probabilistic-nested-design-v7

April 19, 2020

1 Probabilistic Nested Designs with Sensitivity Indices, version 7

1.1 Load packages.

[1]:
```r
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 methods]
Loading required package: rTensor
Loading required package: ggplot2
Loading required package: GGally
Registered S3 method overwritten by 'GGally':
  method from
  +.gg   ggplot2
```

1.2 Function to generate simulations.

[2]:
```r
# 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 time
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:dimension, m))
    functions <- lapply(degrees, single)

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

    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))})
    }

}
```

1.3 Functions for nesting designs

[3]:
```
ssa.digits <- 30
```

[4]:
```
ssa.scale <- 2^ssa.digits
```

[5]:
```
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
}
```

[6]:
```
ssa.depth <- function(i) {
    ssa.digits - ssa.level(i)
}
```

[7]:
```
ssa.corner <- function(i, offset=0){
    d <- ssa.level(i) - offset
    c(i - 2^d, i + 2^d)
}
```

[8]:
```
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), by="d1",␣
 ↪allow.cartesian=TRUE),
        data.table(d2=2, i2=ssa.corner(i2, offset=offset), s2=0:1), by="d2",␣
 ↪allow.cartesian=TRUE),
        data.table(d3=4, i3=ssa.corner(i3, offset=offset), s3=0:1), by="d3",␣
 ↪allow.cartesian=TRUE
    )[,
    .(
        i1,
        i2,
        i3,
        axis=mapply(axis, s1, s2, s3)
    )]
}
```

[9]:
```
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
        )
    ]
}
```

[10]:
```
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"))
}
```

[11]:
```
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
}
```

[12]:
```
ssa.measure <- function(xs, ys, focus=2) {

    result <- merge(
        merge(
            xs[measure == TRUE][, ssa.corners(i1, i2, i3), by=.
 ↪(center=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
}
```

[13]:
```
ssa.probe <- function(xs, alpha=1, maxdepth=-log(sqrt(.Machine$double.eps),2)) {
    choices <- xs[probed == FALSE & !is.na(s), .(sequence, s)]
    if (nrow(choices) == 1)
        choice <- choices$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$sequence, `:=`(compute=TRUE, measure=FALSE,␣
↪probed=TRUE)]
    setkeyv(result, c("i1", "i2", "i3"))
    list(
        sequence=probe$sequence,
        xs=result
    )
```

```
}
```

1.4 Reproducible random numbers.

[14]:
```
RNGkind("Mersenne-Twister", "Inversion", "Rejection")
```

[15]:
```
set.seed(46)
```

1.5 Create a simulation function.

[16]:
```
f <- makeGenerator(c(2, 2, 3), c(0, 1, 2), 3)
```

1.6 Example application

1.6.1 Set time resolution.

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

1.6.2 Initialize experiment at bounds of domain.

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

[19]:
```
xs
```

A data.table: 9 x 15

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

1.6.3 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.

[21]:
```
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))
```

1.6.4 Save results.

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

1. 54744 2. 15

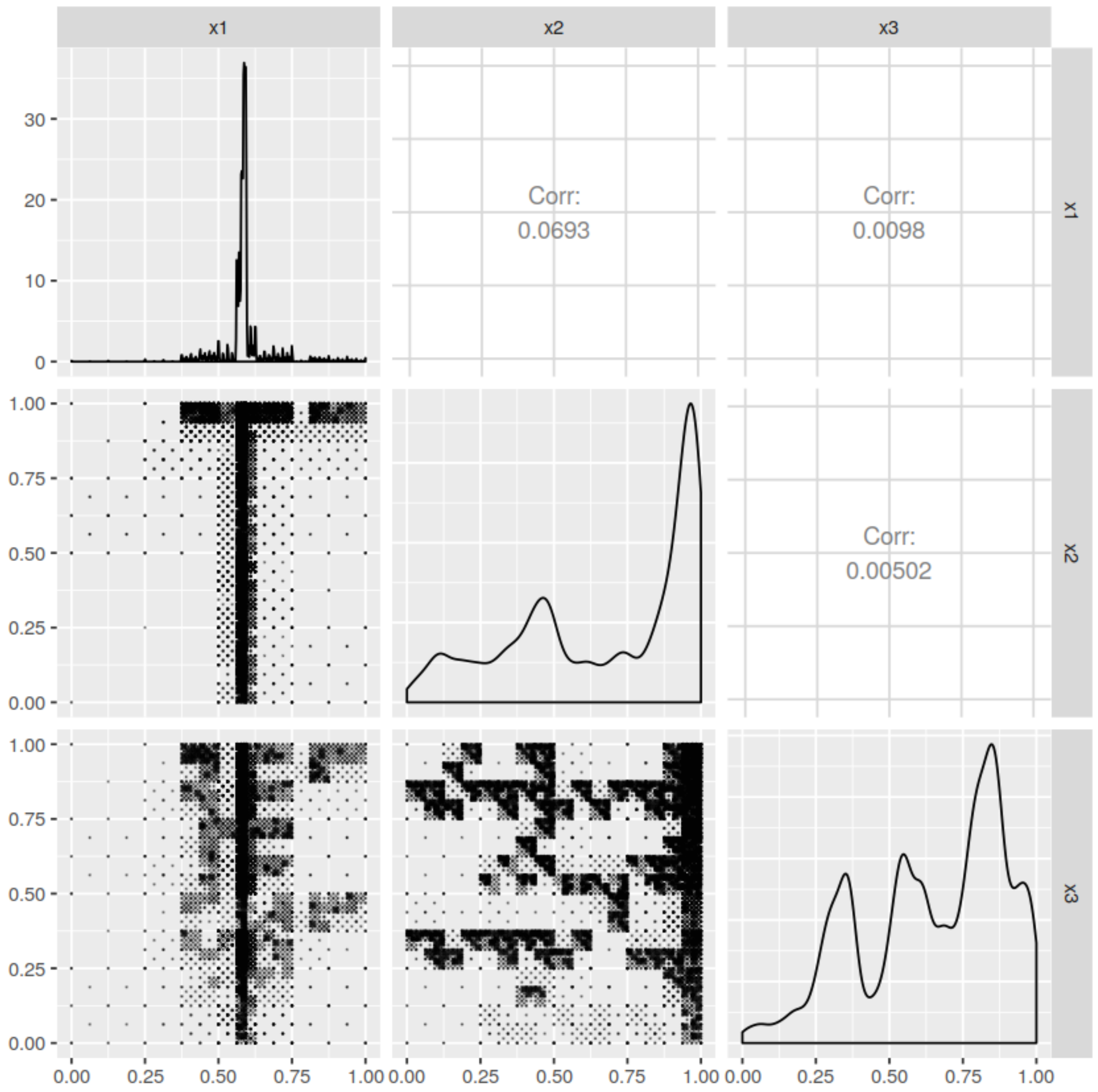
[23]:
```
write.table(ys, file="ys-v7.csv", row.names=FALSE, sep=",")
ys %>% dim
```

1. 782103 2. 5

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

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

1.6.5 Plot sampling pattern.

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



1.6.6 Compute sensitivity indices.

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

[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 <int>	x1 <dbl>	x2 <dbl>	x3 <dbl>	y1 <dbl>	y2 <dbl>	y3 <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.

[41]:
```
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.all)^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.all)^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.

[42]:
```
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.

[43]:
```
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.

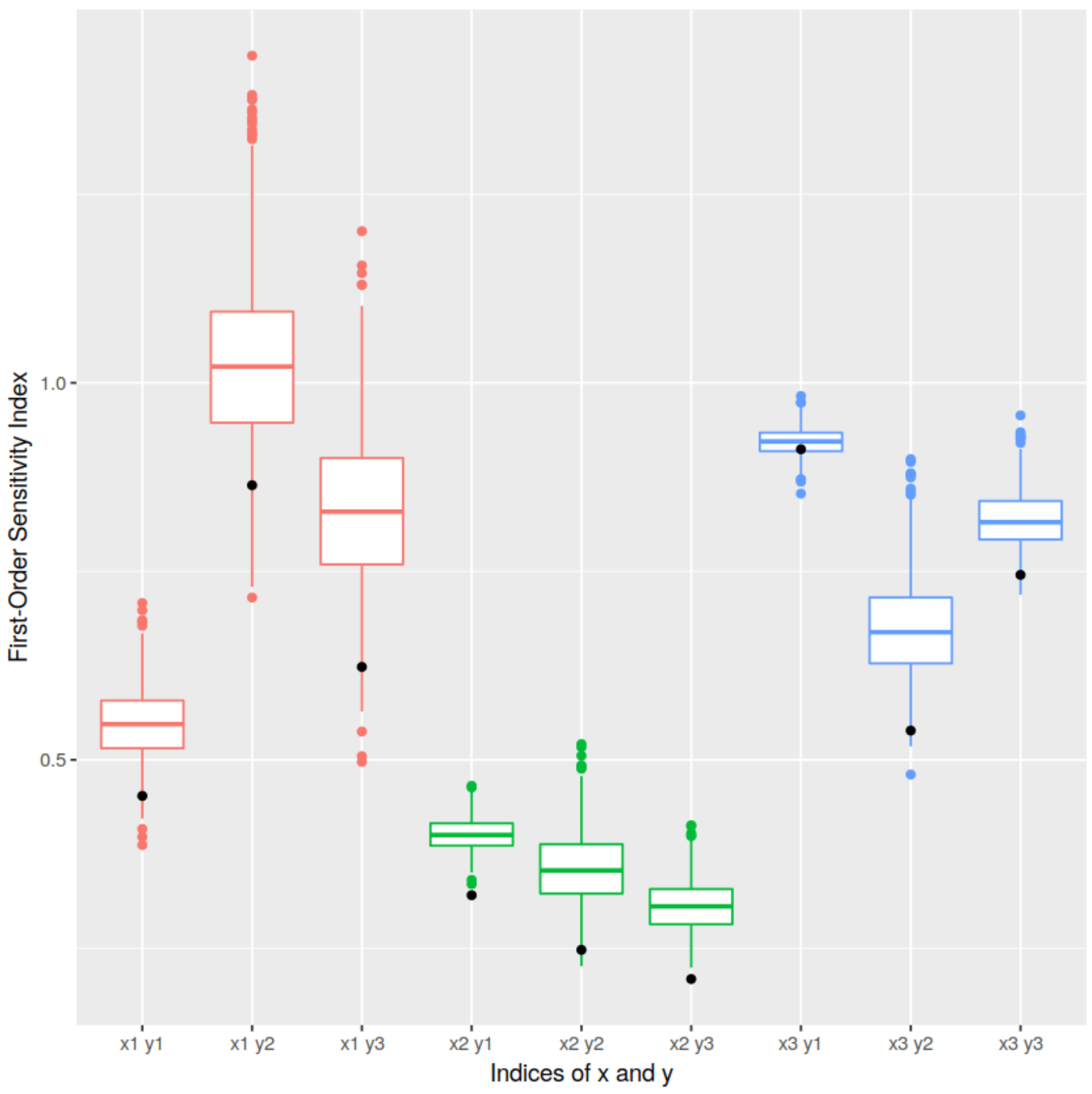
[44]:
```
s.x <- sensitivity_indices_resample(xys.wide, 1000)
s.x[n == 0]
```

A data.table: 9 x 4

n <dbl>	i <fct>	j <fct>	s.x <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.

[45]:
```
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="black")
```



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.

1.6.7 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.

[4]:
```
us <- xs[,
    .(u=round((1:6)/7, 3)),
    by=.(sequence)
][,
    .(k=c("split on x1", "split on x2", "split on x3")),
    by=.(sequence, u)
]
```

[5]:
```
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
```

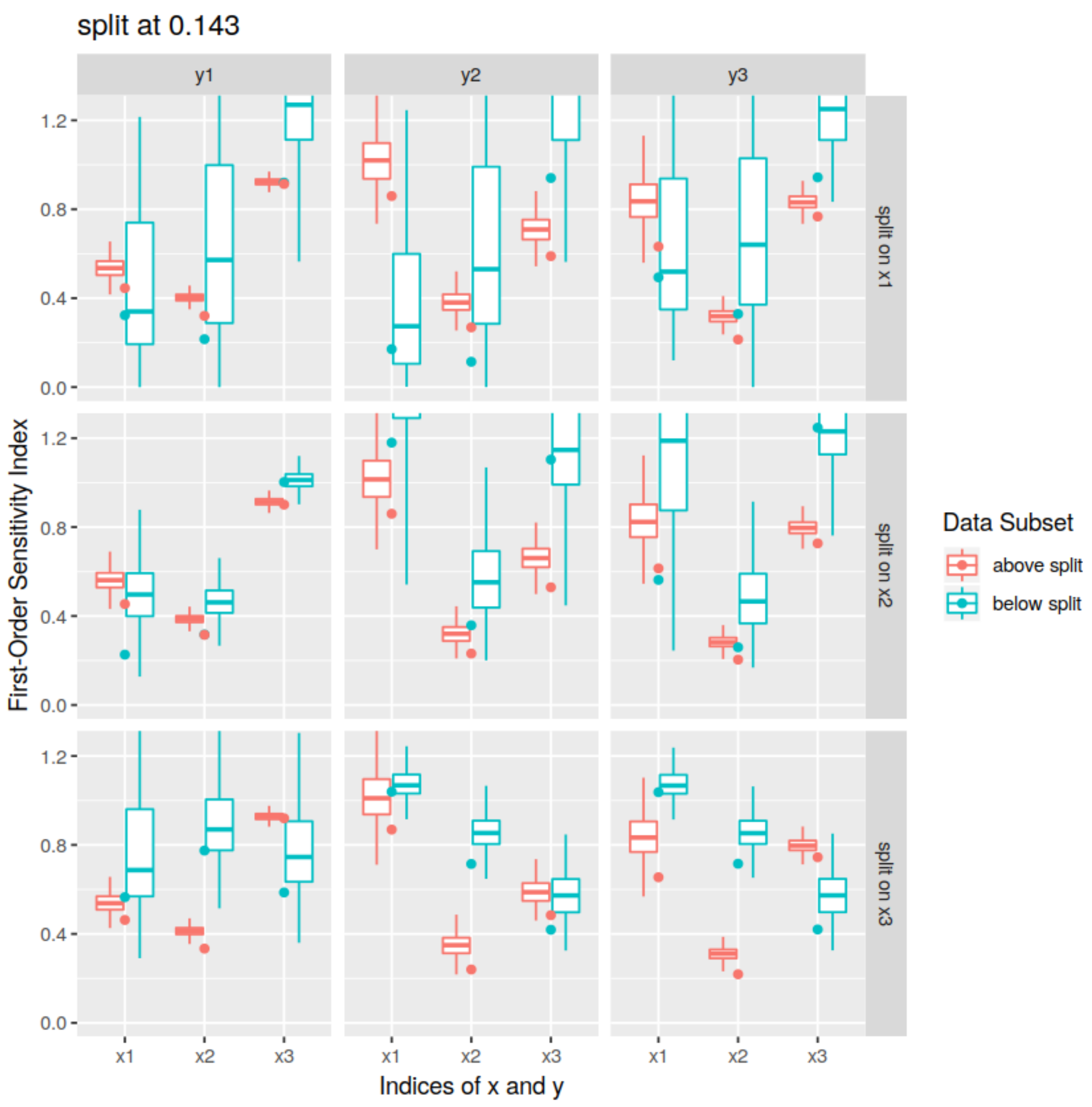
1. 45144 2. 10

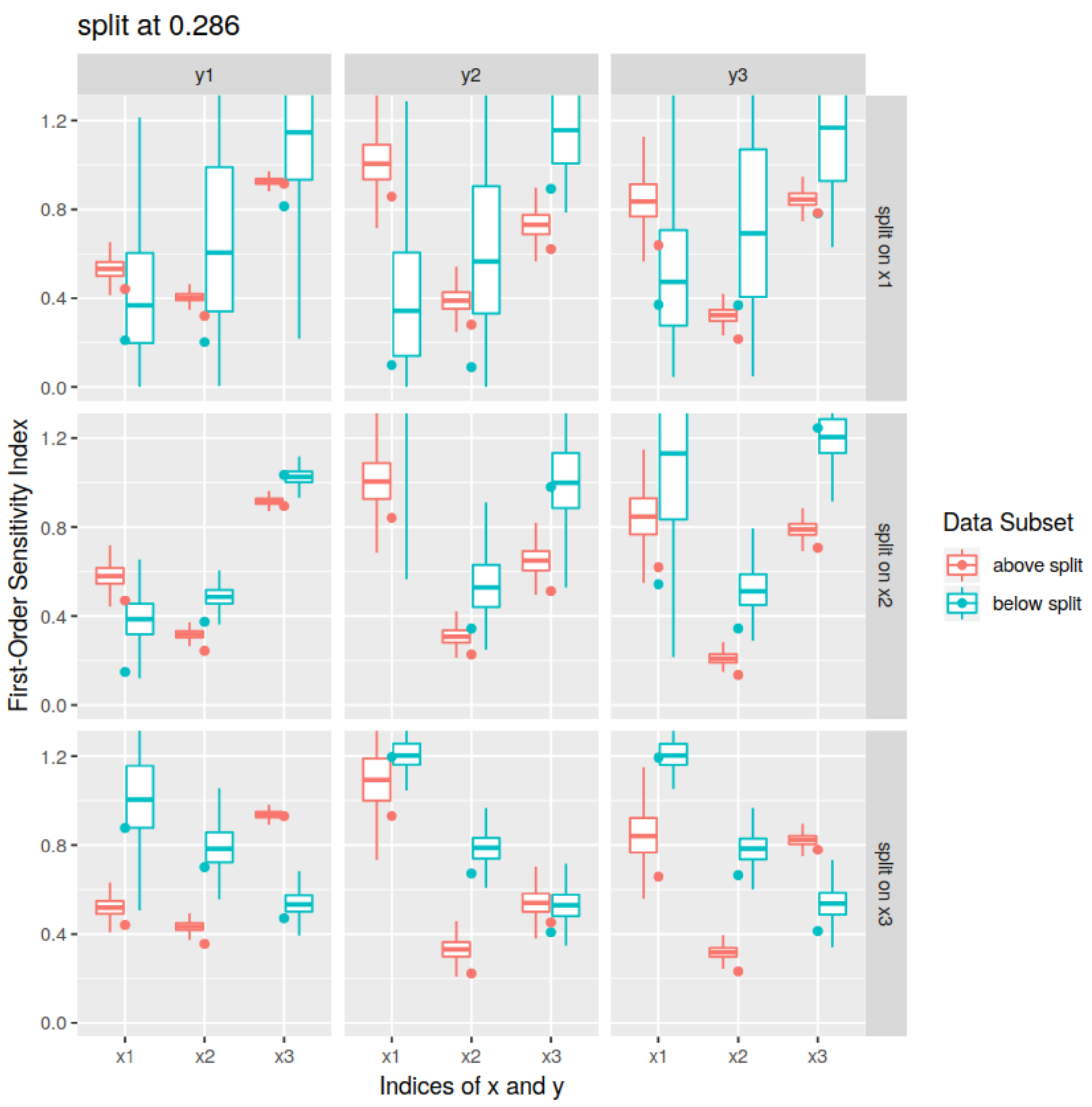
[6]:
```
us <- us[, .(s=c("below split", "above split")), by=.(k, u)]
us.x <- NULL
for (row in 1:nrow(us))
    us.x <- rbind(
        us.x,
        cbind(
            us[row, .(k, u, s)],
            sensitivity_indices_resample(merge(us[row], uxys.wide, by=c("k",␣
↪"u", "s")), 1000)
        )
    )
us.x %>% dim
```

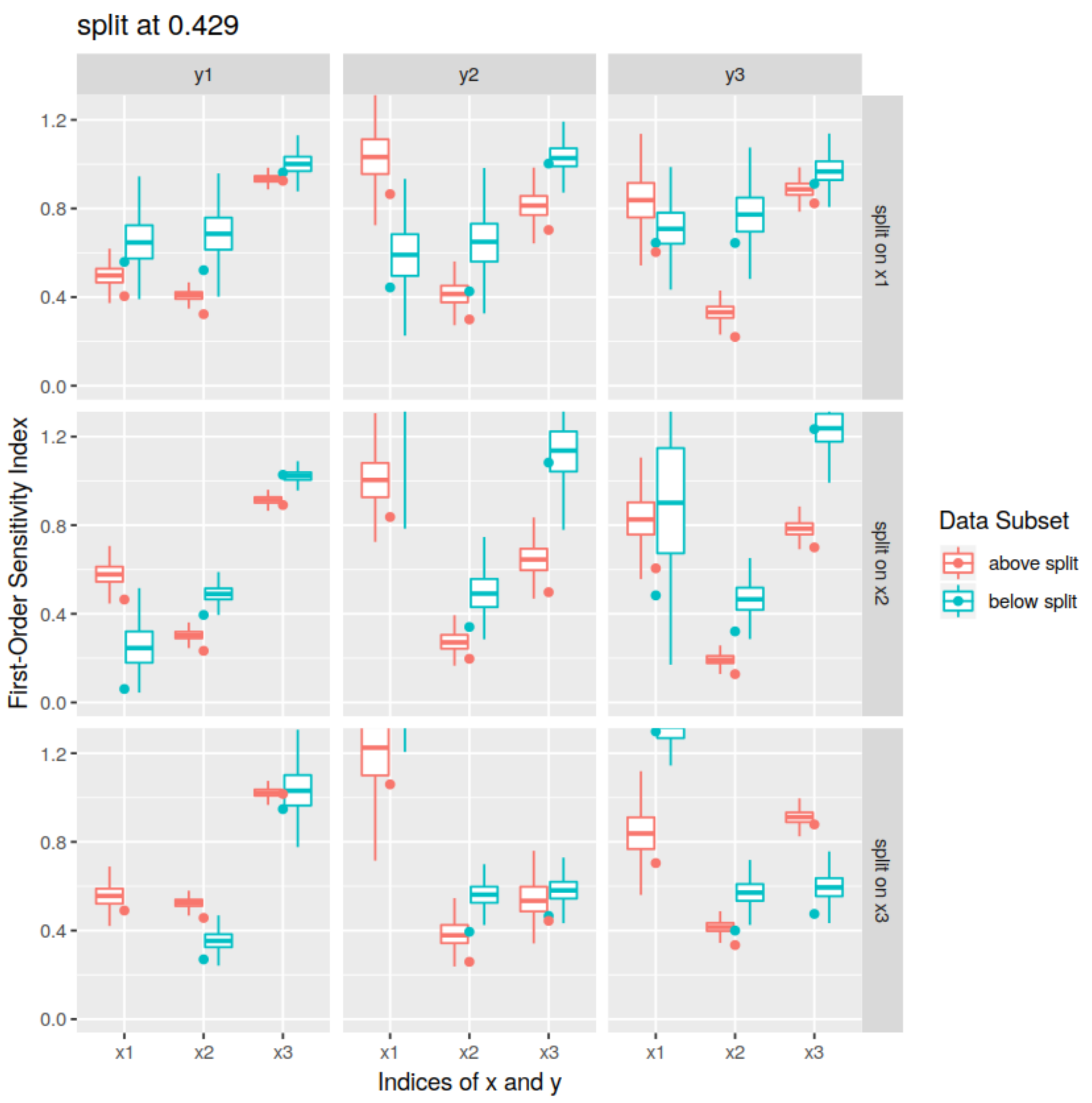
```
        Error in sensitivity_indices_resample(merge(us[row], uxys.wide, by =␣
↪c("k", : could not find function "sensitivity_indices_resample"
    Traceback:
        1. rbind(us.x, cbind(us[row, .(k, u, s)],␣
↪sensitivity_indices_resample(merge(us[row],
    .     uxys.wide, by = c("k", "u", "s")), 1000)))

        2. cbind(us[row, .(k, u, s)], sensitivity_indices_resample(merge(us[row],
    .     uxys.wide, by = c("k", "u", "s")), 1000))
```

[53]:
```
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)
}
```

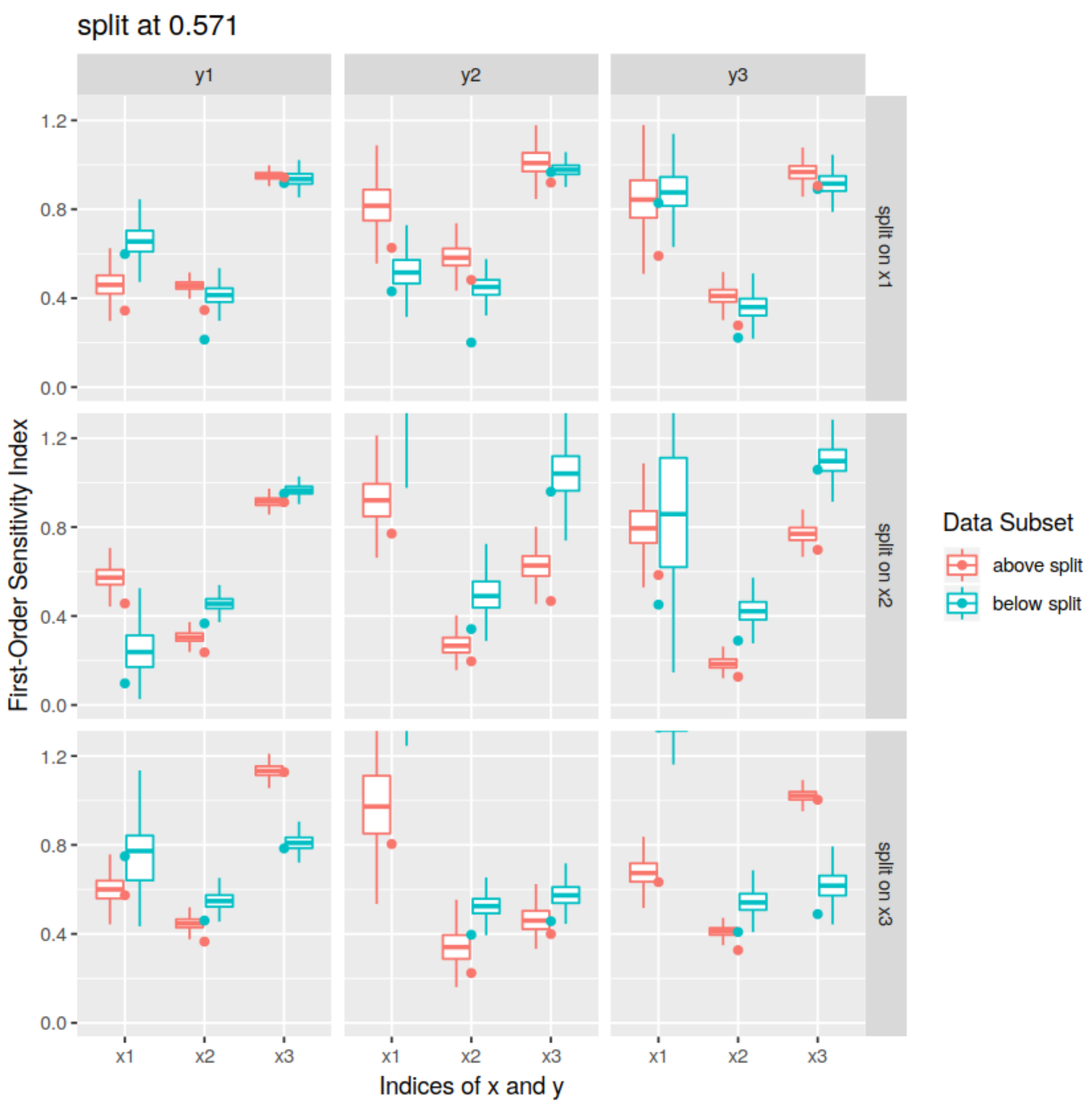
```
Warning message:
Removed 280 rows containing non-finite values (stat_boxplot).Warning message:
```

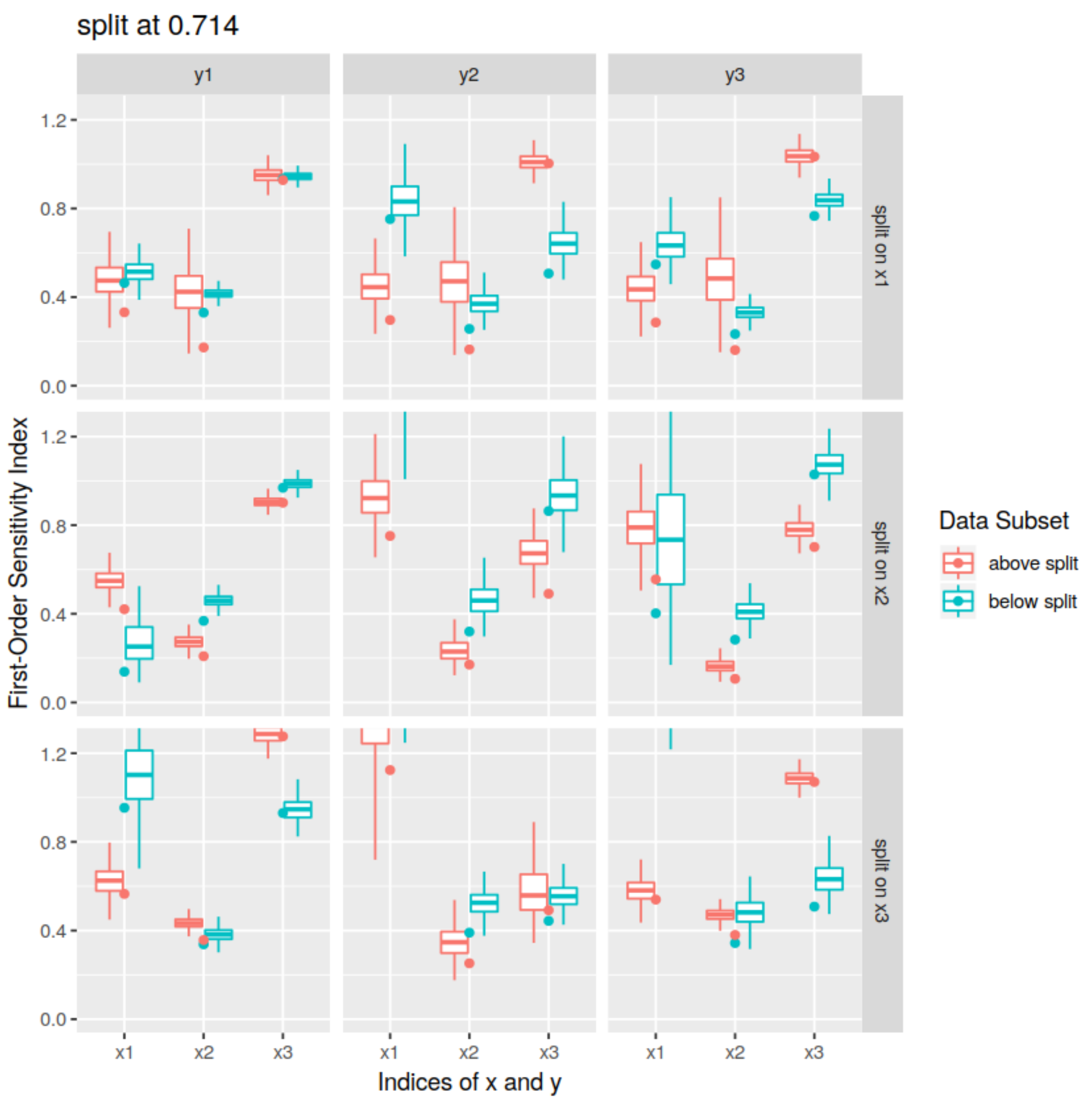

split at 0.143
y1
y2
y3
split on x1
split on x2
split on x3
First-Order Sensitivity Index
1.2
0.8
0.4
0.0
x1
x2
x3
Indices of x and y
Data Subset
above split
below split


split at 0.286
y1
y2
y3
split on x1
split on x2
split on x3
First-Order Sensitivity Index
Indices of x and y
x1
x2
x3
0.0
0.4
0.8
1.2
Data Subset
above split
below split

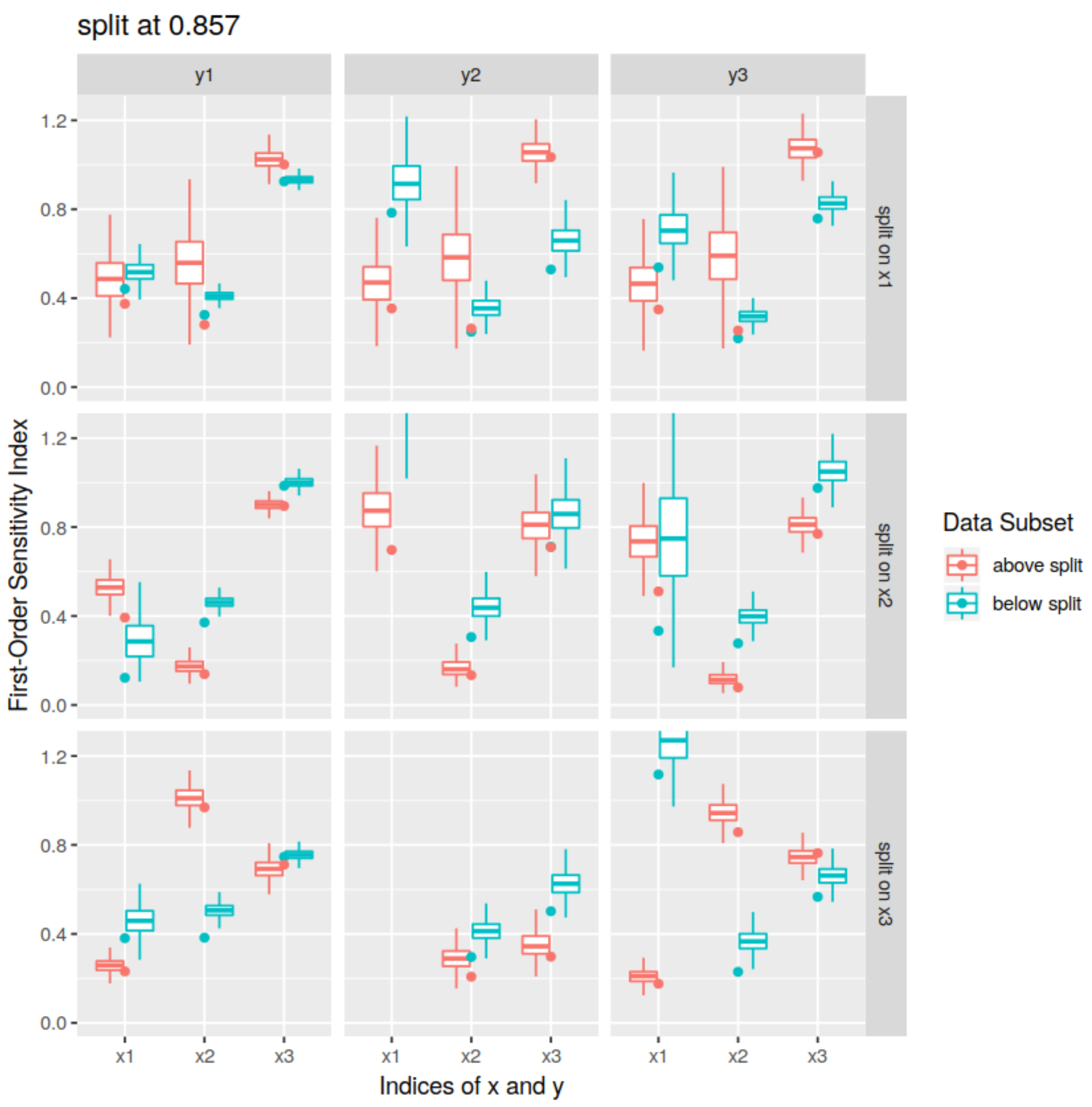


split at 0.429
y1
y2
y3
split on x1
split on x2
split on x3
First-Order Sensitivity Index
Indices of x and y
x1
x2
x3
0.0
0.4
0.8
1.2
Data Subset
above split
below split


split at 0.571
y1
y2
y3
split on x1
split on x2
split on x3
First-Order Sensitivity Index
0.0
0.4
0.8
1.2
x1
x2
x3
Indices of x and y
Data Subset
above split
below split



split at 0.714
y1
y2
y3
split on x1
split on x2
split on x3
First-Order Sensitivity Index
1.2
0.8
0.4
0.0
x1
x2
x3
Indices of x and y
Data Subset
above split
below split



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`.

1.6.8 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.

[41]:
```
tus <- us[, .(1), by=.(k, u)]
une <- NULL
for (row in 1:nrow(tus)) {
```