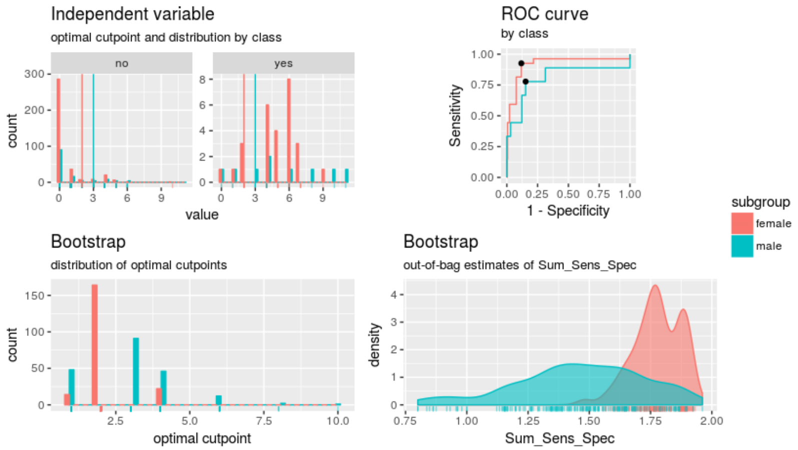
The arguments to `method` and `metric` are actual functions

- `metric` is passed to `method`

```
accuracy <- function(tp, fp, tn, fn) {
    (tp + tn) / (tp + fp + tn + fn)
}
```

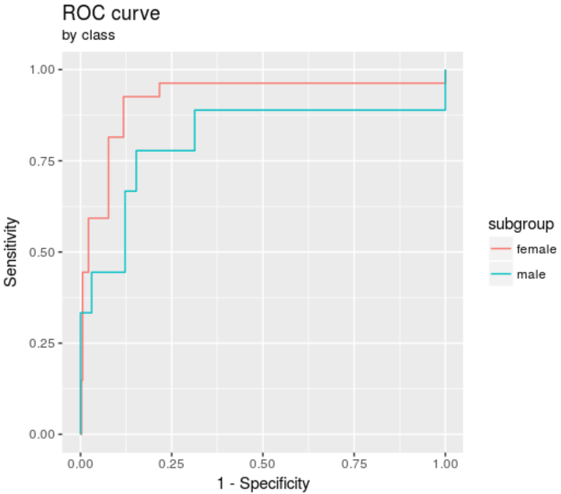
Plots

```
cp <- cutpointr(suicide, dsi, suicide, gender,
                boot_runs = 200,
                direction = ">=", pos_class = "yes")
plot(cp)
```

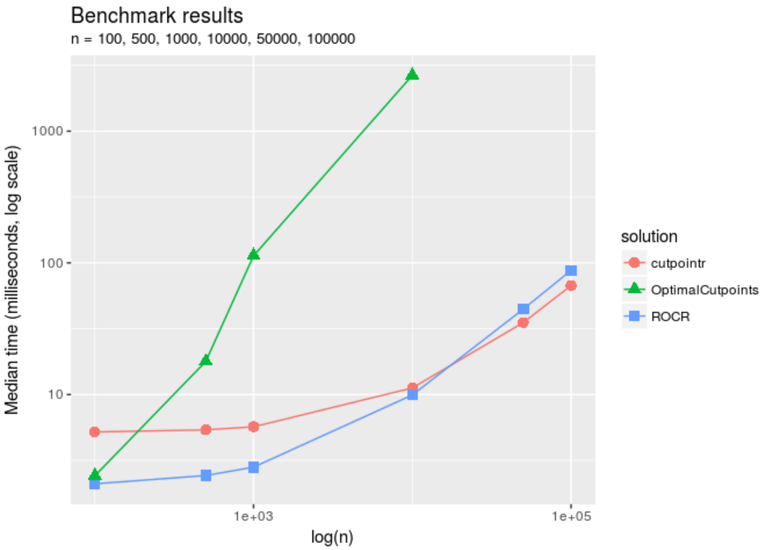


Single plots

```
suicide %>%
    cutpointr(dsi, suicide, gender) %>%
    plot_roc(display_cutpoint = FALSE)
```

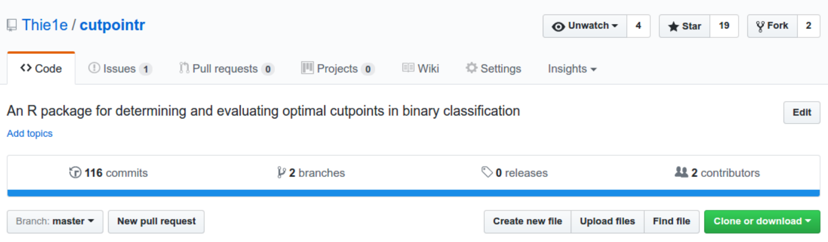


Benchmarks

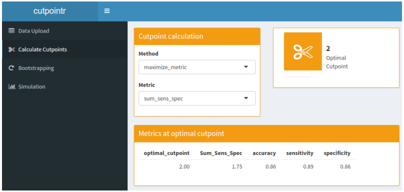

Benchmark results
n = 100, 500, 1000, 10000, 50000, 100000
Median time (milliseconds, log scale)
1000
100
10
1e+03
1e+05
log(n)
solution
cutpointr
OptimalCutpoints
ROCR

Thank you

Not yet on CRAN but on Github: `https://github.com/Thie1e/cutpointr`



Future plans: Shiny



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References

Fluss, R., Faraggi, D., & Reiser, B. (2005). Estimation of the Youden Index and its associated cutoff point. Biometrical Journal, 47(4), 458–472.

Leeflang, M. M., Moons, K. G., Reitsma, J. B., & Zwinderman, A. H. (2008). Bias in sensitivity and specificity caused by data-driven selection of optimal cutoff values: mechanisms, magnitude, and solutions. Clinical Chemistry, (4), 729–738.