

# A Vignette for RCAL (version 1.0)

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## 1 Introduction

The R package RCAL (version 1.0) can be used for two main tasks:

- to estimate the mean of an outcome in the presence of missing data,
- to estimate the average treatment effects in causal inference.

There are 3 high-level functions provided for the first task:

- `mn.nreg`: inference using non-regularized calibrated estimation,
- `mn.regu.cv`: inference using regularized calibrated estimation based on cross validation,
- `mn.regu.path`: inference using regularized calibrated estimation along a regularization path.

The first function `mn.nreg` is appropriate only in relatively low-dimensional settings, whereas the functions `mn.regu.cv` and `mn.regu.path` are designed to deal with high-dimensional data (namely, the number of covariates close to or greater than the sample size). In parallel, there are 3 functions for the second task, `ate.nreg`, `ate.regu.cv`, and `ate.regu.path`. These functions can also be used to perform inference for the average treatment effects on the treated or on the untreated. Currently, the treatment is assumed to be binary (i.e., untreated or treated). Extensions to multi-valued treatments will be incorporated in later versions.

The package also provides lower-level functions, including `glm.nreg` to implement non-regularized M-estimation and `glm.regu` to implement Lasso regularized M-estimation for fitting generalized linear models currently with continuous or binary outcomes. The latter function `glm.regu` uses an active-set descent algorithm, which enjoys a finite termination property for solving least-squares Lasso problems.

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## 2 An example

We illustrate the use of the package on a simulated dataset as in Tan (2019), Section 4. The dataset, `simu.data`, is included as part of the package.

```
> library(RCAL)
> data(simu.data)
```

The following shows the first 10 rows and the first 6 columns of the dataset, which is of size  $800 \times 202$ .

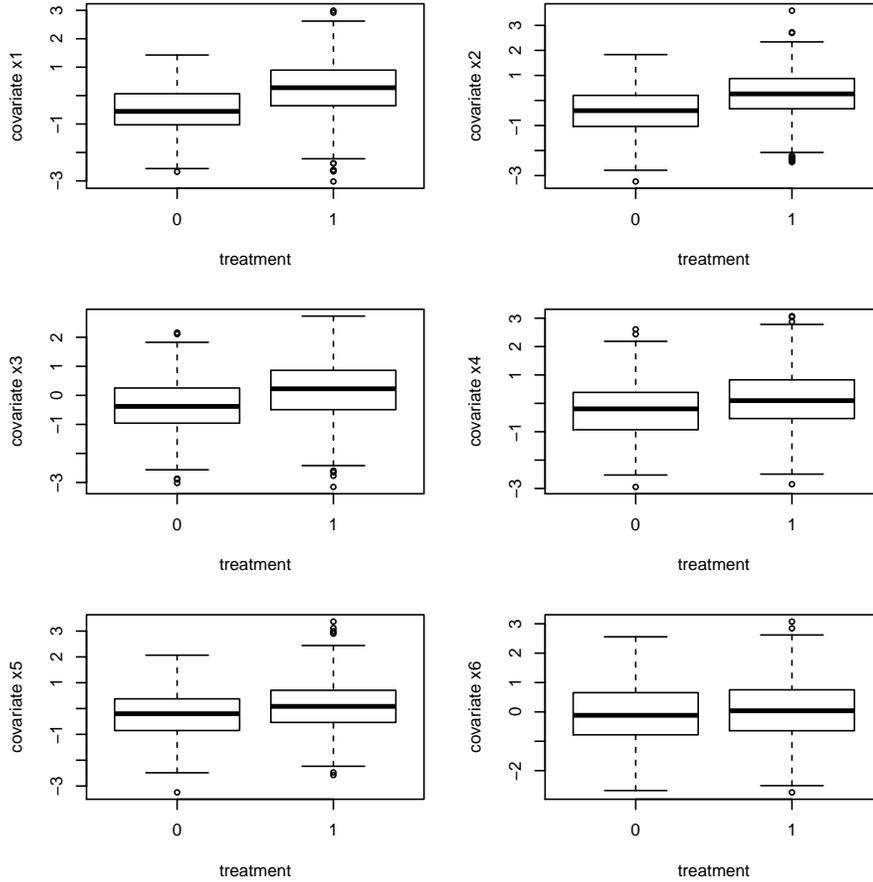
```
> simu.data[1:10, 1:6]
```

```
      y tr
[1,] 0.6032936 1 0.9616951 0.5962625 0.4492321 0.8512571217
[2,] 4.0070254 1 2.3647316 0.3364174 1.8668110 1.1255817363
[3,] 1.3576326 1 0.1563721 -0.2232653 0.4548950 0.9605372221
[4,] 0.9133211 1 0.2015582 1.4384546 -0.1350395 1.5087188960
[5,] 2.5373546 1 1.2350352 1.5431279 1.0112577 0.3531083965
[6,] 3.0240024 1 0.6151206 1.0198704 1.6962577 -0.2750277816
[7,] -1.3507495 0 -1.7719684 -0.6344480 -1.2890632 -1.5098428847
[8,] -2.4126343 0 -1.6242547 -0.1267854 0.7021270 -0.0009029026
[9,] -1.1280024 0 0.1138376 -0.5874306 0.7784352 -0.4486271136
[10,] -1.0314948 0 -0.2667515 0.4259913 -0.3408476 -0.0722745940
```

The first column represents an observed outcome `y`, the second column represents a binary treatment `tr`, and the remaining 200 columns represent covariates.

```
> n <- dim(simu.data)[1]
> p <- dim(simu.data)[2]-2
> y <- simu.data[,1]
> tr <- simu.data[,2]
> x <- simu.data[,2+1:p]
> x <- scale(x)
```

Figure 1: Boxplots of covariates in the untreated and treated groups.

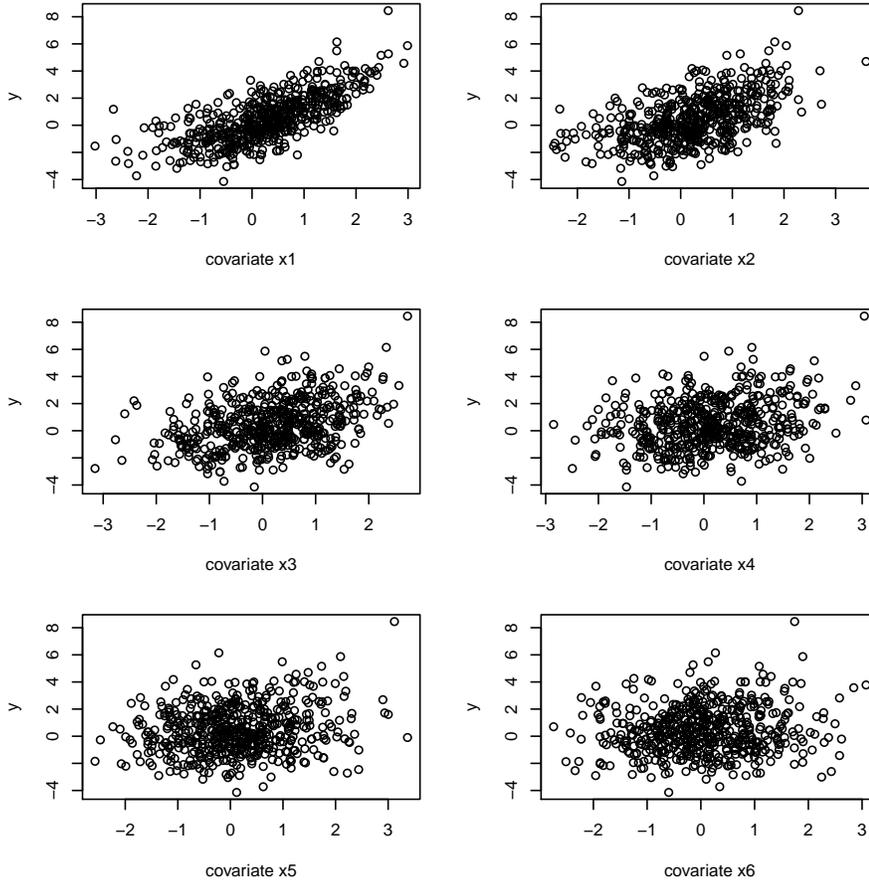


To examine the data, Figure 1 shows the boxplots of the first 6 covariates in the untreated and treated groups, and Figure 2 shows the scatterplots of observed outcomes and the first 6 covariates in the treated group.

## 2.1 Estimation of a population mean with missing data

We use the potential outcome framework for causal inference (Neyman 1923; Rubin 1974). For each individual  $i$ , the potential outcome  $Y_i^1$  with the treatment is the observed outcome  $Y_i$  if treatment variable  $T_i$  is 1, or missing otherwise. Similarly, the potential outcome  $Y_i^0$  without the treatment is observed if treatment variable  $T_i$  is 0, or missing otherwise. To estimate the means of the potential outcomes amounts to estimation of population means with missing data.

Figure 2: Scatterplots of observed outcomes and covariates in the treated group.



In this section, we consider the problem of estimating the mean  $\mu^1$  of potential outcomes  $Y_i^1$  with the treatment, which are observed when  $T_i$  is 1 but missing otherwise. The covariates  $X_i$  are observed on all individuals in the sample, and can be relevant to the estimation of  $\mu^1$  in two distinct ways. On one hand, the covariates  $X_i$  can be associated with the treatment variable  $T_i$ . In other words, individuals with different covariates may differ in their probabilities of receiving the treatment, which are denoted as  $\pi(X_i)$  and called propensity scores (Rosenbaum and Rubin 1983). On the other hand, the covariates  $X_i$  can also be associated with the outcome variable  $Y_i$  in the treated group  $\{T_i = 1\}$ . The conditional mean of  $Y_i$  given  $X_i$  and  $T_i = 1$  is called the outcome regression function in the treated and denoted as  $m^1(X_i)$ . These associations can be seen from Figures 1 and 2.

Ignoring the covariates and using the simple sample average of observed outcomes in the treated yield an estimate 0.47 with standard error 0.076. This inference would be biased, since the true value of  $\mu^1$  is 0 by the design of the simulated data, as described in `help(simu.data)`.

```
> mean(y[tr==1])    # point estimate

[1] 0.4706937

> sqrt(var(y[tr==1]) / sum(tr) )    # standard error

[1] 0.07643911
```

The function `mn.regu.cv` implements a two-step method for estimating  $\mu^1$ . First, propensity score and outcome regression models are fitted. Denote by  $\hat{\pi}^1(X_i)$  and  $\hat{m}^1(X_i)$  the fitted propensity score and outcome regression function respectively. Then the augmented IPW estimator of  $\mu^1$  is applied (Robins et al. 1994):

$$\hat{\mu}_{\text{AIPW}}^1 = \frac{1}{n} \sum_{i=1}^n \left[ \frac{T_i Y_i}{\hat{\pi}^1(X_i)} - \left\{ \frac{T_i}{\hat{\pi}^1(X_i)} - 1 \right\} \hat{m}^1(X_i) \right].$$

For `ploss="cal"`, regularized calibrated estimation is performed with cross validation as in Tan (2017, 2019). The method then leads to model-assisted inference, in which confidence intervals are valid with high-dimensional data if the propensity score model is correctly specified but the outcome regression model may be misspecified. With linear outcome models, the inference is also doubly robust. For `ploss="ml"`, regularized maximum likelihood estimation is used (Belloni et al. 2014; Farrell 2015). In this case, standard errors are only shown to be valid if both the propensity score model and the outcome regression model are correctly specified.

For this example, both the propensity score and outcome regressions models are (slightly) misspecified, by the design of the simulated data; see `help(simu.data)`. Nevertheless, regularized calibrated estimation yields an estimate 0.11 with standard error 0.068, whereas regularized maximum likelihood estimation yields an estimate 0.089 with standard error 0.069. Both estimates are much closer to the true value 0, with smaller standard errors, than the unadjusted estimate.

```

> ## regularized calibrated estimation
> set.seed(0) #this affects random split of data in cross validation
> mn.cv.rcal <-
+ mn.regu.cv(fold=5*c(1,1), nrho=(1+10)*c(1,1), rho.seq=NULL, y, tr, x,
+           ploss="cal", yloss="gaus")
> unlist(mn.cv.rcal$est)

           one           ipw           or           est           var           ze
1.000252762  0.191416564 -0.053716233  0.113076037  0.004640538  1.659917193

> sqrt(mn.cv.rcal$est $var)

[1] 0.06812149

> ## regularized maximum likelihood estimation
> set.seed(0) #this affects random split of data in cross validation
> mn.cv.rml <-
+ mn.regu.cv(fold=5*c(1,1), nrho=(1+10)*c(1,1), rho.seq=NULL, y, tr, x,
+           ploss="ml", yloss="gaus")
> unlist(mn.cv.rml$est)

           one           ipw           or           est           var           ze
0.972338673  0.156331196  0.055241855  0.085678228  0.004824676  1.233492146

> sqrt(mn.cv.rml$est $var)

[1] 0.06945989

```

The following shows how the same results can be obtained as above, but using the lower-level function `glm.regu.cv` to perform regularized M-estimation for fitting propensity score and outcome regression models, and using the function `mn.aipw` to compute the augmented IPW estimates.

```

> ## regularized calibrated estimation
> set.seed(0)
> ps.cv.rcal <-
+ glm.regu.cv(fold=5, nrho=1+10, y=tr, x=x, loss="cal")
> ps.cv.rcal$sel.nz[1]

[1] 11

> fp.cv.rcal <- ps.cv.rcal $sel.fit[,1]
> or.cv.rcal <-
+ glm.regu.cv(fold=5, nrho=1+10, y=y[tr==1], x=x[tr==1,],
+             iw=1/fp.cv.rcal[tr==1]-1, loss="gaus")
> fo.cv.rcal <- c( cbind(1,x)%*%or.cv.rcal$sel.bet[,1] )
> mn.cv.rcal2 <- unlist(mn.aipw(y, tr, fp=fp.cv.rcal, fo=fo.cv.rcal))
> mn.cv.rcal2

           one           ipw           or           est           var           ze
1.000252762  0.191416564 -0.053716233  0.113076037  0.004640538  1.659917193

> ## regularized maximum likelihood estimation
> set.seed(0)
> ps.cv.rml <-
+ glm.regu.cv(fold=5, nrho=1+10, y=tr, x=x, loss="ml")
> ps.cv.rml$sel.nz[1]

[1] 32

> fp.cv.rml <- ps.cv.rml $sel.fit[,1]
> or.cv.rml <-
+ glm.regu.cv(fold=5, nrho=1+10, y=y[tr==1], x=x[tr==1,],
+             iw=NULL, loss="gaus")
> fo.cv.rml <- c( cbind(1,x)%*%or.cv.rml$sel.bet[,1] )
> mn.cv.rml2 <- unlist(mn.aipw(y, tr, fp=fp.cv.rml, fo=fo.cv.rml))
> mn.cv.rml2

```

	one	ipw	or	est	var	ze
	0.972338673	0.156331196	0.055241855	0.085678228	0.004824676	1.233492146

## 2.2 Closer look at propensity score estimation

One of the difficulties in estimating the population mean  $\mu^1$  is that the treated group is, by definition, a selected sub-sample and hence may not be representative of the entire sample. The idea of inverse probability weighting is to reweight individuals in the treated group by the inverse of propensity scores, so that the weighted averages of covariates in the treated group are similar to the simple averages in the entire sample. Hence it is desirable to reduce the following differences as much as possible given the sample size and the number of covariates under study:

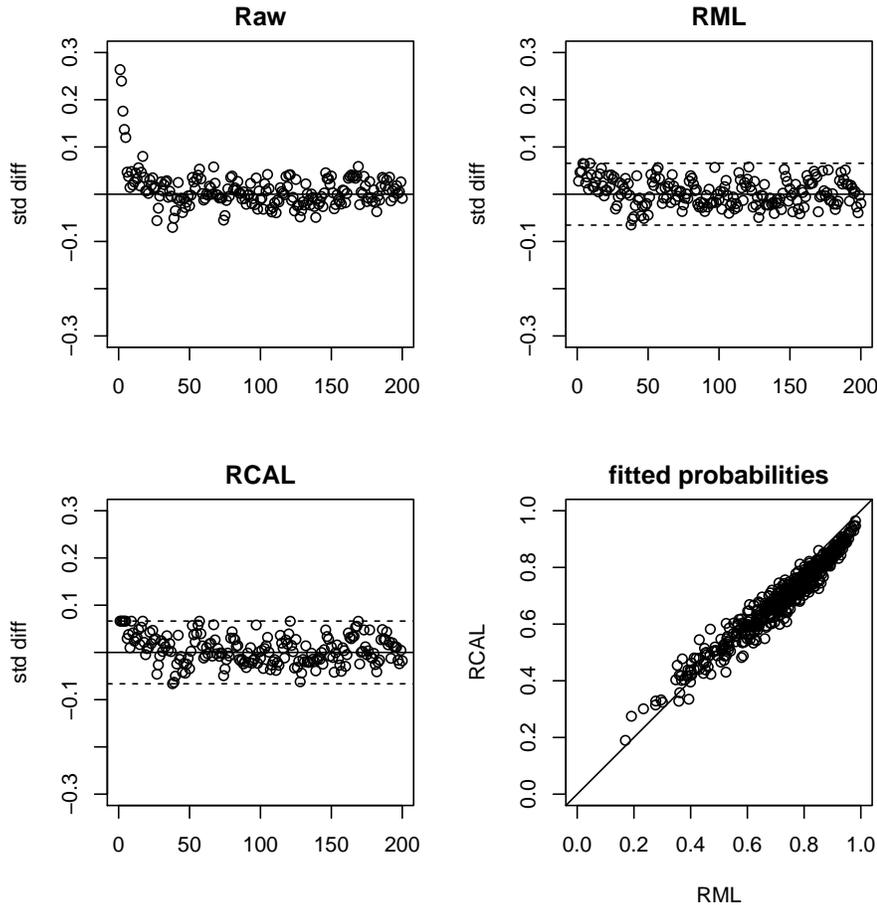
$$\frac{1}{n} \sum_{i=1}^n \left\{ \frac{T_i}{\hat{\pi}^1(X_i)} - 1 \right\} X_{ji} = \sum_{i: T_i=1, 1 \leq i \leq n} \hat{w}_i X_{ji} - \frac{1}{n} \sum_{i=1}^n X_{ji}, \quad j = 1, \dots, p,$$

where  $\hat{w}_i = \{n\hat{\pi}^1(X_i)\}^{-1}$  and  $X_{ji}$  denotes the  $j$ th component of  $X_i$ . If the covariates are standardized with sample means 0 and variances 1, then the above gives the standardized calibration differences as in Tan (2017), Section 5.

The following shows the calculation of such calibration differences using the function `mn.ipw`. The results are plotted in Figure 3.

```
> fp.raw <- rep(mean(tr), n) #constant propensity scores
> check.raw <- mn.ipw(x, tr, fp.raw)
> check.cv.rcal <- mn.ipw(x, tr, fp.cv.rcal)
> check.cv.rml <- mn.ipw(x, tr, fp.cv.rml)
> par(mfrow=c(2,2))
> par(mar=c(4,4,2,2))
> plot(check.raw$est, xlim=c(0,p), ylim=c(-.3,.3),
+       xlab="", ylab="std diff", main="Raw")
> abline(h=0)
> plot(check.cv.rml$est, xlim=c(0,p), ylim=c(-.3,.3),
+       xlab="", ylab="std diff", main="RML")
```

Figure 3: Standardized calibration differences and scattplot of propensity scores.



```

> abline(h=0)
> abline(h=max(abs(check.cv.rml$est)) *c(-1,1), lty=2)
> plot(check.cv.rcal$est, xlim=c(0,p), ylim=c(-.3,.3),
+      xlab="", ylab="std diff", main="RCAL")
> abline(h=0)
> abline(h=max(abs(check.cv.rcal$est)) *c(-1,1), lty=2)
> plot(fp.cv.rml[tr==1], fp.cv.rcal[tr==1], xlim=c(0,1), ylim=c(0,1),
+      xlab="RML", ylab="RCAL", main="fitted probabilities")
> abline(c(0,1))

```

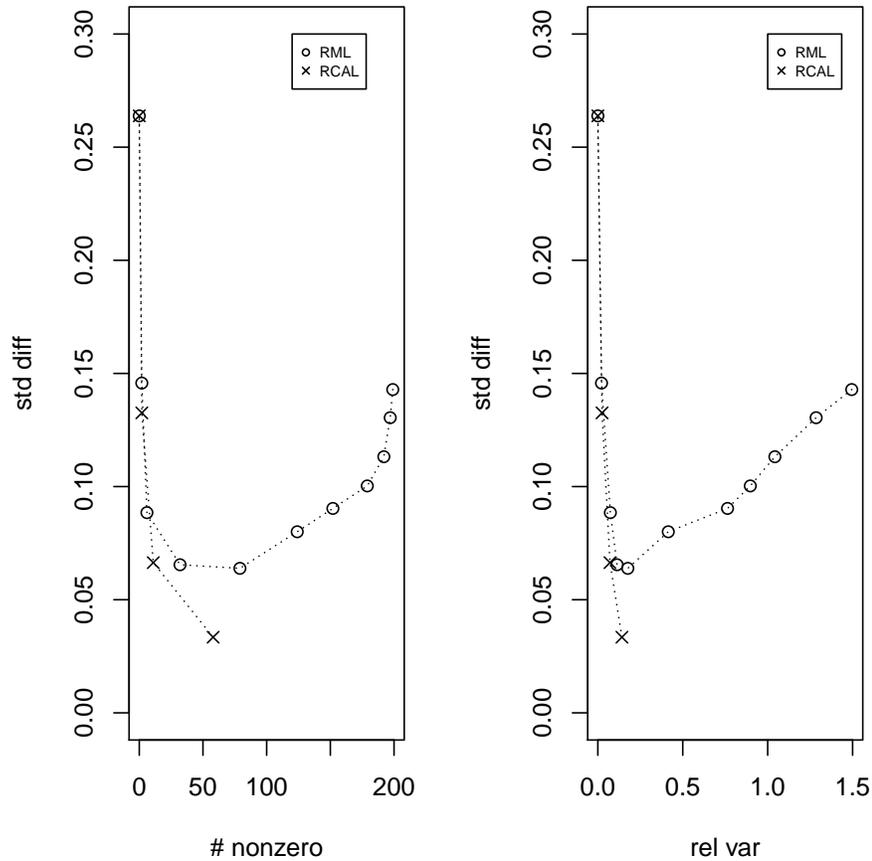
The maximum standardized calibration differences from the two methods appear similar to each other. However, the number of nonzero coefficients estimated out of

a total of 200 is 11 for regularized calibrated estimation, but much larger, 32, for regularized maximum likelihood estimation.

For further comparison, the following uses the function `glm.regu.path` to compute fitted propensity scores over regularization paths. Figure 4 shows how the maximum absolute standardized differences vary against the numbers of nonzero coefficients and relative variances, similarly as in Tan (2017), Section 5. In this example, it seems impossible for regularized maximum likelihood estimation to reduce calibration differences to lower than 0.05, even with decreased Lasso penalties and increased numbers of nonzero coefficients and relative variance.

```
> set.seed(0)
> ps.path.rcal <-
+ glm.regu.path(nrho=1+10, rho.seq=NULL, y=tr, x=x, loss="cal")
> fp.path.rcal <- ps.path.rcal $fit.all[, !ps.path.rcal$non.conv]
> mdiff.path.rcal <- rep(NA, dim(fp.path.rcal)[2])
> rvar.path.rcal <- rep(NA, dim(fp.path.rcal)[2])
> for (j in 1:dim(fp.path.rcal)[2]) {
+   check.path.rcal <- mn.ipw(x, tr, fp.path.rcal[,j])
+   mdiff.path.rcal[j] <- max(abs(check.path.rcal$est))
+   rvar.path.rcal[j] <-
+   var(1/fp.path.rcal[tr==1,j])/mean(1/fp.path.rcal[tr==1,j])^2
+ }
> set.seed(0)
> ps.path.rml <-
+ glm.regu.path(nrho=1+10, rho.seq=NULL, y=tr, x=x, loss="ml")
> fp.path.rml <- ps.path.rml $fit.all[, !ps.path.rml$non.conv]
> mdiff.path.rml <- rep(NA, dim(fp.path.rml)[2])
> rvar.path.rml <- rep(NA, dim(fp.path.rml)[2])
> for (j in 1:dim(fp.path.rml)[2]) {
+   check.path.rml <- mn.ipw(x, tr, fp.path.rml[,j])
+   mdiff.path.rml[j] <- max(abs(check.path.rml$est))
```

Figure 4: Maximum absolute standardized differences against the numbers of nonzero coefficients and relative variances



```
+ rvar.path.rml[j] <-
+ var(1/fp.path.rml[tr==1,j])/mean(1/fp.path.rml[tr==1,j])^2
+ }
```

### 2.3 Estimation of average treatment effects

The following shows the use of the function `ate.regu.cv`, to estimate the two means ( $\mu^0, \mu^1$ ) and the ATE,  $\mu^1 - \mu^0$ .

```
> ## regularized calibrated estimation
> set.seed(0)
```

```

> ate.cv.rcal <-
+ ate.regu.cv(fold=5*c(1,1), nrho=(1+10)*c(1,1), rho.seq=NULL, y, tr, x,
+           ploss="cal", yloss="gaus")
> matrix(unlist(ate.cv.rcal$est), ncol=2, byrow=T,
+ dimnames=list(c("one", "ipw", "or", "est", "var", "ze",
+ "diff.est", "diff.var", "diff.ze"), c("untreated", "treated")))

```

	untreated	treated
one	0.999776665	1.000252762
ipw	-0.368246088	0.191416564
or	-0.197375029	-0.053716233
est	-0.217788745	0.113076037
var	0.008102314	0.004640538
ze	-2.419529353	1.659917193
diff.est	NA	0.330864782
diff.var	NA	0.008956097
diff.ze	NA	3.496158733

```

> ## regularized maximum likelihood estimation

```

```

> set.seed(0)

```

```

> ate.cv.rml <-

```

```

+ ate.regu.cv(fold=5*c(1,1), nrho=(1+10)*c(1,1), rho.seq=NULL, y, tr, x,
+           ploss="ml", yloss="gaus")
> matrix(unlist(ate.cv.rml$est), ncol=2, byrow=T,
+ dimnames=list(c("one", "ipw", "or", "est", "var", "ze",
+ "diff.est", "diff.var", "diff.ze"), c("untreated", "treated")))

```

	untreated	treated
one	0.856202560	0.972338673
ipw	-0.474703750	0.156331196
or	-0.461081789	0.055241855
est	-0.328482703	0.085678228

var	0.007177901	0.004824676
ze	-3.877160574	1.233492146
diff.est	NA	0.414160931
diff.var	NA	0.008834561
diff.ze	NA	4.406326061

## REFERENCES

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- Robins, J.M., Rotnitzky, A., and Zhao, L.P. (1994) Estimation of regression coefficients when some regressors are not always observed, *Journal of the American Statistical Association*, 89, 846-866.
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