Programming I – algorithms and loops

How computers think How to program them to think for you

Computers are dumb but fast

- Computers are literal
 - They will do exactly what you tell them to do
 - They will not do what you don't tell them to do
- Computers are fast
 - They execute millions of instructions millions of times per second
- The trick in programming is telling the computer exactly what it needs to do to accomplish a task

Algorithms

- Computers execute instructions one at a time
- Algorithms are step by step procedures for calculations
- They describe a series of steps for accomplishing a task
- To get a computer to do a task, we need to:
 - Identify the task to be completed
 - Figure out how to do the task using operations the computer knows how to do
 - Write instructions to the computer to do the steps

Example: sorting numbers

- How to sort numbers from 1 to 10 in descending order?
- There are many ways to do this
 - All will accomplish the task
 - Some will take longer than others

"Bubble" sort

- Start with unsorted numbers
- Compare the first and second numbers – if they are out of order swap them



- Continue to second and third number, third and fourth, fourth and fifth, etc. until all comparisons have been made
- Repeat until no more swaps are needed

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Fourth run

Fifth run

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Finished!

Nothing changed in the last run, but needed to confirm that the list is in order

Better bubble sort

- A weakness of the algorithm: numbers can move up rapidly, but down slowly
- An improved algorithm: alternate running up and down between runs

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9. 27 A 14	1.780 F.J. 35T 350 C.M. 40		*******						ふち ボンクリー おだて たいさつぶつ

	439811499
	A
1	Numbers
2	10
3	9
4	8
5	7
6	6
7	5
8	4
9	3
10	2
11	1



Sixth run

Programming a computer

- A program is a series of instructions executed by the computer
- They are written in a programming language
- They are executed in order, first to last

Programming languages

- Many out there, some more "English like" in their syntax than others
- Written as "code" = a series of instructions, with a syntax specific to the language
- Some then execute the code from within an "interpreter" = another program that translates the code into a binary form the computer understands
- Some "compile" the program = convert it into a binary code the computer understands, which can then be run without an interpreter

The language we will use

- The language used to program Excel is "Microsoft Visual Basic for Applications" (VBA)
 - Interpreted language
 - Only runs from within an MS Office application, but can take advantage of the capabilities of Excel
- Visual Basic is fairly simple to use, fairly English-like in its syntax
- Programs that run in Excel are called VBA "macros"

Macros in Excel

Three major uses

- Automating a complex task
- Automating a repetitive task
- Implementing functions/algorithms not already available as functions in Excel
- Simplifies programming
 - Take advantage of Excel for storing data, file input/output, summary, graphing
- Constrained by the way Excel works
 - Need to learn to move around the worksheet, select cells, from within the program

Automating a complex task

- Some operations take multiple steps to complete
- May be faster to:
 - Record yourself doing the task once with the macro recorder
 - Assign the macro to a key
 - Hit the key to run the macro and perform the task
- Example: setting the format on some cells...

Automating a repetitive task

- If you need to do an operation on each cell in your spreadsheet one at a time, it may be faster to record the operation once, then write a "loop" to repeat it
- Repetitive task example another sort algorithm

Random re-ordering

- Let's try another sort algorithm
- The algorithm matters...how would random reorderings work?
 - Start with the numbers
 - Generate random numbers
 - Sort by the random numbers
 - Check if the sort order is correct
- Let's try it once in Excel...

Repeating tasks in a computer – using loops

- Loops are ways of telling the computer to repeat an operation until a condition is met
- The condition can be several different things:
 - A fixed number of repeats
 - A run through a list of arguments
 - A criteria that needs to be satisfied
- Begin and end with key words
- Details of the syntax of loops depends on the programming language

Do loops

- Do loops can have two different forms:
 - Do while
 - loop
 - Do
 - ... loop until
- The criterion can be tested before or after the loop instructions within the loop are executed
- Once the criterion is met the program leaves the loop and continues on to the next instruction

The code that Excel recorded for random sorter

Sub RandSort()

'RandSort Macro

' Show how slow a sorting algorithm that selects random sort orders would be.

'Keyboard Shortcut: Ctrl+Shift+R

```
Range("A1:B11").Select

ActiveWorkbook.Worksheets("RandomSorter").Sort.SortFields.Clear

ActiveWorkbook.Worksheets("RandomSorter").Sort.SortFields.Add Key:=Range("B2:B11") _

, SortOn:=xlSortOnValues, Order:=xlAscending, DataOption:=xlSortNormal

With ActiveWorkbook.Worksheets("RandomSorter").Sort

.SetRange Range("A1:B11")

.Header = xlYes

.MatchCase = False

.Orientation = xlTopToBottom

.SortMethod = xlPinYin

.Apply

End With

End Sub
```

The header

' RandSort Macro

1

' Show how slow a sorting algorithm that selects random sort orders would be.

Keyboard Shortcut: Ctrl+Shift+R

The apostrophes are "comment" characters. Anything after them is ignored by the interpreter.

Used to make notes about what the program does.

Comments are a Good Thing.

Subroutines are marked by Sub, End Sub

Sub RandSort()

Instructions to execute...

End Sub

At least one must be present for the macro to run.



Now, make it run repeatedly

- The rand() function selects a new set of random numbers each time the sheet recalculates
- Sorting recalculates the sheet
- As soon as the numbers are sorted, there are new random numbers for sorting again
- All that's needed is to tell the macro to repeat the operation until the numbers are in order

Do this repeatedly with a Do while...loop

Sub RandSort()
' RandSort Macro ' Show how slow a sorting algorithm that selects random sort orders would be.
Keyboard Shortcut: Ctrl+Shift+R The loop
Do While Range("B13") = False Range("A1:B11").Select ActiveWorkbook.Worksheets("RandomSorter").Sort.SortFields.Clear ActiveWorkbook.Worksheets("RandomSorter").Sort.SortFields.Add Key:=Range("B2:B11") , SortOn:=xlSortOnValues, Order:=xlAscending, DataOption:=xlSortNormal With ActiveWorkbook.Worksheets("RandomSorter").Sort
End With Range("B15").Select ActiveCell.Value = ActiveCell.Value + 1 Loop Count iterations

End Sub

For...next loops

- Useful for executing an operation on a defined list of inputs, or a fixed number of times
- Syntax is:

```
For i in 1 to 10
Things for the loop to do
Next i
```

 We'll use these a lot for randomization testing and bootstrapping

Infinite loops

- Avoid these
- If you use a loop in which the ending condition cannot ever be met, it will run forever
- If this happens, VB allows you to interrupt a running macro
- Childishly easy to create!

An infinite Do...loop

• The following is an infinite Do loop

```
Range("A2").Value = False
Do while Range("A2") = False
Loop
```

- A2 is never changed, so it can never become True
- This will execute forever, until you stop it or the computer dies
- Stop a program with the Escape key (Esc)

Randomization testing

- A "nonparametric" approach to analyzing data
- Generally used when the usual parametric approaches (t-tests, ANOVA, regression, etc.) aren't appropriate because of violated assumptions
- The sampling distribution is derived by randomly shuffling the data

Example: Mantel tests

- Mantel tests are tests of association between two square matrices
- Often these are "distance matrices"
 - Geographic distance between sampled populations, genetic distance between sampled populations
- A measure of association between the matrices is calculated, then the elements of the matrix are randomly shuffled
- The association is re-calculated with each random shuffle
- The observed association is compared with the randomly generated differences to obtain a p-value

Association between geographic distance and genetic distance

- Organisms tend to find mates in their vicinities
- This leads to "isolation by distance"
- Gene pools tend to become more different with increasing distance
- Is this true for humans?
- Let's look at the association between gene frequencies and location from the DNA fingerprint data

The analysis

- Data from 7 states
- Calculate a genetic distance among all possible pairs of states
- Treat the location of the capitol city as the location, calculate distances among them
- Test for association using a Mantel test

Euclidean distance

 As you no doubt recall, the distance between two points with coordinates (x₁,y₁) and (x₂, y₂) is:

$$d = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

 If we have more than two coordinates we just continue to add squared differences:

$$d = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2} \dots$$

Distance between capitols

91.467.97 7	А	∣ ¤	<u>ر</u>	U	E	Г	Ú Ú		217843
1		California	Alabama	Florida	Virginia	New York	Michigan	Minnesota	
2	California		2432.8299	2569.85796	3046.0153	3298.369	2553.161	1964.8485	
3	Alabama			139.48841	613.4105	871.5	132.394	467.9823	
4	Florida				478.3441	740.6782	84.82056	605.4398	
5	Virginia					268.7998	494.7943	1081.2876	
6	New York						746.3383	1336.8301	
7	Michigan							590.5349	
8	Minnesota								
9									

Done in another program – earth is curved, longitude lines are not parallel, need software that knows this

Distances between sets of gene frequencies

California

Alabama

Locus	Allele 1	Allele 2
D3S1358	0.2800	0.2167
VWA	0.2333	0.2800
FGA	0.1500	0.1767
D8S1179	0.3733	0.3733
D21S11	0.1967	0.2321
D18S51	0.1467	0.1600
D5S818	0.3400	0.3600
D13S317	0.3133	0.2767
D7S820	0.2433	0.2233
THO1	0.2200	0.3233
TPOX	0.5267	0.5267
CSF1P0	0.3005	0.3251

Locus	Allele 1	Allele 2
D3S1358	0.2300	0.2567
VWA	0.2133	0.2800
FGA	0.1367	0.1900
D8S1179	0.3133	0.3133
D21S11	0.1867	0.2733
D18S51	0.1567	0.1100
D5S818	0.4167	0.3667
D13S317	0.3200	0.2667
D7S820	0.2967	0.1500
THO1	0.1967	0.3067
TPOX	0.5433	0.5433
CSF1PO	0.3033	0.3200

48.62	M10		- (6	fx {=SUN	M((\$B4;\$B1	5-C4:C15)^	2+(\$B21:\$I	B32-C21:C3	2)^2)}	EV DEVE EV BERKE			24 (A 16 / 19 (A 16 (A 16 (A		2.94 Z.20.65 ¥10201	ANY OF A FORM		5.35 L 83 Z 87 S M	120-201
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1	A Allala 1	В	L.	U	E	F	G	н		J	ĸ	L	IVI	IN I	0	F	Q	К	5
1	Allele I																		
2		<u></u>	01	F 1	1. JA	N D7	5 AL	5 40 1											
3	LOCUS	0.0000	AL	FL	VA	NY 0.0040	IVII												
4	D351338	0.2800	0.2300	0.2736	0.2437	0.2943	0.2844	0.2833											
2	VWA	0.2333	0.2133	0.2093	0.2284	0.2270	0.2188	0.2300											
5	FGA	0.1500	0.1367	0.1592	0.1472	0.1099	0.1656	0.1300			o	-+							
/	D851179	0.3733	0.3133	0.3557	0.3112	0.3156	0.3469	0.3000			Genetica	stances							
8	D21511	0.1967	0.1867	0.2289	0.2117	0.2179	0.2500	0.1867				0-1:6		El - ut -l -	L . H	8.1			
9	D18551	0.1467	0.1567	0.1617	0.1556	0.1879	0.1625	0.1633			- 116 - 1	California	a Alabama	Florida	Virginia	New York	iviicnigan	Minnesota	1
10	D55818	0.3400	0.4167	0.3740	0.3858	0.3794	0.3600	0.3633			California		0.032152	0.01559	0.023229	0.030644	0.016594	0.02409	
11	D135317	0.3133	0.3200	0.3232	0.3173	0.3475	0.3576	0.2967			Alabama			0.022855	0.013359	0.023823	0.024248	0.015337	
12	D7S820	0.2433	0.2967	0.2622	0.3147	0.3156	0.2848	0.2700			Florida				0.023953	0.028312	0.012459	0.021753	
13	THO1	0.2200	0.1967	0.2378	0.2411	0.2113	0.2143	0.2467			Virginia					0.012674	0.01529	0.015625	
14	TPOX	0.5267	0.5433	0.5488	0.5254	0.5458	0.5408	0.5600			New York						0.015094	0.022419	
15	CSF1PO	0.3005	0.3033	0.3679	0.2944	0.2993	0.3151	0.2933			Michigan							0.02146	
16											Minnesota	a							
17																			
18		Allele 2																	
19																			
20	Locus	CA	AL	FL	VA	NY	MI	MN											
21	D3S1358	0.2167	0.2567	0.2338	0.2563	0.2563	0.2482	0.2375											
22	VWA	0.2800	0.2800	0.2967	0.2792	0.2908	0.2844	0.2567											
23	FGA	0.1767	0.1900	0.1642	0.1675	0.1738	0.1625	0.1667											
24	D8S1179	0.3733	0.3133	0.3557	0.3112	0.3156	0.3469	0.3000											
25	D21S11	0.2321	0.2733	0.2786	0.2143	0.2143	0.2156	0.2700											
26	D18S51	0.1600	0.1100	0.1318	0.1480	0.1170	0.1188	0.1167											
27	D5S818	0.3600	0.3667	0.3557	0.3350	0.2801	0.3433	0.3633											
28	D13S317	0.2767	0.2667	0.2541	0.2766	0.2766	0.2881	0.3067											
29	D7S820	0.2233	0.1500	0.2093	0.1777	0.1986	0.1987	0.1833											
30	THO1	0.3233	0.3067	0.2947	0.2944	0.3063	0.2789	0.2900											
31	TPOX	0.5267	0.5433	0.5488	0.5254	0.5458	0.5408	0.5600											
32	CSF1PO	0.3251	0.3200	0.3069	0.3477	0.3345	0.2979	0.3200											
33																			
34																			
35																			

Genetic di	stances						
	California	Alabama	Florida	Virginia	New York	Michigan	Minnesota
California		0.032152	0.01559	0.023229	0.030644	0.016594	0.02409
Alabama			0.022855	0.013359	0.023823	0.024248	0.015337
Florida				0.023953	0.028312	0.012459	0.021753
Virginia					0.012674	0.01529	0.015625
New York						0.015094	0.022419
Michigan							0.02146
Minnesota	a						
Geographi	c distance	(km)					
	California	Alabama	Florida	Virginia	New York	Michigan	Minnesota
California		3915.267	4135.792	4902.095	5308.219	4108.921	3162.122
Alabama			224.4852	987.1902	1402.546	213.0678	753.1457
Florida				769.8215	1192.008	136.5057	974.3626
Virginia					432.5921	796.2956	1740.167
New York						1201.117	2151.423
Michigan							950.3753

The relationship we'll test



Does the genetic distance depend on geographic distance?

Why not just test the correlation?

- The measures aren't independent
- We have only 7 states, but we've generated 21 distances of each type
- Since parametric tests require independence, we can't use them
- But, a randomization test doesn't make this assumption, because any dependence will be accounted for when we randomly shuffle the data

Unfold the data

Genetic di	stances						
	California	Alabama	Florida	Virginia	New York	Michigan	Minnesota
California		0.032152	0.01559	0.023229	0.030644	0.016594	0.02409
Alabama			0.022855	0.013359	0.023823	0.024248	0.015337
Florida				0.023953	0.028312	0.012459	0.021753
√irginia					0.012674	0.01529	0.015625
New York						0.015094	0.022419
Michigan							0.02146
Minnesota	а						
Geographi	ic distance	(km)					
	California	Alabama	Florida	Virginia	New York	Michigan	Minnesota
California		3915.267	4135.792	4902.095	5308.219	4108.921	3162.122
Alabama			224.4852	987.1902	1402.546	213.0678	753.1457
Florida				769.8215	1192.008	136.5057	974.3626
√irginia					432.5921	796.2956	1740.167
New York						1201.117	2151.423
Michigan							950.3753

1		PERCENT A PART A TOP PART A PERCE	1	<u></u>
	А	В	С	
1	Comparison	Geograph	Genetic	
2	California to Minnesota	3162.122	0.02409	
3	Alabama to Minnesota	753.1457	0.015337	
4	Florida to Minnesota	974.3626	0.021753	
5	Virginia to Minnesota	1740.167	0.015625	
6	New York to Minnesota	2151.423	0.022419	
7	Michigan to Minnesota	950.3753	0.02146	
8	California to Michigan	4108.921	0.016594	
9	Alabama to Michigan	213.0678	0.024248	
10	Florida to Michigan	136.5057	0.012459	
11	Virginia to Michigan	796.2956	0.01529	
12	New York to Michigan	1201.117	0.015094	
13	California to New York	5308.219	0.030644	
14	Alabama to New York	1402.546	0.023823	
15	Florida to New York	1192.008	0.028312	
16	Virginia to New York	432.5921	0.012674	
17	California to Virginia	4902.095	0.023229	
18	Alabama to Virginia	987.1902	0.013359	
19	Florida to Virginia	769.8215	0.023953	
20	California to Florida	4135.792	0.01559	
21	Alabama to Florida	224.4852	0.022855	
22	California to Alabama	3915.267	0.032152	

The logic of the test

- Assume no relationship
 - The correlation between them is just random sampling
 - If so, the amount of correlation should be typical of randomly generated data
- If true, randomly shuffled genetic and geographic distances will give correlations as big as observed
- Conversely, if the amount of association we see is big compared to what we see when we randomly shuffle the data, we can conclude the association is real

	Α	В	С	D	E	F		Cat up tha	
1	Comparison	Geograph	Genetic	Randomizer		Sums of p	roducts	- Set up the	
2	California to Minnesota	3162.122	0.02408959	0.918175332					
3	Alabama to Minnesota	753.1457	0.01533667	0.561645718				workahaat	
4	Florida to Minnesota	974.3626	0.02175256	0.083160037		N		worksneel	
5	∨irginia to Minnesota	1740.167	0.01562474	0.213115326					
6	New York to Minnesota	2151.423	0.0224185	0.973133831					
7	Michigan to Minnesota	950.3753	0.02145971	0.048686382			\backslash		
8	California to Michigan	4108.921	0.01659358	0.608297796				Column for toot	
9	Alabama to Michigan	213.0678	0.02424808	0.391236353				Column for test	
10	Florida to Michigan	136.5057	0.01245909	0.429935504				statistic for random	
11	Virginia to Michigan	796.2956	0.01528989	0.068107105	\setminus			shuffles	
12	New York to Michigan	1201.117	0.01509435	0.513797044	-ro	nd()			
13	California to New York	5308.219	0.03064421	0.490451294	-la	inu()			
14	Alabama to New York	1402.546	0.02382347	0.879806774					
15	Florida to New York	1192.008	0.02831232	0.159336885		ι	Use the macro recorder to:		
16	Virginia to New York	432.5921	0.01267416	0.947817755					
17	California to Virginia	4902.095	0.02322859	0.054737555		c	Sort only the genetic		
18	Alabama to Virginia	987.1902	0.01335929	0.273387711		3			
19	Florida to Virginia	769.8215	0.02395328	0.426013632		C	listar	ices by the Randomizer	
20	California to Florida	4135.792	0.01559009	0.651453488		C	olum	n	
21	Alabama to Florida	224.4852	0.02285535	0.805971365					
22	California to Alabama	3915.267	0.03215176	0.957294725		(Conv	the new test statistic and	
23							ooto	anagial to column E	
24	Sum of products		886.3886249	_		4	asie-	special to column F	
25	(the Mantel test statistic)								
26					{=sun	n(produ	ict(h2	$(-1)^{-1}$	
27	Observed sum of products		886.3886249		ູ່ວິດກ	ii(piouc			
28									
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31	CECENTE TO DE SERVICE AND ALSO DE LA PERSON DUPER.		o a una a marcana	MARTIN CONTRACTOR	025301050500	2113 W30 / 702 / 704 1	SNOVEDOUR		
		12121201	A in the second s	A copy of	the ob	served	test	statistic	

Macro as recorded

```
(General)
                                                                    MantelTest
  Sub MantelTest()
   MantelTest Macro
   ' Conduct a Mantel test on the geographic and genetic distances.
    Kevboard Shortcut: Ctrl+Shift+M
      Range("C1:D22").Select
      ActiveWorkbook.Worksheets("Sheet2").Sort.SortFields.Clear
      ActiveWorkbook.Worksheets("Sheet2").Sort.SortFields.Add Key:=Range("D2:D22")
           , SortOn:=xlSortOnValues, Order:=xlAscending, DataOption:=xlSortNormal
      With ActiveWorkbook.Worksheets("Sheet2").Sort
           .SetRange Range("C1:D22")
           .Header = xlYes
           .MatchCase = False
           .Orientation = xlTopToBottom
           .SortMethod = xlPinYin
           .Applv
      End With
      Range("C24").Select
      Selection.Copv
      Range("F2").Select
      Selection.PasteSpecial Paste:=xlPasteValues, Operation:=xlNone, SkipBlanks
           :=False, Transpose:=False
  End Sub
```

Modify the macro to loop

- Two changes:
 - Add a "For...next" loop
 - Each time through the macro, need to store the measure of association
- Currently, copying/pasting measure of association to F2 – looping will make us replace this number each time through
- But, the counter ("i") increases by 1 each iteration – if we paste to cell F(i+1), we will write to a new row each time

Add a loop, record each result

```
Sub MantelTest()
MantelTest Macro
' Conduct a Mantel test on the geographic and genetic distances.
' Keyboard Shortcut: Ctrl+Shift+M
For i = 1 To 1000
    Range("C1:D22").Select
    ActiveWorkbook.Worksheets("Sheet2").Sort.SortFields.Clear
    ActiveWorkbook.Worksheets("Sheet2").Sort.SortFields.Add Key:=Range("D2:D22")
        , SortOn:=xlSortOnValues, Order:=xlAscending, DataOption:=xlSortNormal
    With ActiveWorkbook.Worksheets("Sheet2").Sort
        .SetRange Range("C1:D22")
        .Header = xlYes
        .MatchCase = False
        .Orientation = xlTopToBottom
        .SortMethod = xlPinYin
                                           Select and copy the
        .Apply
                                           Mantel statistic
    End With
    Range("C24").Select
    Selection.Copy 🚽
                                         Select a location to record it
    Range("F" & i + 1).Select
    Selection.PasteSpecial Paste:=xlPasteValues, Operation:=xlNone, SkipBlanks
        :=False, Transpose:=False
Next i
                                         Paste-special the
End Sub
                                         value
```

Run the macro, sort the results

How many exceeded the observed?

We're only interested in whether there was a greater association than observed, so can just look at values bigger than observed (one-tailed test)

2=	F	
8	Sums of products	į
	680, 4899364	
	691 633857	
	694 7970171	
	694,7070141	
	702 5622657	
	703.3632637	
	707.3579128	
<u>8</u> —	/08.6603/44	
	708.7029923	
	709.2008845	
	709.2259746	
9	714.464126	
	716.5807235	
	719.5179922	
1	903.9585579	2
	908.6388034	
	909.1593751	
	909.5246373	
	909.8134634	
	910.7131166	
	912.239676	
	913.8250635	
	914,4788926	
	918,1006404	
	918,1550153	
	921 2731812	
	922,2731012	
9—	922.473072	
	927.1737834	
	932. /133386	
	937.300003	
		Converse de

2	А	6 L	ULF	F	6
27	Observed sum of products	886.388625		729.5221284	이 같은 것 같은 것 같은 것이 같은 것이 같은 것이 같은 것이 같이 같이 많이 많이 많다.
28				729.5840747	
958				882 8188554	
959				883.0791281	
960				885.5101171	Coloulata n
961				886.5968693	
962				886.6395865	
63				886.9566006	
64				887.5672563	
65				887.6931162	
66				888.1998953	
67				888.759341	
68				889.0449391	
69				891.3669924	
70				891.7571737	
71				892.8692841	
72				893.0389275	
73				894.7192509	
74				895.6236515	Number exceeding observed + 1
75				895.8392815	$= n = \frac{n}{n}$
70				096.0020476	- P Number of iterations+1
79				906 4590957	
70				897 1162263	— 7. 19. 19. 19. 19. 19. 19. 19. 19. 19. 19
80				899 7294216	
81				900.0607245	—1997) (1997) - 1997) - 1997) (1997) - 1997) (1997) - 1997)
82				900.2007867	
83				901.6036995	41+1 0.042
84				903.2106488	$p = \frac{1000}{1000} = 1 = 0.042$
85				903.6495732	1000+1
86				903.9585579	
87				908.6388034	
88				909.1593751	
89				909.5246373	Dojact the null there is a (weak
990				909.8134634	Reject the null – there is a (weak
991				910.7131166	but) cignificant accordiation
992				912.239676	Dut) Significant association
993				913.8250635	botwoon agnotic distance and
94				914.4788926	Delween genetic distance and
95				918.1006404	apparanhic distance
96				918.1550153	yeographic distance
197				921.2/31812	
98				922.473072	
99 000				927.1757034	
001				937 300003	
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