Supplementary Information

COmbined Mapping of Multiple clUsteriNg ALgorithms (COMMUNAL): A Robust Method for Selection of Cluster Number, K

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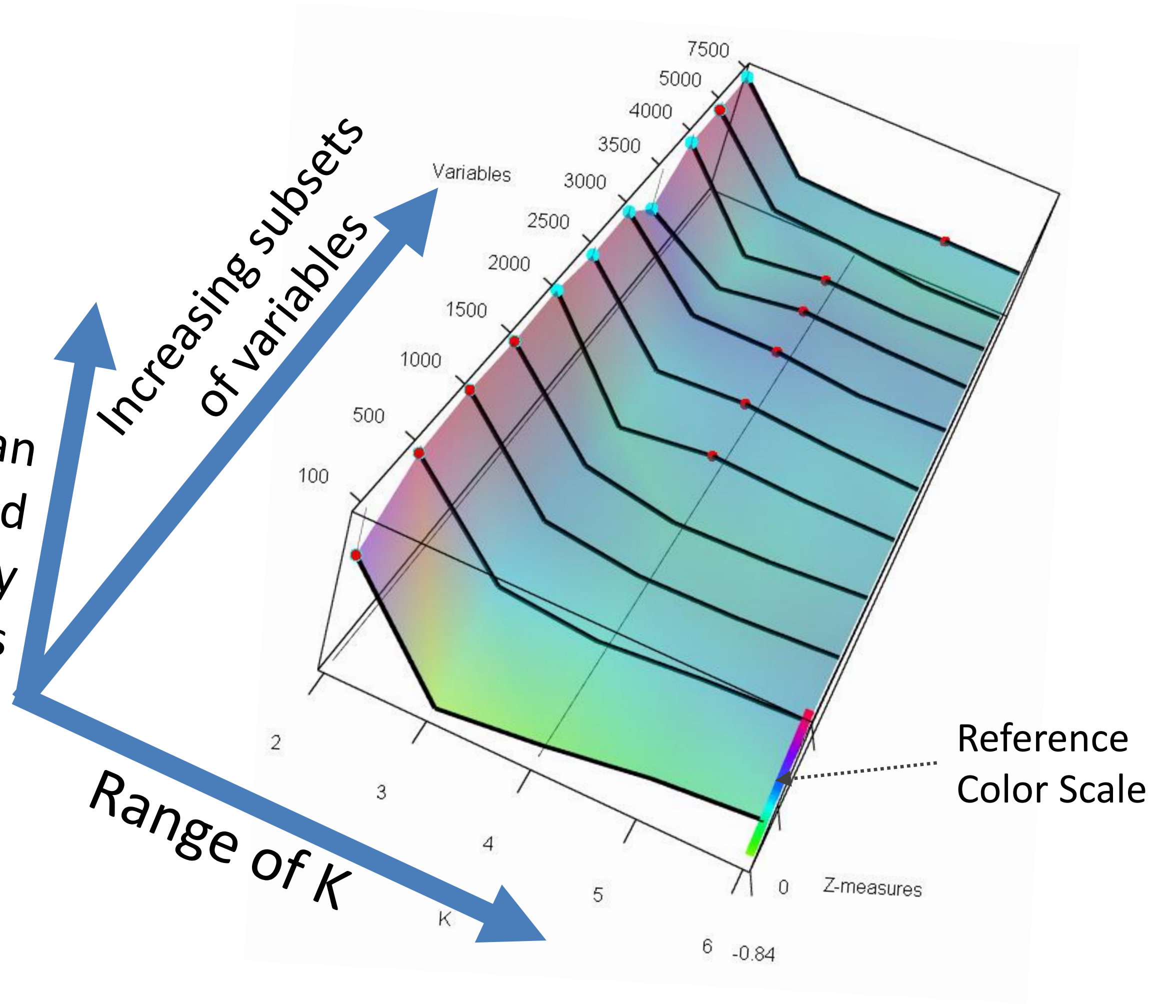
● Steepest non-edge maximum for given gene subset

● Overall maximum for given gene subset

Mean normalized validity measures

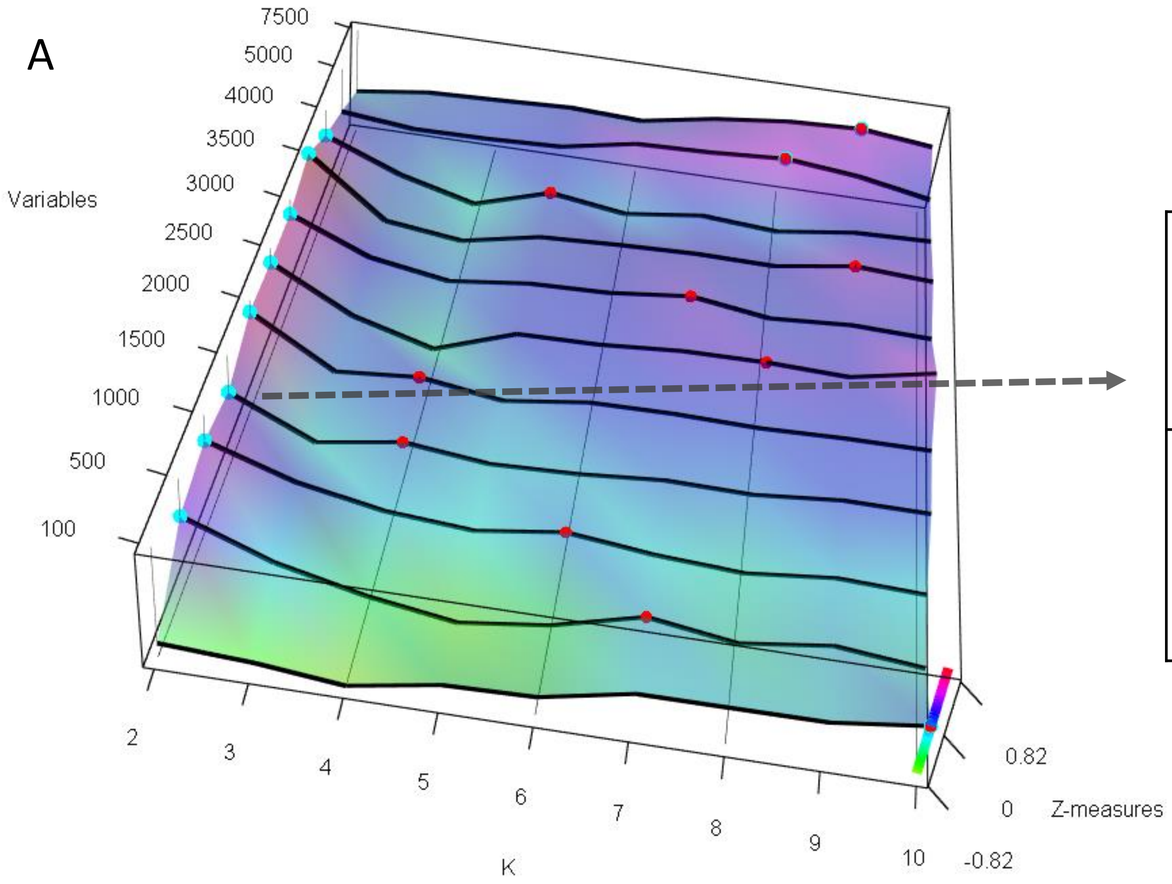


Increasing subsets of variables

Range of K

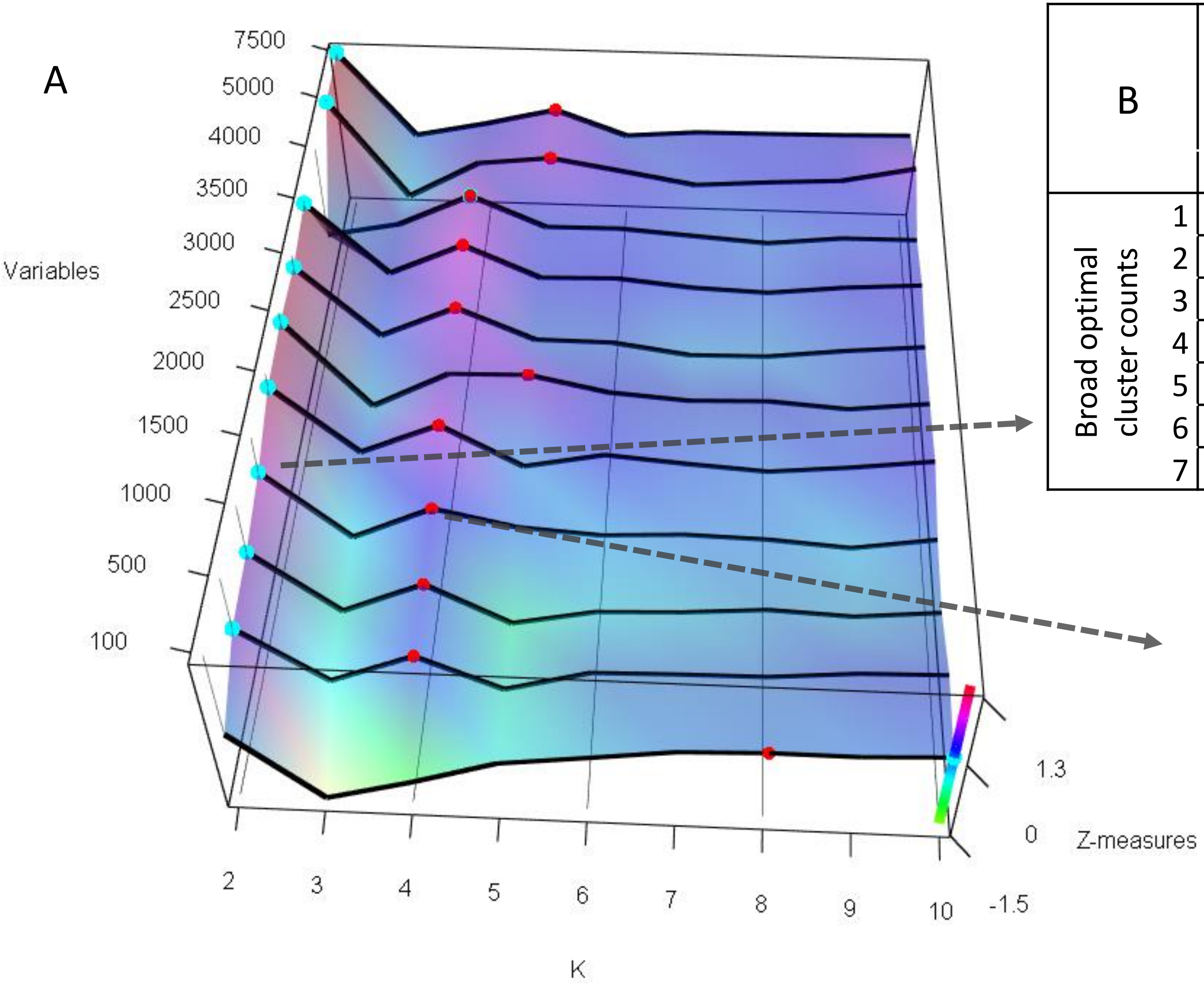
Reference Color Scale

Supplemental Figure S1. Schematic of example COMMUNAL 3D map. Axis labels are shown at left. Red dots indicate steepest non-edge maximum for given gene subset; pale blue dots indicate overall maximum for given subset.



B		COMMUNAL optimal cluster counts at 1500 genes		
		1	2	NA
Broad optimal cluster counts	1	48	2	2
	2	0	41	0
	3	4	72	1
	4	0	52	0

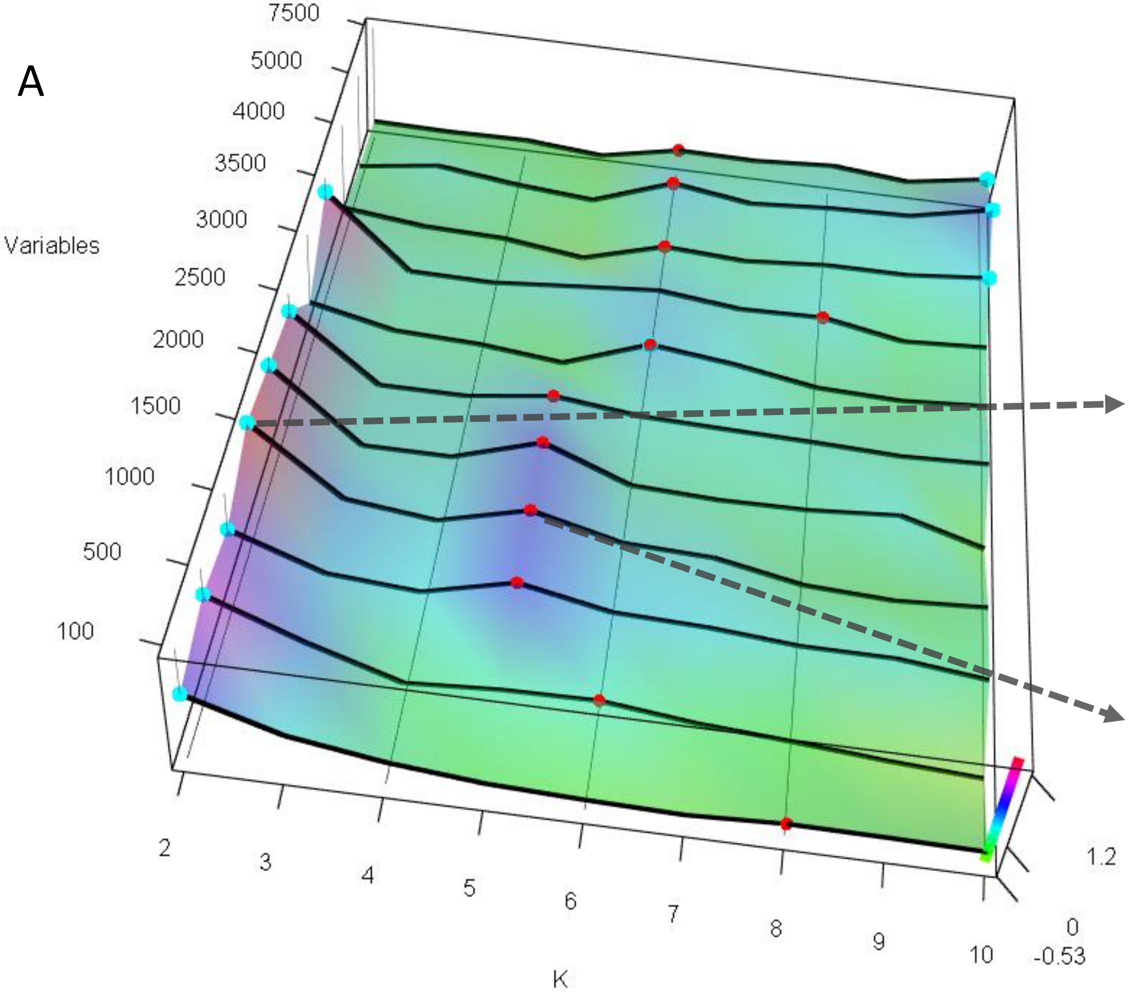
Supplemental Figure S2. COMMUNAL output for the Broad colorectal adenocarcinoma (COADREAD). (A) 3D map of K vs. genes included vs. standardized validity measures showing optima at K=2. (B) Comparison of COMMUNAL core cluster assignment counts vs. Broad CCP-hierarchical cluster assignment counts at 1500 genes for K=2 (lambda= 0.83).



B		COMMUNAL optimal cluster counts at 1500 genes	
		1	2
Broad optimal cluster counts	1	12	0
	2	12	0
	3	4	0
	4	11	0
	5	13	0
	6	9	0
	7	0	11

C		COMMUNAL optimal cluster counts at 1500 genes			
		1	2	3	4
Broad optimal cluster counts	1	12	0	0	0
	2	0	12	0	0
	3	0	0	4	0
	4	0	11	0	0
	5	13	0	0	0
	6	9	0	0	0
	7	0	0	1	10

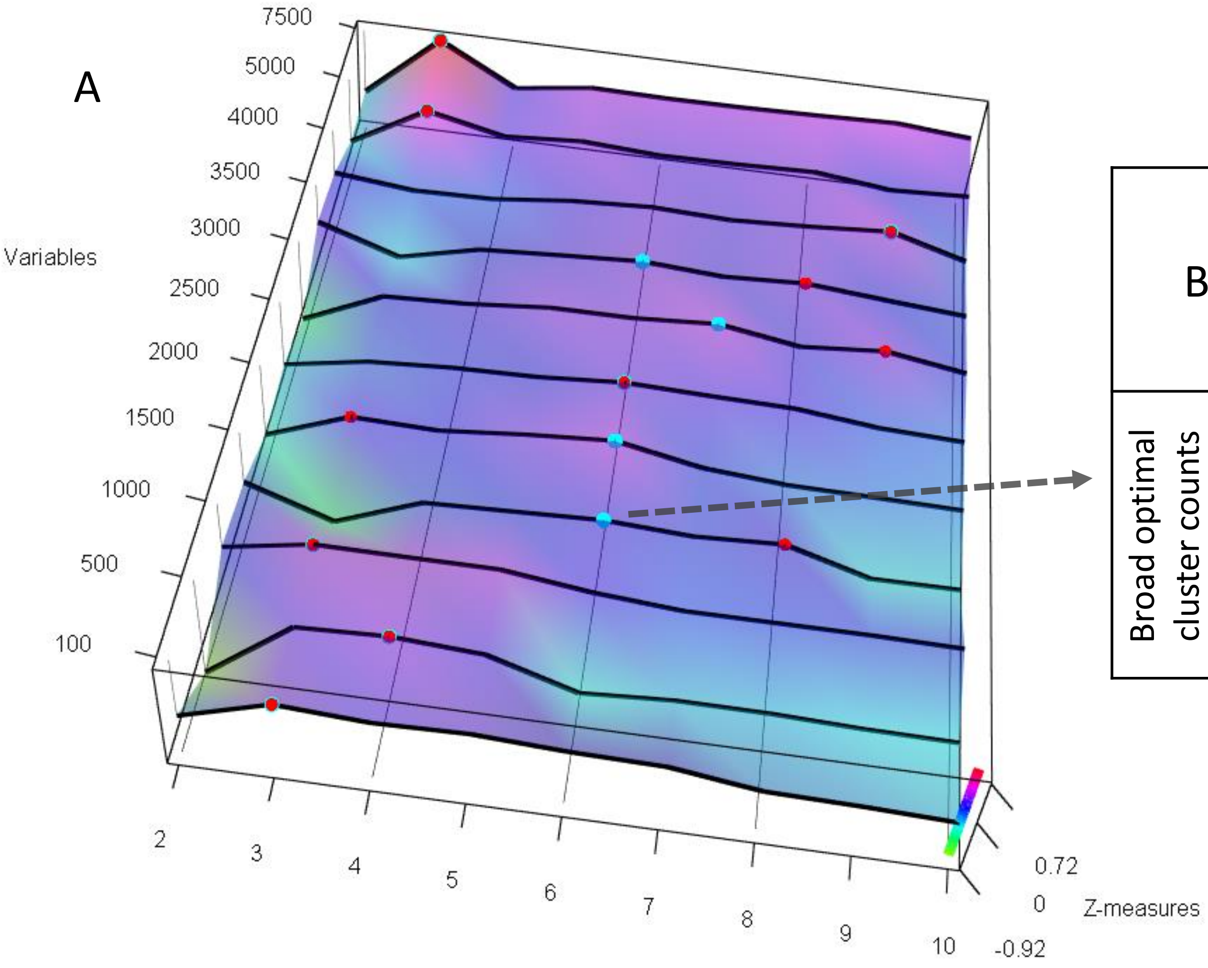
Supplemental Figure S3. COMMUNAL output for the Broad renal cell carcinoma (KIRC). (A) 3D map of K vs. genes included vs. standardized validity measures showing highly stable optima at K=2 and K=4. (B, C) Comparison of COMMUNAL core cluster assignment counts vs. Broad CCP-hierarchical cluster assignment counts at 1500 genes for (B) K=2 (lambda= 1.0) and (C) K=4 (lambda=0.97).



B		COMMUNAL optimal cluster counts at 1500 genes	
		1	2
Broad optimal cluster counts	1	46	1
	2	56	0
	3	24	27

C		COMMUNAL optimal cluster counts at 1500 genes					
		1	2	3	4	5	NA
Broad optimal cluster counts	1	14	0	16	0	0	17
	2	0	53	1	0	0	2
	3	0	0	22	13	9	7

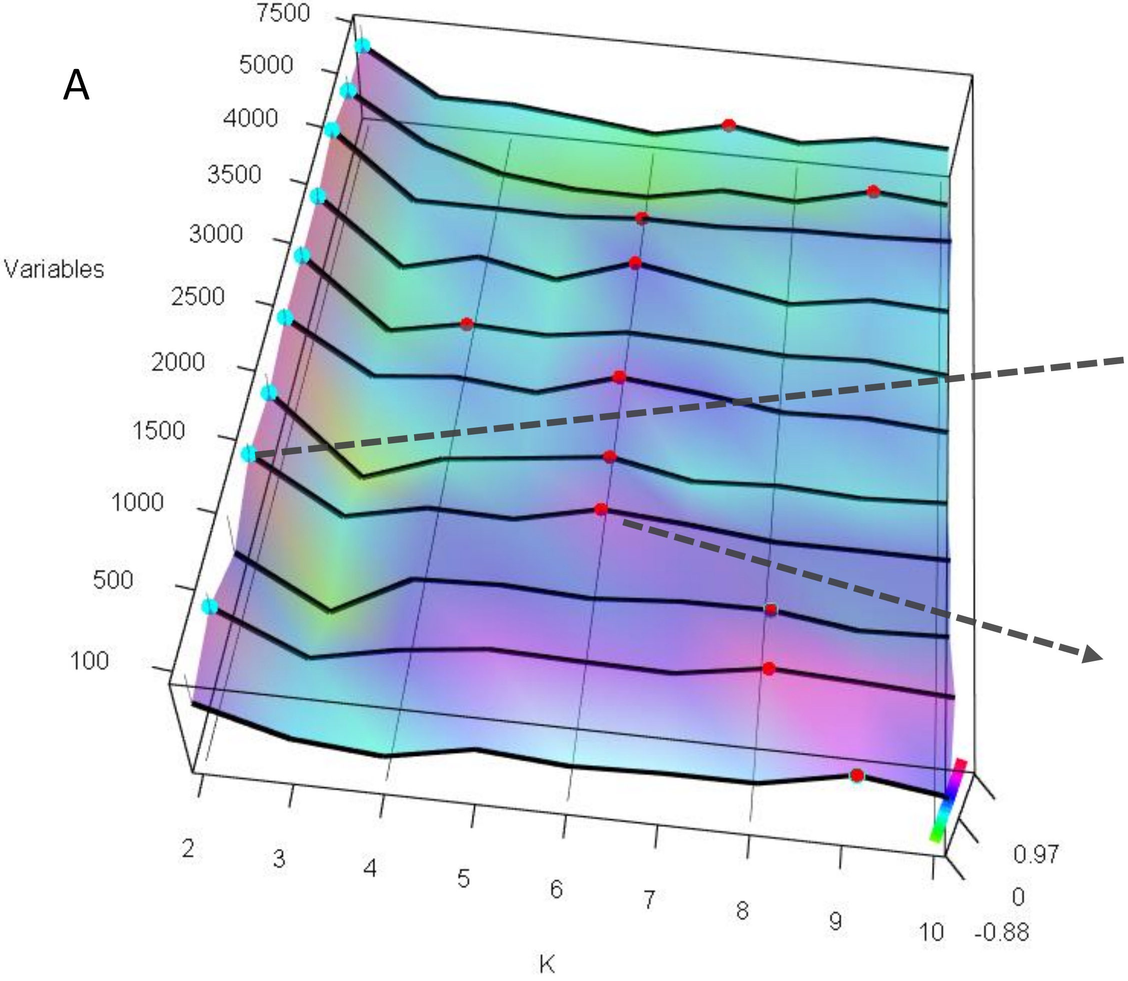
Supplemental Figure S4. COMMUNAL output for lung squamous cell carcinoma (LUSC). (A) 3D map of K vs. genes included vs. standardized validity measures showing stability, at K=2 and then K=5→6. (B, C) Comparison of COMMUNAL core cluster assignment counts vs. Broad CCP-hierarchical cluster assignment counts at 1500 genes; (B) at K=2, lambda=0.27; (C) at K=5, lambda=0.73.



B		COMMUNAL optimal cluster counts at 1500 genes						
		1	2	3	4	5	6	NA
Broad optimal cluster counts	1	106	19	0	10	69	17	96
	2	3	141	0	0	8	0	10
	3	3	5	0	75	0	0	7

Supplemental Figure S5. COMMUNAL output for ovarian cancer (OV). (A) 3D map of K vs. genes included vs. standardized validity measures has no stable clustering, showing the importance of testing over multiple gene sets. (B) Comparison of COMMUNAL core cluster assignment counts vs. Broad CCP-hierarchical cluster assignment counts at 1500 genes; at K=6, lambda=0.74.

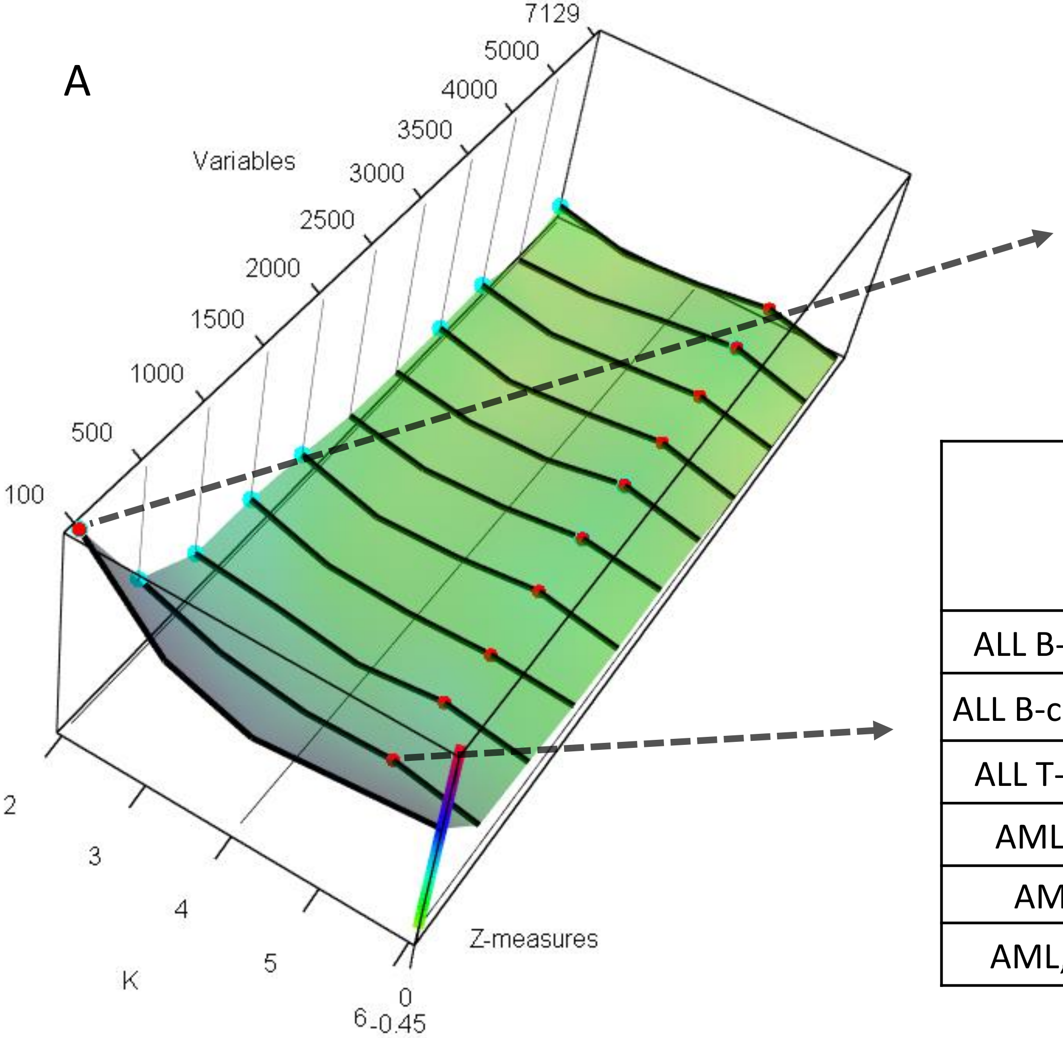
A



B		COMMUNAL optimal cluster	
		1	2
Broad optimal cluster counts	1	9	5
	2	10	0
	3	0	7
	4	0	7
	5	0	16

C		COMMUNAL optimal cluster counts at 1500 genes						
		1	2	3	4	5	6	NA
Broad optimal cluster counts	1	3	4	2	0	0	1	4
	2	0	0	0	0	0	10	0
	3	0	0	6	0	0	0	1
	4	0	0	7	0	0	0	0
	5	0	0	0	12	0	0	4

Supplemental Figure S6. COMMUNAL output for uterine corpus endometrial carcinoma (UCEC). (A) 3D map of K vs. genes included vs. standardized validity measures shows unstable clustering except at K=2. (B, C) Comparison of COMMUNAL core cluster assignment counts vs. Broad CCP-hierarchical cluster assignment counts at 1500 genes for (B) K=2 (lambda= 0.74) and (C) K=6 (lambda=0.63).



B	COMMUNAL optimal cluster counts at 100 genes		
Type	1	2	NA
ALL B-cell	34	3	1
ALL T-cell	7	2	0
AML	16	8	0

C	COMMUNAL optimal cluster counts at 1500 genes					
	1	2	3	4	5	NA
ALL B-cell, DFCI	29	2	2	0	2	0
ALL B-cell, St-Jude	0	3	0	0	0	0
ALL T-cell, DFCI	1	0	1	0	7	0
AML, CALGB	1	1	2	9	0	1
AML, CCG	1	2	1	1	0	0
AML, St-Jude	0	5	0	0	0	0

Supplemental Figure S7. COMMUNAL assessment of the entire Golub leukemia dataset. (A) 3D map of K vs. genes included vs. standardized validity measures showing optima at K=2 and K=4. (B) Core cluster assignment counts at K=2 at 100 genes vs. main leukemia type. (C) Core cluster assignment counts at K=4 at 500 genes vs. leukemia subtypes (AML, ALL-T-Cell and ALL-B-Cell); lambda = 0.15. (D) Core cluster assignment counts at K=5 at 500 genes vs. hospital enrollment sites; lambda = 0.58.

Supplemental Table S1. Listing of algorithms and metrics used in each 3D plot of COMMUNAL.

BRCA	
Algorithms	hierarchical, kmeans, som, sota, pam, agnes
Measures	gap statistic, dunn index 2, dunn index, g3
COADREAD	
Algorithms	hierarchical, kmeans, som, pam, agnes
Measures	gap statistic, dunn index, g3, dunn index 2
GBM	
Algorithms	hierarchical, kmeans, som, pam, clara, agnes
Measures	Widest gap, dunn index, g3, min. separation
KIRC	
Algorithms	hierarchical, kmeans, som, agnes
Measures	gap statistic, avg. between, g2, g3
LUSC	
Algorithms	hierarchical, kmeans, som, pam, agnes
Measures	gap statistic, pearson gamma, dunn index, dunn index 2
OV	
Algorithms	hierarchical, kmeans, som, sota, pam, agnes
Measures	gap statistic, pearson gamma, g3, dunn index 2
UCEC	
Algorithms	hierarchical, kmeans, som, agnes
Measures	gap statistic, g2, dunn index, dunn index 2
Golub	
Algorithms	hierarchical, kmeans, som, pam, clara, agnes
Measures	gap statistic, widest gap, g3, dunn index 2, avg. silhouette