



a Bitlab software

# **Association Rules collaborative tool**

Integrated suite for association rule discovering in medical and molecular data

# **User Manual**



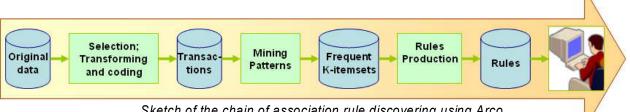
Version v1: 8<sup>th</sup> November 2007. On-line updated information available at: <u>http://chirimoyo.ac.uma.es/arco</u>

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# **ARco** pipeline

As described in the Introduction section, Arco has been organised to fulfil the KDD procedure integrating a diverse gallery of methods with different but combined scope. At the end, or as one important part of KDD, we devise ARco that should take place in the data selection, transforming, processing and high level analysis, including visualization (for human analysis) of the new expressed knowledge in the form of association rules or the co-occurrence of events from which is possible to produce a conclusion with certain degree of confidence. Next picture depict a sketch of this chain as we see it.



Sketch of the chain of association rule discovering using Arco

First step in this chain is the selection of the data relevant to be subject of analysis. Over this selected dataset is necessary, in general, operate on it to focus the processes in particular features. Data transformations, reduction and compacting, hierarchical simplification, diverse alternative coding procedures, etc. are important procedures in this step. A collection of transactions in the form of a list of numbers that represent events that co-occur simultaneously is the resulting output. This output is the input to identify k-itemset (set of "k" items appearing together more frequently than expected by chance). From these frequent k-itemsets it is possible infer rules with certain confidence (estimated from the dataset).

## Steps

ARco is endowed with different algorithms to be applied on the same data set in pipeline fashion. This guided tour will shown each of these procedures, in the following order:

- a) Installation guide
- Load Step which includes filtering and transforming data to produce a transaction dataset b)
- Mining transactions to identify frequent k-itemsets c)
- Ruling the frequent k-itemset to produce rules d)
- e) Analysis procedures.

# **ARco installation guide**

Java support has been chosen with the aim to extend the scope of ARco. Installing a Java virtual machine available for most of the current operating systems is enough to have a full operative environment

# **System Requirements**

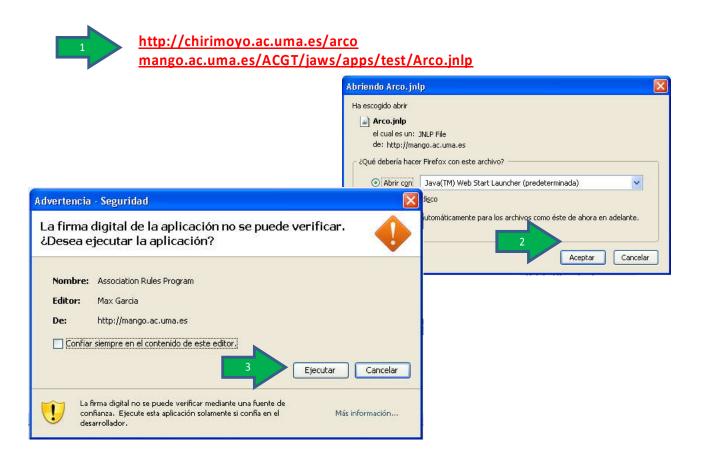
- Java virtual machine 1.50 or latter
- Last version of ARco software

#### Java virtual machine



#### **Download ARco**

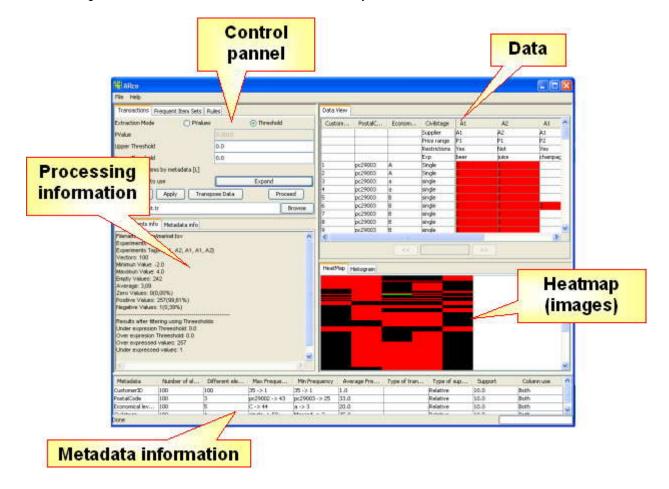
# from http://chirimoyo.ac.uma.es/arco



Note: Since ARco manuscript is in the evaluation process, the software is only available upon request.

# ARco main screen

**ARCO** is organised in five frames, each one with the ability to contain several sub-tabs



The most important is the "Control Pane" in which the main ARco options are available and parameters are settled. The "Data" frame contains original and processed datasets (i.e. gene-expression matrix or association rules). Below the control pane, one frame is devoted to display summarised information about data processing; and also have a tab for graphical displaying of rules. Heatmap frame contains different data representations and on the bottom specific information about selected data sets are provided.

Frame re-sizing is available

# Icons glossary

Common elements are used in ARco with the same behaviour in different contexts:

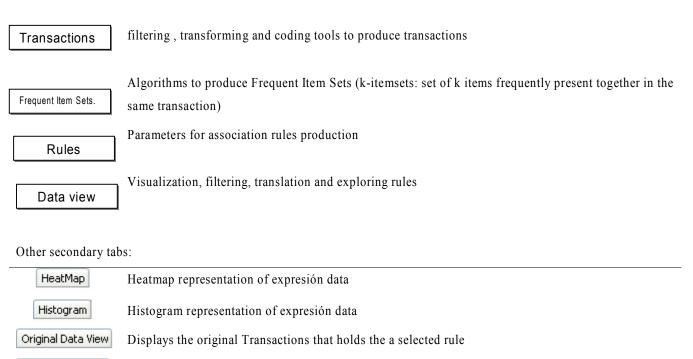
Load	Load button: Used to upload a data file: gene-expression data in the Transaction tab, a Transactions datafile in the "Frequent itemset tab"; and frequent itemset datafile in the Rules Tab
Browse	Browse button: Used to "save" files : transactions, frequent itemsets or rules depending on the tab.
Expand	Expand button: Displays the advanced options in the "transactions generation" tab.
Proceed	Proceed button: Launch the corresponding process.
<< >>	Next / Previous buttons: browse and surfing the multiple-pages tables.

# **ARco organization:**

Tabs: ARco is organised in four main modules; the natural steps in association rule discovering: procedures:

- 1. Data manipulation to produce a set of transactions to be mined
- 2. Finding frequent itemsets in the transactions file
- 3. Produce association rules
- 4. Browsing and exploring results

Following these steps the Control Pane has the next tabs or sub-sections:



Visualization Panel Rule profile display

Info Tabs Different informative tabs associated with a given action

# From original data to Transactions

This section contains the Control Pane with the working options and needed parameters. It contains filtering parameters, items selection and transformation; metadata identifiers, etc.

Transactions Frequent Item	Sets Rule:	s
Extraction Mode (	) PValues	<ul> <li>Threshold</li> </ul>
PValue		0.1
Upper Threshold		0.0
Lower Threshold		-0.0
Replace items by metadat	a [L]	
Show columns to use		Expand
Load Apply	Transpo	ose Data Proceed
C:\tmp2\kobdat\kob.tr		Browse

► Parameters

Extraction Mode	Used to transform expression values into 3-state elements: over- and under-expressed and not
	differentially expressed.
	Two methods are available: Thresholds (under- and over- ) and p-values
pvalue	Maximum p-value to set an expression value as differentially expressed (required when using the p-
	value extraction mode).
	Under this option, the pvalue associated to each expression ratio will be computed from the z-scores
	(normalised ratios, with mean zero and standard deviation 1)
Upper Threshold	Over-expression threshold. Minimum expression value to be set as over-expressed (required when
	using the <i>threshold</i> extraction mode)
Lower Threshold	Under-expression threshold. Maximum expression value to be set as under-expressed (required when
	using the <i>threshold</i> extraction mode)
Relpace items by	Instead of including the item-ID in a transaction, it is replaced with the experiment metadata (sample
metadata [L]	or column metadata).
Apply	Perform the data filtering (using the extraction mode and associated parameters) and up-dates the
	corresponding images.
Transpose Data	Transpose the matrix (row-columns interchanging). Obviously it includes metadata.

Proceed

Generate transaction from filtered data.

Advanced options are displayed when click on expand button

Column ID	Exp	*
Row ID	#ORF	*
Row Metadata	Columns	
🖌 #ORF	🔽 Ex263	
Hierarchical	🔽 Ex264	
🔽 Genes	🔽 ex265	
▼ ×	💌 Ex266	
🗹 у	💌 Ex267	
	🔽 Ex268	
	🔽 Ex269	
	💌 ex270	

Column ID E	Experiment, sample	or column identifier
-------------	--------------------	----------------------

Row ID Gene or row identifier

In the main body of the dialog box, row and column metadata can be activate/inactivate to participate in the mining procedure.

# **Frequent Item Set tab**

Frequent k-itemset production procedure is controlled from this tab. Main parameter are: Support (number of transactions containing a given k-itemset); maximum k value and algorithm.

Transactions Frequent Item Sets	Rules	
Algorithm	💿 Borglet	O Ard
Support Type	() Absolute	Relative
Support Mode	🚫 Unique	<ul> <li>Multiple</li> </ul>
Minimal number of items	1	
Maximal number of items	5	
Minimal support	10.0	
Maximal support	100.0	
Multiple supports		Expand
Load		Run
C:\tmp2\kobdat\kob.fis		Browse

Algorithm	Two options are available:
	Extended (variable support) Borgelt proposal (http://www.borgelt.net/apriori.html)
	Rodriguez et al. (http://www.biomedcentral.com/1471-2105/7/54)
Support Type	In absolute value (number of transactions) or relative percentage.
	When working with multiple supports (by item support) this parameter must be specified for each
	different item.
Support Mode	Unique: the same support for all items
	Multiple: specific support for each item
Minimal number	Minimal k value
ofitems	
Maximal number	Maximum k value
ofitems	
Minimal support	Available for Unique support
Maximal support	Available for Unique support

These options and parameters are needed to produce frequent k-itemset with general support. If individual supports are needed for each item we can use the  $\boxed{\text{Expand}}$  button.

Name	Min support	Max support	Support Type	
Hierarchical	10.0	100.0	Relative	*
Genes	10.0	100.0	Relative	*
×	10.0	100.0	Relative	*
У	10.0	100.0	Relative	*
[+Ex263]	10.0	100.0	Absolute	*
[+Ex264]	10.0	100.0	Absolute	*
[+ex265]	10.0	100.0	Absolute	*
[+Ex266]	10.0	100.0	Absolute	*
Execute 21	10.0	100.0	Abaababa	

All the item labels are displayed and a dialog box can be used to set individual supports both, modes and values. A table with the following parameters is available:

Name	Item-label (it can correspond to an item, an item metadata or sample metadata).
Min support	Minimum support for this item
Max support	Maximum support for this item
Support Type	Absolute (number of transactions) or relative as percentage.

All values can be modified at the same time using right button functionality. Fir instance, to set to "Absolute" all the Support-type you can click right button over any cell in the "Support-type" column (the same is valid for support values).

#### **Rules Tab**

Option and parameter related with rule production

Transactions Frequent Item Sets Ru	es
Confidence	50.0
Improvement	1.0
Minimal consecuent size	1
Appearance	Expand
Load	Run
C:\tmp2\kobdat\kob.rul	Browse

Confidence Minimum rule confidence: rule reliability of X => Y in T is the ratio of the # of transactions in T containing X that also contain Y, versus total # of transactions in T containing X to produce a rule Minimum Improvement Minimal How many items in the consequent side

By default, any element can be at any place in the rule (antecedent or consequent side). Positional

restrictions can be established for each item-type to be in the antecedent, in the consequent, in both or not to be in the rule.

Hierarchical	🚫 Ant.	🚫 Con.	💿 Both	🚫 None
Genes	🚫 Ant.	🚫 Con.	💿 Both	🚫 None
×	🚫 Ant.	🚫 Con.	💿 Both	🚫 None
У	🚫 Ant.	🚫 Con.	💿 Both	🚫 None
[+Ex263]	🚫 Ant.	🚫 Con.	💿 Both	🚫 None
+Ex264]	🚫 Ant.	🚫 Con.	💿 Both	🚫 None
+ex265]	🚫 Ant.	🚫 Con.	💿 Both	🚫 None
+Ex266]	🚫 Ant.	🚫 Con.	💿 Both	🚫 None
+Ex267]	🚫 Ant.	🚫 Con.	💿 Both	🚫 None
+Ex268]	🚫 Ant.	🚫 Con.	💿 Both	🚫 None

Ant. This data type can only be in the antecedent side of the rule

Con This data type can only be in the consequent side of the rule

Both This data type can be both in the antecedent or consequent side of the rule

None Rules with this datatype are discarded

## Data View tab

It becomes available when a data file has been loaded. A table-style is used to display the data set highlighting the cells involved in a transaction production. Some data manipulation tools are available on rightbutton functionality clicking over the column to be modified.

Data View												
#ORF	Hierar	Genes	х	У	170	153	167	186	188	165	175	
	1 1			Height	170	153	167	186	188	165	175	
				Age	32	22	12	21	11	22	55	
				Gender	Male	Female	Female	Female	Male	Male	Female	
				Exp	Ex263	Ex264	ex265	Ex266	Ex267	Ex268	Ex269	1
BG10065	1.2.3 , 2 0	dnaA, dn	1,44	1	-0.550197	10.133	-0.838249	0.0687128	168.182	-134.104	-116.993	
BG10066	1.2.4 , 2 0	dnaN, dn	2,4	1	-0.499571	181.876	Empty	-0.563901	-0.403897	-207.039	-1.822	
BG10077	1.2.3 , 2 9	serS	12	1	0.286304	0.910733	-112.553	0.82852	0.906891	-103.953	-117.754	
BG10078	1.2.4 , 2 0	dck, yaaF	13	1	0.555215	102.975	o	0.347165	-0.765535	-193.587	-119.265	
BG10081	1.2.3 , 2	yaaI	16	1	-168.281	-0.165249	13.516	-118.488	0.247438	-107.039	-0.631355	
BG10100	1.2.4 , 2 a	abrB, cpsX	36	1	-0.519818	-138.466	0.391579	-0.405712	-0.708446	0.930876	0.10276	
BG11565	1.2.3 , 2	ybbA	28	3	-0.670692	0.0718929	-0.289507	-217.856	-0.396517	-1	-0.10188	
BG10837	1.2.4 , 2 1	feuC	29	3	-0.0888093	0.367329	-120.256	-154.649	-168.407	-235.908	-0.135655	
BG10836	1.2.3 , 2 1	feuB	30	3	0.680063	0.64372	-0.698406	-0.969838	0.147104	0.451989	-0.0107264	
BG10833	1.2.4 , 2	ybbC, yzbB	33	3	-141.504	0.0844746	-0.428843	-199.035	-223.704	-112.873	-0.300124	
BG10832	1.2.3 , 2	ybbD, yzbA	34	3	0.294103	-0.563901	-0.0239789	0.159513	-0.744936	-0.150448	-0.00898179	ī
BG11566	1.2.4 , 2	ybbE	35	3	-0.173016	-0.379237	-0.441705	-0.812067	-192.254	-0.471143	-0.0889005	
BG11567	1.2.3 , 2	ybbF	36	3	0.275634	-0.427862	-0.259387	-0.508791	-0.657475	-0.337695	-0.0313155	
BG11569	1.2.4 , 2	уЬЬН	37	3	-0.811143	-0.572694	-0.409185	-110.815	-0.805781	-0.35973	-0.51	1
BG11571	1.2.3 , 2 )	уbbJ	39	3	-159.516	-0.613583	-0.415037	-122.408	-119.265	-0.89743	-0.467126	1
BG11572	1.2.4 , 2	уЬЬК	40	3	0.129283	-0.13493	-0.216423	-0.298179	0.165285	-0.171046	-0.440216	
BG10166	1.2.3 , 2 a	adaA	48	3	0.196397	0.521835	-0.76356	-179.564	-209.311	-182.716	-0.245112	ľ
BG10167	1.2.4 , 2 (	adaB	49	3	0.257158	104.439	-0.571157	-117.544	0.456378	-0.163499	-0.125531	l
BG10949	1.2.3 , 2 1	ndhF, ybxE	50	3	-0.395138	0.246161	-0.90092	-224.236	-217.864	-204.731	-0.337035	
<											>	j

Triming	Keeps the first or last 'n' characters
Hierarchic	Reduce the deep-level value in a hierarchical codification
Interval Equi-Depth	Identify 'n' different groups with equal number of elements (equalization). Valid for numerical
	data)
Interval Equi-Width	Produce "n" different groups with the same range size. Require min and max values and interval
	size
Undo Transformation	Un-do the last transformation
Reload Column	Un-do all transformations performed on a given column (re-load original values)

Annexe 1 contains detailed information for data transforming procedures

# Frequent Items Sets (Visualization) tab

Displays the frequent item sets. It can be explored and ordered by the item support (absolute or relative)

Set	Support	Number of transactions	
[-ex274]	1,80	13,00	
[-Ex264]	2,00	14,00	
[+ex273]	2,40	17,00	
[+ex285]	2,00	14,00	
[+ex270]	2,10	15,00	
[-ex279]	3,70	26,00	
[+ex272]	2,70	19,00	
[-E×267]	2,10	15,00	
[+ex286]	2,40	17,00	
[+ex280]	4,40	31,00	
[+ex283]	3,10	22,00	
[+ex276]	3,40	24,00	
[+ex284]	4,70	33,00	
[+ex279]	6,80	48,00	
[-Ex268]	4,90	35,00	
[-ex270]	5,20	37,00	
[-Ex266]	11,00	78,00	
[+ex283] [+ex286]	2,10	15,00	
[-Ex266] [-Ex268]	2,80	20,00	
[-Ex268] [-ex271]	3,20	23,00	
[-Ex266] [-ex270]	2,30	16,00	
[-ex270] [-ex271]	4,10	29,00	
[-Ex266] [-ex271]	8,10	57,00	
[-Ex266] [-Ex268] [-ex271]	2,10	15,00	

## Rules (Visualization) tab.

Tab used to display rules. Rules can be ordered by any of their numeric columns.

Antecedent	Consecuent	Confidence	Support	ABS Support	Coverage	Improvem	Leverage	Conviction	Entropy	RuleID	
[+181]	[-155]	78,16	9,60	68,00	12,29	1,79	4,22	257,40	0	0	
+186]	[-186]	56,10	9,75	69,00	17,37	1,22	1,77	123,22	0	1	
-170]	[-186]	88,24	12,71	90,00	14,41	1,92	6,10	459,82	0	2	
+181]	[-186]	73,56	9,04	64,00	12,29	1,60	3,40	204,62	0	3	
-176]	[-155]	52,94	5,08	36,00	9,60	1,21	0,88	119,46	0	4	
-176]	[-188]	62,90	5,51	39,00	8,76	2,93	3,63	211,69	0	5	
-196] [-176]	[-155]	90,00	5,08	36,00	5,65	2,06	2,61	562,15	0	6	
-155] [-176]	[-196]	80,00	5,08	36,00	6,36	3,06	3,42	369,35	0	7	
-176]	[-186]	72,58	6,36	45,00	8,76	1,58	2,34	197,29	0	8	
-196]	[-155]	89,73	23,45	166,00	26,13	2,05	12,01	547,35	0	9	
-155]	[-196]	53,55	23,45	166,00	43,79	2,05	12,01	159,03	0	10	
-186] [-176]	[-155]	91,11	5,79	41,00	6,36	2,08	3,01	632,42	0	11	
-155] [-176]	[-186]	91,11	5,79	41,00	6,36	1,98	2,87	608,58	0	12	
-176]	[-186]	57,35	5,51	39,00	9,60	1,25	1,10	126,85	0	13	
-165]	[-155]	91,48	22,74	161,00	24,86	2,09	11,86	659,59	0	14	
-155]	[-165]	51,94	22,74	161,00	43,79	2,09	11,86	156,33	0	15	
-188]	[-155]	80,92	17,37	123,00	21,47	1,85	7,97	294,64	0	16	
-165]	[-196]	64,77	16,10	114,00	24,86	2,48	9,61	209,70	0	17	
-196]	[-165]	61,62	16,10	114,00	26,13	2,48	9,61	195,79	0	18	
-188]	[-196]	66,45	14,27	101,00	21,47	2,54	8,66	220,16	0	19	
-196]	[-188]	54,59	14,27	101,00	26,13	2,54	8,66	172,96	0	20	

Clicking a given rule, all transactions that hold the rule are highlighted in the "Data frame".

Different filters are available

E=>E	Experiment – Experiment rules (only expresión values)
E => M	Experiment values (antecedent) implies a Metadata (consequent)
M=>E	Metadata in the antecedent and experiment value in the consequent
M => M	Metadata – Metadata rules
Show all	Show all rules
Filters	Advanced filters
Hide trivials	Remove trivial rules. A rule is <b>trivial</b> if there is another rule with the same Right-Hand-Side and a subset of the Left-Hand-Side that covers exactly the same cases from the data set. For example, the first of the two rules below is trivial because it has the same coverage as the second. Adding Tomatoes to the LHS of the second rule does not affect it.
	Lettuce & Tomatoes -> Cucumber [Coverage=0.250 (250); Support=0.239 (239); Strength=0.956; Lift=2.91; Leverage=0.1568 (156)]
	Lettuce -> Cucumber [Coverage=0.250 (250); Support=0.239 (239); Strength=0.956; Lift=2.91; Leverage=0.1568 (156)]
	If a rule is trivial then it will have the same support, strength, lift, and leverage as the rule with respect to which it is trivial.
	(see http://www.rulequest.com/MOfiltering.html)
Hide unproductive	Unproductive rules. A rule is <b>unproductive</b> if there is another rule with the same Right-Hand-Side and a subset of the Left-Hand-Side that has equal or higher strength. For example, the first of the rules below is unproductive because it has lower strength than the second. Adding Promotion1=f to the LHS of the second rule decreases its performance.
	Profitability99 < 419 & Promotion1=f -> Spend99 < 2030 [Coverage=0.274 (274); Support=0.248 (248); Strength=0.905; Lift=2.72; Leverage=0.1568 (156)]
	Profitability99 < 419 -> Spend99 < 2030 [Coverage=0.333 (333); Support=0.302 (302); Strength=0.907; Lift=2.72; Leverage=0.1911 (191)]
	If a rule is unproductive then it will have the same or worse support, strength, lift, and leverage as the rule with respect to which it is unproductive.
	(see <u>http://www.rulequest.com/MOfiltering.html</u> )
Custom Filter	Customised filter

Customised filters allow combining different requirements to filter the rules. In the available dialog-box several criterions can be used at the same time (confidence, support, coverage, etc.) and minimum and maximum values must be specified for each criterion. Output is stored in a file

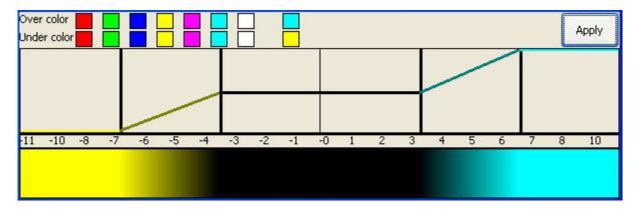
	Min	Max
	0	100
Support Relative	0	100
Support Absolute	0	100
Coverage	0	100
Improvement	0	100
Leverage	0	100
Conviction	0	100
Output Filename		

#### Heat-Map tab

This frame is used to display a visual representation of gene expression values in the form of a coloured matrix. Traditionally expression values have been represented using red for over-expression and green for underexpressed genes. The colour scale also includes a "black" range for values (log2 ratios) close to zero, and red and green scale for different values, including a saturation point from which all the values receive the same colour.

Image can be saved to disk using right-button: "Save image" functionality.

The colour palette and saturation points are customisable. Right-button: Colours Palette

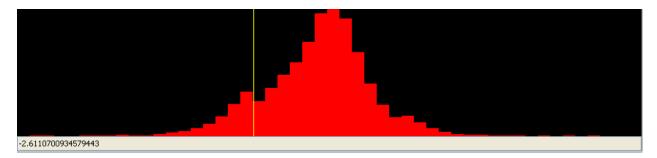


Over and under- colours are used for over-expressed and under-expressed genes. Changes affect Data view representation

In the main body there are 4 vertical lines that can be horizontally moved to define the "non differentially expressed range –around log ratio equal cero)" and under / over expressed points at which the signal become saturated (al values at the left in the under-expression side or all values on the right of the saturation points are coded with the same colour).

#### Histogram tab

Histogram of gene-expression values (original data).



Numerical values are shown on the bottom bar when the mouse moves over the image.

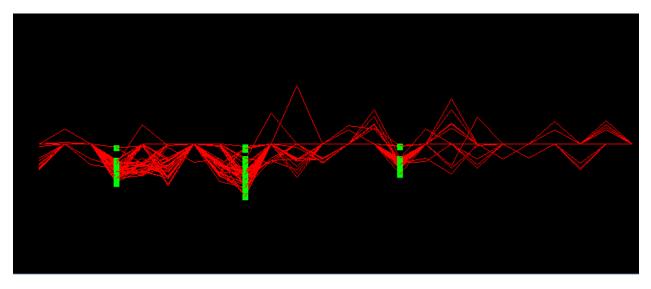
## **Original Data View tab**

This frame is used to display the transactions that hold the rule (selected rule) and only will be available after the rule selection event.

#ORF	Hierarchical	Genes	x	У	170	153	167	186	188	165	
				Height	170	153	167	186	188	165	17
				Age	32	22	12	21	11	22	55
				Gender	Male	Female	Female	Female	Male	Male	Fe
			Exp	Ex263	Ex264	ex265	Ex266	Ex267	Ex268	E:	
BG10081	1.2.3 , 2.3.5	yaaI	16	1	-168.281	-0.165249	13.516	-118.488	0.247438	-107.039	-C
3G10833	1.2.4 , 2.3.7	ybbC, yzbB	33	3	-141.504	0.0844746	-0.428843	-199.035	-223.704	-112.873	-C
3G11571	1.2.3 , 2.3.8	убЬЭ	39	3	-159.516	-0.613583	-0.415037	-122.408	-119.265	-0.89743	-C
BG12711	1.2.3, 2.3.10	ybcL	56	3	-170.044	0.274507	-0.303781	-213.993	-196.963	-247.249	-C
BG11504	1.2.4 , 2.3.12	csgA	12	4	-119.265	0.539159	0.0	-198.793	-147.089	-0.793549	-C
3G10173	1.2.4 , 2.3.19	ycxB	30	6	-147.732	0.0792633	-0.053638	-188.604	-124.691	-0.527247	-C
3G12053	1.2.3 , 2.3.21	ydaE	31	7	-196.963	0.184233	138.215	-12.555	-0.406424	-135.669	-C
BG12067	1.2.3 , 2.3.22	ydaT	49	7	-119.465	0.12063	116.046	-148.843	0.201634	-144.057	-C
3G12804	1.2.3, 2.3.30	ydjN	46	10	-130.812	0.461179	0.571313	-167.807	-0.464963	-133.985	-0
3G12841	1.2.3 . 2.3.33	verO	27	11	-129.399	-0.31034	-0.304855	-139.734	10.889	0.0687128	-0 🔪
<											>

### Visualization tab

For E-E rules, displays the gene-expression profile (or the sample-profile for transposed matrices) with red lines; and the experiments that hold the rule (green boxes)

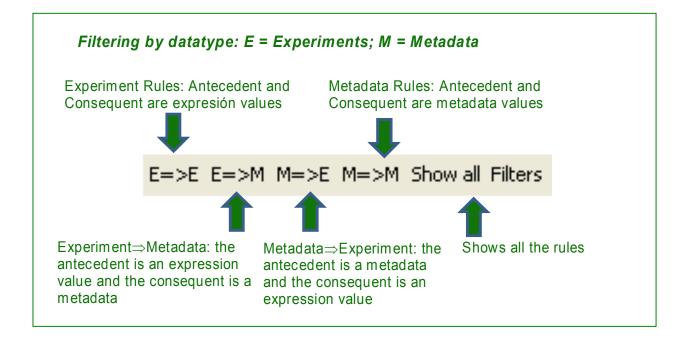


Options to modify the representation are available on right-buttom: "Change View"

Show backgroundgrid	Displays a grid
Show all profiles	OFF: displays the gene-expression-profile of those genes holding the rule.
	ON: displays all the gene-expression profiles as a background image, the gene-expression profile
	of those genes holding the rule coloured in the foreground and the green boxes for items
	involved in the rule
Draw lines/Draw dots	Displays only the green-boxes or also draws a "rule profile" (joint with a line all the points)

## Filtering rules

Antecedent	Consecuent	Confidence	Support	ABS Support	Coverage	Improvement	Leverage	Conviction	Entropy	RuleID	
[Economical le	[PostalCode.2	66,67	16,00	16,00	24,00	2,08	8,32	204,00	0	0	
[PostalCode.2	[Economical le	50,00	16,00	16,00	32,00	2,08	8,32	152,00	0	1	
[Economical le	[PostalCode.p	61,36	27,00	27,00	44,00	1,43	8,08	147,53	0	2	
[PostalCode.p	[Economical le	62,79	27,00	27,00	43,00	1,43	8,08	150,50	0	3	
[Economical le	[PostalCode.p	61,90	13,00	13,00	21,00	2,48	7,75	196,88	0	4	
[PostalCode.p	[Economical le	52,00	13,00	13,00	25,00	2,48	7,75	164,58	0	5	
[PostalCode.2	[Civilstage.ma	53,13	17,00	17,00	32,00	1,15	2,28	115,20	0	6	
[PostalCode.p	[Civilstage.sin	55,81	24,00	24,00	43,00	1,12	2,50	113,16	0	7	
[Economical le	[Civilstage.ma	70,83	17,00	17,00	24,00	1,54	5,96	185,14	0	8	
[Economical le	[PostalCode.2	76,47	13,00	13,00	17,00	2,39	7,56	289,00	0	9	
[PostalCode.2	[Economical le	76,47	13,00	13,00	17,00	3,19	8,92	323,00	0	10	
[PostalCode.2	[Civilstage.ma	81,25	13,00	13,00	16,00	1,77	5,64	288,00	0	11	
[Civilstage.sin	[Economical le	50,00	25,00	25,00	50,00	1,14	3,00	112,00	0	12	
[Economical le	[Civilstage.sin	56,82	25,00	25,00	44,00	1,14	3,00	115,79	0	13	
[PostalCode.2	[Economical le	66,67	10,00	10,00	15,00	1,52	3,40	168,00	0	14	
[PostalCode.2	[Civilstage.sin	71,43	10,00	10,00	14,00	1,43	3,00	175,00	0	15	
[+champagne]	[PostalCode.2	57,14	32,00	32,00	56,00	1,79	14,08	158,67	0	16	
[PostalCode.2	[+champagne]	100,00	32,00	32,00	32,00	1,79	14,08	Infinity	0	17	
[+beer]	[PostalCode.p	64,00	16,00	16,00	25,00	2,56	9,75	208,33	0	18	
[PostalCode.p	[+beer]	64,00	16,00	16,00	25,00	2,56	9,75	208,33	0	19	
Economical le	[PostalCode.p	60,00	15,00	15,00	25,00	1,40	4,25	142,50	0	20	
PostalCode.p	[Economical le	62,50	15,00	15,00	24,00	1,42	4,44	149,33	0	21	
[PostalCode.p	[Civilstage.sin	55,56	15,00	15,00	27,00	1,11	1,50	112,50	0	22	
[PostalCode.2	[+wine High Q]	100,00	32,00	32,00	32,00	1,33	8,00	Infinity	0	23	
Economical le	[Civilstage.ma	52,38	11,00	11,00	21,00	1,14	1,34	113,40	0	24	
	F	100.00	05 00	05.00		le or	r. 00		6	05	_
.=>E E=>M M=	=>E M=>M Shov	v all Filters		<<	[0 - 306				>	>	



### Filtering by values

	E=>E E=	>M M=>E M=>M Sho	w all Filters
Custom filter			Hide Trivials Hide Unproductive
	Min	Max	Custom Filter
	0	100	
Support Relative	0	100	
Support Absolute	0	100	
Coverage	0	100	
Improvement	0	100	
Leverage	0	100	
Conviction	0	100	
Output Filename C:\gu	uia\market[0].rul		
Accept		Cancel	

#### Set filtering parameters

	Min	Max		
	0	100		
Support Relative	0	100		Maximun and
Support Absolute	0	100		minimum parameter
Coverage	0	100	2	value
Improvement	0	100		
Leverage	0	100		
Conviction	0	100		
Output Filename C:\gu	uia\market[0].r	ul		File pathname to
Accept		Cancel	3	store filtered rules



# Visualization of transactions that hold the rule

Antecedent	Consecuent	Confidence	Support	ABS Sup	Coverage	Improve	Lever	Conviction	Entropy	RuleID	
[Economical level(ABCD).D]	[PostalCode.29001]	66,67	16,00	16,00	24,00	2,08	8,32	204,00	0	0	~
[PostalCode.29001]	[Economical level(	50,00	16,00	16,00	32,00	2,08	8,32	152,00	0	1	
[Economical level(ABCD).C]	[PostalCode.pc29	61,36	27,00	27,00	44,00	1,43	8,08	147,53	0	2	
[PostalCode.pc29002]	[Economical level(	62,79	27,00	27,00	43,00	1,43	8,08	150,50	0	3	
[Economical level(ABCD).B]	[Posta 1 .pc29	61,90	13,00	13,00	21,00	2,48	7,75	196,88	0	4	1
[PostalCode.pc29003]	[Econd level(	52,00	13,00	13,00	25,00	2,48	7,75	164,58	0	5	-
[PostalCode.29001]	[Civils arried]	53,13	17,00	17,00	32,00	1,15	2,28	115,20	0	6	
[PostalCode.pc29002]	[Civilstays.single]	55,81	24,00	24,00	43,00	1,12	2,50	113,16	0	7	
[Economical level(ABCD).D]	[Civilstage.married]	70,83	17,00	17,00	24,00	1,54	5,96	185,14	0	8	
[Economical level(ABCD).D]	[PostalCode.29001]	76,47	13,00	13,00	17,00	2,39	7,56	289,00	0	9	
[PostalCode.29001] [Civilst	[Economical level(	76,47	13,00	13,00	17,00	3,19	8,92	323,00	0	10	
[PostalCode.29001] [Econo	[Civilstage.married]	81,25	13,00	13,00	16,00	1,77	5,64	288,00	0	11	1
[Civilstage.single]	[Economical level(	50,00	25,00	25,00	50,00	1,14	3,00	112,00	0	12	
[Economical level(ABCD).C]	[Civilstage.single]	56,82	25,00	25,00	44,00	1,14	3,00	115,79	0	13	
[PostalCode.29001] [Civilst	[Economical level(	66,67	10,00	10,00	15,00	1,52	3,40	168,00	0	14	
[PostalCode.29001] [Econo	[Civilstage.single]	71,43	10,00	10,00	14,00	1,43	3,00	175,00	0	15	~
E=>E E=>M M=>E M=>M S	Show all Filters		<<	[0 - 3	06]				>>		

#### Original Data View

CustomerID	PostalCode	Economic	Civilstage	A1	A2	A1	A1	A2	<u>^</u>
			Supplier	A1	A2	A1	A1	<b>A</b> 2	
		2	Price range	P1	P1	P2	P2	P1	
			Restrictions	Yes	Not	Yes	Yes	Yes	
			Exp	beer	juice	champagne	wine High Q	wine X	
49	pc29002	D	married	Empty	Empty	3.0	3.0	Empty	
50	pc29002	D	married	Empty	Empty	3.0	3.0	Empty	
65	pc29002	D	married	Empty	3.0	Empty	3.0	Empty	
66	pc29002	D	married	Empty	4.0	4.0	4.0	Empty	
69	29001	D	married	Empty	4.0	4.0	4.0	Empty	
70	29001	D	married	Empty	4.0	4.0	4.0	Empty	
73	29001	D	married	Empty	4.0	4.0	4.0	Empty	
74	29001	D	married	Empty	4.0	4.0	4.0	Empty	
92	29001	D	married	Empty	Empty	4.0	4.0	Empty	
93	29001	D	married	Empty	Empty	4.0	4.0	Empty	
94	29001	D	married	Empty	Empty	4.0	4.0	Empty	
95	29001	D	married	Empty	Empty	4.0	4.0	Emoty	<u>×</u>





#### a Bitlab software

# **Association Rules collaborative tool**

Integrated suite for association rule discovering in medical and molecular data

# Annexes



Version v1: 8<sup>th</sup> November 2007. On-line updated information available at: http://chirimoyo.ac.uma.es/arco

Comments to: ots@ac.uma.es

# Annexe 1: Data transformation tools

Before producing transactions, it is possible to perform some data transformations with the aim to increase the probability of discovering new knowledge. For instance, if we have extremely descriptive metadata (e.g. patient age) it will be difficult to incorporate this metadata in a frequent itemset. Therefore it could be better to define some categories or groups with similar metadata (e.g. age ranges: {0-10; 11-20; 21-40; 41-60; 61-85; 86-+}).

After rule generation to allow a better analysis, the original data are shown in the "Original Data View" tab.

The following transformations are available for metadata:

#### Trimming: Kept the first T characters.

Protein Annotations					
ACETATE KINASE					
ACETOIN_DEHYDROGENASE	Trimming: reduce the metadata space in descriptive fields				
ACETOIN_DEHYDROGENASE_E1_COMPON	IENT(TPP_DEPENDENT_ALPHA_SUBUNIT)				
ACETOIN_DEHYDROGENASE_E1_COMPON					
	IENT(DIHYDROLIPOAMIDE_ACETYLTRANSFERASE) IENT(DIHYDROLIPOAMIDE_DEHYDROGENASE)				
ACETOLACTATE_SYNTHASE_(ACETOHYDH ACETOLACTATE_SYNTHASE_(ACETOHYDH ACETYL COA ACETYLTRANSFERASE					
ACETYL_COA_CARBOXYLASE_(ALPHA_SU	BUNIT)				
ACETYL_COA_CARBOXYLASE_SUBUNIT_(E					
ACETYL_COA_CARBOXYLASE_SUBUNIT_(E	BIOTINGARBOXYLASE_SUBUNIT)				
ACETYL_COA_SYNTHETASE					

Example: Trimming the 20 first characters will code the boxes metadatas into the general "ACETOIN\_ DEHYDROGENAS".

#### Hierarchical:

Items are often organised in hierarchical way, and some transformations also produce hierarchical data. This characteristic has effect in the expected support of item (items at the lower level are expected to have lower support). Since, some fields of the transactions database have this structure; ARco provides a way to re-code the level at which the metadata are annotated

Uniform suppo Level 1 min_sup = 5%	M	lilk t = 10%]	Flexible support Level 1 min_sup = 5%		
Level 2	2% Milk	Skim Milk	Level 2		
min_sup = 5%	[support = 6%]	[support = 4%]	min_sup = 3%		

Distance-based data transformations (Interval Equi-Depth & equi-width)

Price	Equi- width	Equi- depth	Distance- based
7	[0,10]	[7,20]	[7,7]
20	[11,20]	[22,50]	[20,22]
22	[21,30]	[51,53]	
50	[31,40]		
51	[41,50]	4	[50,53]
53	[51,60]		

Binning methods do not always capture semantic of data intervals. In these situations a distance-based partitioning can be used, this is to say, numeric attributes can be dynamically discretised to maximise the confidence or compactness of the rules. This discretization can be done by accounting the number of points in a given interval or by "closeness" of points in an interval (distance function)

# Triming

Keep the first or last 'n' characters and it is available for all data types (all datatypes are taken as string data).

ID
CETATE_KINASE
CETOIN_DEHYDROGENASE
CETOIN_DEHYDROGENASE
CETOIN_DEHYDROGENASE
CETOIN_DEHYDROGENASE_E1_COMPONENT(TPP_DEPENDENT_ALPHA_SUBUNIT)
CETOIN_DEHYDROGENASE_E1_COMPONENT(TPP_DEPENDENT_BETA_SUBUNIT)
CETOIN_DEHYDROGENASE_E2_COMPONENT(DIHYDROLIPOAMIDE_ACETYLTRANSFERASE)
CETOIN_DEHYDROGENASE_E3_COMPONENT(DIHYDROLIPOAMIDE_DEHYDROGENASE)
CETOLACTATE_SYNTHASE_(ACETOHYDROXY_ACIDSYNTHASE)_(LARGE_SUBUNIT)
CETOLACTATE_SYNTHASE_(ACETOHYDROXY_ACIDSYNTHASE)_(SMALL_SUBUNIT)

In this example we can devise three main groups of annotations with at different level of detail. One of the main purposes of data transformation is to increase the probability of a given itemset to be part of a frequent itemset. However, a disperse space of metadata can go on the converse direction. This transformation allows to joint similar data under the same category increasing the support of the categories

🚟 Triming Parameters 🛛 🛛 🕅		ID ID
	a state of the second	ACETATE_KINASE
Length	21	ACETOIN_DEHYDROGENASE
From	Left 💊	ACETOIN_DEHYDROGENASE
		ACETOIN_DEHYDROGENASE
Accept Cancel		ACETOIN_DEHYDROGENASE
		ACETOLACTATE_SYNTHASE
		ACETOLACTATE_SYNTHASE

In the example, the first 21 characters on the left are used to describe the category. As result, the descriptor keeps the main power, but additionally, several items will contain it.

Important note: When a trimmed item is part of a rule, ARco will display the original value of the item.

## Hierarchical

This type of data transformation is used to reduce the deep level in a hierarchical metadata (the metadata must be in the form of {XsYsZ, where X, Y and Z are a category and 's' is a separator

genName	Functional category	FC_level3
aceE	Metabolism	4
aceF	pyruvate dehydrogenase E2 component	4.2.1
ackA	acetate kinase	4.2
асрР	carrier protein	4.5.1
acpS	holo-[acyl-carrier protein] synthase	4.5.1
adk	adenylate kinase	4.6.2
ahpC	hydroperoxide reductase, C22 subunit, thioredoxin-like	3.3
alaS	alanyl-tRNA synthetase	1.2.2
amiB	Peptidoglycan biosynthesis	5.2
ansA	L-asparaginase I	4.4.2
араН	diadenosine tetraphosphatase	4.6.2
apbE	thiamine biosynthesis lipoprotein ApbE precursor	4.8.11

In the example, the functional category of genes is shown togeter with the geneName in the first row and the numeroc level of the category. The deper the level is, the more specific the description is. Reduce specificity can be obtained by Hierarchical transformation

🎬 Hierarchic Parameters 🛛 🔯					
Level	2				
Level Separator	4				
Accept	Cancel				

In this case we set a retdution to the second level (those annotation whose original category is lower than 2 maintain their initial values).

Result of data transformation are displayed in the picture

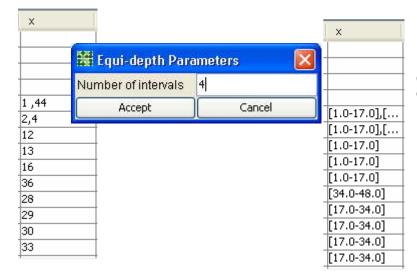
genName	Functional category	FC_level3
aceE	Metabolism	4
aceF	pyruvate dehydrogenase E2 component	4.2
ackA	acetate kinase	4.2
acpP	carrier protein	4.5
acpS	holo-[acyl-carrier protein] synthase	4.5
adk	adenylate kinase	4.6
ahpC	hydroperoxide reductase, C22 subunit, thioredoxin-like	3.3
alaS	alanyl-tRNA synthetase	1.2
amiB	Peptidoglycan biosynthesis	5.2
ansA	L-asparaginase I	4.4
араН	diadenosine tetraphosphatase	4.6
apbE	thiamine biosynthesis lipoprotein ApbE precursor	4.8

## Data categorization

These transformations allow to group numerical values into a reduced set of categories (partitioning). The next options are available:

#### Equi-Depth interval transformation.

Each partition (interval) has the same number of items.



In the example 4 groups have been created with similar number of elements

## Equi-Width intervals transformation

×			×
1,44 2,4	Equi-wig	lth Par 🔀	[-Inf-3.0),[4
12	and Eddinatio		[-Inf-3.0),[3
	Lower limit	3	[8.0-13.0)
13	Linn on lineit	60	[13.0-18.0)
16	Upper limit	60	[13.0-18.0)
36	Interval size	5	[33.0-38.0)
28		1 <u></u>	[28.0-33.0)
29	Accept	Cancel	· · · · · · · · · · · · · · · · · · ·
30		200	
33			[28.0-33.0)
			[33.0-38.0)

Each partition (interval) has the same size (range and interval sizes are required)

Groups values between 3 and 60 in intervals of size 5  $\,$ 

# Annexe 2: File formats

#### engene© format (\*.dat) <u>http://chirimoyo.ac.uma.es/engenet</u>)



An **engene** data file is a table. This table is stored in the file as a set of fields separated by TAB, and along several lines. This text format may be worked out by Excel. So, an Excel table as follows will generate a file as shown below, when it is saved-as-text.

	A	В	С	1	16	72
1	1	16	72	123 151	15 15	1 23
2	123	15	1	32	15 516	23 53
3	151	15	23			
4	32	516	53	No. of Concession, Name		
-			۸	-	D	

Data are a collection of vectors, one vector a row. All vectors have the same number of *variables*, one variable a column. Some values may be unknown; in this case, the respective field may be a non numeric string o may be null. These values are

	A	В	С		
1	NAN	16	72		
2	123	15	UNK		
3	151		23		
4	32	516	23 53		

called NaN (Not A Number). In the picture, these values are red marked.

It is possible to append notes to data. This kind of information is called metadata. There are three types of metadata: global labels, row labels and column labels. All labels have two parts: the label\_name and the label\_values. For each global labels name there is only one-value.Row labels have one-value for each data-row; and column labels have one\_value for each data column. Next picture shows how to put labels to data.

	A	В	С		E)	)		E	e red, and the
1		CTag1Name	CTag1Val1	CTa	ag1\	/al2	CT	ag1Val3	abels names e blue. Global
2		CTag2Name	CTag2Val1	CTa	ag2	Val2	CT	ag2Val3	d the values
3	RTag1Name								
4	RTag1Val1		1			16		72	etween
5	RTag1Val2		123			15		1	pace in next
a (	DTaa4Val2		454			45			ave fields
	A	B	C			D		E	v and column
1		CTag1Name	CTag1Val1	C	СТа	g1Val2	2	CTag1Va	n next figure), ling after the
2		CTag2Name	CTag2Val1	C	CTag	g2Val2	2	CTag2Va	in the figure).
3	RTag1Name								Excel, you must
4	RTag1Val1			1			16	ia	on used to
5	RTag1Val2		11	23			15		ne works with ds separation and
6	RTag1Val3		1(	51			15		lecimal separator

	А	В	С	D	E	F	G	Н		J
1					Supplier	A1	A2	A1	A1	A2
2					Price range	P1	P1	P2	P2	P1
3					Restrictions	Yes	Not	Yes	Yes	Yes
4					Exp	beer	juice	champagne	wine High Q	wine X
5	CustomerID	PostalCode	Economical I	Civilstage						
6		pc29003	A	Single		2	2			2
7		pc29003	A	Single		2	2			2
8		pc29003	a	single		2	2			2
9		pc29003	a	single		2	2			2
10		pc29003	В	single		2	2			2
11		pc29003	В	single		2	2	2	2	
12		pc29003	В	single		2	3			
13		pc29003	В	single		2	2		2	
14		pc29003	В	single		2	2		2	
15		pc29003	A	single		2	2		2	
16		pc29003	A	single		2	2		2	
17		pc29003	а	single		2	2		2	
18		pc29003	A	single		2	3		2	
19		pc29003	A	Married			2		2	
20		pc29003	С	Married			2		2	
21		pc29003	С	married			2			2
22		pc29003	С	married			2			2
23		pc29003	В	married			2	2		
24		pc29003	В	married		2	2	-2		
25		pc29003	В	married			4		2	
26		pc29003	В	married			4			2
27		pc29003	В	married		2	4			
28		pc29003	В	married			2	2	2	
29		pc29003	В	married		2	4			
30	25	pc29003	В	married			2	2	2	

Gene (or row) Metadata labels are shown in red and data in orange. Dark green represents sample (or experiment / column) metadata labels; and light green column metadata values. Gene-expression ratios are shown in blue.

The same format is valid as \*.xls (Excel file); or TSV -text tabulated- / CVS -comma separated) files

	А	В	С	D	E	F	G	Н	
1				Supplier	A1	A2	A1	A1	A2
2				Price range	P1	P1	P2	P2	P1
3				Restrictions	Yes	Not	Yes	Yes	Yes
4		PostalCode	Economical I		beer	juice	champagne	wine High Q	wine X
5		pc29003	A	Single	2	2			2
6		pc29003	A	Single	2	2			2
7		pc29003	а	single	2	2			2
8		pc29003	а	single	2	2			2
9		pc29003	В	single	2	2			2
10		pc29003	В	single	2	2	2	2	
11		pc29003	В	single	2	3			
12		pc29003	В	single	2	2		2	
13		pc29003	В	single	2	2		2	
14		pc29003	A	single	2	2		2	
15		pc29003	A	single	2	2		2	
16		pc29003	а	single	2	2		2	
17		pc29003	A	single	2	3		2	
18		pc29003	A	Married		2		2	
19		pc29003	С	Married		2		2	
20		pc29003	С	married		2			2
21		pc29003	С	married		2			2
22		pc29003	В	married		2	2	2	
23		pc29003	В	married	2	2	-2		
24		pc29003	В	married		4		2	
25			В	married		4			2
26			В	married	2	4			
27		pc29003	В	married		2	2	2	
28		pc29003	В	married	2	4			
29		pc29003	В	married		2	2	2	
30		pc29002	В	single	3				3
31		pc29002	A	single	3				3
32		pc29002	С	single	3				3
33		pc29002	С	single	3				3
34		pc29002	С	single		4	3		
35		pc29002	В	single		4	3		
36	32	pc29002	В	married		4	3	3	

Gene (or row) Metadata labels are shown in red and data in orange. Dark green represents sample (or experiment / column) metadata labels; and light green column metadata values. Gene-expression ratios are shown in blue.