nested-design-v6

April 12, 2020

1 Nesting Designs, version 6

1.1 Load packages.

[1]:

```
require(abind)
require(data.table)
require(deSolve)
require(magrittr)
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: 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]:

```
# 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(xs)) {
        ys <- rbind(
            ys,
            data.table(f(as.numeric(xs[row, .(x1, x2, x3)]), ts))[,
                .(
                    sequence = xs[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) {
    probe <- xs[
        probed == FALSE,
        .(sequence, i1, i2, i3, rank=frank(-s, ties.method="random"))
    ][
        rank == 1,
        .(sequence, i1, i2, i3)
    ]
    candidates <- ssa.candidates(probe$i1, probe$i2, probe$i3)
    setkeyv(candidates, c("i1", "i2", "i3"))
    candidates <- candidates[!xs]
    candidates <- candidates[, .(
        sequence = xs[, max(sequence)] + (1:nrow(candidates)),
        generation = NA,
        i1, i2, i3,
        x1, x2, x3,
        compute = TRUE ,
        measure = FALSE,
        probed  = FALSE,
        s1 = 0. / 0.,
        s2 = 0. / 0.,
        s3 = 0. / 0.,
        s  = 0. / 0.
    )]
    probes <- ssa.corners(probe$i1, probe$i2, probe$i3, offset=1)
    probes <- probes[, .(
        sequence = max(candidates$sequence) + (1:nrow(probes)),
        generation = NA,
        i1, i2, i3,
        x1 = i1 / ssa.scale,
        x2 = i2 / ssa.scale,
        x3 = i3 / ssa.scale,
        compute = FALSE,
        measure = TRUE ,
        probed  = FALSE,
        s1 = 0. / 0.,
        s2 = 0. / 0.,
        s3 = 0. / 0.,
        s  = 0. / 0.
    )]
    result <- rbind(
        xs,
        candidates,
        probes
    )
    result[sequence == probe$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	generation	i1	i2	i3	x1	x2	x3
<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<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.

[20]:

```
ys <- NULL
sequences <- NULL
```

[21]:

```
for (k in 1:250) {
    # Perform pending computations.
    ys <- ssa.compute(f, ts, xs, NULL)
    # Measure divergences.
    ssa.measure(xs, ys, focus = 1)
    # Select where to probe further.
    result <- ssa.probe(xs)
    # Tally results.
    sequences <- rbind(
        sequences,
        xs[
            sequence == result$sequence,
            .(
                sequence,
                x1, x2, x3,
                generation,
                depth=mapply(ssa.depth, i1))
        ]
    )
    # Update grid.
    xs <- result$xs
}
sequences
```

A data.table: 250 x 6

sequence	x1	x2	x3	generation	depth
<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
9	0.5000	0.5000	0.5000	1	1
33	0.7500	0.2500	0.7500	2	2
35	0.7500	0.7500	0.7500	2	2
56	0.6250	0.3750	0.6250	3	3
55	0.6250	0.1250	0.8750	3	3
76	0.6250	0.6250	0.8750	4	3
78	0.6250	0.8750	0.8750	4	3
57	0.6250	0.3750	0.8750	3	3
58	0.8750	0.1250	0.6250	3	3
77	0.6250	0.8750	0.6250	4	3
79	0.8750	0.6250	0.6250	4	3
34	0.7500	0.7500	0.2500	2	2
233	0.5625	0.9375	0.6875	11	4
104	0.5625	0.4375	0.6875	5	4
105	0.6875	0.3125	0.5625	5	4
234	0.6875	0.8125	0.5625	11	4
32	0.7500	0.2500	0.2500	2	2
230	0.5625	0.8125	0.5625	11	4
101	0.5625	0.3125	0.5625	5	4
232	0.5625	0.9375	0.5625	11	4
103	0.5625	0.4375	0.5625	5	4
278	0.8750	0.6250	0.1250	13	3
398	0.6250	0.3750	0.3750	18	3
396	0.6250	0.1250	0.3750	18	3
275	0.6250	0.6250	0.3750	13	3
174	0.5625	0.9375	0.8125	8	4
129	0.5625	0.1875	0.9375	6	4
189	0.6875	0.3125	0.8125	9	4
187	0.5625	0.4375	0.8125	9	4
128	0.5625	0.1875	0.8125	6	4
...	...	...	...	...	...
2252	0.578125	0.109375	0.796875	103	6
1561	0.578125	0.265625	0.796875	73	6
2386	0.578125	0.609375	0.796875	111	6
2250	0.578125	0.078125	0.796875	103	6
2266	0.578125	0.453125	0.796875	104	6
2384	0.578125	0.578125	0.796875	111	6
1587	0.609375	0.421875	0.765625	74	6
1659	0.609375	0.203125	0.796875	77	6
2270	0.609375	0.453125	0.796875	104	6
1582	0.578125	0.390625	0.796875	74	6
2372	0.609375	0.359375	0.765625	110	6
2367	0.578125	0.328125	0.796875	110	6
1912	0.609375	0.953125	0.796875	88	6
1935	0.578125	0.984375	0.921875	89	6
1934	0.578125	0.984375	0.890625	89	6
2607	0.578125	0.421875	0.890625	122	6
2013	0.578125	0.234375	0.921875	92	6
2012	0.578125	0.234375	0.890625	92	6
2608	0.578125	0.421875	0.921875	122	6
3418	0.578125	0.734375	0.484375	158	6

1.6.4 Save results.

[22]:

```
write.table(xs, file="xs-v6.csv", row.names=FALSE, sep=",")
xs %>% dim
```

1. 5403 2. 15

[23]:

```
write.table(ys, file="ys-v6.csv", row.names=FALSE, sep=",")
ys %>% dim
```

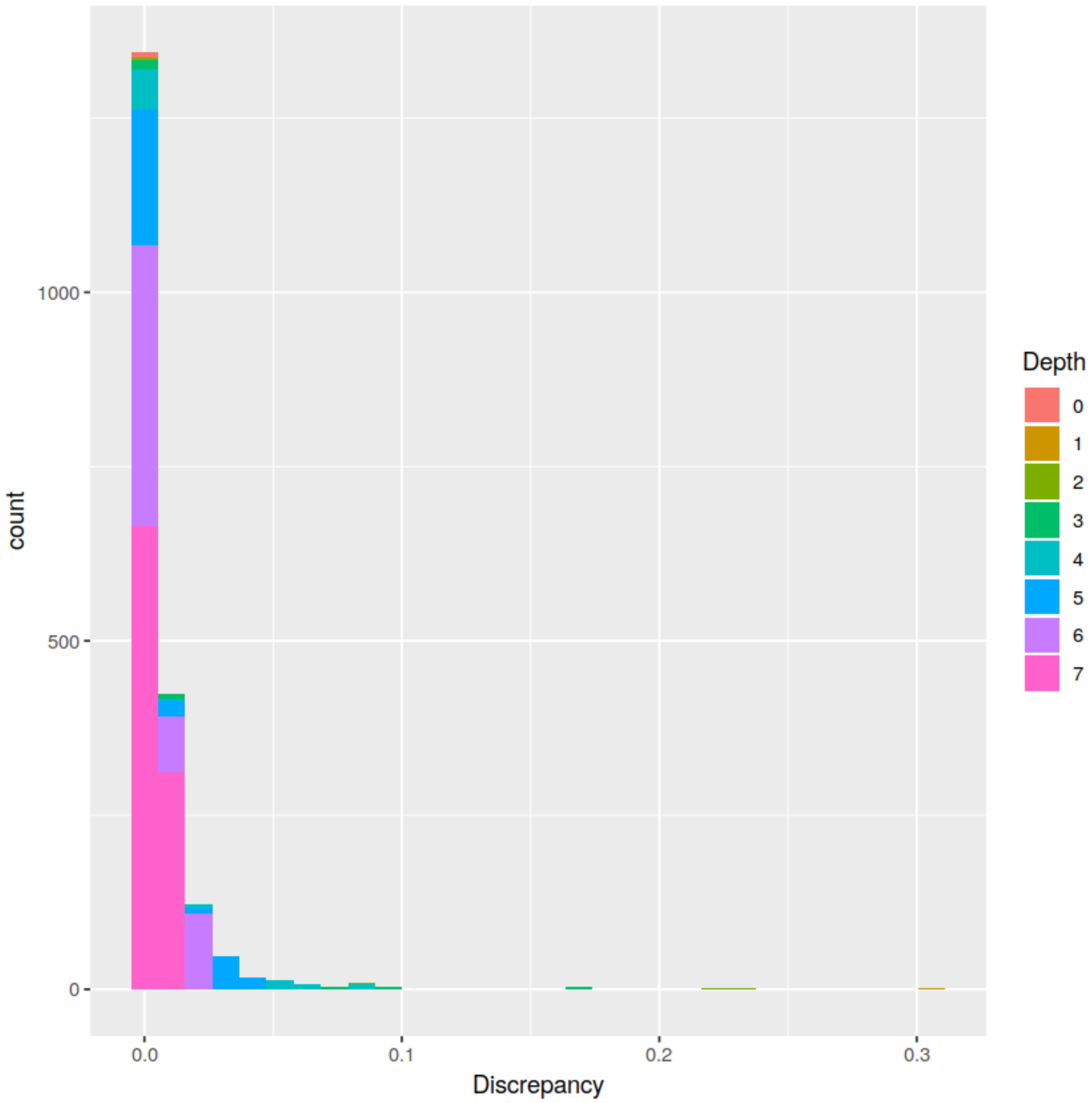
1. 112917 2. 5

1.6.5 Plot sampling pattern.

Distribution of discrepancies, distinguished by depth.

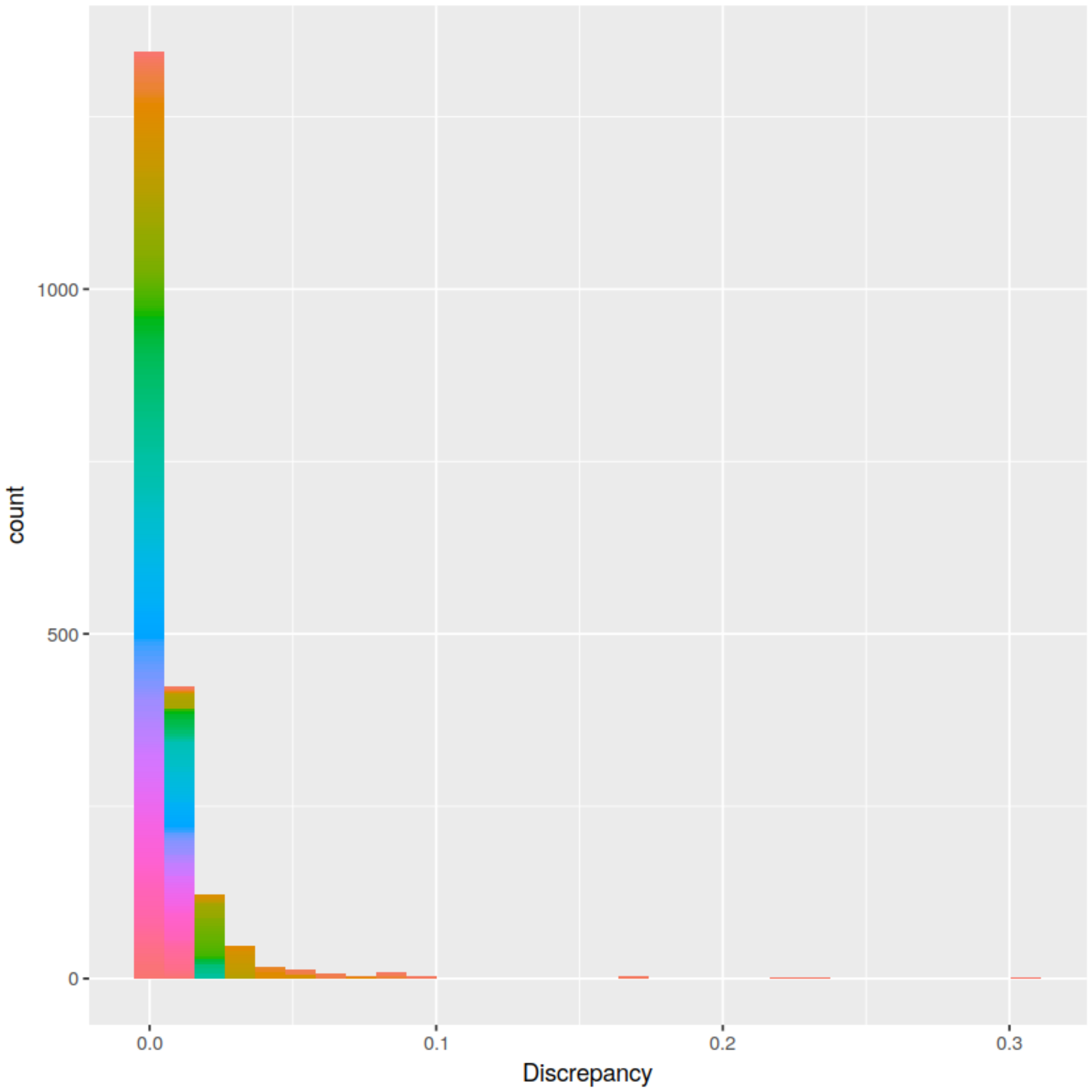
[24]:

```
ggplot(
    xs[!is.na(generation), .(Generation=factor(generation), Discrepancy=s,␣
 ↪Depth=factor(mapply(ssa.depth, i1)))],
    aes(x=Discrepancy, fill=Depth)
) + geom_histogram(bins = 30)
```



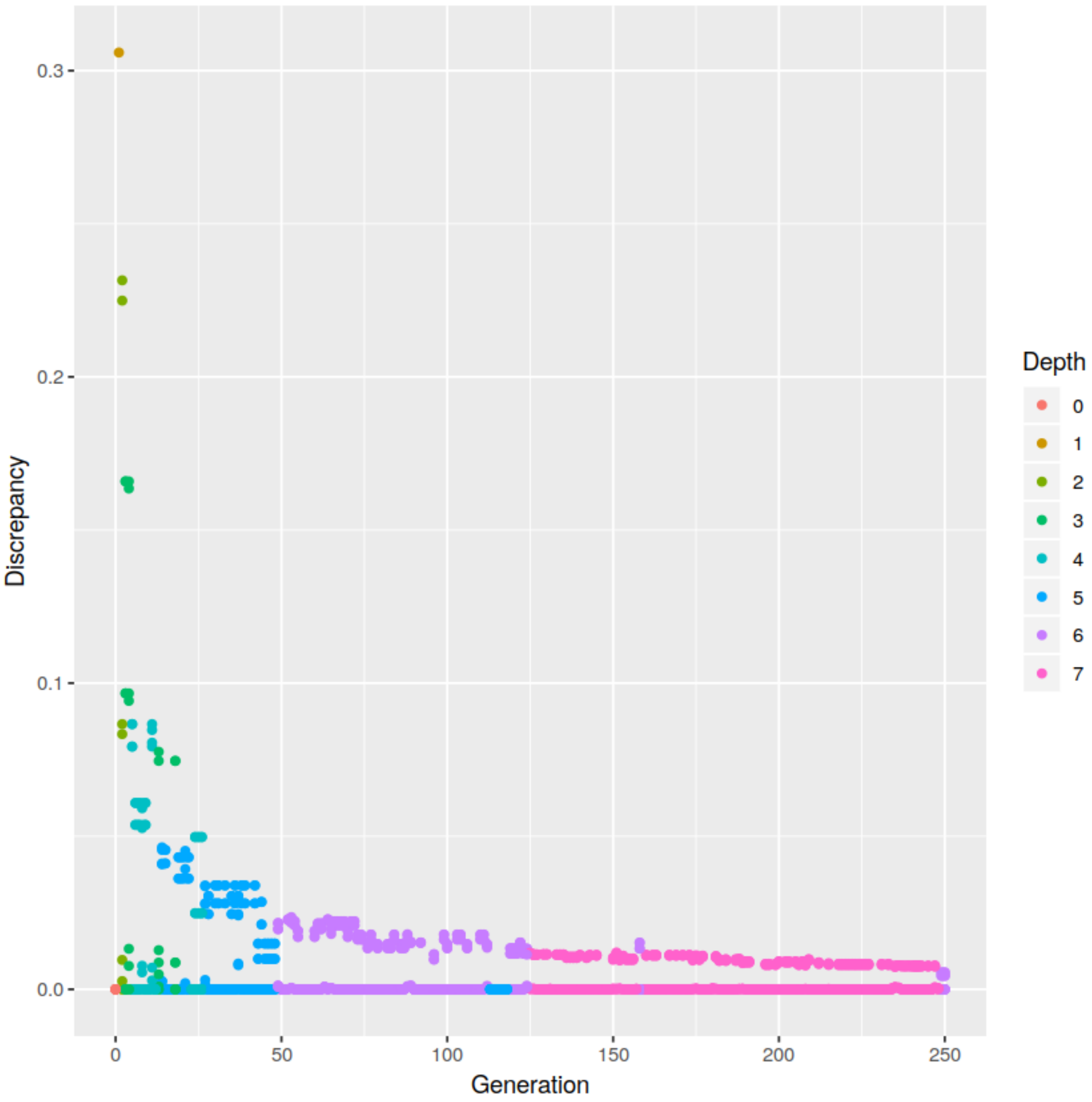
Distribution of discrepancies, distinguished by generation.

[25]:
```
ggplot(
    xs[!is.na(generation), .(Generation=factor(generation), Discrepancy=s,␣
 ↪Depth=factor(mapply(ssa.depth, i1)))],
    aes(x=Discrepancy, fill=Generation)
) + geom_histogram(bins = 30)  + theme(legend.position = "none")
```



Discrepancies and depth as a function of generation.

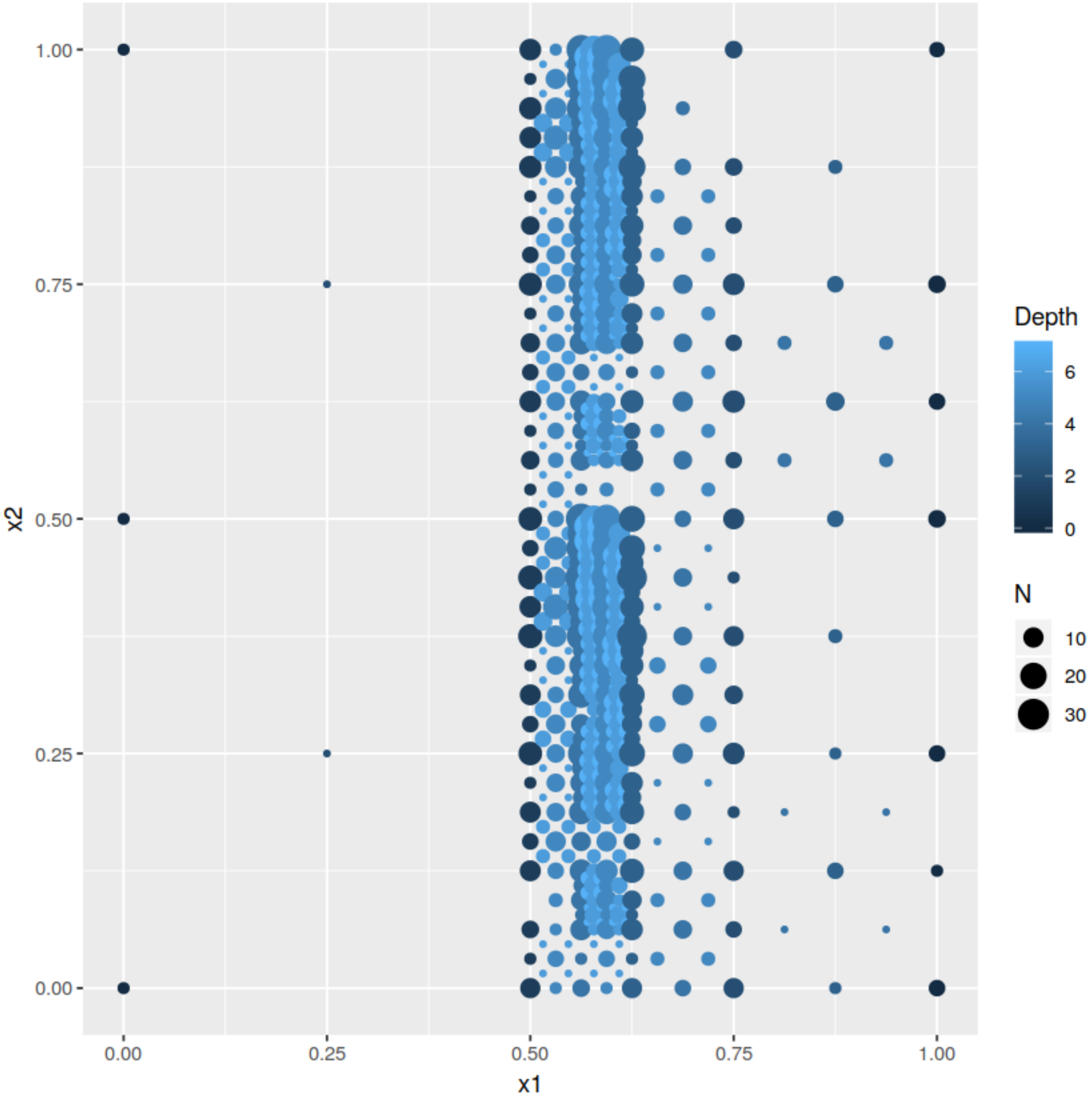
```
[26]: ggplot(
          xs[!is.na(generation), .(Generation=generation, Discrepancy=s,␣
       ↪Depth=factor(mapply(ssa.depth, i1)))],
          aes(x=Generation, y=Discrepancy, color=Depth)
      ) + geom_point()
```



Marginal densities of sampling.

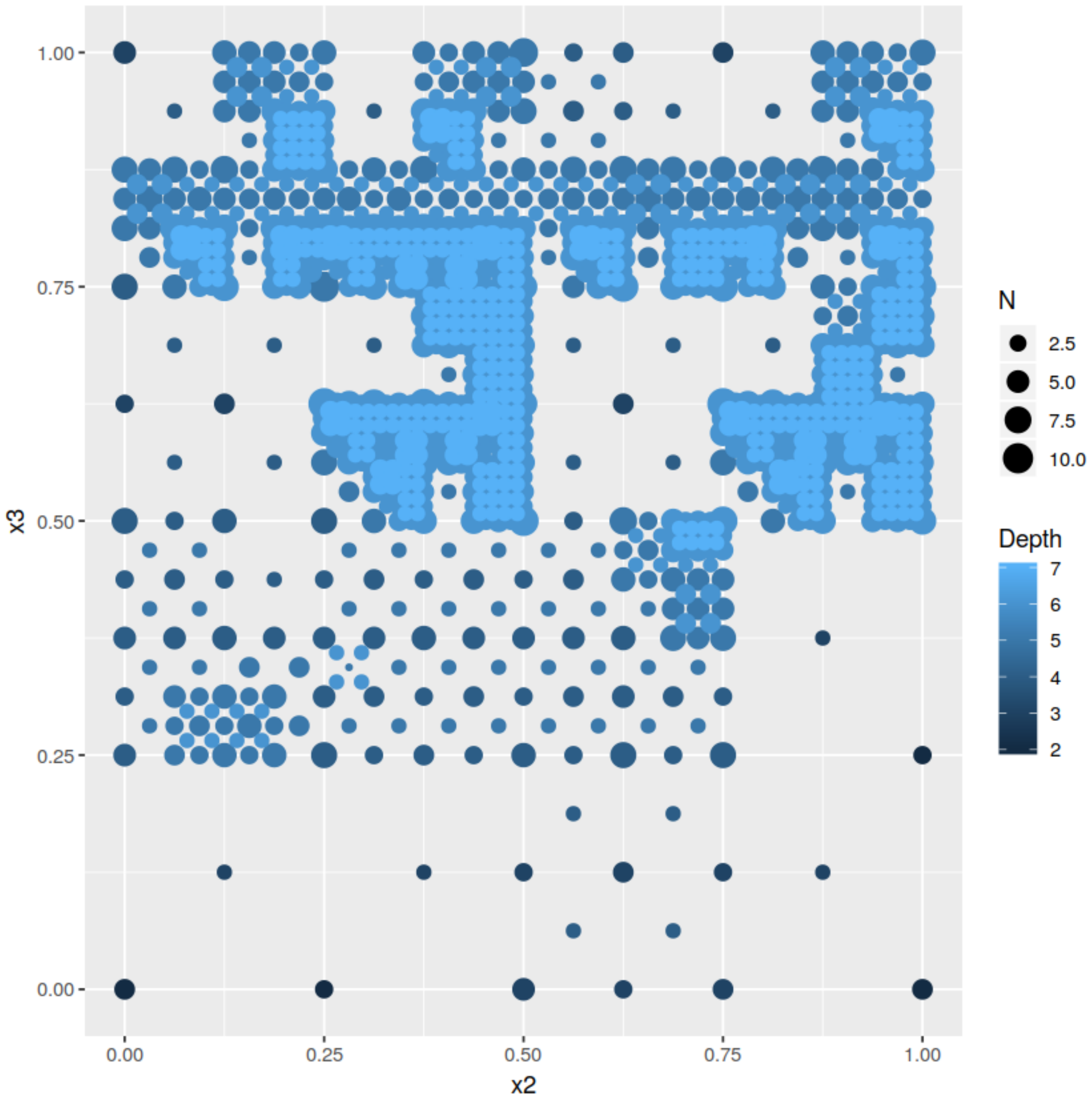
x1 vs x2.

[27]:
```
ggplot(
    xs[compute == FALSE, .(N=.N, Depth=max(mapply(ssa.depth, i1))), by=.(x1,␣
 ↪x2)],
    aes(x=x1, y=x2, size=N, color=Depth)
) + geom_point()
```



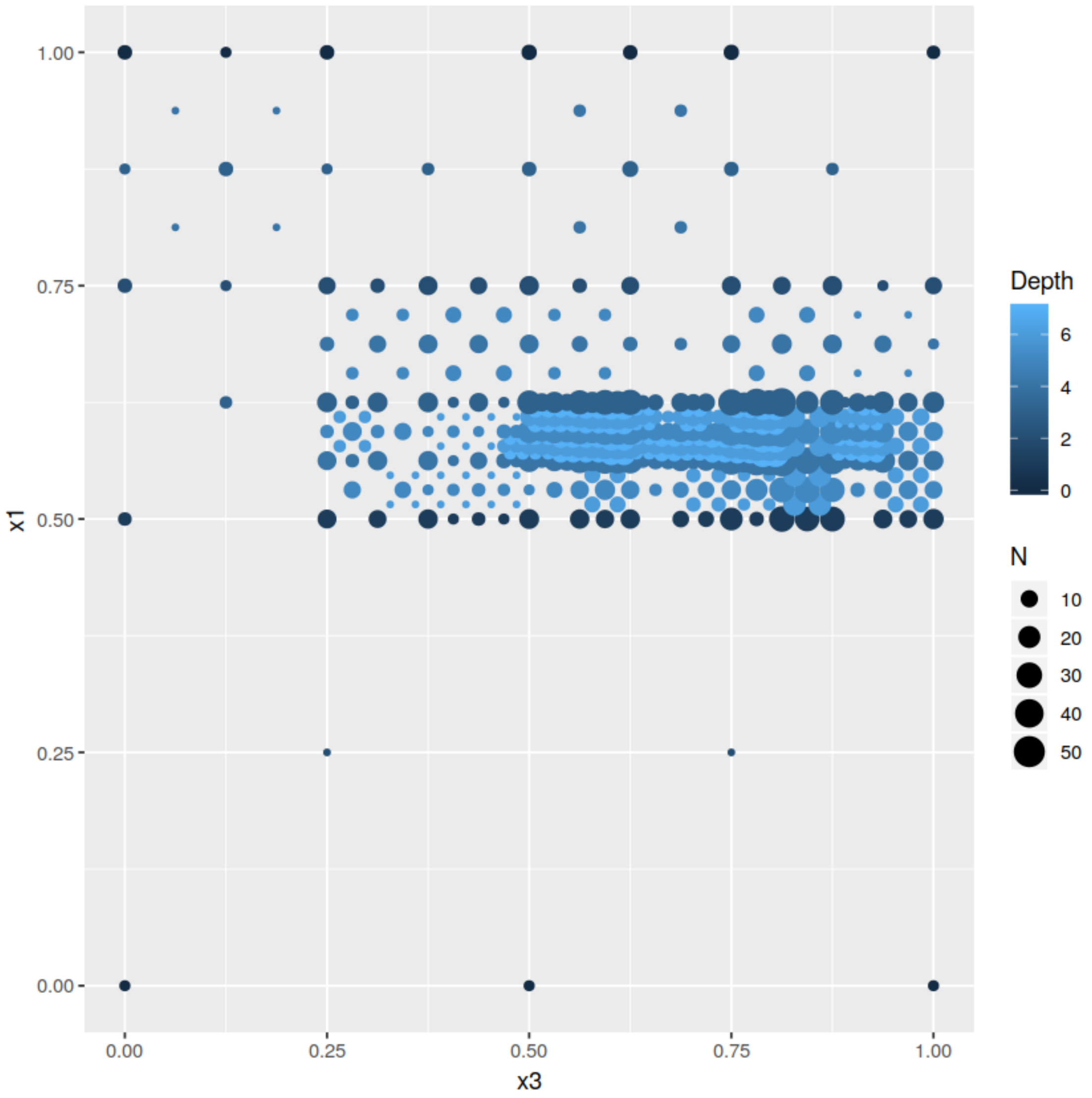
x2 vs x3.

[28]:
```
ggplot(
    xs[compute == FALSE, .(N=.N, Depth=max(mapply(ssa.depth, i1))), by=.(x2,␣
↪x3)],
    aes(x=x2, y=x3, size=N, color=Depth)
) + geom_point()
```



x3 vs x1.

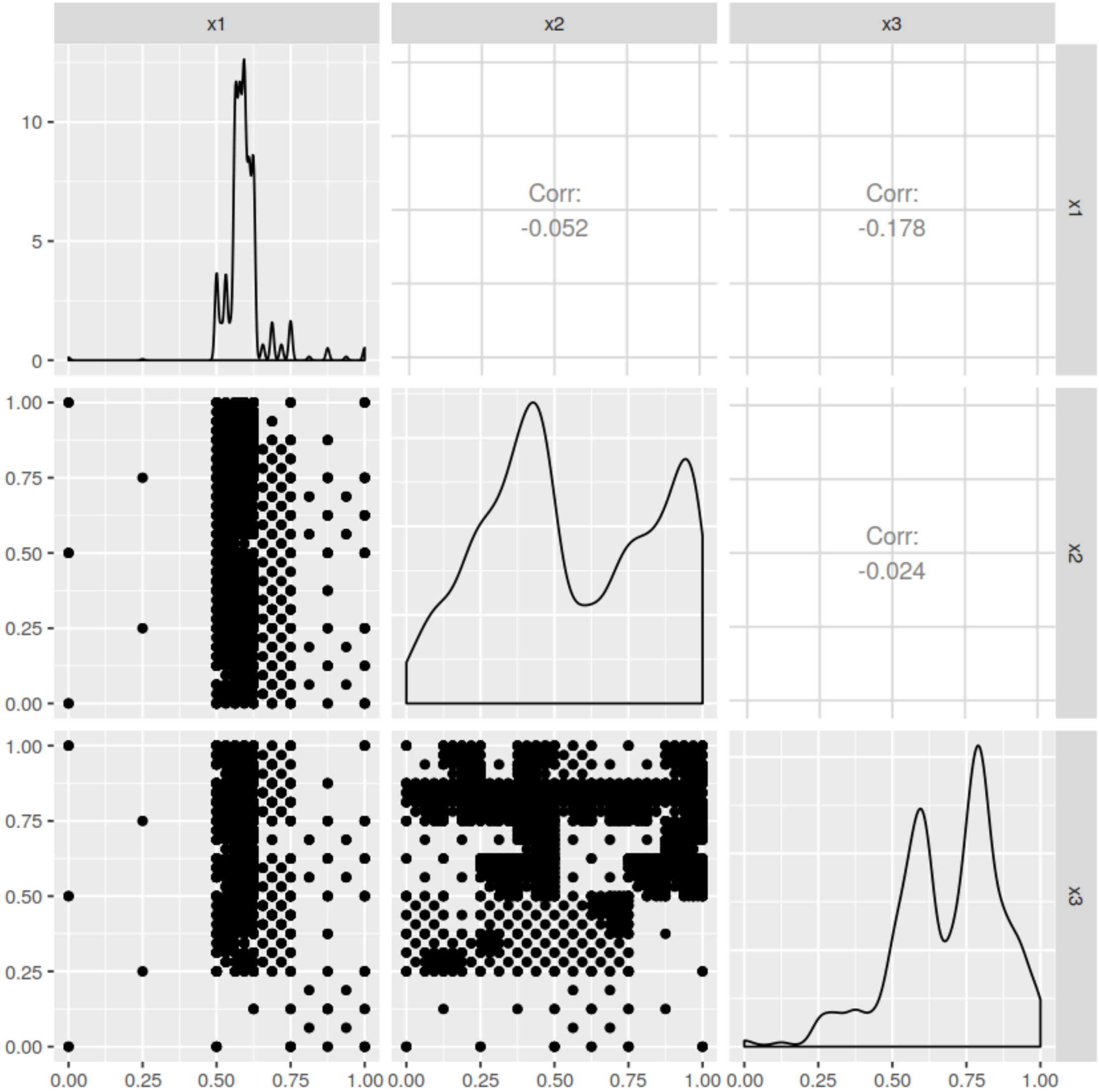
[29]:
```
ggplot(
    xs[compute == FALSE, .(N=.N, Depth=max(mapply(ssa.depth, i1))), by=.(x3,␣
 ↪x1)],
    aes(x=x3, y=x1, size=N, color=Depth)
) + geom_point()
```



Pairs.

[30]:

```
ggpairs(xs, 6:8)
```


x1
x2
x3
Corr:
-0.052
Corr:
-0.178
Corr:
-0.024
x1
x2
x3
10
5
0
1.00
0.75
0.50
0.25
0.00
0.00
0.25
0.50
0.75
1.00