

Optimal Pi and Importance Sampling Analysis

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Overview

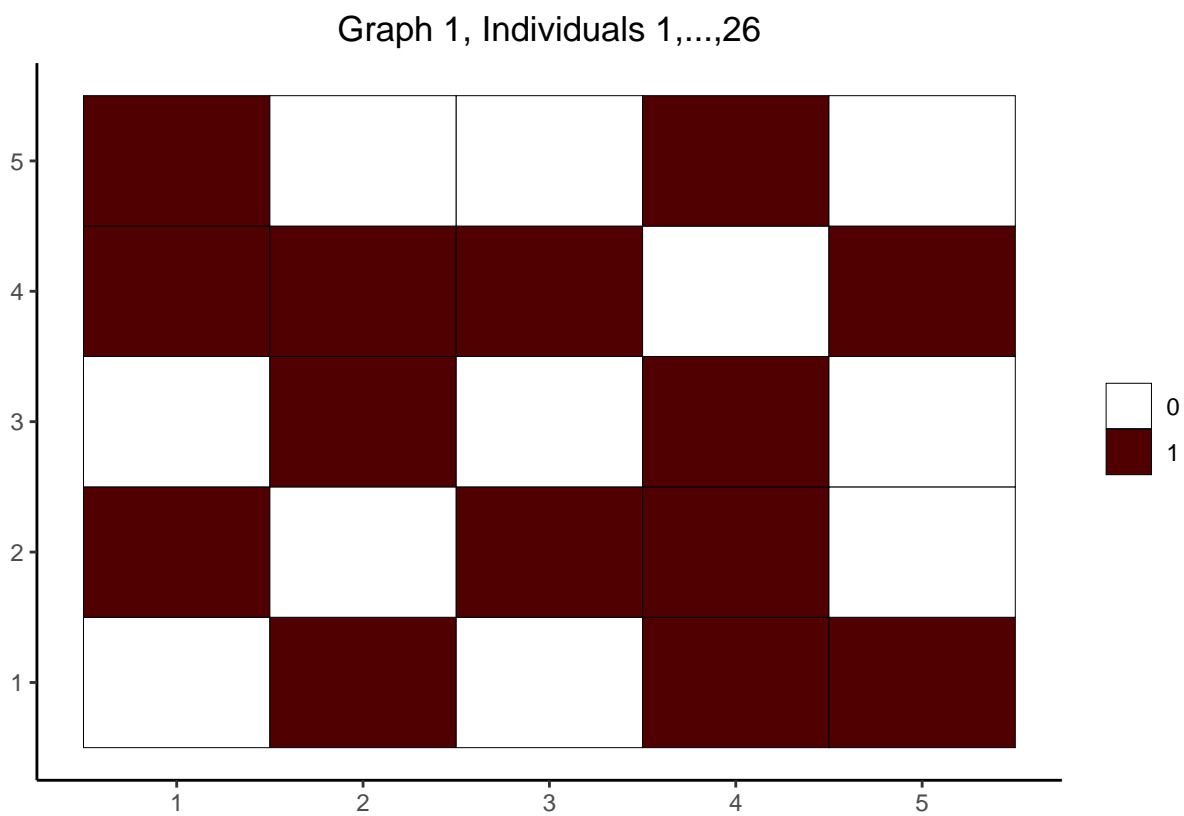
In this document, I present the results of two experiments. The first describes the distribution of the optimal hyperparameters selected by grid search. In the second, I compare the results of a novel importance sampling - grid search hybrid scheme for hyperparameter specification.

The first two main sections contain the results of these experiments, while the third describes the data and extraneous covariate generation.

Optimal Π

Hyperparameter specification

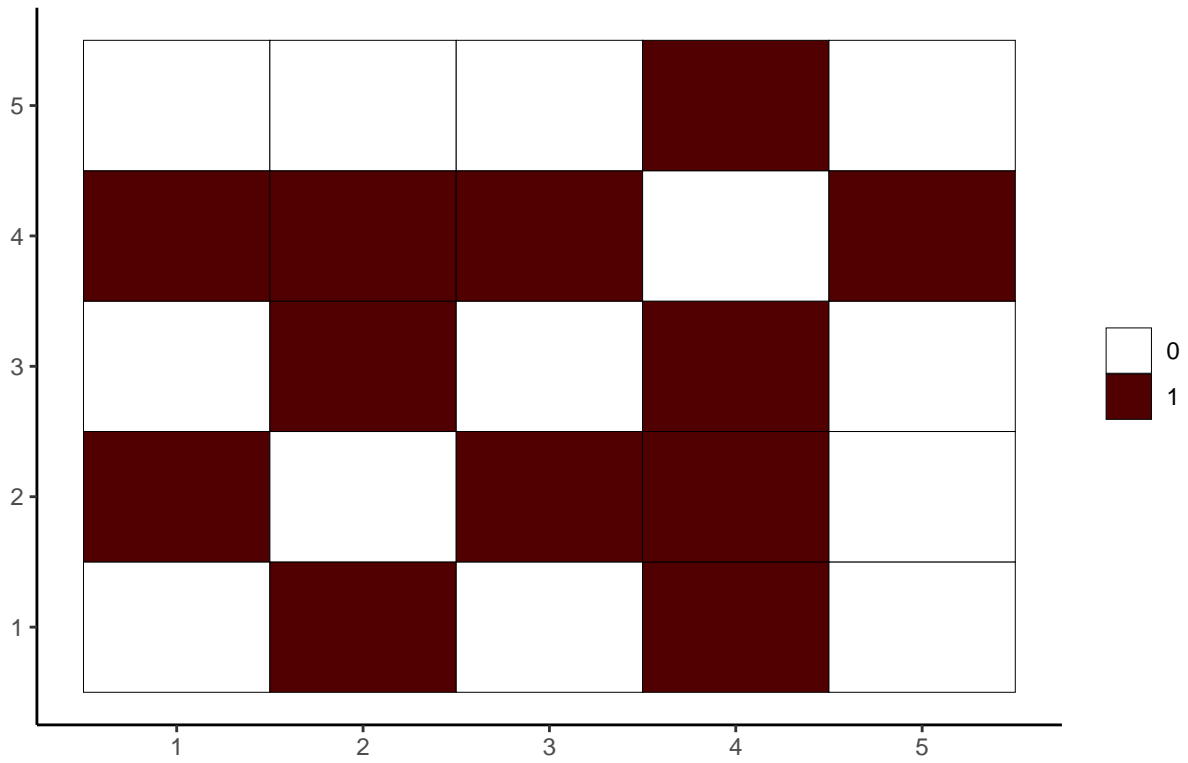
[[1]]



##

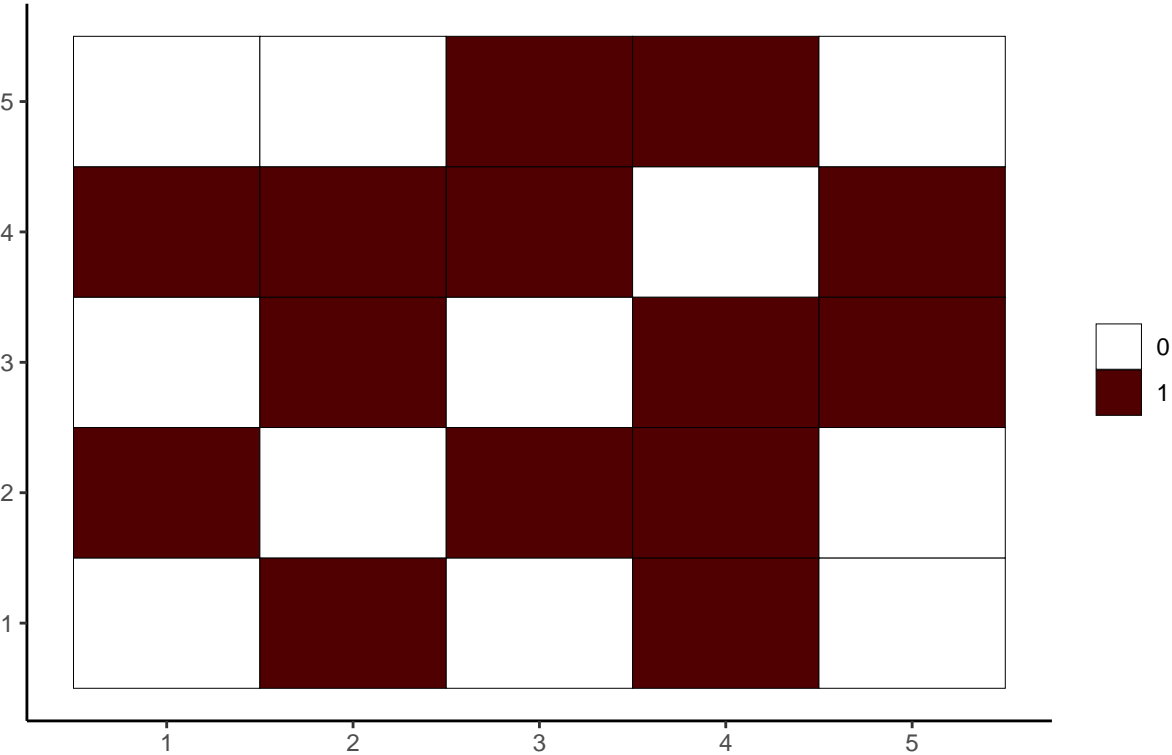
[[2]]

Graph 2, Individuals 27,...,44,50,...,53



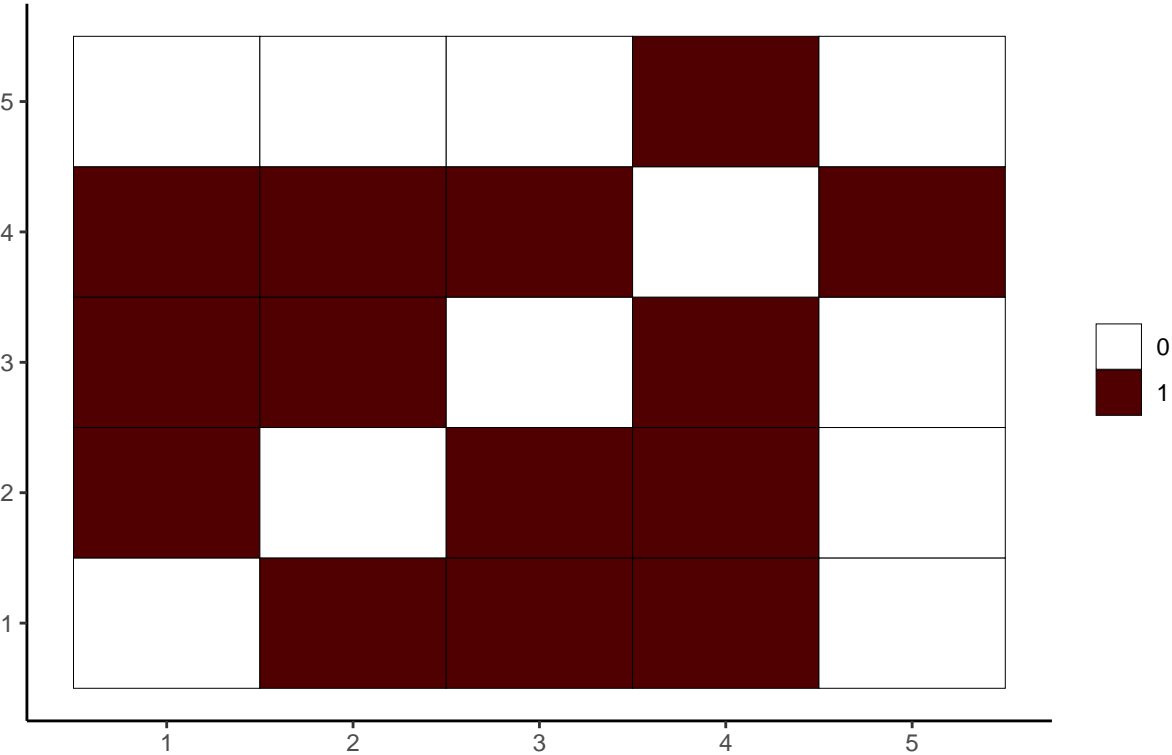
```
##  
## [[3]]
```

Graph 3, Individuals 45,...,49



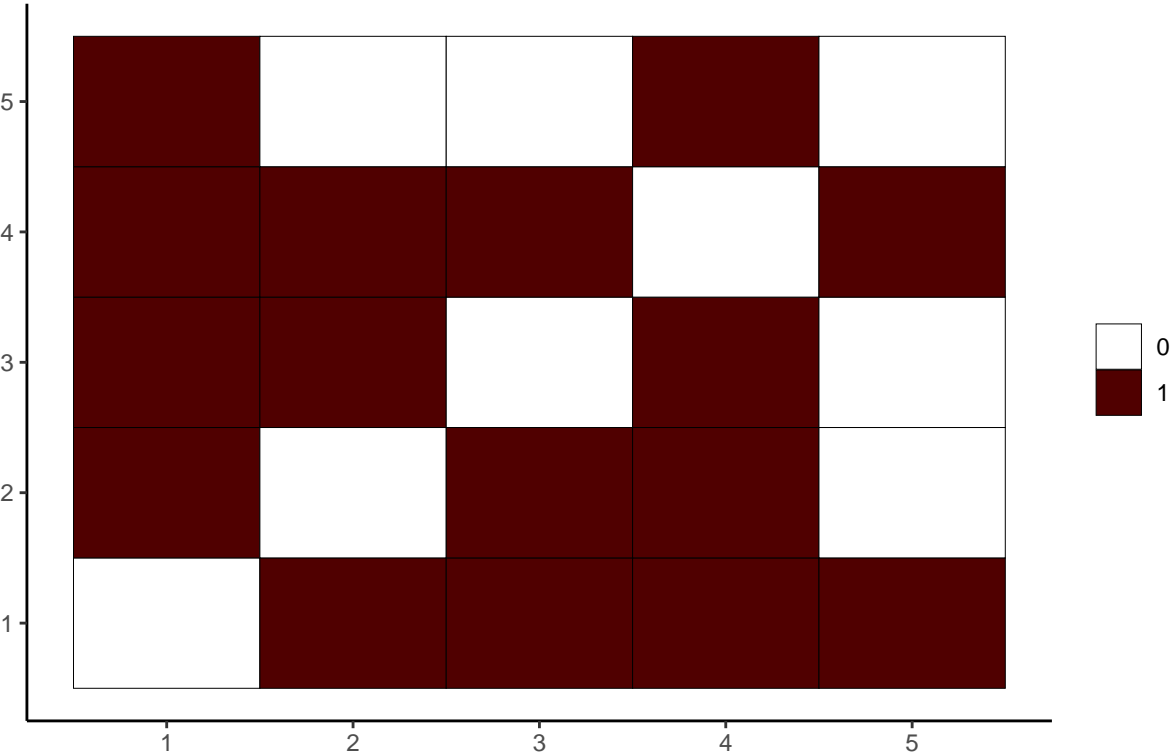
[[4]]

Graph 4, Individuals 54,...,82



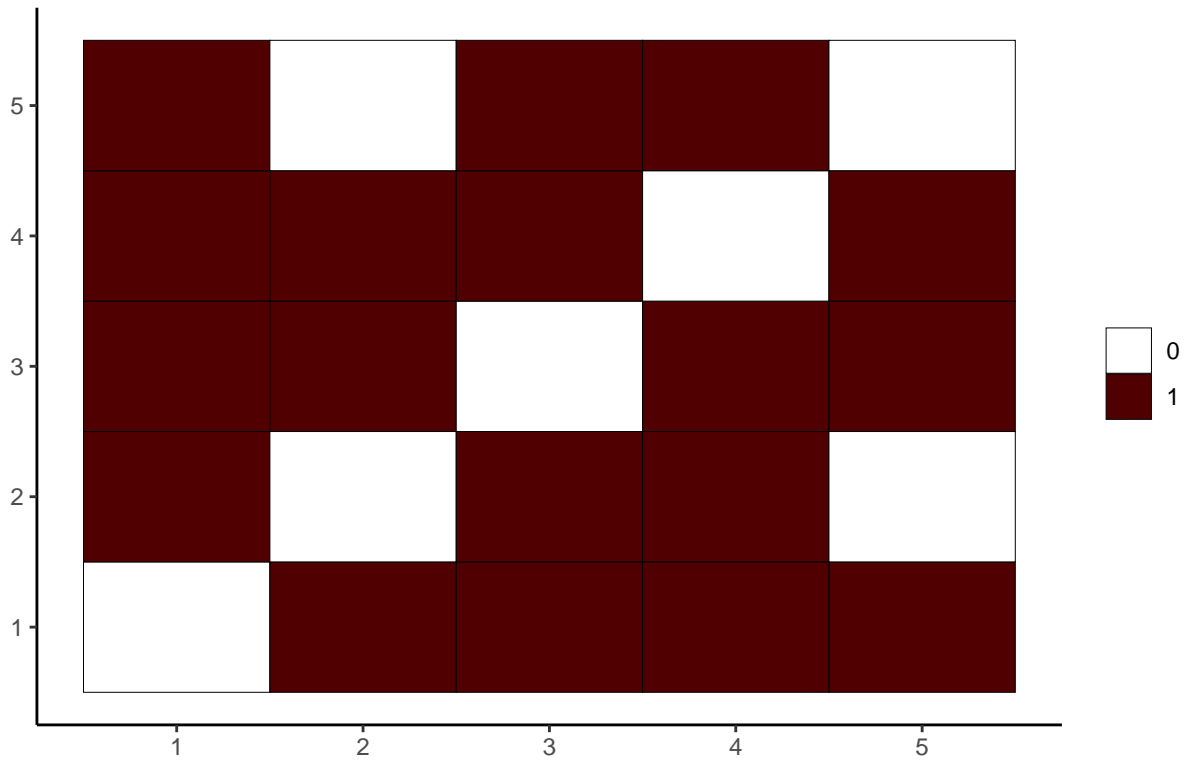
[[5]]

Graph 5, Individuals 83,...,116



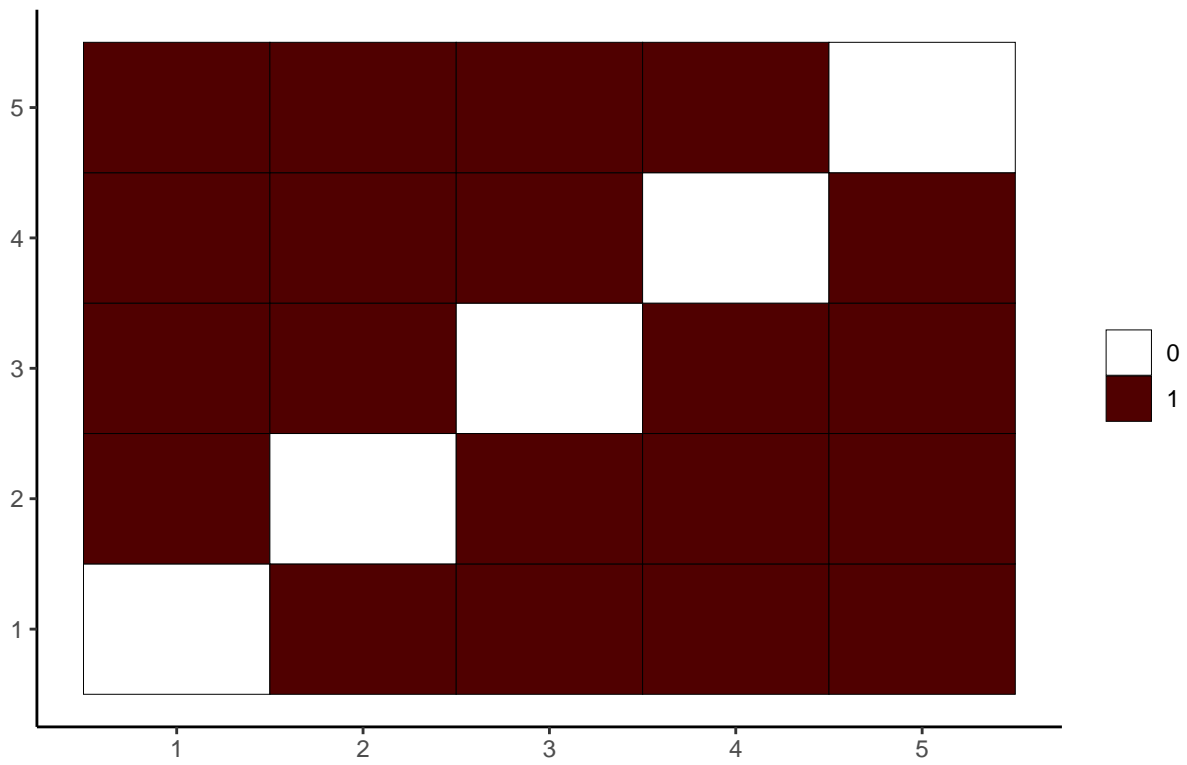
[[6]]

Graph 6, Individuals 117,...,131



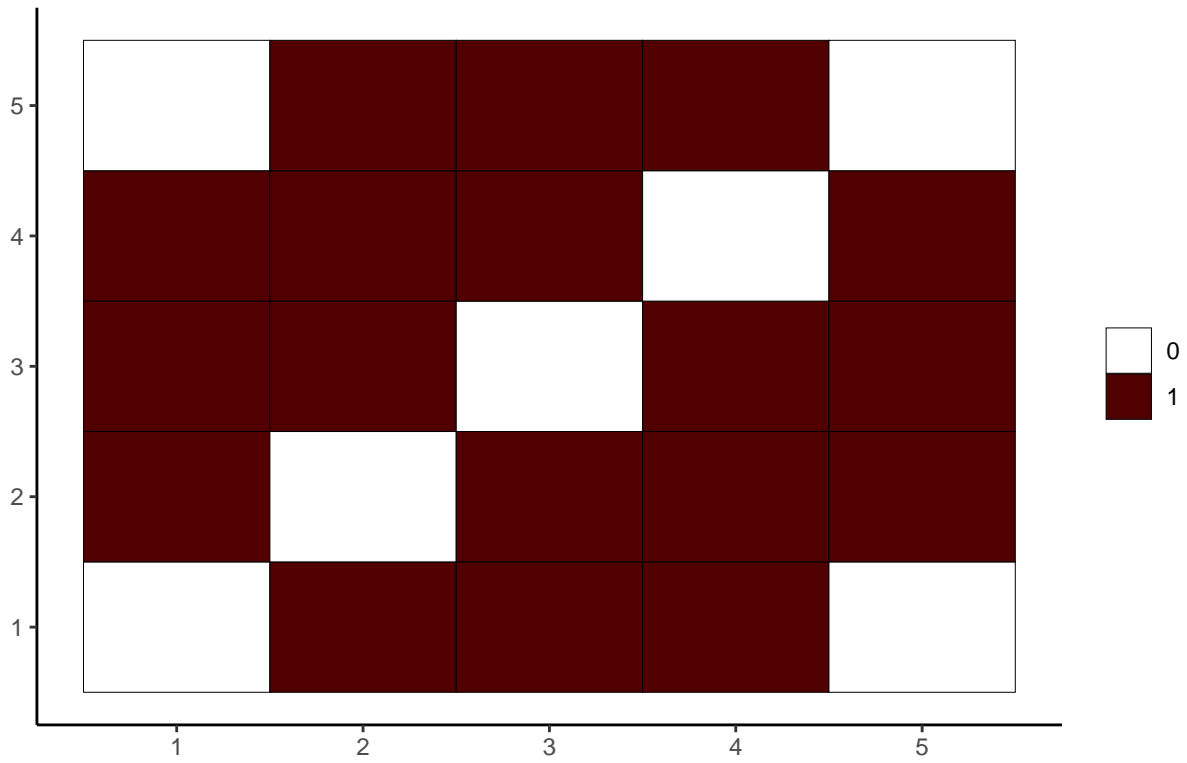
```
##  
## [[7]]
```

Graph 7, Individuals 132,...,143



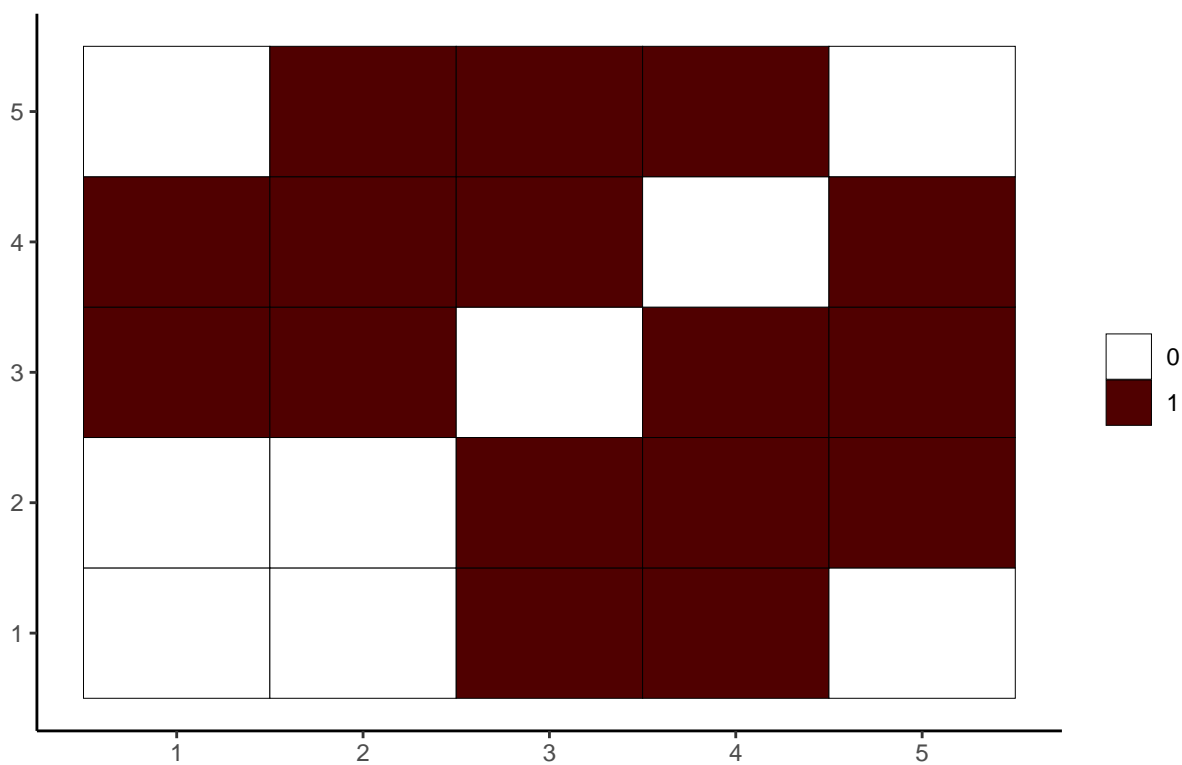
[[8]]

Graph 8, Individuals 144,...,150



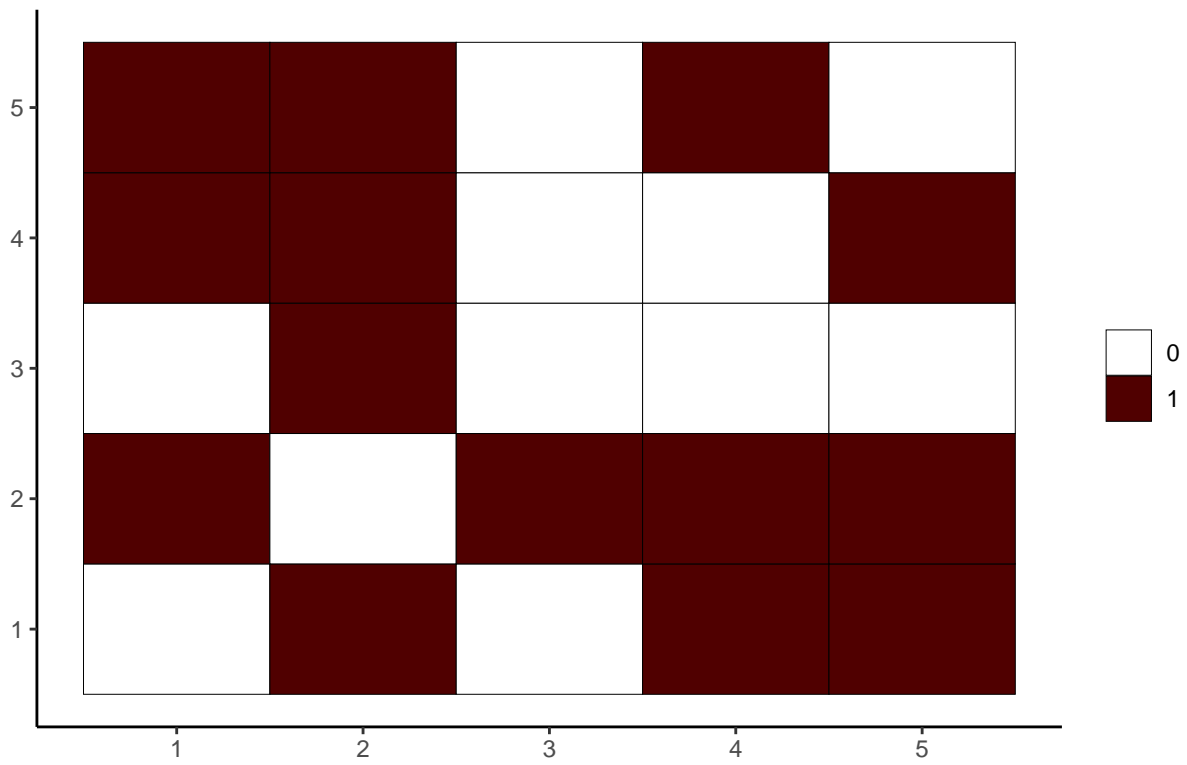
[[9]]

Graph 9, Individuals 151,...,180



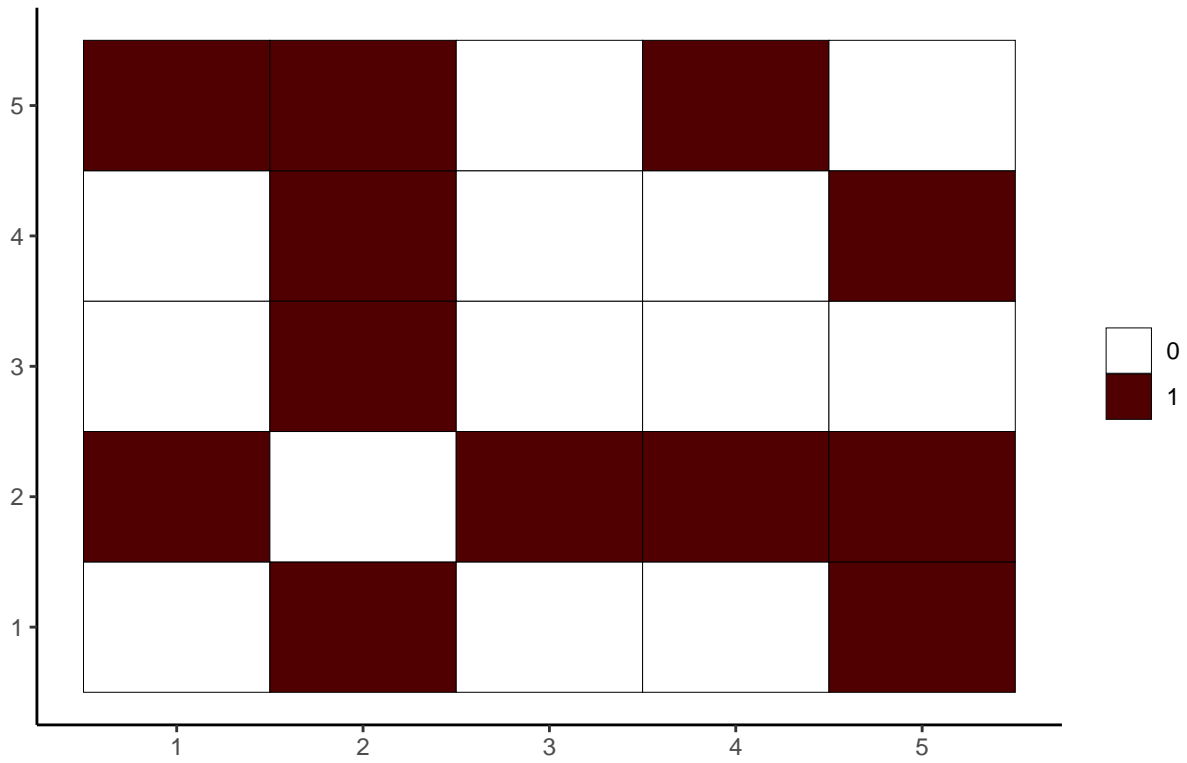
[[1]]

Graph 1, Individuals 1,...,33



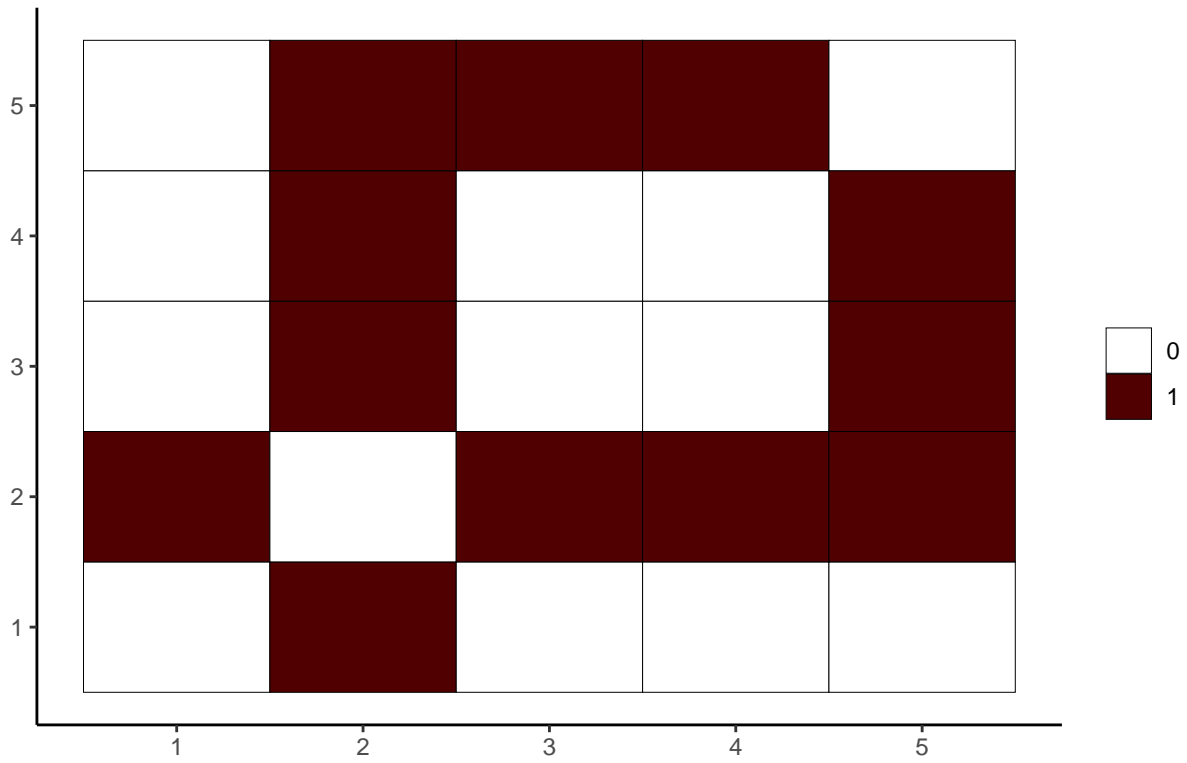
```
##  
## [[2]]
```

Graph 2, Individuals 34,...,60



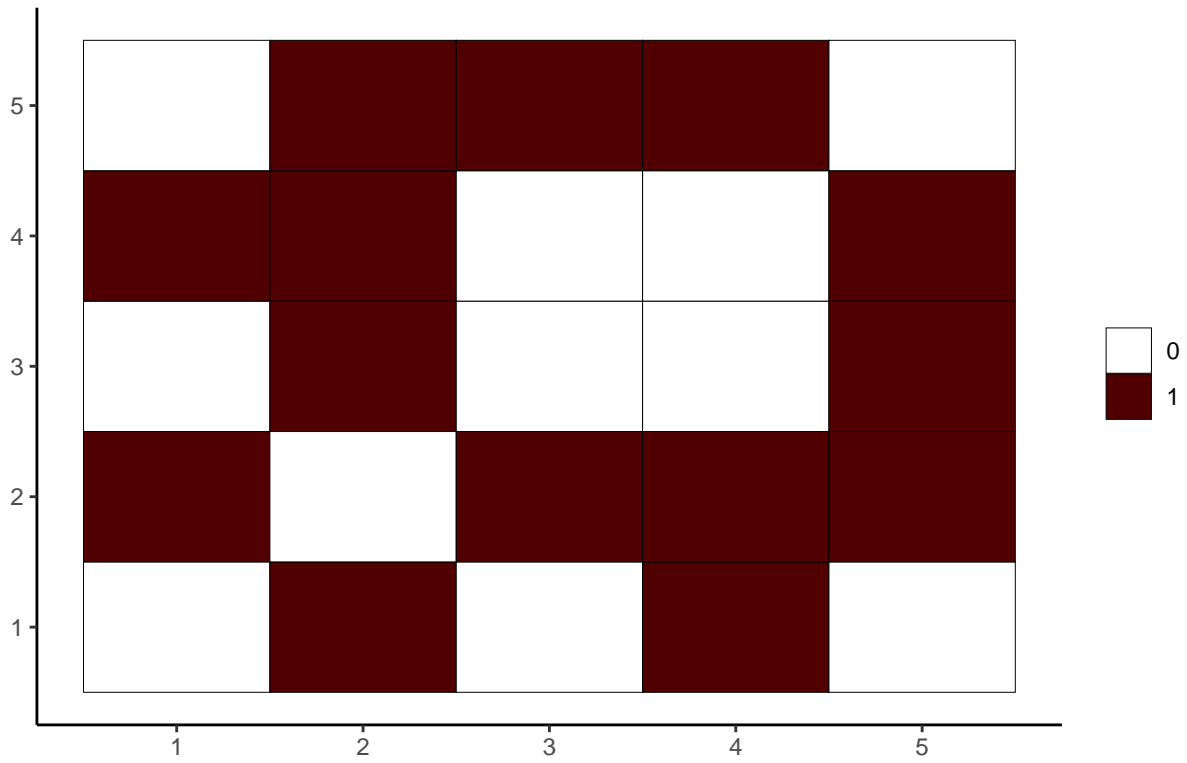
```
##  
## [[3]]
```

Graph 3, Individuals 61,...,66



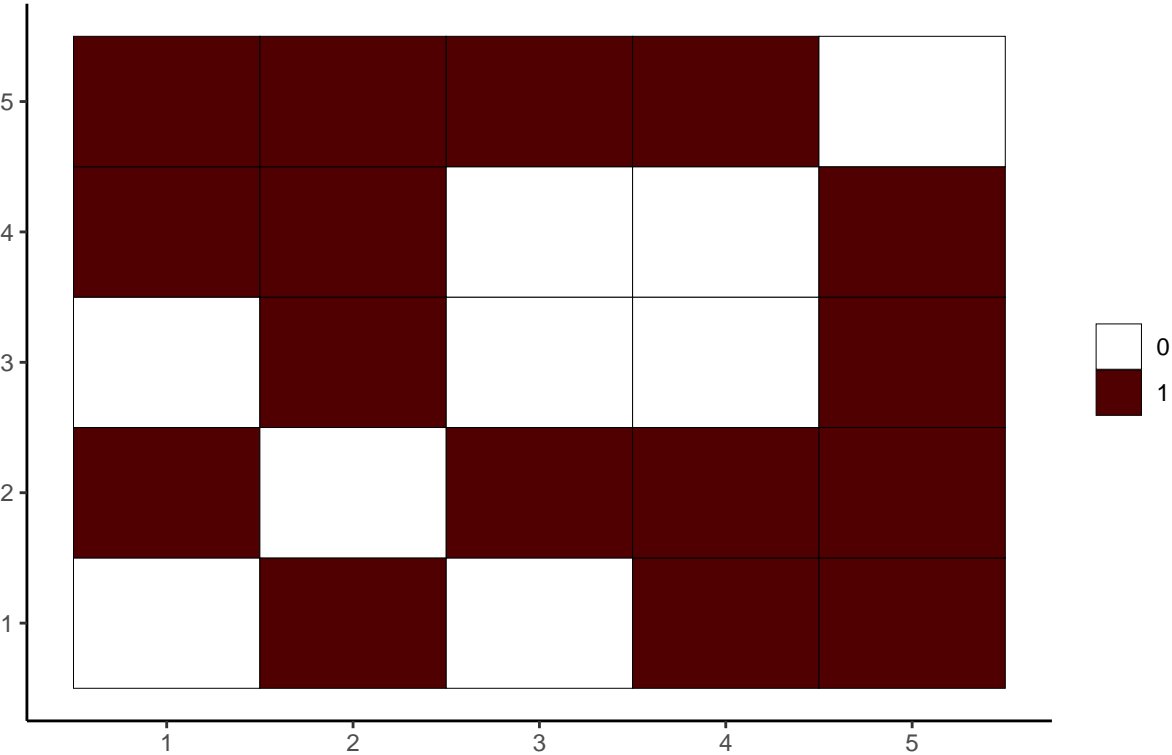
```
##  
## [[4]]
```

Graph 4, Individuals 67,...,71



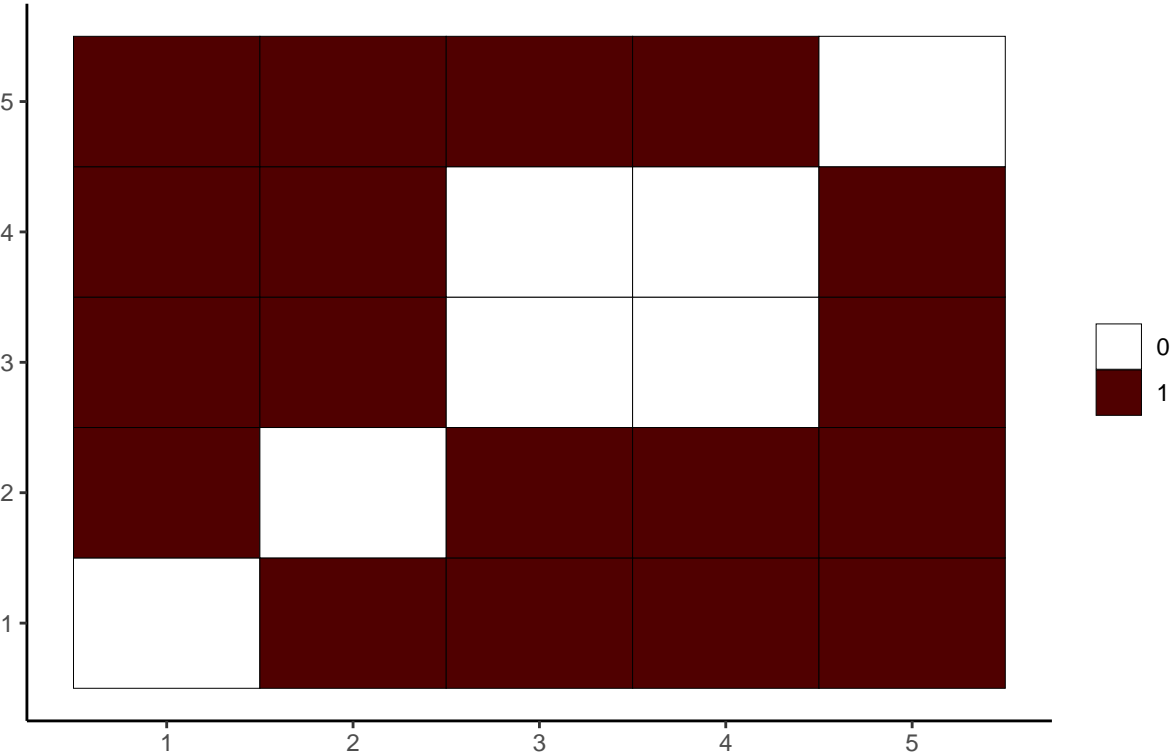
```
##  
## [[5]]
```

Graph 5, Individuals 72,73



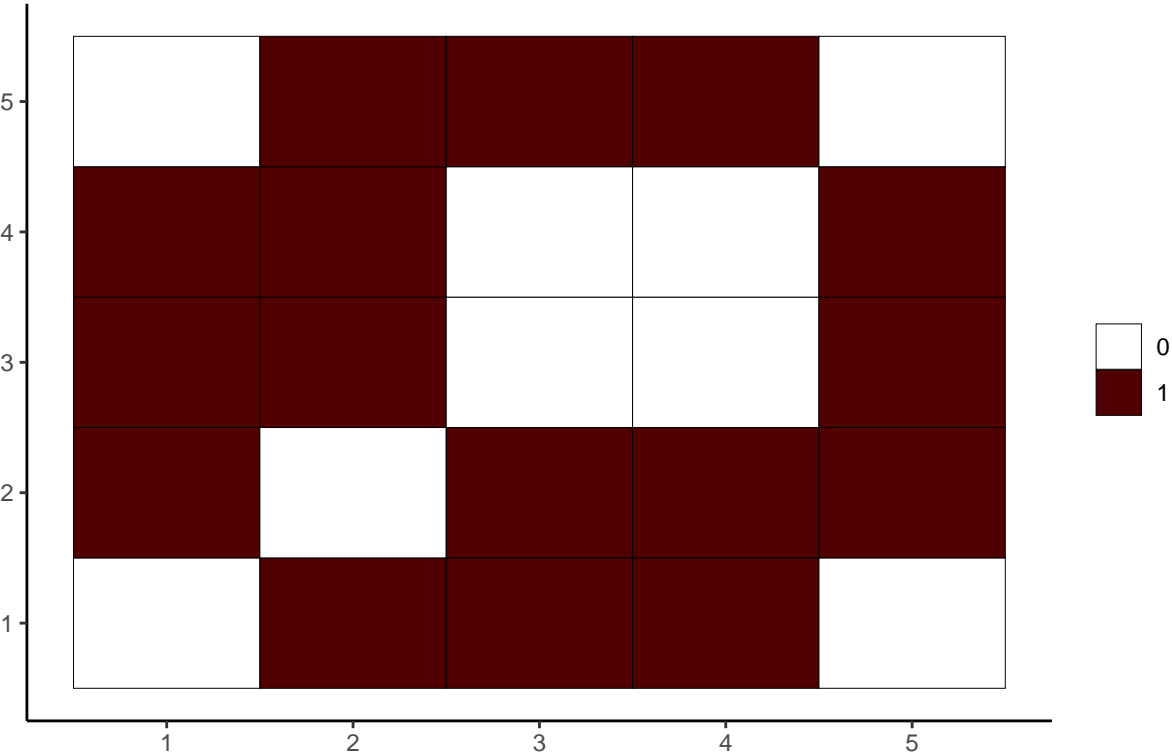
[[6]]

Graph 6, Individuals 74,...,96



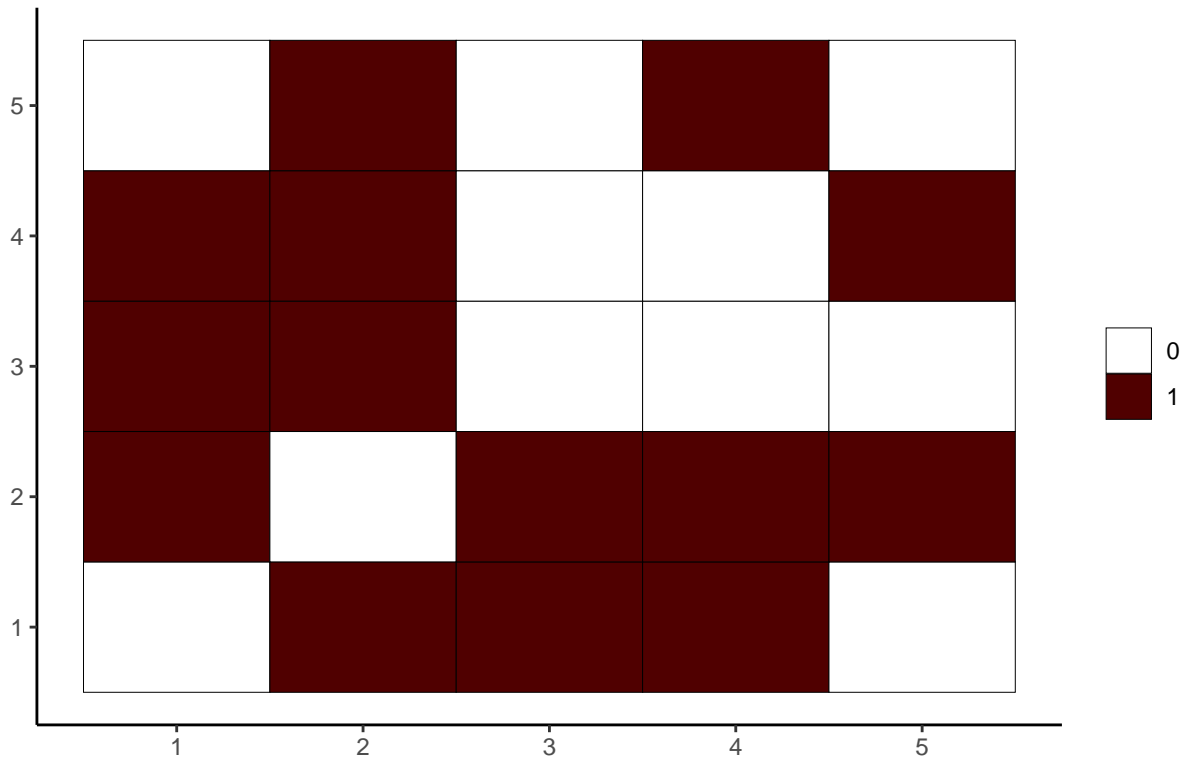
```
##  
## [[7]]
```


Graph 7, Individuals 97,...,106



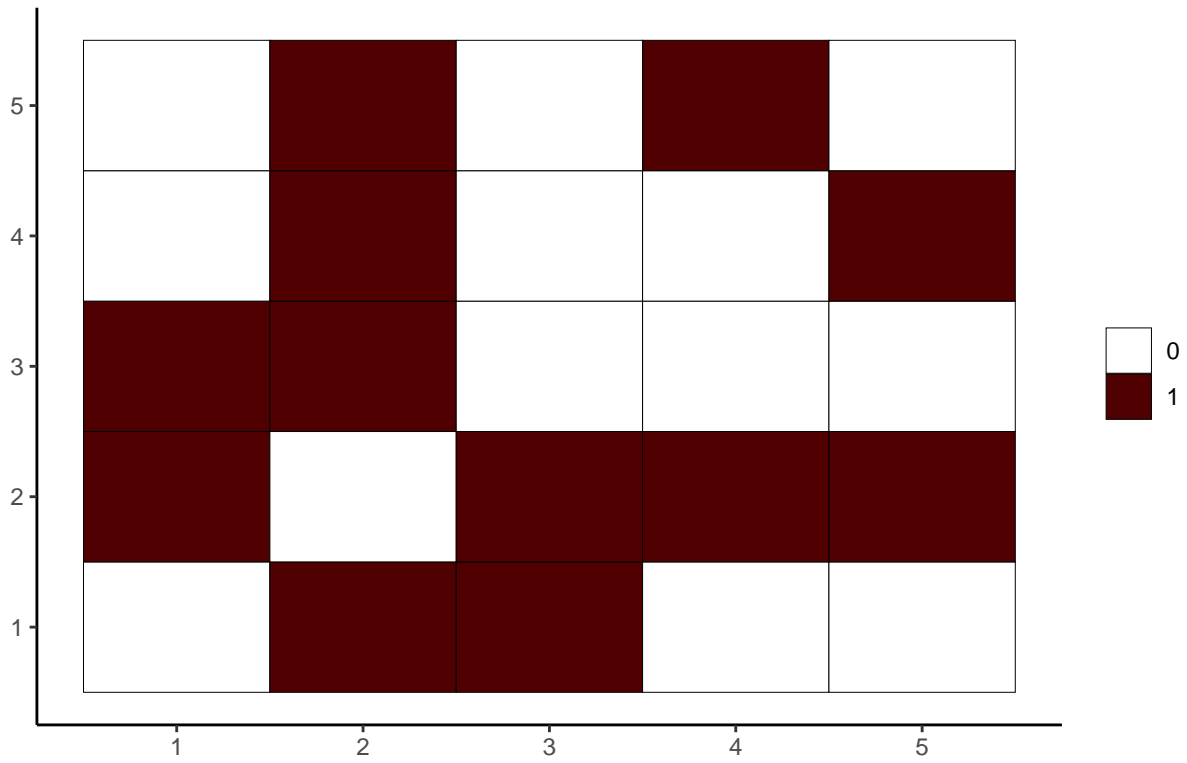
[[8]]

Graph 8, Individuals 107,...,109



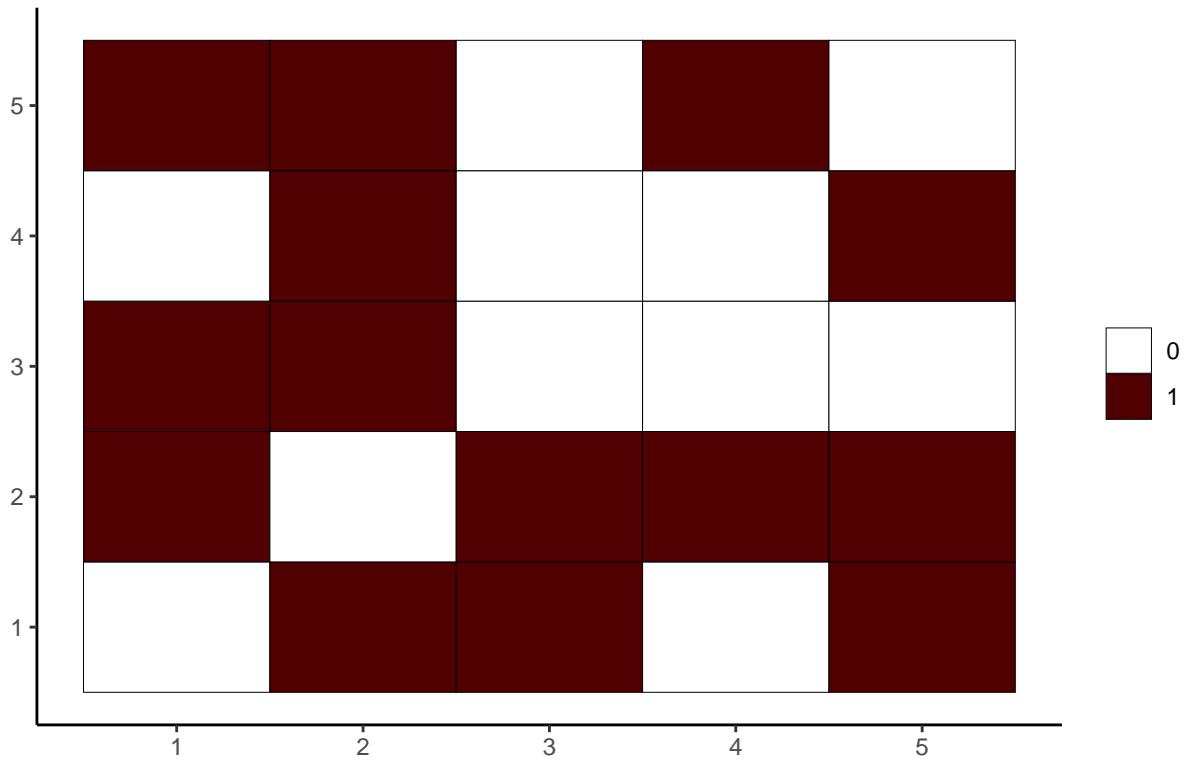
```
##  
## [[9]]
```

Graph 9, Individuals 110,...,119



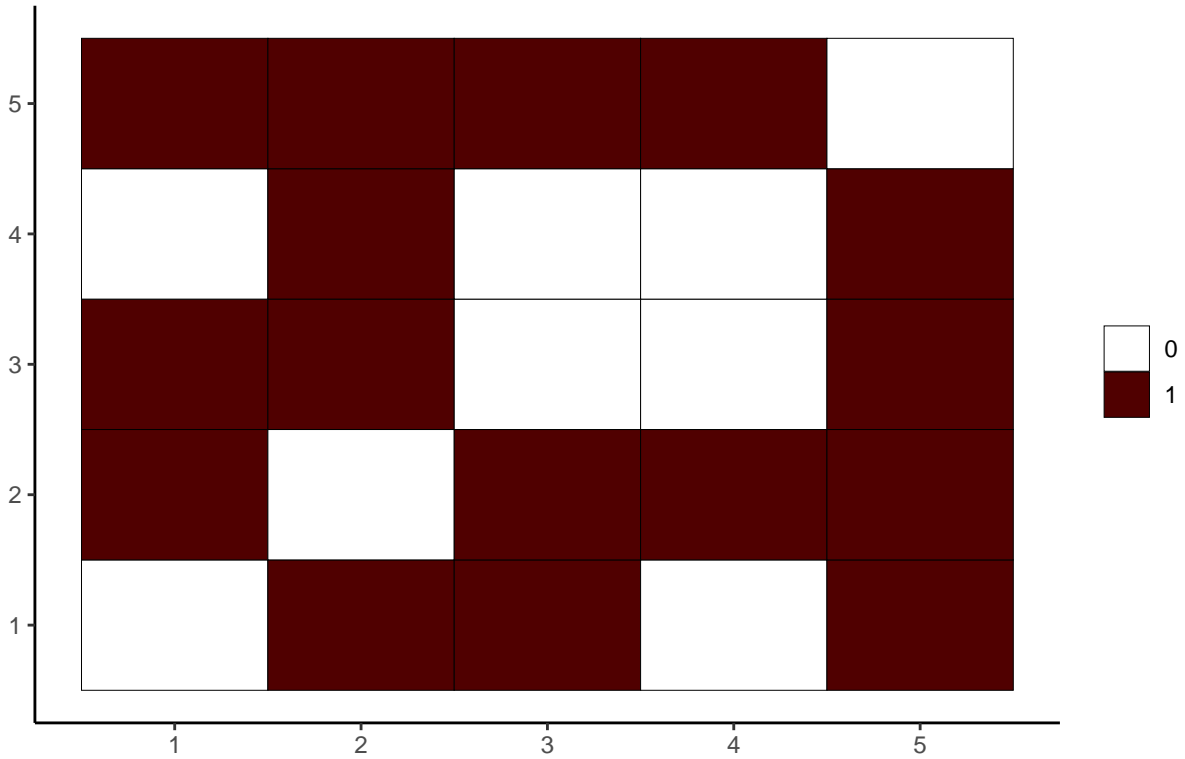
```
##  
## [[10]]
```

Graph 10, Individuals 120,...,156



```
##  
## [[11]]
```

Graph 11, Individuals 157,...,180



In this experiment, I applied the grid search algorithm in 100 trials. I generated the grid from the cartesian product of the following marginal grids:

marginal grids

`marg_grids`

`## $pip`

`## [1] 0.00001 0.00010 0.00100 0.01000 0.02500 0.05000 0.15000 0.25000 0.35000`

`## [10] 0.45000 0.55000 0.65000 0.75000 0.85000 0.95000 0.99000 0.99900 0.99990`

`## [19] 0.99999`

`##`

`## $ssq`

`## [1] 1.0e-05 1.0e-04 1.0e-03 1.0e-02 2.5e-02 5.0e-02 1.0e-01 1.5e-01 2.0e-01`

`## [10] 2.5e-01 3.0e-01 3.5e-01 4.0e-01 4.5e-01 5.0e-01 5.5e-01 6.0e-01 6.5e-01`

`## [19] 7.0e-01 7.5e-01 8.0e-01 8.5e-01 9.0e-01 9.5e-01 1.0e+00 1.5e+00 2.0e+00`

`## [28] 2.5e+00 3.0e+00 5.0e+00 1.0e+01`

`##`

`## $sbsq`

`## [1] 1.0e-05 1.0e-04 1.0e-03 1.0e-02 2.5e-02 5.0e-02 1.0e-01 1.5e-01 2.0e-01`

`## [10] 2.5e-01 3.0e-01 3.5e-01 4.0e-01 4.5e-01 5.0e-01 5.5e-01 6.0e-01 6.5e-01`

`## [19] 7.0e-01 7.5e-01 8.0e-01 8.5e-01 9.0e-01 9.5e-01 1.0e+00 1.5e+00 2.0e+00`

`## [28] 2.5e+00 3.0e+00 5.0e+00 1.0e+01`

number of grid points in the cartesian product

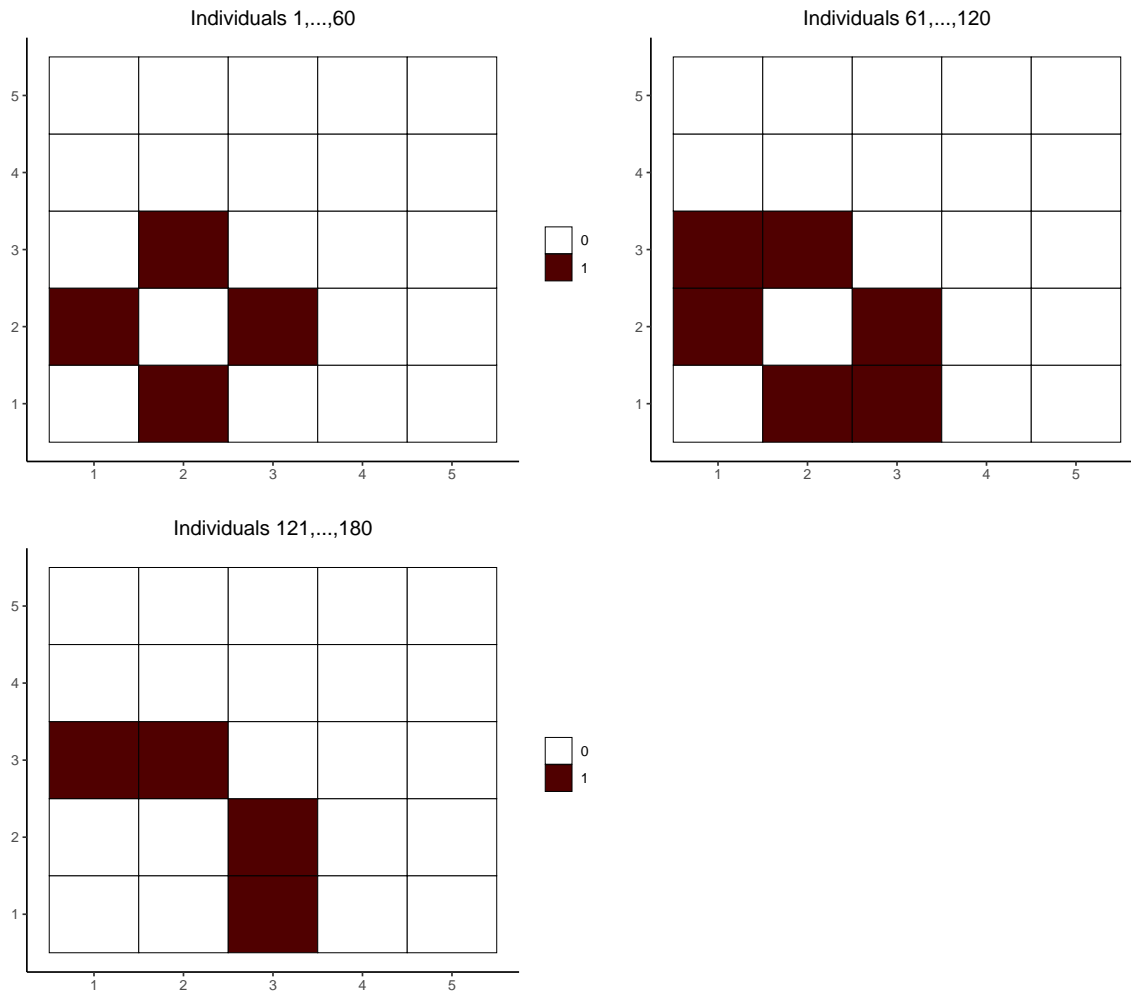
`nrow(expand.grid(marg_grids))`

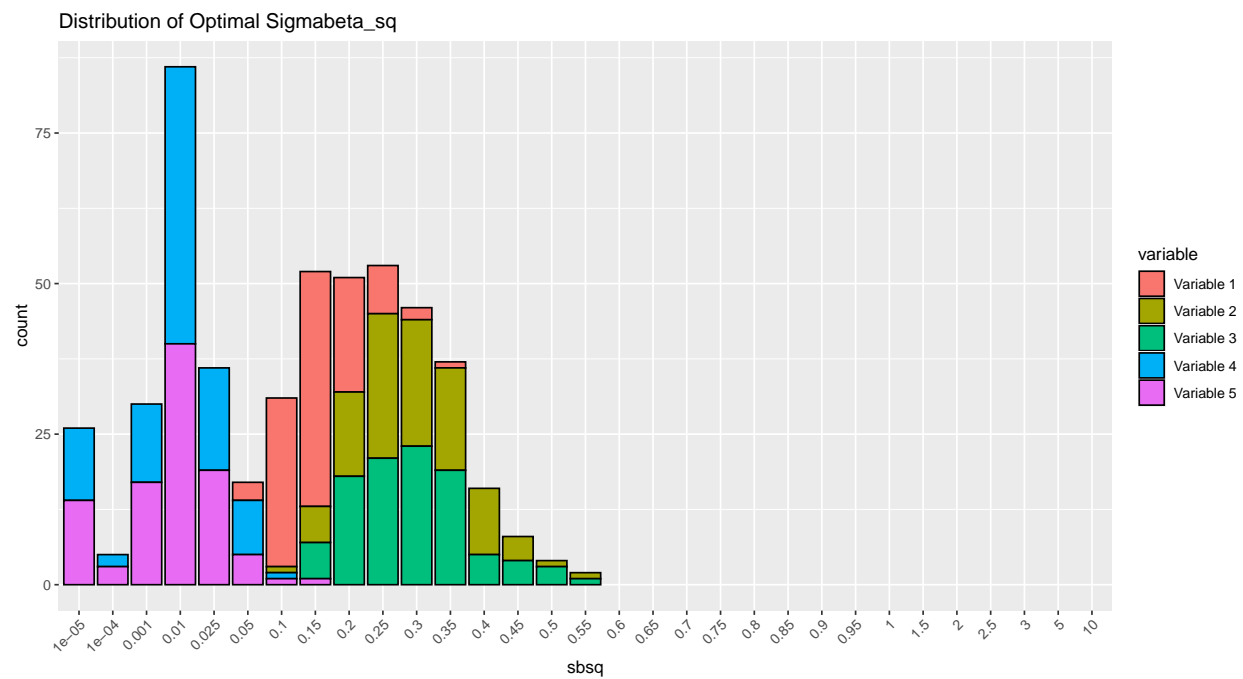
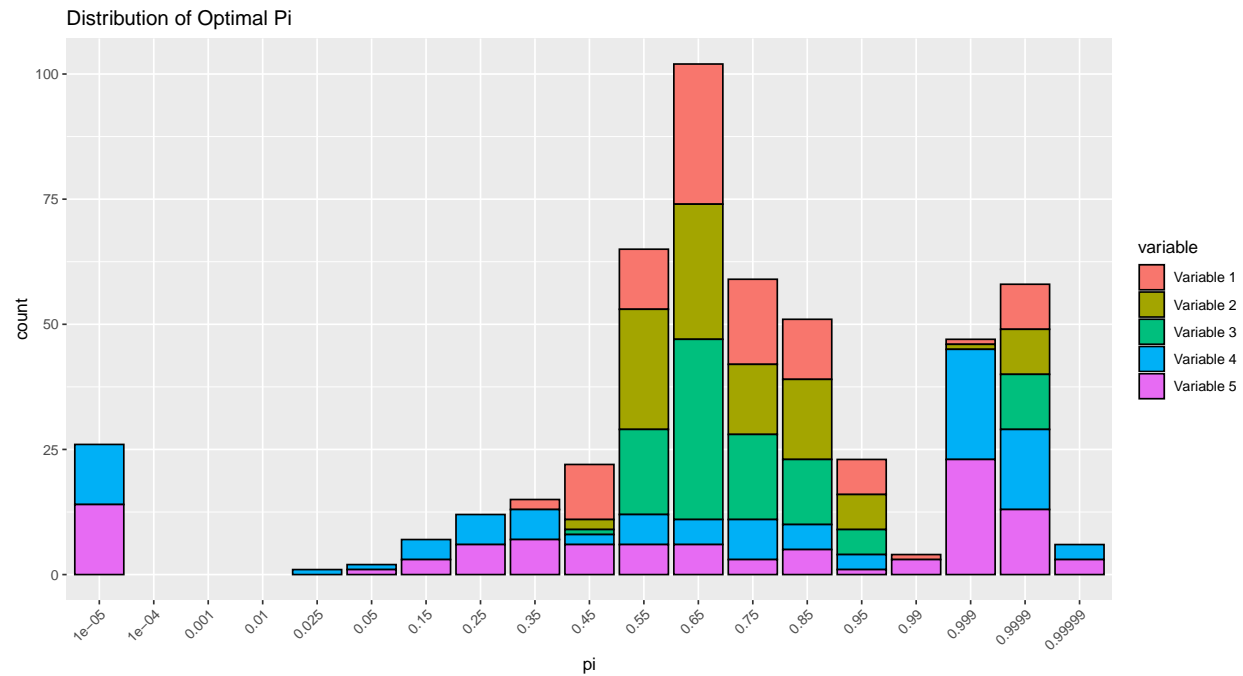
[1] 18259

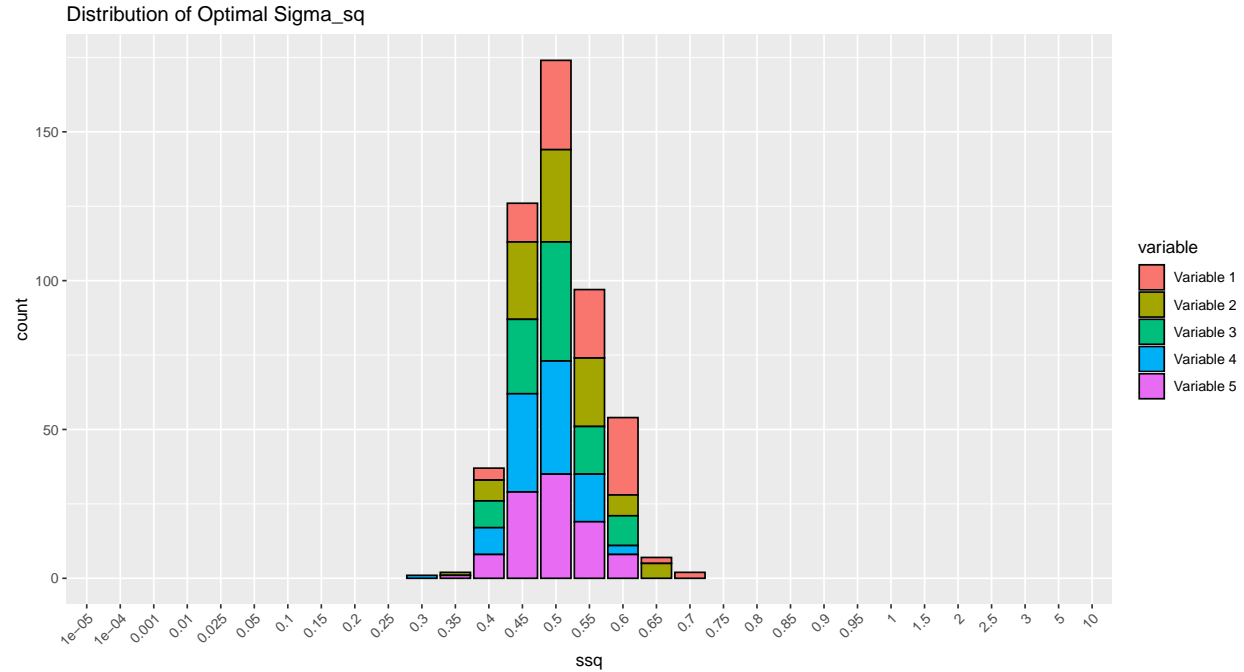
Optimal Hyperparameter Distribution

In this section, I display the distribution of optimal hyperparameters aggregated across all variables. Since a unique point in the hyperparameter grid was selected for each of the 5 variables, a total of 500 grid points are represented in each figure.

I begin by displaying the true underlying precision structures to provide context for the optimal pi.





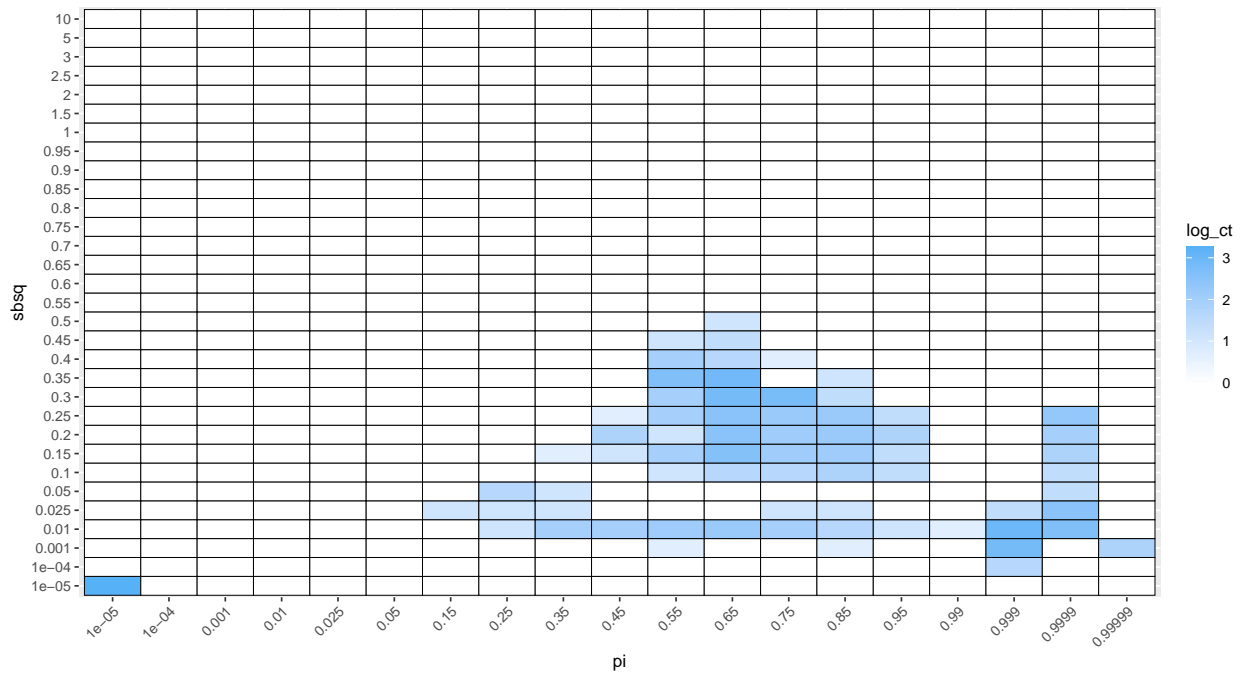


Optimal Sigmabeta_sq as a function of Pi

Here, I visualize the optimal sigmabeta_sq as a function of pi. Note that the count is on the log scale.

##		1e-05	1e-04	0.001	0.01	0.025	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45			
##	1e-05	26	0	0	0	0	0	0	0	0	0	0	0	0	0			
##	1e-04	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
##	0.001	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
##	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
##	0.025	0	0	0	1	0	0	0	0	0	0	0	0	0	0			
##	0.05	0	0	0	0	0	1	0	1	0	0	0	0	0	0			
##	0.15	0	0	1	1	3	1	1	0	0	0	0	0	0	0			
##	0.25	0	0	0	3	3	5	1	0	0	0	0	0	0	0			
##	0.35	0	0	0	7	3	3	0	2	0	0	0	0	0	0			
##	0.45	0	0	0	7	1	0	0	3	6	2	1	0	1	1			
##	0.55	0	0	2	8	1	1	3	7	3	7	7	14	7	3			
##	0.65	0	0	1	9	1	1	5	13	12	12	17	18	5	4			
##	0.75	0	0	1	7	3	0	5	8	8	9	16	0	2	0			
##	0.85	0	0	2	5	3	1	6	8	9	9	4	3	1	0			
##	0.95	0	0	0	3	1	0	4	4	6	4	0	1	0	0			
##	0.99	0	0	0	2	1	0	1	0	0	0	0	0	0	0			
##	0.999	0	5	17	19	4	0	1	0	0	0	0	1	0	0			
##	0.9999	0	0	0	14	12	4	4	6	7	10	1	0	0	0			
##	0.99999	0	0	6	0	0	0	0	0	0	0	0	0	0	0			
##		0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1	1.5	2	2.5	3	5	10
##	1e-05	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
##	1e-04	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
##	0.001	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
##	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

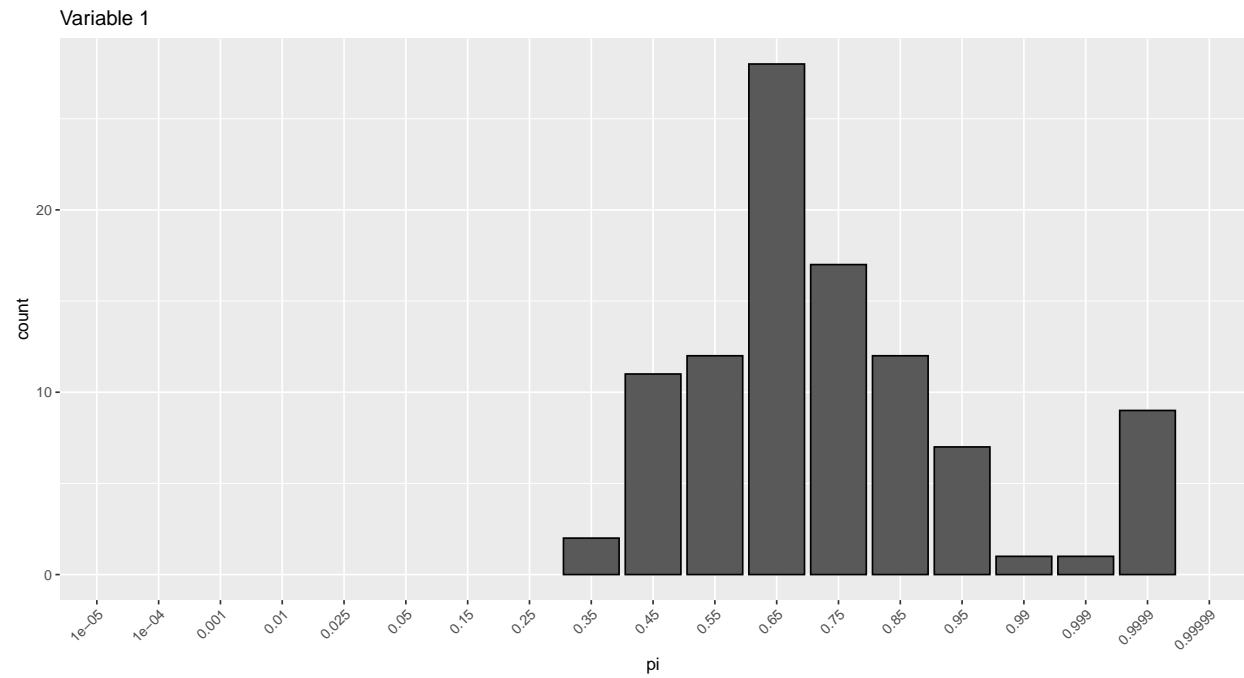

```
## 0.025 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.05 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.15 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.25 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.35 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.45 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.55 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.65 3 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.75 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.85 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.95 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.99 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.999 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.9999 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
## 0.99999 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```



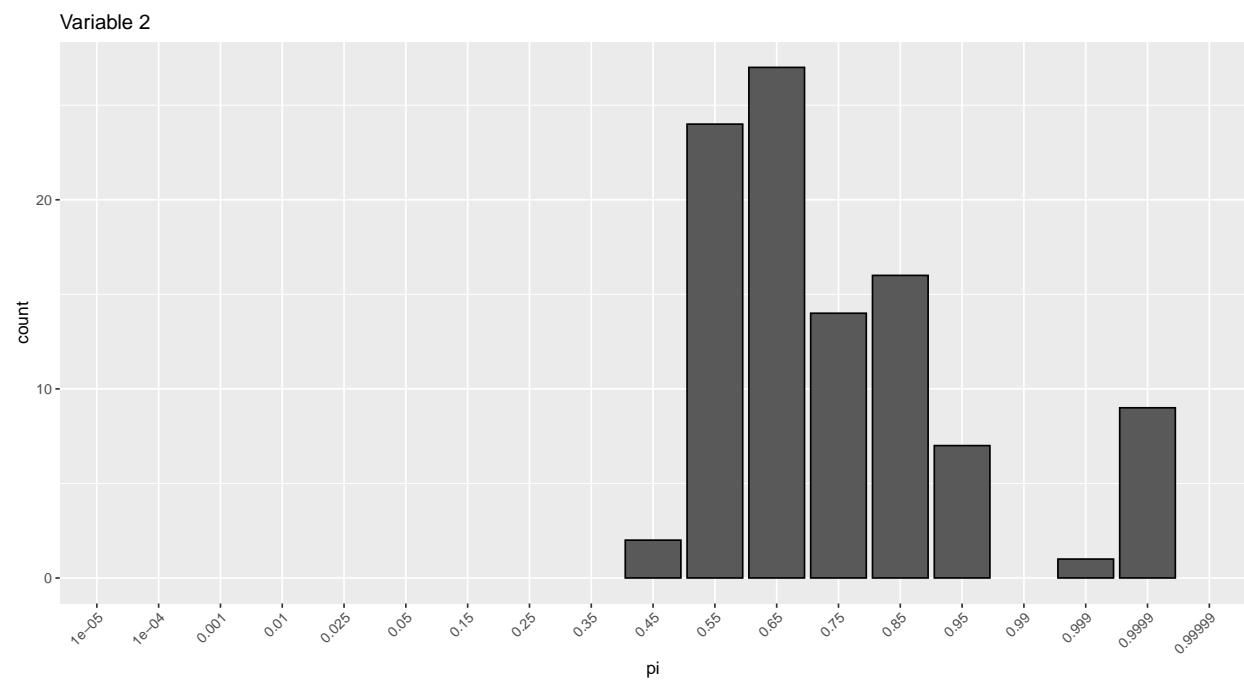
Optimal Pi by variable

In this section, I visualize the optimal pi by variable.

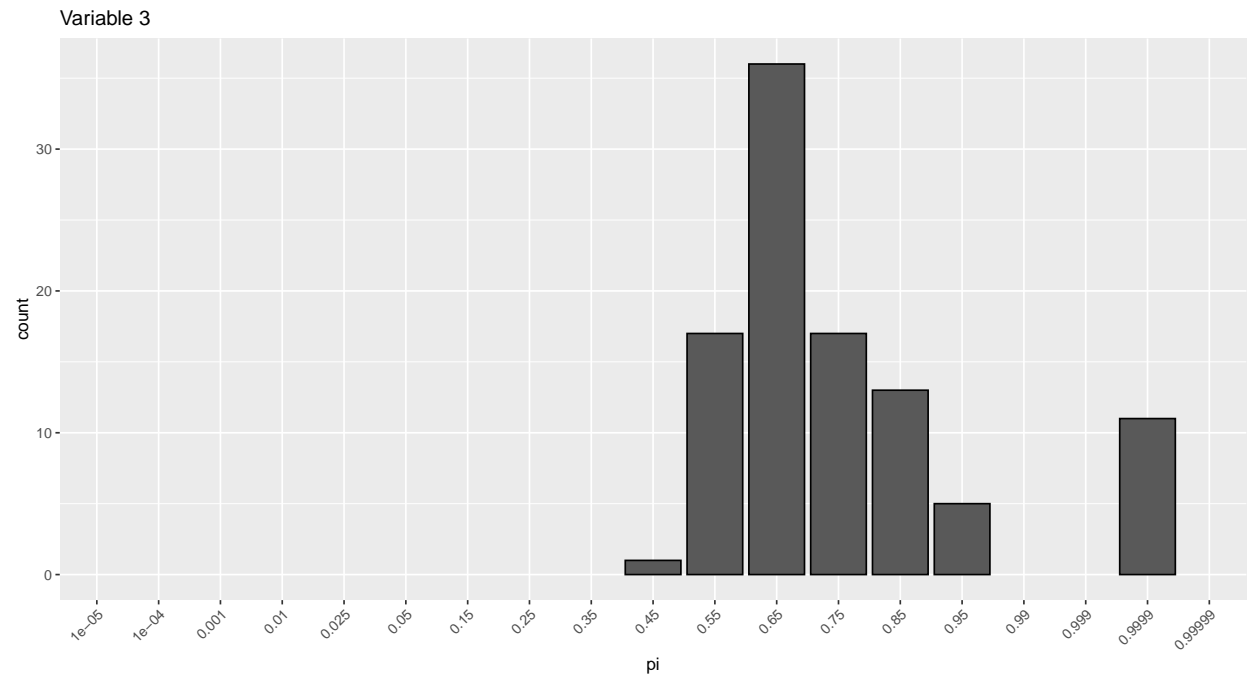
```
## [[1]]
```



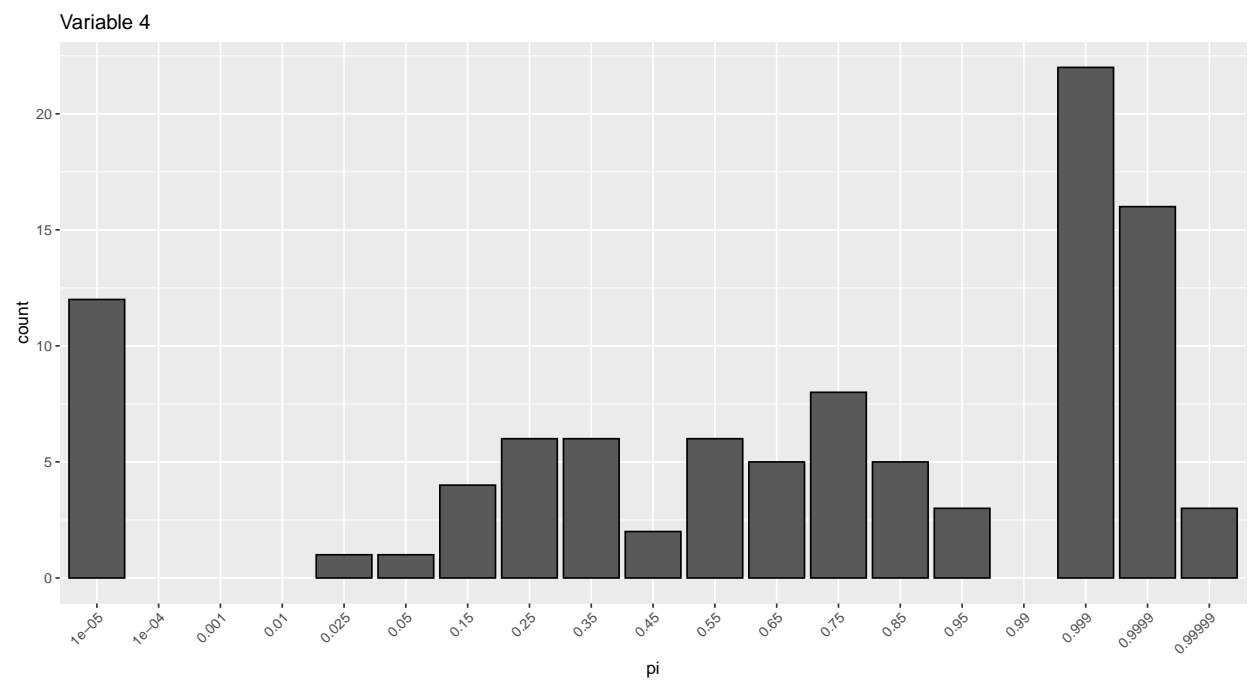
```
##
## [[2]]
```



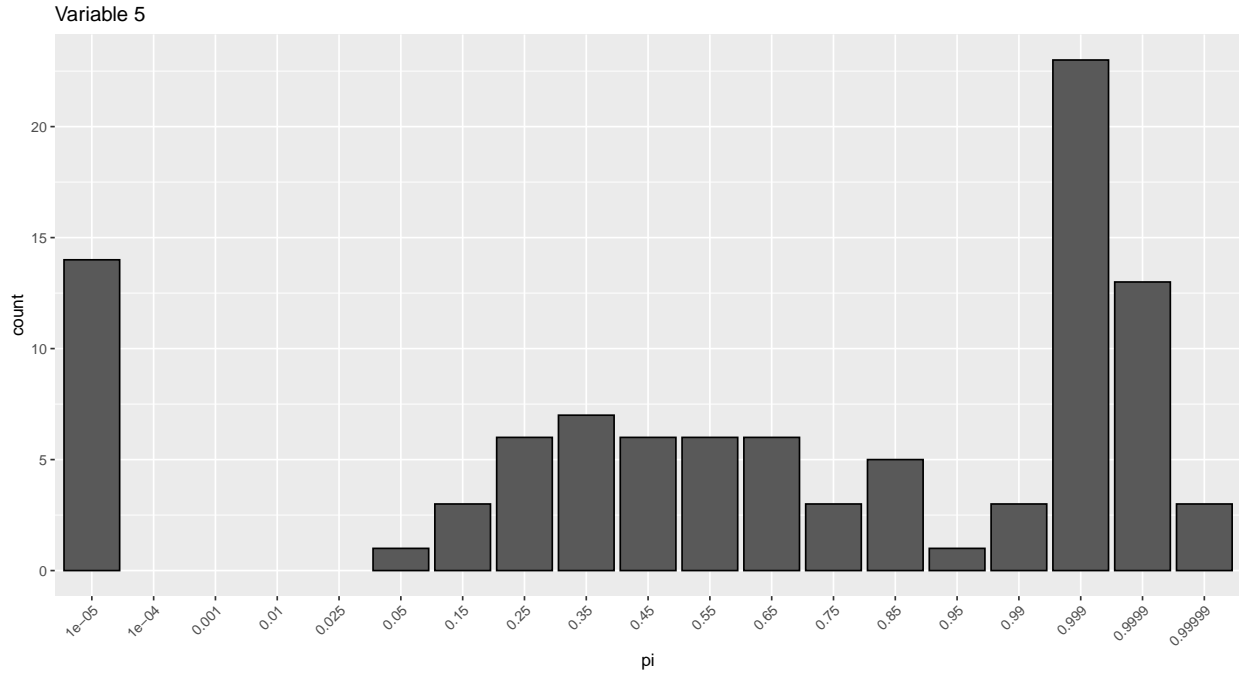
```
##
## [[3]]
```



```
##  
## [[4]]
```



```
##  
## [[5]]
```



$p = 20$

In this section, I present the same analyses as above for a dataset with $p = 20$.

The marginal grids are:

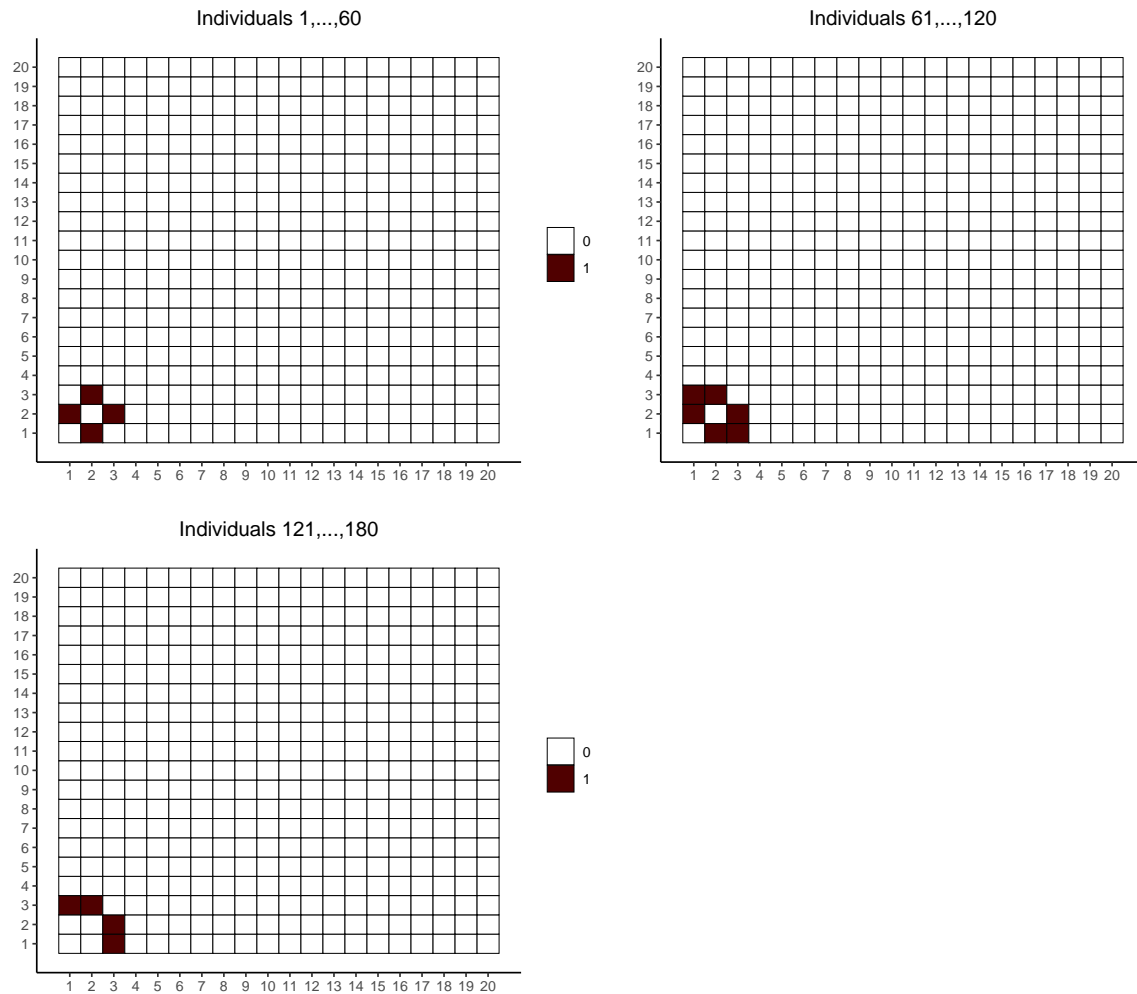
```
# marginal grids
marg_grids
```

```
##      pip      ssq      sbsq
## 1  0.00001  1.0e-05  1.0e-05
## 2  0.00010  1.0e-04  1.0e-04
## 3  0.00100  1.0e-03  1.0e-03
## 4  0.01000  1.0e-02  1.0e-02
## 5  0.02500  2.5e-02  2.5e-02
## 6  0.05000  5.0e-02  5.0e-02
## 7  0.15000  2.0e-01  2.0e-01
## 8  0.25000  3.5e-01  3.5e-01
## 9  0.35000  5.0e-01  5.0e-01
## 10 0.45000  6.5e-01  6.5e-01
## 11 0.55000  8.0e-01  8.0e-01
## 12 0.65000  9.5e-01  9.5e-01
## 13 0.75000  1.0e+00  1.0e+00
## 14 0.85000  1.5e+00  1.5e+00
## 15 0.95000  2.0e+00  2.0e+00
## 16 0.99000  2.5e+00  2.5e+00
## 17 0.99900  3.0e+00  3.0e+00
## 18 0.99990  5.0e+00  5.0e+00
## 19 0.99999  1.0e+01  1.0e+01
```

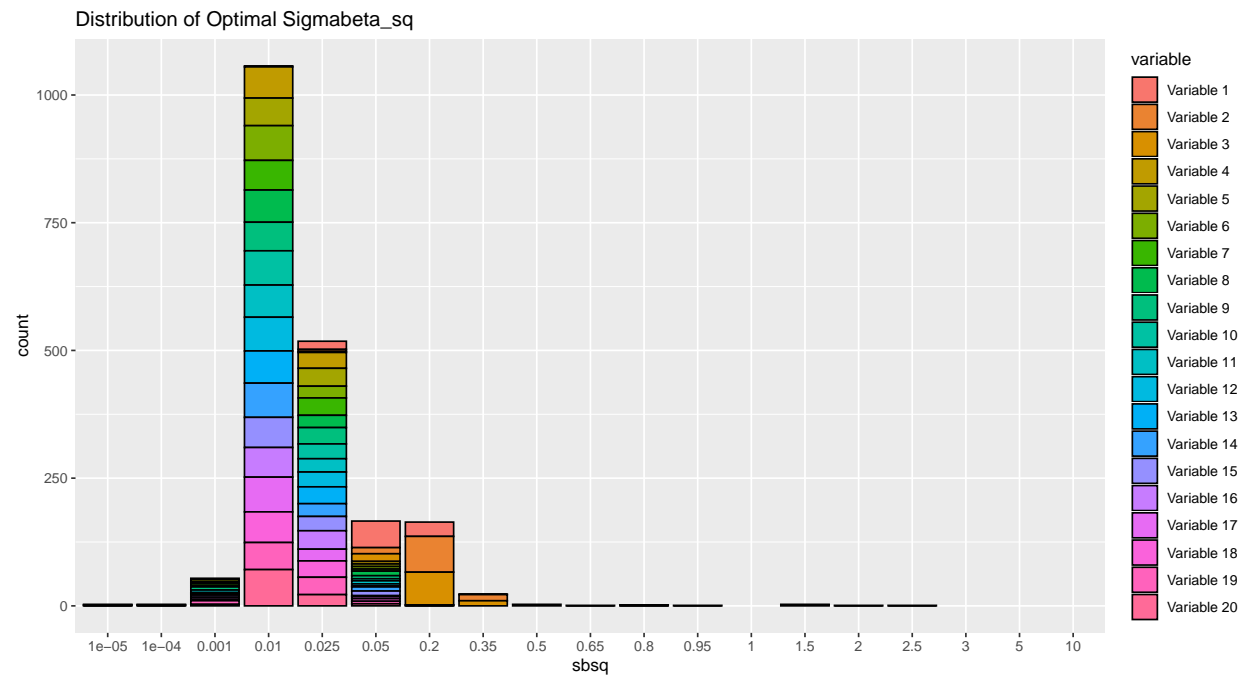
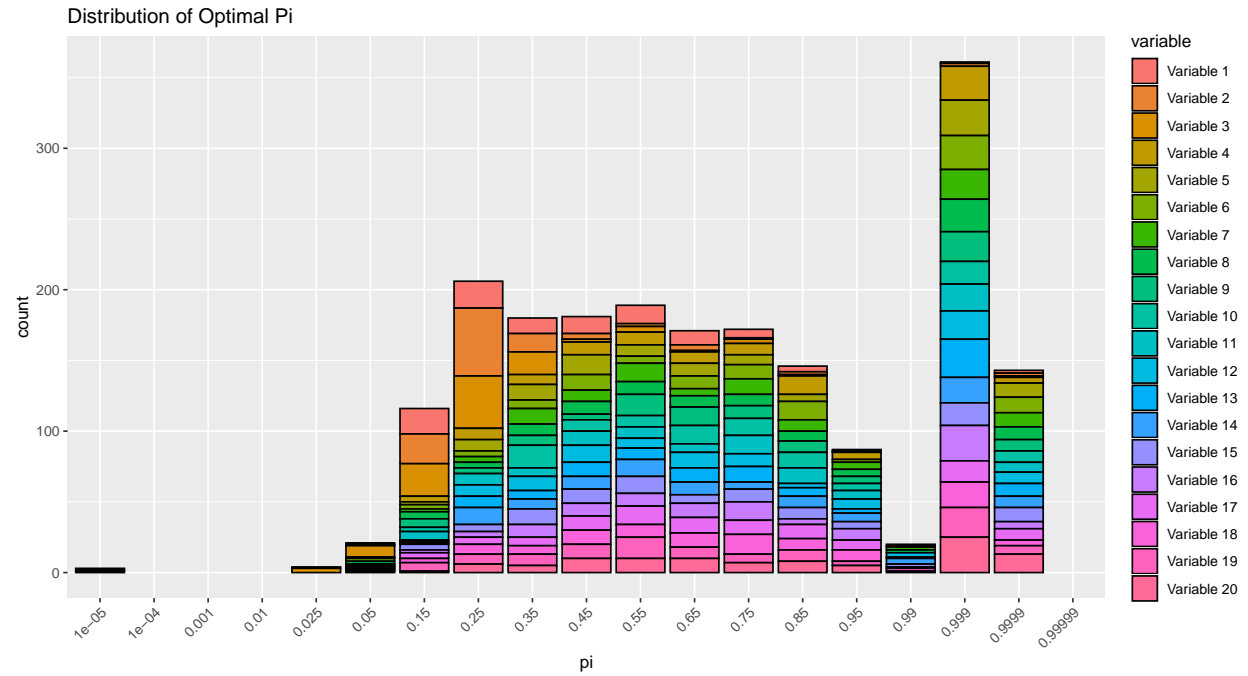
```
# number of grid points in the cartesian product
nrow(expand.grid(marg_grids))
```

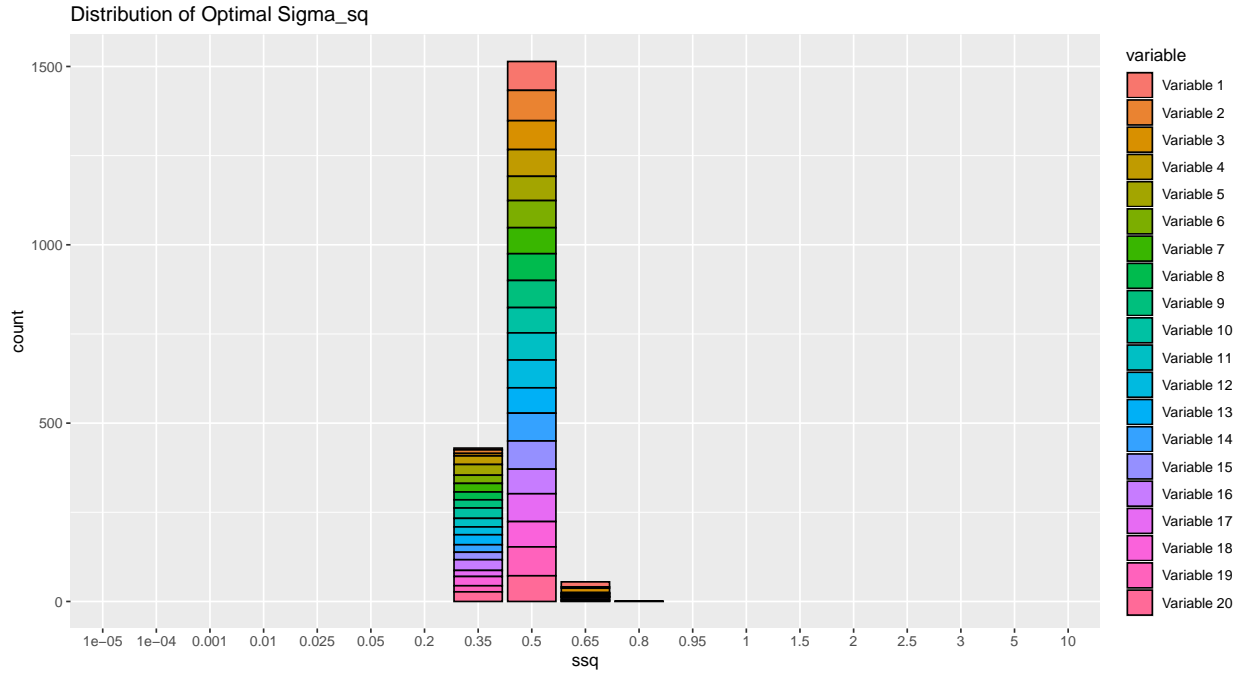
```
## [1] 6859
```

The true precision structures are given below:



Below is the distribution of the optimal hyperparameters aggregated across all variables.

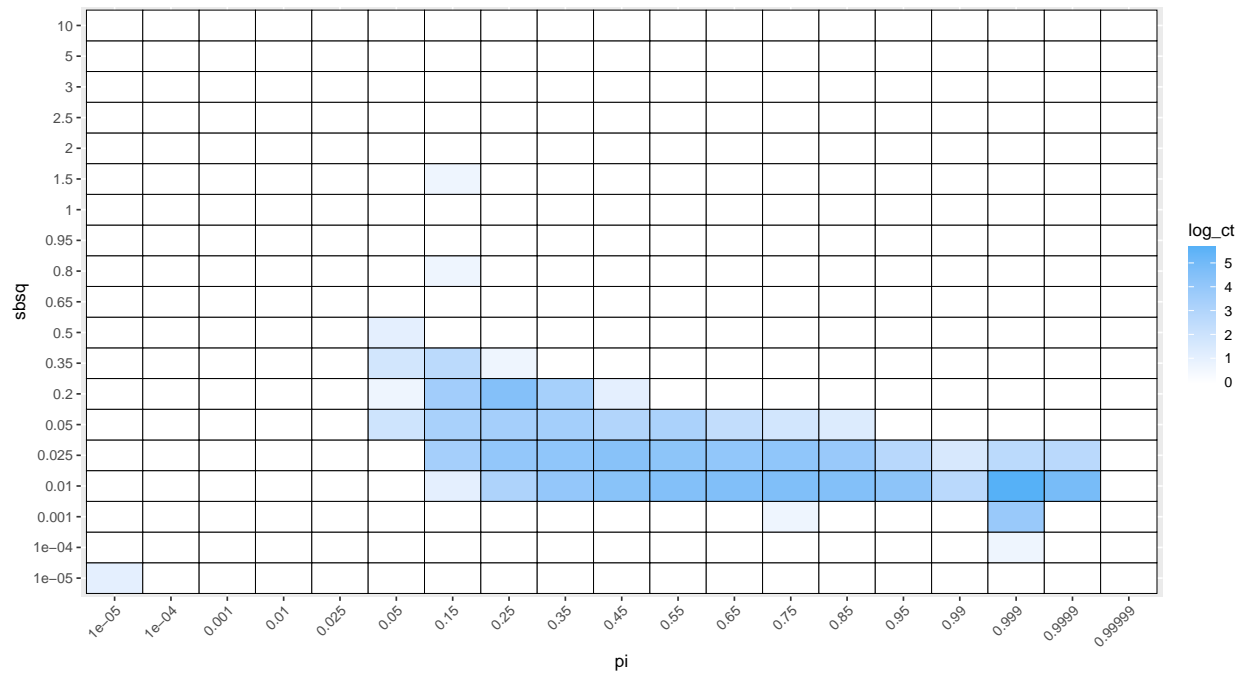




The optimal value of sbsq as a function of pi is visualized below.

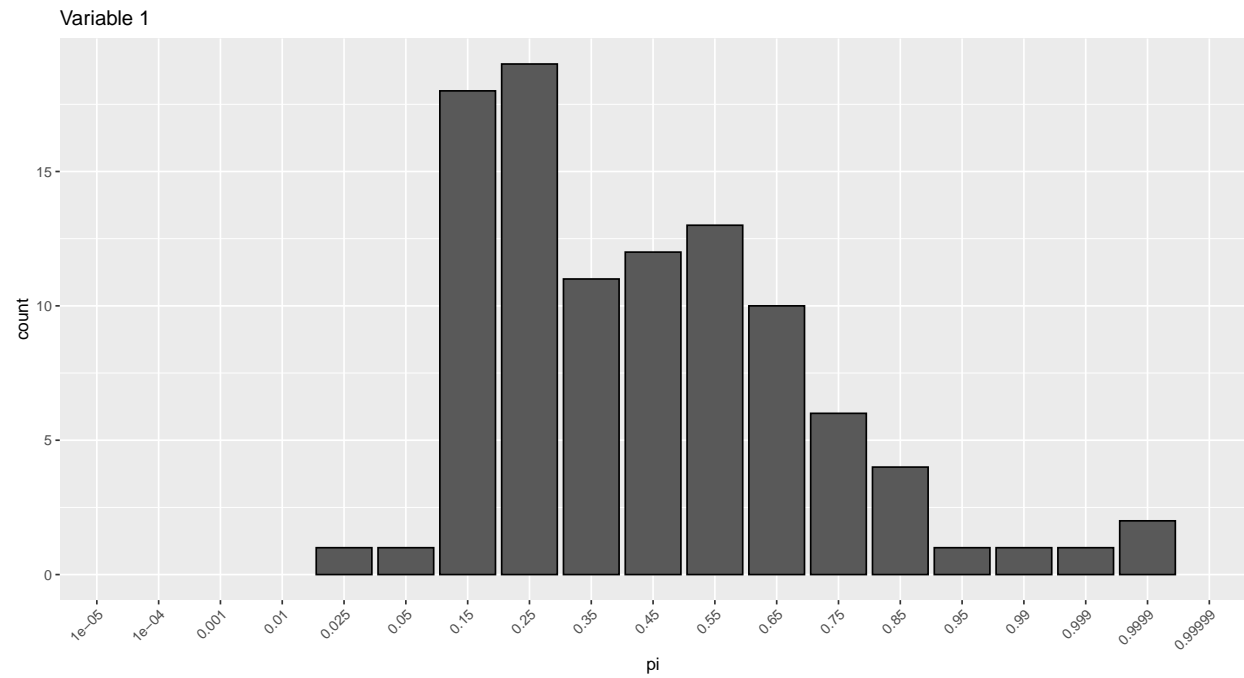
##	##	1e-05	1e-04	0.001	0.01	0.025	0.05	0.2	0.35	0.5	0.65	0.8	0.95	1	1.5
##	1e-05	3	0	0	0	0	0	0	0	0	0	0	0	0	0
##	1e-04	0	0	0	0	0	0	0	0	0	0	0	0	0	0
##	0.001	0	0	0	0	0	0	0	0	0	0	0	0	0	0
##	0.01	0	0	0	0	0	0	0	0	0	0	0	0	0	0
##	0.025	0	0	0	0	0	0	1	1	0	0	0	0	0	1
##	0.05	0	0	0	1	1	7	2	6	3	1	0	0	0	0
##	0.15	0	0	0	3	31	27	35	14	0	0	2	1	0	2
##	0.25	0	0	1	23	57	31	92	2	0	0	0	0	0	0
##	0.35	0	0	1	55	62	32	30	0	0	0	0	0	0	0
##	0.45	0	0	0	77	81	20	3	0	0	0	0	0	0	0
##	0.55	0	1	1	94	68	25	0	0	0	0	0	0	0	0
##	0.65	0	0	1	100	58	11	1	0	0	0	0	0	0	0
##	0.75	0	0	2	101	63	6	0	0	0	0	0	0	0	0
##	0.85	0	0	0	95	47	4	0	0	0	0	0	0	0	0
##	0.95	0	0	1	69	16	1	0	0	0	0	0	0	0	0
##	0.99	0	0	0	15	5	0	0	0	0	0	0	0	0	0
##	0.999	0	2	47	297	14	1	0	0	0	0	0	0	0	0
##	0.9999	0	0	0	127	15	1	0	0	0	0	0	0	0	0
##	0.99999	0	0	0	0	0	0	0	0	0	0	0	0	0	0
##	##	2	2.5	3	5	10									
##	1e-05	0	0	0	0	0									
##	1e-04	0	0	0	0	0									
##	0.001	0	0	0	0	0									
##	0.01	0	0	0	0	0									
##	0.025	0	1	0	0	0									
##	0.05	0	0	0	0	0									
##	0.15	1	0	0	0	0									

```
## 0.25      0 0 0 0 0
## 0.35      0 0 0 0 0
## 0.45      0 0 0 0 0
## 0.55      0 0 0 0 0
## 0.65      0 0 0 0 0
## 0.75      0 0 0 0 0
## 0.85      0 0 0 0 0
## 0.95      0 0 0 0 0
## 0.99      0 0 0 0 0
## 0.999     0 0 0 0 0
## 0.9999    0 0 0 0 0
## 0.99999   0 0 0 0 0
```

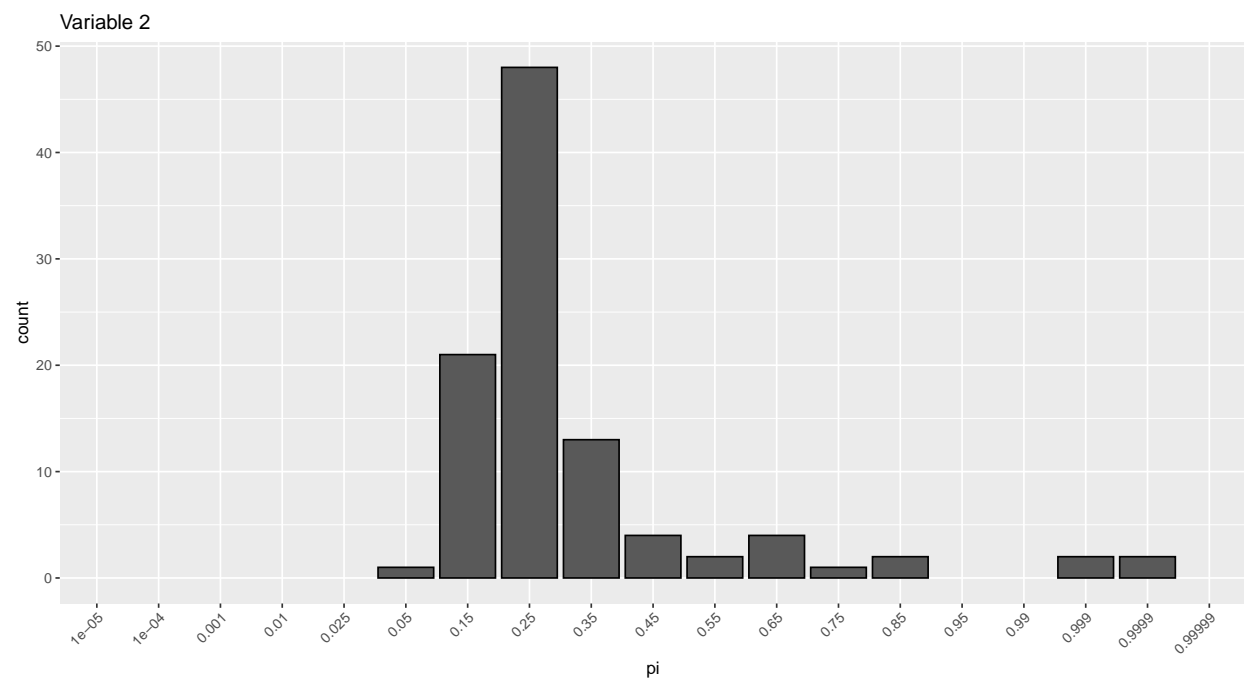


Here the distribution of the optimal π is visualized by variable.

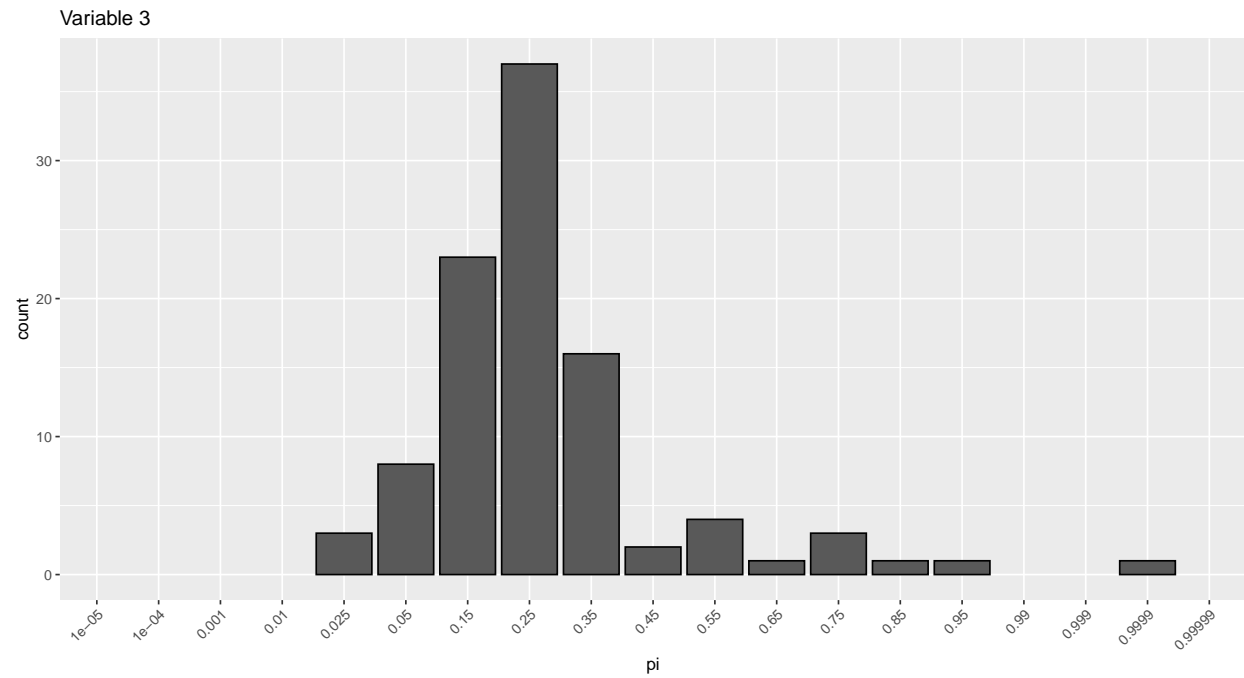
```
## [[1]]
```

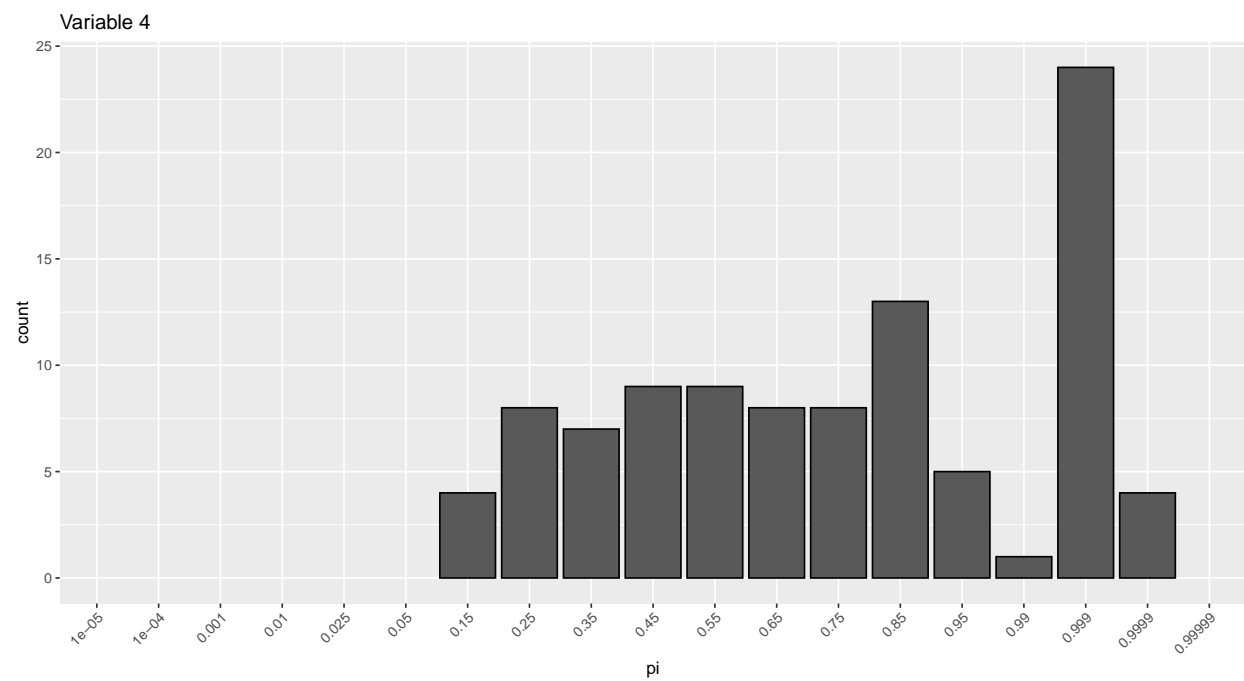
```
##
## [[2]]
```



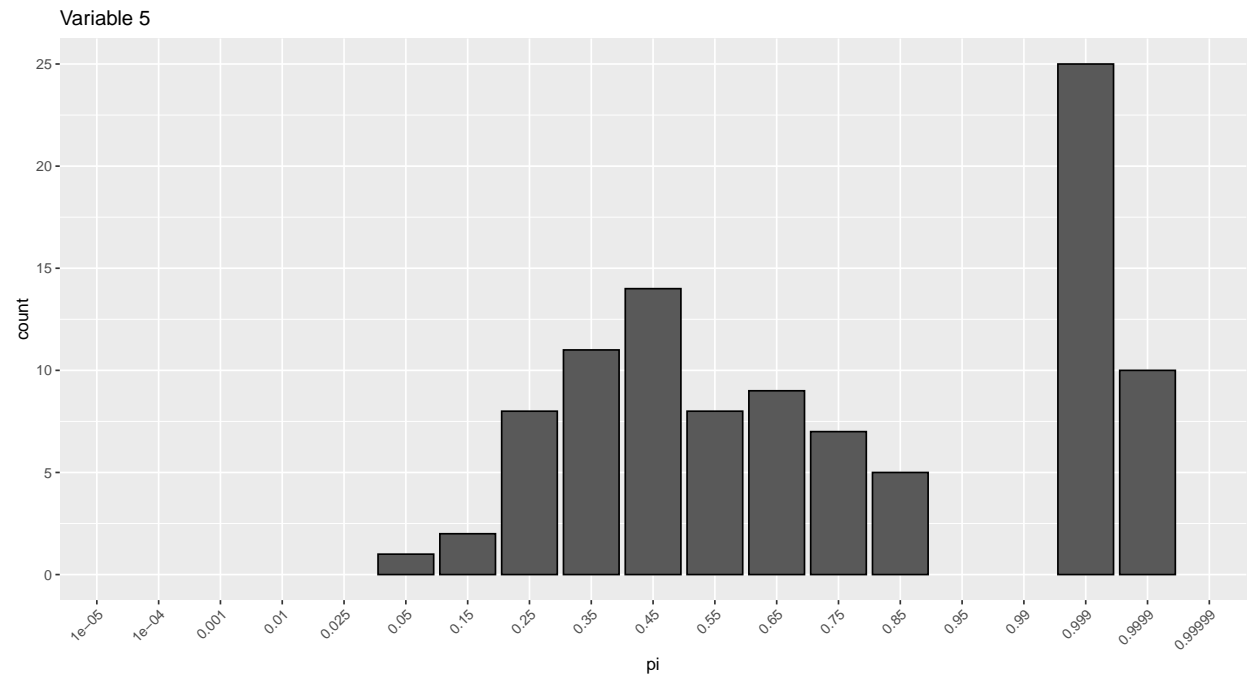
```
##
## [[3]]
```



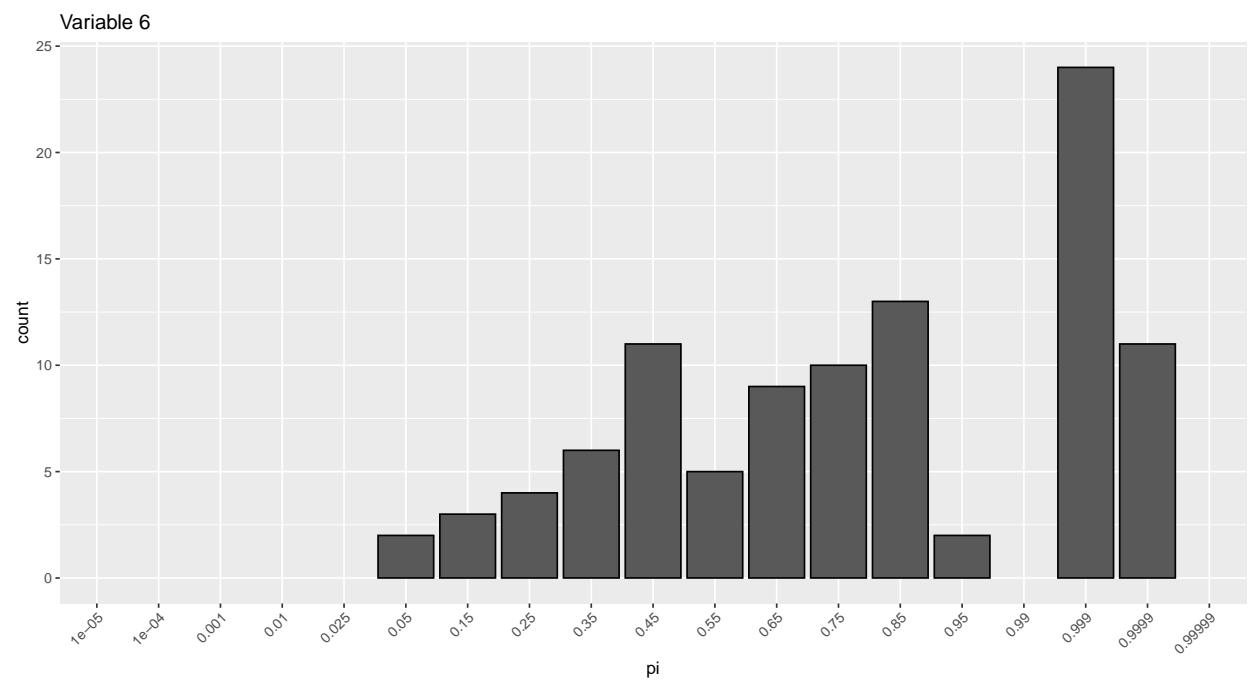
```
##
## [[4]]
```



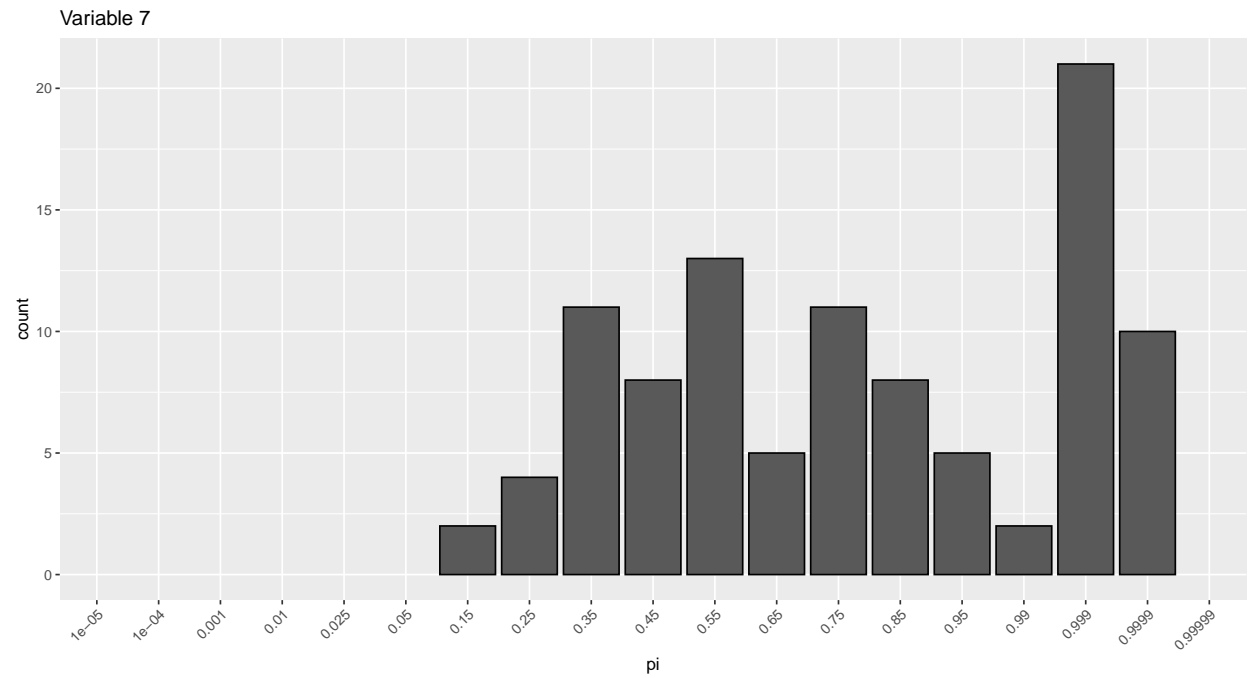
```
##
## [[5]]
```



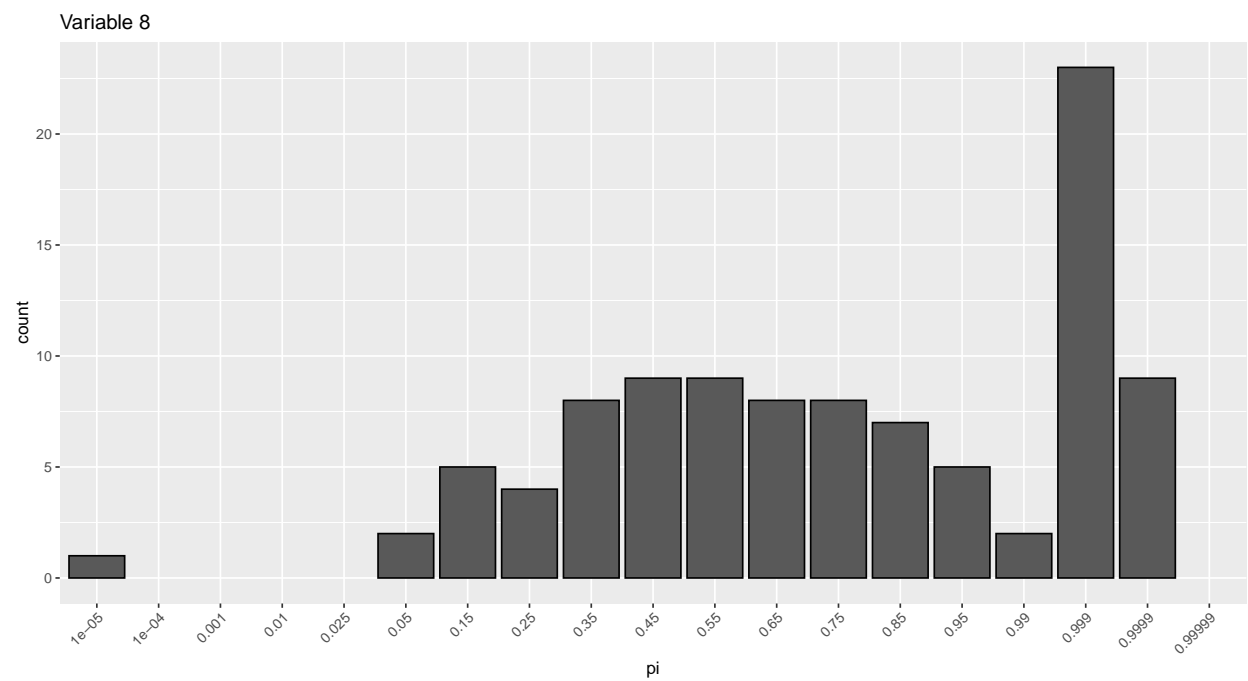
```
##
## [[6]]
```



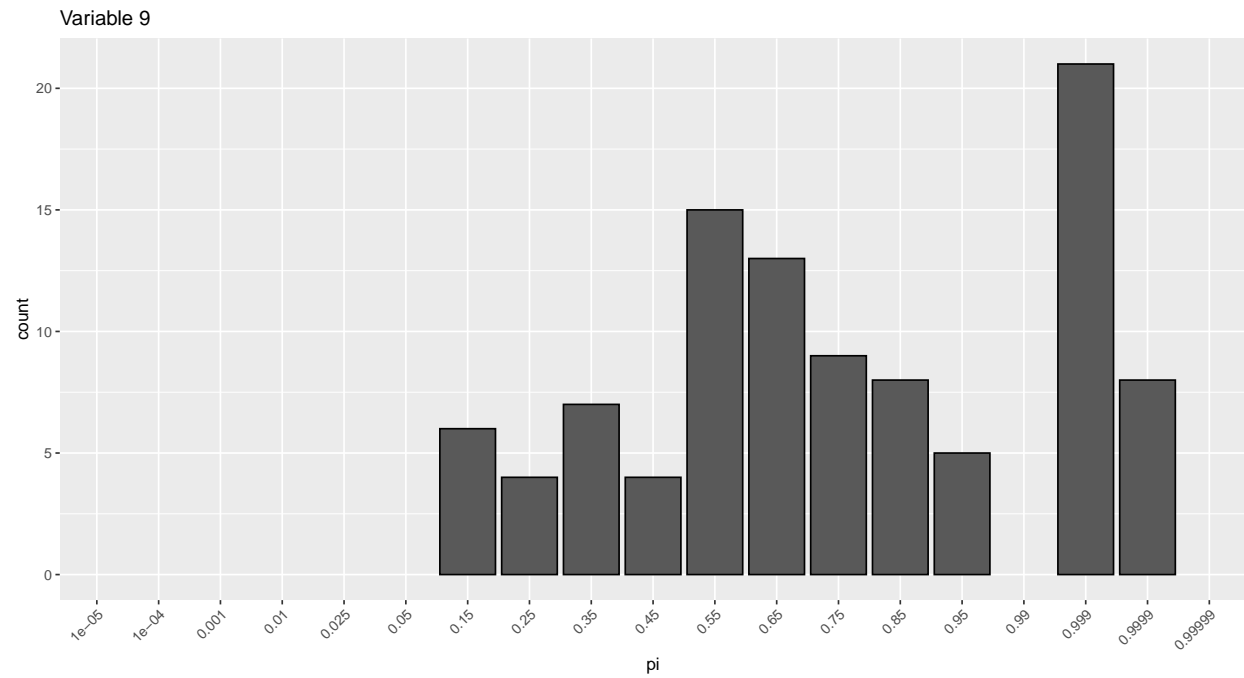
```
##
## [[7]]
```



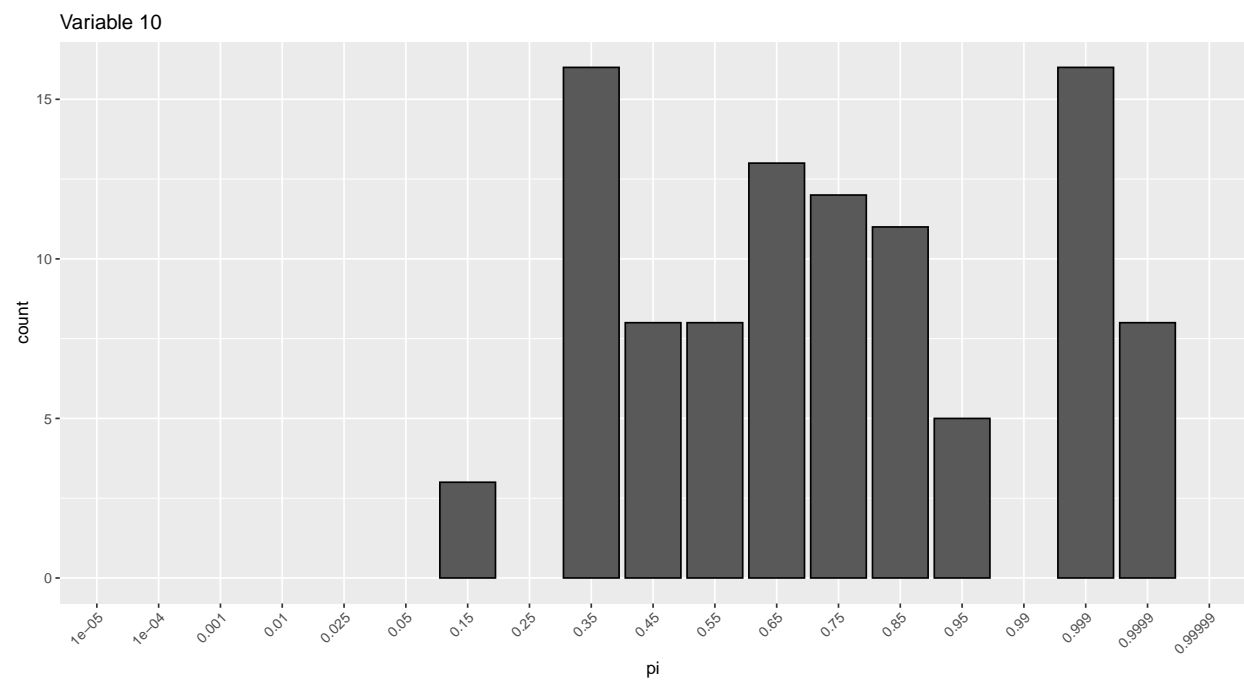
```
##
## [[8]]
```



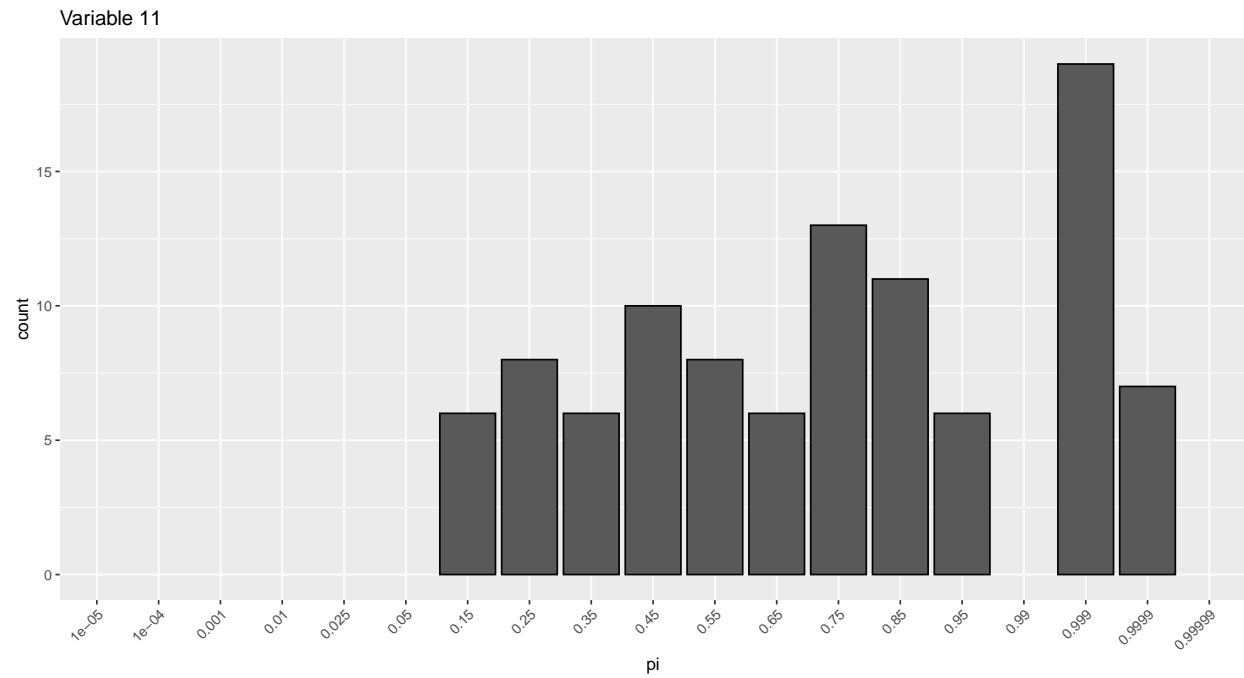
```
##
## [[9]]
```



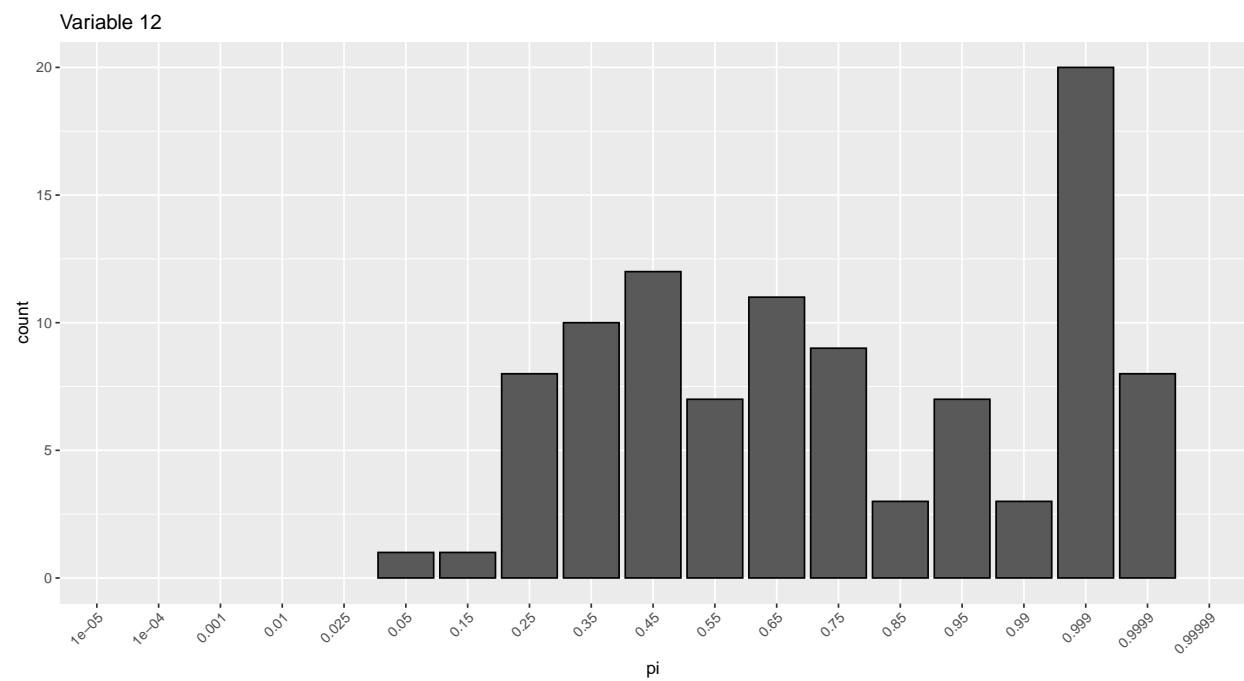
```
##  
## [[10]]
```



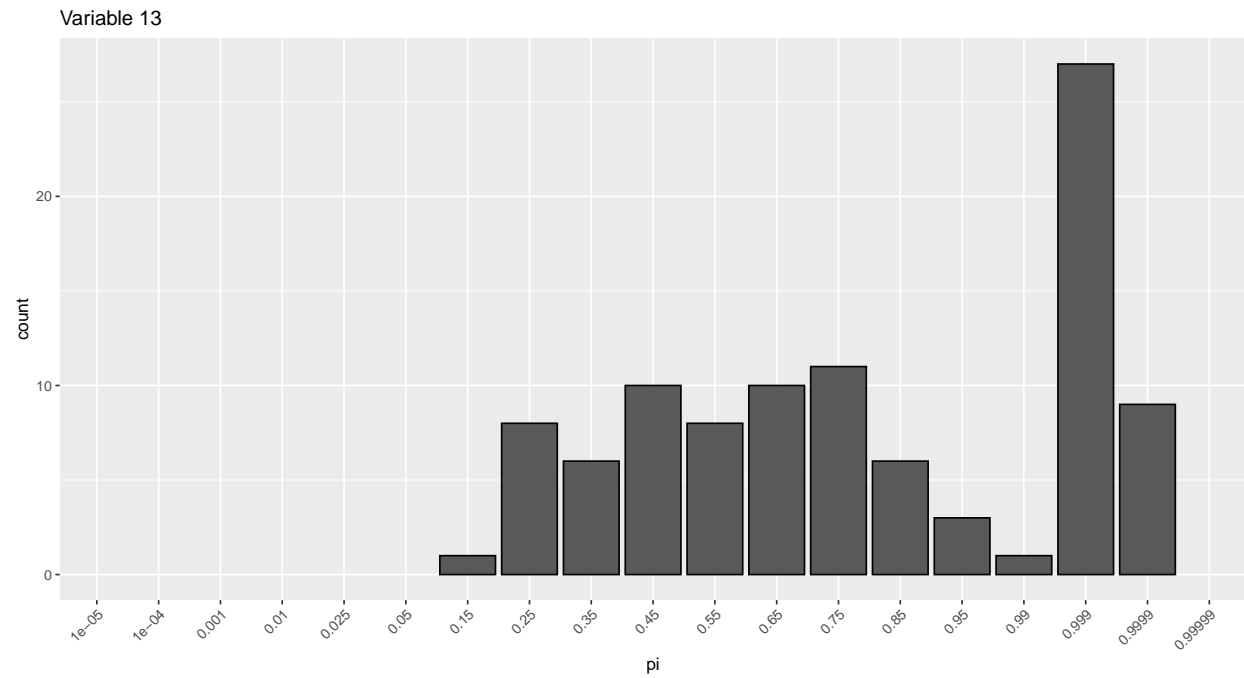
```
##  
## [[11]]
```



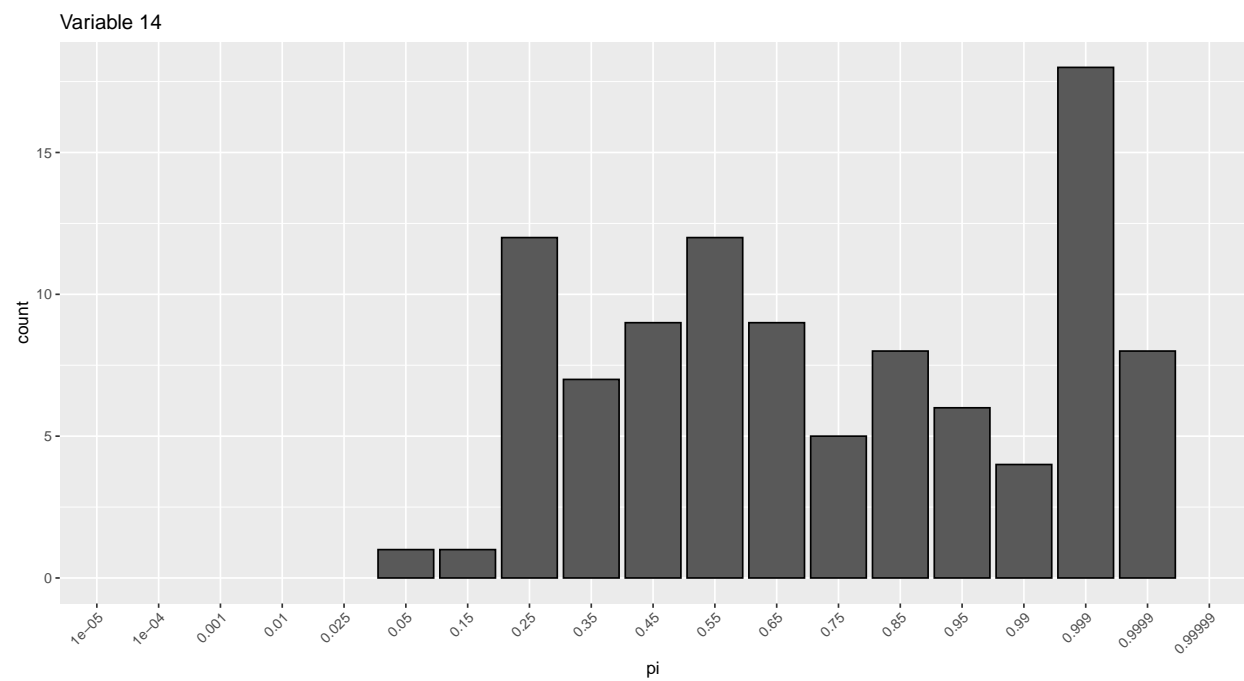
```
##  
## [[12]]
```



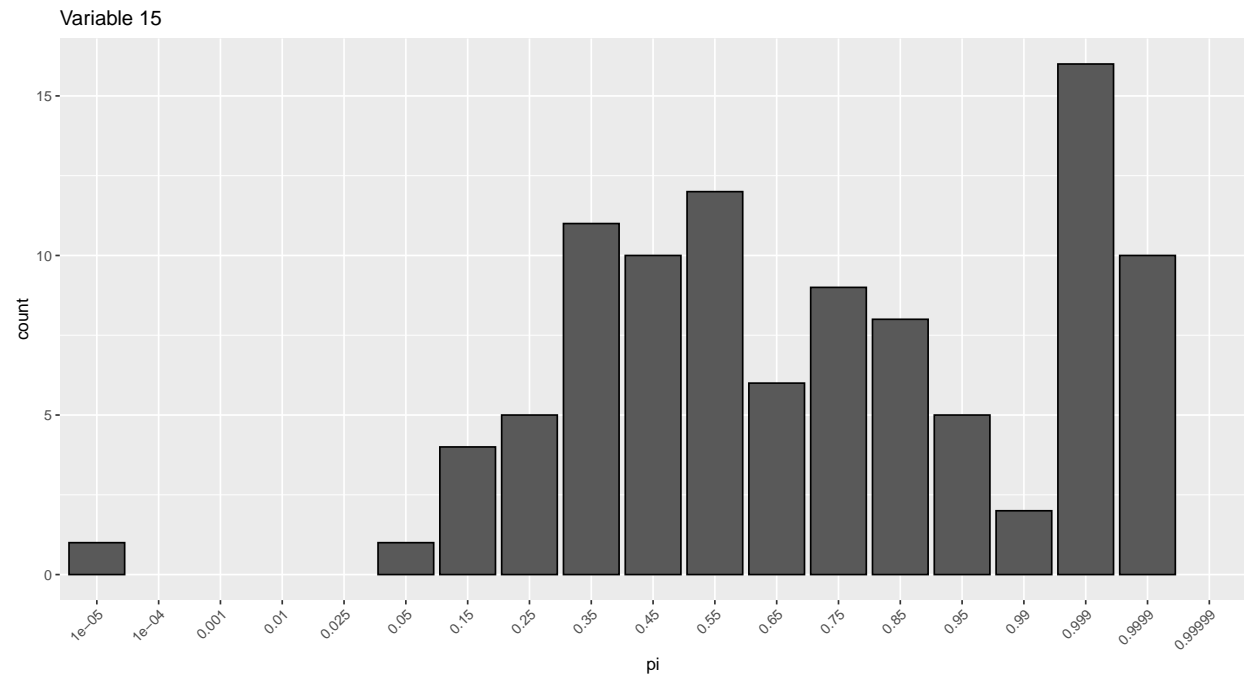
```
##  
## [[13]]
```



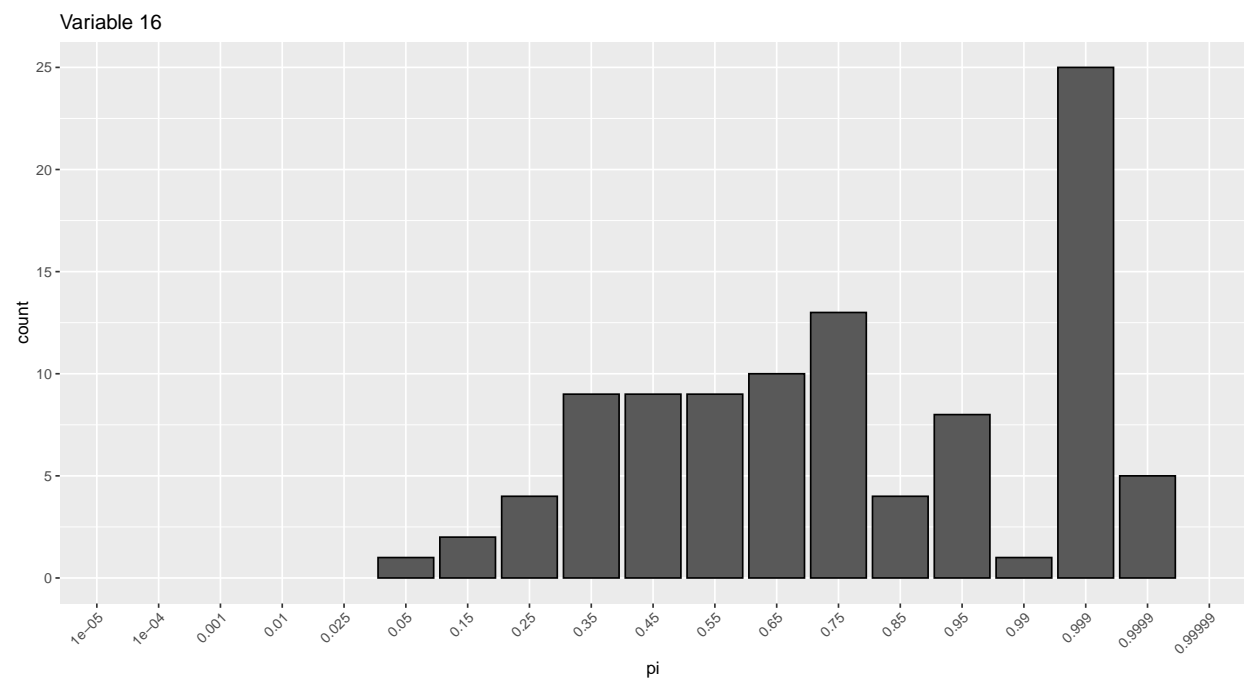
```
##  
## [[14]]
```



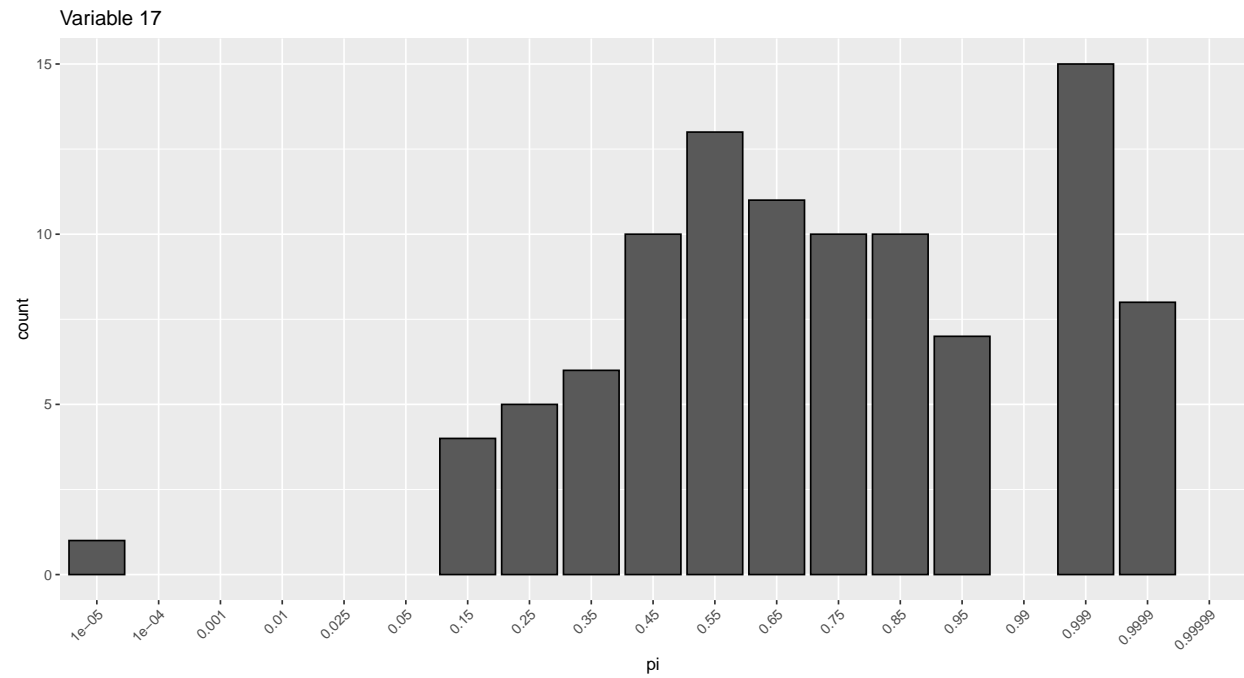
```
##  
## [[15]]
```



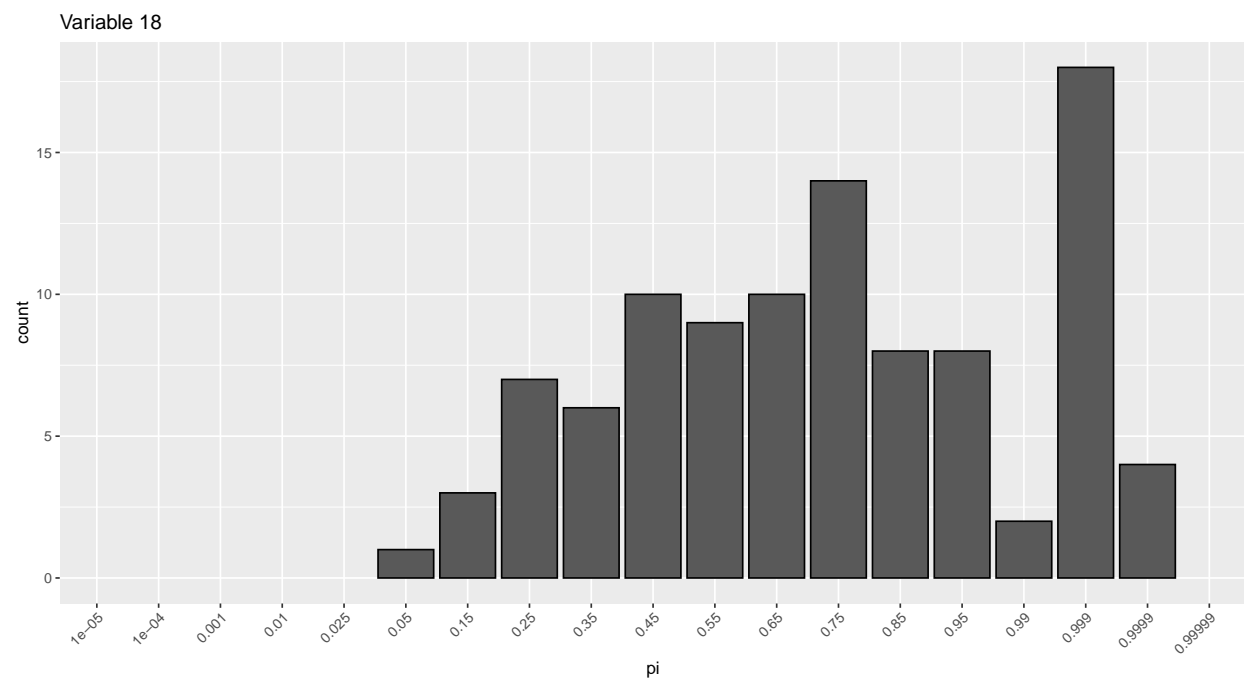
```
##
## [[16]]
```



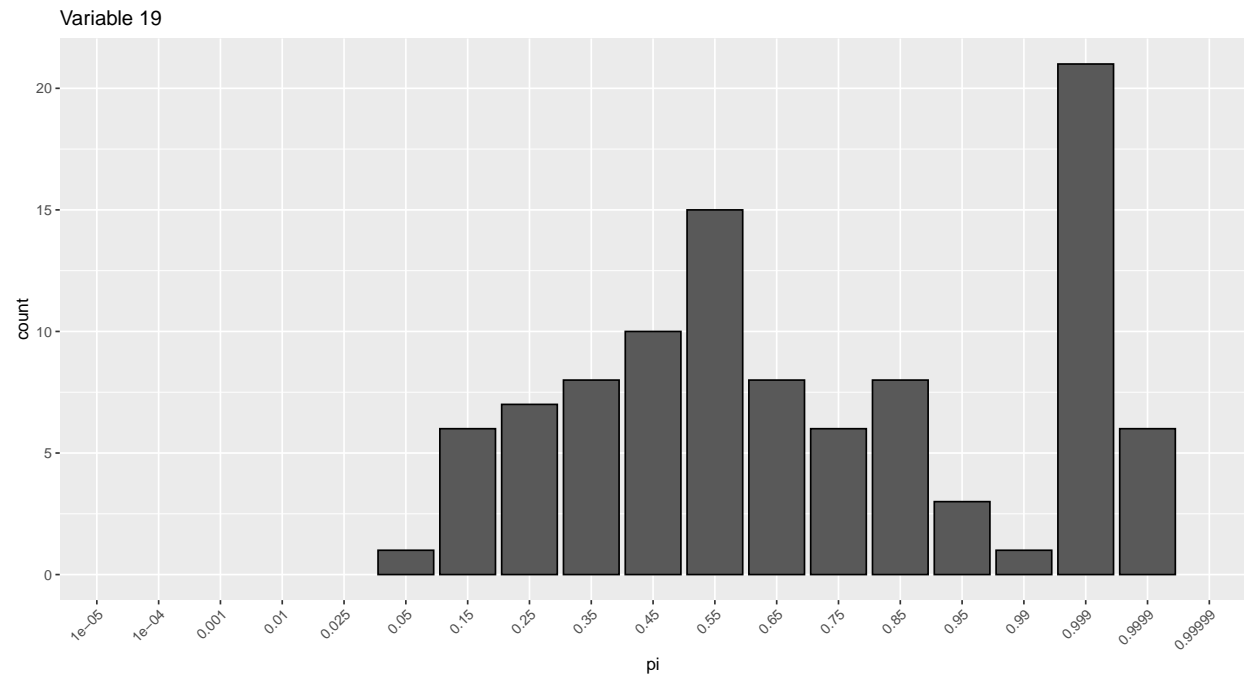
```
##
## [[17]]
```

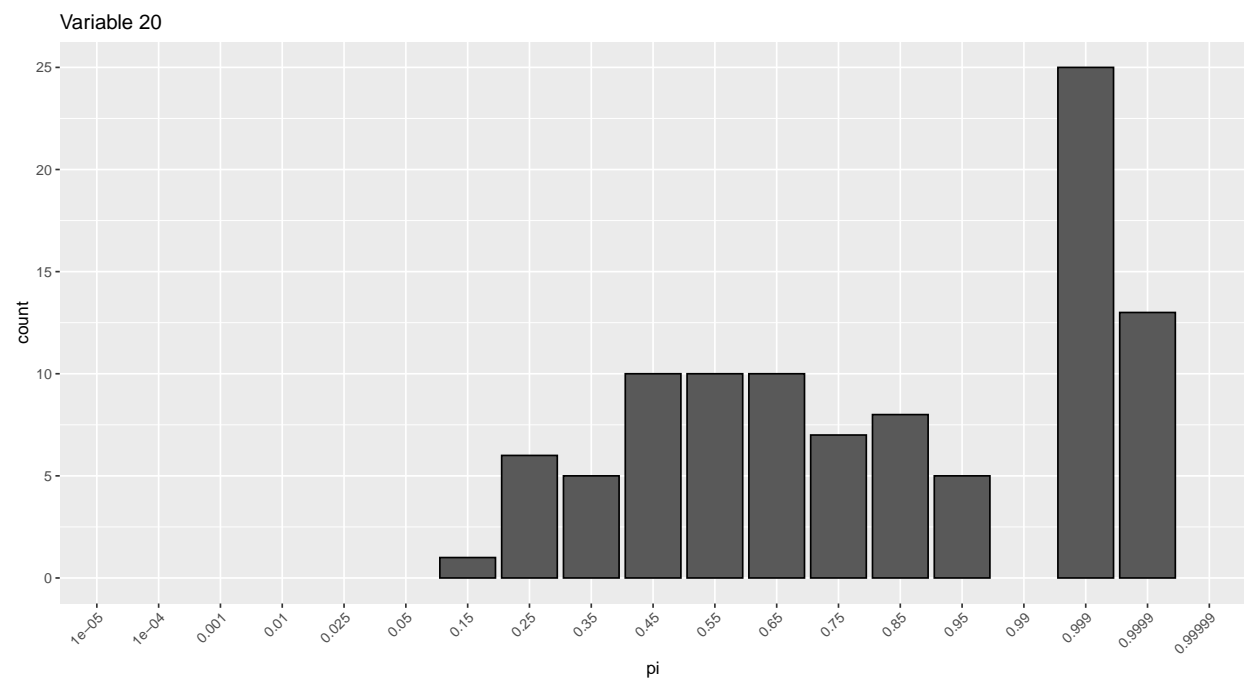
```
##
## [[18]]
```



```
##
## [[19]]
```



[[20]]



Importance Sampling Hybrid

Algorithm Overview

This algorithm averages over a deterministic grid of π . For each value of π , the values of σ_{sq} and $\sigma_{\text{sq_beta}}$ are chosen using grid search. The importance weights are calculated by assigning a uniform prior to each value of π and approximating the marginal likelihood using the ELBO.

Hyperparameter Grid

Below, I display the grid of π that are averaged over, as well as the marginal grids for σ_{sq} and $\sigma_{\text{sq_beta}}$.

```
## $pip
## [1] 0.1 0.2 0.3 0.4 0.5
##
## $ssq
## [1] 0.001 0.010 0.050 0.100 0.250 0.500 0.750 1.000 2.000 3.000
##
## $bsq
## [1] 1.0e-05 1.0e-03 1.0e-02 1.0e-01 2.5e-01 5.0e-01 1.0e+00 3.0e+00 5.0e+00
## [10] 1.0e+01
```

Sensitivity and Specificity

In this section, I compare the sensitivity and the specificity for the two methods.

```
# grid sensitivity
summary(grid_sens)
```

```
##      Min. 1st Qu.  Median      Mean 3rd Qu.      Max.
## 0.4286  0.7732  0.8083  0.8041  0.8571  0.9738
```

```
# importance sensitivity
summary(impt_sens)
```

```
##      Min. 1st Qu.  Median      Mean 3rd Qu.      Max.
## 0.4286  0.7065  0.7476  0.7379  0.7911  0.8929
```

```
# difference in the sensitivities
summary(grid_sens - impt_sens)
```

```
##      Min. 1st Qu.  Median      Mean 3rd Qu.      Max.
## -0.002381 0.023810 0.069048 0.066190 0.091071 0.216667
```

```
# grid specificity
summary(grid_spec)
```

```
##      Min. 1st Qu.  Median      Mean 3rd Qu.      Max.
## 0.9672  1.0000  1.0000  0.9991  1.0000  1.0000
```

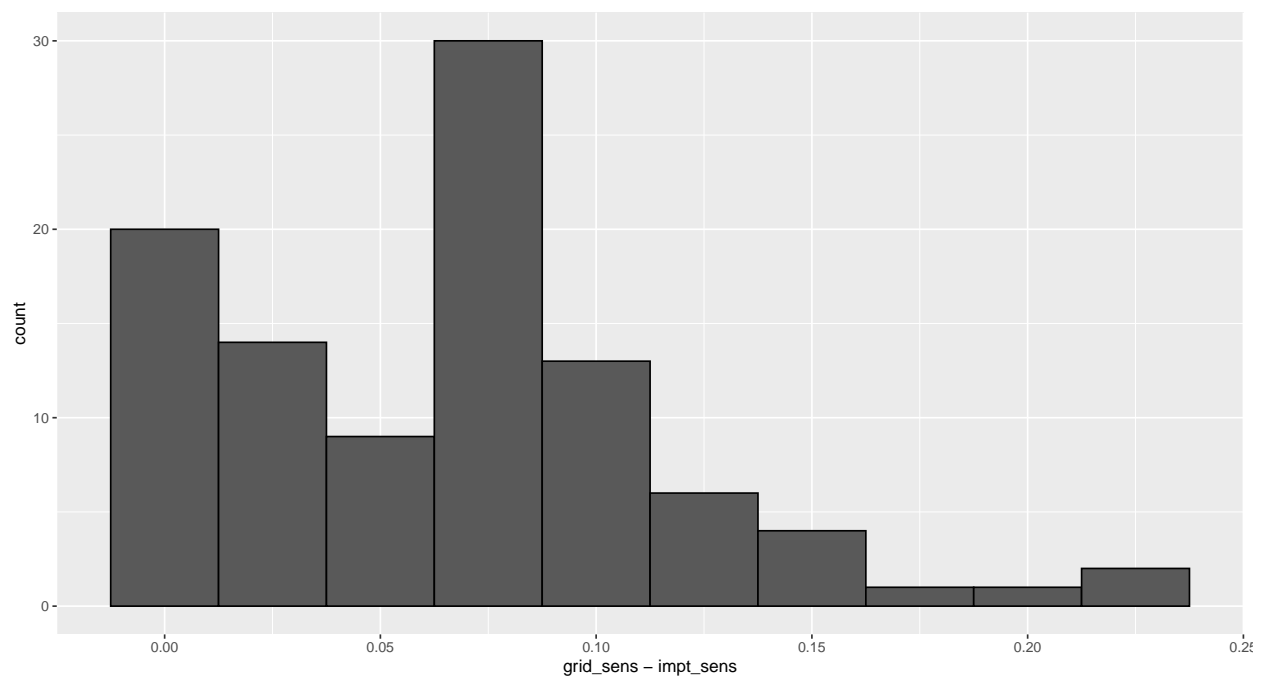
```
# importance specificity
summary(impt_spec)
```

```
##      Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
## 0.9885  1.0000  1.0000  0.9999  1.0000  1.0000
```

```
# difference in the specificities
summary(grid_spec - impt_spec)
```

```
##      Min.    1st Qu.    Median      Mean   3rd Qu.      Max.
## -0.0256831  0.0000000  0.0000000 -0.0007432  0.0000000  0.0005464
```

```
# visualize the difference in the sensitivity
ggplot() + geom_histogram(aes(grid_sens - impt_sens), binwidth = 0.025, color = "black")
```



Case Study

Here, I present the graphs estimated by the two methods in two cases; the first case represents the performance of the methods in the trial wherein the hybrid method had its maximum sensitivity. The second case represents the performance of the methods in the trial where the difference in the sensitivity of the two methods was maximal.

I also display the importance weights for variables 2 and 3 for individual 90 in both cases.

Case 1: Optimal Importance Performance

```
good_ind <- which.max(impt_sens)
```

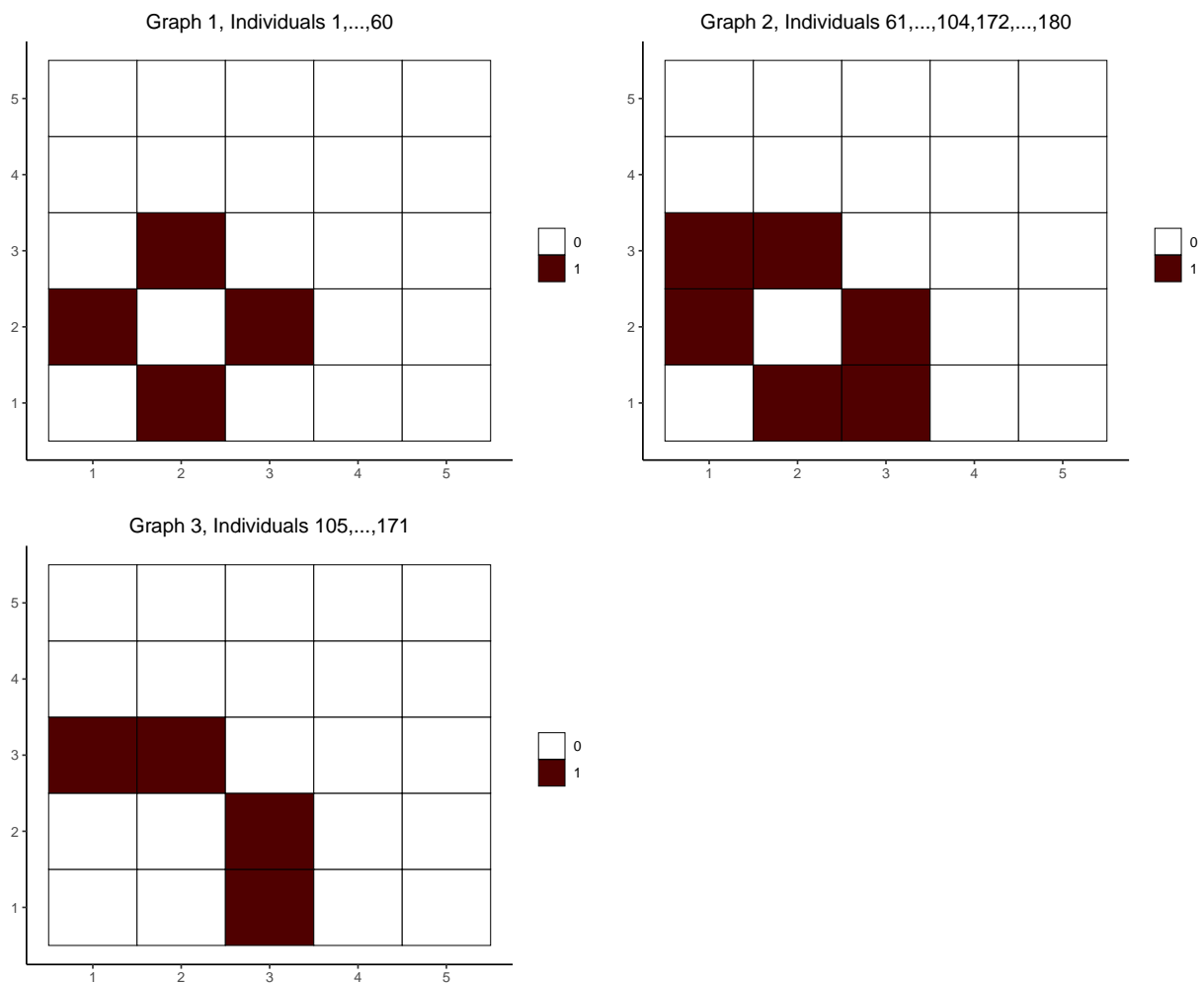
```
# sensitivity for grid search  
grid_sens[good_ind]
```

```
## [1] 0.9619048
```

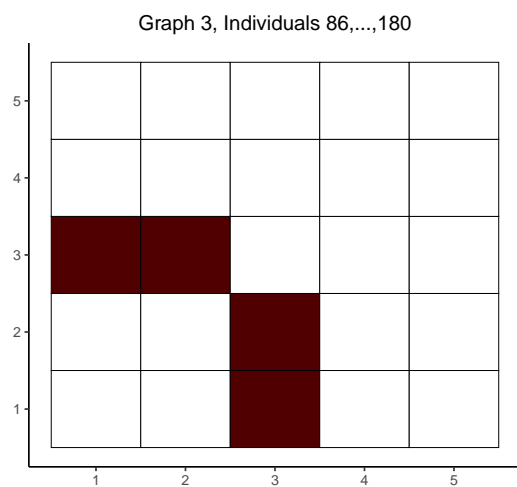
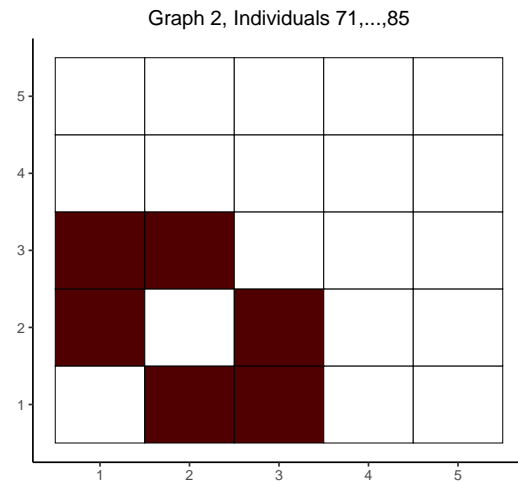
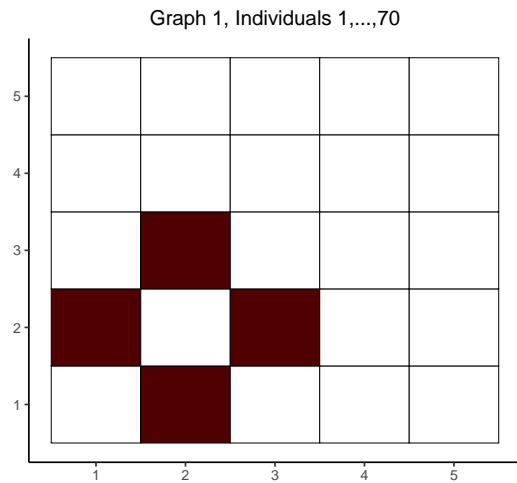
```
# sensitivity for importance sampling  
impt_sens[good_ind]
```

```
## [1] 0.8928571
```

```
# graphs estimated by grid search  
ggarrange(plotlist = plot(res[[good_ind]]$grid))
```



```
# graphs estimated by importance sampling  
ggarrange(plotlist = plot(res[[good_ind]]$impt))
```



```
# visualize the weights for individual 90

# variable 2
res[[good_ind]]$impt$hyperparameters$`Variable 2`$weights[90, ]
```

Importance Weights

```
##           0.1      0.2      0.3      0.4      0.5
## 90 0.07772511 0.1478517 0.2096107 0.2595237 0.3052888
```

```
# variable 3
res[[good_ind]]$impt$hyperparameters$`Variable 3`$weights[90, ]
```

```
##           0.1      0.2      0.3      0.4      0.5
## 90 0.04692807 0.1146042 0.1937813 0.2763521 0.3683344
```

Case 2: Greatest Grid Search Margin

```
diff_ind <- which.max(grid_sens - impt_sens)
```

```
# sensitivity for grid search
```

```
grid_sens[diff_ind]
```

```
## [1] 0.7785714
```

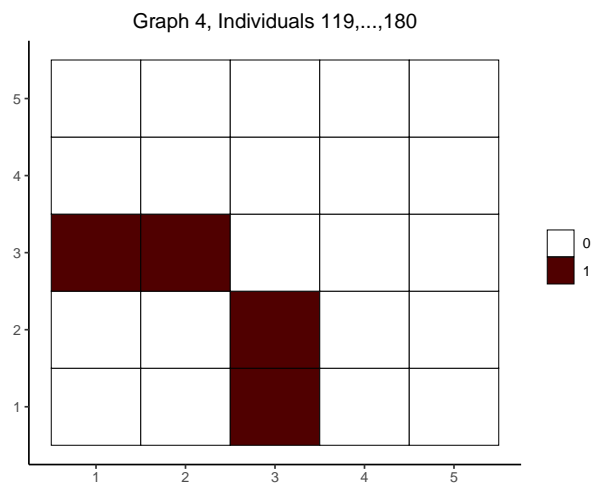
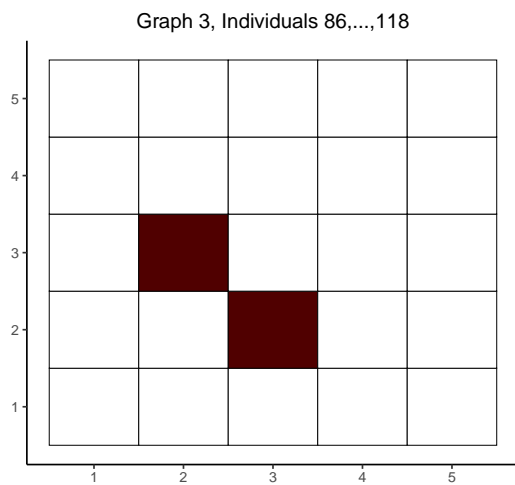
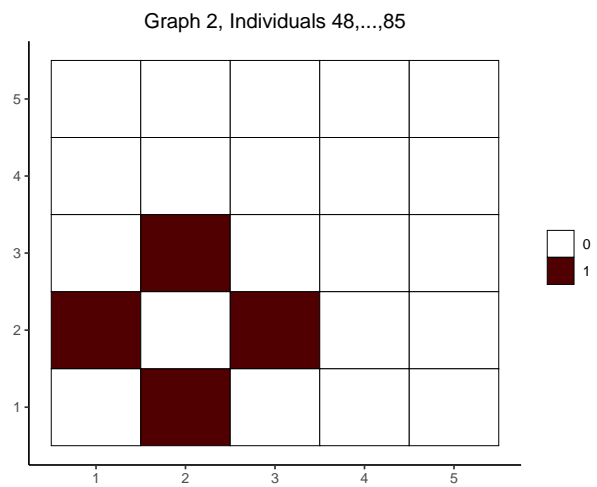
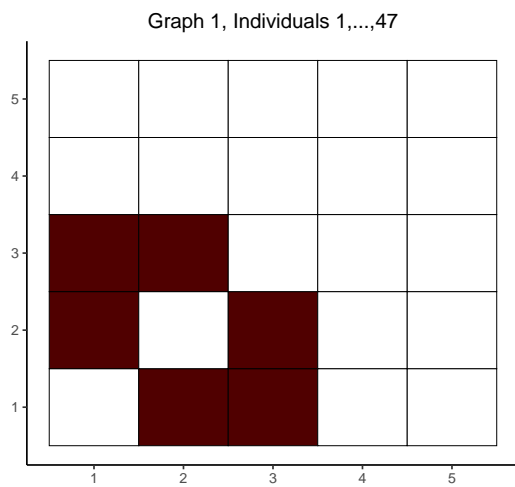
```
# sensitivity for importance sampling
```

```
impt_sens[diff_ind]
```

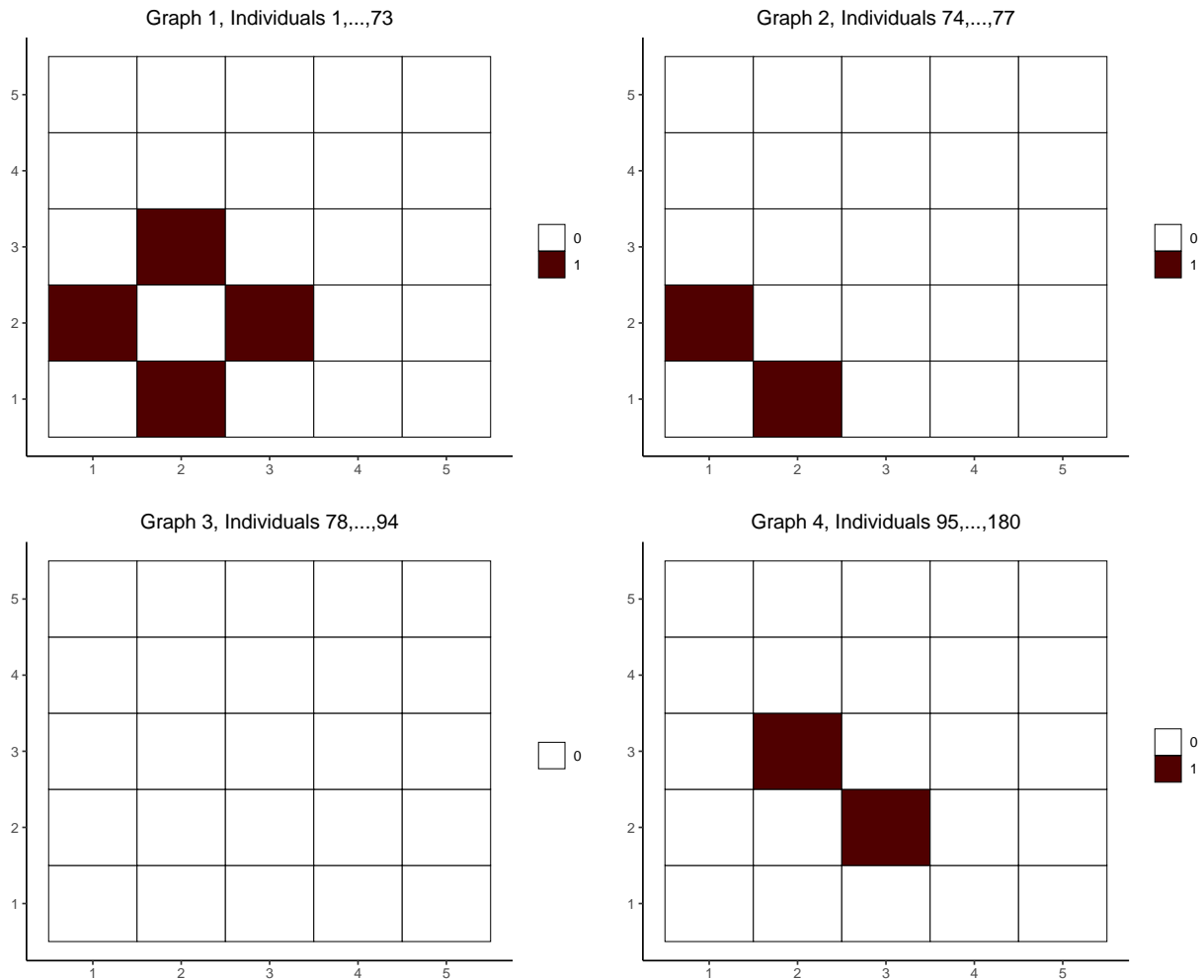
```
## [1] 0.5619048
```

```
# graphs estimated by grid search
```

```
ggarrange(plotlist = plot(res[[diff_ind]]$grid))
```



```
# graphs estimated by importance sampling
ggarrange(plotlist = plot(res[[diff_ind]]$impt))
```



```
# visualize the weights for individual 90
```

```
# variable 2
```

```
res[[diff_ind]]$impt$hyperparameters$`Variable 2`$weights[90, ]
```

Importance Weights

```
##          0.1          0.2          0.3          0.4          0.5
## 90 0.1891123 0.2086809 0.2077903 0.2020615 0.192355
```

```
# variable 3
```

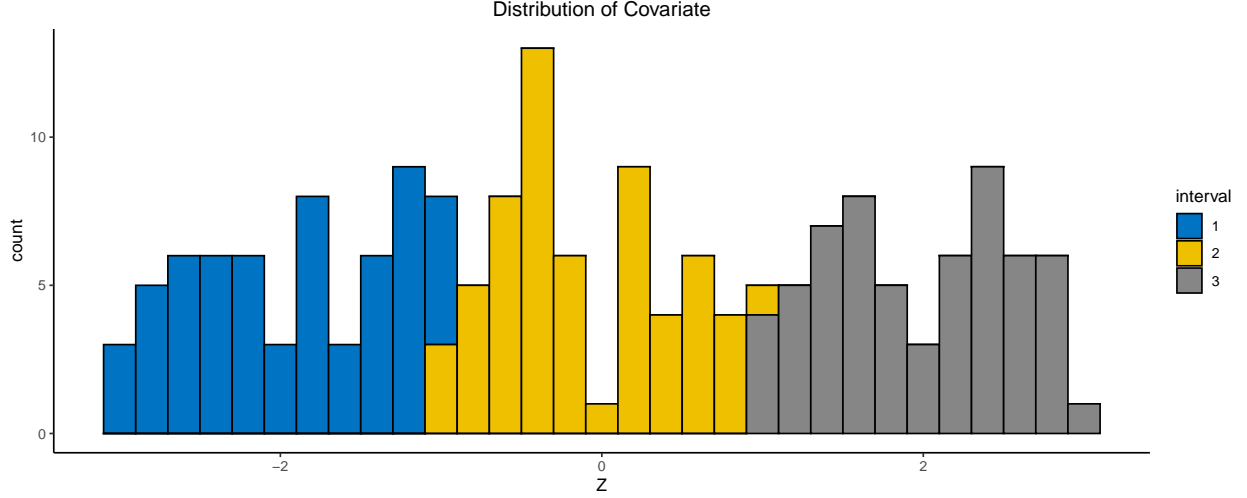
```
res[[diff_ind]]$impt$hyperparameters$`Variable 3`$weights[90, ]
```

```
##          0.1          0.2          0.3          0.4          0.5
## 90 0.2293057 0.2037865 0.1780152 0.1526882 0.2362043
```


Data Generation

Extraneous Covariate

I generated the covariate, Z , as the union of three almost disjoint intervals of equal measure. That is, $Z = Z_1 \cup Z_2 \cup Z_3$ with $Z_1 = (-3, -1)$, $Z_2 = (a, b) = (-1, 1)$, $Z_3 = (1, 3)$. Within each interval, I generated 60 covariate values from a uniform distribution. For example:



Precision Matrix

All of the individuals in interval 1 had the same precision matrix, $\Omega^{(1)}$:

$$\Omega_{i,j}^{(1)} = \begin{cases} 2 & i = j \\ 1 & (i, j) \in \{(1, 2), (2, 1), (2, 3), (3, 2)\} \\ 0 & o.w. \end{cases}$$

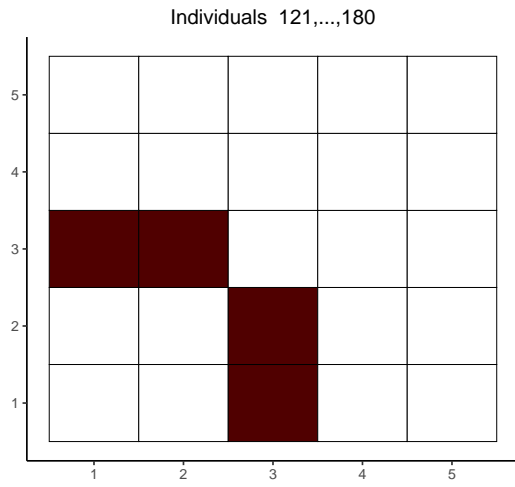
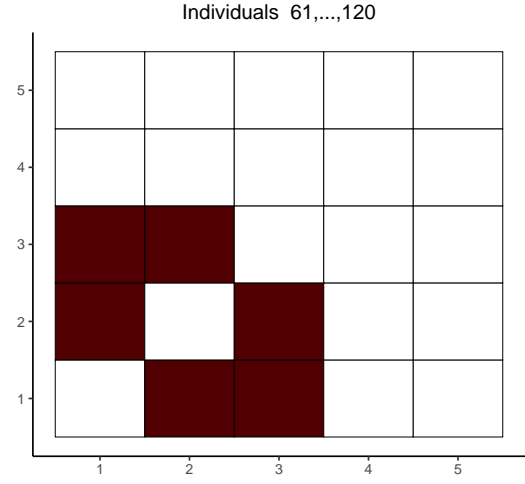
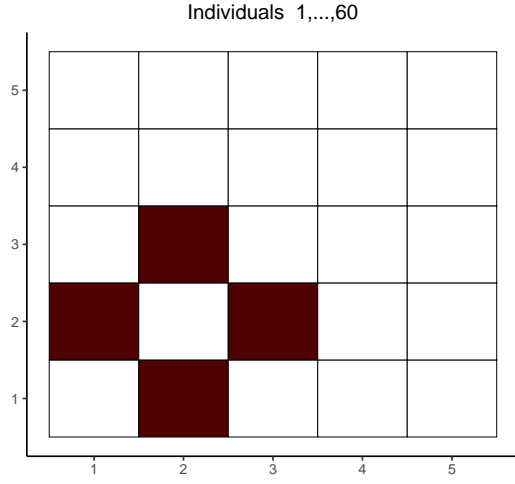
Also, all of the individuals in interval 3 had the same precision matrix, $\Omega^{(3)}$:

$$\Omega_{i,j}^{(3)} = \begin{cases} 2 & i = j \\ 1 & (i, j) \in \{(1, 3), (3, 1), (2, 3), (3, 2)\} \\ 0 & o.w. \end{cases}$$

However, the individuals in interval 2 had a precision matrix that was dependent upon Z and (a, b) . Let $\beta_0 = -a/(b - a)$ and $\beta_1 = 1/(b - a)$. Then:

$$\Omega_{i,j}^{(2)}(z) = \begin{cases} 2 & i = j \\ 1 & (i, j) \in \{(2, 3), (3, 2)\} \\ 1 - \beta_0 - \beta_1 z & (i, j) \in \{(1, 2), (2, 1)\} \\ \beta_0 + \beta_1 z & (i, j) \in \{(1, 3), (3, 1)\} \\ 0 & o.w. \end{cases}$$

Thus, $\Omega^{(2)}(a) = \Omega^{(1)}$ and $\Omega^{(2)}(b) = \Omega^{(3)}$. That is, an individual on the left or right boundary of Z_2 would have precision matrix $\Omega^{(1)}$ or $\Omega^{(3)}$, respectively. The conditional dependence structures corresponding to each of these precision matrices are visualized below.



Data matrix

Let z_l be the extraneous covariate for the l -th individual. To generate the data matrix for the l -th individual, I took a random sample from $\mathcal{N}(0, \{\Omega_l(z_l)\}^{-1})$, where:

$$\Omega_l(z_l) = \begin{cases} \Omega^{(1)} & z_l \in Z_1 \\ \Omega^{(2)}(z_l) & z_l \in Z_2 \\ \Omega^{(3)} & z_l \in Z_3 \end{cases}$$