Performing Comparisons in BioNumerics



Erik W. Coleman May 2009





Overview

Create a Comparison and Perform a Cluster Analysis

Cluster Analysis Parameters Position Tolerance and Optimization Dice Coefficient with UPGMA Dendrogram Similarity within dendrograms ■ Change the look of the dendrogram Manage Comparisons ■ Save, Open, Delete ■ Cut, Copy, Paste in Comparison windows Print Comparisons Change Settings/Views, Copy to Clipboard Compare One Pattern to Others Compare Two Entries Compare Raw Images





Create New Comparison



Create New Comparison





CDC

Comparisons: View Patterns





Comparisons: Perform Cluster Analysis







Comparisons: Perform Cluster Analysis

Comparison													
File Edit Layout Groups Clus	stering Dimensioning Ba	ndmatching Character:	s Sequence Trend	Data Composite Wir	ndow								
😂 🖯 🎒 🛪 😫	1 1 1 +	PFGE	E-Xbal	💧 🖆 🕼		I	2	111 3	1 1 2	3	111		2
Experiments					_			5995					
🗄 PFGE-Bini 👔 D	endrogram E	xperiment data			Info	rmation	n fields		Simi	laritie	s		
FGE-Spel	8	PFGE-Xbal											
🐔 PFGE-Xbal													
🐮 antibio									PFGE	-Xbal (E)ice (Opl	:1.50%)	(Tol 1.5%-
🐮 biochem 🛛 🛛 P	FGE-Xbal 78.93%					Indou	Kau	LabiD	0		40	60	80 1
📲 test 👘 📲		11.81				muex	ney						
	ſ	44 451			7	1	034292						
		11.111		1000	1	3	034293	TN					(
		1 11	1111 1111		-	4	00-06	TN					
		Û W		101	•	5	00-06	TN					
Г		11 1	11 111	10 11	+	6	034390	TN					
		11			•	7	034559	TN				•	
•		11		11111	•	8	035137	TN				٠	
						9	04-09	TN					•
					*	10	034273	TN					
Resultir	ng Dend	rogram						si	m	la	rity	/ m	natri

Overview

Create a Comparison and Perform a Cluster Analysis <u>Cluster Analysis Parameters</u> Position Tolerance and Optimization Dice Coefficient with UPGMA Dendrogram Similarity within dendrograms ■ Change the look of the dendrogram Manage Comparisons ■ Save, Open, Delete Cut, Copy, Paste in Comparison windows Print Comparisons Change Settings/Views, Copy to Clipboard Compare One Pattern to Others Compare Two Entries Compare Raw Images





Cluster Analysis Parameters

PulseNet Parameters for Cluster Analysis

Comparison settings:

- Dice coefficient
- UPGMA dendrogram
- Position tolerance settings
 - Optimization: 1.50
 - Tolerance setting: 1.50
 - Choose to ignore uncertain bands

		Compari	son settings (Fingerp	rint)	×
		Similarity	y coefficient	Dendrogram type	
n ngs .50		Curve I Pe- Cor Band ba Jac Dic Jef	based: arson correlation sine coefficient ased: ccard ce frey's x	 UPGMA Ward Neighbor Joining Single linkage Complete linkage Advanced Settings 	
ition tolerance	setti	ings		Position tolerances	
Optimization: and comparison Position tolerance:	1.50	*	Uncertain bands Ignore Include	OK Cancel	
Change towards and of fingerprint:	0.00	%			
Minimum height:	0.00	~	ОК		
Minimum surface:	0.00	%	Cancel		



Cluster Analysis Parameters: Position Tolerance

Computer Interpretation of Band Positions

- To the computer a band is not a band, but a band plus a window surrounding the band
- When comparing band positions of two profiles the computer will consider the band position identical if the band position in one of the profiles falls within a window around a band in the other profile
- The size of this window is called the <u>Position</u> <u>Tolerance</u> (set at 1.5% of the run length of the band)







Cluster Analysis Parameters: Position Tolerance Set Too High

The computer will interpret some unique profiles as being identical!

Dice (Opt:1.50%) (Tol 2.0%-2.0%) (H⊳0.0% S>0.0%) [10.8%-97.0%] PFGE-Xbal PFGE-Xbal







Cluster Analysis Parameters: UPGMA



Note! In UPGMA clustering the similarity value at each branching in the dendrogram represents the average similarity of the profiles in the branches





Comparisons: Dendrograms







Comparisons: Dendrograms

PFGE-Xbal PFGE-Xbal	You can also right-click on the branches for additional options, such as to collapse or expand a branch
Here, we have	 718 ECOS COC 719 2005 IL 720 ECOS 721 2005 IL 722 WA WA 723 493-89 724 CB2755 CDC Cluster analysis (similarity matrix) (PFGE-XbaI) Show dendrogram (PEGE-XbaI)
Contapsed time branch Size Name Cluster analysis (similarity matrix) (PFGE-XbaI) Select root Swap branches Reroot tree Collapse/expand branch Calculate error flags Calculate cophenetic correlations Calculate cophenetic correlations Calculate cluster cutoff values Bootstrap analysis Select branch into list	Select root Swap branches Reroot tree Collapse/expand branch Calculate error flags Calculate cophenetic correlations Calculate cluster cutoff values

Select branch into list



Overview

Create a Comparison and Perform a Cluster Analysis Cluster Analysis Parameters Position Tolerance and Optimization Dice Coefficient with UPGMA Dendrogram Similarity within dendrograms Change the look of the dendrogram Manage Comparisons ■ Save, Open, Delete Cut, Copy, Paste in Comparison windows Print Comparisons Change Settings/Views, Copy to Clipboard Compare One Pattern to Others Compare Two Entries Compare Raw Images









đ	BioNur	nerics											
File	e Edit	Database	e Subsets Experiments	Comparison Identification Pu	ulseNet Scripts Wind	low							
100	X 🛐	2	M M Comple	ete view	8 8 4	In		6					
4		0. 10-	10. 10 1					11	~	_			
	4 14	r Va	VA VC III III			_	_	_		-11			
Da	itabase	entries	5			_			_	Exp	eriments	_	
	Index	Key	LabID	SourceCountry	SourceSt -	1 3	234	5 (3		XXA		_
	1	014754		USA	MD	é			^		Name	Type	×
	2	0147		USA	MD					Expe	riments Entry re	elations	
_	3	07-18		USA	VA		٠			Links			
_	4	07-690			FL					File	S		
	5	07-794			FL	•					XXA		
	6	07-828			FL						Nama	Created	Madifier
_	7	07BC		USA	W	•					Name	created	Mudille
_	8	07EN	-							H	K		>
_	9	07EN	Vou car	v manado v	our					Con	marieone		
_	10	07EN		i manaye y	our		•			Con	iparisons	_	
-	11	08-084	compar	isons in the	e		•			13	> 🗡 🕺 🕅	I	
-	12	08-35	"Compo	ricone" wi	ndow						Name	Created	Modifie
-	13	08-70		a1150115 WI	nuow.						2007	2008-09-25 14h01r	n2 2008-09-251
-	14	08-70	Create	New: 🔼							2008	2008-09-25 14h01n	n4 2008-09-251
-	10	0000	Onon				•						
				<u> </u>									
			Delete:	X									
VICES-US			Soorah	44									
			Search:	ana									



- If you want to add patterns to a comparison window: Click "Copy selection" in main window or another comparison
 - window
- Click "Paste selection..." in comparison window





If you want to take patterns out of a comparison window: Select the patterns Click "Cut selection..." in comparison window Click "OK"

🖪 2008 (Comp	parison)							-
File Edit Layou	t Groups Clustering Di	mensioning Bandmat	ching Characters	Sequenc	e Trendi	Data Co	mposite	Window
<i>2</i>		<u>} 🕇 🕂 🖂</u>	PFGE	-Xbal			년 100 99	×
Experi	Cut selection fi	om comparison						
PFGE-Bini	👔 Dendrogr	Experiment dat	a	Info	ormation	fields		
PFGE-Spel		PFGE-Xbal						
🚰 PFGE-Xbal								
📫 antibio								
i biochem				-	Indou	Kau	LahiD	
💡 test					Index	пеу	Lann	
			1 11111	- I	4	01E0		
					5	03X0		
	· •				6	07-03		
				•	7	07-180		
			1 101 111 1	181 ->	8	07-271		
Groups			1 1 1 1 1 1		9	07-287		
Size Nat					10	07-579		
		11			11	07-65		
0					12	07-65		
0					13	07-65		
0					14	07-65		
0 🗸				1	15	07-65		





OK

Are you sure you want to remove the current selection from this comparison?

Cancel

Comparisons: Print



Comparisons: Print

Comparisons: Arrange by Serotype

Comparison			
File Edit Layout	Groups Clustering Dimensioning Bandmatching Seq		
	× \$% \$_ \$ \	1 99% ***	
Ś	PFGE-Xbal	95 entries	
		•Se	protype Outbreak odc.id
		🔿 Ty	phimurium Arrange entries by field (numerical)
		He He	eidelberg Set database field length
	1 1 3414 33 311	Ha Ha	idar Freeze left pane
		He	Idelberg Create groups from database field
			nbinurium
		→ Tv	phinurium
		🗢 En	teritidis
1		🔿 Mir	
		⇒ Ja ⇒ Ty ⇒ Pa	Right-click on "Serotype"
		🗢 Ty	📲 and choose "Arrange 🔰 🗖
	and there is a	En	teri
		Ja Ja	🗒 entries by field"
		Su	
		⇒ Pu	
		🔿 Pa	ratyphi B
		🗢 Ту	phinurium
	<	> 🗢 <	
PFGE-Xbal	NOTE: Arrange b	y serc	otype to see clusters more
1	easily before crea	ating	dendrogram

Overview

Create a Comparison and Perform a Cluster Analysis Cluster Analysis Parameters Position Tolerance and Optimization Dice Coefficient with UPGMA Dendrogram Similarity within dendrograms ■ Change the look of the dendrogram Manage Comparisons ■ Save, Open, Delete Cut, Copy, Paste in Comparison windows Print Comparisons Change Settings/Views, Copy to Clipboard Compare One Pattern to Others Compare Two Entries Compare Raw Images

🖪 2008 (Comparison)						_ P X
File Edit Layout Groups Clustering Dimensioning Bandmatching Characters	s Sequence TrendData Composi	te Window				
🖙 🖶 🎒 🗙 🗱 👔 🚉 🕇 🗍 💌 🐋 🛛 PFGE	E-Xbal	100× 100× 100× 10	1 🎸	s III 🗠		<u>8</u>
Experiments	\sim	Arrange by decreasi	ng similari	ty		
PFGE-Bini Dendrogram Experiment da	ta 🔰	Informati	on field	s	Similarities	
PFGE-Spel	\sim					
PFGE-Xbal						
🕂 antibio						
E biochem					_	
		Index	Key	LabID	-	
		→	1 07-65		100.0	^
Slick on "Arrange by			2 07-65		100.0	≡
			3 07-65		100.0	_
ecreasing similarity —			4 07-65		100.0	
			5 07-65		100.0	
compare the selected			7 07 65		100.0	
			8 07-65		100.0	
attern to all others within			9 07-65		100.0	
			10 07-65		100.0	
he comparison window			11 07-65		97.6	
			12 07-65		95.2	
			13 2007		92.7	
			14 EC08-		92.7	

🖻 2008 (Comparison)			
File Edit Layout Groups Clustering Dimensioning Bandr	natching Characters Sequence TrendData Composite W	/indow	
🚔 🖬 🗁 🛪 🔱 😩 🕇 🖊	🗻 🛌 PFGE-Xbal 🛕 🖆 💵	🐜 🏭 🕰 ី 🐇 🕍	
Experiments	Arra	nge by decreasing similarity	
💷 PFGE-Bini 💿 Dendrogram	Experiment data	Information fields	Similarities
II PFGE-Spel	PFGE-Xbal		
Y PFGE-Xbal	_		
antibio			
-			
Now your patterns		Index Key LabiD	
Now, your patterns		➡ 1 07-65	100.0
are arranged by		2 07-65	100.0
are arranged by		3 07-65	
docroasina		4 07-65	1000 II% Similarity
decreasing		5 07-65	100.0
similarity to the		7 07 65	100.0
Similarity to the		8 07-65	100.0
nattern vou		9 07-65	100.0
pattern you		10 07-65	100.0
selected		11 07-65	97.6
		12 07-65	95.2
		13 2007	92.7
		14 EC08	92.7

Comparisons: Compare Two Entries

1. Select two isolates in your database to compare

æ	BioNun	nerics												
File	e Edit I	Database	Subsets	Experiments	Comparison	Identification	PulseNet	Scripts	Windov	w				
Image: Solution of the second seco			e Load com Create no Delete co Comparis Alignmen	parison ew comparison mparison on list ts	Alt+C	, , ,	(]	1 2	34	5 6	<u> </u>			
+	1	07-65		5	Compare Analyze v	two entries with GeneMaths.	Ctrl+Al	t+C		-	•	_	^	
1	3	FL 352			Chart / S	tatistics		2 5	مام	ct				
	4	0001			USA					UL				
	5	0001			USA			'Co	mp	Dar	'e			
	7	0160			USA					1 m i .	~~	,, L		
	8	07-03			USA		U	.wo	en	UT I	es		IOIII	i
	9	07-180			USA			com	าทอ	ris	50	n n	neni	U
	10	07-271			USA				<u>. b a</u>					
	11	07-287			USA		1	FL	•	•	•			
	<								>	•	•		~	-
All	levels													
	Database:	Ecoli-clie	nt 8114 e	ntries 6 exp	eriments Vico	dc\project\CCID_	NCZVED_E	FBMD_P	ulseNet/E	DataVEc	coli-cli	ent		

Comparisons: Compare Two Entries

Also called a Pairwise comparison or 2x2 comparison

Comparisons: Compare Two Entries

A REAL PROPERTY OF THE PROPERT

Shows matching bands and non-matches

