A   EXPERIMENTAL SETTINGS

In this section, we introduce the details of the settings in our experiments. Firstly, Table 7 is the number of neural datasets from three brain regions and Fig. 5 illustrates the training image of the neural stimuli. Secondly, the Table 8 and Table 9 are the settings of the hyperparameters for image reconstruction and neural similarity experiments, respectively. Thirdly, the Table 10 is the setting of the hyperparameters of different DAE-NR variants for image reconstruction experiments for image reconstruction on region 3 . Fourthly, the Table 11, Table 12 and Table 13 are the settings the hyperparameters of different DAE-NR variants for neural similarity experiments on Region 1,2 and 3, respectively.

Table 7: The neural dataset containing neural responses in three brain regions under visual stimulation Antolík et al. (2016). The number in bracket is the repeated times.

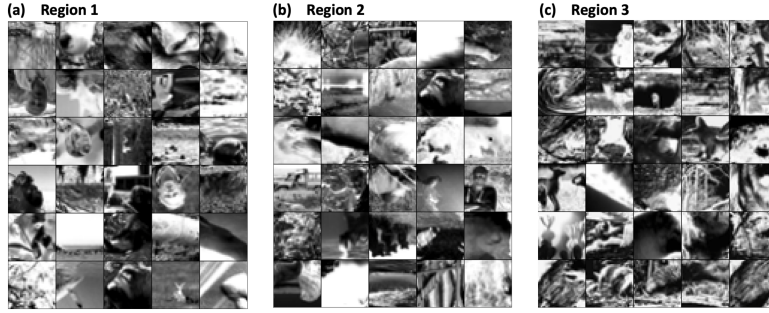|	Number of train images	Number of test images	Number of neurons
Region 1	1800 (1)	50 (10)	103
Region 2	1260 (1)	50 (8)	55
Region 3	1800 (1)	50 (12)	102

Figure 5: The examples of training stimuli in each brain region.

Table 8: The settings of the hyperparameters for image reconstruction experiments.

	Region 1	Region 2	Region 3
Models	$\alpha : \beta$	$\alpha : \beta$	$\alpha : \beta$
CAE-FR$_1$	1e-0:1e-5	1e-0:1e-3	1e-0:1e-4
CAE-FR$_2$	1e-0:1e-5	1e-0:1e-4	1e-0:1e-3
CAE-FR$_3$	1e-0:1e-4	1e-0:1e-3	1e-0:1e-5
CAE-FR$_4$	1e-0:1e-5	1e-0:1e-4	1e-0:1e-4

B   ADDITIONAL EXPERIMENTS

In this section, we provide results from additional experiments. Fig. 6 and Fig. 7 display the results of image reconstruction using the neural responses on the region 1 and 2. Fig. 8 shows the number of significant neurons and insignificant neurons of regions 1 and 2 in the image reconstruction experiments, respectively.

Table 9: The settings the hyperparameters for neural similarity experiments.

Models	Region 1 $\alpha : \beta$	Region 2 $\alpha : \beta$	Region 3 $\alpha : \beta$
CAE-FR$_1$	1e-0:9e-1	7e-1:1e-0	8e-1:1e-0
CAE-FR$_2$	7e-1:1e-0	1e-0:1e-2	4e-1:1e-0
CAE-FR$_3$	1e-0:6e-1	1e-4:1e-0	1e-0:4e-1
CAE-FR$_4$	1e-0:9e-1	1e-0:1e-2	1e-0:9e-1

Table 10: The settings the hyperparameters of different DAE-NR variants for image reconstruction experiments on region 3.

Models	h_1 $\alpha : \beta$	h_2 $\alpha : \beta$	h_3 $\alpha : \beta$	h_4 $\alpha : \beta$
CAE-FR	1e-0:1e-4	1e-0:5e-3	1e-0:1e-3	1e-0:1e-3
CAE-FC	1e-0:1e-4	1e-0:1e-4	1e-0:1e-4	1e-0:1e-4
CAE-FM	1e-0:2e-1	1e-0:1e-3	1e-0:1e-4	1e-0:1e-4
VAE-FR	1e-0:2e-2	1e-0:1e-2	1e-0:2e-1	1e-0:5e-3
VAE-FC	1e-0:1e-2	1e-0:5e-3	1e-0:1e-3	1e-0:1e-1
VAE-FM	1e-0:5e-3	1e-0:5e-2	1e-0:2e-1	1e-0:5e-3
VQ-VAE-FR	1e-0:2e-2	1e-0:2e-1	1e-0:1e-2	1e-0:1e-3
VQ-VAE-FC	1e-0:1e-3	1e-0:1e-4	1e-0:1e-4	1e-0:1e-4
VQ-VAE-FM	1e-0:2e-1	1e-0:1e-3	1e-0:1e-2	1e-0:1e-3

Table 11: The settings the hyperparameters of different DAE-NR variants for neural similarity experiments on Region 1

Models	h_1 $\alpha : \beta$	h_2 $\alpha : \beta$	h_3 $\alpha : \beta$	h_4 $\alpha : \beta$
CAE-FR	1e-0:5e-1	1e-0:5e-2	1e-0:5e-2	1e-0:1e-2
VAE-FR	1e-3:1e-0	2e-2:1e-0	1e-3:1e-0	1e-1:1e-0
VQ-VAE-FR	1e-0:2e-2	1e-0:2e-1	1e-0:5e-3	1e-0:2e-1
CAE-FC	5e-3:1e-0	1e-3:1e-0	2e-2:1e-0	1e-2:1e-0
VAE-FC	2e-2:1e-0	1e-0:1e-2	2e-1:1e-0	1e-3:1e-0
VQ-VAE-FC	1e-0:1e-1	1e-0:5e-1	1e-4:1e-0	1e-2:1e-0
CAE-FM	1e-2:1e-0	5e-1:1e-0	1e-0:1e-1	1e-0:5e-1
VAE-FM	1e-4:1e-0	1e-3:1e-0	1e-1:1e-0	1e-1:1e-0
VQ-VAE-FM	1e-1:1e-0	1e-1:1e-0	1e-0:1e-2	1e-0:1e-0

Table 12: The settings the hyperparameters of different DAE-NR variants for neural similarity experiments on Region 2

Models	h_1 $\alpha : \beta$	h_2 $\alpha : \beta$	h_3 $\alpha : \beta$	h_4 $\alpha : \beta$
CAE-FR	1e-0:2e-1	1e-0:2e-2	5e-3:1e-0	1e-0:5e-3
VAE-FR	5e-3:1e-0	2e-1:1e-0	5e-2:1e-0	5e-1:1e-0
VQ-VAE-FR	1e-0:1e-1	2e-1:1e-0	1e-0:1e-2	1e-0:2e-1
CAE-FC	1e-2:1e-0	5e-3:1e-0	1e-0:5e-2	1e-4:1e-0
VAE-FC	1e-2:1e-0	5e-3:1e-0	1e-0:5e-1	1e-4:1e-0
VQ-VAE-FC	1e-0:1e-0	5e-3:1e-0	1e-3:1e-0	1e-3:1e-0
CAE-FM	1e-0:1e-1	1e-0:1e-2	1e-0:5e-3	1e-0:5e-3
VAE-FM	5e-2:1e-0	1e-4:1e-0	5e-3:1e-0	2e-2:1e-0
VQ-VAE-FM	1e-0:5e-2	5e-2:1e-0	1e-0:1e-1	1e-0:5e-1

Table 13: The settings the hyperparameters of different DAE-NR variants for neural similarity experiments on Region 3

	h_1	h_2	h_3	h_4
Models	$\alpha : \beta$	$\alpha : \beta$	$\alpha : \beta$	$\alpha : \beta$
CAE-FR	1e-0:1e-1	1e-0:1e-0	1e-0:5e-2	1e-0:1e-2
VAE-FR	1e-0:1e-4	5e-1:1e-0	1e-2:1e-0	1e-0:1e-0
VQ-VAE-FR	1e-0:2e-1	1e-0:2e-2	1e-0:1e-0	1e-4:1e-0
CAE-FC	1e-0:2e-1	5e-2:1e-0	1e-0:1e-1	1e-0:2e-1
VAE-FC	1e-3:1e-0	1e-2:1e-0	5e-3:1e-0	2e-1:1e-0
VQ-VAE-FC	1e-1:1e-0	1e-3:1e-0	1e-2:1e-0	1e-4:1e-0
CAE-FM	5e-3:1e-0	1e-0:5e-3	1e-0:5e-1	1e-2:1e-0
VAE-FM	1e-3:1e-0	1e-0:2e-1	2e-2:1e-0	5e-2:1e-0
VQ-VAE-FM$_4$	1e-0:5e-1	1e-4:1e-0	1e-3:1e-0	1e-3:1e-0
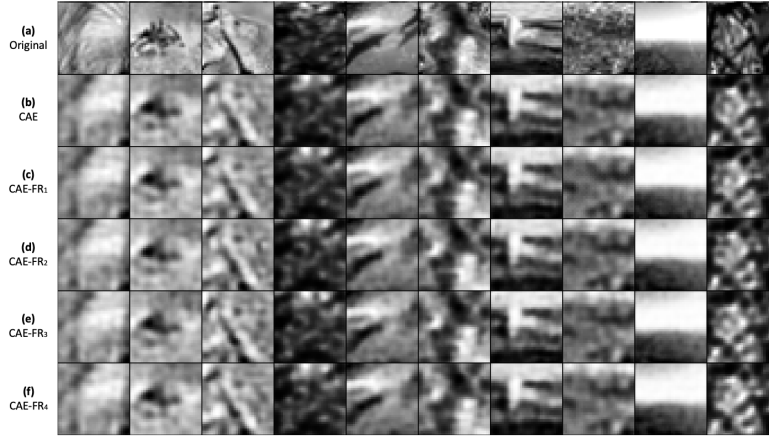
Figure 6: The reconstructed images with neurons in Region 1. From top to bottom, each row displays the original images (a), the images reconstructed by CAE (b), CAE-FR$_1$ (c), CAE-F$_2$ (d), CAE-F$_3$ (e), CAE-FR$_4$ (f), respectively.
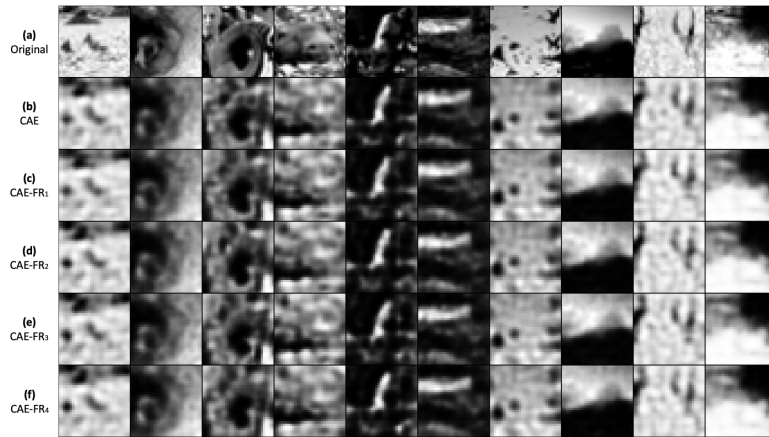
Figure 7: The reconstructed images with neurons in Region 2. From top to bottom, each row displays the original images (a), the images reconstructed by CAE (b), CAE-FR$_1$ (c), CAE-F$_2$ (d), CAE-F$_3$ (e), CAE-FR$_4$ (f), respectively.
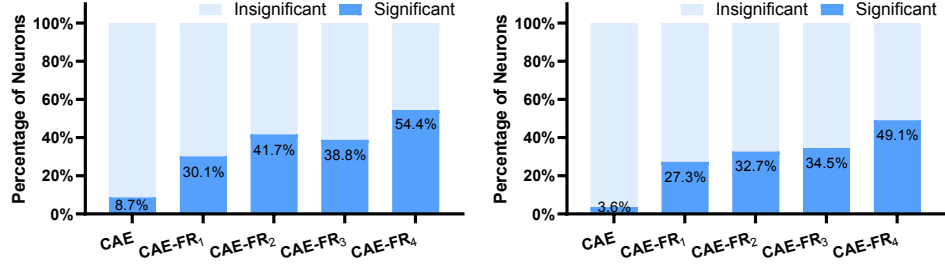
Figure 8: The number of significant neurons and insignificant neurons in region 1 and 2 in the image reconstruction experiments. The threshold for significance is $p \leq 0.05$.

Table 14: Network architecture. This architecture was used for DAE-NR.

Operation	kernel	stride	Features
Convolution	3×3	2×2	32
Convolution	3×3	1×1	32
Convolution	3×3	2×2	32
Convolution	3×3	1×1	32
Deconvolution	3×3	1×1	32
Deconvolution	3×3	2×2	32
Deconvolution	3×3	1×1	32
Deconvolution	3×3	2×2	1