

Project

Transplant kidney rejection

High Dimensional Data Analysis

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Executive summary

This research examines whether some genes are responsible for a patient's likelihood of rejecting a kidney after transplantation, for the Gene Expression Omnibus (GEO) dataset. This dataset consists of gene expression levels of 54675 genes from 282 patients. The variability of the gene expression is ... From the 54675 genes, 18080 genes are identified as having a differential expression between the group of rejected and the group of accepted kidneys. The list of these genes can be found in ... (insert appendix) Kidney rejection can be predicted sufficiently from the gene expressions with 17 genes. The most important genes in predicting rejection are in ... (insert appendix). The prediction model (insert which model is best) performs the best and (say something about the performance)

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1 Abbreviations

abbreviation	meaning
AUC	Area under the curve
IQR	Interquartile range
LDA	Linear discriminant analysis
LLE	Locally linear embedding
PCA	Principle component analysis
sd	Standard deviation

2 Exploratory Analysis

In this section general descriptive statistics are given and multiple methods for high dimensional data exploration are used.

2.1 Basic descriptive summary

In this study 54675 gene expression levels of 282 samples were analysed. In total, 76 or 27% of the transplanted kidneys were rejected.

Several descriptive statistics (mean, sd, median, iqr, min, and max) were calculated for every gene and kidney rejection status combination. This resulted in 2 (accepted vs. rejected) distributions of every statistic across genes. Note that these statistics were only calculated to perform a visual inspection.

The resulted plot is presented in figure 1. From this figure we can see there are, at least on this level, differences between the two groups. Most notable are the mean and median expression levels which tend to be closer to the overall mean (across groups) expression levels in the *accepted* group and more varying

in the *rejected* group. There seems to be more variability in the measures of dispersion in the *rejected* group. Finally there are minimal differences between the min/max expression level distributions, perhaps suggesting that gene expression levels in the *rejected* group are slightly less extreme than in the *accepted* group.

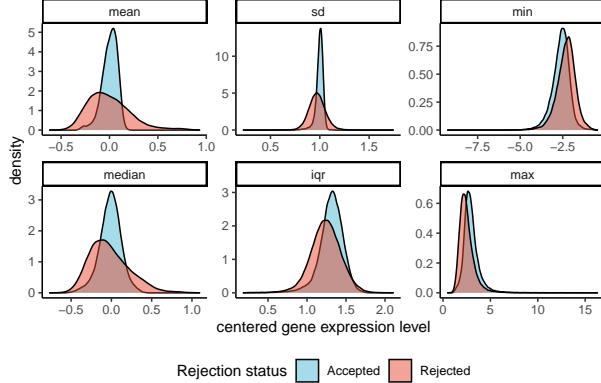


Figure 1: Descriptive statistics across genes and between groups.

2.2 Advanced exploratory analyses

Multiple methods for exploration and visualisation of high dimensional data were applied (sparse PCA, MDS, sparse LDA, LLE, ISOMAP, Sammon Mapping, Diffusion maps, and t-SNE), yet without clear results. Because the sparse LDA gave the best results we discuss the results here and refer to the appendices ?? to ?? for the results of the other techniques.

The sparse LDA was performed to find potential candidate genes for future investigation. Due to computational constraints (our system ran out of memory) we needed to split the data set in 3 parts (each part consisting of 282 observations on 18225 genes). We considered this approach to be valid since we only used it as an exploratory tool. In total 116 genes (or 0.2%) had non-zero loadings.

Because this is still a substantial amount, only the genes with loadings in absolute value larger than two standard deviations were further considered ($|v_i| > 2sd(v)$, with $i = \{1, \dots, 116\}$, where v_i is the i th loading). This resulted in a list of 10 genes. The list of genes can be found in appendix ??.

By using these gene's loadings we calculated the scores of the linear discriminant for every sample and used these to construct the following graph.

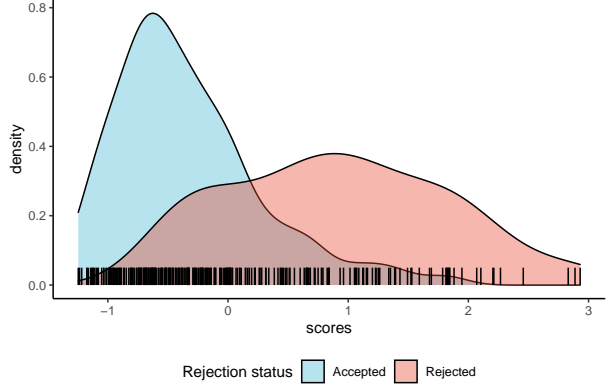


Figure 2: Density plot of linear discriminant scores based on the selected subset of genes.

From this graph we can see that to a degree a distinction can be made, albeit with a substantial overlap.

2.3 Conclusions Exploratory Analysis

Although differences between groups could be found within the data, no articulate distinction between the rejection status groups could be made with any of the used methods. This finding suggests there is relevant information at the genetic level w.r.t. transplant kidney rejection, but more factors need to be taken into account in order to arrive at a better understanding.

The main directions of variability in the gene expression dataset do not coincide with the separation between the rejection status groups. Nevertheless, certain genes were identified as potentially closely related to the differentiation between the two groups using sparse LDA.

3 Differentially expressed genes between kidney rejection groups

In order to find out which genes are differentially expressed between rejection status groups null hypotheses were tested against alternative hypotheses as follows.

$$\left. \begin{array}{l} H_{0,i} : \mu_{rejected,i} = \mu_{accepted,i} \\ H_{a,i} : \mu_{rejected,i} \neq \mu_{accepted,i} \end{array} \right\} \quad \text{with } i = \{1, \dots, 54675\}$$

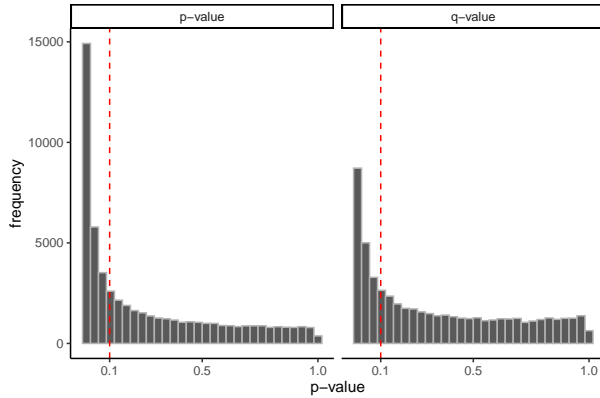
In these hypotheses $\mu_{rejected,i}$ and $\mu_{accepted,i}$ are the population means of the gene expression level of the

ith gene in the rejected and accepted kidney rejection group respectively. Before testing, a visual inspection of 30 QQ plots, from 15 randomly drawn variables, was done to assess whether the variables follow a normal distribution for both groups separately. These QQ plots showed that some genes were normally distributed, but also that many genes were not.

Nevertheless, two-sided Welch t-tests were performed on the uncentered data to determine whether the two groups can be differentiated based on the gene expression level for every gene. The choice for the Welch t-test is motivated by the presence of unequal variances between the two groups, even though not all genes were normally distributed. We included a small random subset 6 QQ plots in the appendix so the reader, if she/he wishes, can have a rough idea of the divergence from normality.

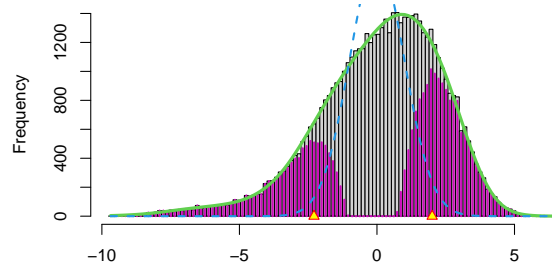
To address the multiple testing problem at this large scale (54675 simultaneous tests), the FDR is controlled at 0.10 through application of the method of Benjamini and Hochberg (1995).

To summarise the results we constructed a histogram of both the regular and adjusted p-values or q-values.



Both histograms reveal non-uniform distributions. More importantly, they have many small values, indicating that for many genes the null hypothesis was rejected. Based on the q-values, there were 18081 rejected null hypotheses. As such we conclude that the mean gene expression differs between the accepted and rejected kidney groups for those 18081 genes. As the FDR is controlled at 10%, it is expected to have around 1808 false discoveries.

Next, the normalised test statistics (z-scores) are plotted and compared to the local false discovery rate.

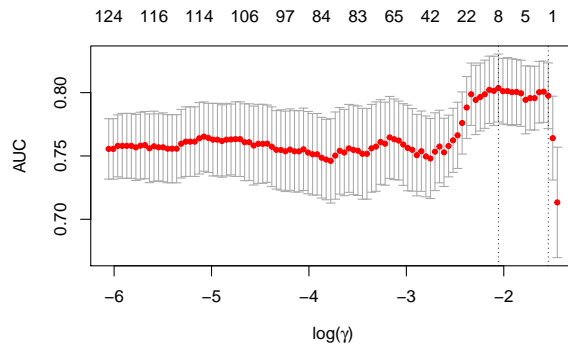


From the figure ?? can be concluded that a small lfrd can be obtained for small and large z-scores (a lfrd smaller than 0.2 for z-scores smaller than -2 and larger than 2). For these z-scores, it is more likely that when rejecting the null hypotheses, a true discovery is made.

4 Prediction of kidney transplant rejection

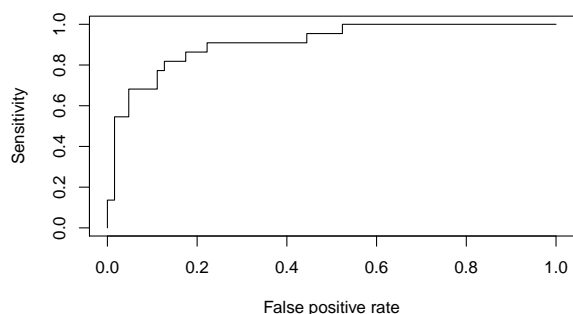
The objective of this final part is to construct a classifier for kidney acceptance or rejection based on the measured gene expressions. Three approaches are compared: lasso, ridge regression and principle component regression. These approaches will be compared based on the AUC. The final modelling approach is chosen as the one that shows the largest cross-validated AUC. The cutoff is chosen based on the F1-score. The dataset is split into a training and test dataset.

4.1 Lasso regression

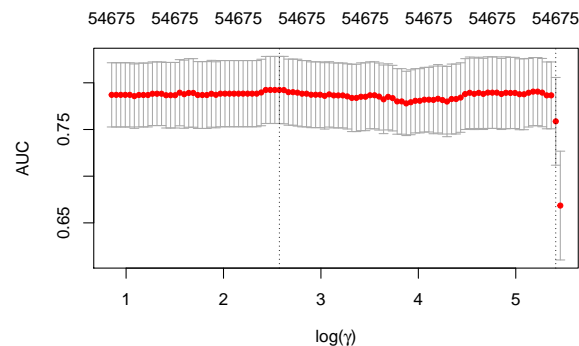


In the figure above, one can see that for γ equal to 0.1280675, the area under the curve (AUC) is maximal (0.909) for the train dataset based on a 10-fold cross-validation over the train dataset.

The ROC curve, estimated with the cross-validation dataset, is shown below:

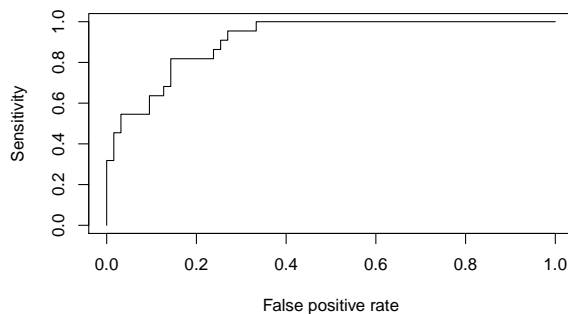


4.2 Ridge regression

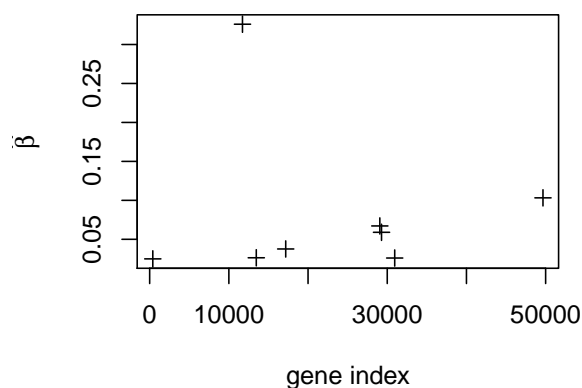


Likewise as for the Lasso regression, for γ equal to 13.1081041, the optimal AUC (0.911) is obtained.

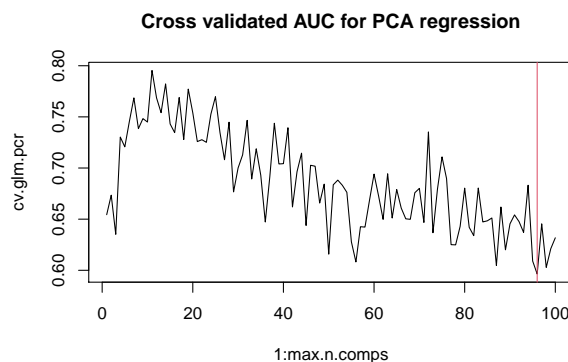
The ROC curve, estimated with the cross-validation dataset, is shown below:

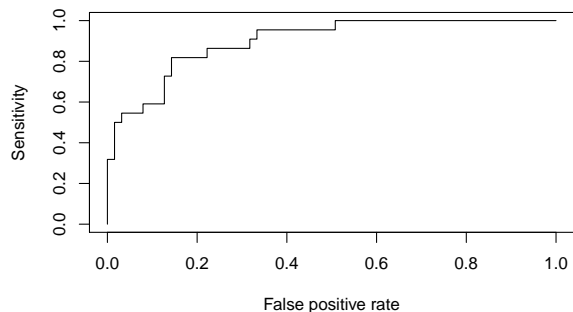


This model only uses 8 of the genes: 396, 11720, 13463, 17178, 29063, 29276, 30941, 49664. Compared to the interesting genes found with the Sparse LDA method: This is a considerable dimensional reduction. This is illustrated below. This figure shows the loadings of the 8 selected values.



4.3 Principal component regression



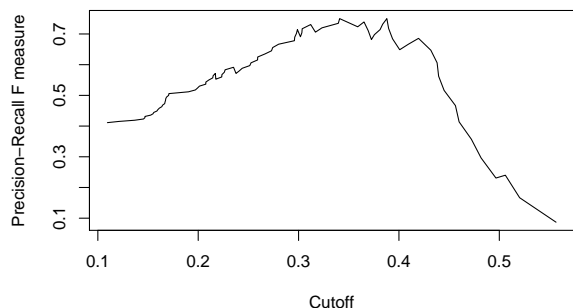


AUC is 0.899.

4.4 Final model evaluation

The model performance in terms of AUC is extremely similar for the 3 models. Since LASSO regression is the simplest model, this is preferred. By choosing cutoff $c = 0.23$, we can achieve a F1-score of over 0.7. This is represented on the following graph. Below, the F1 graph, the confusion matrix for the PCR model with cutoff $c = 0.21$ is shown.

The confusion matrix shows no false negatives at all, but the number of false positives is high.



	accept predicted	reject predicted
accept observed	35	28
reject observed	1	21

This confusionmatrix clearly shows a sensitivity of 0.4285714, and a specificity of 0.9722222. In short, this predictor seems to strike a balance between both, but the performance is not perfect. If a person tests positive, there is still a considerable chance the kidney will not be rejected.

This behaviour could be *explained* (or at least understood a little better) when looking back at the exploratory analysis. Here it was already clear that

the gene expressions of the patients with rejected kidneys overlap with those of the patients with accepted kidneys. Both are not perfectly separable.

5 Conclusions

From the 54675 genes in the dataset, 18080 genes are differentially expressed between the two kidney groups, based on multi-scale Welch t-test at an FDR of 10%.

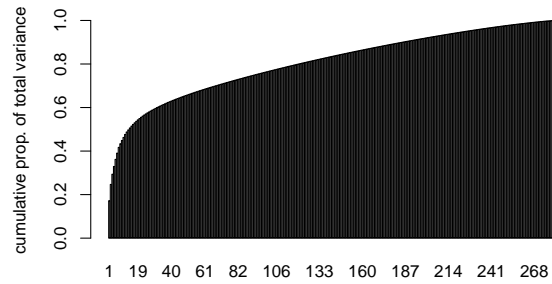
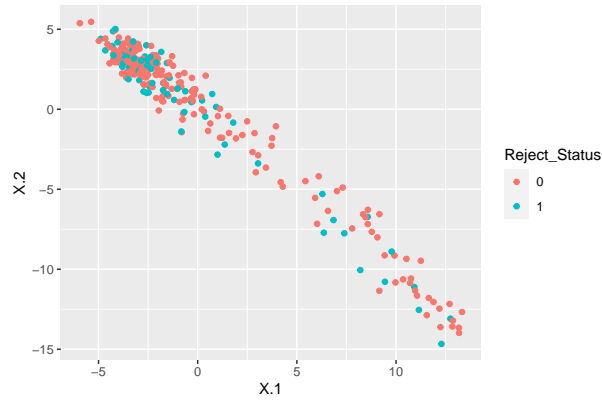
6 Appendices

6.1 Exploration methods for high dimensional data

6.1.1 Sparse principle components analysis

```
## Fold 1 out of 5
## Fold 2 out of 5
## Fold 3 out of 5
## Fold 4 out of 5
## Fold 5 out of 5

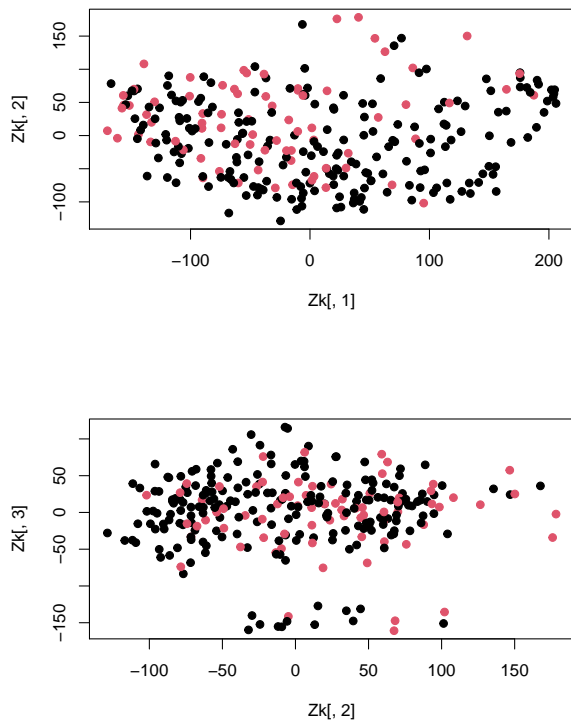
## Call:
## SPC.cv(x = GeneExpression_C)
##
##
## Cross-validation errors:
##      Sumabsvs CV Error  CV S.E. # non-zero v's
## 1      1.200  3072720 1069.866           2.8
## 2      1.622  3072688 1067.905           4.2
## 3      2.044  3072646 1066.778           7.4
## 4      2.467  3072600 1065.211           9.4
## 5      2.889  3072540 1062.144          13.6
## 6      3.311  3072476 1061.874          16.8
## 7      3.733  3072400 1061.760          22.0
## 8      4.156  3072305 1060.237          27.4
## 9      4.578  3072197 1061.406          32.6
## 10     5.000  3072079 1063.205          40.0
##
## Best sumabsv value (lowest CV error): 5
##
## Smallest sumabsv value that has CV error within 1 SE of
## 1234567891011121314151617181920
## 1234567891011121314151617181920
```



Unfortunately, naive sparse principle component analysis cannot be used to make a distinction between the accepted and rejected kidneys.

In the scree plot ?? it can be seen that the two first dimensions account for only 25% of the total variance in the dataset and the first three dimensions for 29%. To account for 80% of the total variance, 120 dimensions are needed.

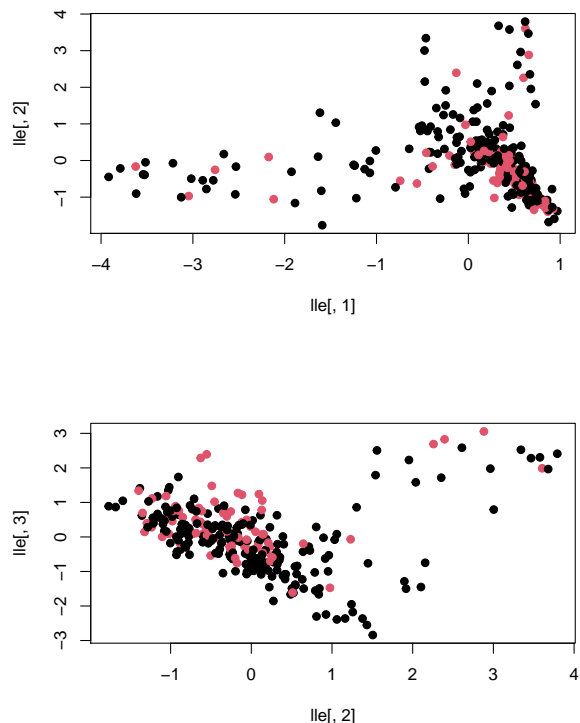
6.1.2 Multi-dimensional scaling:



In the biplots of the three first dimensions of the svd (??), no distinction can be made between rejected and accepted kidneys.

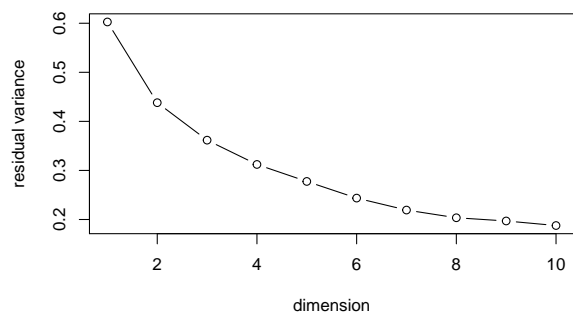
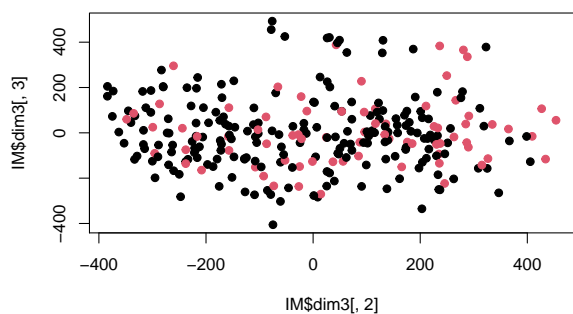
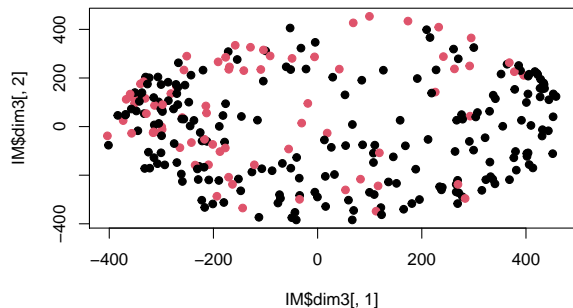
6.1.3 LLE (locally linear embedding)

Locally linear embedding described by Roweis and Saul (2000) was performed. From figures ?? can be seen that no distinction between the accepted and rejected kidneys can be made.



6.1.4 ISOMAP

ISOMAP presented by Tenenbaum, Silva and Langford in 2000 is performed. The parameter k is varied manually so that the maps are optimal. From figure ?? can be seen that with ISOMAP, it is also not possible to make a distinction between the group of accepted and rejected kidneys.



```
## $dim1
##           [,1]
## [1,] -314.1028796
## [2,] -178.5069763
## [3,] -323.2510524
## [4,]  -34.4197998
## [5,] -229.1546177
```

```
## [6,] -367.4564935
## [7,] -312.9434498
## [8,]  165.2027211
## [9,]   66.5079017
## [10,] 409.5497921
## [11,] -193.3700888
## [12,] -330.1639781
## [13,] -332.9836016
## [14,]  121.4722130
## [15,] -209.4631047
## [16,]  241.4702215
## [17,]  292.7259347
## [18,]  -49.4973261
## [19,]  270.8730645
## [20,] -243.0286392
## [21,]  323.0164012
## [22,] -126.0720974
## [23,]  107.1095177
## [24,] -216.7127311
## [25,] -305.2144802
## [26,] -212.3889306
## [27,]  266.0971501
## [28,]   99.6126225
## [29,] -107.0766273
## [30,]   14.7881550
## [31,] -259.8686912
## [32,] -264.3668825
## [33,] -219.9460331
## [34,]  431.6331879
## [35,] -299.2561426
## [36,] -109.0230284
## [37,] -328.7268674
## [38,]  145.2956150
## [39,]  395.8184512
## [40,]  268.8006127
## [41,]  -71.3304477
## [42,] -221.7744362
## [43,] -373.2328713
## [44,] -315.7794113
## [45,]  332.0505723
## [46,]  340.5174219
## [47,] -256.8365046
## [48,]  -43.4671356
## [49,] -287.0680713
## [50,]  391.3377513
## [51,]  428.1785456
## [52,]  -51.7256135
## [53,] -208.8748509
## [54,] -189.6074640
## [55,] -213.1829751
## [56,] -281.6506228
## [57,] -271.1127136
## [58,]  118.6013139
## [59,] -297.9074383
```

```

## [60,] -217.1270573
## [61,] 191.3678204
## [62,] -180.0051055
## [63,] 266.0859625
## [64,] 381.4247041
## [65,] 26.3096565
## [66,] -112.6305195
## [67,] 431.1168804
## [68,] 68.4159350
## [69,] -351.1747398
## [70,] -34.7013518
## [71,] -222.3594027
## [72,] -201.2167170
## [73,] 306.8804443
## [74,] -293.4143429
## [75,] -340.0853997
## [76,] 268.7629909
## [77,] 158.4469753
## [78,] 151.4755733
## [79,] -225.3371722
## [80,] -331.9266008
## [81,] 173.4858357
## [82,] 195.5382508
## [83,] 263.8736932
## [84,] 352.1953097
## [85,] -256.5585288
## [86,] -171.5822183
## [87,] -49.0506119
## [88,] -251.1853863
## [89,] -298.4607588
## [90,] -55.6056997
## [91,] 451.3391674
## [92,] -298.8159335
## [93,] -313.5842187
## [94,] -330.9729084
## [95,] 402.0091478
## [96,] 232.4368471
## [97,] -99.6403996
## [98,] 86.3956676
## [99,] -227.5266881
## [100,] -313.0899217
## [101,] -324.7203917
## [102,] 444.0081343
## [103,] -176.5497614
## [104,] -169.2234365
## [105,] 299.4631051
## [106,] -300.8953490
## [107,] 341.2819749
## [108,] -214.4808259
## [109,] -188.7399314
## [110,] -5.2825372
## [111,] -40.2311254
## [112,] -5.8458283
## [113,] 225.8590474

```

```

## [114,] -237.3994989
## [115,] 376.6681888
## [116,] 291.3627358
## [117,] -268.3497190
## [118,] 278.0418794
## [119,] -158.1680035
## [120,] 400.8194756
## [121,] 234.2260077
## [122,] -4.5763931
## [123,] 99.4927733
## [124,] 237.7666073
## [125,] -22.2201406
## [126,] -104.2705723
## [127,] 66.7557298
## [128,] 261.0053914
## [129,] 389.5590396
## [130,] -267.2623138
## [131,] 368.3700258
## [132,] 299.8743238
## [133,] 434.7989844
## [134,] 168.5124197
## [135,] 377.6649451
## [136,] 209.2934724
## [137,] 239.3638335
## [138,] 363.7145404
## [139,] 336.2083026
## [140,] 315.3260615
## [141,] 218.8835830
## [142,] -170.4641018
## [143,] -201.3959864
## [144,] -30.5554548
## [145,] -306.4843257
## [146,] 457.6836130
## [147,] 406.1350547
## [148,] 404.3001863
## [149,] 385.9788309
## [150,] 294.7909067
## [151,] 435.6373131
## [152,] 417.1734761
## [153,] -52.7450258
## [154,] -176.6462864
## [155,] 355.4683895
## [156,] 188.3752320
## [157,] 427.0515489
## [158,] 215.7810252
## [159,] 421.2936091
## [160,] 430.9276022
## [161,] 413.2716687
## [162,] 378.3986130
## [163,] 29.0351306
## [164,] 321.5591494
## [165,] -60.2323200
## [166,] 422.5442571
## [167,] 368.0314815

```



```

## [168,] 404.0366007
## [169,] 433.8085574
## [170,] -300.6115501
## [171,] 442.9987520
## [172,] 41.6430651
## [173,] 107.2173211
## [174,] -103.9872689
## [175,] 291.9080525
## [176,] -342.4364570
## [177,] 330.1455720
## [178,] -181.6727585
## [179,] 303.6014043
## [180,] 427.1817794
## [181,] -73.1121904
## [182,] -31.9220460
## [183,] -314.6532574
## [184,] -271.8323572
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## [186,] -141.6711560
## [187,] 227.4490519
## [188,] -91.1447168
## [189,] -352.9479020
## [190,] -235.1368154
## [191,] -383.6293883
## [192,] -128.8738382
## [193,] -115.4508750
## [194,] 452.4845988
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## [201,] 283.2445842
## [202,] -270.1651894
## [203,] 406.1611580
## [204,] 452.1406041
## [205,] 330.7963841
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## [212,] -259.6144386
## [213,] -244.6806937
## [214,] -0.3317219
## [215,] 126.2310542
## [216,] 53.7925424
## [217,] -217.8936230
## [218,] 136.0076614
## [219,] -276.5265373
## [220,] 180.9438573
## [221,] -146.3105678

```

```

## [222,] 108.7031491
## [223,] -357.6668717
## [224,] -275.3591797
## [225,] -322.2842725
## [226,] -299.4964775
## [227,] -345.0650789
## [228,] -151.9827010
## [229,] -87.3603740
## [230,] -307.3923011
## [231,] -261.6726892
## [232,] -163.4387376
## [233,] -76.1201413
## [234,] 262.7134386
## [235,] -230.7967725
## [236,] 69.2202574
## [237,] -254.6002148
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## [239,] -247.2658667
## [240,] -401.5311139
## [241,] -268.2710532
## [242,] -143.8674990
## [243,] -337.2357934
## [244,] -350.7517998
## [245,] -35.2415336
## [246,] 32.3745886
## [247,] 15.4249389
## [248,] -342.1229033
## [249,] -270.2633454
## [250,] 116.0770490
## [251,] -121.4925822
## [252,] -51.4163007
## [253,] -368.8986567
## [254,] -315.0727190
## [255,] -170.8632371
## [256,] -334.1535062
## [257,] -67.6511790
## [258,] -304.8235545
## [259,] -286.5117118
## [260,] -242.2894075
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## [262,] -190.9826871
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## [264,] 53.5116037
## [265,] 84.8116829
## [266,] -326.6657820
## [267,] -297.8135980
## [268,] -260.7456828
## [269,] 59.2643610
## [270,] -187.4033825
## [271,] -368.6581565
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##	[105,]	299.4631051	-96.8899434	-150.4039105	[155,]	B8586552936091	218.7928241	-9.5648347	-21.2288
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##	[109,]	-188.7399314	0.8613576	136.3721924	[162,]	A17140940351306	203.1774983	-335.2108703	-53.0626
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##	[261,]	13.0288750	-55.0037015	-95.9111964	[32,]	196136320438173368554192708921		
##	[262,]	-190.9826871	266.3895054	143.6679987	[33,]	03279501888259273829461044393		
##	[263,]	-18.7852365	95.4143027	91.5569642	[38,]	30228801175609475499451916699		
##	[264,]	53.5116037	-260.6675624	295.6927307	[35,]	666063008274931635464655881051		
##	[265,]	84.8116829	190.7389553	157.8606284	[36,]	32131087781301572128702847601448		
##	[266,]	-326.6657820	175.0991076	95.8577185	[38,]	7587267122356277508034795153		
##	[267,]	-297.8135980	90.2728385	227.5872920	[35,]	34956299036604869334406083574		
##	[268,]	-260.7456828	31.3646360	202.1645588	[33,]	1106746457844012375871147301841		
##	[269,]	59.2643610	-302.7353778	186.6740840	[40,]	10484016683925152539437233842		
##	[270,]	-187.4033825	-102.9807237	13.7039205	[48,]	03674247406826721165556076049		
##	[271,]	-368.6581565	50.1774236	-68.2585108	[42,]	08363948689304445295145927479		
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##	[274,]	-300.4407498	172.9034552	-73.5090848	[42,]	074392463337693412893116271931		
##	[275,]	112.2556436	-348.1876582	59.8850974	[46,]	0177828925800495995843751628		
##	[276,]	-359.8506464	133.7095280	-7.7685576	[45,]	23958241794663493816127700887		
##	[277,]	122.7994222	-362.7710489	3.3727564	[49,]	0608872717173170146524091431		
##	[278,]	-347.9676775	64.1974973	6.6840502	[43,]	36638506690804052958000918136		
##	[279,]	-403.5457960	-38.1085328	-11.3181368	[56,]	1653405734327479898301669506		
##	[280,]	270.0435415	278.9812580	181.8486045	[58,]	16336305209725933116874440205		

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## [77,]	-0.5544988	59.637292037	## [131,]	-116.7128175	-117.979251435
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## [114,]	173.5979768	91.931493302	11.91611591624D	757297359567	-44.403667298	30.1082280	-62.37
## [115,]	15.7481594	67.577901385	-40.39689021693D	973415831885	41.951913315	-25.7311059	-38.50
## [116,]	110.4517418	-32.265627791	-28.82767211701B	440174512696	116.293288383	-121.8339140	-0.26
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## [118,]	9.7746440	-253.656900657	49.379741311726B	604282133350	22.527855355	-61.4963257	10.98
## [119,]	9.4287677	-109.830562485	-23.525558617371	349607623993	-93.162116556	112.2540296	-172.84
## [120,]	157.0914508	-22.599256775	132.60479901747D	30839296566	119.960759275	51.9510758	139.27
## [121,]	46.8955488	135.631854806	28.002770711754D	858126276390	193.305705823	124.1180147	-86.02
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## [123,]	66.6125633	119.042098055	5.901928117721	782379670146	-49.511178312	-54.5114810	-60.28
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## [125,]	-66.4553858	-167.493057231	83.09867571792B	567810877034	92.551517004	-41.3635651	87.03
## [126,]	172.6023676	-10.041492658	-154.42050321801D	566273624917	-126.540039188	-19.5214986	-68.01
## [127,]	103.0539698	197.301739450	165.576994418161	190236617803	147.603464901	-110.8500676	-139.43
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## [129,]	61.8990052	113.047106905	51.83878881836B	79888854130	-57.230907734	-5.4236325	-26.68
## [130,]	55.3449712	-124.418420095	-7.86784151841B	703813285972	45.667519774	-33.5582436	-0.38
## [131,]	-116.7128175	-117.979251435	-3.6029415185, D	4147318716447	-158.164576369	135.0159740	19.71
## [132,]	72.4147393	-100.673888033	-70.91187891864B	962515754910	41.475642212	226.0106756	231.38
## [133,]	-73.4776113	59.911605867	-4.1865612187, B	075810506996	-103.940419292	182.3691359	-71.36
## [134,]	-10.4602458	47.386281648	-157.91314916188, B	102512984318	60.373919085	-1.9831908	108.41
## [135,]	-134.3305244	87.232924044	26.8057789218901	332827892796	63.977858410	-127.3149681	-30.01
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## [137,]	77.2108296	-28.005929992	-44.430599119161	642968238761	6.525665593	-57.3347838	-60.00
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## [139,]	24.1855632	16.012946959	88.81642561933B	525862624023	144.025799857	-26.0342390	64.66
## [140,]	-106.8168046	-141.481220660	54.7597744194, D	4787152874336	21.947424445	39.4870610	25.30
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## [142,]	-88.3649351	59.386877402	-82.58298491965D	72748955218	-36.392668526	-61.6048127	-48.48
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## [144,]	-64.4962797	-87.957789440	-117.786891919811	595125678794	-53.339508260	-58.7644908	-35.20
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## [150,]	-44.1211024	48.342580324	-74.08577652048D	707272659136	108.976256348	-11.3329896	23.65
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## [153,]	25.7397896	50.843776441	4.90194197207, J	5165789218231	-48.982855405	-70.5430207	-33.36
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## [156,]	-15.3004594	144.298971505	-89.5356581210, B	801329225522	-99.453056894	-32.9112222	103.16
## [157,]	-71.6992173	14.262788497	7.758448652111D	312830261174	31.608886788	-38.4528258	45.07

##	[212,]	4.5669822	113.727687546	130.2177783126687	156.629733116	-101.824459170	42.0609076	-130.36
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##	[214,]	-70.4871769	215.801272427	-171.404682126822	-128.572810637	-227.229491828	15.5235075	-67.85
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##	[221,]	-168.8273855	222.293998253	-46.939403627554	6.159152919069	-29.811556781	171.2335936	108.09
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##	[223,]	80.2470323	133.234328409	252.474755727739	8.24595669736	0.009894055	-64.8680347	202.45
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##	[229,]	-297.6682664	119.749817734	93.4584450	-116.3289834			
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##	[231,]	-80.9203100	164.800151031	-123.8745411	-7.7207303	[,1]	[,2]	[,3]
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##	[258,]	-27.2674875	-170.025862991	15.9840619	[27,6]	2.260509171501	-268.8811530	-1.6054155
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##	[78,]	151.4755733	-233.6249824	-116.7827242	[124,]	1364289287432381152361296671	-156.9393887	-11.8500
##	[79,]	-225.3371722	-24.3999570	-43.6054548	[133,]	13682247579884190277373919182	32.0206634	22.8833
##	[80,]	-331.9266008	-172.2448464	-77.3848806	[134,]	1272068551246992525990720122	-272.3926897	-224.4842
##	[81,]	173.4858357	434.1026820	-115.9371471	[135,]	13662718664955845258208680	28.4397892	146.0152
##	[82,]	195.5382508	-300.1504512	-125.3085288	[136,]	17442058293722493354976675157	-15.9810350	145.6051
##	[83,]	263.8736932	-102.3498716	43.7899680	[137,]	1117239136284337228858996689	-183.1020461	-50.0634
##	[84,]	352.1953097	216.2053543	-71.8931464	[138,]	118032767144049829655450974	19.4462430	155.5194
##	[85,]	-256.5585288	232.7859436	21.6657300	[130,]	1158324820838269416933682321	-109.7093123	-70.7276
##	[86,]	-171.5822183	308.4522268	-156.4575528	[140,]	137731252324067157876242819762	-53.9052676	-22.9664
##	[87,]	-49.0506119	280.6587447	365.7519980	[149,]	11622240883583049158778598301	-246.8862597	29.3288
##	[88,]	-251.1853863	289.9141204	-63.3888482	[142,]	1272788246485188368407520331	-134.5155849	-2.7112

## [143,]	-201.3959864	-73.3731029	-234.2181792	[156,]	1384220606064	80945287874553	425.1054138	-22.1711
## [144,]	-30.5554548	14.3611305	-270.4564615	[157,]	33927082371205	509643804344712	420.8904976	-14.7904
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## [146,]	457.6836130	123.8589418	60.8592156	[207,]	3992319175632	27533109609137	70.2232381	-272.5359
## [147,]	406.1350547	215.5225132	61.4317168	[201,]	3422832244584	224238707776887	-90.3653266	75.1535
## [148,]	404.3001863	207.5467140	-24.7003708	[202,]	12427015165189	471169810362694	229.4767940	17.3499
## [149,]	385.9788309	251.3387144	-44.1876524	[203,]	3604068161458	00625302926023	-9.4618446	-65.0607
## [150,]	294.7909067	364.7917793	16.9048416	[204,]	3914572514060	74115808443592391	117.8297384	-13.4030
## [151,]	435.6373131	157.1212806	33.9916207	[205,]	1563494796834	652074120703295	24.6129345	-128.6220
## [152,]	417.1734761	226.4886496	-33.4129008	[206,]	2573526616831	49183015342589	408.2831240	-104.4336
## [153,]	-52.7450258	405.5815367	-127.3260874	[207,]	0872465906233	59062681806505	418.4193189	-48.5745
## [154,]	-176.6462864	94.1533865	-42.9166588	[208,]	7432430658700	6709270544972651	110.0911381	-222.8618
## [155,]	355.4683895	1.3180293	-276.8164347	[209,]	2404786561372	53525412325592	-84.7525741	113.7955
## [156,]	188.3752320	-175.3507271	-236.2421454	[210,]	1742620743229	621723808016715	-135.9266386	-193.8787
## [157,]	427.0515489	157.9114676	-0.3827645	[251,]	1545491883436	7268476843462379	492.7489291	135.2838
## [158,]	215.7810252	366.5216904	-35.7881894	[212,]	790268661413	61822817950644	-38.0997756	18.1407
## [159,]	421.2936091	218.7928241	-9.5648347	[213,]	2282448680693	55639235866810	133.6293423	92.7890
## [160,]	430.9276022	-38.7619244	-152.8507288	[215,]	7793194331721	95328967702113	-105.7519188	-101.5949
## [161,]	413.2716687	-170.1318151	155.0949298	[216,]	3798261231084	271231219319276	179.1104509	269.8108
## [162,]	378.3986130	153.1810603	-103.4773188	[219,]	5447582792562	45352651835103	455.3898533	-77.8054
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## [164,]	321.5591494	-45.8530908	-242.8817856	[214,]	1531899007661	40025388239841	118.6675188	107.2360
## [165,]	-60.2323200	245.9507705	-92.7730469	[206,]	367282852653	732403244971256	-77.3856639	-170.4993
## [166,]	422.5442571	213.6896658	-25.2100402	[220,]	1151898943867	54436906917004	11.0618652	-221.7663
## [167,]	368.0314815	263.0564199	-18.2726089	[225,]	500146231058	759239196616892	-17.9377329	233.2643
## [168,]	404.0366007	-108.1274101	-124.7029847	[222,]	7278750703149	144028976543745	202.1970701	-68.7070
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## [175,]	291.9080525	249.5861771	252.4362940	[220,]	1392744361354	67795745631812	91.0555223	71.9165
## [176,]	-342.4364570	130.2714338	98.4009820	[236,]	0453081392361	80488235756727	-26.7595137	103.3679
## [177,]	330.1455720	63.0050581	354.4879895	[238,]	063088672689	215749851555363	44.3112852	61.1235
## [178,]	-181.6727585	45.5517991	397.1008190	[232,]	7436735438257	6955307352148	-74.5396995	91.0100
## [179,]	303.6014043	39.6397088	-212.8674564	[233,]	3415765120141	38488855415571	-70.1529854	119.7474
## [180,]	427.1817794	122.2076337	131.9807244	[235,]	3942327713488	68865134350495	-46.9950525	-156.4805
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## [187,]	227.4490519	233.2781965	-184.9152788	[249,]	3452635271083	252161615543308	-202.5484343	1.0418
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##	[251,]	-121.4925822	-157.2499276	110.9051500	-122.59775507634324569708949899095	24.5523820	115.99		
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##	[259,]	-286.5117118	106.7899024	76.2427925	230.346267699083149945629407359014	81.1239581	-145.00		
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##	[261,]	13.0288750	-55.0037015	-95.9111961	339.149613632043873368554192708921	77.7872434	-116.39		
##	[262,]	-190.9826871	266.3895054	143.6679987	331.0327950188259273879461044393	-50.6466531	18.27		
##	[263,]	-18.7852365	95.4143027	91.5569612	334.3302288011856947549451916699	-30.8197638	-95.31		
##	[264,]	53.5116037	-260.6675624	295.6927307	131.366063008274931635454655881051	-32.8779363	114.99		
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##	[266,]	-326.6657820	175.0991076	95.8577185	378.75812971228353277508034795153	-126.5387341	52.40		
##	[267,]	-297.8135980	90.2728385	227.5872929	135.34958299031604869334406083574	94.9453949	-30.85		
##	[268,]	-260.7456828	31.3646360	202.1645588	333.1100776457844023753071147301841	-9.0215121	-6.84		
##	[269,]	59.2643610	-302.7353778	186.6740810	400.104840316688925152569437233842	52.2710903	-46.10		
##	[270,]	-187.4033825	-102.9807237	13.7039205	148.336174247406826721165556076049	13.7560414	-14.45		
##	[271,]	-368.6581565	50.1774236	-68.2585108	142.083637486893044445295145927479	-29.9875603	122.36		
##	[272,]	-154.3304020	276.0828062	154.5688486	147.73411422610425232232635000192	7.6729032	-38.71		
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##	[274,]	-300.4407498	172.9034552	-73.5090848	142.374432463337269341293116271931	-104.9264754	-132.85		
##	[275,]	112.2556436	-348.1876582	59.8850974	140.0177828925800495905843751628	76.6727191	-66.86		
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##	[278,]	-347.9676775	64.1974973	6.6840502	143.36638506690804052458000918136	36.5226354	8.90		
##	[279,]	-403.5457960	-38.1085328	-11.3181368	506.31653405734327479898301669506	-51.2407961	60.00		
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##	[281,]	403.8422720	134.2462045	-40.2680381	252.369010706604553225730418990636	-98.9811834	183.25		
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##	[,6]		[,7]	##	[54,]	106.0705104	-60.1331157268	-50.8974607	115.63
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##	[2,]	-249.5716627	-124.019946438	80.9635247	56.55.0645198242348.665359170600312	-205.9290741	92.04		
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##	[5,]	125.9039204	-157.823137136	107.1820618	59.99.209220542922.28115587221164	-115.6603959	51.24		
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##	[10,]	-154.7596822	63.202464635	87.8555809	64.11.908435906162.03941565812517	-87.4196661	-33.80		
##	[11,]	97.2356175	34.011995985	87.28484137	65.49.3320821599470.05806342160718	-122.2351369	-109.90		
##	[12,]	56.2732700	-110.728852358	-17.3738785	66.0.6413924450615.57206251960279	36.4809213	-51.25		
##	[13,]	-30.2255196	-286.361352426	79.6564448	67.49.4751543129748.26366927375598	21.1355399	49.51		
##	[14,]	72.2528442	258.475612977	177.0570829	68.24.052204007102.63794565747517	19.0794605	-12.45		
##	[15,]	-3.5202989	26.808827763	3.7575269	69.85.6187267686645.60892380935539	-83.2918188	-23.09		
##	[16,]	120.4210917	37.396288311	6.2116485	70.55.542758606665.29634939166681	5.9093126	75.47		
##	[17,]	172.1558524	-40.373423921	-69.378148	71.45.71569629684670.89759275482833	11.3194303	-48.59		
##	[18,]	49.6612020	172.138050724	-114.6682620	72.54.209254344203.79690967615503	8.2720885	-8.73		
##	[19,]	-138.1885558	127.032584332	20.9396117	73.07.9278189364573.60127207658994	-78.2153634	-25.06		
##	[20,]	47.3956249	-182.687897621	-44.6788164	74.24.2086510296545.03075285682753	39.9988386	9.20		
##	[21,]	-108.1748277	-36.996457657	-73.9776258	75.19.050346971669.599762929000250	-42.9890835	-20.63		

##	[76,]	-120.7789899	9.642372965	-3.531667213064	4.44533949786	-9829468420095	-7.8673158	-15.70
##	[77,]	-0.5544988	59.637292037	42.323510013111	3.316750028175	-55888979251435	-3.6029158	0.41
##	[78,]	25.2829571	-154.374528076	-49.185681013213	0.30247047396	-87087673888033	-70.9118789	-46.96
##	[79,]	2.6240521	-99.917078738	-0.210006613150	9.972597976173	2.6801911605867	-4.1865612	8.07
##	[80,]	31.3011271	63.142076101	83.463051213441	7.57669202453	8.8867386281648	-157.9131916	4.10
##	[81,]	109.8733299	-39.950209385	-29.267551713543	8.630434305244	9.98592632924044	26.8057892	104.33
##	[82,]	23.0817951	-135.349772794	-19.8700075213624	5.82421880646	3.112125641319136	63.7228324	-76.04
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##	[84,]	167.7110624	-67.621608190	-15.253876213830	6.829370032135	4.671966291791756	31.4332019	86.47
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##	[90,]	-41.1692092	197.740237972	-51.741224514443	4.354245627874	0.48178937789440	-117.7868919	11.59
##	[91,]	68.7996642	-89.392986085	-9.847900014594	1.984796349338	5.83665178856140	18.8894596	-164.81
##	[92,]	-120.2311434	15.848191730	-144.50784901463	7.237362656455	2.75056398787934	-3.6974039	16.69
##	[93,]	-38.1666216	-143.724936936	-29.3290851414772	5.1607504195730	1.6742036025742	-28.8709838	-19.13
##	[94,]	-43.5160263	47.757835244	-168.182687514851	7.269781253470	9.99258772441350	-6.9367372	74.84
##	[95,]	109.6569267	-79.300502360	-155.5894471314201	8.63031832284	6.709728376056968	39.2187797	45.48
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##	[97,]	32.7363142	-54.414971975	39.243225915160	0.768971499175	1.54851071675184	4.3260468	-8.33
##	[98,]	158.2823995	20.688156165	64.6518906915275	8.983270093747	5.26622944879616	9.3440292	9.55
##	[99,]	148.7067194	-41.288824370	-48.18268915324	2.226971297896	4.0528543776441	4.9019197	-7.51
##	[100,]	46.6449090	-34.248218634	46.5000411515497	3.63478808971	3.8033864766902	-60.7787349	12.63
##	[101,]	39.1573319	-138.482434203	-54.0674460715502	6.052846981009	7.7283391344823	74.2755483	-28.35
##	[102,]	-38.8899061	35.443829384	33.817652015600	6.73836904554	5.82452928971505	-89.5356581	5.80
##	[103,]	44.6421950	93.561623006	-160.9307766151755	8.421169921734	5.6543062788497	7.7584865	19.31
##	[104,]	13.1602841	-249.347793549	-181.732823815812	6.240741009718	3.8954660862521	96.7936620	-118.31
##	[105,]	-8.3419998	-56.756611611	-159.105061515959	3.1748746629102	8.0270684954580	-10.9918799	38.73
##	[106,]	76.5529128	82.125153170	-54.9937718116036	4.0246704630877	0.2816839635942	-66.2564658	-5.41
##	[107,]	-126.0392262	-45.971092334	55.8194464316143	2.552078863524	8.8529880845603	53.8558726	-38.64
##	[108,]	58.4828588	73.032831964	-48.635869216212	5.54479490466	6.27127482920196	-41.7161206	93.39
##	[109,]	127.5030608	-275.902659048	52.54288016341	4.256482734729	8.51029265684974	163.2003114	-249.30
##	[110,]	90.1910317	110.832273968	49.22908951642	9.97504316453	1.0359078446273	146.5864461	-163.85
##	[111,]	-90.8897547	-52.772510540	95.30882831653	5.245914346435	4.0884827228371	10.1703402	6.52
##	[112,]	35.4703188	29.905176426	-239.7594455160223	9.28806888945	3.52753027950736	-2.5999364	30.56
##	[113,]	-235.3815272	205.553429854	27.074860716253	9.24834241623	2.4568324964485	-51.4838634	52.04
##	[114,]	173.5979768	91.931493302	11.9161459116240	7.572975595674	7.45614953667298	30.1082280	-62.37
##	[115,]	15.7481594	67.577901385	-40.396890216930	9.734158318875	6.70444851913315	-25.7311059	-38.50
##	[116,]	110.4517418	-32.265627791	-28.827672117013	4.401745126916	2.07642943288383	-121.8339140	-0.26
##	[117,]	145.7182631	43.931015812	-63.533669117194	6.539887738939	1.45675015018742	-63.8736648	-142.05
##	[118,]	9.7746440	-253.656900657	49.3797743117263	6.042821333158	8.3203527855355	-61.4963257	10.98
##	[119,]	9.4287677	-109.830562485	-23.525558517374	3.496076223953	7.68304262116556	112.2540296	-172.84
##	[120,]	157.0914508	-22.599256775	132.6047799017470	3.68392396566	2.9427960759275	51.9510758	139.27
##	[121,]	46.8955488	135.631854806	28.0027707117542	8.581282763904	7.8048305705823	124.1180147	-86.02
##	[122,]	153.8728934	-86.769642072	53.558260517675	2.30792628588	1.8234045835217	-65.7322065	-2.58
##	[123,]	66.6125633	119.042098055	5.901922817724	7.20779670146	4.8672551178312	-54.5114810	-60.28
##	[124,]	122.0835201	-136.125163483	-7.511851217855	8.21876154558	1.1034357033695	-91.4256940	-60.65
##	[125,]	-66.4553858	-167.493057231	83.098675717923	5.658108770374	7.89235521517004	-41.3635651	87.03
##	[126,]	172.6023676	-10.041492658	-154.420503218010	5.66273824917	5.92817540039188	-19.5214986	-68.01
##	[127,]	103.0539698	197.301739450	165.5766044518161	1.902366178065	6.22761653464901	-110.8500676	-139.43
##	[128,]	-42.6379985	275.803481092	205.147255318257	7.060936075644	4.31284166988591	-73.4073252	-43.39
##	[129,]	61.8990052	113.047106905	51.838778818363	7.928886541304	3.87704230907734	-5.4236325	-26.68

## [184,]	81.3285972	45.667519774	-33.5582436238,-1.382789201506,3.087158179107302	-13.5864615	-21.80
## [185,]	-143.8216447	-158.164576369	135.0150740239,19,-7115694038745,-64854282105032	-27.5073552	-36.49
## [186,]	-125.7754910	41.475642212	226.010675624031,1.388588919710,141720278624962	49.4582904	35.08
## [187,]	55.1506996	-103.940419292	182.36941859241-71,3.67235217475,-448045321844660	-97.0144180	-138.06
## [188,]	125.2084318	60.373919085	-1.9834190824208,414267091327,697262759569807	158.8761439	-2.03
## [189,]	21.0392796	63.977858410	-127.314068124330,0.0154163135114,894598076196400	148.6864191	-82.54
## [190,]	-211.5624460	17.506631188	66.8030885244,10,08491060415242,57517921194580	173.3137041	-52.02
## [191,]	20.5238761	6.525665593	-57.3347783824560,-0.053125014172,-98764038326259	42.6277371	-61.92
## [192,]	-70.7883420	-37.765767387	44.9917701824625,8.6527743910328,46682035194810	-23.2827096	23.21
## [193,]	-257.2624023	144.025799857	-26.034289024761,6.62542682783,712108678683954	-1.4685389	-69.88
## [194,]	-87.4874336	21.947424445	39.487061024825,3.083287101113,82236783438690	224.6431561	-111.58
## [195,]	-127.2788706	45.535042847	156.686570524987,6.652326143482,842605630420269	-153.0460601	-23.66
## [196,]	154.5255218	-36.392668526	-61.604812725043,-4295214657293,299291657189864	-98.9755677	28.90
## [197,]	80.6010151	16.570875049	-108.2274146025100,-426696836685,-32488536785281	72.3310036	8.65
## [198,]	171.7678794	-53.339508260	-58.764490825235,2.052127353853,46873389593642	28.0614002	-46.80
## [199,]	202.8504784	-63.229767426	-72.72646225328,4.376068956327,1736761717114	10.7334982	-33.92
## [200,]	31.2401799	-8.736398548	-128.5098630254,-8,0930082083708,475393574961075	40.2498594	142.25
## [201,]	104.9367353	-29.884861503	-106.262468925541,4.351962357810,27844938798464	-90.6596223	6.48
## [202,]	-9.4281870	-30.996253780	10.785485725617,8.043768789897,472815279396821	49.0639185	15.86
## [203,]	-28.3043277	-17.040304841	80.186426225757,9.8023358666910,02729296839673	-34.2617109	15.09
## [204,]	-72.2359136	108.976256348	-11.332989625828,6.521228174871,-10000245862991	15.9840519	-63.22
## [205,]	-200.2639938	-192.995377821	176.1777417525971,9.0247103466310,07891682201259	224.1385565	-12.72
## [206,]	178.4656918	-36.629516955	55.9620800126025,5.932286137998,46551085108737	172.5830233	-30.96
## [207,]	165.7218231	-48.982855405	-70.543020726138,3.653105220325,55243588024557	-9.4074062	-152.53
## [208,]	-10.1786643	21.439318926	-13.201898826240,2.2006158896349,35486841869139	32.0771379	13.16
## [209,]	44.1878170	-188.473335524	-20.5936291263100,-676262461800,-298893174701850	122.0754258	19.33
## [210,]	-43.7725522	-99.453056894	-32.911222226408,1.836107647222,34233216553342	27.2518291	110.02
## [211,]	10.0261174	31.608886788	-38.452825826545,-07346715154711,54559057471770	136.7883171	-42.24
## [212,]	4.5669822	113.727687546	130.217783126687,1.540269733176,886174824459170	42.0609076	-130.36
## [213,]	-135.7831838	-28.657002230	12.097623926717,2.19528640236,75257462686270	-29.0630068	-49.73
## [214,]	-70.4871769	215.801272427	-171.404682126820,-128572810637,-328758219491828	15.5235075	-67.85
## [215,]	-258.6951297	177.062745350	109.752782226982,0.0321675033384,37287382640876	249.5896373	126.66
## [216,]	78.6153983	-95.808409452	-16.2610899270,7,225210326374,53681508214145	312.0639801	119.90
## [217,]	-182.0295669	137.792369550	-135.138511527191,1.424028112769,983038470383625	11.3410519	-28.96
## [218,]	-85.5768881	237.487019082	-141.6974111527212,0.004187477420,85281245242779	133.2650677	-53.82
## [219,]	129.0295413	162.745886883	119.673668627390,0.070882039382,46397658678586	12.2499574	20.13
## [220,]	67.5145246	114.464591842	-96.53246427488,1.25839602648,15863080678175	106.2580861	32.68
## [221,]	-168.8273855	222.293998253	-46.939403627551,6.159152919069,89253851556781	171.2335936	108.09
## [222,]	-53.0496850	5.788167049	60.92827827679,2.98526325480,37027051618214	30.0256155	-8.83
## [223,]	80.2470323	133.234328409	252.474755727739,8.29592569736,00416309894055	-64.8680347	202.45
## [224,]	175.6902614	-113.123356968	204.6997419278120,7.26685251125,12729225984928	141.1587209	-2.66
## [225,]	131.1139411	-12.838450948	187.0214414627965,8.023542915207,13650839884988	-66.2084719	23.10
## [226,]	-114.8063488	-9.009035503	-85.37386928011,0.834308154938,05675385156164	-42.2134320	-45.92
## [227,]	-92.9685767	156.442116963	-69.600770281,-2,945237290140,1185459717388	-19.9970339	87.90
## [228,]	-173.1025521	65.260614595	-105.112095028105,5.23929872725,67293924525856	-34.6338670	-41.07
## [229,]	-297.6682664	119.749817734	93.4584450	-116.3289834	-75.3671649
## [230,]	30.4214819	183.432422579	-29.8351515	46.3113795	-60.9887469
## [231,]	-80.9203100	164.800151031	-123.8745411	-7.7207303	-26.7834636
## [232,]	-50.4892789	51.348423638	-113.7807789	32.2073291	7.4818186
## [233,]	-89.1339264	196.635470137	-42.1226390	99.688749	26.061827
## [234,]	-121.2246129	-40.448982165	36.6824621	247.5524617	37.5805642
## [235,]	-221.2461035	3.071774256	-70.8341536	-38.0511873	-24.3641237
## [236,]	-173.2122133	103.870018650	-132.1486132	-109.2876068	72.7407036
## [237,]	-259.2037099	62.114203838	21.3530581	-75.7349064	75.2163388

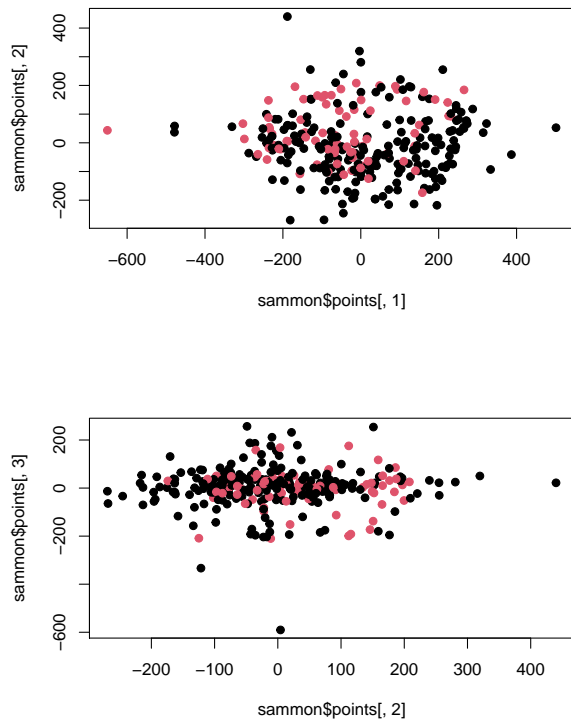
6.1.5 Sammon mapping

Sammon (1969). The
 does not is an iterative process. The
 between the 52 groups.

Initial stress : 0.28532
 ## stress after 10 iters: 0.21735, magic = 0.004
 ## stress after 20 iters: 0.16971, magic = 0.009

```
## stress after 28 iters: 0.13928
```

6.1.7 t-SNE



t-stochastic neighbor embedding is presented by Van Den Maaten and Hilton (2008). The resulting plot can be seen in figure ?? and indicates again that a simple distinction between the two groups cannot be made. Yet, there seems to be roughly two groups that differ in heterogeneity: one largely heterogeneous group and one group that is less heterogeneous, though far from homogeneous.

6.1.6 Diffusion maps

Diffusion mapping was presented by Nadler et al (2006) and LAfon and Lee (2006). From figure ??, no distinction between the two groups can be made with diffusion maps.

```
## Performing eigendecomposition
## Computing Diffusion Coordinates
## Used default value: 3 dimensions
## Elapsed time: 134.1 seconds
```

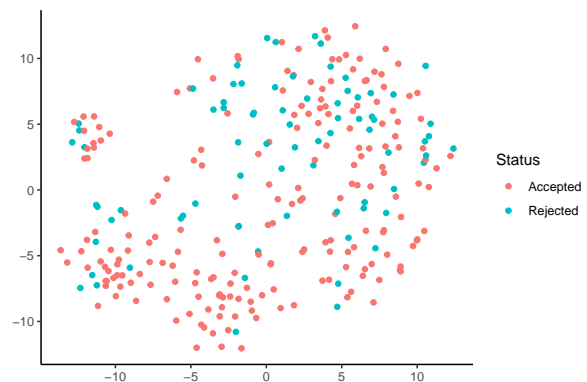
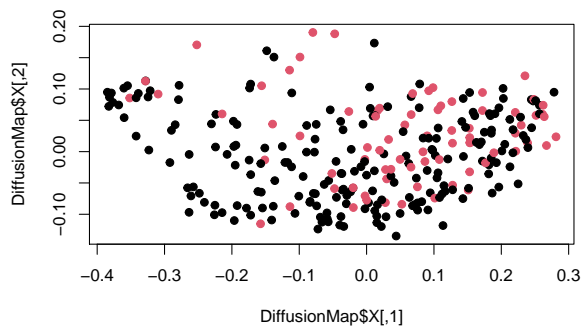
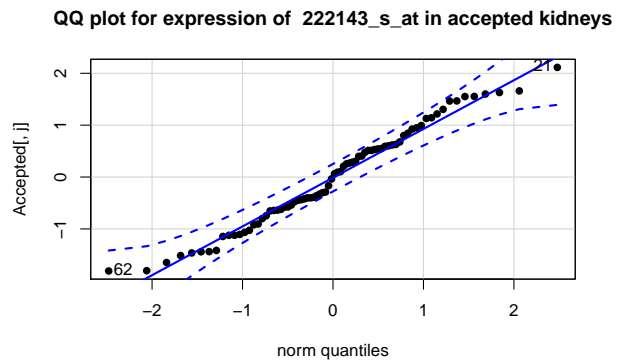
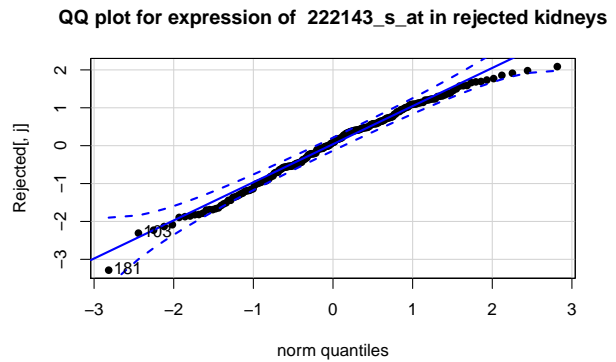
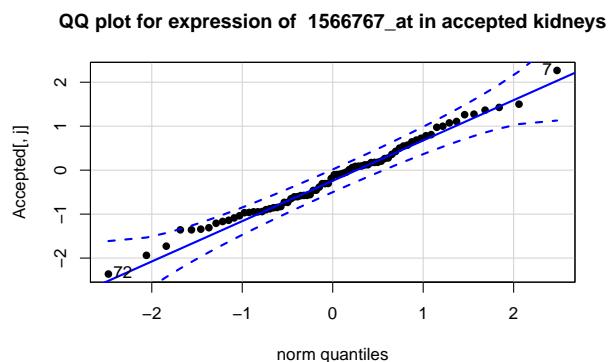
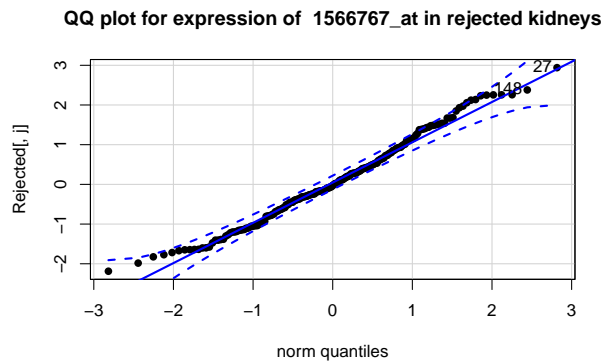
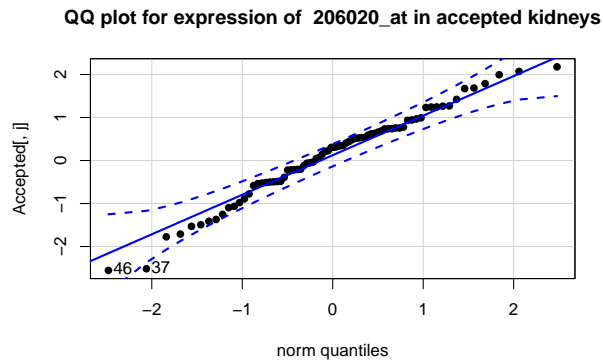
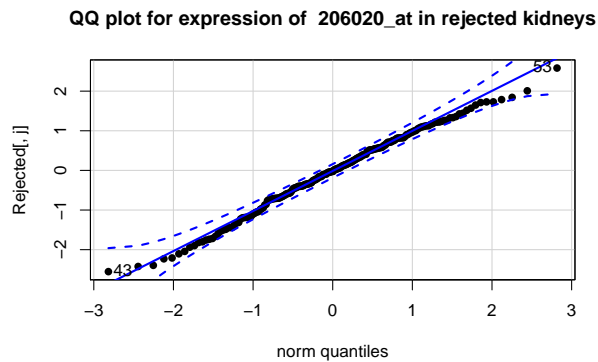


Figure 3: Two dimensional representation of the data through application of t-SNE

6.2 QQ-plots



7 References

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