Negative eigenvectors, long paths and p*

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ABSTRACT

We will discuss the roles of positive and negative eigenvalues of the Normal spectrum in identifying long paths in a network. These roles may be understood in terms of the "vibrational modes" of the associated eigenvectors. Nodes clustered together in an off-diagonal (almost bipartite) blockmodel may in fact be quite far apart in either graph-theoretic or random walk distance, especially in large sparse networks. We use p* as a tool to evaluate the blockmodels based on eigenvector partitions. We will also discuss fitting p* models large networks, recently added to MultiNet.

INTRODUCTION

The main purpose of this paper is to discuss the role and interpretation of negative eigenvalues (and associated eigenvectors) of the Normal Spectrum of a (binary, symmetric) graph. The Normal spectrum (defined below) is closely related to Correspondence Analysis, which for such graphs is eigendecomposition of the χ^2 (actually, χ) matrix, treating the adjacency matrix as a contingency table. We have viewed partitions of a graph based on the eigenvectors belonging to the largest eigenvalues as a way of approximately maximising χ^2 , a hard combinatorial problem (Chung, Graham, Yau, 1996). That is, simple polynomials based on the signs of the eigenvector components can be used to permute the rows and columns of an adjacency matrix so that a few "blocks" contain most of the links, while the rest are mainly empty. This approximate procedure usually works quite well, even for directed graphs, though the partitions are based on undirected graphs. (Normal eigendecomposition can be easily extended to multi-graphs or edge-weighted graphs, but there is currently no agreement on how to extend the procedure to directed graphs, except in certain special cases (Chung, Faber, Manteuffel, 1994)). Comparing the quality of partitions based on the largest eigenvectors by looking at χ^2 leads to difficulties when the number of blocks changes. More importantly, a partition based on the largest eigenvectors can fail for reasons to be discussed, although very good partitions can still be found by looking at smaller eigenvalues. We recently implemented a version of p* in MultiNet (Seary, Richards, 2000), because p* promised to be a

completely independent way of assessing the goodness (actually, badness) of a fit using different permutations with different numbers of "blocks". Since p* (as we have implemented it, based on the work of Frank & Strauss (1986)) focusses on local structure and the Normal eigenvectors provide global structure via blocking, it seems that p* and eigendecomposition are complimentary. As we shall see, the Normal spectrum *also* provides information about local structure, and this comes from the negative eigenvalues.

PHYSICAL ANALOGY

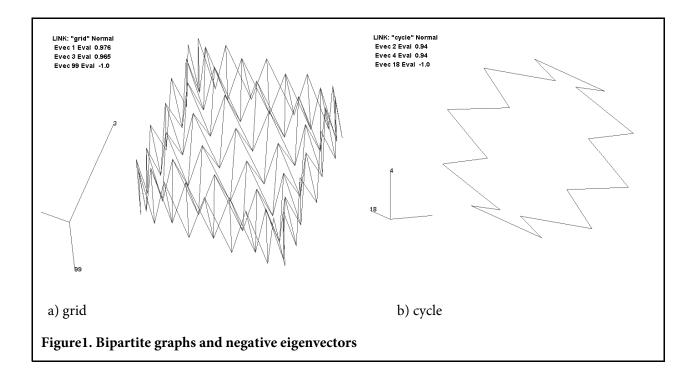
To discuss the role of negative eigenvalues, we consider the following physical analogy. The analogy is quite good: it is the basis of Markov Chain Monte Carlo (MCMC) methods, and has stirred much recent research into graph spectra. In physics, problems such as wave propagation and diffusion are generally solved by considering the spatial and time-dependent parts of the problem separately. The spatial part leads to consideration of the eigenvalues and eigenfunctions of the Laplacian operator ∇^2 .

The resulting eigenfunctions generally have a close relationship with the geometry of the space under consideration. In the discrete case, where the "space" is a set of nodes connected byedges - a graph - the Laplacian operator has a discrete version with a very simple form: it is a square matrix which acts on vectors which have dimension equal to the number of nodes, with definition (see Seary & Richards, 1995, for some alternative derivations).

Laplacian(G) = D(G) - A(G)

where D(G) is a diagonal matrix of node degrees, and A(G) is the adjacency matrix of a graph G. It is easy to show that the eigenvalues of **D**-**A** are non-negative, with a lowest value of 0, and highest possible value of maximum degree. The second-smallest eigenvalue plays an important role in spectral graph theory, since it provides a measure of how "random" the graph is. The largest possible eigenvalue is only attained when the graph is bipartite semi-regular. The eigenvalues may be considered as the amount of energy required to stimulate each mode of vibration (eigenvector). The highest frequency vibrations correspond to highest amount of energy. Figures 1a and b show the highest vibration for an even cycle, and a rectangular grid. In each case, the vibration is the largest possible, because in each case the graphs are bipartite. But this can be viewed as a *local* property! Graphs that, locally, look like a path (or cycle, or tree) are, locally, bipartite. In each case, we know that, because the highest frequency is attained, the graphs must be triangle free - the type of count that p* makes.

As mentioned, the second-smallest eigenvalue is important (Alon, 1986). The corresponding eigenvector can be used to partition the graph with few edges between the two parts. If this eigenvalue is far from 0, the corresponding edge-cut will be poor, and all distances in the graph are short (see below). These properties are generally associated with random graphs. Conversely, a value close to 0 corresponds to a graph with structure.



We now introduce the Normal spectrum by performing a simple operation to the Laplacian:

$$CombLap(G) = D^{-1} (D - A)$$

= I - D⁻¹ A = I - Markov(G)

This has the form of a Laplacian (it is sometimes called the Combinatorial Laplacian (Dodziuk & Kendall, 1985), where the second term is a matrix of transition probabilities: the Markov chain matrix for a simple random walk on the graph G. Since the eigenvalues of **Markov**(G) can between -1 and 1, the eigenvalues of **CombLap**(G) can be between 0 and 2. Again, the highest value is only attained for bipartite graphs, and the second-lowest is large for graphs with short distances. Such graphs are the basis of MCMC methods.

The matrix used to define the Normal spectrum is

Normal(G) =
$$D^{-1/2} A D^{-1/2}$$

This should look familiar to users of Correspondence Analysis (CA). In CA, we generally go on to remove a "trivial" eigenvector (the χ^2 expected) before performing an SVD, then further adjust the length of the resulting singular vectors by singular values. Symmetrising means that singular values and vectors are eigen-values and -vectors. Some implementations of CA ignore eigenvalue signs (they are absorbed in one or other of the eigenspaces), while others implicitly weight the diagonal with row/column degrees which supresses all negative eigenvectors (this is the method used by the MultiNet CorrAnal procedure). The Normal eigendecomposition does very little pre- or post-

processing: no trivial vector is removed (this destroys sparsity), eigenvalue signs are preserved, and the vectors are merely normalised to length 1.

It turns out that **Normal**(G) has exactly the same eigenvalues as **Markov**(G), and the eigenvectors differ by a simple transformation which does not affect the signs. We can map between:

 $\{\lambda_{0},...\lambda_{n-1}\}$, the eigenvalues of **CombLap**(G) and

 $\{\mathbf{v}_{0},...\mathbf{v}_{n-1}\}$, the eigenvalues of **Normal**(G) very simply:

 $\{ \lambda_i \} = 0, \dots, 2 \qquad i=1, \dots, n-1 \\ \{ \nu_i \} = 1, \dots, -1$

That is, the positive eigenvalues of **Normal**(G) correspond to low-frequencies and the negative eigenvalues correspond to high frequencies. Since **Markov**(G) = D^{-1} **A** is the matrix for simple random walks on a graph, the i,jth entry of **Markov**(G)]^p is the probability that a random walk from i will reach j in p steps (Cvetkovic, Doob, Sachs, 1980). This observation can be used to find bounds on distances between subsets of the graph, including a bound on the diameter of the graph (Chung, 1995). The proofs involve finding powers o**Markov**(G) from the eigenvalues and eigenvectors, and lead to the following set of bounds:

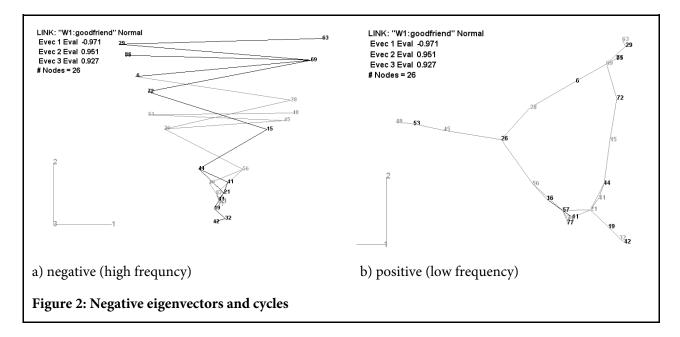
$$Dist(X_{i}, X_{j}) \leq \frac{\ln(n-1)}{\ln\frac{\lambda_{n-1} + \lambda_{k}}{\lambda_{n-1} - \lambda_{k}}}$$

for distances between (k+1)-subsets of the graph. This is simplified version of the formula proved in Chung (1995). A much better bound can be found for the diameter (k = 1).

A very similar formula shows that distance bounds can be found from other pairs of large and small eigenvalues besides the largest and second-smallest. The important point to note is that for *pairs* of eigenvalues near their extreme values (0 and 2, respectively), the denominator is near 0, which gives very large distances. This will be the case when G contains a long path (or cycle). When we map this to the Normal spectrum, we can see that pairs of large eigenvalues of opposite sign correspond to large distances. They also correspond to large oscillations in the corresponding negative eigenvector.

As an example of this, see figure 2, which is taken from actual data (as are the rest of the examples in this paper). This network comes from data collected by Stork.

and represents who nominated who as a "good friend". Two views are given: 2a shows the largest negative eigenvector along the x-axis. In 2b, the view has been rotated to show the largest positive eigenvector. The network is clearly dominated by a cycle. The partition from 2a puts 48 in the same

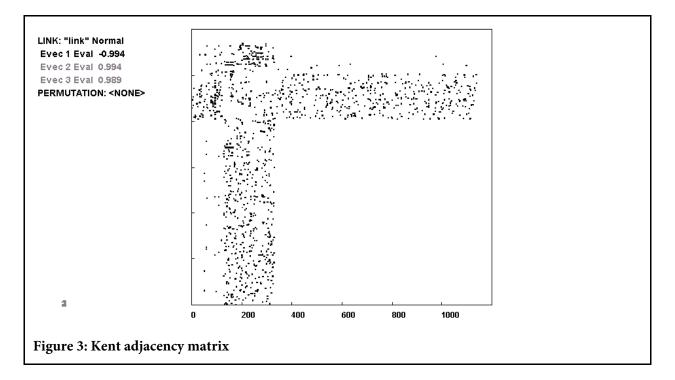


part as 15, even though they are far apart. We suggest that this can be understood by considering the two off-diagonal blocks - which always occur in pairs - as a single *anti-block*. A partition based on the first (negative) and second (positive) eigenvectorapproximately maximises χ^2 and also gives a "significantly" better (smaller) -2*LogPseudoLikelihood (-2LogPL) from a p* fit when compared to the partition from the first two positive eigenvectors (tables 1a and 1b). (The statement about "significance" assumes that differences in -2*LogPL are distributed approximately as χ^2 with the appropriate degrees of freedom (Crouch & Wasserman, 1998). We will put such statements about "significance" in quotes. As of this writing, the actual distribution remains unclear; perhaps it should be called pseudo-significance.) In fact, it gives a "significantly" better p* fit than *any* of the node attributes that come with this dataset. We must also note that the actual *number* of links correctly predicted by p* is rather small at the 0.5 probability level, and at lower probability level, p* "predicts" the predefined *blocks* more than anything else.

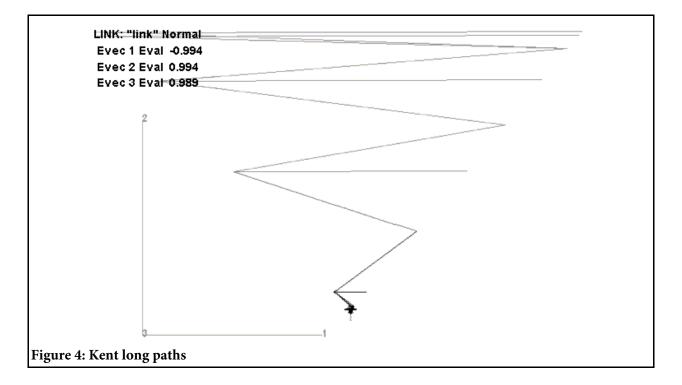
KENT DATA

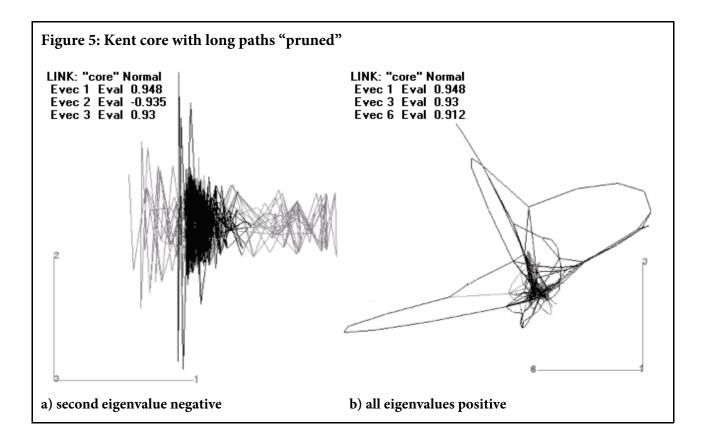
The adjacency matrix for this data is shown in figure 3. It has the appearance of a core-periphery network: nodes in the two peripheries can only reach each other by passing through the "core". This network is very directed: only 6 (0.5%) of the links are reciprocated. It is also very sparse, with 1332 nodes and 1139 links. In particular, the "core" itself is quite sparse. We might expect that, with few connections within the "core", there may be long paths or cycles from the two "peripheries" through the core and back again. Because the "core" is so sparse we suggest calling this an *intersection-periphery* network.

The three largest eigenvectors are shown in figure 4. This view is dominated by a long path from top to bottom of length 17 (and this is the diameter of the large component of this network). Note the



oscillations in the x-axis from the first, negative, eigenvalue. Views of 2nd, 3rd, 4th eigenvectors are similar: in each case the views are dominated by a long path, whose length can be upper-bounded by the corresponding eigenvalues. Not until the 13th eigenvector do we see a picture that is not dominated by a long path. How do we find this representation?



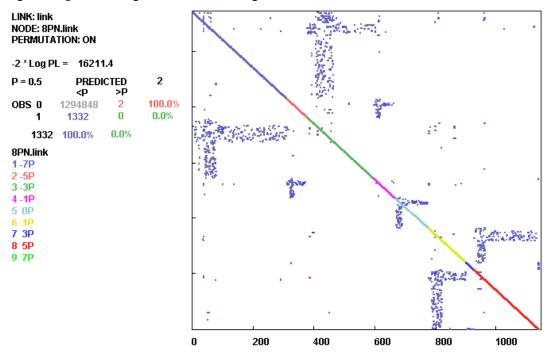


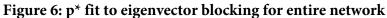
One simple method is to recursively remove nodes with 0 or 1 links. The effectis to shorten all the long paths and results in figure 5a. By rotating along the y-axis and then the x-axis, we see in figure 5b a number of long cycles. These cycles are present in figure 5a as the oscillations across the x-axis coming from the second eigenvector with negative eigenvalue. As in the example above, the partition based on these three (positive, negative, positive) eigenvectors give larger χ^2 and "significantly" better -2LogPL than a partition based on the first three positive eigenvectors (tables 2a and 2b). Note that each bipartite anti-block pair all the nodes in one of the bipartitions belong to the "core". The blockmodel used is based on permutations to successively smaller $2^n x 2^n$ blocks of an identity matrix:

8 x 8 positive (no change),	4 x 4 negative	2 x 2 positive (no change)
1 0 0 0 0 0 0 0	0 0 1 0 0 0 0 0	0 0 1 0 0 0 0 0
0 1 0 0 0 0 0 0	0 0 0 1 0 0 0 0	0 0 0 1 0 0 0 0
0 0 1 0 0 0 0 0	1 0 0 0 0 0 0 0	1 0 0 0 0 0 0 0
0 0 0 1 0 0 0 0 ->	0 1 0 0 0 0 0 0 ->	0 1 0 0 0 0 0 0
0 0 0 0 1 0 0 0	0 0 0 0 0 0 1 0	0 0 0 0 0 0 1 0
0 0 0 0 0 1 0 0	0 0 0 0 0 0 0 1	0 0 0 0 0 0 0 1
0 0 0 0 0 0 1 0	0 0 0 0 1 0 0 0	0 0 0 0 1 0 0 0
0 0 0 0 0 0 0 1	0 0 0 0 0 1 0 0	0 0 0 0 0 1 0 0

Now we are ready to examine the larger network. We find by taking inner products that eigenvectors 13-15 correspond to eigenvectors 1-3 of the "pruned" network, with the same positive, negative, positive sequence of eigenvalues. The partition is presented in table 3a, and appears to be rather good.

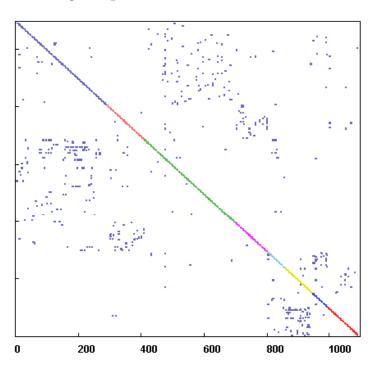
Figure 6a shows this view of the network. The view involving only positive eigenvectors is shown in figure 6b. The blockmodel is as for the smaller network. Again, this partition gives higher χ^2 and "significantly" lower -2LogPL in a p* fit than the all-positive eigenvalue partition. These results are shown in tables 2c and 2d.











DISCUSSION

There are a number of features about this analysis that concern us. The fact that we need to look at the 13th and higher eigenvectors is one of them. We see that the lower eigenvectors are dominated by long paths in this very articulated network, where pairs of positive and negative eigenvalues give estimates of the path length. However, this interpretation requires *viewing* the eigenvector representation, and even for the one involving 13-15 it is not immediately clear from the view that this will give approximately correct results, since both paths and cycles are present, and the former are more obvious. The use of "pruning" to remove long paths was important in recognising the correct eigenvectors for the large network. The conclusion that these actually *are* correct is based on the χ^2 and p^{*} results (but see below) as well as on some knowledge of the network (the intersection-periphery structure).

There is also the problem that results from symmetrisation: some of the "cycles" are really "weak cycles" where direction is ignored. That this does not seem to be important here is no guarantee against problems with other networks.

Another concern is the apparent reliance on 2^n blocks, but this is not really necessary. Blocks can easily be combined. For example, for the small ("pruned") network, the lower right 4 x 4 section (see figure 7 for the motivation) can be combined as

0	0	1	0
0	0	0	1
1	1	0	0
1	1	0	0

without "significant" loss of -2LogPL (from 4279 to 4271). The full network has 9 blocks, one of them coming from a number of disconnected dyads and 2-stars. If we view the bipartite anti-block pairs as *single* blocks, the numbers are reduced to 4 for the pruned network, and 5 for the full network.

Finally, there is the quality of the p* fits. While the -2LogPL results confirm our χ^2 results (and intuition), the fact remains that *no* links were correctly predicted, and very few even at the lowest probability level (0.0625). Even these are largely the result of "predicting" the predefined block structure. This is an unusual network in some respects: it is much larger than ones usually analysed in p* presentations; there is almost no reciprocation; there are few transitive triads and *no* cyclic triads. We have looked at networks much larger than this (over 4000 nodes) with even lower densities where p* does a fairly good job of predicting links (about 1/3 correctly) but these networks also have much more reciprocation and triads, as well as a strong *cohesive* (on-diagonal) block structure with much shorter paths. We suspect it is the long paths (and associated off-diagonal block structure) that causes the fit problems. A similar problem was noticed for the much smaller (n=57) "good friend" networks.

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Tables

Table 1A. MultiNet PSTAR REPORT ON "STORK2.MNW" 7/04/2000 05:10:46 ITERATIONS = 11 LINK = "goodfriend" LINKS = 52 ORDER = 44 (DIAGONAL NOT INCLUDED) NODE = "4PN.goodfriend" BLOCKING 0 1 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 0 0 1 0 0 0 0 1 -2 Log PseudoLikelihood = Goodness of Fit = Model Chi-squared = 266.495 1008.880 2356.374 df = 13 FIT AT P = 0.5PRED <P | >P 15 -----0 | 1836 | 4 26.7% -----OBS ----1 41 11 73.3% 78.8% 21.2% 52 -----Table 1B. MultiNet PSTAR REPORT ON "STORK2.MNW" 7/04/2000 05:12:34 ITERATIONS = 9 LINK = "goodfriend" LINKS = 52 ORDER = 44 (DIAGONAL NOT INCLUDED) NODE = "4PP.goodfriend" BLOCKING 0 0 0 1 0 0 0 0 0 1 -2 Log PseudoLikelihood = Goodness of Fit = 293.842 904.230 2329.027 df = 13 Model Chi-squared = FIT AT P = 0.5PRED 12 <P | >P ------0 | 1836 | 4 33.3% OBS |----- |----- -----44 8 66.7% 1 84.6% 15.4% 52

Table	2A.
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MultiNet 2-D NETWORK XTABS REPORT ON "KENT.MNW" 9/04/2000 22:40:54 Crosstabulation of FROM 8PN.link with TO 8PN.link COUNT

COUNT ROW % COL %	ROWS = FROM 8PN.link COLS = TO 8PN.link -5P -1P							5.5		
-	-7P		-3P			1P	3P		7P	TOTAL
-7P	19 5.15% 5.38%		326 88.35% 93.68%		0.0 %			8 2.17% 13.11%		369 27.7 %
-5P	1 2.44% 0.28%	1 2.44% 1.56%	7.32%		0.0 %	0.0 %		0.0 %	2.44%	3.08%
-3P	312 91.76% 88.39%	0 0.0 % 0.0 %	3.82%	0 0.0 % 0.0 %	0.0 %	9 2.65% 13.64%	0.88%	0.29%	0.59%	25.53%
-1P		61 79.22% 95.31%	1 1.3 % 0.29%	0 0.0 % 0.0 %	0.0 %	0 0.0 % 0.0 %			0 0.0 % 0.0 %	
0 P	0 0.0 % 0.0 %	0 0.0 % 0.0 %	0 0.0 % 0.0 %	0.0 %	92 100.0 % 100.0 %	0.0 %	0.0 %	0 0.0 % 0.0 %		92 6.91%
1P	0 0.0 % 0.0 %	1 1.82% 1.56%	3 5.45% 0.86%	0.0 %	0 0.0 % 0.0 %	1.82%	1.82%	45 81.82% 73.77%		
3 P	3 2.33% 0.85%	0 0.0 % 0.0 %	0 0.0 % 0.0 %		0.0 %		3.1 %	3 2.33% 4.92%	92.25%	
5P	5 7.46% 1.42%	0 0.0 % 0.0 %	2 2.99% 0.57%	0 0.0 % 0.0 %	0.0 %	54 80.6 % 81.82%	4.48%	2.99%	1.49%	
7P	2 1.23% 0.57%	0 0.0 % 0.0 %		0 0.0 % 0.0 %	0.0 %	0.62%	147 90.74% 89.63%	0.62%		
TOTAL	353	64	348	45	92	66	164	61	139	1332
	26.5 %	4.8 %	26.13%	3.38%	6.91%	4.95%	12.31%	4.58%	10.44%	

CHI-SQUARE = 7941.131 D.F. = 64

Table 2B.

MultiNet PSTAR REPORT ON "KENT.MNW" 9/04/2000 22:24:29 ITERATIONS = 12

LINK = "link" LINKS = 1332 ORDER = 1139 (DIAGONAL NOT INCLUDED) NODE = "8PN.link" BLOCKING FIT AT P = 0.50 0 0 0 0 0 0 0 PRED 0 0 0 0 <P | >P 0 0 0 0 0 0 0 1 0 0 0 0 0 _____ 0 | 1294848 | 2 100.0% 0 0.0% OBS |----i 0 0 0 0 0 1 0 0 100.0% 0.0% 0 1 0 0 0 -2 Log PseudoLikelihood = 16194.490 Goodness of Fit = 720984.365 Model Chi-squared = 1780695.307 df = 11

Table 2C.

MultiNet 2-D NETWORK XTABS REPORT ON "KENT.MNW" 9/04/2000 22:45:54 Crosstabulation of FROM 8PP.link with TO 8PP.link COUNT DOWC - EDOM ODD link

COUNT ROW % COL %		CO	WS = FRO LS = TO	8PP.lin						
	-7P		-3P		0 P	1P	3P	5P	7 P	TOTAL
-7P	455 90.82% 92.67%	18 3.59%	7 1.4 %	1	0.0 %	12	2 0.4 %	4	2 0.4 %	
-5P	12 5.77% 2.44%	88.94%	2 0.96% 3.03%	1 0.48% 2.33%	0.0 %		4 1.92% 16.67%	0.96%	0.48%	208 15.62%
-3P	12 16.22% 2.44%	0.0 %	56 75.68% 84.85%	2 2.7 % 4.65%	0.0 %	1 1.35% 0.97%			2.7 %	
-1P	2 4.55% 0.41%	2 4.55% 0.95%			0 0.0 % 0.0 %	0 0.0 % 0.0 %		0 0.0 % 0.0 %	2.27%	44 3.3 %
0₽	0 0.0 % 0.0 %	0 0.0 % 0.0 %	0 0.0 % 0.0 %	0.0 %	92 100.0 % 100.0 %	0 0.0 % 0.0 %	0 0.0 % 0.0 %		0 0.0 % 0.0 %	92 6.91%
1P	6 6.0 % 1.22%	2 2.0 % 0.95%	0 0.0 % 0.0 %	1 1.0 % 2.33%	0.0 %		1.0 %	4.0 %		100 7.51%
ЗP	0 0.0 % 0.0 %	2 9.09% 0.95%	0 0.0 % 0.0 %	0 0.0 % 0.0 %	0.0 %		16 72.73% 66.67%		18.18%	22 1.65%
5P	1 1.64% 0.2 %	0 0.0 % 0.0 %	0 0.0 % 0.0 %	0 0.0 % 0.0 %	0.0 %	2 3.28% 1.94%		54 88.52% 79.41%	6.56%	61 4.58%
7P	3 1.3 % 0.61%	1 0.43% 0.48%	0 0.0 % 0.0 %	0 0.0 % 0.0 %	0.0 %	2 0.87% 1.94%	0.43%	3 1.3 % 4.41%		230 17.27%
TOTAL	 491 	210	66	43	92	103	24	68	235	1332
	36.86%	15.77%	4.95%	3.23%	6.91%	7.73%	1.8 %	5.11%	17.64%	
CHI-SQUAN	RE =	7787.392	D.F	. = 64						

Table 2D.

0

0 0

0

0

MultiNet PSTAR REPORT ON "KENT.MNW" 9/04/2000 06:55:14 ITERATIONS = 12

LINK = "link" LINKS = 1332 ORDER = 1139 (DIAGONAL NOT INCLUDED) NODE = "8PP.link" BLOCKING 1 0 FIT AT P = 0.50 1 0 0 0 0 0 0 0

1

-2 Log PseudoLikelihood = 16950.531 Goodness of Fit = 772892.889 Model Chi-squared = 1779939.266 df = 11

0 0 0

0 0 0 0 1 0 0 0 0 0 0 0 1 0

0 0 0

<P | >P 0 | 1294850 | 0 0.0% OBS 0 0.0% 1 | 1332|