
Supplement of “A Network of Networks Approach for Modeling Interconnected Brain Tissue-Specific Networks”

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1 DESCRIPTION OF GOSPEL OPTIMIZATION PROBLEM

GOSPEL optimization Eq. (1) consists of the squared Frobenius norm term, the *graph-guided-fused-lasso* regularization term and the *lasso* regularization term. If $R_{j,k}^{(i)}$ of the *graph-guided-fused-lasso* regularization term is zero, the equation becomes solely dependant on the *lasso* regularization term. In order to better understand the regularizers in this equation, let us inspect the behavior of regression coefficients in the specific cases where $R_{j,k}^{(i)} = 0$ and $R_{j,k}^{(i)} = 1$.

The first term of Eq. (1) can be rewritten as

$$\begin{aligned} \|\tilde{\mathbf{K}}^{(i)} - \sum_{j=1}^p \beta_j^{(i)} \tilde{\mathbf{K}}^{(j)}\|_F^2 = & \text{CKA}(\tilde{\mathbf{K}}^{(i)}, \tilde{\mathbf{K}}^{(i)}) \\ & - 2 \sum_{j=1}^p \beta_j^{(i)} \text{CKA}(\tilde{\mathbf{K}}^{(i)}, \tilde{\mathbf{K}}^{(j)}) + \sum_{j,k=1}^p \beta_j^{(i)} \beta_k^{(i)} \text{CKA}(\tilde{\mathbf{K}}^{(j)}, \tilde{\mathbf{K}}^{(k)}). \end{aligned} \quad (1)$$

In Eq. (1), the first term $\text{CKA}(\tilde{\mathbf{K}}^{(i)}, \tilde{\mathbf{K}}^{(i)}) = 1$, and thus it does not influence the GOSPEL optimization problem. The second term $\text{CKA}(\tilde{\mathbf{K}}^{(i)}, \tilde{\mathbf{K}}^{(j)})$ expresses the correlation between $\tilde{\mathbf{K}}^{(i)}$ and $\tilde{\mathbf{K}}^{(j)}$ which are associated with the response network and the j -th predictor network respectively.

If $\tilde{\mathbf{K}}^{(i)}$ and $\tilde{\mathbf{K}}^{(j)}$ are highly correlated and $R_{j,k}^{(i)} = 0$, $\beta_j^{(i)}$ takes any real value except zero. This means that the response and the j -th predictor have a relationship. On the other hand, when $\tilde{\mathbf{K}}^{(i)}$ and $\tilde{\mathbf{K}}^{(j)}$ are uncorrelated, and further $R_{j,k}^{(i)} = 0$, $\beta_j^{(i)}$ tends to be zero and is eliminated because of the *lasso* regularizer. This shows that the response and the j -th predictor have no relationship.

The third term in Eq. (1) indicates the correlation between $\tilde{\mathbf{K}}^{(j)}$ and $\tilde{\mathbf{K}}^{(k)}$ which respectively correspond to the j -th and the k -th predictor networks. In cases where $\tilde{\mathbf{K}}^{(j)}$ and $\tilde{\mathbf{K}}^{(k)}$

are highly correlated, i.e. $R_{j,k}^{(i)} = 1$, the *graph-guided-fused-lasso* regularization works so that $\beta_j^{(i)}$ and $\beta_k^{(i)}$ take similar values. Specifically, when $\tilde{\mathbf{K}}^{(i)}$ and $\tilde{\mathbf{K}}^{(j)}$ are highly correlated and further $R_{j,k}^{(i)} = 1$, both $\beta_j^{(i)}$ and $\beta_k^{(i)}$ tend to be similar values excluding zero. This indicates that both the j -th and the k -th predictors are related to the response. To the contrary, when $\tilde{\mathbf{K}}^{(i)}$ and $\tilde{\mathbf{K}}^{(j)}$ are uncorrelated and $R_{j,k}^{(i)} = 1$, both $\beta_j^{(i)}$ and $\beta_k^{(i)}$ tend to take zero. This means that both the j -th and the k -th predictors are unrelated to the response.

2 SUPPLEMENT FOR SECTION 3.2

2.1 COMPARISON BETWEEN THE NETWORK GRAPHS CONSTRUCTED BY THE NON MODEL AND BY CKA PAIR

In the process of performing GOSPEL, we must first compute a correlation between every pair of networks (CKA pair). If we examine the results of this computation without performing GOSPEL, we can observe how the results of real data changes.

Figure 1 shows the network graphs constructed by the NoN model (GOSPEL), and by CKA pair. The result of CKA pair is not sparse, and thus interpreting the obtained network becomes difficult.

Next, in order to quantitatively compare the results, we compute the link consistency between BTO, TC, and CKA pair. Table 1 indicates the results of the link consistency, and it shows that result of CKA pair is not similar to either BTO or TC. This lack of similarity is caused by large numbers of false positive, namely the non-sparsity of the CKA pair result. One of the reasons for this non-sparsity may be related to how the threshold of the CKA values is determined.

In GOSPEL, CKA pair is used to create a correlation matrix \mathbf{R} in the computation process, and \mathbf{R} is automatically optimized by the Bayesian optimization. CKA pair should be calculated by the optimal kernel parameter, γ , and the threshold of correlation matrix, τ , which must both be determined appropriately to ensure the fused lasso regularization term works properly.

The optimization of τ can be substituted by conducting an independence test on CKA pair, however, the independence test takes a huge computation time and is therefore expensive. Moreover, the optimization of the kernel parameter, γ , may be impossible in CKA pair. Taking these issues into consideration, the benefit of using of GOSPEL becomes clear.

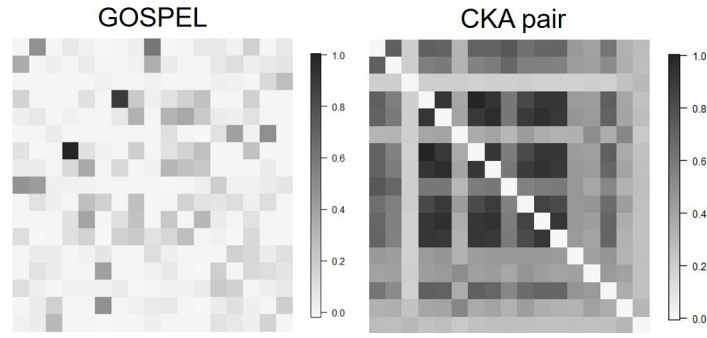


Figure 1: Network graphs constructed by the Non model (GOSPEL), and CKA pair. The left image is a network graph created by the coefficients obtained by GOSPEL. The right image is a network graph created by CKA values. Both network graphs are normalized, and the diagonal elements of the CKA pair result are changed from 1 to 0, for easy visibility. The kernel parameter of CKA is fixed to an optimum value selected by GOSPEL.

Table 1: Link consistency between BTO, TC, and CKA pair. The CKA values below 0.7 are set to 0 prior to calculation.

	#Regions	TP	FP	TN	FN	Consistency
BTO	17	18	100	14	4	0.235
TC	14	8	55	20	8	0.308

2.2 FIGURES, TABLES, AND LISTS

Table 2: Regression coefficients obtained by performing GOSPEL. In Figure 1 of the paper, edges below the 70-th percentile of the whole coefficients are removed for easy visibility.

	Amygdala	Caudate nucleus	Caudate putamen	Cerebellar cortex	Dentate gyrus	Frontal lobe	Hippocampus	Hypophysis	Hypothalamus
Amygdala	0	0.226	0.005	0.016	0	0.02	0.036	0.062	0.027
Caudate nucleus	0.264	0	0.013	0	0	0.033	0.091	-0.003	0
Caudate putamen	0.006	0	0	0.014	0	0.328	0	0.01	0.133
Cerebellar cortex	0.004	0	0.007	0	0.285	0	0	0.091	0.134
Dentate gyrus	0	0	0	0.29	0	0	0	0.011	0.06
Frontal lobe	0.009	0.016	0.426	0.014	-0.014	0	0	0.121	0.037
Hippocampus	0.061	0.131	0	0	0.01	0.06	0	0.165	0
Hypophysis	0.009	-0.008	0.003	0.116	0.012	0.083	0.03	0	0.144
Hypothalamus	0.006	0.001	0.081	0.123	0.052	0.004	0	0.099	0
Nucleus accumbens	0	0.008	0.026	0.07	0.34	0	0	0.017	0.033
Occipital lobe	0.025	0.006	0.244	0.08	-0.001	0.25	0	0.021	0.043
Parietal lobe	0	0	0.006	0.01	0.009	0	0	0	0.016
Pons	0	0	0.02	0.035	-0.009	0.006	0	0.021	0.056
Substantia nigra	0.274	0.167	0.003	0	0	0	0.067	0.064	0.027
Subthalamic nucleus	0.184	0.175	0	0.079	0.118	0	0.001	0.019	0.052
Temporal lobe	0.059	0.139	0.023	0	0	0.114	0.635	0.121	0
Thalamus	0.106	0.136	0.059	-0.012	-0.008	0.079	0.119	0.094	0.008

	Nucleus accumbens	Occipital lobe	Parietal lobe	Pons	Substantia nigra	Subthalamic nucleus	Temporal lobe	Thalamus
Amygdala	0	0.041	0	0.004	0.26	0.221	0.009	0.14
Caudate nucleus	0.03	0.027	0	0.001	0.172	0.214	0.094	0.15
Caudate putamen	0.032	0.303	0.018	0.051	0	-0.009	0.01	0.016
Cerebellar cortex	0.08	0.058	0.029	0.052	0	0.038	0.004	-0.011
Dentate gyrus	0.352	0	0.035	0	0	0.065	0	-0.008
Frontal lobe	0	0.335	0.004	0.036	0	-0.01	0.037	0.037
Hippocampus	0	-0.014	0	0	0.115	0.061	0.707	0.175
Hypophysis	0.017	0.023	0	0.037	0.011	0.011	0.009	0.028
Hypothalamus	0.032	0.029	0.03	0.07	0.002	0.016	0	0
Nucleus accumbens	0	0.03	0.118	0.127	0	0.036	0	-0.007
Occipital lobe	0.042	0	0.019	0.054	0	0.031	0	0
Parietal lobe	0.088	0.002	0	0.189	0	0.004	0	0
Pons	0.107	0.026	0.199	0	0	0	0	0
Substantia nigra	0	-0.001	0	0	0	0.155	0.055	0.21
Subthalamic nucleus	0.076	0.056	0.019	0	0.108	0	0.002	0.056
Temporal lobe	0	-0.004	0	0	0.121	0.062	0	0.166
Thalamus	-0.004	-0.012	0	0	0.187	0.101	0.071	0

Table 3: The Gyral regions in Table 1 of Yahata *et al.*, (2016) and its corresponding subregions used in our experiment. ‘N/A’ means ‘not Applicable’. The colored lines indicate abnormal functional connections corresponding to our experiment.

ID	Gyral region		Subregion		ID	Gyral region		Subregion	
1	(4)	— (6)	Frontal lobe	— Frontal lobe	9	(1)	— (15)	Frontal lobe	— Parietal lobe
2	(21)	— (22)	N/A	— N/A	10	(26)	— (20)	Caudate nucleus	— N/A
3	(28)	— (23)	Thalamus	— N/A	11	(8)	— (17)	Frontal lobe	— Occipital lobe
4	(24)	— (25)	Amygdala	— Caudate nucleus	12	(27)	— (9)	N/A	— Temporal lobe
5	(12)	— (8)	Hippocampus	— Frontal lobe	13	(29)	— (9)	N/A	— Temporal lobe
6	(11)	— (3)	Temporal lobe	— Frontal lobe	14	(14)	— (7)	Parietal lobe	— Frontal lobe
7	(10)	— (13)	Temporal lobe	— Temporal lobe	15	(5)	— (18)	Frontal lobe	— Occipital lobe
8	(13)	— (2)	Temporal lobe	— Frontal lobe	16	(3)	— (19)	Frontal lobe	— Occipital lobe

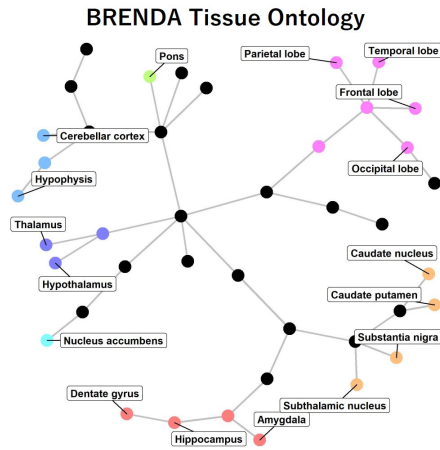


Figure 2: The hierarchical structure of tissues determined by BTO. The color of the nodes are associated with Table 3 in the paper. Black nodes are not included in our experiment, since they represent higher subregions than the 17 subregions in the hierarchy utilized by our experiment.

Path from the amygdala to the occipital lobe

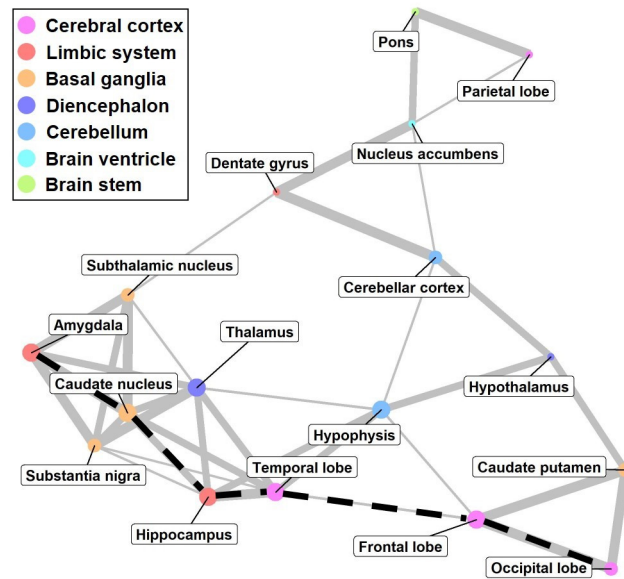


Figure 3: The path from the amygdala to the occipital lobe containing the 4 abnormal connections consistent with NoN and *Yahata et al., 2016*.



Figure 4: Plots for the diffusion kernels of subregions where the response subregion is the amygdala. For this plot, we shift the values of the diffusion kernels so that they have positive values, and compute the base 2 logarithm of these positive values. Then, we assign 0 to all values below the 75-th percentile of the values of the logarithm, and normalize the values above the 75-th percentile of the values of the logarithm. The rows and columns of the diffusion kernels are sorted according to the result of the community extraction (*Pons and Latapy, 2006*) conducted for the adjacency matrix of the amygdala. This means that we display these plots after rearranging the genes in descending order of the community sizes. The predictors are sorted in descending order of coefficients.



Figure 5: Plots for the diffusion kernels of subregions where the response subregion is the caudate nucleus. For this plot, we shift the values of the diffusion kernels so that they have positive values, and compute the base 2 logarithm of these positive values. Then, we assign 0 to all values below the 75-th percentile of the values of the logarithm, and normalize the values above the 75-th percentile of the values of the logarithm. The rows and columns of the diffusion kernels are sorted according to the result of the community extraction (*Pons and Latapy, 2006*) conducted for the adjacency matrix of the caudate nucleus. This means that we display these plots after rearranging the genes in descending order of the community sizes. The predictors are sorted in descending order of coefficients.

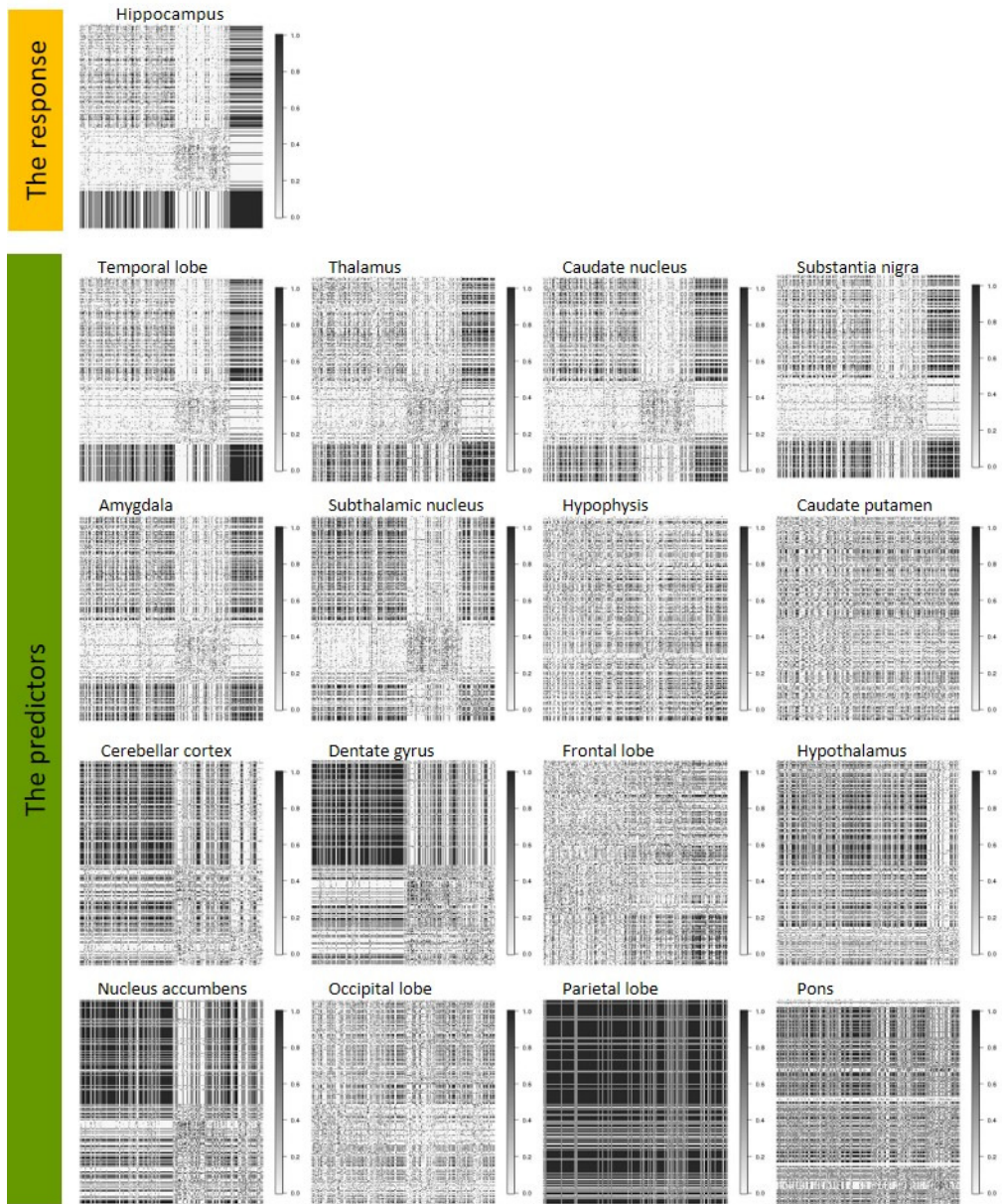


Figure 6: Plots for the diffusion kernels of subregions where the response subregion is the hippocampus. For this plot, we shift the values of the diffusion kernels so that they have positive values, and compute the base 2 logarithm of these positive values. Then, we assign 0 to all values below the 75-th percentile of the values of the logarithm, and normalize the values above the 75-th percentile of the values of the logarithm. The rows and columns of the diffusion kernels are sorted according to the result of the community extraction (*Pons and Latapy, 2006*) conducted for the adjacency matrix of the hippocampus. This means that we display these plots after rearranging the genes in descending order of the community sizes. The predictors are sorted in descending order of coefficients.

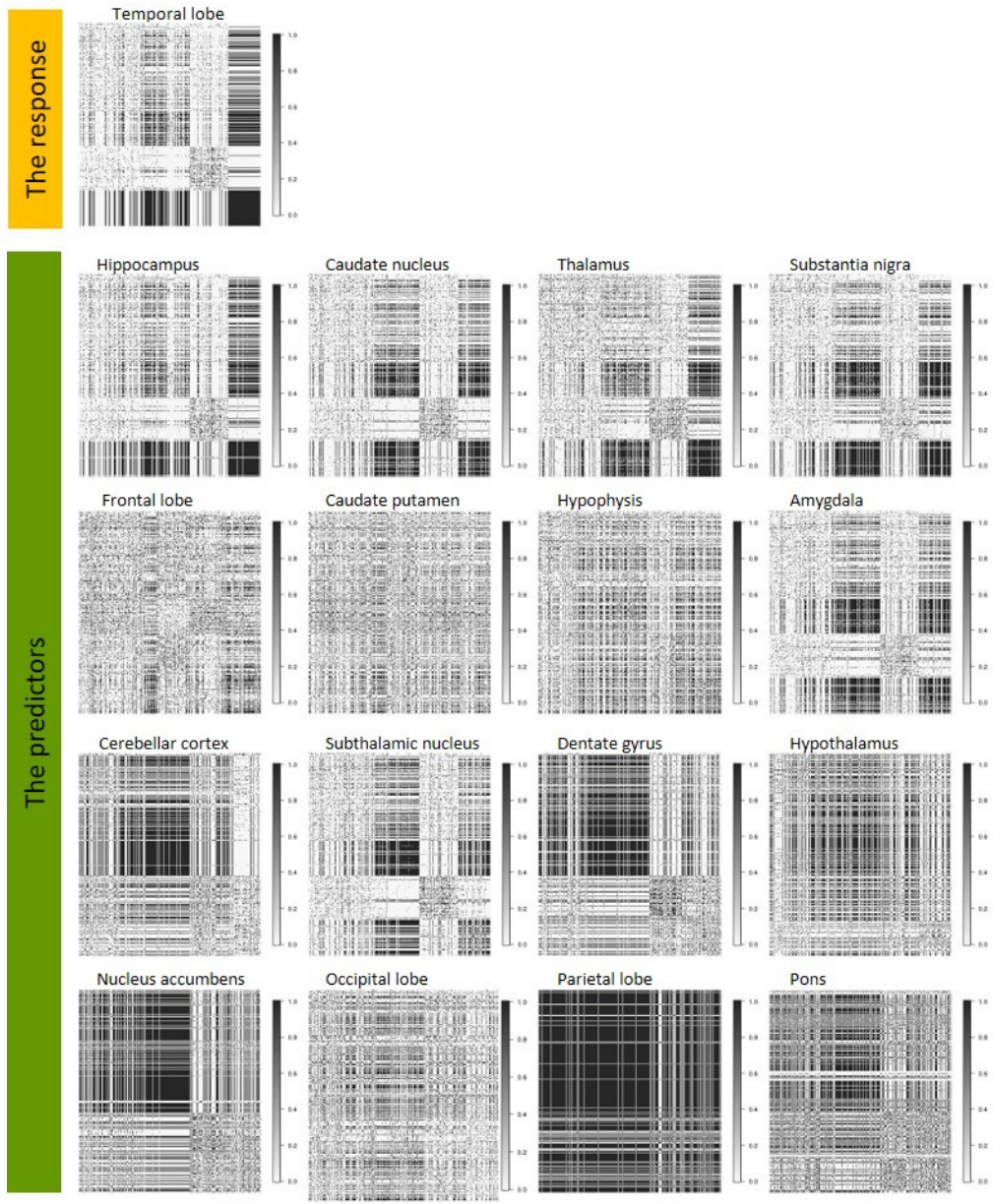


Figure 7: Plots for the diffusion kernels of subregions where the response subregion is the temporal lobe. For this plot, we shift the values of the diffusion kernels so that they have positive values, and compute the base 2 logarithm of these positive values. Then, we assign 0 to all values below the 75-th percentile of the values of the logarithm, and normalize the values above the 75-th percentile of the values of the logarithm. The rows and columns of the diffusion kernels are sorted according to the result of the community extraction (*Pons and Latapy, 2006*) conducted for the adjacency matrix of the temporal lobe. This means that we display these plots after rearranging the genes in descending order of the community sizes. The predictors are sorted in descending order of coefficients.

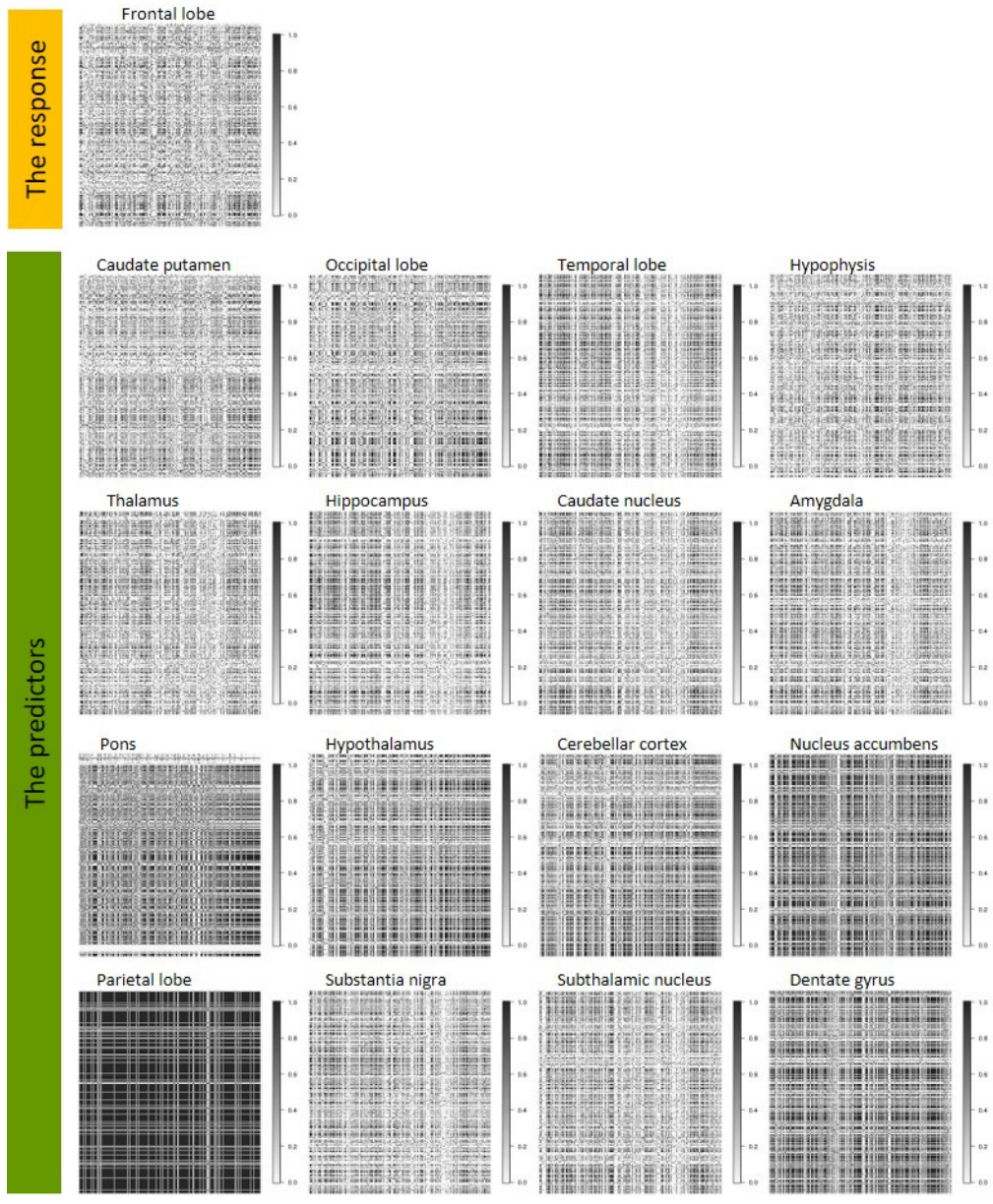


Figure 8: Plots for the diffusion kernels of subregions where the response subregion is the frontal lobe. For this plot, we shift the values of the diffusion kernels so that they have positive values, and compute the base 2 logarithm of these positive values. Then, we assign 0 to all values below the 75-th percentile of the values of the logarithm, and normalize the values above the 75-th percentile of the values of the logarithm. The rows and columns of the diffusion kernels are sorted according to the result of the community extraction (*Pons and Latapy, 2006*) conducted for the adjacency matrix of the frontal lobe. This means that we display these plots after rearranging the genes in descending order of the community sizes. The predictors are sorted in descending order of coefficients.

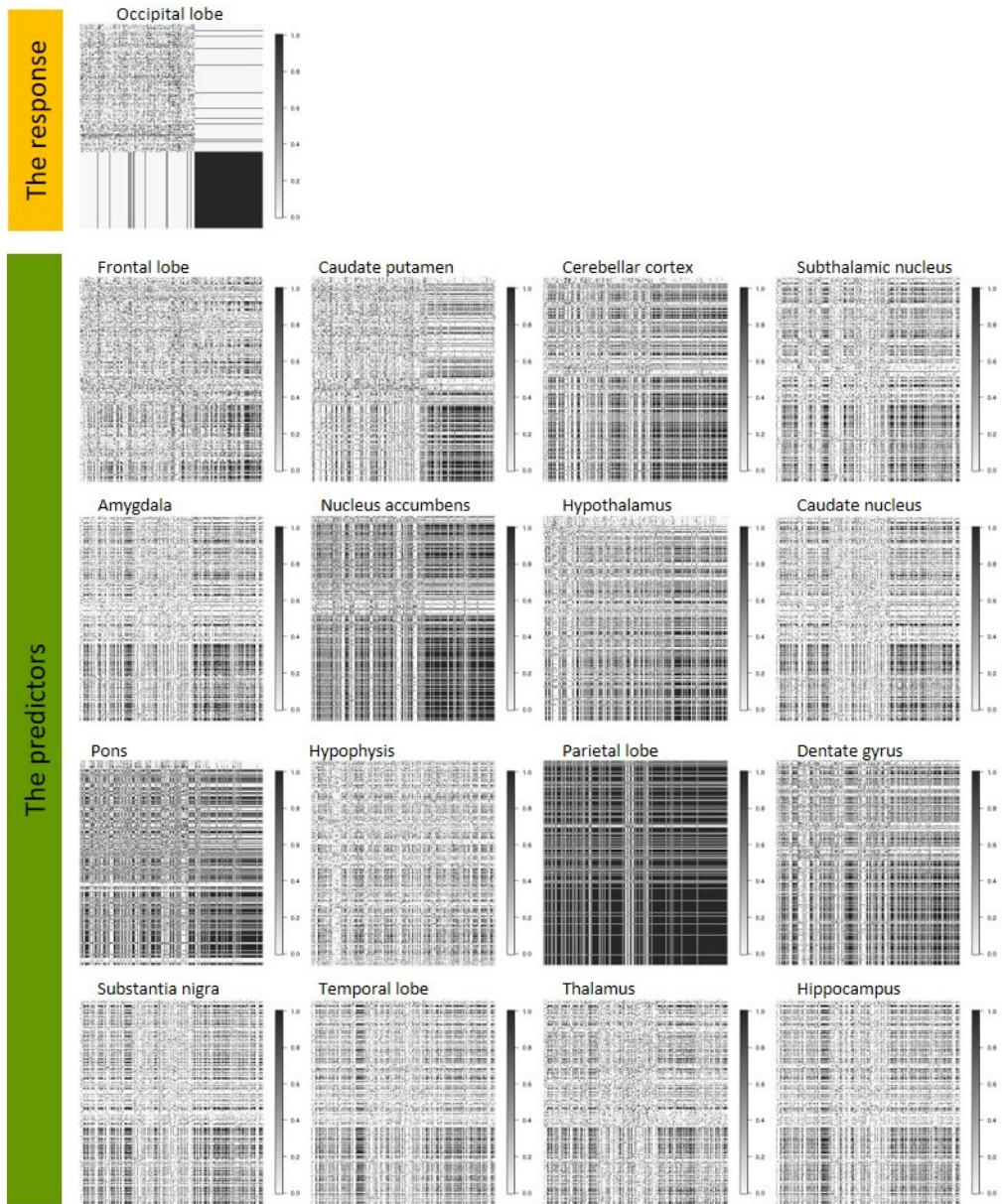


Figure 9: Plots for the diffusion kernels of subregions where the response subregion is the occipital lobe. For this plot, we shift the values of the diffusion kernels so that they have positive values, and compute the base 2 logarithm of these positive values. Then, we assign 0 to all values below the 75-th percentile of the values of the logarithm, and normalize the values above the 75-th percentile of the values of the logarithm. The rows and columns of the diffusion kernels are sorted according to the result of the community extraction (*Pons and Latapy, 2006*) conducted for the adjacency matrix of the occipital lobe. This means that we display these plots after rearranging the genes in descending order of the community sizes. The predictors are sorted in descending order of coefficients.

List 1: Gene ID for autism risk genes introduced in Entrez Databases (<https://www.ncbi.nlm.nih.gov/Class/MACourse/Original8Hour/Entrez/>).

1030, 2, 344752, 19, 10349, 26154, 154664, 20, 10347, 340273, 94160, 25890, 32, 653857, 100, 53616, 80332, 111, 115, 266977, 84059, 23394, 158, 159, 2334, 116986, 84871, 55750, 392636, 26523, 192670, 64902, 79026, 113146, 57491, 11214, 10142, 220, 7915, 226, 8092, 262, 270, 275, 10393, 287, 288, 29123, 23294, 124401, 63982, 203859, 8125, 84168, 301, 26, 8120, 321, 51107, 345, 9870, 83478, 257106, 9743, 50649, 9459, 23229, 57492, 10865, 151188, 410, 416, 347527, 153642, 170302, 51665, 55870, 438, 444, 23245, 80816, 57205, 23200, 84239, 344905, 481, 23439, 493, 550, 26053, 552, 126792, 2683, 582, 53335, 10018, 9774, 63035, 627, 139105, 57448, 55589, 128861, 675, 23774, 8019, 9024, 54014, 696, 699, 147685, 148345, 26005, 54980, 718, 339883, 55262, 57685, 775, 776, 777, 8912, 55799, 93589, 783, 23705, 93664, 814, 821, 11132, 4076, 113201, 8573, 9139, 867, 8535, 57805, 64770, 343099, 317762, 440193, 60492, 10344, 977, 283316, 146722, 9578, 55536, 1008, 1009, 1012, 1016, 1003, 1006, 6792, 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List 2: Gene ID for schizophrenia risk genes introduced in Entrez Databases (<https://www.ncbi.nlm.nih.gov/Class/MLACourse/Original8Hour/Entrez/>).

844, 10157, 154664, 20, 23461, 26090, 3983, 390110, 2532, 48, 50, 2182, 51703, 59, 10880, 87, 6868, 8756, 9510, 81794, 170689, 170691, 9508, 11174, 57188, 115, 221393, 27245, 221264, 10142, 207, 64400, 211, 214, 126133, 160428, 7915, 7840, 246, 155185, 51433, 286, 29123, 118932, 57182, 56899, 316, 8943, 9907, 321, 348, 80831, 351, 116985, 10565, 9826, 22899, 57492, 196528, 415, 421, 427, 50807, 8853, 55870, 431705, 23245, 171023, 9140, 477, 481, 488, 493, 51606, 6310, 6311, 26053, 558, 27087, 10458, 580, 586, 607, 29760, 84446, 7809, 695, 56244, 122525, 284756, 65250, 647024, 389384, 203228, 56934, 23523, 774, 775, 8912, 8911, 779, 781, 9254, 93589, 783, 785, 10369, 811, 815, 816, 6650, 726, 10753, 84869, 23468, 57332, 387707, 64753, 728621, 57003, 284001, 886, 150160, 929, 9332, 283316, 998, 9578, 83879, 55536, 1003, 29965, 1033, 1036, 1952, 1951, 22897, 9859, 80184, 64781, 283848, 1108, 26038, 57680, 11200, 1114, 1116, 10752, 27243, 89832, 1139, 1145, 1146, 22856, 23152, 148113, 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List 3: Gene ID for neurodegenerative diseases risk genes introduced in Entrez Databases (<https://www.ncbi.nlm.nih.gov/Class/MLACourse/Original8Hour/Entrez/>).

334, 2, 19, 20, 10347, 5243, 9429, 176, 130013, 8754, 126, 154, 340351, 177, 221264, 57679, 258, 51434, 283, 88455, 328, 51107, 348, 351, 367, 23237, 64283, 387715, 9474, 10533, 23400, 540, 148229, 6310, 6311, 8312, 23621, 627, 274, 642, 342346, 84077, 203228, 8912, 255022, 857, 23607, 945, 1012, 1000, 1026, 55835, 118491, 3075, 1103, 400916, 51142, 1114, 25978, 1128, 1137, 1142, 170482, 1191, 1262, 23019, 1303, 1310, 1363, 56265, 1378, 1385, 1400, 1428, 1436, 1471, 29119, 1509, 8722, 1588, 1565, 10858, 1610, 1639, 163259, 1719, 196385, 146754, 1770, 23317, 1804, 1809, 1815, 1778, 340900, 1889, 1936, 253314, 1981, 2036, 2041, 2044, 285220, 83481, 79956, 2130, 100129583, 64839, 25793, 55277, 9896, 2318, 2332, 1112, 2357, 2358, 80144, 2495, 2521, 2580, 79690, 85569, 2617, 2629, 2643, 26058, 2717, 2733, 64689, 55668, 11250, 2904, 2896, 2932, 2947, 2952, 2968, 2976, 10013, 113802, 55008, 3074, 3077, 3163, 3176, 3178, 3181, 3184, 3303, 3313, 3315, 27429, 3552, 3553, 3569, 3570, 3709, 169522, 85449, 22920, 54758, 3816, 58508, 3920, 3929, 3938, 8994, 4023, 4036, 4040, 79705, 120892, 4060, 260425, 4129, 9479, 4137, 162333, 57787, 9782, 4223, 79091, 23269, 54903, 4311, 931, 64231, 245802, 58475, 4524, 84073, 8735, 140469, 4671, 10135, 23385, 4729, 4744, 4741, 4772, 123606, 22871, 84166, 51314, 64127, 4842, 4864, 10577, 4835, 4929, 4968, 4973, 10133, 390081, 5009, 135138, 167153, 11315, 55486, 5184, 5216, 84547, 8301, 5300, 65018, 5309, 8605, 8398, 5333, 23646, 57449, 91584, 6490, 10908, 5428, 5444, 5445, 5446, 5521, 5578, 5621, 5630, 5663, 5664, 55851, 5695, 5728, 2185, 5794, 57111, 116442, 5890, 8786, 126432, 25897, 10900, 950, 51156, 12, 23064, 10280, 23411, 6573, 6506, 7781, 254428, 55065, 200010, 6532, 57152, 6606, 6607, 6609, 6622, 9627, 27044, 6647, 6653, 6683, 80208, 6710, 8878, 10847, 26039, 27148, 9900, 23345, 8867, 8148, 138474, 23435, 29110, 6908, 6949, 7018, 10342, 80731, 80213, 29058, 7124, 8711, 7143, 10452, 7157, 66008, 54209, 79865, 285852, 205860, 54822, 8295, 146057, 7267, 7277, 7305, 29978, 7345, 23074, 23025, 8633, 7399, 9217, 7415, 7422, 7436, 55737, 55275, 7443, 9277, 11180, 7494, 7515, 7517, 57473, 9726