Conditional average treatment effect estimation

```
#> Loading required package: glmnet
#> Loading required package: Matrix
#> Loaded glmnet 4.1-8
```

0.1 Background: CATE estimation and pretraining

In causal inference, we are often interested in predicting the treatment effect for individual observations; this is called the conditional average treatment effect (CATE). For example, before prescribing a drug to a patient, we want to know whether the drug is likely to work well *for that patient* - not just whether it works well on average. One tool to model the CATE is the R-learner (Nie and Wager (2021)), which minimizes the R loss:

$$\hat{L}_n\{\tau(\cdot)\} = \arg\min_{\tau} \frac{1}{n} \sum \Big[(y_i - m^*(x_i)) - (W_i - e^*(x_i))\tau(x_i)\Big]^2.$$

Here, x_i and y_i are the covariates and outcome for observation i, $e^*(x_i)$ is the treatment propensity and W_i the treatment assignment, and $m^*(x_i)$ is the conditional mean outcome ($E[y_i \mid x = x_i]$). Then, $\hat{\tau}$ is the estimate of the heterogeneous treatment effect function.

This is fitted in stages: first, the R-learner fits m^* and e^* to get $\hat{m}^*$ and $\hat{e}^*$; then plugs in $\hat{m}^*(x_i)$ and $\hat{e}^*(x_i)$ to fit τ. A minor detail is that cross-fitting (or prevalidation) is used in the first stage so that the plugin value for e.g. $\hat{m}^*(x_i)$ comes from a model trained without using x_i.

When τ is a linear function, then the second stage of fitting is straightforward. The values $\hat{m}^*(x_i)$ and $\hat{e}^*(x_i)$ are known, and we can use linear regression to model $y_i - \hat{m}^*(x_i)$ as a function of the weighted feature vector $(W_i - \hat{e}^*(x_i))x_i$. This is what we will do in the following example.

How can pretraining be useful here? Well, we are separately fitting models for m^* (the conditional mean) and τ (the heterogeneous treatment effect), and these two functions are likely to share support. We can use pretraining by (1) training a model for m^* and (2) using the support from this model to guide the fitting of τ. Note that the offset is not used in this case; m^* and τ are designed to predict different outcomes.

0.2 A simulated example

Here is an example. We will simplify the problem by assuming treatment has been randomized – the true $e^*(x_i) = 0.5$ for all i.

```r
set.seed(1234)

n = 600; ntrain = 300
p = 20

x = matrix(rnorm(n*p), n, p)

# Treatment assignment
w = rbinom(n, 1, 0.5)

# m^*
m.coefs = c(rep(2,10), rep(0, p-10))
m = x %*% m.coefs
```

```r
# tau
tau.coefs = runif(p, 0.5, 1)*m.coefs
tau = 1.5*m + x%*%tau.coefs

mu = m + w * tau
y  = mu + 10 * rnorm(n)
cat("Signal to noise ratio:", var(mu)/var(y-mu))
#> Signal to noise ratio: 2.301315

# Split into train/test
xtest = x[-(1:ntrain), ]
tautest = tau[-(1:ntrain)]
wtest = w[-(1:ntrain)]

x = x[1:ntrain, ]
y = y[1:ntrain]
w = w[1:ntrain]

# Define training folds
nfolds = 10
foldid = sample(rep(1:10, trunc(nrow(x)/nfolds)+1))[1:nrow(x)]
```

We begin model fitting, starting with our estimate of e^* (the probability of receiving the treatment). To fit τ, we will also need to record the prevalidated $\hat{e}^*$.

```r
e_fit = cv.glmnet(x, w, foldid = foldid,
                  family="binomial", type.measure="deviance",
                  keep = TRUE)

e_hat = e_fit$fit.preval[, e_fit$lambda == e_fit$lambda.1se]
e_hat = 1/(1 + exp(-e_hat))
```

Now, we are ready for stage one of pretraining: fit a model for m^* and record the support. As before, we also record $\hat{m}^*$.

```r
m_fit = cv.glmnet(x, y, foldid = foldid, keep = TRUE)

m_hat = m_fit$fit.preval[, m_fit$lambda == m_fit$lambda.1se]

bhat = coef(m_fit, s = m_fit$lambda.1se)
support = which(bhat[-1] != 0)
```

To fit τ, we will regress $\tilde{y} = y_i - \hat{m}^*(x_i)$ on $\tilde{x} = (w_i - \hat{e}^*(x_i))x_i$; we'll define them here:

```r
y_tilde = y - m_hat
x_tilde = cbind(as.numeric(w - e_hat) * cbind(1, x))
```

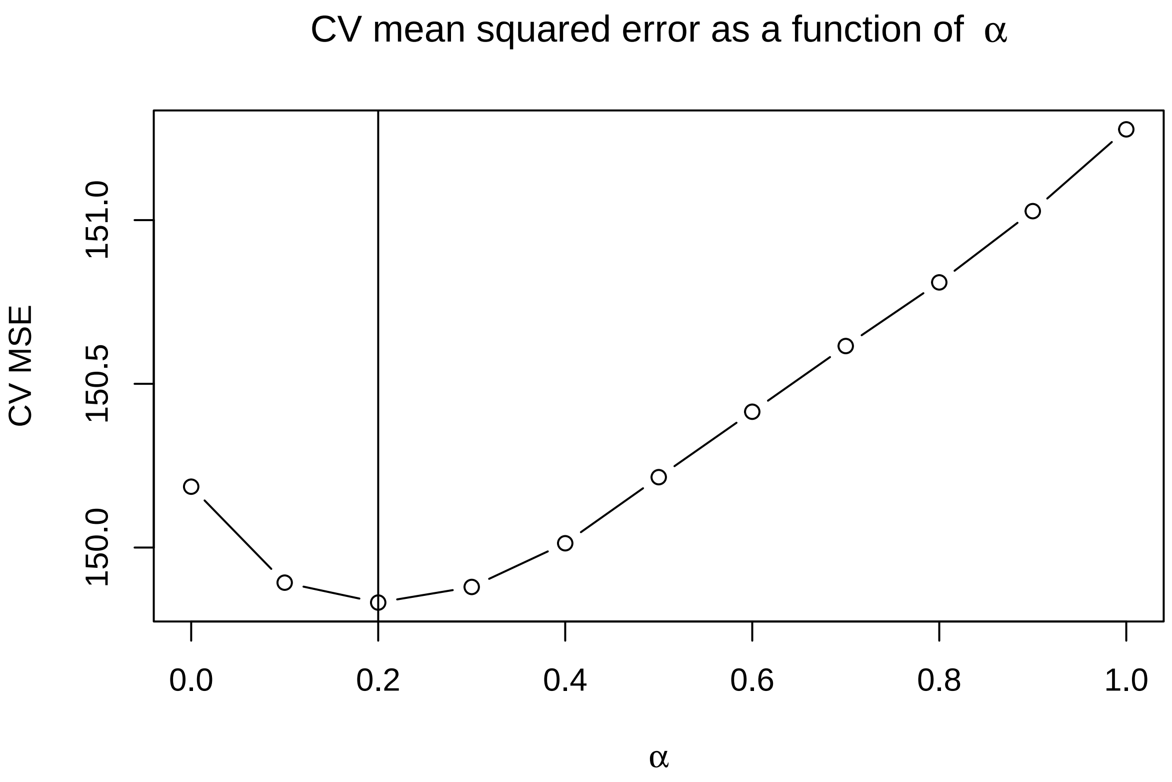
And now, pretraining for τ. Loop over $\alpha = 0, 0.1, \ldots, 1$; for each α, fit a model for τ using the penalty factor defined by the support of $\hat{m}$ and α. We'll keep track of our CV MSE at each step so that we can choose the α that minimizes the MSE.

```r
cv.error = NULL
alphalist = seq(0, 1, length.out = 11)

for(alpha in alphalist){
  pf = rep(1/alpha, p)
  pf[support] = 1
  pf = c(0, pf) # Don't penalize the intercept

  tau_fit = cv.glmnet(x_tilde, y_tilde,
                      foldid = foldid,
                      penalty.factor = pf,
                      intercept = FALSE, # already include in x_tilde
                      standardize = FALSE)
  cv.error = c(cv.error, min(tau_fit$cvm))
}


plot(alphalist, cv.error, type = "b",
     xlab = expression(alpha),
     ylab = "CV MSE",
     main = bquote("CV mean squared error as a function of " ~ alpha))
abline(v = alphalist[which.min(cv.error)])
```



In the plot above, the value at $\alpha = 1$ corresponds to the usual R learner, which makes no assumption about a shared support between τ and m^*. Based on the plot, we choose $\alpha = 0.2$ as our best performing model:

```
best.alpha = alphalist[which.min(cv.error)]
cat("Chosen alpha:", best.alpha)
#> Chosen alpha: 0.2

pf = rep(1/best.alpha, p)
pf[support] = 1
pf = c(0, pf)
tau_fit = cv.glmnet(x_tilde, y_tilde, foldid = foldid,
                    penalty.factor = pf,
                    intercept = FALSE,
                    standardize = FALSE)
```

To concretely compare the pretrained R-learner with the usual R-learner, we'll train the usual R-learner here:

```
tau_rlearner = cv.glmnet(x_tilde, y_tilde, foldid = foldid,
                          penalty.factor = c(0, rep(1, ncol(x))),
                          intercept = FALSE,
                          standardize = FALSE)
```

As anticipated, pretraining improves performance over the R learner – this is how we designed our simulation:

```
rlearner_preds   = predict(tau_rlearner, cbind(1, xtest), s = "lambda.min")
cat("R-learner prediction squared error: ",
    round(mean((rlearner_preds - tautest)^2), 2))
#> R-learner prediction squared error:  45.85

pretrained_preds = predict(tau_fit, cbind(1, xtest), s = "lambda.min")
cat("Pretrained R-learner prediction squared error: ",
    round(mean((pretrained_preds - tautest)^2), 2))
#> Pretrained R-learner prediction squared error:  37.63
```

0.3 What if the pretraining assumption is wrong?

Here, we repeat everything from above, only now there is no overlap in the support of m^* and τ.

```
x = matrix(rnorm(n*p), n, p)

# Treatment assignment
w = rbinom(n, 1, 0.5)

# m^*
m.coefs = c(rep(2,10), rep(0, p-10))
m = x %*% m.coefs

# tau
tau.coefs = c(rep(0, 10), rep(2, 10), rep(0, p-20))
tau = x%*%tau.coefs

mu = m + w * tau
y  = mu + 10 * rnorm(n)
cat("Signal to noise ratio:", var(mu)/var(y-mu))
#> Signal to noise ratio: 0.6938152

# Split into train/test
xtest = x[-(1:ntrain), ]
tautest = tau[-(1:ntrain)]
wtest = w[-(1:ntrain)]

x = x[1:ntrain, ]
y = y[1:ntrain]
w = w[1:ntrain]

# Model fitting: e^*
e_fit = cv.glmnet(x, w, foldid = foldid,
                  family="binomial", type.measure="deviance",
                  keep = TRUE)
e_hat = e_fit$fit.preval[, e_fit$lambda == e_fit$lambda.1se]
e_hat = 1/(1 + exp(-e_hat))

# Model fitting: m^*
m_fit = cv.glmnet(x, y, foldid = foldid, keep = TRUE)

m_hat = m_fit$fit.preval[, m_fit$lambda == m_fit$lambda.1se]

bhat = coef(m_fit, s = m_fit$lambda.1se)
support = which(bhat[-1] != 0)

# Pretraining: tau
y_tilde = y - m_hat
x_tilde = cbind(as.numeric(w - e_hat) * cbind(1, x))

cv.error = NULL
alphalist = seq(0, 1, length.out = 11)

for(alpha in alphalist){
  pf = rep(1/alpha, p)
  pf[support] = 1
  pf = c(0, pf) # Don't penalize the intercept

  tau_fit = cv.glmnet(x_tilde, y_tilde,
                      foldid = foldid,
                      penalty.factor = pf,
                      intercept = FALSE, # already include in x_tilde
                      standardize = FALSE)
  cv.error = c(cv.error, min(tau_fit$cvm))
}

# Our final model for tau:
best.alpha = alphalist[which.min(cv.error)]
cat("Chosen alpha:", best.alpha)
#> Chosen alpha: 1

pf = rep(1/best.alpha, p)
pf[support] = 1
pf = c(0, pf)
tau_fit = cv.glmnet(x_tilde, y_tilde, foldid = foldid,
                    penalty.factor = pf,
                    intercept = FALSE,
                    standardize = FALSE)

# Fit the usual R-learner:
tau_rlearner = cv.glmnet(x_tilde, y_tilde, foldid = foldid,
                         penalty.factor = c(0, rep(1, ncol(x))),
                         intercept = FALSE,
                         standardize = FALSE)

# Measure performance:
```

```r
rlearner_preds = predict(tau_rlearner, cbind(1, xtest), s = "lambda.min")
cat("R-learner prediction squared error: ",
    round(mean((rlearner_preds - tautest)^2), 2))
#> R-learner prediction squared error:  31.11

pretrained_preds = predict(tau_fit, cbind(1, xtest), s = "lambda.min")
cat("Pretrained R-learner prediction squared error: ",
    round(mean((pretrained_preds - tautest)^2), 2))
#> Pretrained R-learner prediction squared error:  31.11
```

Pretraining has not hurt our performance, even though the support of m^* and τ are not shared. Why? Recall that we defined $y = m^*(x) + W * \tau(x) + \epsilon$, so the relationship between y and x is a function of the supports of both m^* and τ. In the first stage of pretraining, we fitted m^* using `y ~ x` – so the fitted support *should* include the support of τ. As a result, using pretraining with the R-learner should not harm predictive performance on average.

Nie, Xinkun, and Stefan Wager. 2021. "Quasi-Oracle Estimation of Heterogeneous Treatment Effects." *Biometrika* 108 (2): 299–319.