

## Data S2

Demo\_CAM\_MDL.R:

```
rm(list=ls())
setwd('F:/Niya Wang/DCE-MRI')

library(compositions)
library(apcluster)
library(geometry)
library(nnls)

source('measure_conv.R')

#####
X <- read.table('MouseData.txt')
X <- matrix(unlist(X),1609,24)
X <- t(X)

max_pixel <- max(X)
X <- X/max_pixel
X <- X*2^12

data_size<- dim(X)[2]
L <- dim(X)[1]

##### use APC to cluster the observation #####
cat("Performing APC to cluster data\n")

denom <- as.matrix(colSums(X))
num <- dim(X)[1]
denom <- t(denom[,rep(1,num)])

X_proj <- X/denom

sim <- negDistMat(t(X_proj),r=2)
apres <- apcluster(sim,q=0.1)
cluster <- as.vector(unlist(apres@exemplars))

small_cluster <- matrix(numeric(0),0,0)
for (k in 1:length(cluster)){
  if
  (length(as.vector(unlist(apres@clusters[k])))<0.1*dim(X)[2]/length(cluster))
  small_cluster <- c(small_cluster,k)
}

if (length(small_cluster)==0){
  cluster <- cluster
} else {
  cluster <- cluster[-small_cluster]
}
```

```

J <- length(cluster)

J_out <- J
corner <- c(1:J)

##### estimate A and S and calculate MDL#####
cat("Calculating MDL\n")
MDL1 <- matrix(numeric(0), 0,0)
likelihood_all1 <- matrix(numeric(0), 0,0)
penalty_all1 <- matrix(numeric(0), 0,0)
sigma_all1 <- matrix(numeric(0), 0,0)

likelihood_all2 <- matrix(numeric(0), 0,0)
penalty_all2 <- matrix(numeric(0), 0,0)
sigma_all2 <- matrix(numeric(0), 0,0)
MDL2 <- matrix(numeric(0), 0,0)

for (K_est in 2:6){
  if (K_est==J_out){
    A_est <- X_proj[,cluster[corner]]
    ind <- cluster[corner]
  }
  else {
    cornerResult <- measure_conv(X_proj[,cluster[corner]], K_est)

    A_est <- cornerResult[[1]]
    ind <- cornerResult[[2]]
  }

  S_est <- matrix(0,nrow=dim(A_est)[2],ncol=dim(X_proj)[2])
  for (i in 1:ncol(X_proj)){
    S_est[,i] <- coef(nnls(A_est,X[,i]))
  }

  likelihood1 <- (L*J)/2*log(var(as.vector(X[,cluster]-
A_est**S_est[,cluster])))
  likelihood2 <- (L*data_size)/2*log(var(as.vector(X-A_est**S_est)))
  sigma_all1 <- c(sigma_all1,var(as.vector(X[,cluster]-
A_est**S_est[,cluster])))
  sigma_all2 <- c(sigma_all2,var(as.vector(X-A_est**S_est)))

  likelihood_all1 <- c(likelihood_all1,likelihood1)
  likelihood_all2 <- c(likelihood_all2,likelihood2)

  penalty1 <- (K_est*L)/2*log(J)+(K_est*J)/2*log(L) #+log(J*L)/2
  penalty2 <- (K_est*L)/2*log(data_size)+(K_est*data_size)/2*log(L)
#+log(J*L)/2

  penalty_all1 <- c(penalty_all1,penalty1)

```

```
penalty_all2 <- c(penalty_all2,penalty2)
MDL1 <- c(MDL1,(likelihood1+penalty1))
MDL2 <- c(MDL2,(likelihood2+penalty2))
}

rm(sim)
save(list=ls(all=TRUE),file="DCEMRIresult.RData")
```

## Measure\_conv.R:

```
measure_conv <- function(X,N){
  # This function needs the "nnls" package in R, you can use the
  # command:
  # install.packages("nnls")
  # in R interface to install that package if you don't have it.
  require("nnls")

  M <- nrow(X); L <- ncol(X)
  total_index <- t(combn(1:L,N))
  comb <- nrow(total_index)

  error <- matrix(0,comb,1)
  for (p in 1:comb) {
    A <- X[,total_index[p,]]
    Others <- X[,-total_index[p,]]
    Ae <- rbind(1e-5*A, matrix(1,1,N))
    Oe <- rbind(1e-5*Others, matrix(1,1,L-N))
    alpha <- matrix(0,N,L-N)
    for (i in 1:(L-N))
      alpha[,i] <- nnls(Ae, Oe[,i])$x
    error[p] <- norm(Others - A %*% alpha, 'f')^2
  }
  val <- min(error)
  ind <- which.min(error)

  eA <- X[,total_index[ind,]]
  cornerind <- total_index[ind,]
  return(list(eA,cornerind))
}
```

MouseData:

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4.3414834e-004 4.1615205e-004 4.2322060e-004 3.8803644e-004  
4.0360192e-004 4.3456825e-004 4.3404195e-004 4.3012617e-004  
3.9772473e-004 4.1962319e-004 3.7701386e-004 4.1308729e-004

MouseDataResult

A=[ 0.0366 0.0532 0.0352

0.0387 0.0551 0.035

0.0434 0.0513 0.0365

0.0443 0.0527 0.0402

0.0465 0.0503 0.0365

0.0468 0.0487 0.0347

0.0502 0.0447 0.0355

0.0454 0.0433 0.04

0.0442 0.0414 0.0402

0.0447 0.0425 0.0366

0.0439 0.0427 0.037

0.043 0.0393 0.0402

0.0426 0.0371 0.0412

0.0413 0.0376 0.0424

0.04 0.0367 0.0456

0.0412 0.0372 0.0434

0.0399 0.039 0.0422

0.0376 0.0368 0.0473

0.0409 0.0358 0.0447

0.038 0.0376 0.049

0.0376 0.0336 0.0477

0.0376 0.0338 0.0496

0.0372 0.0349 0.0496

0.0381 0.0347 0.0497];

Aorg=[ 0.035 0.051 0.0333

0.037 0.0528 0.0331

0.0419 0.0498 0.035

0.0421 0.0502 0.0379

0.0447 0.0484 0.0348

0.0434 0.0453 0.0319

0.0487 0.0435 0.0342

0.0436 0.0417 0.038

0.0428 0.0402 0.0386

0.0429 0.0409 0.0348

0.0434 0.0424 0.0363

0.0432 0.0396 0.0401

0.0421 0.0368 0.0404

0.0414 0.0378 0.0422

0.0421 0.0387 0.0475

0.0425 0.0385 0.0445

0.0404 0.0397 0.0424

0.0396 0.0389 0.0494

0.0422 0.0371 0.0458

0.0404 0.04 0.0516

0.0402 0.036 0.0505

0.0406 0.0366 0.0531

0.0392 0.0368 0.0518

0.0408 0.0373 0.0528];



eCf=[ 0.0263 0.0405 0.0473 0.0501 0.0505 0.0498 0.0486 0.0472 0.0457 0.0444 0.0432 0.0421  
0.0411 0.0402 0.0395 0.0389 0.0383 0.0378 0.0374 0.0371 0.0368 0.0365 0.0363 0.0361];

eCs=[ 0.0114 0.0208 0.0283 0.034 0.0383 0.0413 0.0434 0.0448 0.0456 0.046 0.0461 0.046  
0.0458 0.0454 0.045 0.0445 0.0441 0.0436 0.0432 0.0427 0.0424 0.042 0.0416 0.0413];

eCp=[ 0.0532 0.0541 0.0532 0.0514 0.0495 0.0476 0.0458 0.0442 0.0428 0.0416 0.0405 0.0396  
0.0388 0.0381 0.0375 0.037 0.0366 0.0362 0.0358 0.0356 0.0353 0.0351 0.0349 0.0347];

eKtrans=[ 0.1897 0.0524];

eKep=[ 0.6521 0.2053];

del\_t=5;