

Package mactivate

Examples II

Dave Zes

November 9, 2024

1 Example: Medium Data, Numerical Inputs, Numerical Response

```
library(mactivate)
set.seed(777)
d <- 56
N <- 100000
X <- matrix(rnorm(N*d, 0, 1), N, d) ####
colnames(X) <- paste0("x", 1:(d))
##### primary effects
b <- rep_len( c(-1/4, 1/4), d )
#####

ystar <-
  X %*% b +
  1/3 * (X[, 11]+1) * (X[, 12]-1) * (X[, 33]+1) -
  1/2 * (X[, 30]+0) * (X[, 44]+1) * (X[, 45]-0) * (X[, 56]-1) +
  1/3 * (X[, 6]+1) * (X[, 47]-1) -
  1/2 * (X[, 1]-1) * (X[, 32]+0) * (X[, 33]+1) * (X[, 34]-0) *
  (X[, 45]-0) * (X[, 51]-1)
m_tot <- 12
#####

xs1 <-
```

```

"y ~ . + x11:x12:x33 + x30:x44:x45:x56 + x6:x47 + x1:x32:x33:x34:x45:x51"
xs2 <-
"y ~ . + x11*x12*x33 + x30*x44*x45*x56 + x6*x47 + x1*x32*x33*x34*x45*x51"
xnotQuiteTrue_formula <- eval(parse(text=xs1))
xtrue_formula <- eval(parse(text=xs2))
xnoint_formula <- eval(parse(text="y ~ ."))
yerrs <- rnorm(N, 0, 3)
y <- ystar + yerrs
## y <- (y - mean(y)) / sd(y)

##### standardize X
Xall <- t( ( t(X) - apply(X, 2, mean) ) / apply(X, 2, sd) )
yall <- y
Nall <- N
##### fold index
xxfoldNumber <- rep_len(1:2, N)
ufolds <- sort(unique(xxfoldNumber)) ; ufolds
##### predict
##### predict

dfx <- data.frame("y"=yall, Xall)
##### incorrectly fit LM: no interactions

xlm <- lm(xnoint_formula , data=dfx)
summary(xlm)
yhat <- predict(xlm, newdata=dfx)
sqrt( mean( (yall - yhat)^2 ) )
##### incorrectly fit LM: no lower-order interactions
xlm <- lm(xnotQuiteTrue_formula , data=dfx)
summary(xlm)
yhat <- predict(xlm, newdata=dfx)
sqrt( mean( (yall - yhat)^2 ) )
##### correctly fit LM
xlm <- lm(xtrue_formula, data=dfx)
summary(xlm)
yhat <- predict(xlm, newdata=dfx)
sqrt( mean( (yall - yhat)^2 ) )
##### fit using hybrid m-activation

```

```

##### takes about 1.5-3 hours

xcmact_hybrid <-
  f_control_mactivate(
    param_sensitivity = 10^12,
    bool_free_w = TRUE,
    w0_seed = 0.01,
    w_col_search = "alternate",
    max_internal_iter = 500, #####
    ss_stop = 10^(-14), ###
    escape_rate = 1.003, ##### 1.002,
    Wadj = 1/1,
    force_tries = 0,
    lambda = 0/10000, ### hybrid only
    tol = 10^(-14) ### hybrid only
  )
##### Fit

Uall <- Xall
xthis_fold <- ufolds[ 1 ]
xndx_test <- which( xxfoldNumber %in% xthis_fold )
xndx_train <- setdiff( 1:Nall, xndx_test )
X_train <- Xall[ xndx_train, , drop=FALSE ]
y_train <- yall[ xndx_train ]
xxnow <- Sys.time()
xxls_out <-
  f_fit_hybrid_01(
    X = X_train,
    y = y_train,
    m_tot = m_tot,
    U = X_train,
    m_start = 1,
    mact_control = xcmact_hybrid,
    verbosity = 1
  )
cat( difftime(Sys.time(), xxnow, units="mins"), "\n" )
##### check test error

```

```

U_test <- Xall[ xndx_test, , drop=FALSE ]
X_test <- Xall[ xndx_test, , drop=FALSE ]
y_test <- yall[ xndx_test ]
yhatTT <- matrix(NA, length(xndx_test), m_tot+1)
for(iimm in 0:m_tot) {
  yhat_fold <- predict(object=xxls_out, X0=X_test, U0=U_test, mcols=iimm )
  yhatTT[ , iimm + 1 ] <- yhat_fold
}
errs_by_m <- NULL
for(iimm in 1:ncol(yhatTT)) {
  yhatX <- yhatTT[ , iimm]
  errs_by_m[ iimm ] <- sqrt(mean( (y_test - yhatX)^2 ))
  cat(iimm, ":", errs_by_m[ iimm ])
}
##### plot test RMSE vs m

plot(0:(length(errs_by_m)-1), errs_by_m, type="l", xlab="m", ylab="RMSE Cost")
#### 11 best

```

```

##### known 'true' for non zero-centered is
xtrue_formula_use <- xtrue_formula
xthis_fold <- ufolds[ 1 ]
xndx_test <- which( xxfoldNumber %in% xthis_fold )
xndx_train <- setdiff( 1:Nall, xndx_test )
xlm <- lm(xtrue_formula_use , data=dfx[ xndx_train, ])
yhat <- predict(xlm, newdata=dfx[ xndx_test, ])
sqrt( mean( (y_test - yhat)^2 ) )
#####

```

```

##### Let's dig in
##### We can use train W to construct test Xstar
##### Check which columns drive our response, y

```

```
X_test <- Xall[ xndx_test, ]
y_test <- yall[ xndx_test ]
Xstar_test <- f_mactivate(U=X_test, W=xxls_out[[ length(xxls_out) ]][[ "What" ]])
Xi <- cbind(X_test, Xstar_test)
xlm <- lm(y_test ~ Xi)
sumxlm <- summary(xlm)
```

```
print(sumxlm)
```

Call:

```
lm(formula = y_test ~ Xi)
```

Residuals:

Min	1Q	Median	3Q	Max
-12.6721	-2.0218	-0.0189	2.0268	17.8341

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	2.706e+00	3.882e+00	0.697	0.485760	
Xix1	-2.529e-01	5.311e-02	-4.762	1.92e-06	***
Xix2	2.928e-01	4.076e-02	7.183	6.93e-13	***
Xix3	-2.394e-01	6.772e-02	-3.535	0.000409	***
Xix4	2.901e-01	5.291e-02	5.482	4.22e-08	***
Xix5	-1.933e-01	8.021e-02	-2.409	0.015983	*
Xix6	-5.480e-02	3.740e-02	-1.465	0.142835	
Xix7	-2.412e-01	5.105e-02	-4.725	2.31e-06	***
Xix8	2.832e-01	4.973e-02	5.694	1.25e-08	***
Xix9	-2.380e-01	4.192e-02	-5.677	1.38e-08	***
Xix10	2.814e-01	4.999e-02	5.629	1.82e-08	***
Xix11	-3.069e-01	6.118e-02	-5.017	5.27e-07	***
Xix12	3.381e-01	4.511e-02	7.495	6.74e-14	***
Xix13	-2.237e-01	5.192e-02	-4.308	1.65e-05	***
Xix14	2.723e-01	3.932e-02	6.924	4.46e-12	***
Xix15	-2.244e-01	4.134e-02	-5.427	5.75e-08	***
Xix16	2.955e-01	5.092e-02	5.803	6.54e-09	***
Xix17	-2.419e-01	4.757e-02	-5.085	3.69e-07	***
Xix18	2.535e-01	6.801e-02	3.728	0.000193	***
Xix19	-2.004e-01	8.207e-02	-2.442	0.014614	*
Xix20	3.012e-01	4.416e-02	6.821	9.12e-12	***
Xix21	-2.099e-01	5.010e-02	-4.190	2.79e-05	***
Xix22	2.854e-01	6.367e-02	4.482	7.42e-06	***
Xix23	-2.280e-01	5.350e-02	-4.261	2.04e-05	***
Xix24	2.858e-01	4.097e-02	6.975	3.09e-12	***
Xix25	-2.216e-01	4.775e-02	-4.642	3.46e-06	***
Xix26	2.855e-01	4.316e-02	6.615	3.77e-11	***
Xix27	-1.908e-01	7.456e-02	-2.560	0.010482	*

Xix28	3.146e-01	6.579e-02	4.781	1.75e-06	***
Xix29	-2.218e-01	4.379e-02	-5.065	4.09e-07	***
Xix30	2.936e-01	5.358e-02	5.480	4.26e-08	***
Xix31	-2.128e-01	4.253e-02	-5.003	5.65e-07	***
Xix32	2.775e-01	3.978e-02	6.977	3.06e-12	***
Xix33	-3.369e-01	3.928e-02	-8.576	< 2e-16	***
Xix34	2.802e-01	4.295e-02	6.524	6.91e-11	***
Xix35	-2.099e-01	6.172e-02	-3.401	0.000672	***
Xix36	2.902e-01	5.601e-02	5.180	2.22e-07	***
Xix37	-2.130e-01	6.445e-02	-3.305	0.000951	***
Xix38	3.002e-01	8.099e-02	3.707	0.000210	***
Xix39	-2.601e-01	5.574e-02	-4.666	3.08e-06	***
Xix40	2.896e-01	6.015e-02	4.815	1.48e-06	***
Xix41	-2.460e-01	4.160e-02	-5.913	3.38e-09	***
Xix42	3.086e-01	5.391e-02	5.725	1.04e-08	***
Xix43	-2.435e-01	4.662e-02	-5.222	1.77e-07	***
Xix44	2.848e-01	5.467e-02	5.209	1.91e-07	***
Xix45	-2.204e-01	5.974e-02	-3.689	0.000225	***
Xix46	2.473e-01	5.917e-02	4.179	2.93e-05	***
Xix47	5.280e-01	6.007e-02	8.791	< 2e-16	***
Xix48	2.576e-01	4.636e-02	5.557	2.76e-08	***
Xix49	-2.533e-01	6.713e-02	-3.774	0.000161	***
Xix50	2.834e-01	5.838e-02	4.855	1.21e-06	***
Xix51	-2.187e-01	4.951e-02	-4.417	1.00e-05	***
Xix52	2.511e-01	4.219e-02	5.952	2.67e-09	***
Xix53	-2.323e-01	4.953e-02	-4.691	2.73e-06	***
Xix54	2.729e-01	5.590e-02	4.881	1.06e-06	***
Xix55	-2.274e-01	3.979e-02	-5.714	1.11e-08	***
Xix56	2.814e-01	5.066e-02	5.554	2.81e-08	***
Xi	1.746e-01	2.384e-03	73.242	< 2e-16	***
Xi	2.684e-01	5.615e-03	47.809	< 2e-16	***
Xi	-1.977e-04	8.386e-04	-0.236	0.813601	
Xi	-1.414e-01	5.993e-03	-23.589	< 2e-16	***
Xi	2.328e-04	7.586e-03	0.031	0.975514	
Xi	-4.343e-02	4.186e-04	-103.753	< 2e-16	***
Xi	-2.076e-02	1.866e-02	-1.113	0.265808	
Xi	3.501e-03	8.045e-03	0.435	0.663476	
Xi	3.621e+04	3.032e+05	0.119	0.904920	
Xi	-8.776e+04	9.212e+05	-0.095	0.924103	

```

Xi          5.259e+04  8.601e+05   0.061 0.951251
Xi          -1.046e+03  2.450e+05  -0.004 0.996593
Xi          -4.014e-03  1.411e-02  -0.284 0.776060
Xi           1.569e-02  1.524e-02   1.030 0.302984

```

```
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Residual standard error: 3.019 on 49929 degrees of freedom

Multiple R-squared: 0.4611, Adjusted R-squared: 0.4603

F-statistic: 610.2 on 70 and 49929 DF, p-value: < 2.2e-16

```

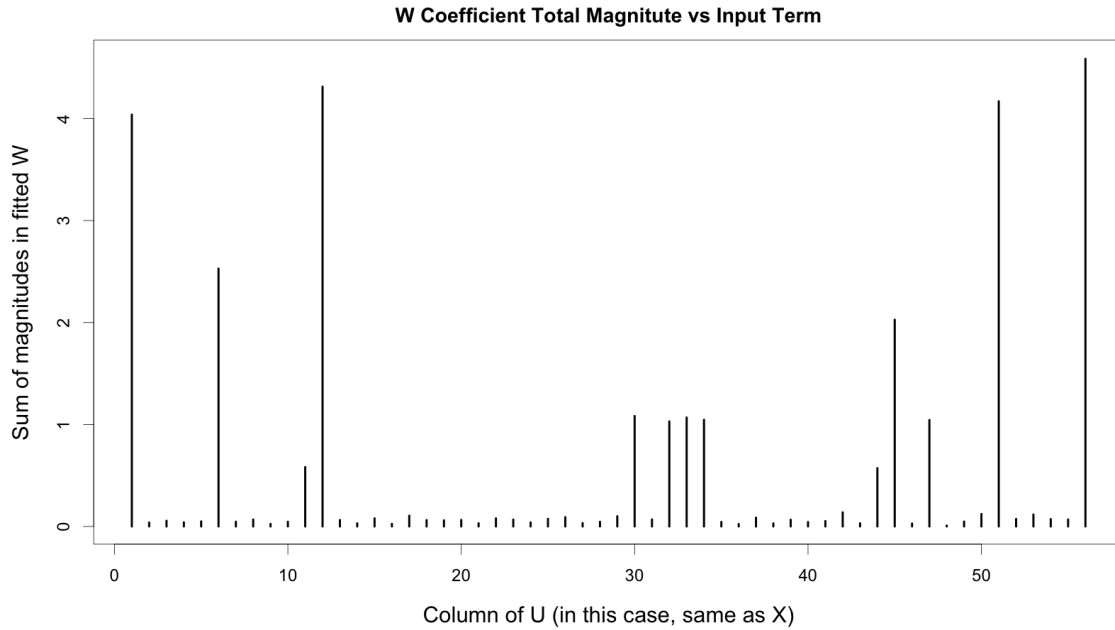
##### Looks like cols 1,2,4,6 are where all the action is
##### (in other word, mactivate didn't track signal on passes 3 and 5)

```

```

bWhat <- xxls_out[[ length(xxls_out) ]][[ "What" ]][[ , c(1,2,4,6) ]
bWhat
wwmag <- apply(bWhat, 1, function(x) { return(sum(abs(x)))} ) ; wwmag
plot(wwmag, type="h", lwd=4,
     main="W Coefficient Total Magnitude vs Input Term",
     xlab="Column of U (in this case, same as X)",
     ylab="Sum of magnitudes in fitted W",
     cex.lab=1.3
    )

```

```
#####
```

```
##### these are the terms in X that
##### appear to have a polynomial contribution
##### to our response, y
```

```
xxhigh <- which(wwmag > 0.5) ; xxhigh
```

```
#####
```

2 Example: Orthopedic Sales Data, Numerical Inputs, Numerical Response, 10-Fold CV

```
data(df_hospitals_ortho)
xvars <- attr(df_hospitals_ortho, "modelvars")
xmx <- as.matrix(df_hospitals_ortho[, xvars])
old_par <- par(mfrow=c(3,4))
for(jj in 1:ncol(xmx)) {
  hist(xmx[,jj], main=colnames(xmx)[jj])
}
```

```

    }
##### pause and look

##### transform

xlog_list <-
  c(
    "tot_sales",
    "tot_knee",
    "tot_hip",
    "beds",
    "rehab_beds",
    "outpatient_visits",
    "adm_costs",
    "revenue_inpatient"
  )
ymx <- xmx
for(jj in 1:ncol(xmx)) {
  ymx[,jj] <- log( xmx[,jj] + 1 )
}
for(jj in 1:ncol(ymx)) {
  hist(ymx[,jj], main=colnames(ymx)[jj])
}
##### pause and look

#### standardize

ymx_stnd <- t( ( t( ymx ) - apply(ymx, 2, mean)) / apply(ymx, 2, sd) )
for(jj in 1:ncol(ymx_stnd)) {
  hist(ymx_stnd[,jj], main=colnames(ymx_stnd)[jj])
}
##### pause and look

##### let's fit an MLR model (in place, no train-test)
ydf_stnd <- as.data.frame(ymx_stnd)

```

```

xlm <- lm( tot_sales ~ . , data=ydf_stnd )
summary(xlm)
yhat <- xlm$fitted
yy <- ydf_stnd[ , "tot_sales" ]
rmse <- sqrt( mean( (yy - yhat)^2 ) ) ; rmse
1 - rmse^2 / 1 ##### r-squared
##### now let's break out m-activation using 10-fold CV

```

```

library(mactivate)
yall <- ymx_stnd[ , "tot_sales" ]
Xall <- ymx_stnd[ , -1 ]
Uall <- Xall
xfolds <- rep_len( 1:10, length(yall) ) ## 10-fold CV
m_tot <- 5
xmcont <-
  f_control_mactivate(
    param_sensitivity = 10^11,
    w0_seed = 0.1,
    max_internal_iter = 500,
    w_col_search = "one",
    bool_headStart = FALSE,
    ss_stop = 10^(-11),
    escape_rate = 1.001,
    step_size = 1/100,
    Wadj = 1/1,
    force_tries = 0,
    lambda = 0,
    tol = 10^(-8)
  )
ufolds <- sort(unique(xfolds))
yout <- numeric(length(yall))
##### takes about 5-10 minutes

for(iif in 1:length(ufolds)) {

  xmask_fold <- xfolds %in% ufolds[ iif ]

  xxls_out <-

```

```

f_fit_hybrid_01(
X=Xall[ !xmask_fold, ],
y=yall[ !xmask_fold ],
m_tot=m_tot,
U = Xall[ !xmask_fold, ],
m_start = 1,
mact_control = xmcont,
verbosity = 0
)

xxls_out

yhatG <- predict(
  object=xxls_out,
  X0=Xall[ xmask_fold, ],
  U0=Uall[ xmask_fold, ],
  mcols=m_tot
)

yout[ xmask_fold ] <- yhatG

cat("Done this fold:", iif, "\n\n")

}

mact_rmse <- sqrt( mean( (yall - yout)^2 ) ) ; mact_rmse
cat("TT R2:", 1 - mact_rmse^2 / 1, "\n") #### m-activation R^2
par(old_par)

```

3 Example: Medium Data, Numerical Inputs, Dichotomous Response

```

library(mactivate)
set.seed(777)
d <- 25
N <- 100000

```

```

X <- matrix(rnorm(N*d, 0, 1), N, d) ####
colnames(X) <- paste0("x", I(1:d))
##### primary effects
b <- rep_len( c(-1/4, 1/4), d )
ystar <-
  X %*% b +
  1/3 * (X[ , 1]+1) * (X[ , 2]-1) * (X[ , 3]+1) -
  1/2 * (X[ , 3]+0) * (X[ , 4]+1) * (X[ , 5]-0) * (X[ , 6]-1) +
  1/3 * (X[ , 6]+1) * (X[ , 7]-1) -
  1/2 * (X[ , 1]-1) * (X[ , 2]+0) * (X[ , 3]+1) * (X[ , 4]-0) *
  (X[ , 5]-0) * (X[ , 7]-1)
m_tot <- 10
#####

xs1 <- "y ~ . + x1:x2:x3 + x3:x4:x5:x6 + x6:x7 + x1:x2:x3:x4:x5:x7"
xs2 <- "y ~ . + x1*x2*x3 + x3*x4*x5*x6 + x6*x7 + x1*x2*x3*x4*x5*x7"
xnotQuiteTrue_formula <- eval(parse(text=xs1))
xtrue_formula <- eval(parse(text=xs2))
xnoint_formula <- eval(parse(text="y ~ ."))
ysigmoid <- 1 / (1 + exp(-ystar))
range(ysigmoid)
y <- rbinom(size=1, n=N, prob=ysigmoid)
##### standardize X
Xall <- t( ( t(X) - apply(X, 2, mean) ) / apply(X, 2, sd) )
yall <- y
Nall <- N
##### fold index
xxfoldNumber <- rep_len(1:2, N)
ufolds <- sort(unique(xxfoldNumber)) ; ufolds
##### predict
##### predict

dfx <- data.frame("y"=yall, Xall)
#####

xglm <- glm(xnoint_formula , data=dfx, family=binomial(link="logit"))
summary(xglm)
yhat <- predict(xglm, newdata=dfx, type="response")

```

```

mean( f_logit_cost(y=yall, yhat=yhat) )
##### known true when zero centered
xglm <- glm(xnotQuiteTrue_formula , data=dfx, family=binomial(link="logit"))
summary(xglm)
yhat <- predict(xglm, newdata=dfx, type="response")
mean( f_logit_cost(y=yall, yhat=yhat) )
##### known true when not zero centered
xglm <- glm(xtrue_formula , data=dfx, family=binomial(link="logit"))
summary(xglm)
yhat <- predict(xglm, newdata=dfx, type="response")
mean( f_logit_cost(y=yall, yhat=yhat) )
##### alternate
##### alternate -- about 1.5 hours

xcmact_gradient <-
  f_control_mactivate(
    param_sensitivity = 10^9,
    bool_free_w = TRUE,
    w0_seed = 0.05,
    w_col_search = "alternate",
    bool_headStart = TRUE,
    ss_stop = 10^(-9), ###
    escape_rate = 1.003,
    Wadj = 1/1,
    force_tries = 0
  )
Uall <- Xall
xthis_fold <- ufolds[ 1 ]
xndx_test <- which( xfoldNumber %in% xthis_fold )
xndx_train <- setdiff( 1:Nall, xndx_test )
X_train <- Xall[ xndx_train, , drop=FALSE ]
y_train <- yall[ xndx_train ]
xxnow <- Sys.time()
xxls_out <-
  f_fit_gradient_logistic_01(
    X = X_train,
    y = y_train,
    m_tot = m_tot,
    U = X_train,

```

```

m_start = 1,
mact_control = xcmact_gradient,
verbosity = 1
)
cat( difftime(Sys.time(), xxnow, units="mins"), "\n" )
U_test <- Xall[ xndx_test, , drop=FALSE ]
X_test <- Xall[ xndx_test, , drop=FALSE ]
y_test <- yall[ xndx_test ]
yhatTT <- matrix(NA, length(xndx_test), m_tot+1)
for(iimm in 0:m_tot) {
  yhat_fold <- predict(object=xxls_out, X0=X_test, U0=U_test, mcols=iimm )
  yhatTT[ , iimm + 1 ] <- yhat_fold[[ "p0hat" ]]
}
errs_by_m <- NULL
for(iimm in 1:ncol(yhatTT)) {
  yhatX <- yhatTT[ , iimm]
  errs_by_m[ iimm ] <- mean( f_logit_cost(y=y_test, yhat=yhatX) )
  cat(iimm, ":", errs_by_m[ iimm ])
}
##### plot test Logit vs m

plot(0:(length(errs_by_m)-1), errs_by_m, type="l", xlab="m", ylab="Logit Cost")
##### use known 'true' in glm()

xglm <- glm(xtrue_formula , data=dfx[ xndx_train, ], family=binomial(link="logit"))
yhat <- predict(xglm, newdata=dfx[ xndx_test, ], type="response")
mean( f_logit_cost(y=y_test, yhat=yhat) )

```