Probabilistic Nested Designs with Sensitivity Indices, version 7

Load packages.

```
In [1]:  require(abind)
         require(data.table)
         require(deSolve)
         require(magrittr)
         require(np)
         require(rTensor)

         require(ggplot2)
         require(GGally)
```

```
Loading required package: abind
Loading required package: data.table
Loading required package: deSolve
Loading required package: magrittr
Loading required package: np
Nonparametric Kernel Methods for Mixed Datatypes (version 0.60-9)
[vignette("np_faq",package="np") provides answers to frequently asked
questions]
[vignette("np",package="np") an overview]
[vignette("entropy_np",package="np") an overview of entropy-based met
hods]
Loading required package: rTensor
Loading required package: ggplot2
Loading required package: GGally
Registered S3 method overwritten by 'GGally':
  method from
  +.gg   ggplot2
```

Function to generate simulations.

```
In [51]:  # Create a multivariate function with specified properties:
          #    tmax: maximum time
          #    multiplicities: number of correlations each parameter has
          #    degrees: polynomial degree of each parameter
          #    dimension: the dimension of the output
          #    returns a multivariate function of the vector of parameters and t
          ime
          makeGenerator <- function(multiplicities, degrees, dimension) {

              single <- function(degree) {
                x0 <- runif(1)
                z0 <- runif(1)
                function(x) {
                    if (x < x0)
                        0
                    else
                        z0 * (x - x0)^degree
                }
              }

              locations <- lapply(multiplicities, function(m) sample(1:dimensio
          n, m))
              functions <- lapply(degrees, single)

              start <- runif(dimension, -0.25, 0.75)
              coefs <- matrix(runif(dimension^2, -0.25, 0.75), dimension, dimen
          sion)
              shift <- matrix(runif(dimension^2, -0.25, 0.75), dimension, dimen
          sion)

              function(x, ts) {
                  z <- rep(0, dimension)
                  for (i in 1:length(locations))
                      for (j in locations[[i]])
                          z[j] <- z[j] + functions[[i]](x[i])
                  ode(start, ts, function(t, y, params) {list((coefs %*% y) * z
          * (1 - ((shift %*% y) * z)))})
              }

          }
```

Functions for nesting designs

```
In [52]:  ssa.digits <- 30
```

```
In [53]:  ssa.scale <- 2^ssa.digits
```

```
In [54]: ssa.level <- function(i) {
             if (i == 0)
                 return(ssa.digits)
             n <- 0
             while (bitwAnd(i, 1) == 0) {
                 n <- n + 1
                 i <- bitwShiftR(i, 1)
             }
             n
         }
```

```
In [55]: ssa.depth <- function(i) {
             ssa.digits - ssa.level(i)
         }
```

```
In [56]: ssa.corner <- function(i, offset=0){
             d <- ssa.level(i) - offset
             c(i - 2^d, i + 2^d)
         }
```

```
In [57]: ssa.corners <- function(i1, i2, i3, offset=0) {
             axis <- function(s1, s2, s3) {
                 if (s1 == 0)
                     4 * s1 + 2 * s2 + s3
                 else
                     4 * (1 - s1) + 2 * (1 - s2) + (1 - s3)
             }
             merge(merge(merge(
                 data.table(
                     d1 = 1,
                     d2 = 2,
                     d3 = 4
                 ),
                 data.table(d1=1, i1=ssa.corner(i1, offset=offset), s1=0:1), b
         y="d1", allow.cartesian=TRUE),
                 data.table(d2=2, i2=ssa.corner(i2, offset=offset), s2=0:1), b
         y="d2", allow.cartesian=TRUE),
                 data.table(d3=4, i3=ssa.corner(i3, offset=offset), s3=0:1), b
         y="d3", allow.cartesian=TRUE
             )[,
             .(
                 i1,
                 i2,
                 i3,
                 axis=mapply(axis, s1, s2, s3)
             )]
         }
```

```
In [58]: ssa.candidates <- function(i1, i2, i3) {
    CJ(
        i1=c(i1, ssa.corner(i1)),
        i2=c(i2, ssa.corner(i2)),
        i3=c(i3, ssa.corner(i3))
    )[,
        .(
            i1,
            i2,
            i3,
            x1 = i1 / ssa.scale,
            x2 = i2 / ssa.scale,
            x3 = i3 / ssa.scale
        )
    ]
}
```

```
In [59]: ssa.start <- function() {
             result <- CJ(
                 i1=c(0, ssa.scale),
                 i2=c(0, ssa.scale),
                 i3=c(0, ssa.scale)
             )[,
                 .(
                     sequence = 1:8      ,
                     generation = 0      ,
                     i1                  ,
                     i2                  ,
                     i3                  ,
                     x1 = i1 / ssa.scale,
                     x2 = i2 / ssa.scale,
                     x3 = i3 / ssa.scale,
                     compute = TRUE      ,
                     measure = FALSE     ,
                     probed  = TRUE      ,
                     s1 = 0              ,
                     s2 = 0              ,
                     s3 = 0              ,
                     s  = 0
                 )
             ]
             result <- rbind(
                 result,
                 data.table(
                     sequence = 9        ,
                     generation = NA     ,
                     i1 = ssa.scale / 2,
                     i2 = ssa.scale / 2,
                     i3 = ssa.scale / 2,
                     x1 = 0.5            ,
                     x2 = 0.5            ,
                     x3 = 0.5            ,
                     compute = FALSE     ,
                     measure = TRUE      ,
                     probed  = FALSE     ,
                     s1 = 0. / 0.        ,
                     s2 = 0. / 0.        ,
                     s3 = 0. / 0.        ,
                     s  = 0. / 0.
                 )
             )
             setkeyv(result, c("i1", "i2", "i3"))
         }
```

```
In [60]: ssa.compute <- function(f, ts, xs, ys) {
    needed <- xs[compute == TRUE]
    for (row in 1:nrow(needed)) {
        ys <- rbind(
            ys,
            data.table(f(as.numeric(needed[row, .(x1, x2, x3)]), ts))
[,
                .(
                    sequence = needed[row, sequence],
                    t = time,
                    y1 = `1`,
                    y2 = `2`,
                    y3 = `3`
                )
            ]
        )
    }
    xs[compute == TRUE, compute := FALSE]
    ys
}
```

```r
ssa.measure <- function(xs, ys, focus=2) {

    result <- merge(
        merge(
            xs[measure == TRUE][, ssa.corners(i1, i2, i3), by=.(cente
r=sequence)],
            xs,
            by=c("i1", "i2", "i3"),
            allow.cartesian=TRUE
        )[, .(center, axis, sequence)],
        ys,
        by="sequence",
        allow.cartesian=TRUE
    )[,
        .(y1 = mean(y1), y2 = mean(y2), y3 = mean(y3)), by=.(sequence
=center, axis, t)
    ][,
        .(s1 = sd(y1), s2 = sd(y2), s3 = sd(y3)), by=.(sequence, t)
    ][,
        .(s1 = max(s1), s2 = max(s2), s3 = max(s3)), by=sequence
    ]

    xs[
        sequence %in% result$sequence,
        `:=`(
            s1=result$s1,
            s2=result$s2,
            s3=result$s3,
            generation=xs[, 1 + max(generation, na.rm=TRUE)]
        )
    ]

    y1min = min(ys$y1)
    y1max = max(ys$y1)
    y2min = min(ys$y2)
    y2max = max(ys$y2)
    y3min = min(ys$y3)
    y3max = max(ys$y3)

    normalize <- function (i, s1, s2, s3)
        max(s1 / (y1max - y1min), s2 / (y2max - y2min), s3 / (y3max -
y3min)) * focus^ssa.depth(i)
    xs[, `:=`(measure = FALSE, s = mapply(normalize, i1, s1, s2, s3))
]

    result
}
```

```r
In [62]: ssa.probe <- function(xs, alpha=1, maxdepth=-log(sqrt(.Machine$doubl
         e.eps),2)) {
             choices <- xs[probed == FALSE & !is.na(s), .(sequence, s)]
             if (nrow(choices) == 1)
                 choice <- choices$sequence
             else
                 choice <- sample(choices$sequence, 1, prob = choices$s^alpha)
             probe <- xs[sequence == choice, .(sequence, i1, i2, i3)]
             xs[
                 probed == FALSE & mapply(ssa.depth, i1) < maxdepth,
                 .(sequence, i1, i2, i3, rank=frank(-s, ties.method="random"))
             ][
                 rank == 1,
                 .(sequence, i1, i2, i3)
             ]
             candidates <- ssa.candidates(probe$i1, probe$i2, probe$i3)
             setkeyv(candidates, c("i1", "i2", "i3"))
             candidates <- candidates[!xs]
             n <- xs[, max(sequence)]
             if (nrow(candidates) > 0) {
                 candidates <- candidates[, .(
                     sequence = n + (1:nrow(candidates)),
                     generation = NA,
                     i1, i2, i3,
                     x1, x2, x3,
                     compute = TRUE ,
                     measure = FALSE,
                     probed  = FALSE,
                     s1 = 0. / 0.,
                     s2 = 0. / 0.,
                     s3 = 0. / 0.,
                     s  = 0. / 0.
                 )]
                 n <- candidates[, max(sequence)]
             }
             probes <- ssa.corners(probe$i1, probe$i2, probe$i3, offset=1)
             probes <- probes[, .(
                 sequence = n + (1:nrow(probes)),
                 generation = NA,
                 i1, i2, i3,
                 x1 = i1 / ssa.scale,
                 x2 = i2 / ssa.scale,
                 x3 = i3 / ssa.scale,
                 compute = FALSE,
                 measure = TRUE ,
                 probed  = FALSE,
                 s1 = 0. / 0.,
                 s2 = 0. / 0.,
                 s3 = 0. / 0.,
                 s  = 0. / 0.
             )]
             if (nrow(candidates) > 0)
                 result <- rbind(
                     xs,
                     candidates,
                     probes
```

```
            )
        else
            result <- rbind(
                xs,
                probes
            )
        result[sequence == probe$sequence, `:=`(compute=TRUE, measure=FAL
SE, probed=TRUE)]
        setkeyv(result, c("i1", "i2", "i3"))
        list(
            sequence=probe$sequence,
            xs=result
        )
}
```

Reproducible random numbers.

```
In [63]:  RNGkind("Mersenne-Twister", "Inversion", "Rejection")
```

```
In [64]:  set.seed(46)
```

Create a simulation function.

```
In [65]:  f <- makeGenerator(c(2, 2, 3), c(0, 1, 2), 3)
```

Example application

Set time resolution.

```
In [17]:  ts <- (0:20) / 2
```

Initialize experiment at bounds of domain.

```
In [18]:  xs <- ssa.start()
```

`xs`

A data.table: 9 x 15

sequence	generation	i1	i2	i3	x1	x2	x3	compute	m
<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<lgl>	
1	0	0	0	0	0.0	0.0	0.0	TRUE	
2	0	0	0	1073741824	0.0	0.0	1.0	TRUE	
3	0	0	1073741824	0	0.0	1.0	0.0	TRUE	
4	0	0	1073741824	1073741824	0.0	1.0	1.0	TRUE	
9	NA	536870912	536870912	536870912	0.5	0.5	0.5	FALSE	
5	0	1073741824	0	0	1.0	0.0	0.0	TRUE	
6	0	1073741824	0	1073741824	1.0	0.0	1.0	TRUE	
7	0	1073741824	1073741824	0	1.0	1.0	0.0	TRUE	
8	0	1073741824	1073741824	1073741824	1.0	1.0	1.0	TRUE	

Iterate several times.

There are two adjustable parameters: `focus` and `alpha`. The `focus` parameter controls the emphasis on depth, with `focus = 0` ignoring depth and `focus = 2` being neutral with respect to depth. The `alpha` parameter controls how peaked the probability of selecting an area to probe is on the nonlinearity there, with `alpha = 0` for no sensitivity to nonlinearity and `alpha = 1` for probability of selection proportional to the amount of nonlinearity.

In [21]:
```r
ys <- NULL
for (k in 1:2500) {
    # Perform pending computations.
    ys <- rbind(ys, ssa.compute(f, ts, xs, NULL))
    # Measure divergences.
    ssa.measure(xs, ys, focus = 0.25)
    # Select where to probe further.
    result <- ssa.probe(xs, alpha = 1)
    # Update grid.
    xs <- result$xs
}
ys <- rbind(ys, ssa.compute(f, ts, xs, NULL))
```

Save results.

```
In [22]: write.table(xs, file="xs-v7.csv", row.names=FALSE, sep=",")
         xs %>% dim
```

54744   15

```
In [23]: write.table(ys, file="ys-v7.csv", row.names=FALSE, sep=",")
         ys %>% dim
```

782103 5

```
In [2]: xs <- fread("xs-v7.csv")
        setkeyv(xs, c("i1", "i2", "i3"))

        ys <- fread("ys-v7.csv")
        setkeyv(ys, c("sequence", "t"))
```

Plot sampling pattern.

```
In [24]: ggpairs(
             xs,
             6:8,
         #   mapping = aes(color=factor(mapply(ssa.depth, i1))),
             lower = list(continuous = wrap("points", alpha = 0.2, size=0.05))
         )
```
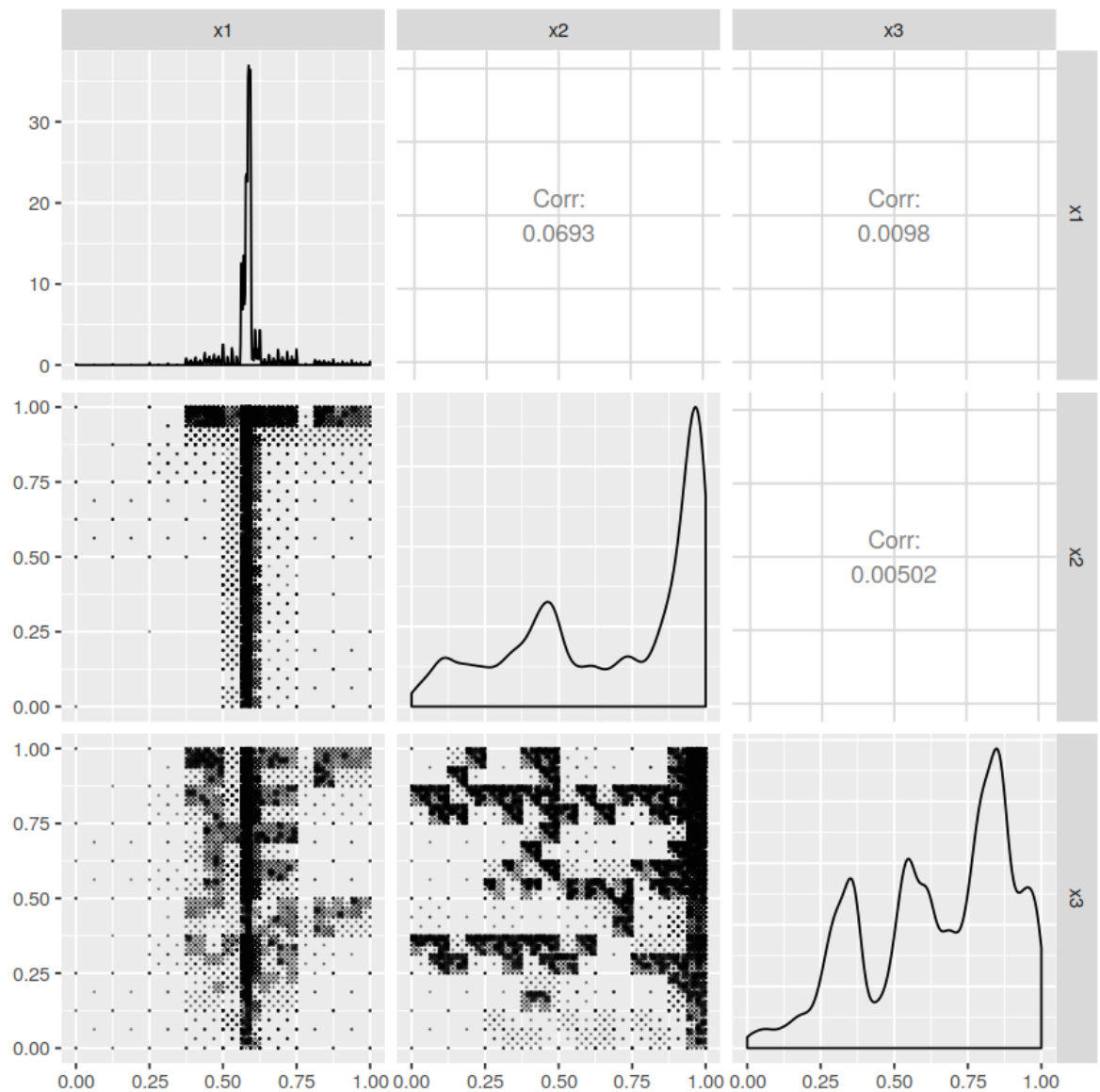

Compute sensitivity indices.

Organize the data for sensitivity analysis, just using the final timestep.

```
In [3]: xys.wide <- merge(
    xs[probed == TRUE, .(sequence, x1, x2, x3)],
    ys[t == 10, .(sequence, y1, y2, y3)]
)
xys.wide %>% head
```

A data.table: 6 x 7

sequence	x1	x2	x3	y1	y2	y3
<int>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
1	0	0	0	-0.1900320	0.5144967	0.4093612
2	0	0	1	5.0782072	1.9488670	2.2320137
3	0	1	0	-0.1437119	0.5511418	0.4093612
4	0	1	1	4.9929679	1.9513684	2.2540234
5	1	0	0	-0.1900320	8.2070979	-1.8065843
6	1	0	1	5.2555080	1.3837551	1.9296318

Function for computing first-order sensitivity index.

Saltelli's method.

This sometimes yields values above one or below zero, but the bootstrapping seems to work better.

```
In [70]:  sensitivity_indices <- function(xy) {
              # Convert to long format.
              xy.tall <- melt(
                  melt(
                      xy,
                      id.vars=c("sequence", "y1", "y2", "y3"),
                      measure.vars=c("x1", "x2", "x3"),
                      variable.name="i",
                      value.name="x"
                  ),
                  id.vars=c("sequence", "i", "x"),
                  measure.vars=c("y1", "y2", "y3"),
                  variable.name="j",
                  value.name="y"
              )
              # Compute `E[y_j]`.
              ybar.all <- xy.tall[, .(ybar.all=mean(y)), by=.(i, j)]
              # Computer `Var[y_j]`.
              var.all <- merge(ybar.all, xy.tall)[, .(var.all=mean((y - ybar.al
          l)^2)), by=.(i, j)]
              # Compute `E[y_j | x_i = x]`.
              ybar.x <- xy.tall[, .(ybar.x=mean(y)), by=.(i, j, x)]
              # Compute `Var[ E[y_j | x_i = x] ]`.
              var.x <- merge(ybar.all, ybar.x)[, .(var.x=mean((ybar.x - ybar.al
          l)^2)), by=.(i, j)]
              # Compute the first-order sensitivity `Var[E[y_j|x_i=x]] / Var[y]
          `.
              s.x <- merge(var.all, var.x)[, .(i, j, s.x=var.x/var.all)]
              # Return the result.
              s.x
          }
```

Literal method.

This yields values between zero and one, but the bootstrapping doesn't seem to work well.

```
In [71]: sensitivity_indices <- function(xy) {
             # Convert to long format.
             xy.tall <- melt(
                 melt(
                     xy,
                     id.vars=c("sequence", "y1", "y2", "y3"),
                     measure.vars=c("x1", "x2", "x3"),
                     variable.name="i",
                     value.name="x"
                 ),
                 id.vars=c("sequence", "i", "x"),
                 measure.vars=c("y1", "y2", "y3"),
                 variable.name="j",
                 value.name="y"
             )
             # Computer `Var[y_j]`.
             var.all <- xy.tall[, .(var.all=var(y)), by=.(i, j)]
             # Compute `E[y_j | x_i = x]`.
             ybar.x <- xy.tall[, .(ybar.x=mean(y)), by=.(i, j, x)]
             # Compute `Var[ E[y_j | x_i = x] ]`.
             var.x <- ybar.x[, .(var.x=var(ybar.x)), by=.(i, j)]
             # Compute the first-order sensitivity `Var[E[y_j|x_i=x]] / Var[y]
         `.
             s.x <- merge(var.all, var.x)[, .(i, j, s.x=var.x/var.all)]
             # Return the result.
             s.x
         }
```

Function to resample sensitivity indices.

This is a very simple bootstrap, just resampling with replacement. It looks like it is biased.

```
In [72]: sensitivity_indices_resample <- function(xy, n) {
             rows <- nrow(xy)
             result <- cbind(n=0, sensitivity_indices(xy))
             for (i in 1:n) {
                 xy.sample <- xy[sample(1:rows, rows, replace=TRUE)]
                 xy.sample[, sequence:=1:rows]
                 result <- rbind(
                     result,
                     cbind(n=i, sensitivity_indices(xy.sample))
                 )
             }
             result
         }
```

Compute the indices.

```
In [73]: s.x <- sensitivity_indices_resample(xys.wide, 1000)
         s.x[n == 0]
```

A data.table: 9 x 4

n	i	j	s.x
<dbl>	<fct>	<fct>	<dbl>
0	x1	y1	0.4521335
0	x1	y2	0.8641704
0	x1	y3	0.6232122
0	x2	y1	0.3204271
0	x2	y2	0.2479287
0	x2	y3	0.2092908
0	x3	y1	0.9118776
0	x3	y2	0.5387907
0	x3	y3	0.7453109

Plot the indices.

```
In [74]: ggplot(s.x[n != 0], aes(x=paste(i, j), y=s.x, color=i)) +
             geom_boxplot() +
             xlab("Indices of x and y") +
             ylab("First-Order Sensitivity Index") +
             guides(color=FALSE) +
             geom_point(data=s.x[n == 0], aes(x=paste(i, j), y=s.x), color="bl
         ack")
```
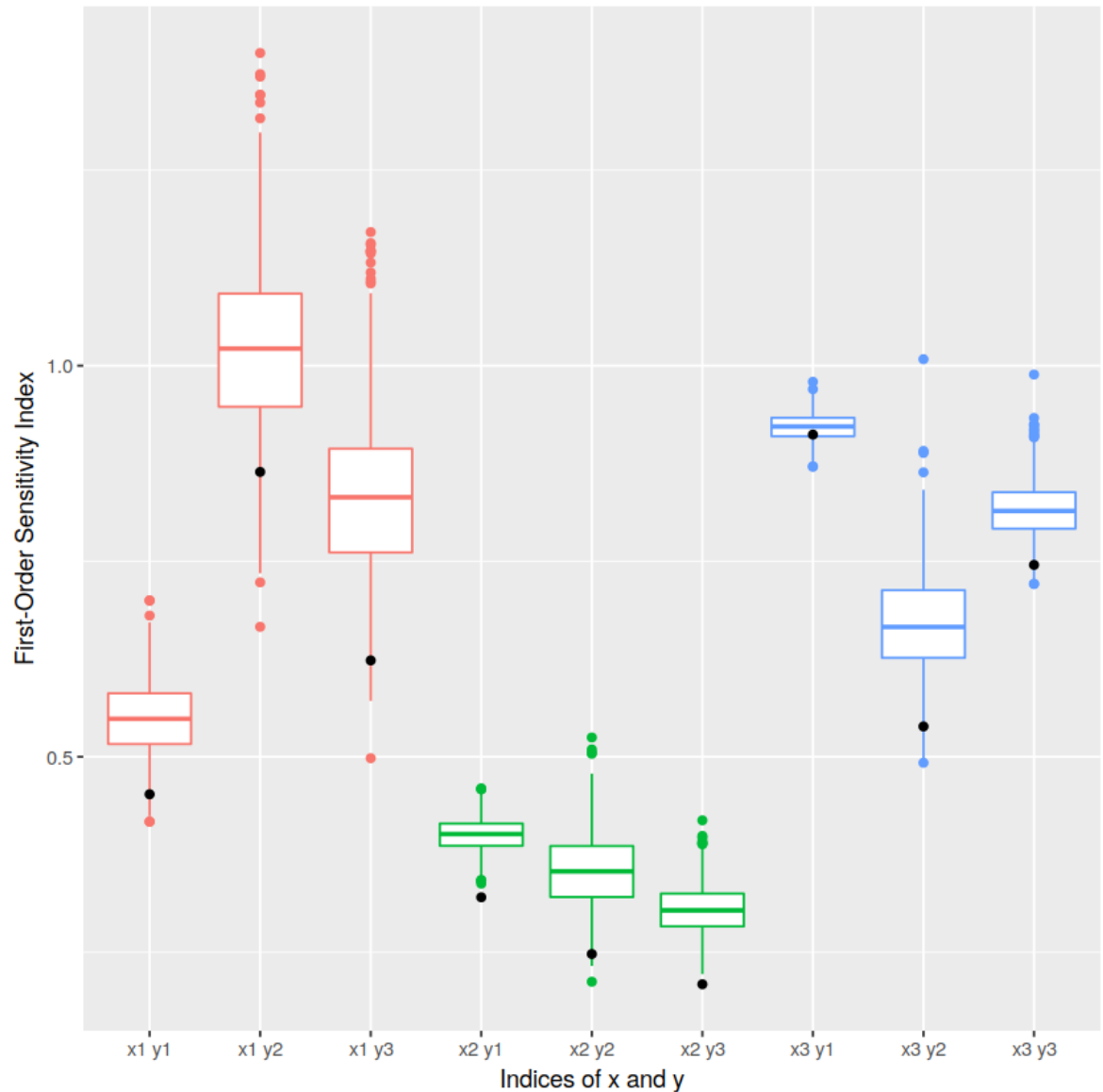

The first-order sensitivity index is `s_ij = Var[ E[y_j | x_i ] ] / Var[ y_j ]`.

The solid black dots show the unbootstrapped estimates. **It is suspicious that the bootstrapped estimates are almost always higher by more than one quartile.**

It looks like `y2` and `y3` have strong dependence on `x1`, and `y1` and `y3` have strong dependence on `x3`. The results do not seem dependenceof `x2`. The dependence of `y1` on `x1` and of `y2` on `x3` is moderate.

Experiment with partitioning data into two contiguous sets and then computing sensitivity indices.

Even though there are the global sensitivities listed above, there might be regions of $(x1, x2, x3)$ where some of those sensitivities disappear or others appear. To investigate this, let's try partitioning $(x1, x2, x3)$ by hyperplanes of constant $x1$, $x2$, or $x3$ and then computing the sensitivity indices on either side of partition. (This is somewhat like Monte-Carlo filtering.)

This is an attempt to find boundaries in the phase diagram of $(x1, x2, x3)$.

Separate by x values into a left and right partition.

```
In [75]: us <- xs[,
             .(u=round((1:6)/7, 3)),
             by=.(sequence)
         ][,
             .(k=c("split on x1", "split on x2", "split on x3")),
             by=.(sequence, u)
         ]
```

```
In [76]: uxys.wide <- merge(us, xys.wide, by="sequence", allow.cartesian=TRUE)
         uxys.wide <- rbind(
             uxys.wide[k == "split on x1" & x1 <  u, .(k, u, s='below split',
         sequence, x1, x2, x3, y1, y2, y3)],
             uxys.wide[k == "split on x1" & x1 >= u, .(k, u, s='above split',
         sequence, x1, x2, x3, y1, y2, y3)],
             uxys.wide[k == "split on x2" & x2 <  u, .(k, u, s='below split',
         sequence, x1, x2, x3, y1, y2, y3)],
             uxys.wide[k == "split on x2" & x2 >= u, .(k, u, s='above split',
         sequence, x1, x2, x3, y1, y2, y3)],
             uxys.wide[k == "split on x3" & x3 <  u, .(k, u, s='below split',
         sequence, x1, x2, x3, y1, y2, y3)],
             uxys.wide[k == "split on x3" & x3 >= u, .(k, u, s='above split',
         sequence, x1, x2, x3, y1, y2, y3)]
         )
         uxys.wide %>% dim
```

```
45144   10
```

```
In [77]: us <- us[, .(s=c("below split", "above split")), by=.(k, u)]
         us.x <- NULL
         for (row in 1:nrow(us))
             us.x <- rbind(
                 us.x,
                 cbind(
                     us[row, .(k, u, s)],
                     sensitivity_indices_resample(merge(us[row], uxys.wide, by
         =c("k", "u", "s")), 1000)
                 )
             )
         us.x %>% dim
```

324324   7

```
In [78]: for (u1 in unique(us$u)) {
             g <- ggplot(us.x[u1 == u & n != 0], aes(x=i, y=s.x, color=s)) +
                 geom_boxplot(outlier.shape=NA) +
                 coord_cartesian(ylim = c(0, 1.25))  +
                 xlab("Indices of x and y") +
                 ylab("First-Order Sensitivity Index") +
                 guides(color=guide_legend(title="Data Subset")) +
                 geom_point(data=us.x[u1 == u & n == 0], aes(x=i, y=s.x, color
         =s)) +
                 facet_grid(k ~ j) +
                 ggtitle(paste("split at", u1))
             print(g)
         }
```
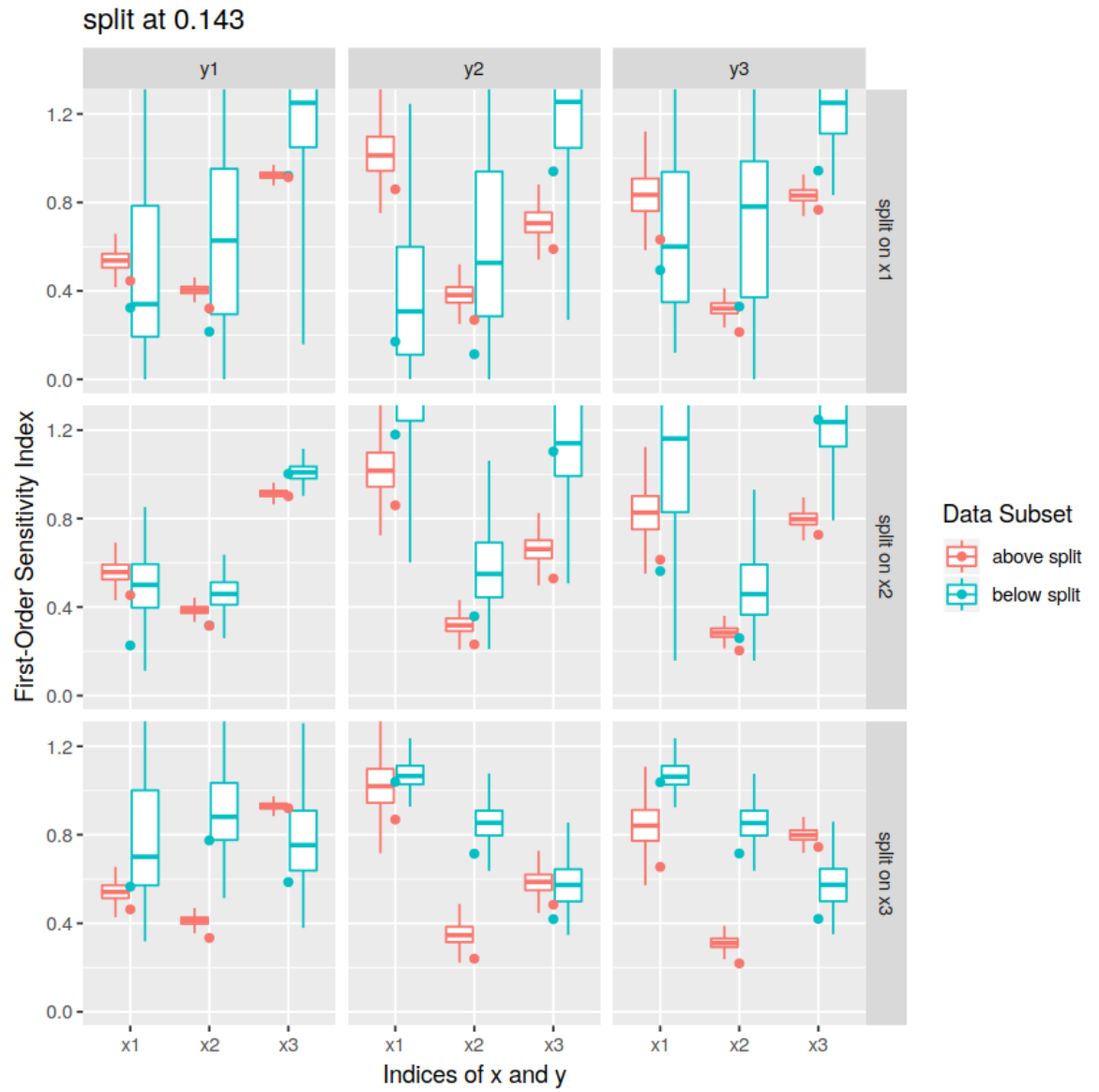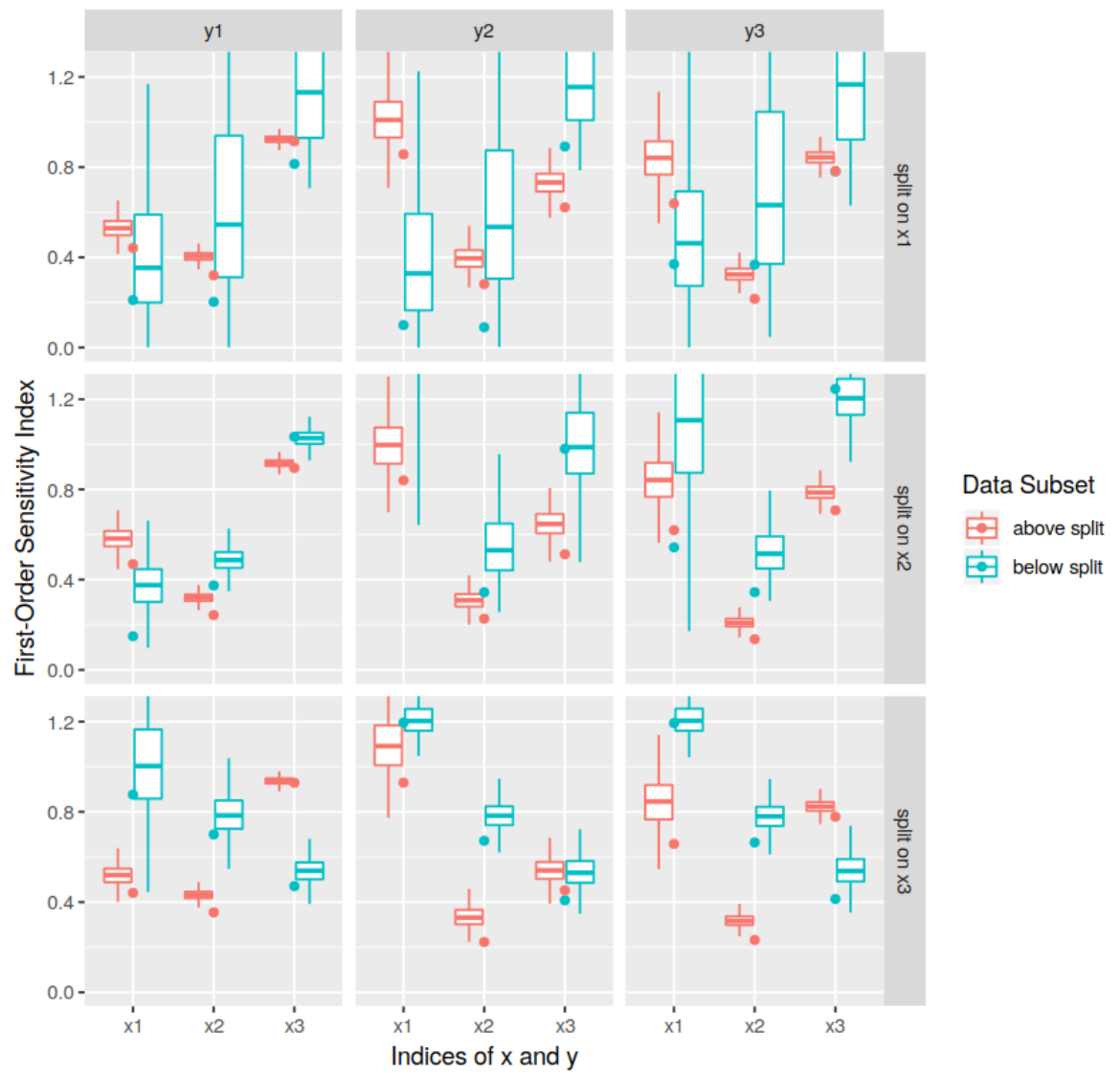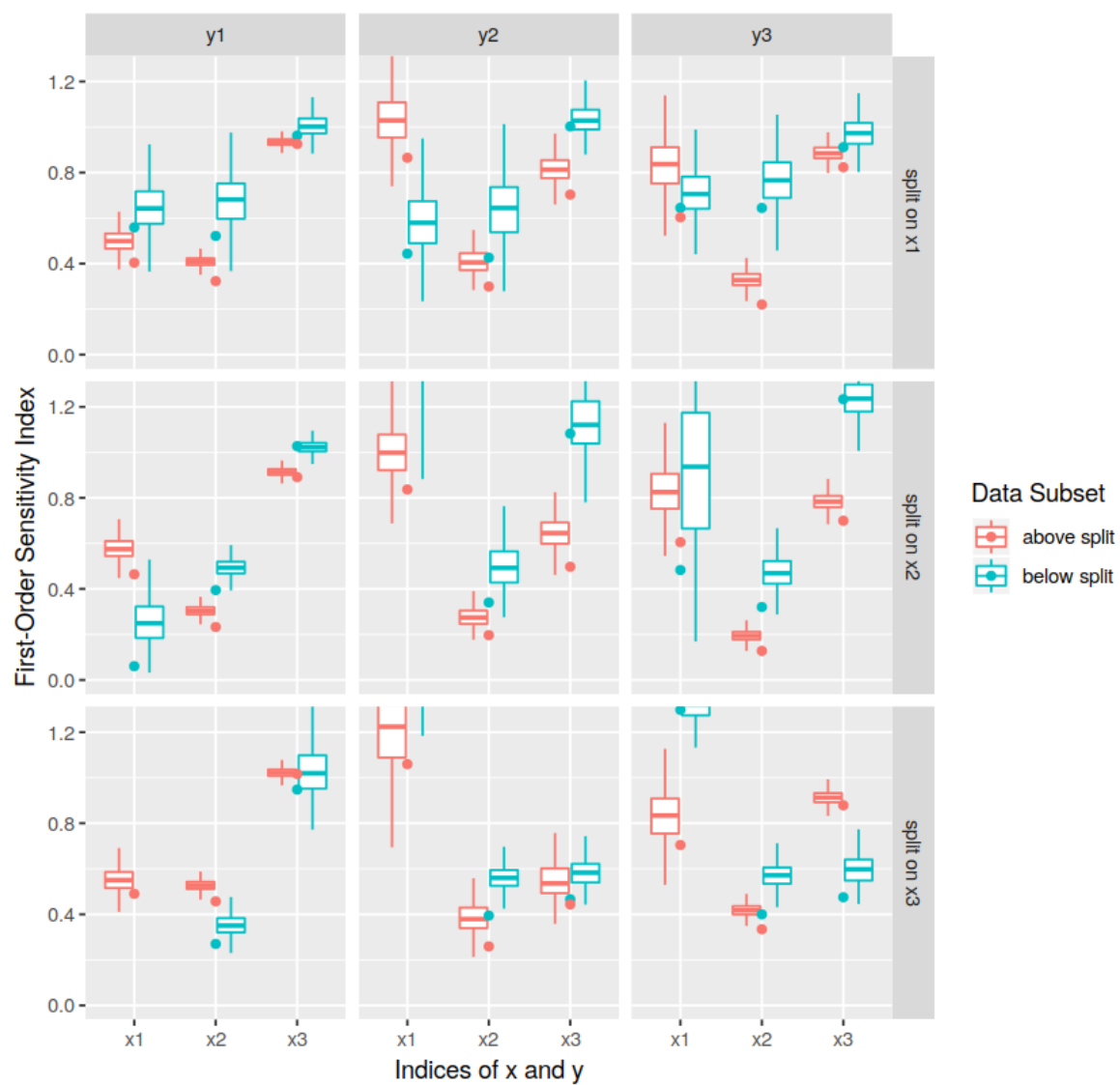
split at 0.286
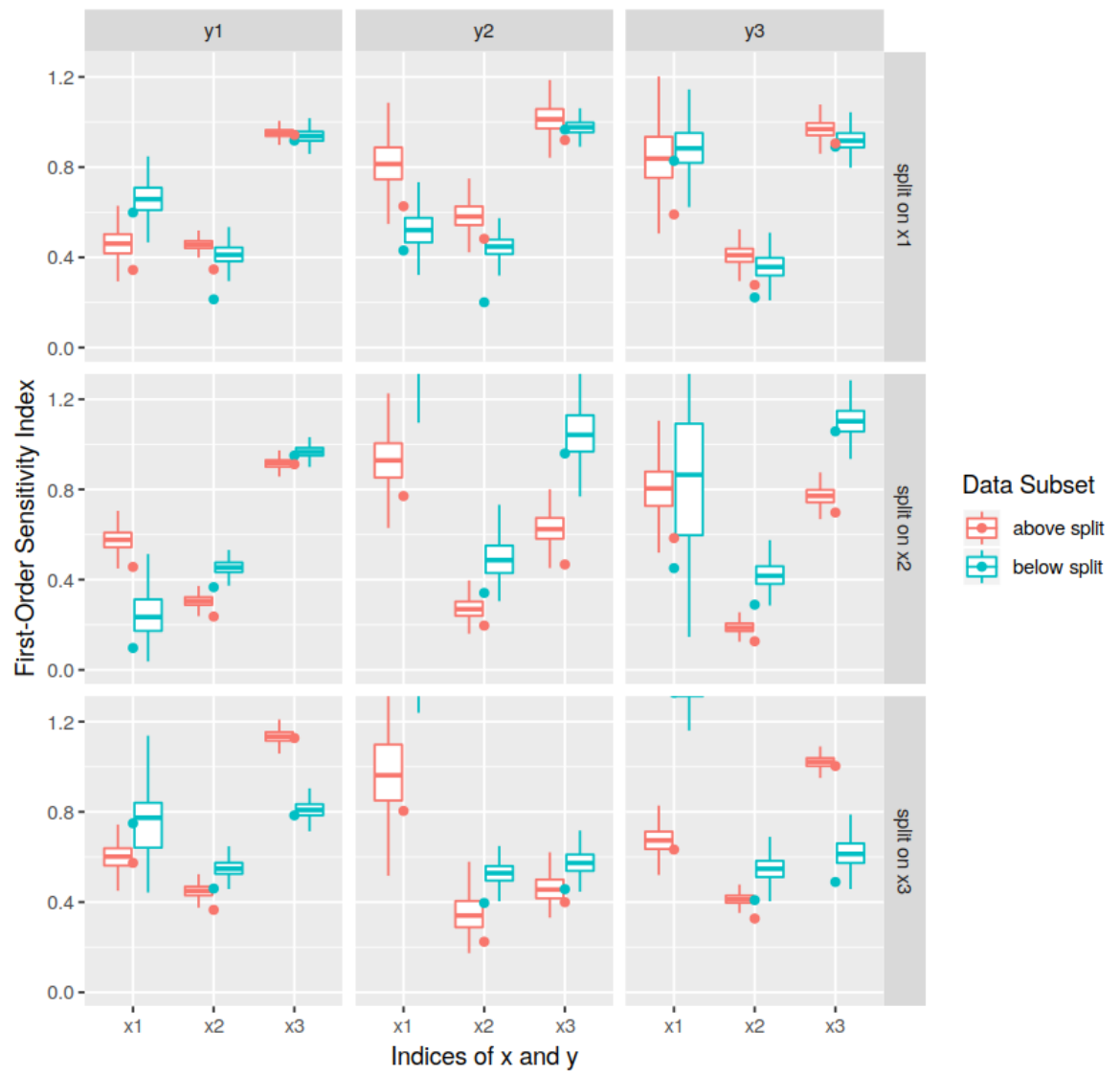
split at 0.714

split at 0.857
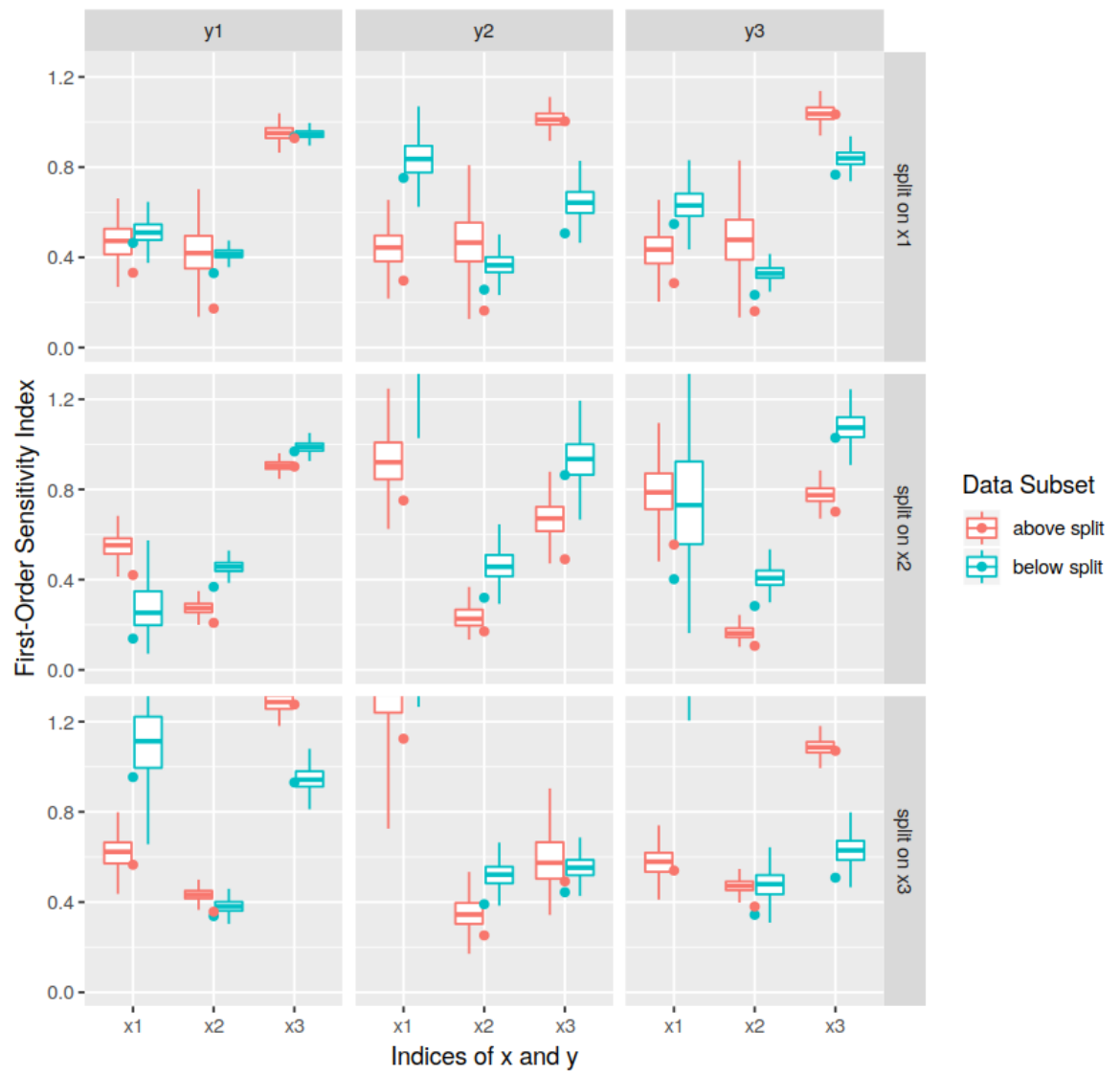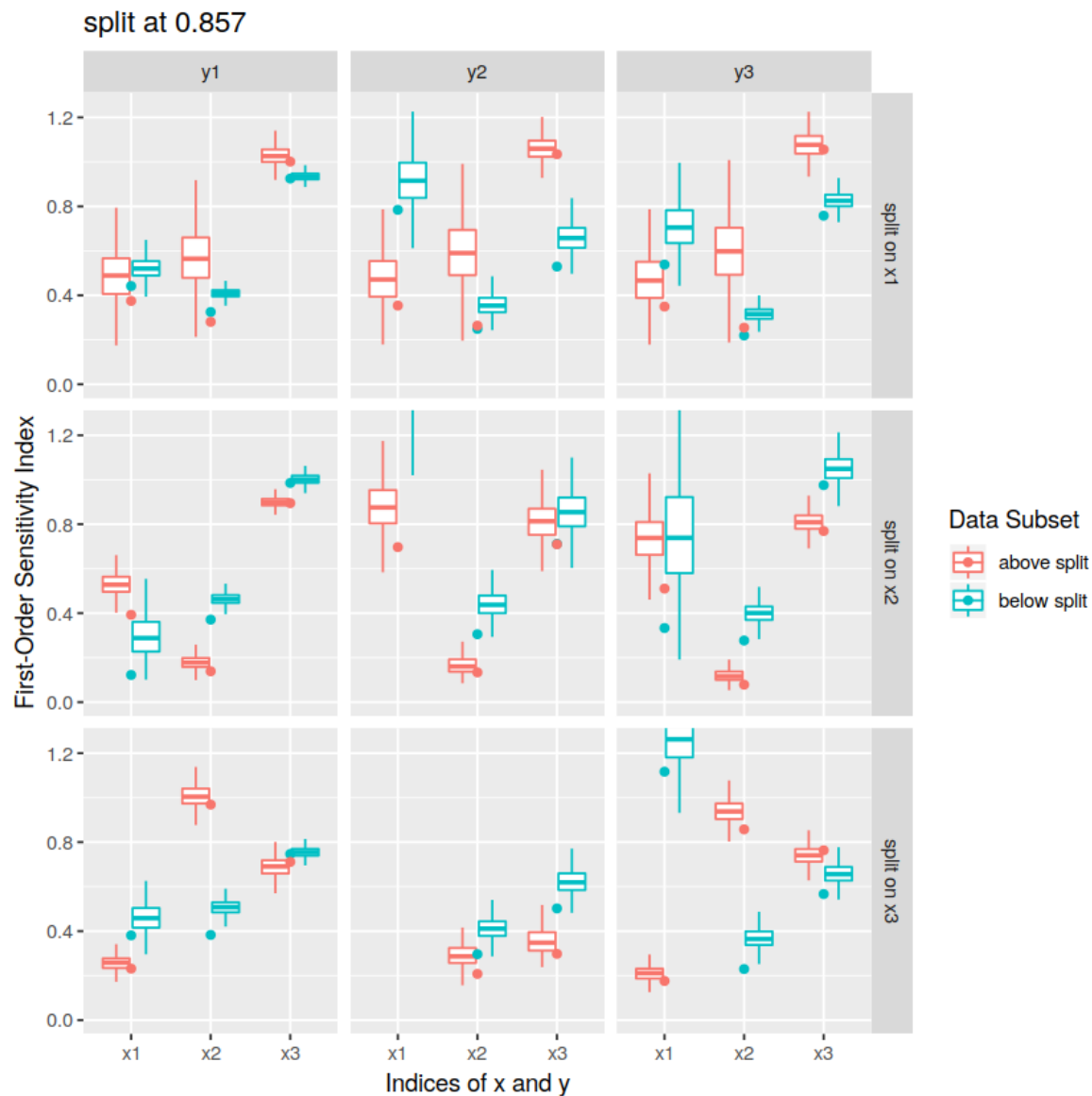
The solid dots show the unbootstrapped estimates.

Splitting `x1`, `x2`, or `x3` at `1/7` doesn't yield significant differences in the sensitivity indices on either side of the split. By the time the split reaches beyond `2/7`, significant differences appear. For example, that of `y3` on `x1` when split into the insignificant `x3 > 6/7` vs the significant `x3 < 6/7`.

Instead of computing the sensitivity indices for each split, just test whether the probability densities on either side of the split are different.

There doesn't seem to be a multivariate KS test available in R, so instead use `npdeneqtest` from the `np` package.

```
In [41]:  tus <- us[, .(1), by=.(k, u)]
          une <- NULL
          for (row in 1:nrow(tus)) {
              z <- merge(tus[row], uxys.wide, by=c("k", "u"))
              une <- rbind(
                  une,
                  cbind(
                      tus[row, .(k, u)],
                      Tn=npdeneqtest(
                          z[s == "below split", .(y1, y2, y3)],
                          z[s == "above split", .(y1, y2, y3)],
                          boot.num=250
                      )$Tn
                  )
              )
          }
          une %>% dim
```

```
Bootstrap replication 1/250...                                    Bootstrap
replication 2/250...                            Bootstrap replicati
on 3/250...                           Bootstrap replication 4/25
0...                            Bootstrap replication 5/250...
Bootstrap replication 6/250...                                    Bootstrap
replication 7/250...                            Bootstrap replicati
on 8/250...                           Bootstrap replication 9/25
0...                            Bootstrap replication 10/250...
Bootstrap replication 11/250...                                        Bootstr
ap replication 12/250...                                Bootstrap repl
ication 13/250...                             Bootstrap replication
14/250...                             Bootstrap replication 15/25
0...                            Bootstrap replication 16/250...
Bootstrap replication 17/250...                                        Bootstr
ap replication 18/250...                                Bootstrap repl
ication 19/250...                             Bootstrap replication
20/250...                             Bootstrap replication 21/25
0...                            Bootstrap replication 22/250...
Bootstrap replication 23/250...                                        Bootstr
ap replication 24/250...                                Bootstrap repl
ication 25/250...                             Bootstrap replication
26/250...                             Bootstrap replication 27/25
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Bootstrap replication 29/250...                                        Bootstr
ap replication 30/250...                                Bootstrap repl
ication 31/250...                             Bootstrap replication
32/250...                             Bootstrap replication 33/25
0...                            Bootstrap replication 34/250...
Bootstrap replication 35/250...                                        Bootstr
ap replication 36/250...                                Bootstrap repl
ication 37/250...                             Bootstrap replication
38/250...                             Bootstrap replication 39/25
0...                            Bootstrap replication 40/250...
Bootstrap replication 41/250...                                        Bootstr
ap replication 42/250...                                Bootstrap repl
ication 43/250...                             Bootstrap replication
44/250...                             Bootstrap replication 45/25
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Bootstrap replication 47/250...                                        Bootstr
ap replication 48/250...                                Bootstrap repl
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ication 61/250...                             Bootstrap replication
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0...                            Bootstrap replication 64/250...
Bootstrap replication 65/250...                                        Bootstr
ap replication 66/250...                                Bootstrap repl
ication 67/250...                             Bootstrap replication
68/250...                             Bootstrap replication 69/25
```

```
0...
Bootstrap replication 71/250...
ap replication 72/250...
ication 73/250...
74/250...
0...
Bootstrap replication 77/250...
ap replication 78/250...
ication 79/250...
80/250...
0...
Bootstrap replication 83/250...
ap replication 84/250...
ication 85/250...
86/250...
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Bootstrap replication 89/250...
ap replication 90/250...
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Bootstrap replication 109/250...
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cation 112/250...
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Bootstrap replication 117/250...
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replication 119/250...
cation 120/250...
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Bootstrap replication 125/250...
trap replication 126/250...
replication 127/250...
cation 128/250...
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Bootstrap replication 133/250...
trap replication 134/250...
replication 135/250...

Bootstrap replication 70/250...
                       Bootstr
              Bootstrap repl
          Bootstrap replication
       Bootstrap replication 75/25
Bootstrap replication 76/250...
                       Bootstr
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```

```
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8/250...                                           Bootstrap replication 139/25
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trap replication 142/250...                                             Bootstrap
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replication 175/250...                                          Bootstrap repli
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trap replication 182/250...                                             Bootstrap
replication 183/250...                                          Bootstrap repli
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Bootstrap replication 189/250...                                           Boots
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replication 191/250...                                          Bootstrap repli
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trap replication 198/250...                                             Bootstrap
replication 199/250...                                          Bootstrap repli
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```

```
n 201/250...                              Bootstrap replication 20
2/250...                          Bootstrap replication 203/25
0...                         Bootstrap replication 204/250...
Bootstrap replication 205/250...                            Boots
trap replication 206/250...                             Bootstrap
replication 207/250...                            Bootstrap repli
cation 208/250...                          Bootstrap replicatio
n 209/250...                          Bootstrap replication 21
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n 217/250...                          Bootstrap replication 21
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Bootstrap replication 221/250...                            Boots
trap replication 222/250...                             Bootstrap
replication 223/250...                            Bootstrap repli
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n 225/250...                          Bootstrap replication 22
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Bootstrap replication 229/250...                            Boots
trap replication 230/250...                             Bootstrap
replication 231/250...                            Bootstrap repli
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n 233/250...                          Bootstrap replication 23
4/250...                          Bootstrap replication 235/25
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Bootstrap replication 237/250...                            Boots
trap replication 238/250...                             Bootstrap
replication 239/250...                            Bootstrap repli
cation 240/250...                          Bootstrap replicatio
n 241/250...                          Bootstrap replication 24
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0...                         Bootstrap replication 244/250...
Bootstrap replication 245/250...                            Boots
trap replication 246/250...                             Bootstrap
replication 247/250...                            Bootstrap repli
cation 248/250...                          Bootstrap replicatio
n 249/250...                          Bootstrap replication 25
0/250...

18  3
```

```
In [42]: ggplot(une, aes(x=u, y=Tn, color=k)) +
            geom_point() +
            geom_line() +
            xlab("split location") +
            ylab("test statistic (standardized)")
```
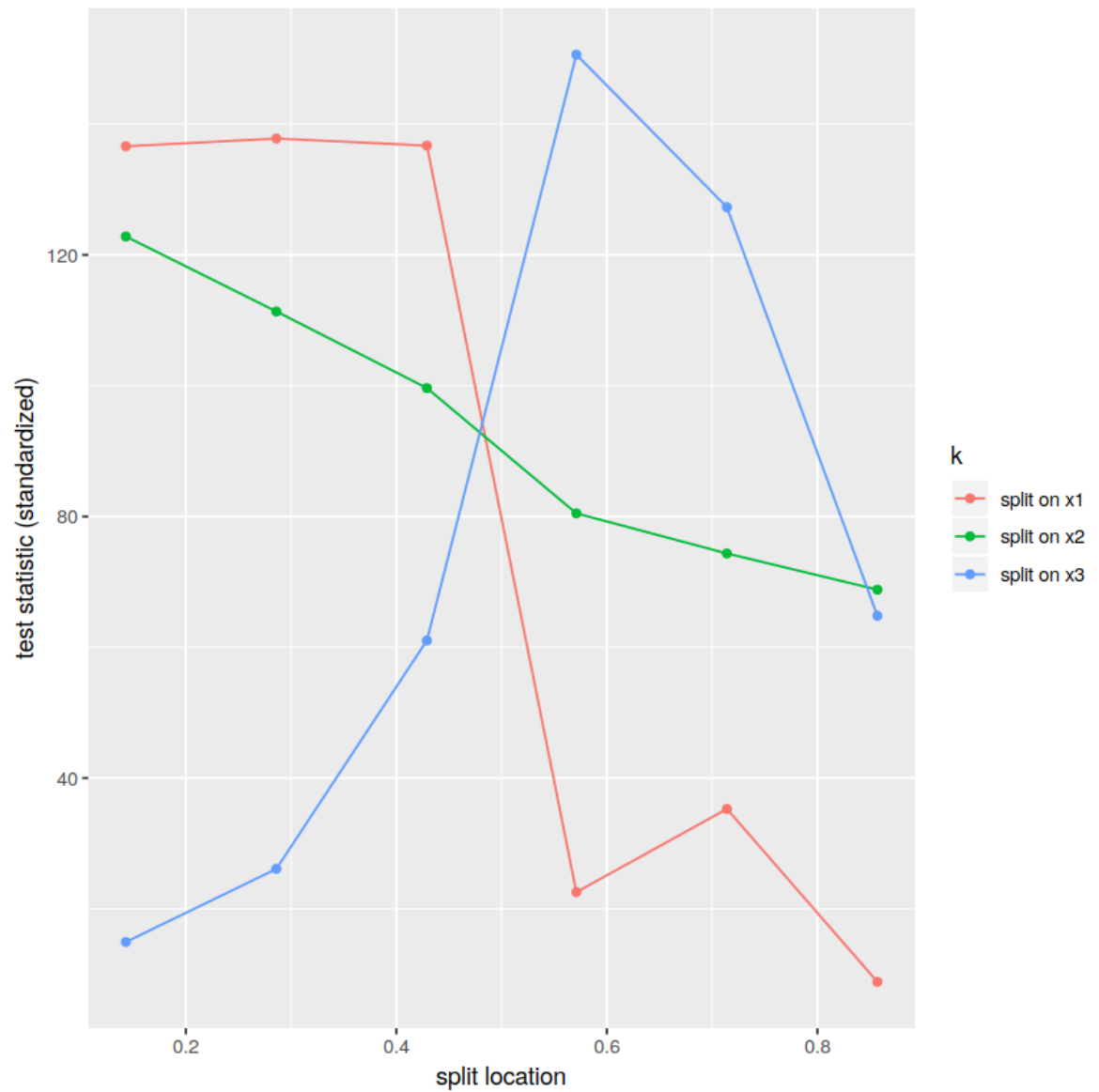

This clearly identifies the phase boundary near $x2 = 1/2$.

Repeat with bootstrap confidence intervals.

```r
In [46]: twosample_test_resample <- function(xy, n) {
    rows <- nrow(xy)
    result <- cbind(
        n=0,
        Tn=npdeneqtest(
            xy[s == "below split", .(y1, y2, y3)],
            xy[s == "above split", .(y1, y2, y3)],
            boot.num=250
        )$Tn
    )
    for (i in 1:n) {
        xy.sample <- xy[sample(1:rows, rows, replace=TRUE)]
        xy.sample[, sequence:=1:rows]
        xy.sample <- merge(tus[row], xy.sample, by=c("k", "u"))
        result <- rbind(
            result,
            cbind(
                n=i,
                Tn=npdeneqtest(
                    xy.sample[s == "below split", .(y1, y2, y3)],
                    xy.sample[s == "above split", .(y1, y2, y3)],
                    boot.num=250
                )$Tn
            )
        )
    }
    result
}
```

```
In [47]: tus <- us[, .(1), by=.(k, u)]
         une <- NULL
         for (row in 1:nrow(tus))
             une <- rbind(
                 une,
                 cbind(
                     tus[row, .(k, u)],
                     twosample_test_resample(merge(tus[row], uxys.wide, by=c(
         "k", "u")), 15)
                 )
             )
         une %>% dim
```

```
Bootstrap replication 1/250...                                    Bootstrap
replication 2/250...                               Bootstrap replicati
on 3/250...                                Bootstrap replication 4/25
0...                                    Bootstrap replication 5/250...
Bootstrap replication 6/250...                                    Bootstrap
replication 7/250...                               Bootstrap replicati
on 8/250...                                Bootstrap replication 9/25
0...                                    Bootstrap replication 10/250...
Bootstrap replication 11/250...                                    Bootstr
ap replication 12/250...                               Bootstrap repl
ication 13/250...                                Bootstrap replication
14/250...                                Bootstrap replication 15/25
0...                                    Bootstrap replication 16/250...
Bootstrap replication 17/250...                                    Bootstr
ap replication 18/250...                               Bootstrap repl
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20/250...                                Bootstrap replication 21/25
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Bootstrap replication 23/250...                                    Bootstr
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ication 43/250...                                Bootstrap replication
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Bootstrap replication 47/250...                                    Bootstr
ap replication 48/250...                               Bootstrap repl
ication 49/250...                                Bootstrap replication
50/250...                                Bootstrap replication 51/25
0...                                    Bootstrap replication 52/250...
Bootstrap replication 53/250...                                    Bootstr
ap replication 54/250...                               Bootstrap repl
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56/250...                                Bootstrap replication 57/25
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ap replication 60/250...                               Bootstrap repl
ication 61/250...                                Bootstrap replication
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0...                                    Bootstrap replication 64/250...
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ap replication 66/250...                               Bootstrap repl
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68/250...                                Bootstrap replication 69/25
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```
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ap replication 72/250...                                       Bootstrap repl
ication 73/250...                                     Bootstrap replication
74/250...                                   Bootstrap replication 75/25
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ication 79/250...                                     Bootstrap replication
80/250...                                   Bootstrap replication 81/25
0...                                       Bootstrap replication 82/250...
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ap replication 84/250...                                       Bootstrap repl
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trap replication 126/250...                                         Bootstrap
replication 127/250...                                       Bootstrap repli
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```
cation 136/250...                                Bootstrap replicatio
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2/250...                                    Bootstrap replication 203/25
0...                                    Bootstrap replication 204/250...
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cation 208/250...                                    Bootstrap replicatio
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replication 215/250...                                    Bootstrap repli
cation 216/250...                                    Bootstrap replicatio
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```

Warning message in EssDee(dcon):
"variable 1 appears to be constantvariable 2 appears to be constantva
riable 3 appears to be constant"Warning message in min(x[x > 0]):
"no non-missing arguments to min; returning Inf"Warning message in mi
n(x[x > 0]):
"no non-missing arguments to min; returning Inf"Warning message in mi
n(x[x > 0]):
"no non-missing arguments to min; returning Inf"

```
Error in system.time(myout <- .C("np_density_bw", as.double(duno), a
s.double(dord), : NA/NaN/Inf in foreign function call (arg 4)
Traceback:

1. rbind(une, cbind(tus[row, .(k, u)], twosample_test_resample(merge
(tus[row],
.        uxys.wide, by = c("k", "u")), 15)))
2. cbind(tus[row, .(k, u)], twosample_test_resample(merge(tus[row],
.        uxys.wide, by = c("k", "u")), 15))
3. twosample_test_resample(merge(tus[row], uxys.wide, by = c("k",
.        "u")), 15)
4. rbind(result, cbind(n = i, Tn = npdeneqtest(xy.sample[s == "below
split",
.        .(y1, y2, y3)], xy.sample[s == "above split", .(y1, y2, y3)],
.        boot.num = 250)$Tn))   # at line 15-25 of file <text>
5. cbind(n = i, Tn = npdeneqtest(xy.sample[s == "below split", .(y1,
.        y2, y3)], xy.sample[s == "above split", .(y1, y2, y3)], boot.n
um = 250)$Tn)   # at line 15-25 of file <text>
6. npdeneqtest(xy.sample[s == "below split", .(y1, y2, y3)], xy.sampl
e[s ==
.        "above split", .(y1, y2, y3)], boot.num = 250)   # at line 15-
25 of file <text>
7. npudensbw(dat = x, ...)
8. npudensbw.NULL(dat = x, ...)
9. npudensbw.default(dat = dat, bws = bws, ...)
10. eval(parse(text = paste("npudensbw.bandwidth(dat=dat, bws=tbw",
.        ifelse(any.m, ",", ""), paste(mc.names[m], ifelse(any.m,
.            "=", ""), mc.names[m], collapse = ", "), ")")))
11. eval(parse(text = paste("npudensbw.bandwidth(dat=dat, bws=tbw",
.        ifelse(any.m, ",", ""), paste(mc.names[m], ifelse(any.m,
.            "=", ""), mc.names[m], collapse = ", "), ")")))
12. npudensbw.bandwidth(dat = dat, bws = tbw)
13. system.time(myout <- .C("np_density_bw", as.double(duno), as.doub
le(dord),
.        as.double(dcon), as.double(mysd), as.integer(myopti), as.doub
le(myoptd),
.        bw = c(bws$bw[bws$icon], bws$bw[bws$iuno], bws$bw[bws$iord]),
.        fval = double(2), fval.history = double(max(1, nmulti)),
.        timing = double(1), PACKAGE = "np")[c("bw", "fval", "fval.his
tory",
.        "timing")])
```
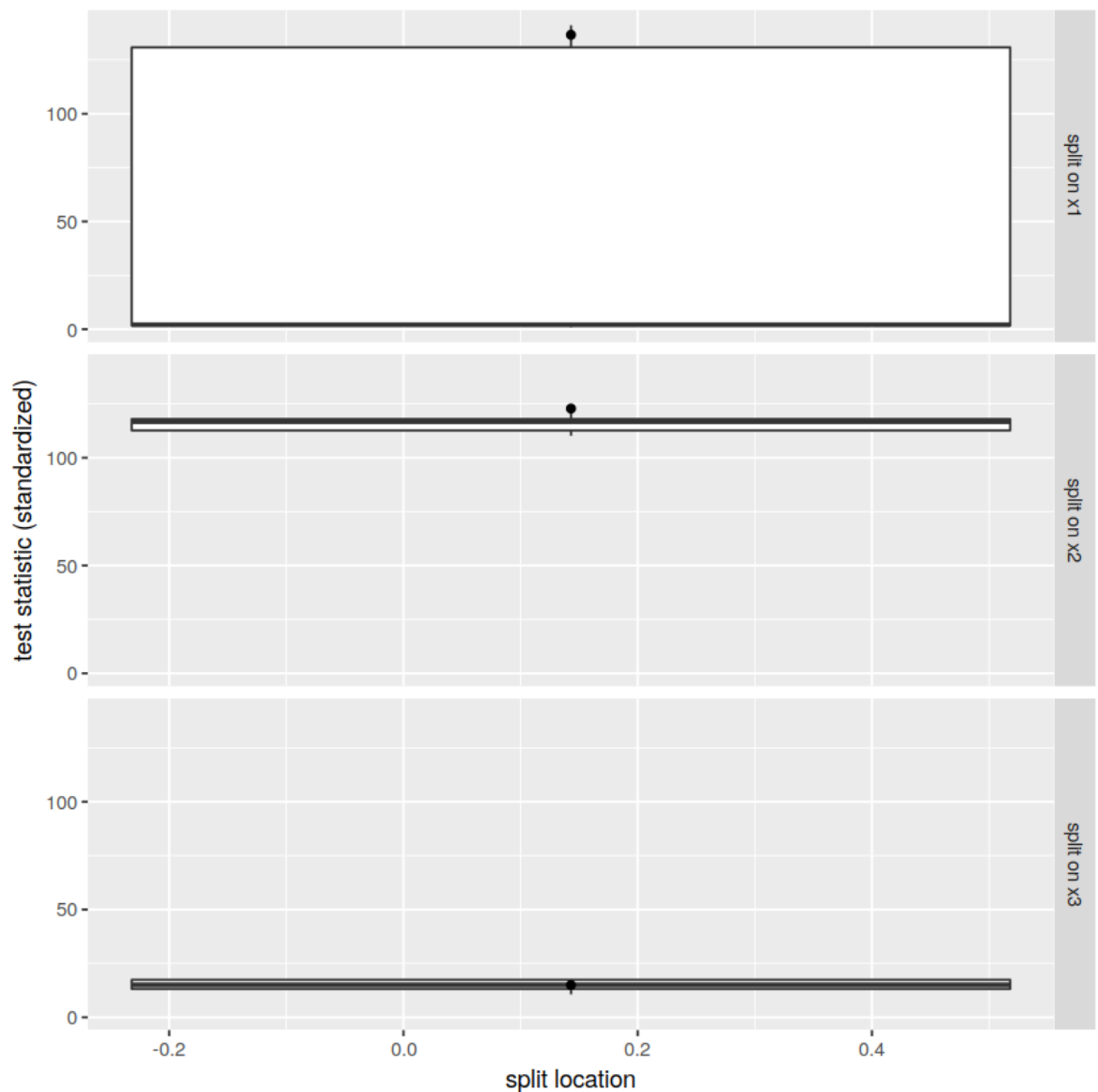
Timing stopped at: 0.005 0 0.005

FIXME: Look into why this failed.

`une %>% summary`

```
        k                  u                 n                Tn
 Length:48         Min.   :0.143     Min.   : 0.00     Min.   :  1.034
 Class :character  1st Qu.:0.143     1st Qu.: 3.75     1st Qu.: 11.409
 Mode  :character  Median :0.143     Median : 7.50     Median : 30.714
                   Mean   :0.143     Mean   : 7.50     Mean   : 61.100
                   3rd Qu.:0.143     3rd Qu.:11.25     3rd Qu.:117.182
                   Max.   :0.143     Max.   :15.00     Max.   :141.062
```

In [81]:
```
ggplot(une[n != 0], aes(x=u, y=Tn)) +
    geom_boxplot(outlier.shape=NA) +
    geom_point(data=une[n == 0], aes(x=u, y=Tn)) +
    facet_grid(k ~ .) +
    guides(color=guide_legend(title="Data Subset")) +
    xlab("split location") +
    ylab("test statistic (standardized)")
```


In [ ]: