

ALA 4.5 Estimating genetic relationships from molecular marker data.Files:

QG\_Mod4\_ALA4.5\_eval dist metrics.csv (note: .xlsx file also provided)  
QG\_Mod4\_ALA4.5\_eval dist metrics.xlsx  
QG\_Mod4\_ALA4.5\_dist eval.R

Goal:

Develop the ability to evaluate R functions based on known mathematical metrics.

Purpose:

Demonstrate and have the students participate in the evaluation of R “dist” functions using known genetic relationships.

ALA:

In ALAs from Chapter 3 and ALAs 4.2, 4.3, and 4.4 genetic diversity among the lines is based on pedigree information. Since the development of genome-wide molecular markers, it has become possible to determine realized relationships among lines, hybrids, individuals, etc.

The “dist” function in the R-code will determine the following distance metrics that can be used with clustering and dendrogram packages to visualize the relationships:

1. Euclidean:

Usual distance between the two vectors (2 norm aka  $L_2$ ),  $\sqrt{\text{sum}((x_i - y_i)^2)}$ .

2. Manhattan:

Absolute distance between the two vectors (1 norm aka  $L_1$ ).

3. Canberra:

$\sum |x_i - y_i| / (|x_i| + |y_i|)$ . Terms with zero numerator and denominator are omitted from the sum and treated as if the values were missing. This is intended for non-negative values (e.g., counts), in which case the denominator can be written in various equivalent ways; Originally, R used  $x_i + y_i$ , then from 1998 to 2017,  $|x_i + y_i|$ , and then the correct  $|x_i| + |y_i|$ .

4. Binary (aka asymmetric binary):

The vectors are regarded as binary bits, so non-zero elements are ‘on’ and zero elements are ‘off’. The distance is the *proportion* of bits in which only one is on amongst those in which at least one is on.

5. Minkowski:

The p norm, the pth root of the sum of the pth powers of the differences of the components.

Ask students to consider which of these metrics provides the most accurate estimate of relationships among doubled haploid or recombinant inbred lines. Have them devise approaches to answer this question.

Provide a demonstration of how to evaluate metrics that you have never seen before by using a small data set consisting of a few individuals and a few markers.

For example, create a set of backcross series to each of the parents, such as found in "ALA 4.5 eval dist metrics.csv". Then observe the calculated distance measures and decide which most accurately reflects the true distances.

## 1. Euclidean distance

The screenshot shows the RStudio interface. The script editor contains the following R code:

```

7 gettwo()
8
9 #####
10 # Use data with known relationships #
11 # to evaluate various distance metrics #
12 #####
13
14
15 EVAL<-read.csv("ALA 4.5 eval dist metrics.csv",header=T)
16 lines = EVAL$line
17 scores<-EVAL[,2:21]
18 row.names(scores) = lines
19 realized = as.matrix(scores)
20
21 euc1 <- round(dist(realized, method="euclidean"),digits=2)
22 euc1
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```

The console output shows the following distance matrix:

```

BC2P2-2  2.24
> euc1
      P1  P2  F1  F2 BC1P1-1 BC1P1-2 BC1P2-1 BC1P2-2 BC2P1-1 BC2P1-2 BC2P2-1
P2      8.94
F1      4.47 4.47
F2      5.48 5.48 3.16
BC1P1-1 2.24 8.06 3.87 3.87
BC1P1-2 2.24 8.06 3.87 5.00 3.16
BC1P2-1 8.06 2.24 3.87 3.87 7.07 7.07
BC1P2-2 8.06 2.24 3.87 5.00 7.07 7.35 3.16
BC2P1-1 1.73 8.43 4.12 4.58 1.41 2.83 7.48 7.48
BC2P1-2 1.41 8.60 4.24 5.29 2.65 1.73 7.68 7.68 2.24
BC2P2-1 8.60 1.41 4.24 4.90 7.68 7.68 1.73 2.65 8.06 8.25
BC2P2-2 8.43 1.73 4.12 5.20 7.48 7.62 2.83 1.41 7.87 8.06 2.24

```

The Environment pane on the right shows the following objects:

- Data
  - EVAL: 12 obs. of 21 vari...
  - realized: int [1:12, 1:20] ~
  - scores: 12 obs. of 20 vari...
- Values
  - euc1: 'dist' num [1:66] 8...
  - lines: Factor w/ 12 levels ~

2. Manhattan

```

7 getTwoLJ
8
9 #####
10 # Use data with known relationships #
11 # to evaluate various distance metrics #
12 #####
13
14
15 EVAL<-read.csv("ALA 4.5 eval dist metrics.csv",header=T)
16 lines = EVAL$line
17 scores<-EVAL[,2:21]
18 row.names(scores) = lines
19 realized = as.matrix(scores)
20
21 manhat <- round(dist(realized, method="manhattan"),digits=2)
22 manhat
23

```

```

> manhat
> manhat
      P1 P2 F1 F2 BC1P1-1 BC1P1-2 BC1P2-1 BC1P2-2 BC2P1-1 BC2P1-2 BC2P2-1
P2    40
F1    20 20
F2    20 20 10
BC1P1-1  5 35 15 15
BC1P1-2  5 35 15 15      10
BC1P2-1 35 5 15 15      30      30
BC1P2-2 35 5 15 15      30      30      10
BC2P1-1  3 37 17 17      2      8      32      32
BC2P1-2  2 38 18 18      7      3      33      33      5
BC2P2-1 38 2 18 18      33      3      7      35      36
BC2P2-2 37 3 17 17      32      32      8      2      34      35      5

```

Note: Manhattan gives the most accurate sets of relationships based on what is known about the individuals.

There is always a reference line, in this case our reference line is Parent 2; 1 represents the homozygote for parent 2 at individual loci.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1		L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	L12	L13	L14	L15	L16	L17	L18	L19	L20	
2	P2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
3																						
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Next, to translate the information of unrelated line (P1) in relation to the reference line; -1 represents the homozygote for parent 1; which is the alternate allele of parent 2 at individual loci.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1		L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	L12	L13	L14	L15	L16	L17	L18	L19	L20	
2	P1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
3																						
4																						
5																						

Next, to translate the information of F1 in relation to the reference line; 0 represents the heterozygote at individual loci

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1		L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	L12	L13	L14	L15	L16	L17	L18	L19	L20	
2	P1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
3	P2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
4	F1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5																						
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7																						

Next, to translate the information of F2 in relation to the reference line; 1 represents the homozygote for parent 2 at individual loci -1 represents the homozygote for parent 1; 0 represent heterozygote at individual loci

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1		L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	L12	L13	L14	L15	L16	L17	L18	L19	L20	
2	P1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
3	P2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
4	F1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	F2	-1	-1	-1	-1	-1	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1
6																						
7																						

Next, to translate the information of BC1P1-1 in relation to the reference line; 1 represents the homozygote for parent 2 at individual loci; -1 represents the homozygote for parent 1; 0 represent heterozygote at individual loci







Next, to translate the information of BC2P2-2 in relation to the reference line; 1 represents the homozygote for parent 2 at individual loci; -1 represents the homozygote for parent 1; 0 represent heterozygote at individual loci.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
1		L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	L12	L13	L14	L15	L16	L17	L18	L19	L20
2	P1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
3	P2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
4	F1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	F2	-1	-1	-1	-1	-1	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1
6	BC1P1-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	0	0	0	0	0
7	BC1P1-2	-1	-1	-1	-1	-1	-1	-1	-1	0	0	0	0	0	-1	-1	-1	-1	-1	-1	-1
8	BC1P2-1	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
9	BC1P2-2	1	1	1	1	1	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1
10	BC2P1-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	0	0	-1	-1	0
11	BC2P1-2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	0	0	-1	-1	-1	-1	-1	-1	-1
12	BC2P2-1	1	0	1	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
13	BC2P2-2	1	1	1	1	1	0	0	1	1	0	1	1	1	1	1	1	1	1	1	1
14																					

Save this final file as "QG\_Mod4\_ALA4.5\_eval dist metrics.csv" (provided).