Slide 1: Kernel canonical correlation analysis, or KCCA, is an efficient way to detect brain activation globally with less computational complexity. In this presentation, we will introduce a new algorithm based on KCCA which allows us to get the activation pattern from general types of kernels.

Slide 2: We claim that there is no conflict of interest, the data is publicly accessible with patients' information properly protected, and this work is supported by NIH.

Slide 3: Here we summarized three common correlation-based methods to detect brain activation from fMRI. Single voxel smoothing computes the correlation on each voxel after a uniform spatial smoothing. Canonical correlation analysis works for multiple variables and can encode nonlinear relationships through constraints, but it has drawbacks for computational efficiency. KCCA is a global method that detects activation in single steps but is limited to a linear kernel. Our newly proposed nonlinear KCCA algorithm works for nonlinear kernels, so it preserves all three of these desired features.

Slide 4: Here we show a schematic diagram for the proposed method. Suppose the fMRI data is labeled with Y, and the design signal labeled with X. We want to find a voxel-specific parameter alpha to characterize the relationship between this voxel and the design signal. KCCA solves this problem by mapping X and Y to the kernel space and then finding the weights called wx and wy to maximize the correlation. To map it back to the original space, we propose a general assumption shown in the square by dimensional matching, then use two different ways to solve this equation. The first way is to compute the derivative from kernel space to the original space, with alpha measuring the importance of each voxel's contribution to the signal in kernel space. The second way is to solve this equation directly using pseudo inverse. Our analytical result shows for linear kernel, both methods give the same result up to a constant, which is equivalent to the previously published method.

Slide 5: The next step is choosing the kernel function. Here, we propose 8 types of common kernel functions, covering linear and nonlinear, bounded and unbounded, with the corresponding unknown hyperparameters shown on the right.

Slide 6: To optimize these hyperparameters, we propose an algorithm based on self-supervised learning, which does not need any ground truth. The idea is that isolated activated voxels are rare, therefore a good method will try to maintain the prediction results even after the voxel location has changed. First, we compute activation alpha from one kernel based on hyperparameter p, and we divide the voxels into two clusters. 10% of them with higher alpha values are activated, and 90% of them are nonactivated. Second, we change the voxel location inside each cluster based on its alpha value. For example, in the activated cluster, we exchange the location between voxels with the highest alpha and lowest alpha, then between voxels with the second highest and second lowest alpha, and so on. The same shuffling is repeated for nonactivated clusters. After shuffling the new fMRI data labeled with Y prime, we can then compute the activation pattern alpha prime based on the same p. Finally, the ROC curve is used to characterize the similarity between alpha and alpha prime, and we optimized p to maximize the area under the curve, or AUC.

Slide 7: We start from the simulated fMRI data generated from the HCP dataset. With a given ground truth shown in the top left corner. The activation pattern from 4 different kernels is shown in the middle, with the color indicating the top 10% of voxels with the highest alpha values. We can observe that the mixed hyperbolic tangent can avoid false activation, also proven by the ROC curve shown on the right. At the bottom, we compute the AUC ratio between different kernels and single voxel smoothing. Results based on 87 subjects show that mixed hyperbolic tangent has a 42% increment, while linear kernel only has a 12% increment compared with single voxel smoothing.

Slide 8: Here we show an example of real fMRI taken from the HCP dataset. The activation pattern is computed using different kernels and different back reconstruction algorithms. As activations usually appear the gray matter than non gray matter area. In the bottom right, we use ROC to show the overlap between activated voxels and gray matter, with the gray shading area indicating the results from single voxel smoothing. The mixed hyperbolic tangent has the maximum AUC, indicating it can mostly prevent activations in undesired regions.

Slide 9: We also do the group-level accuracy by computing the gray matter overlapping ratio between the different kernels and single voxel smoothing. The results based on 87 subjects show that the best kernel is the Mixed hyperbolic tangent under the second back construction algorithm, which on average gives us 23% more under the metric of gray matter overlapping.

Slide 10: To summarize our findings, we proposed a general way to compute activation patterns based on nonlinear kernels. We found that a nonlinear bounded kernel, such as a mixed hyperbolic tangent, can avoid activations outside gray matter. This result is proven by a group-level study on the HCP dataset.

We thank NIH for research support.

Thank you for your attention.