Multivariate Analysis in fMRI
功能性磁共振成像中的多变量分析

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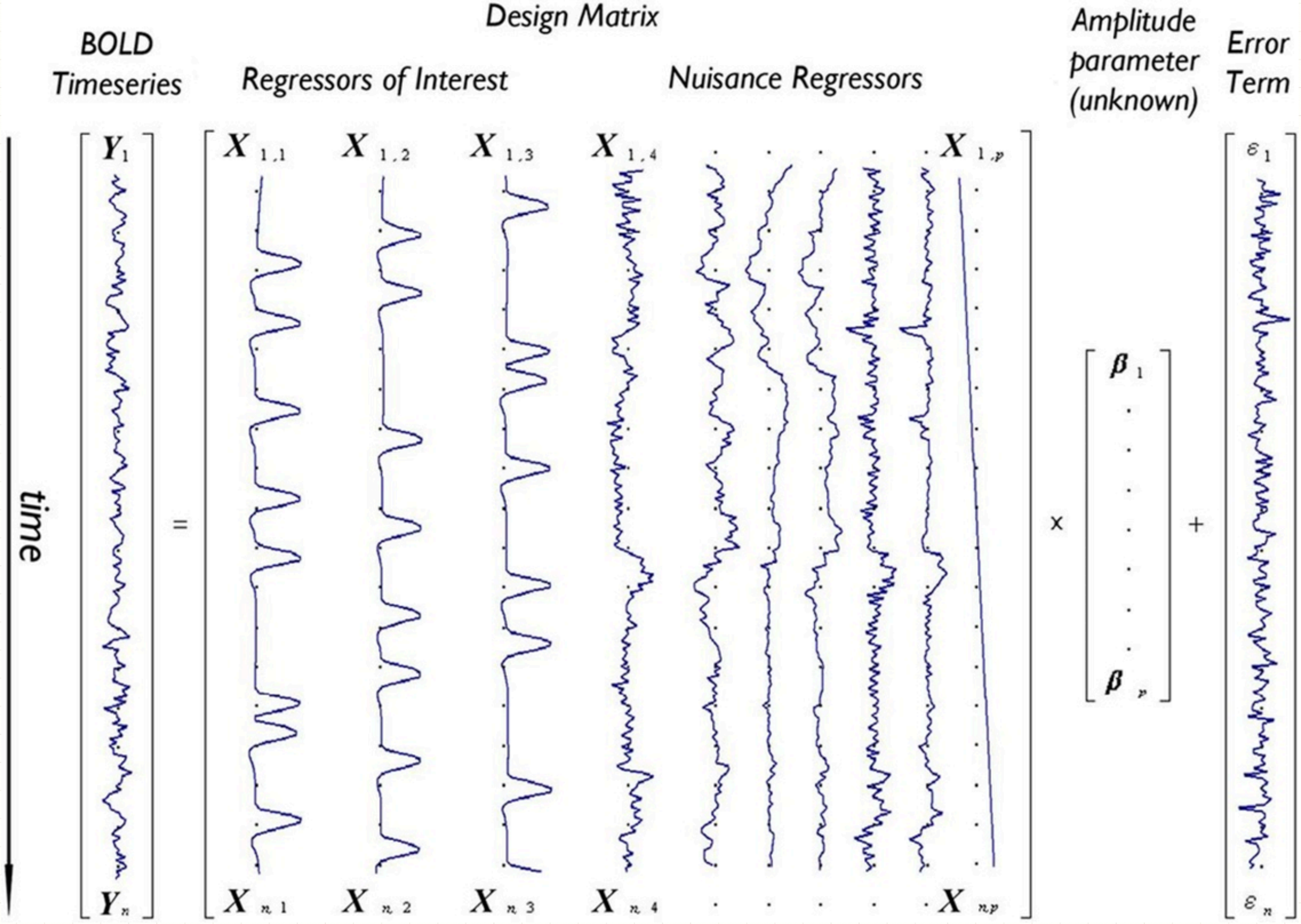
复习：一般线性模型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Error Term
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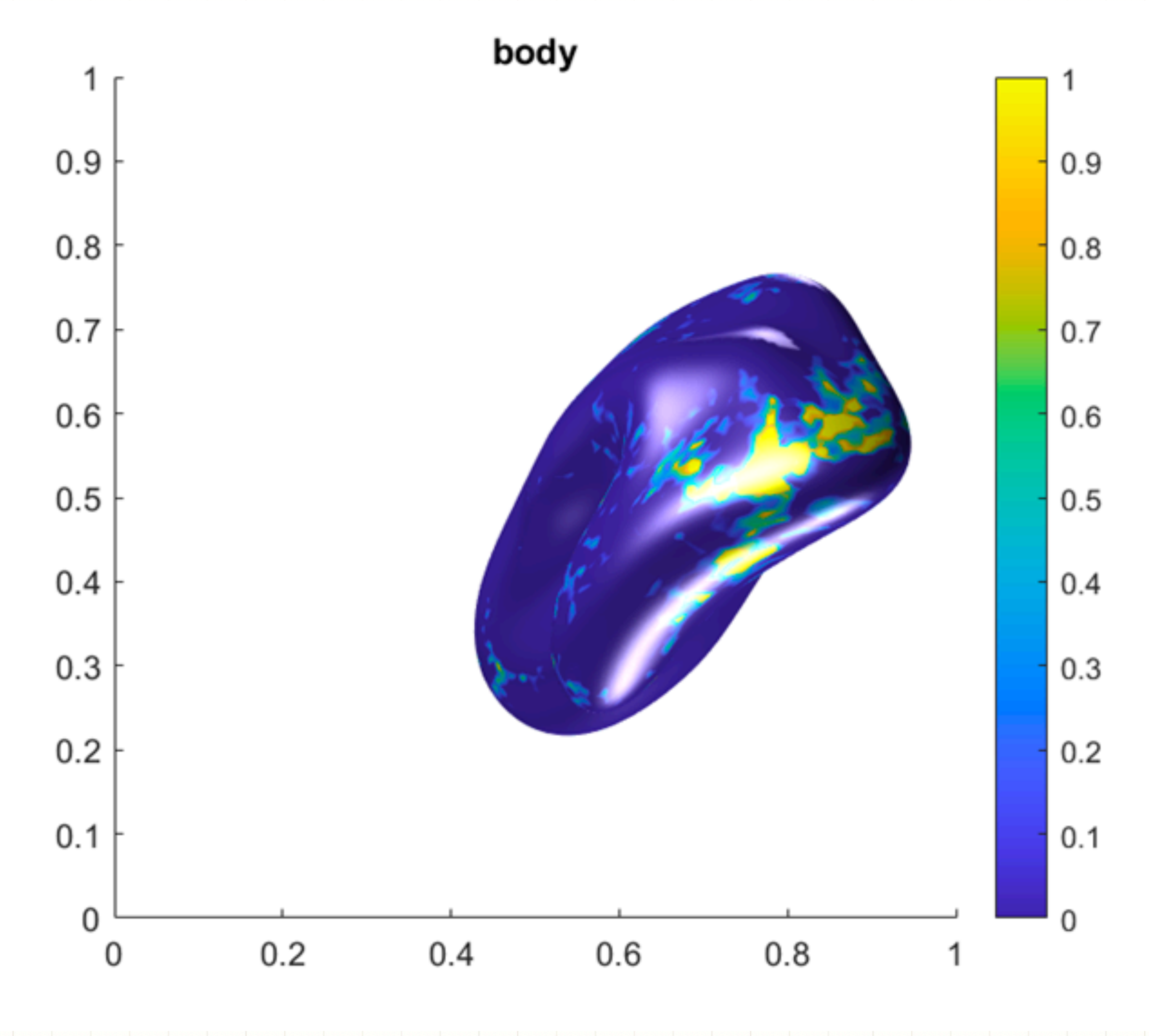
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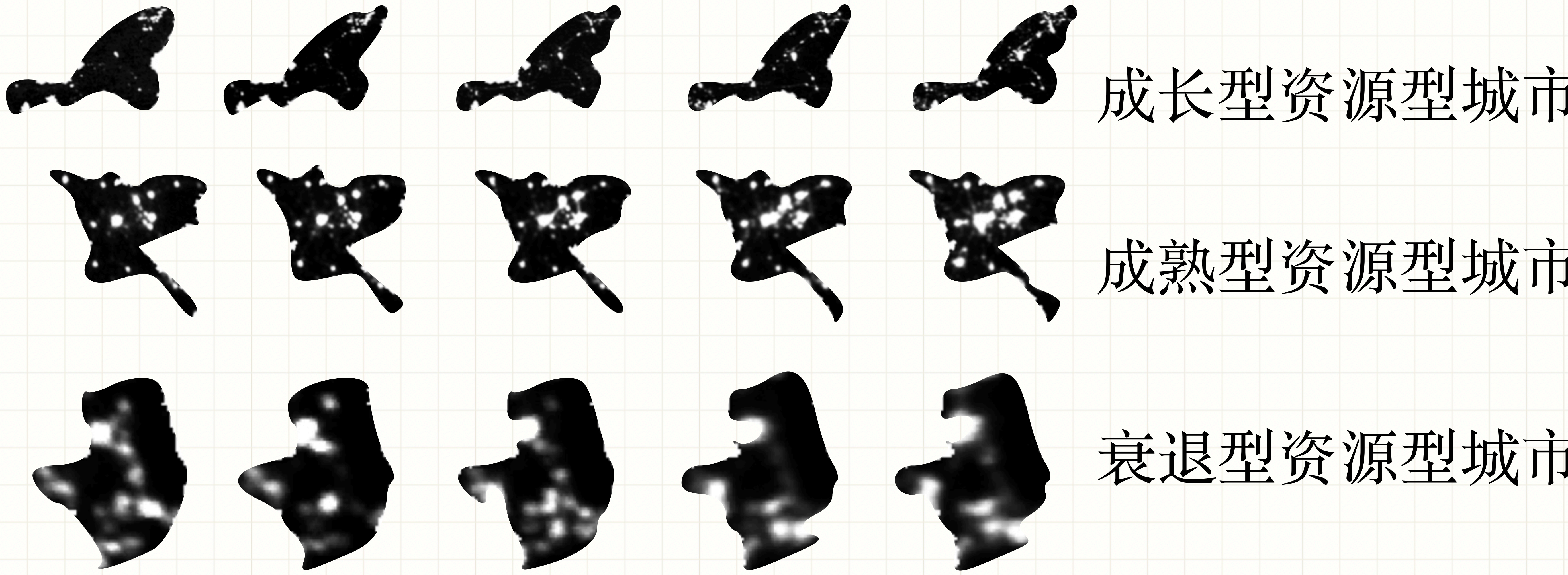
Multivariate Analysis Concept

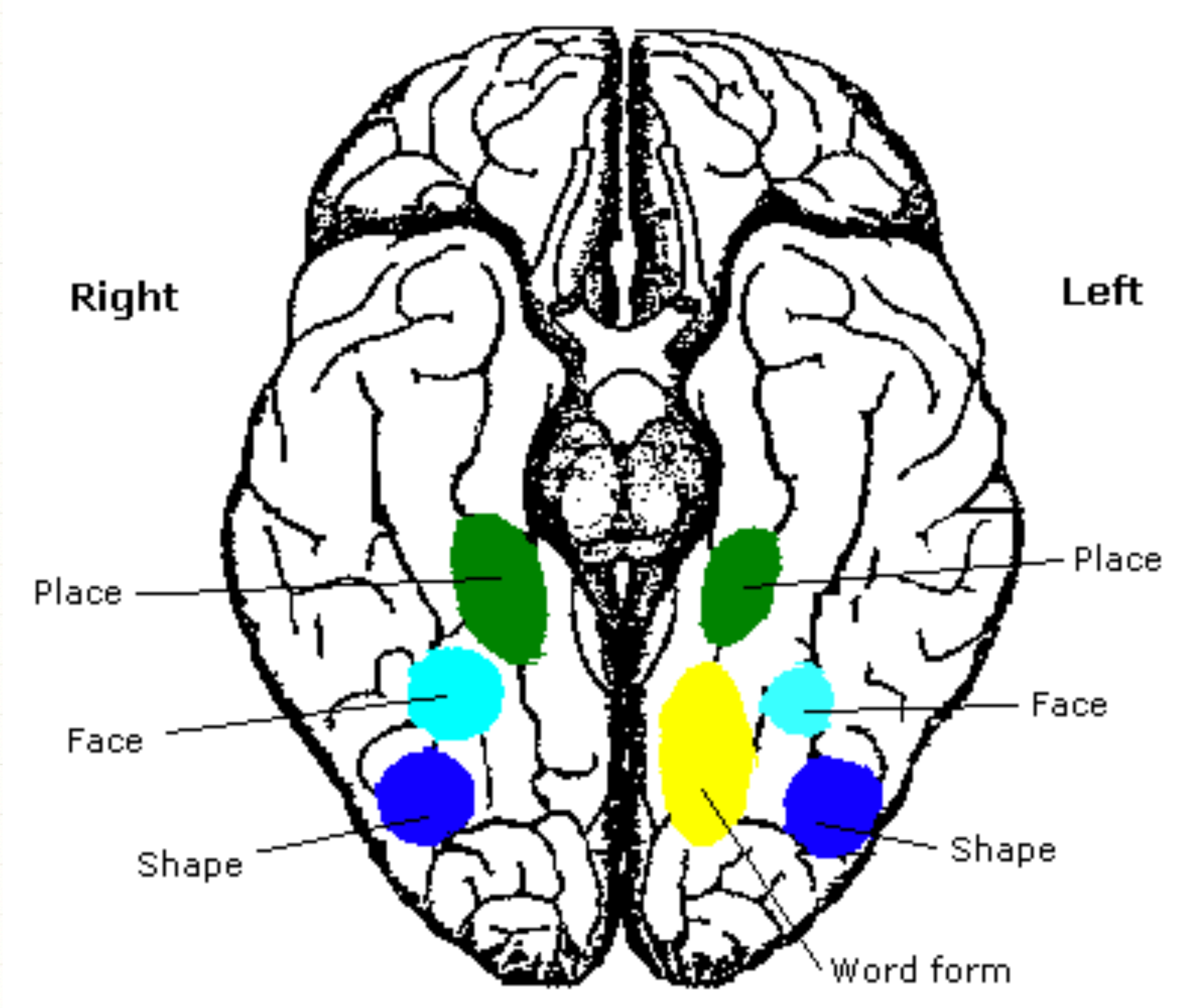
基于 OLS 夜间灯光的全国资源型城市空间结构时空演化研究

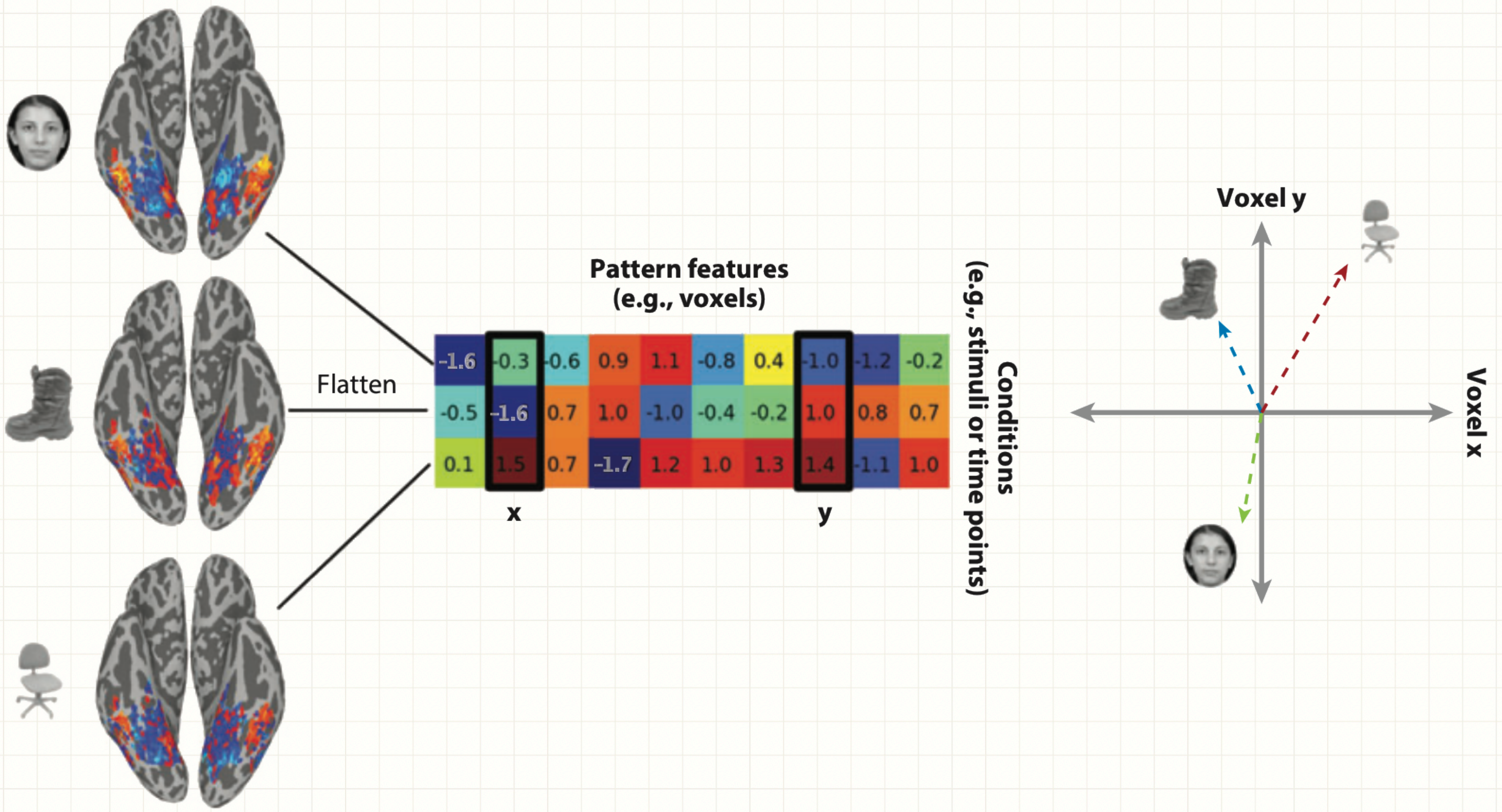


Univariate Analysis
Where is the area?
How strong the light is?

Multivariate Analysis
The **Structure** of the light.
The **Information** represented in a region!

Multivariate Analysis Concept





相同的步骤在每一个体素重复一次

Univariate fMRI

Where is the area?

How strong its response is?

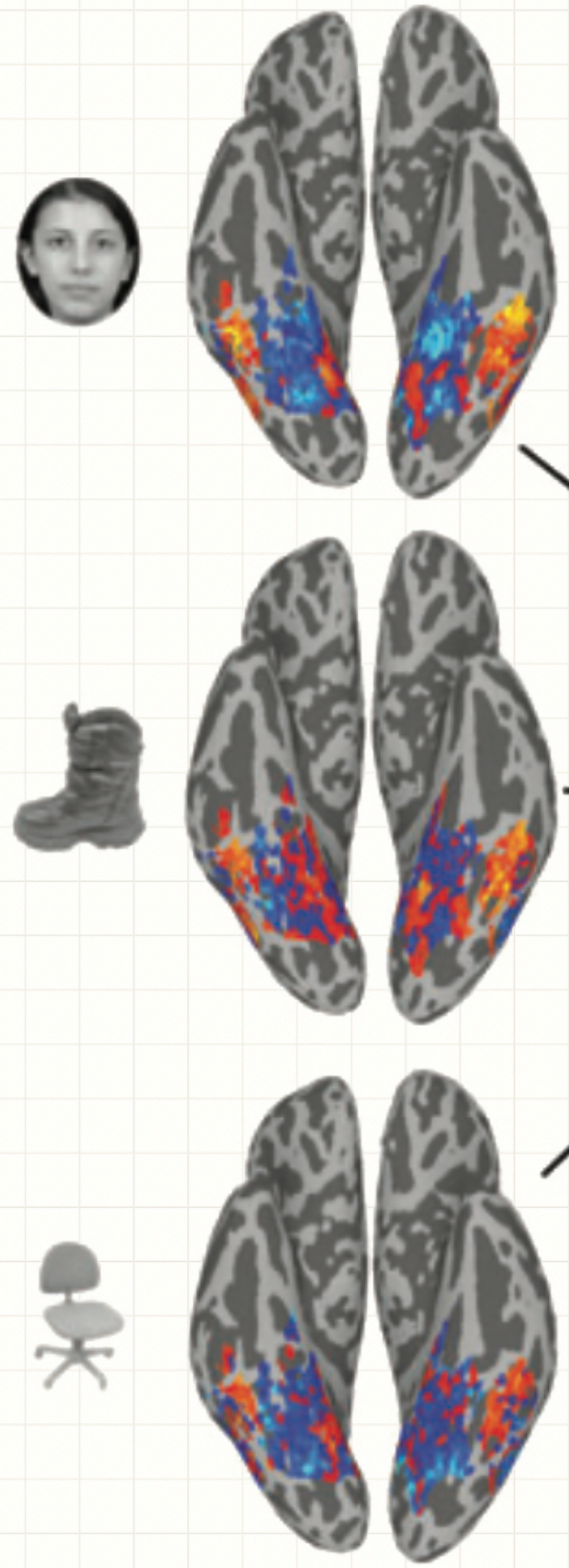
Multivariate Analysis in fMRI

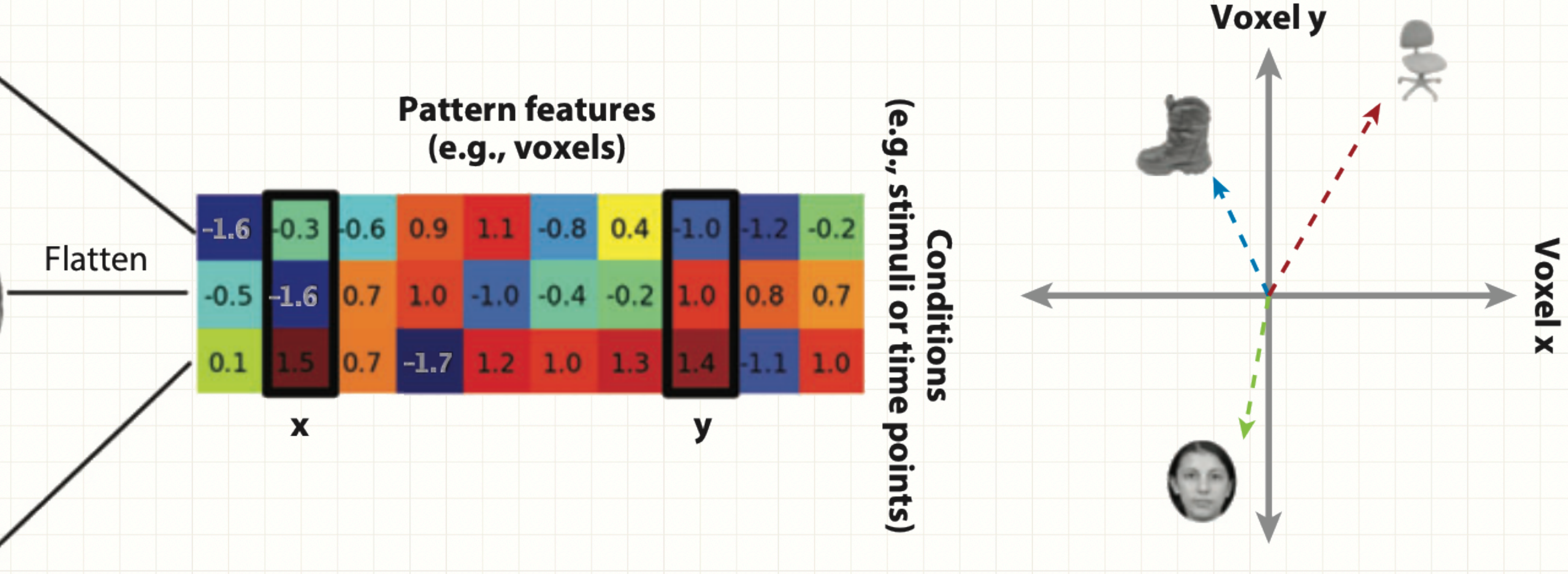
The **Structure** of the response! 激活模式

The **Information** represented in a region!

Multivariate Analysis Concept

REPRESENTATIONAL SPACES





有几行，就有几种观测值，在这里是对三张图片的Beta

有几列，就有几个纬度，在这里是皮层的体素数

Why Multivariate Analysis?

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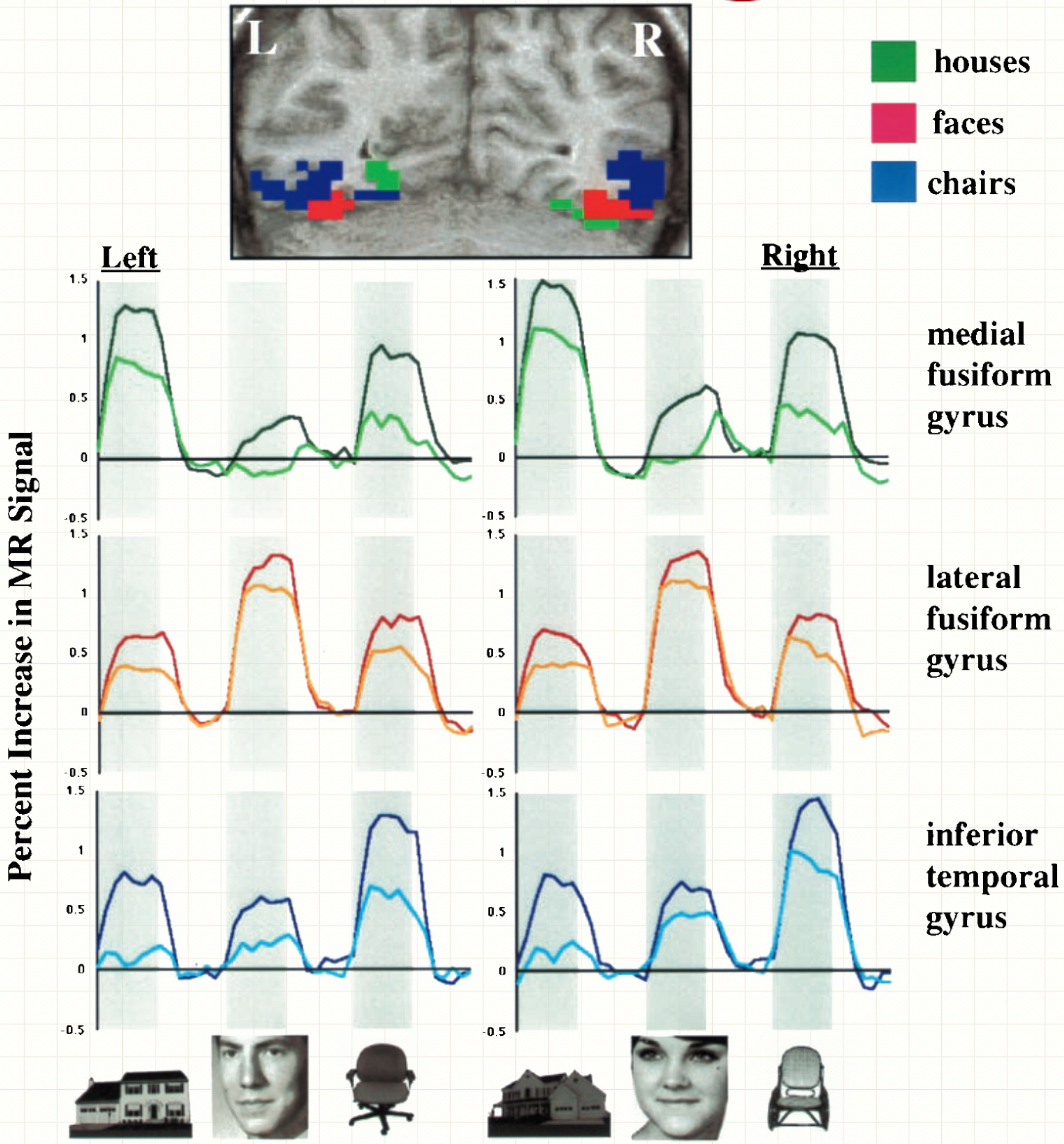
The representation of an object is not restricted to a region that responds maximally to that object, but rather is **distributed** across a broader expanse of cortex.



Why Multivariate Analysis?

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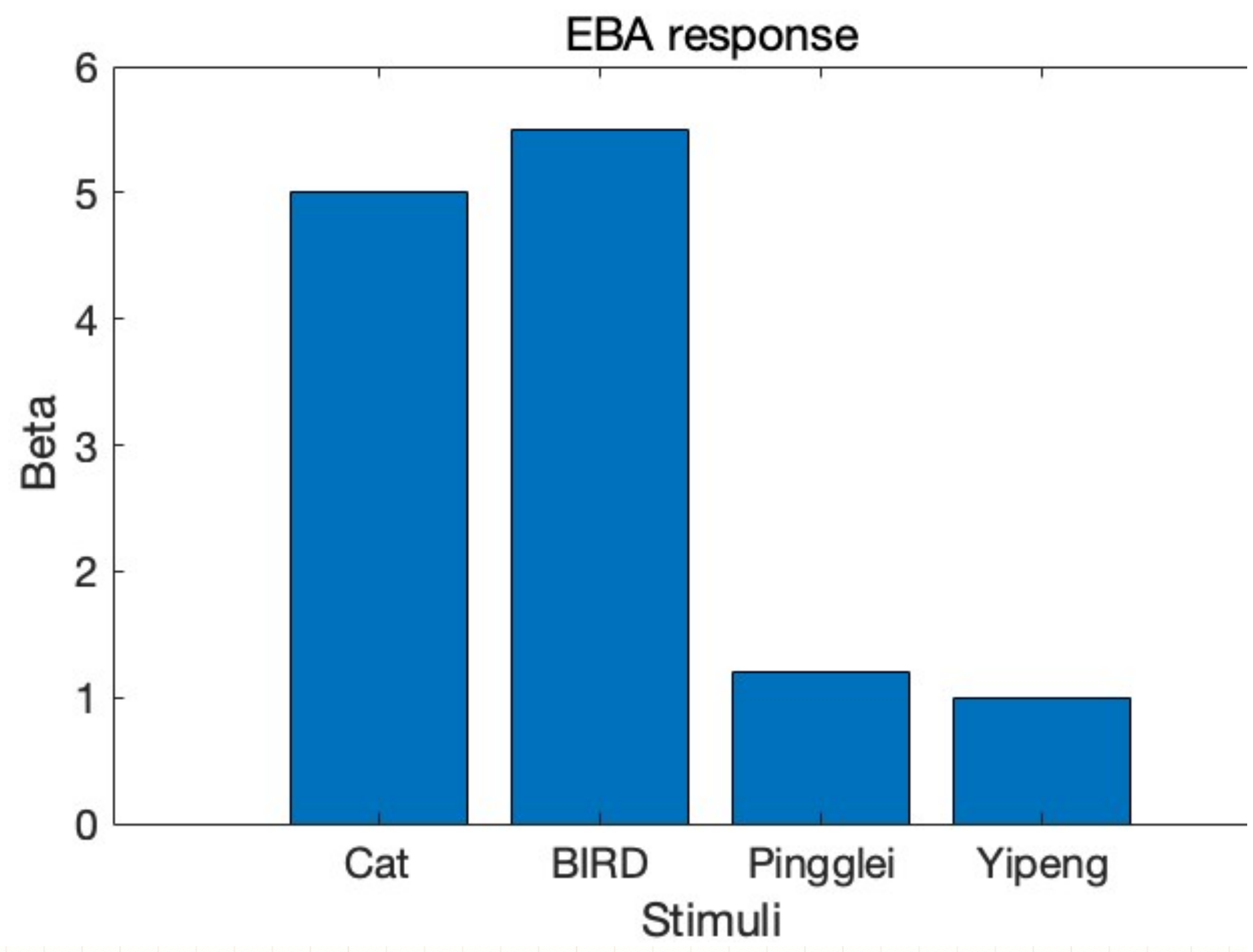
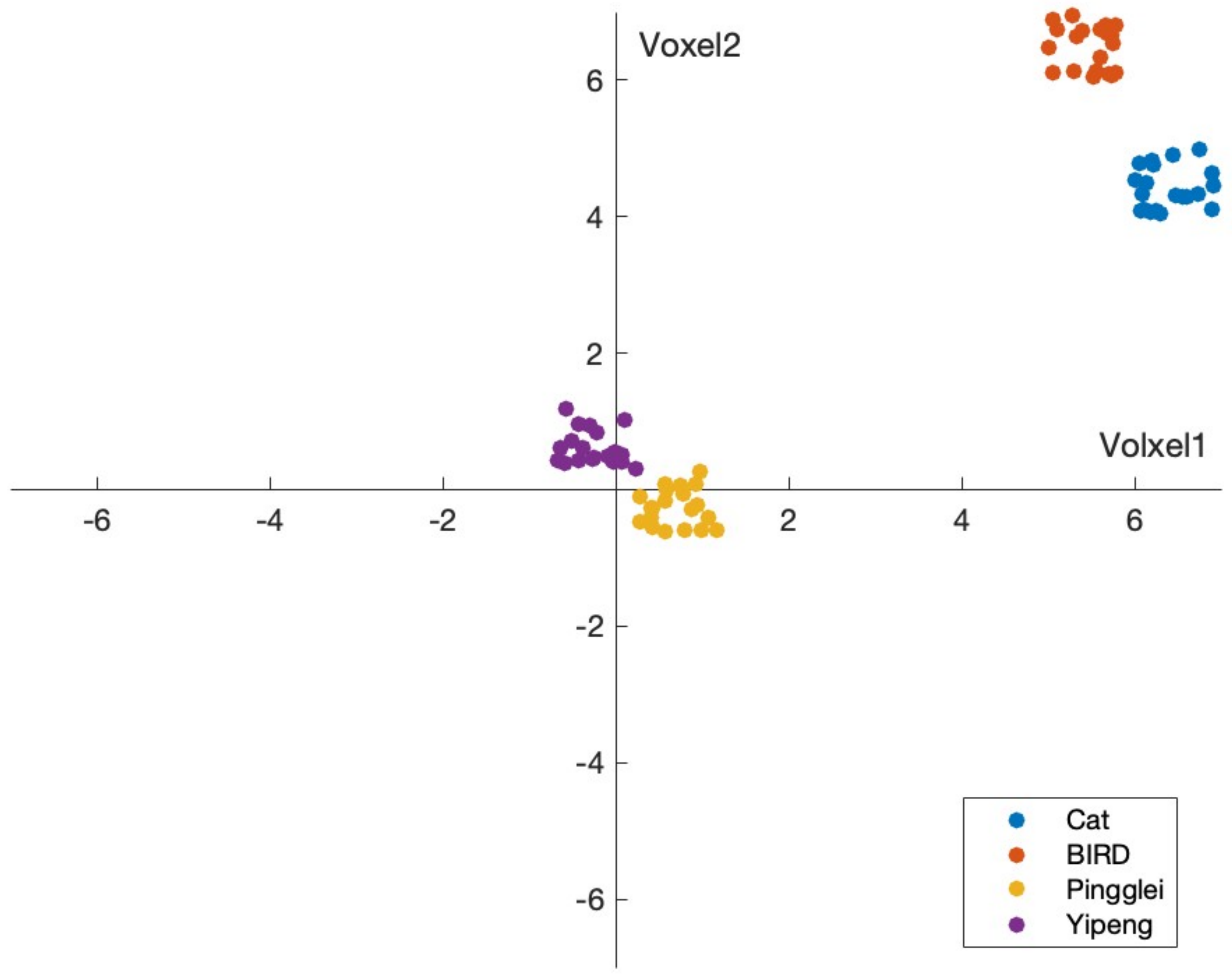
Information lost in Univariate analysis



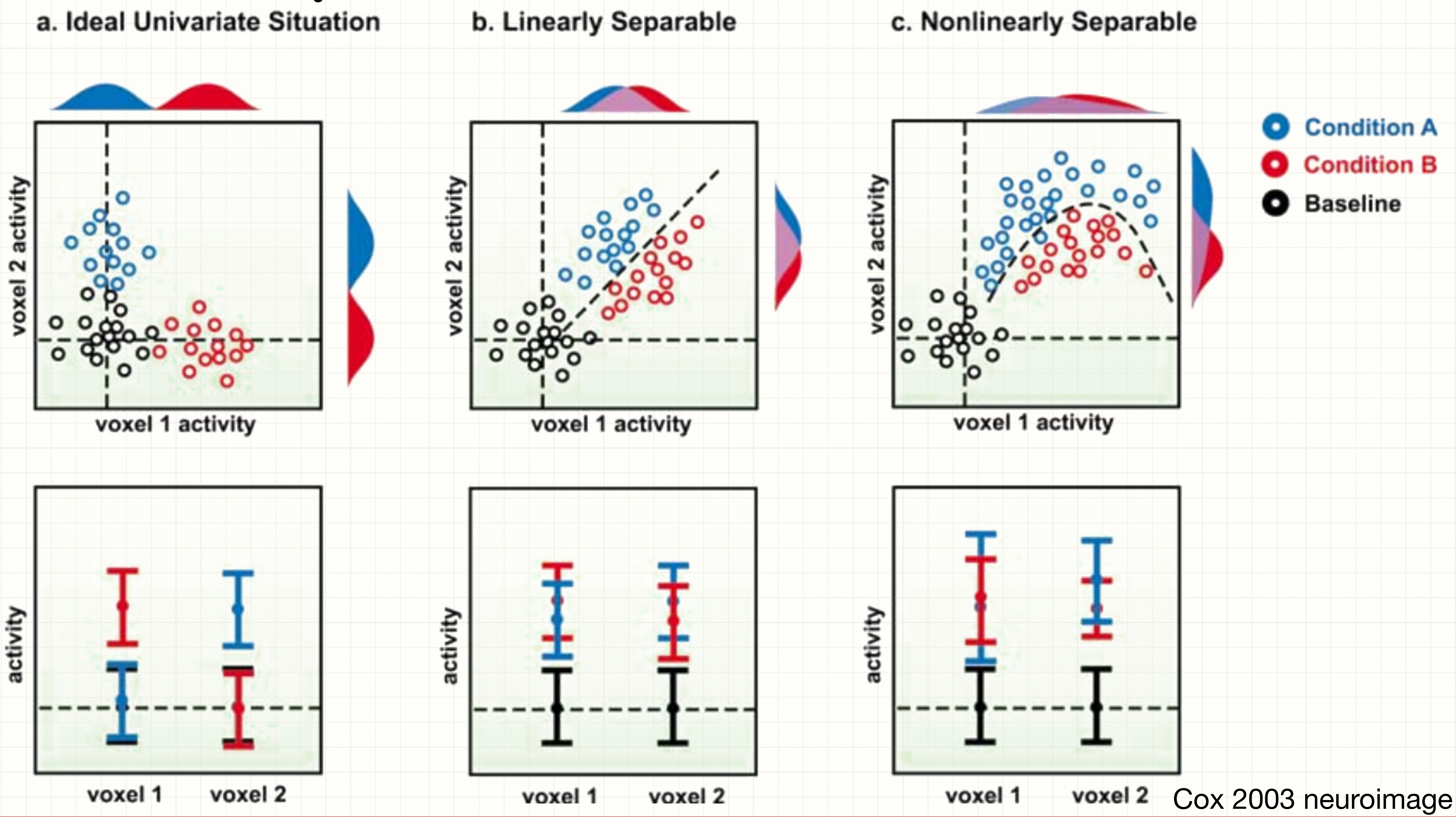


A region's function was identified by determining which task activated it most strongly

what information is represented in a region, in terms of brain states associated with distinct patterns of activity, and how that information is encoded and organized

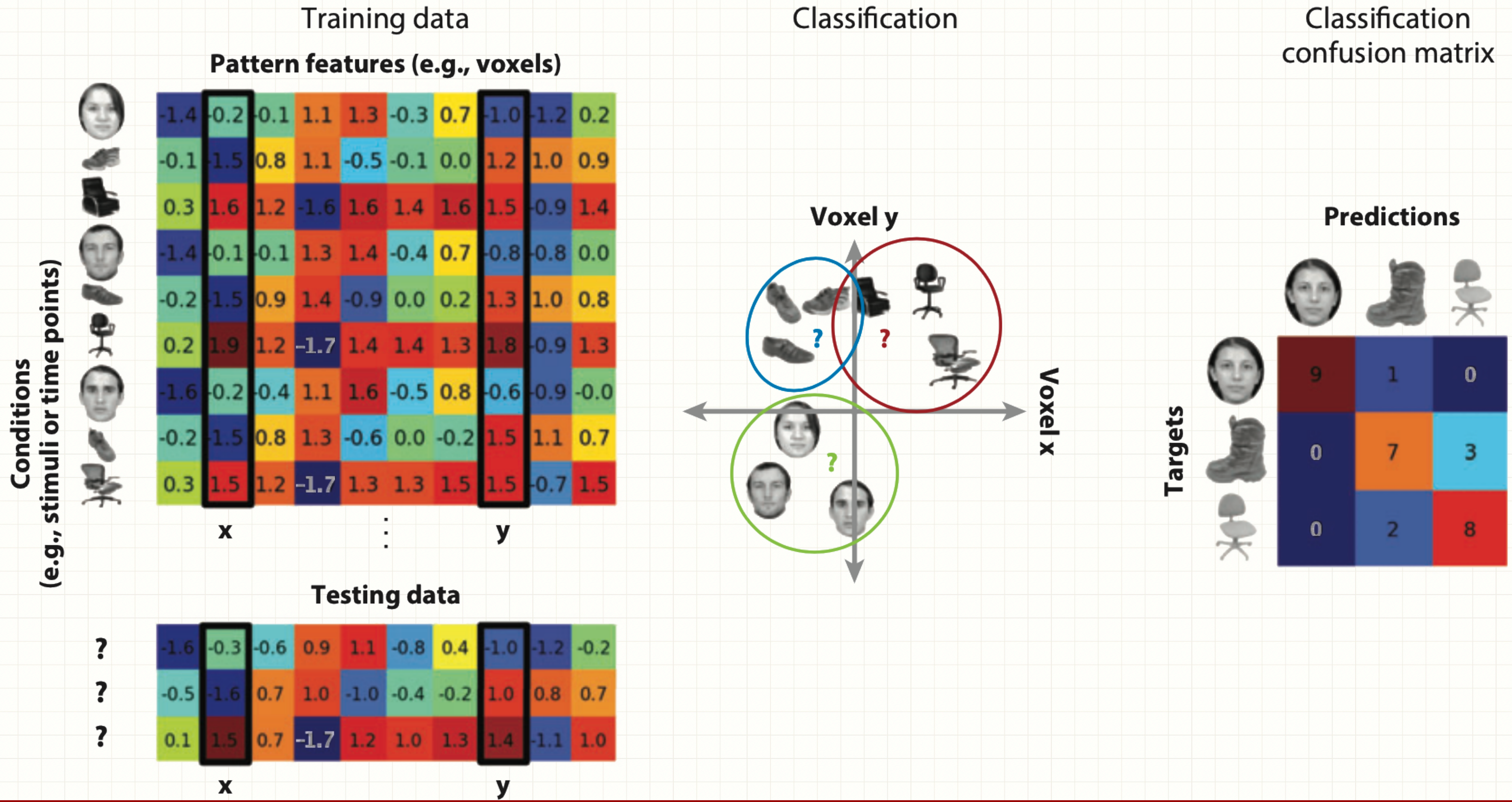
Why Multivariate Analysis?

Information lost in Univariate analysis



Cox 2003 neuroimage

Multivariate Analysis - Classification



Multivariate Analysis - Classification

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- One-nearest-neighbor(1NN): classified a test response vector as the category for the training data vector that was closest in the neural representational space
- Support vector machine(SVM): fine-tune the position of the decision surface on the basis of the vectors that are closest to the surface, i.e., the support vectors, by maximizing the distances from the surface to these borderline cases
- Linear discriminant analysis (LDA), K-nearest-neighbor(KNN)…

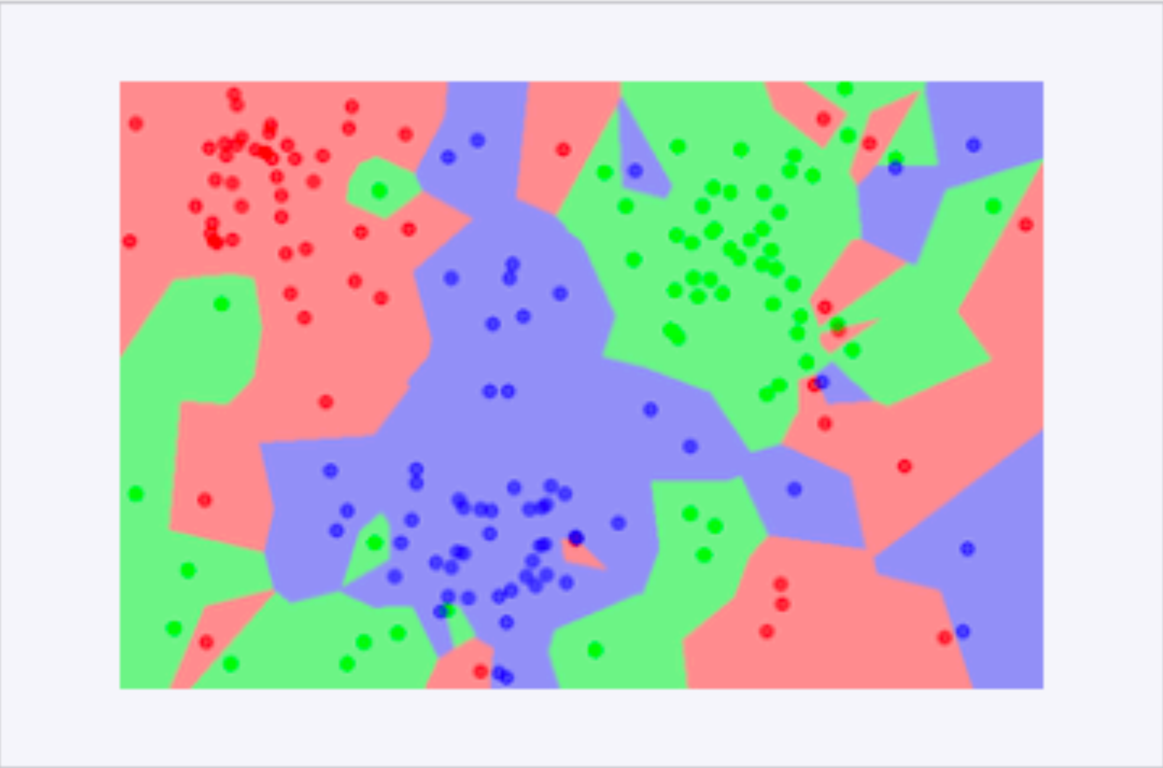


Fig. 2. The 1NN classification map.

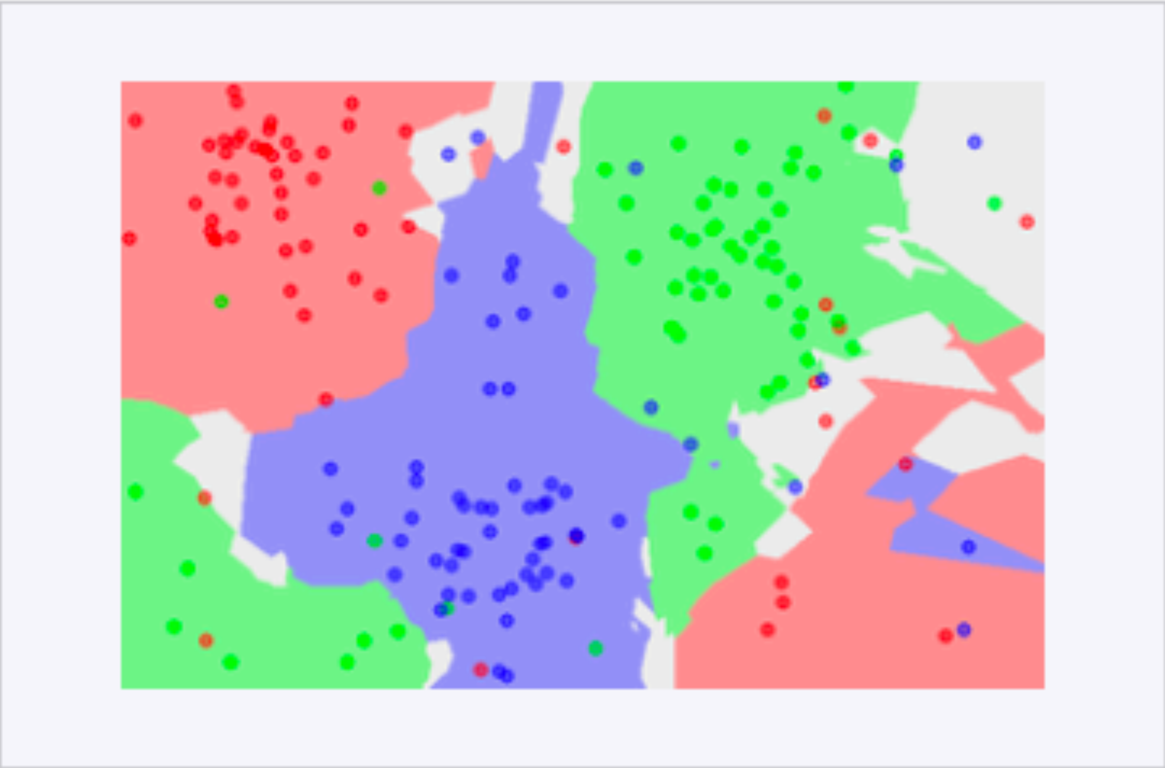
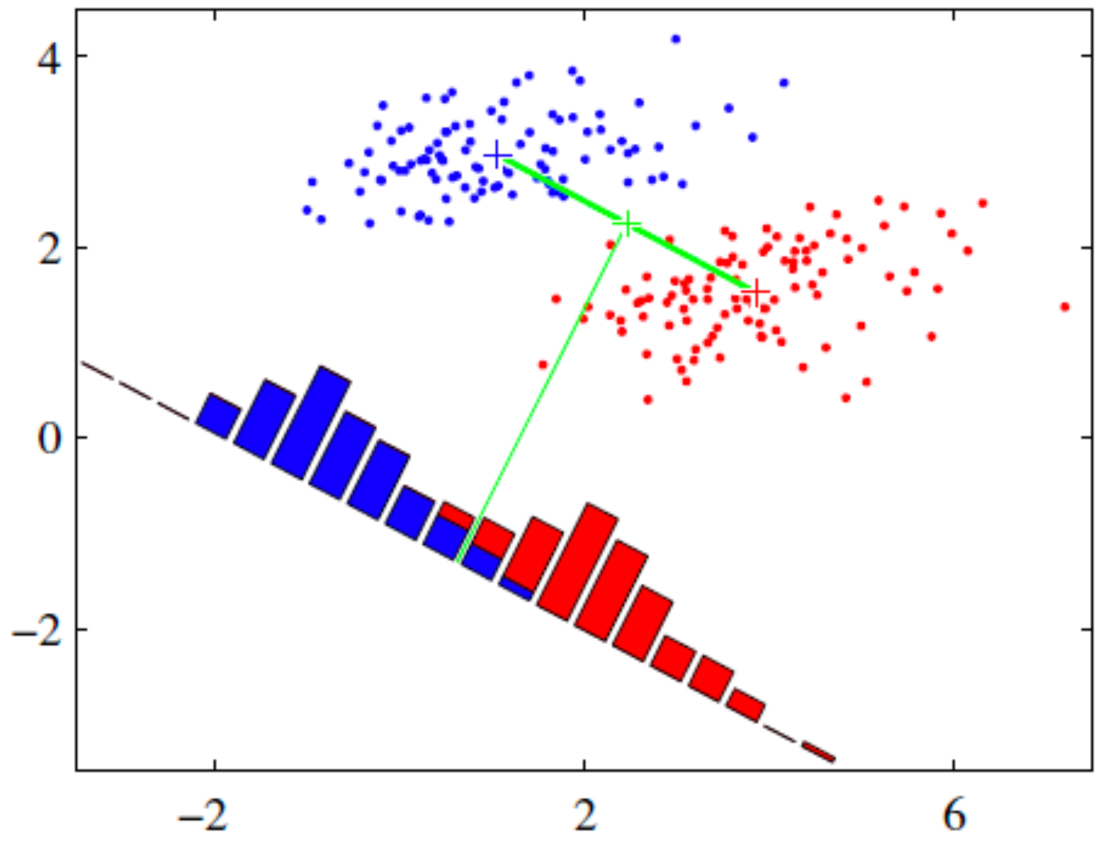
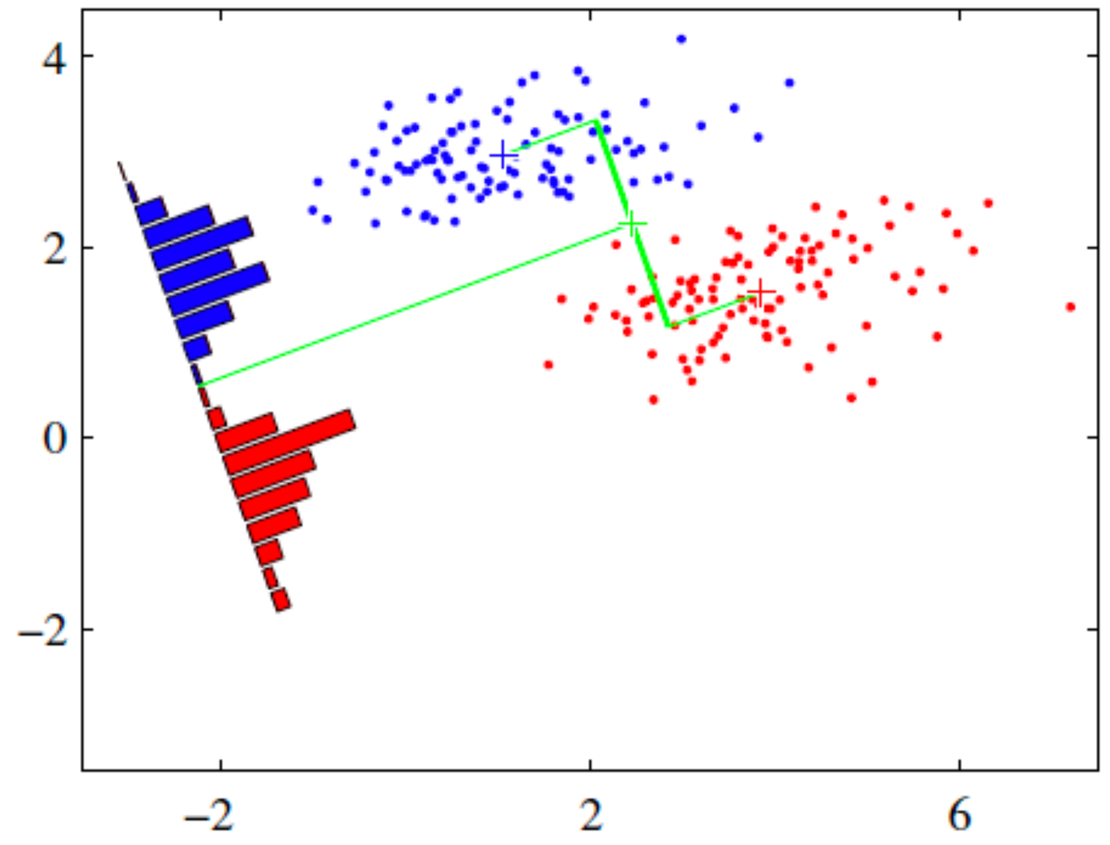


Fig. 3. The 5NN classification map.





Multivariate Analysis - Classification

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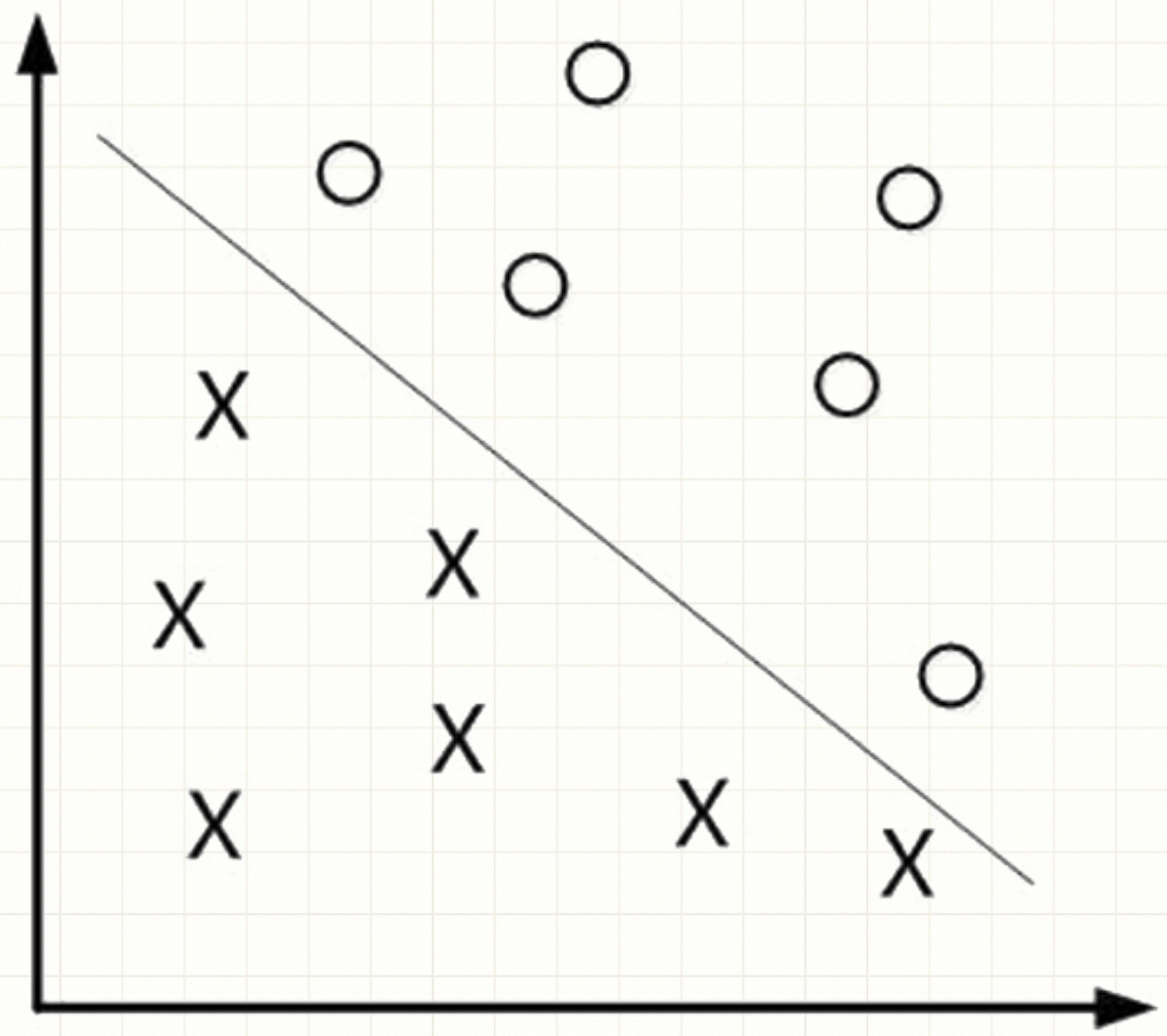
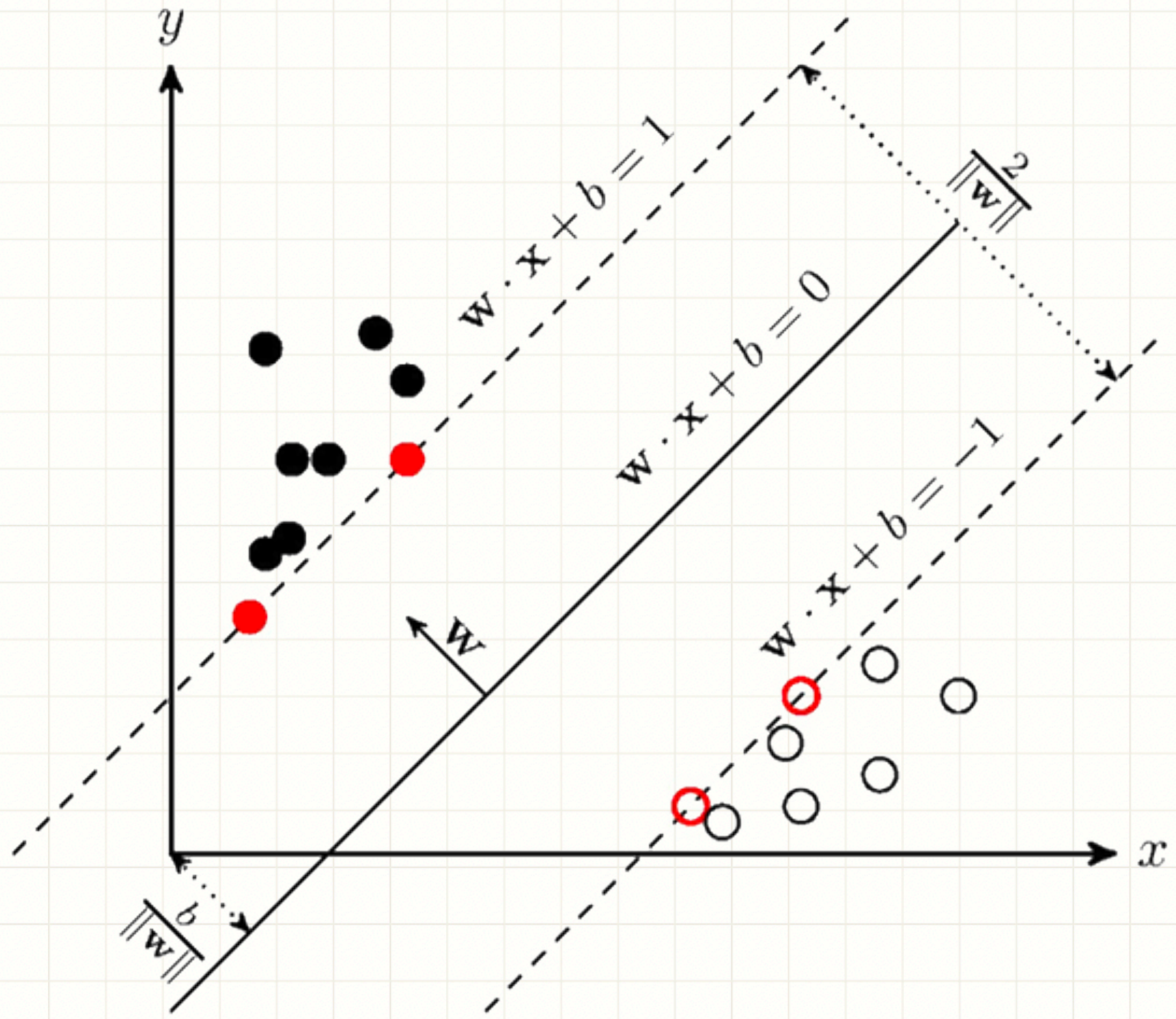
SVM的数学模型

一个线性分类器的学习目标便是要在n维的数据空间中找到一个超平面（hyper plane），这个超平面的方程可以表示为：

$$w^T x + b = 0$$





这个超平面可以用分类函数$f(x) = w^T x + b$表示，当f(x)=0的时候，x便是位于超平面上的点，而f(x)>0的点对应 y=1 的数据点，f(x)小于0的点对应y=-1的点

svm PPT来源：刘燮仪

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SVM的数学模型

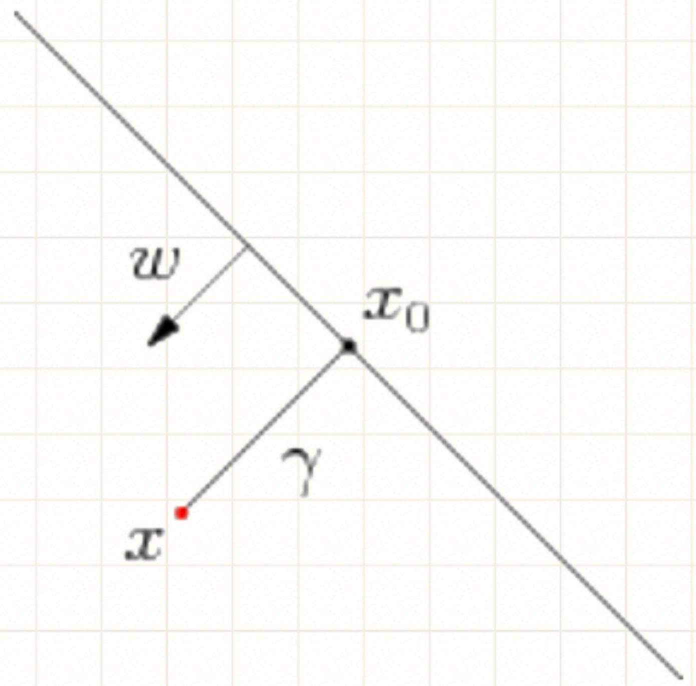
在超平面$w^Tx+b=0$确定的情况下，$|w^Tx+b|$能够表示点x到距离超平面的远近

定义函数间隔为： $\hat{\gamma} = y(w^Tx+b) = yf(x)$

而超平面(w,b)关于T中所有样本点(xi,yi)的函数间隔最小值（其中x是特征，y是结果标签，i表示第i个样本），便为超平面(w, b)关于训练数据集T的函数间隔：

$$\hat{\gamma} = \min \hat{\gamma}_{\mathbf{i}}(\mathbf{i} = \mathbf{1}, \ldots \mathbf{n})$$

因为x_0在超平面上： $w^Tx_0 + b = 0$ $w^Tx_0 = -b$



式子 $x = x_0 + \gamma \frac{w}{\|w\|}$ （$\|w\|$为w的二阶范数） 两边同时乘以w^T

根据 $w^Tx_0 = -b$ 和 $w^Tw = \|w\|^2$ 得到：$\gamma = \frac{w^Tx+b}{\|w\|} = \frac{f(x)}{\|w\|}$

二阶范数：向量元素绝对值的平方和再开方，空间上两个向量矩阵的直线距离

svm PPT来源：刘夔仪

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SVM的数学模型

$$\gamma = \frac{w^T x + b}{\|w\|} = \frac{f(x)}{\|w\|}$$

上式两边乘上对应的类别 y，即可得出几何间隔：$\tilde{\gamma} = y\gamma = \frac{\hat{\gamma}}{\|w\|}$

最大间隔分类器（maximum margin classifier）的目标函数可以定义为：$\max \tilde{\gamma}$

如果令函数间隔为1（方便计算）：$\tilde{\gamma} = \frac{1}{\|w\|}$

目标函数转化为：$\max \frac{1}{\|w\|}, \quad \text{s.t.}\ , y_i\left(w^T x_i + b\right) \geq 1, i = 1, \ldots, n$

求$\frac{1}{\|\omega\|}$的最大值相当于求 $\frac{1}{2}\|\omega\|^2$ 的最小值

定义拉格朗日函数：$\mathcal{L}(w, b, \alpha) = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{n} \alpha_i \left(y_i\left(w^T x_i + b\right) - 1\right)$

svm PPT来源：刘燮仪

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SVM的数学模型

定义拉格朗日函数：$\mathcal{L}(w,b,\alpha)=\frac{1}{2}\|w\|^2-\sum_{i=1}^{n}\alpha_i\left(y_i\left(w^Tx_i+b\right)-1\right)$

$$\theta(w)=\max_{\alpha_i\geq 0}\mathcal{L}(w,b,\alpha)$$

$$\min_{w,b}\theta(w)=\min_{w,b}\max_{\alpha_i\geq 0}\mathcal{L}(w,b,\alpha)=p^*$$

$$\max_{\alpha_i\geq 0}\min_{w,b}\mathcal{L}(w,b,\alpha)=d^*$$

KKT条件就是指上面最优化数学模型的标准形式中的最小点 x* 必须满足下面的条件：

1. $h_j(\mathbf{x}_*)=0, j=1,\ldots,p, g_k(\mathbf{x}_*)\leq 0, k=1,\ldots,q,$
2. $\nabla f(\mathbf{x}_*)+\sum_{j=1}^{p}\lambda_j\nabla h_j(\mathbf{x}_*)+\sum_{k=1}^{q}\mu_k\nabla g_k(\mathbf{x}_*)=\mathbf{0},$

$\lambda_j\neq 0, \mu_k\geq 0, \mu_k g_k(\mathbf{x}_*)=0$

在满足上述条件下，问题转换为对偶问题，首先要让L(w，b，α)关于 w 和 b 最小化，然后求对α的极大，最后利用SMO算法求解对偶问题中的拉格朗日乘子。

svm PPT来源：刘燮仪

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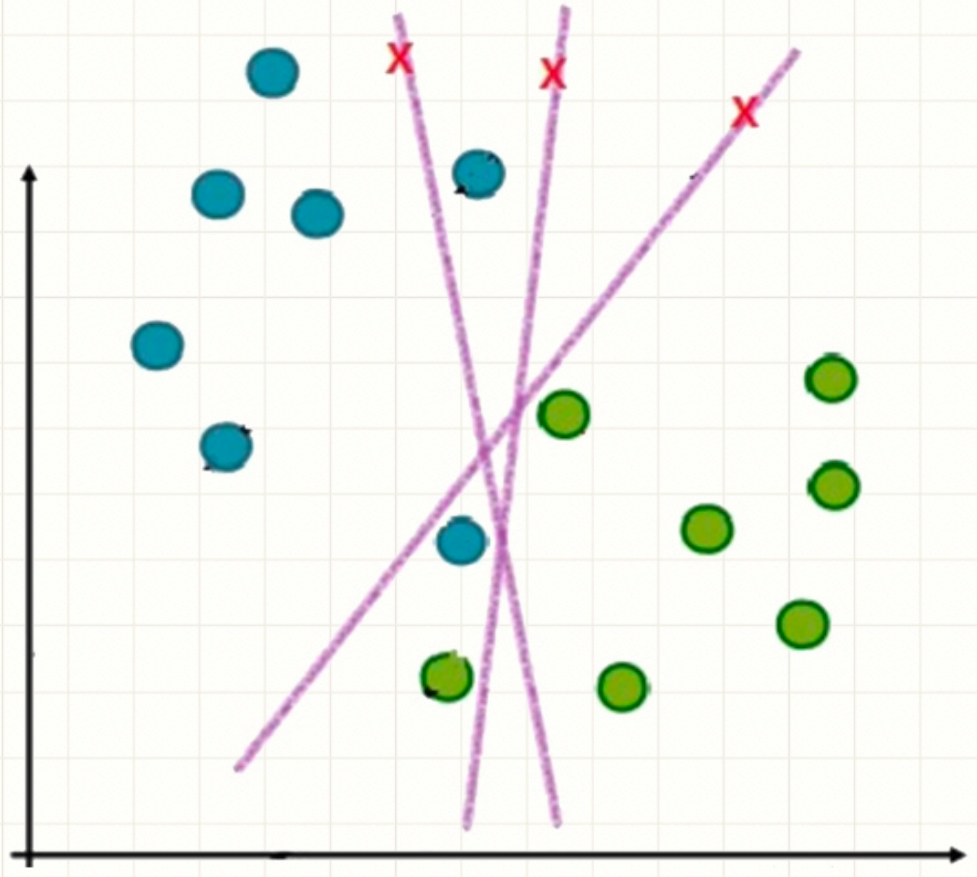
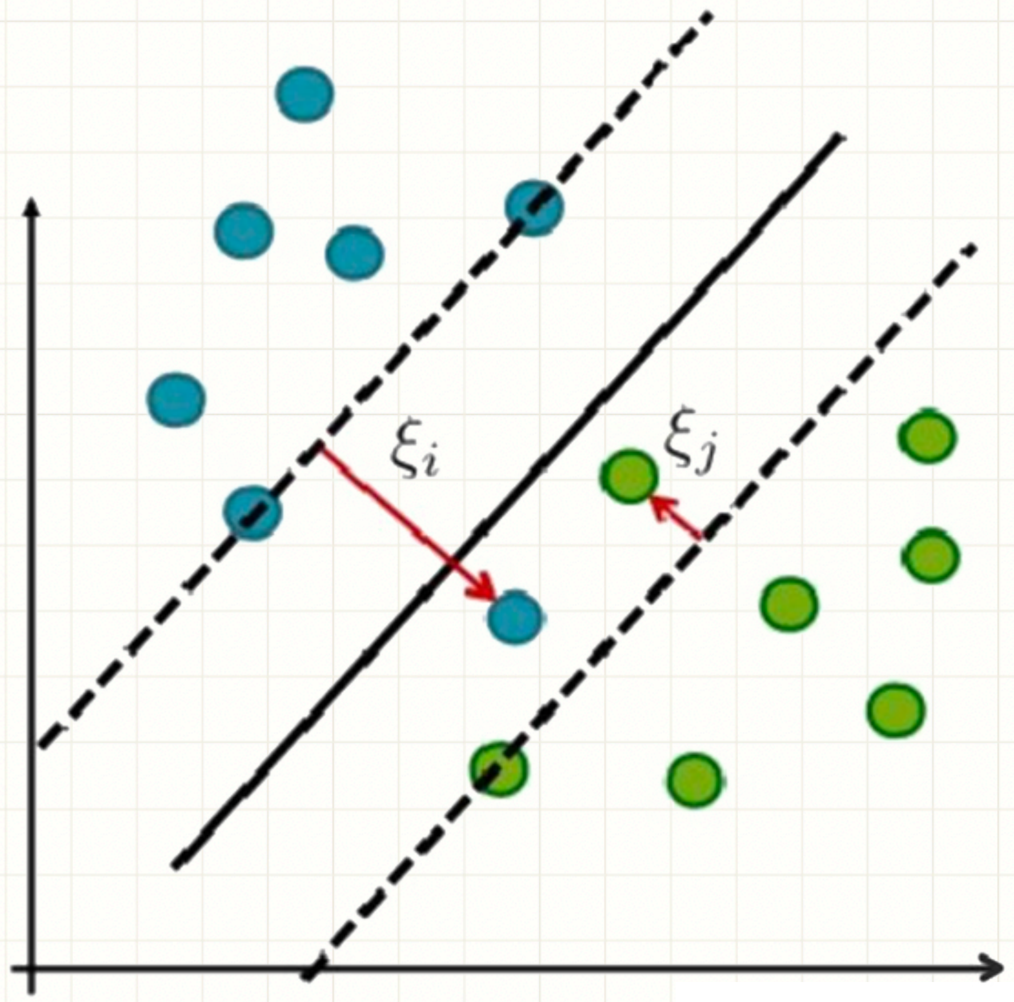
SVM扩展

不完全线性可分





允许部分样本点不满足约束条件： $1 - y_i\left(w^T x_i + b\right) \leq 0$

引入一个松弛变量ξ_i

优化目标：

$$\min_{\mathbf{w},b,\xi\geq 0} \frac{1}{2}\mathbf{w}^\top \mathbf{w} + C\sum_i \xi_i$$

$$\text{s.t. } y_i\left(\mathbf{w}^\top \mathbf{x}_i + b\right) \geq 1 - \xi_i, \quad i = 1, \dots, n$$

$$\xi_i \geq 0$$

其中 C 是一个大于 0 的常数，可以理解为错误样本的惩罚程度

构造拉格朗日函数：$\min_{w,b,\xi} \max_{\lambda,\mu} L(w,b,\xi,\lambda,\mu) = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^m \xi_i + \sum_{i=1}^n \lambda_i\left[1 - \xi_i - y_i\left(w^T x_i + b\right)\right] - \sum_{i=1}^n \mu_i \xi_i$
s.t. $\lambda_i \geq 0 \quad \mu_i \geq 0$

对偶问题转化为： $\max_{\lambda,\mu} \min_{w,b,\xi} L(w,b,\xi,\lambda,\mu)$

svm PPT来源：刘燮仪

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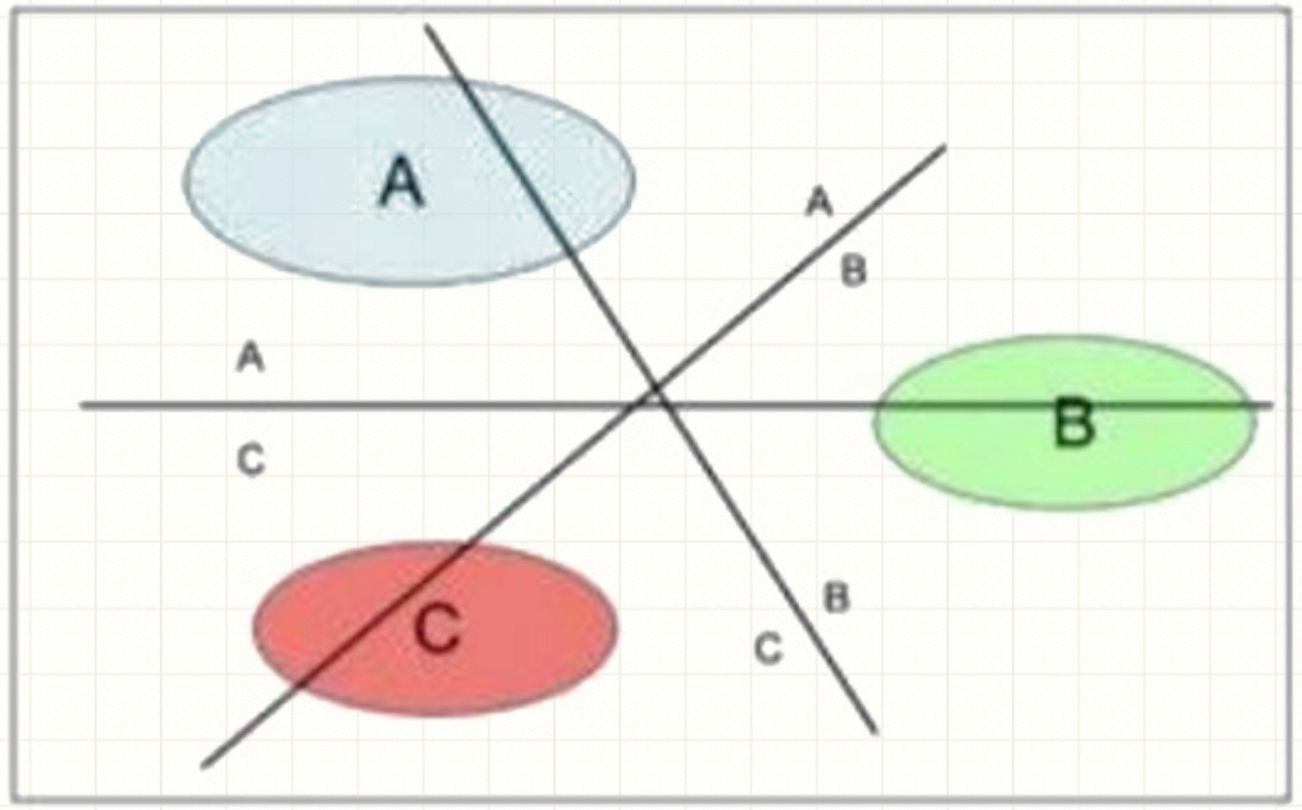
SVM扩展

扩展为多分类的方法有：

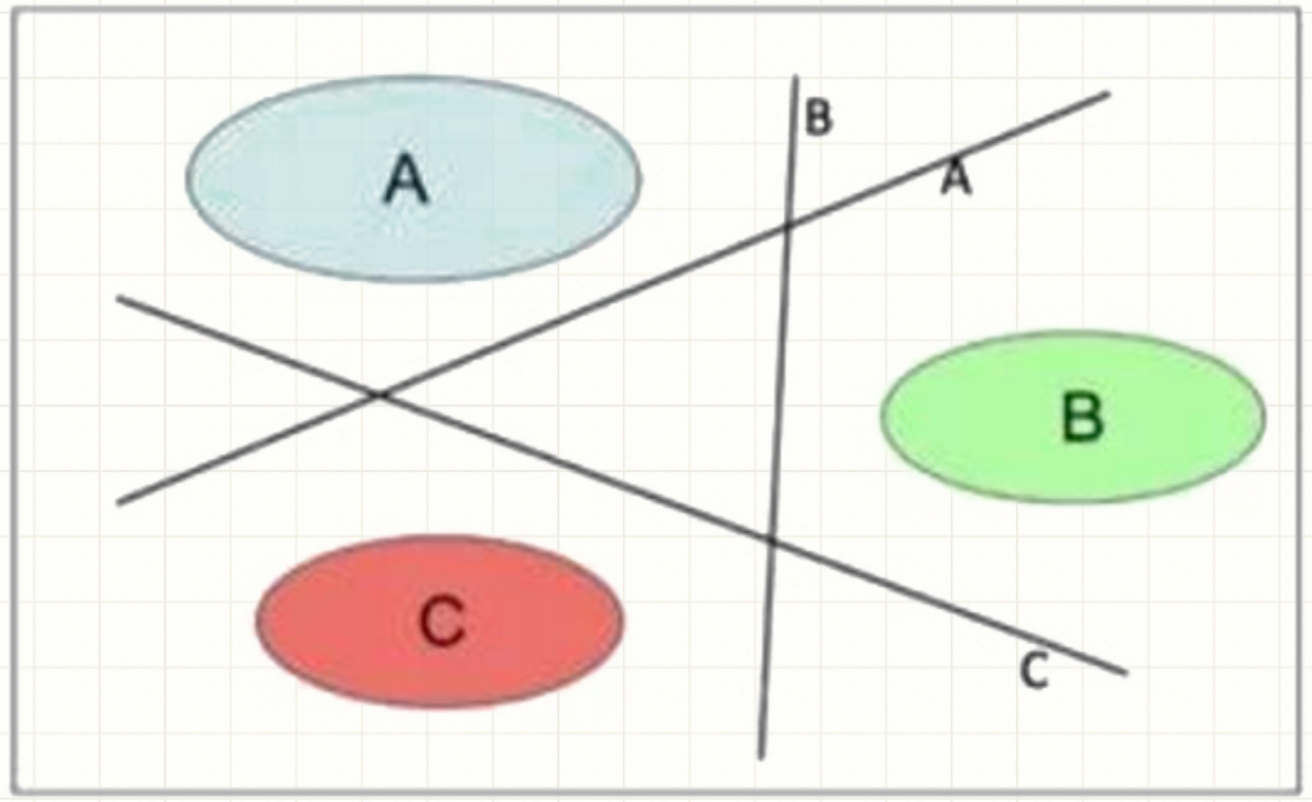
<u>**一对一（one-versus-one, OVO SVMs）方法：**</u>

训练时对于任意两类样本都会训练一个二分类器，最终得到k(k-1)/2个二分类器，共同组成k分类器。对未知样本分类时，使用所有的k(k-1)/2个分类器进行分类，将出现最多的那个类别作为该样本最终的分类结果。



<u>**一对多（one-versus-rest, OVR SVMs）方法：**</u>

训练时依次把k类样本中的某个类别归为一类，其它剩下的归为另一类，使用二分类的SVM训练处一个二分类器，最后把得到的k个二分类器组成k分类器。对未知样本分类时，分别用这k个二分类器进行分类，将分类结果中出现最多的那个类别作为最终的分类结果。



svm PPT来源：刘夔仪

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- **SVM in Matlab & scikit-learn**

fitcsvm

训练用于一类和二类分类的支持向量机 (SVM) 分类器

语法

```
Mdl = fitcsvm(Tbl,ResponseVarName)
Mdl = fitcsvm(Tbl,formula)
Mdl = fitcsvm(Tbl,Y)
```

```
Mdl = fitcsvm(X,Y)
```

```
Mdl = fitcsvm(___,Name,Value)
```

```python
from sklearn.svm import LinearSVC
linearsvc = LinearSVC(C=1e9)
linearsvc.fit(X_stand, y)
```

LIBSVM -- A Library for Support Vector Machines

Chih-Chung Chang and Chih-Jen Lin

Example Data

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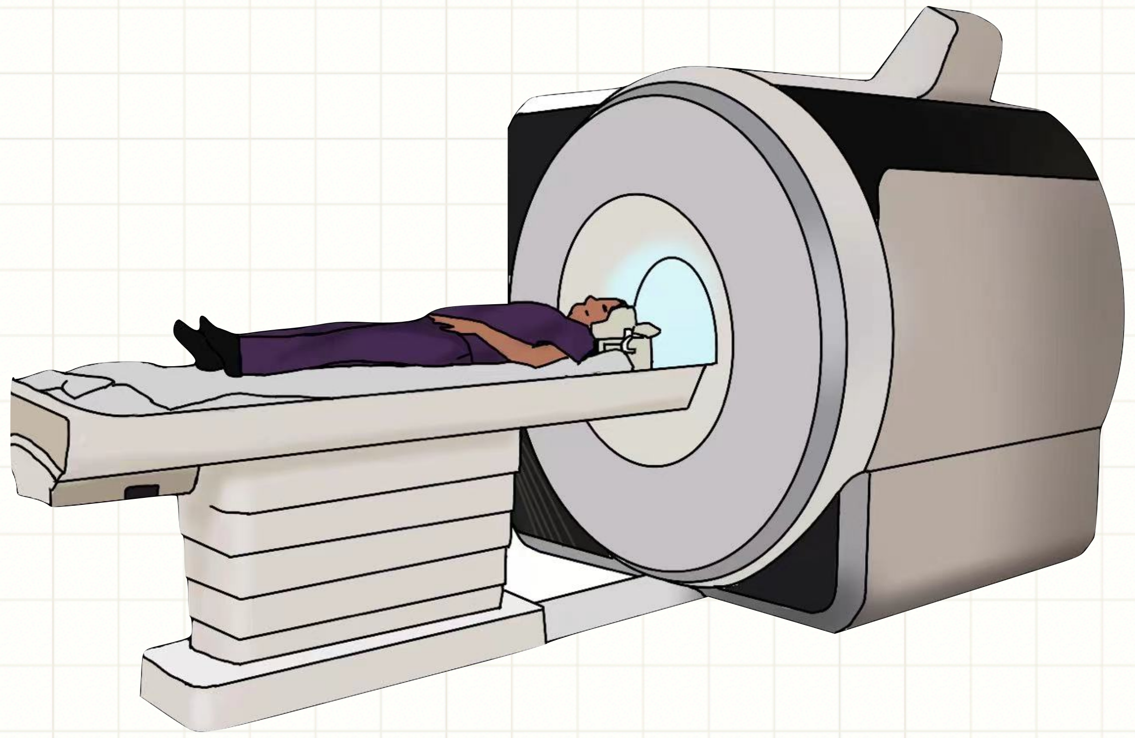
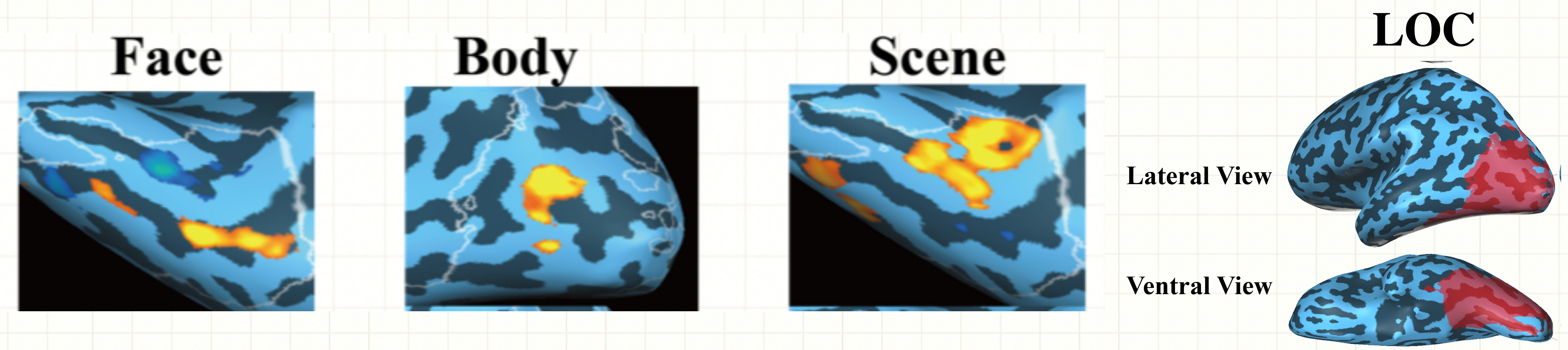
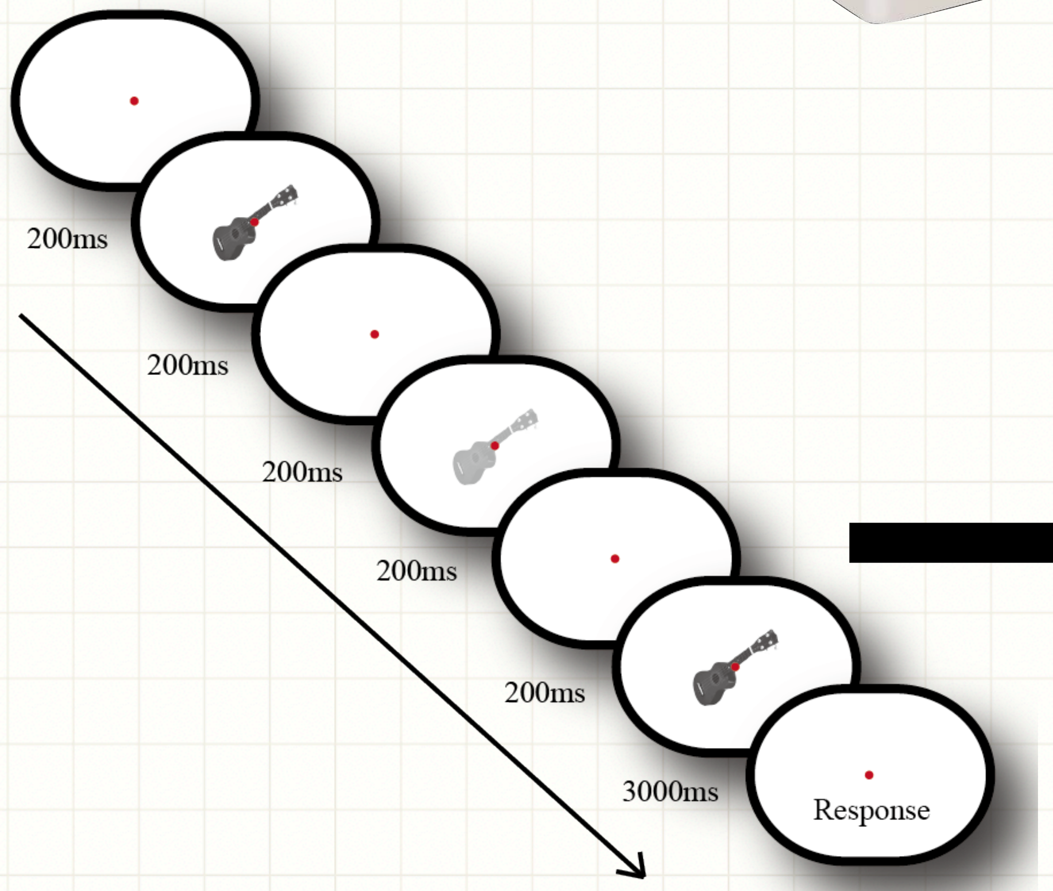
1 subjects, passively viewing 500 images, 10 trials per image, event-related design



A. Contrast Change Detection



Vertice Selection



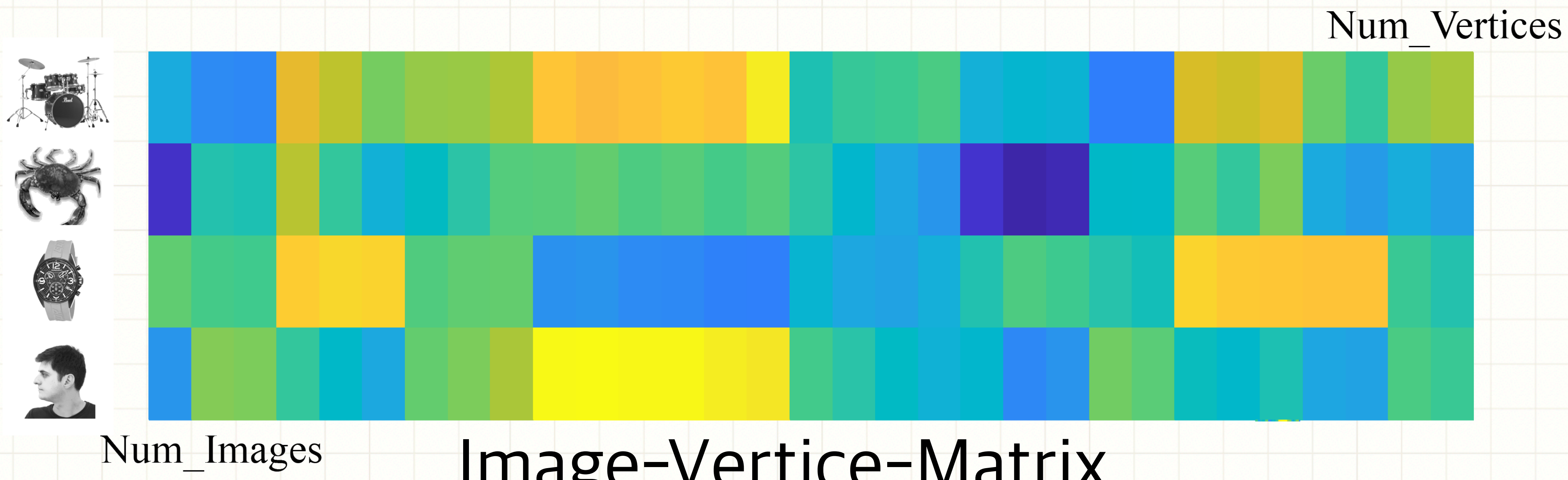
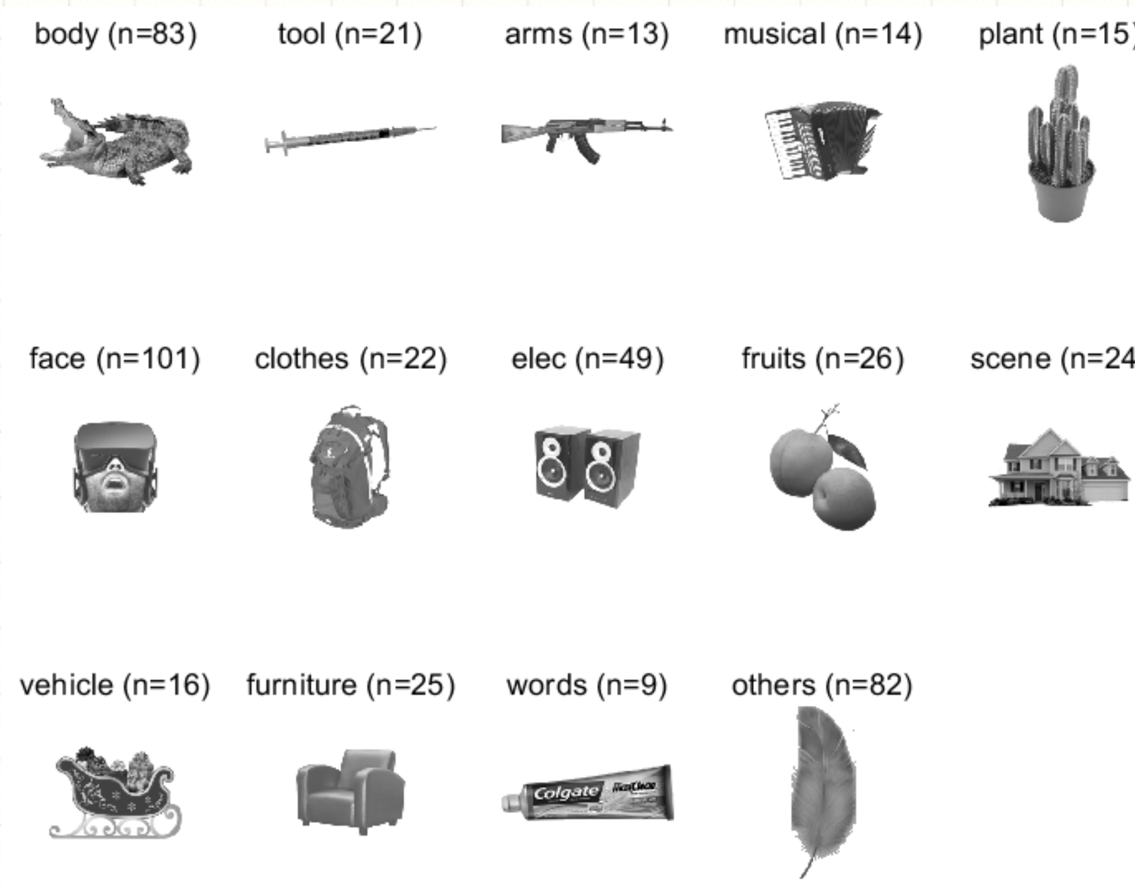


Image-Vertice-Matrix



https://disk.pku.edu.cn:443/link/881109A849EEC661C89691E77B99A949

Multivariate Analysis - Classification

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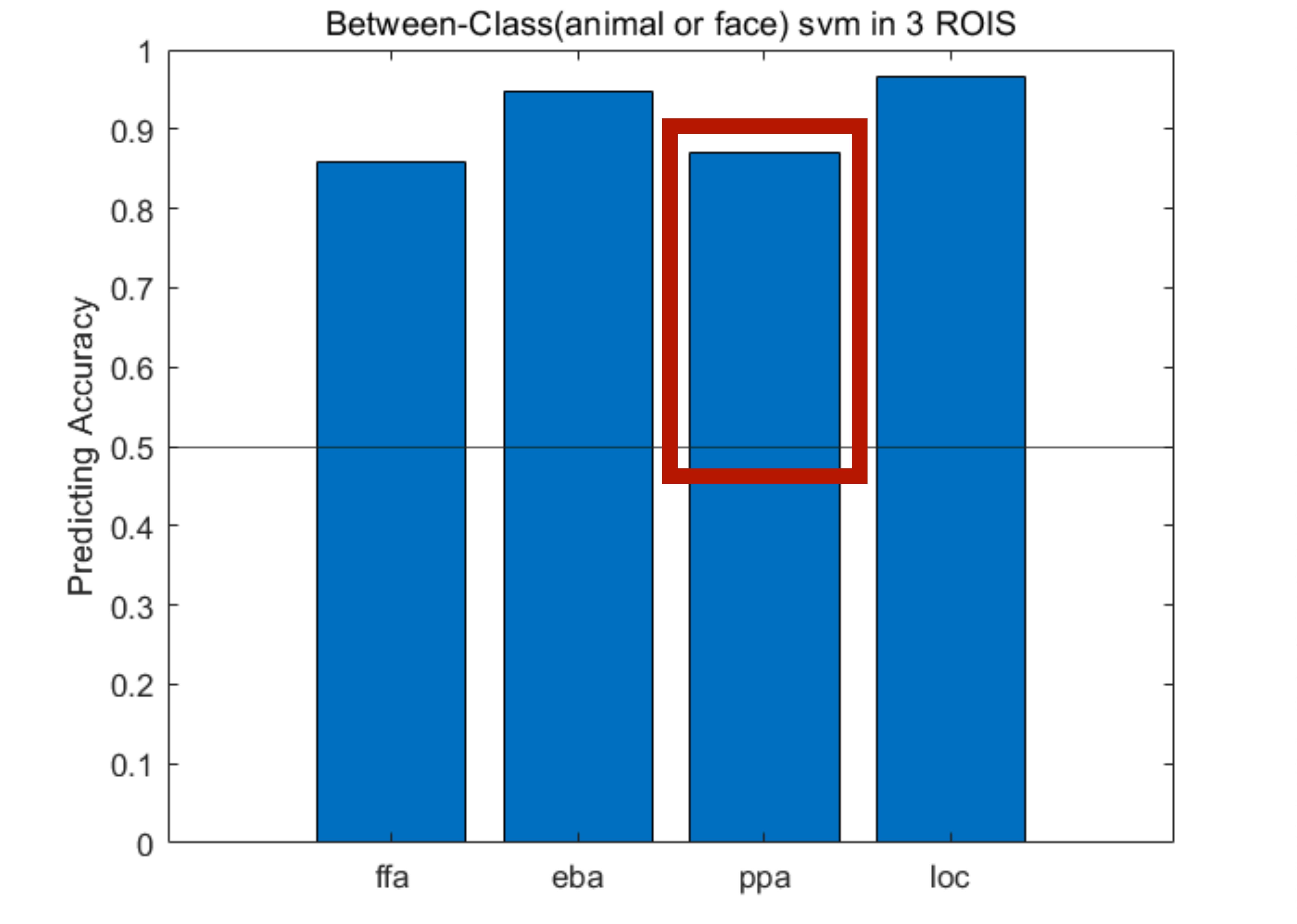
- Q1 - Can we read(decode) image category through the response of non-selective area?
- e.g. Can PPA (scene preferencing area) distinguish Animal & Face?

```
%% 2-calss svm in 3 rois
interested_idx = [image_category(1).picset, image_category(6).picset]; % decode animal or face?
all_image = length(interested_idx);
leave_out_num = 20;
for bb = 1:boot_times
    animal_idx = image_category(1).picset;
    label_array = zeros(1,all_image);
    label_array(animal_idx)=1; % 1 is animal and 0 is face

    leave_out_idx = randperm(all_image,leave_out_num); % split data into train and test sets
    train_idx = setdiff(1:all_image, leave_out_idx);
    for rr = 1:length(average_beta)
        roi_now = average_beta{rr,2};
        mdl = fitcsvm(average_beta{rr,1}(train_idx, :), label_array(train_idx)); % train a svm model
        predicted_label = predict(mdl, average_beta{rr,1}(leave_out_idx, :)); % predict test data
        predicted_acc(rr,bb) = length(find(predicted_label'==label_array(leave_out_idx)))./leave_out_num; %check accuracy
        roi_legend{rr} = roi_now;
    end
end
```

Multivariate Analysis - Classification

- Q1 - Can we read(decode) image category through the response of non-selective area?
- e.g. Can PPA (scene preferencing area) distinguish Animal & Face?
- ——Yes



Multivariate Analysis - Classification

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- **Q2 - Can we read(decode) any categories through the response pattern?**
- **Decoding 4 categories (animal, face, man-made object, natural object)**

```
tic
load('roi_beta.mat') % beta in 3 rois for 6 trials
load("category_label.mat") % category label
% load('toy_data.mat') % beta in LOC for 6 trials

% sort categories into 4 sets
image_category(3).name = 'man-made object';
image_category(3).picset = [image_category(2).picset, image_category(3).picset, image_category(4).picset,
image_category(2)=image_category(6);
image_category(4).name='natural object';
image_category(4).picset = [image_category(5).picset, image_category(9).picset];
image_category(5:end)=[];
category_legend={};
```

Multivariate Analysis - Classification

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- **Q2 - Can we read(decode) any categories through the response pattern?**
- **Decoding 4 categories (animal, face, man-made object, natural object)**

```
confuse_matrix = zeros(boot_times, 4, length(image_category), length(image_category));
for bb = 1:boot_times % we do this for boot_times

    % combine 6 trials, and pick data
    pooled_response{1}=[];pooled_response{2}=[];pooled_response{3}=[];pooled_response{4}=[];label_array=[];
    for cc = 1:length(image_category)
        sample_image = randperm(length(image_category(cc).picset), 40);
        image_idx = image_category(cc).picset(sample_image);
        for trial_num = 1:length(roi_beta)
            pooled_response{1} = [ pooled_response{1};roi_beta{trial_num}.ffa(image_idx, :)];
            pooled_response{2} = [ pooled_response{2};roi_beta{trial_num}.eba(image_idx, :)];
            pooled_response{3} = [ pooled_response{3};roi_beta{trial_num}.ppa(image_idx, :)];
            pooled_response{4} = [ pooled_response{4};roi_beta{trial_num}.loc(image_idx, :)];
        end
        label_array = [label_array, cc*ones(1,trial_num*40)];
        category_legend{cc}=image_category(cc).name;
    end
    % split data into train & test sets
    test_idx = randperm(length(label_array),leave_out_num);
    train_idx = setdiff(1:length(label_array), test_idx);
    for rr = 1:4 % do this for 4 rois
            train_data = double(pooled_response{rr}(train_idx, :));
            train_label = label_array(train_idx);
            test_data = double(pooled_response{rr}(test_idx, :));
            test_label = label_array(test_idx);
            % train a multi-label svm model and predict labels for test sets
            model=svmtrain(train_label', train_data);
            [pred, acc, ~] = svmpredict(test_label', test_data,model);
            acc_save(rr,bb)= acc(1); % save accuracy
            % save confuse matrix
            for sample_now = 1:length(test_label)
                confuse_matrix(bb, rr ,test_label(sample_now), pred(sample_now))=confuse_matrix(bb, rr ,test_label(sample_now), pred(sample_now))+1;
            end
    end
    waitbar(bb/boot_times)
end
```

Balance the data

Save decode pattern

Multivariate Analysis - Classification

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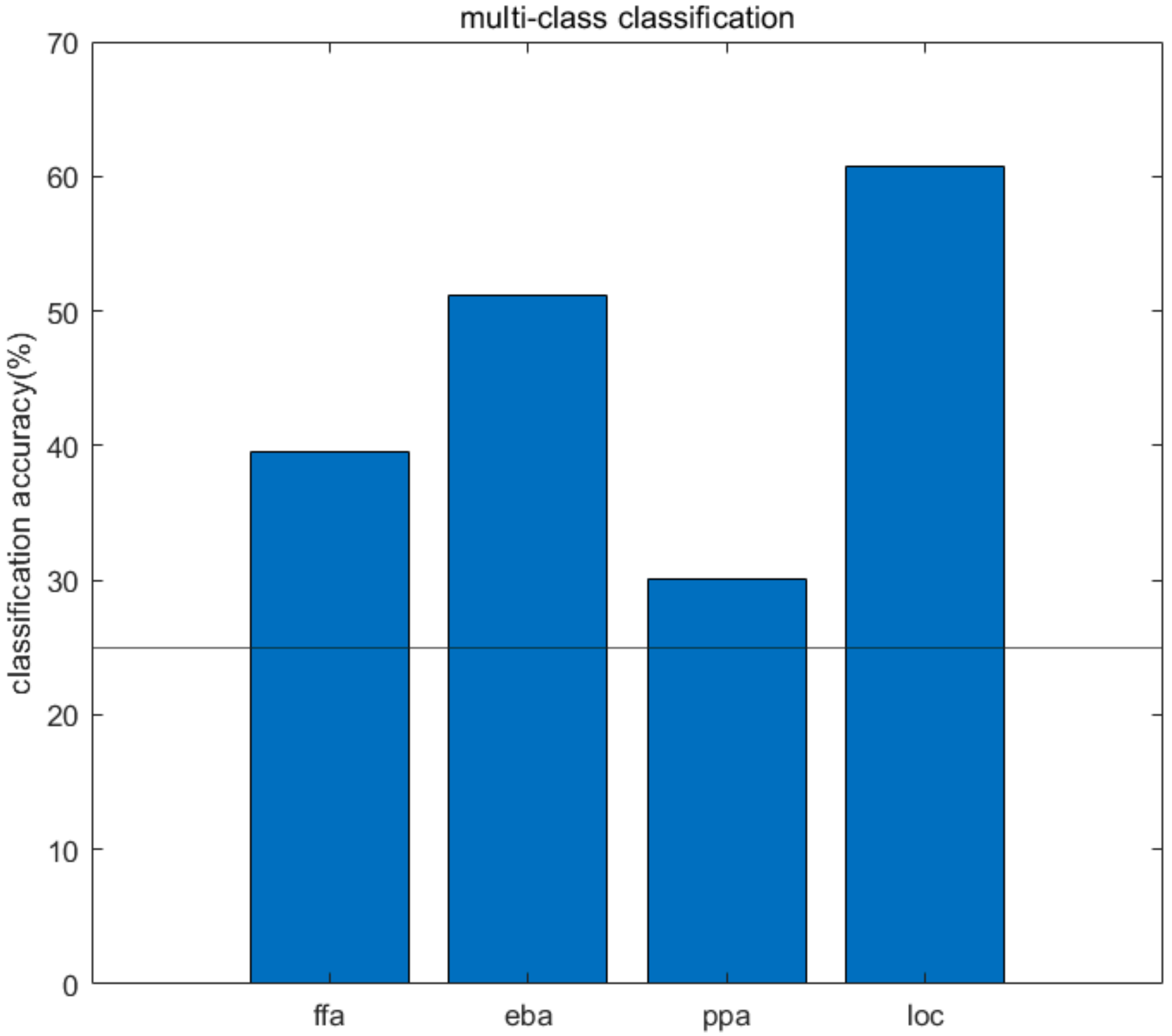
- Q2 - Can we read(decode) any category through the response pattern?
- Decoding 4 categories (animal, face, man-made object, natural object)



Multivariate Analysis - Classification

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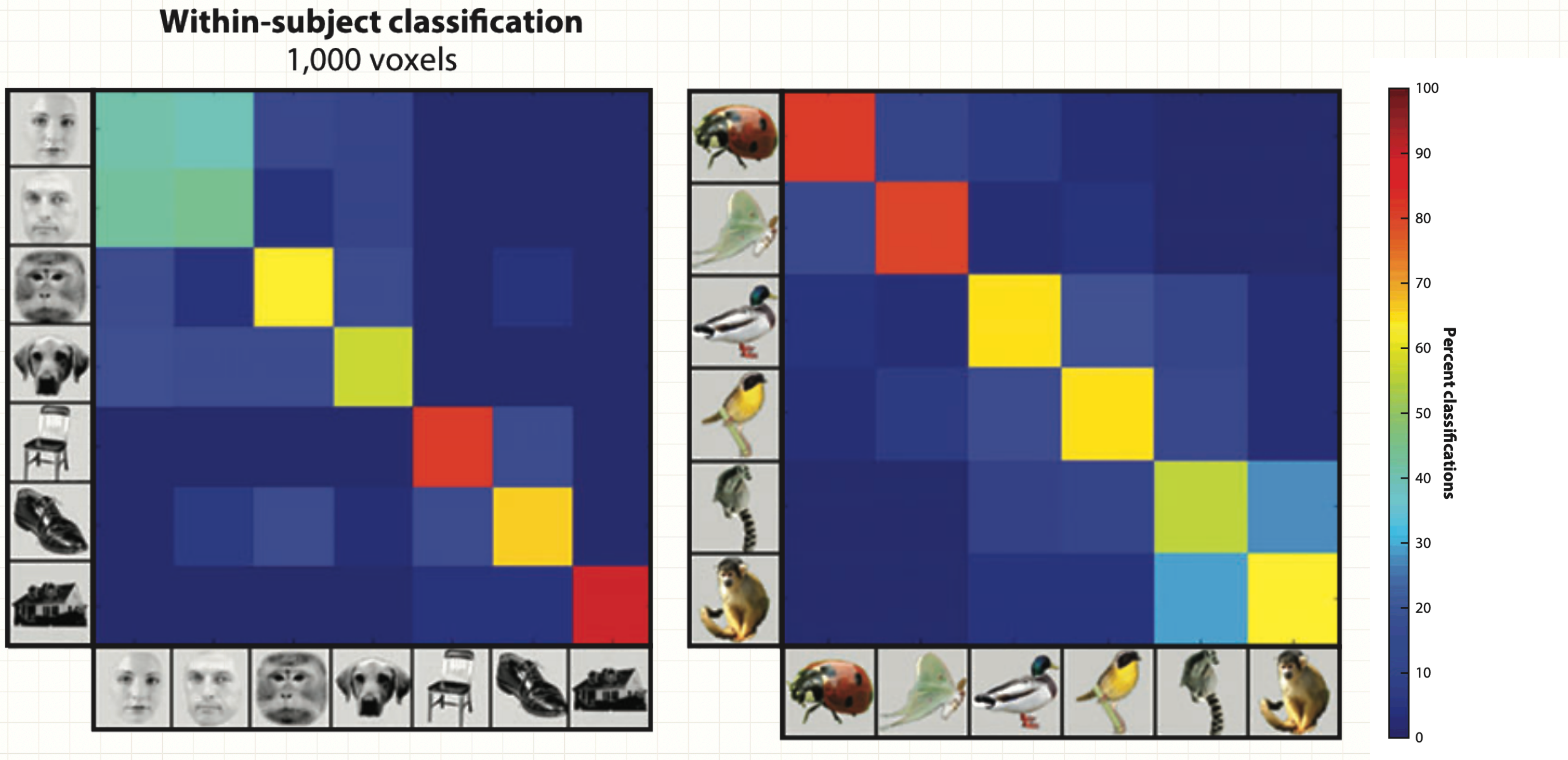
- **Q3 - Which categories are misidentified as what?**
- **Confuse Matrix (error pattern) reveals the discriminability between any two categories**



Multivariate Analysis - Classification

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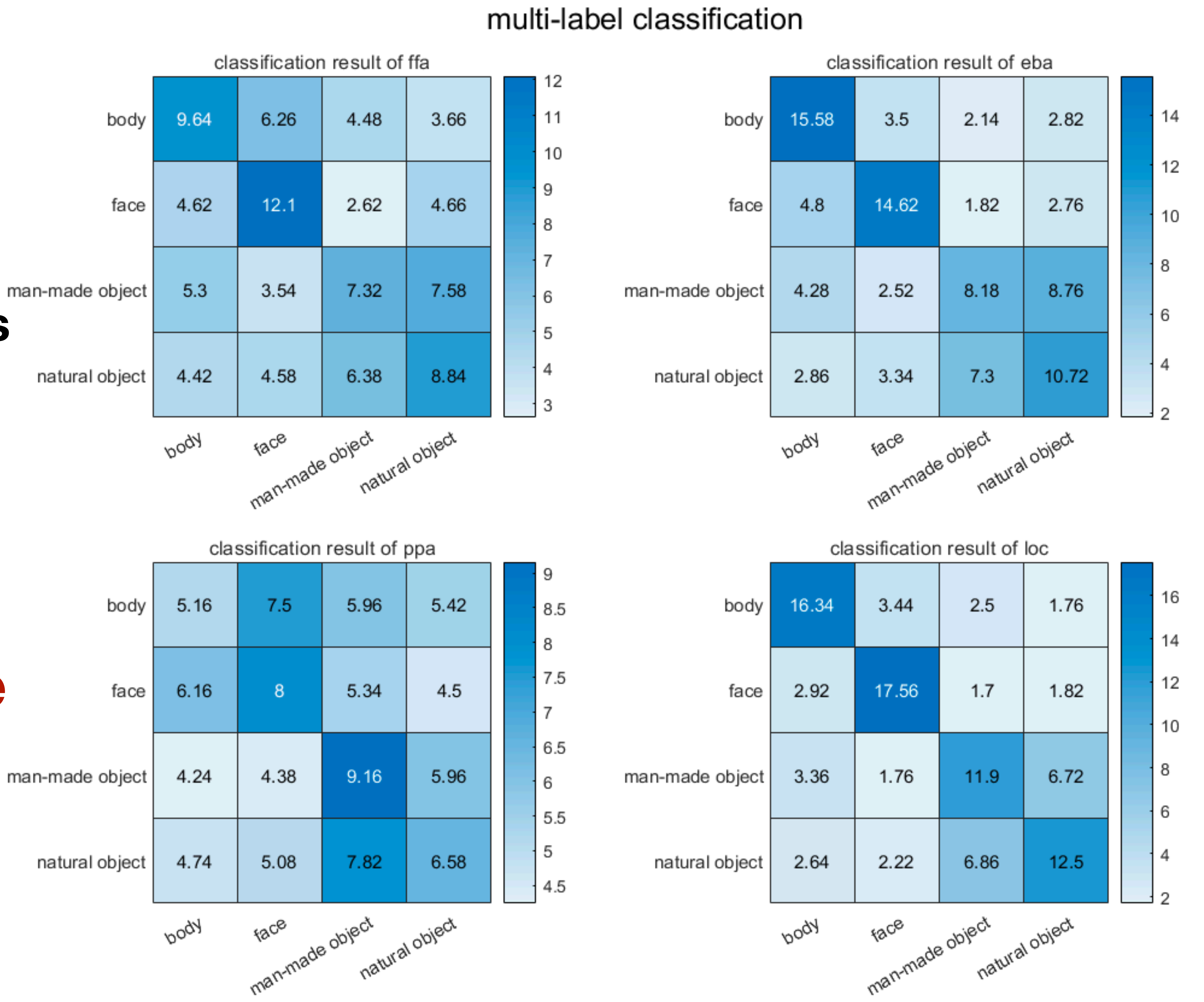
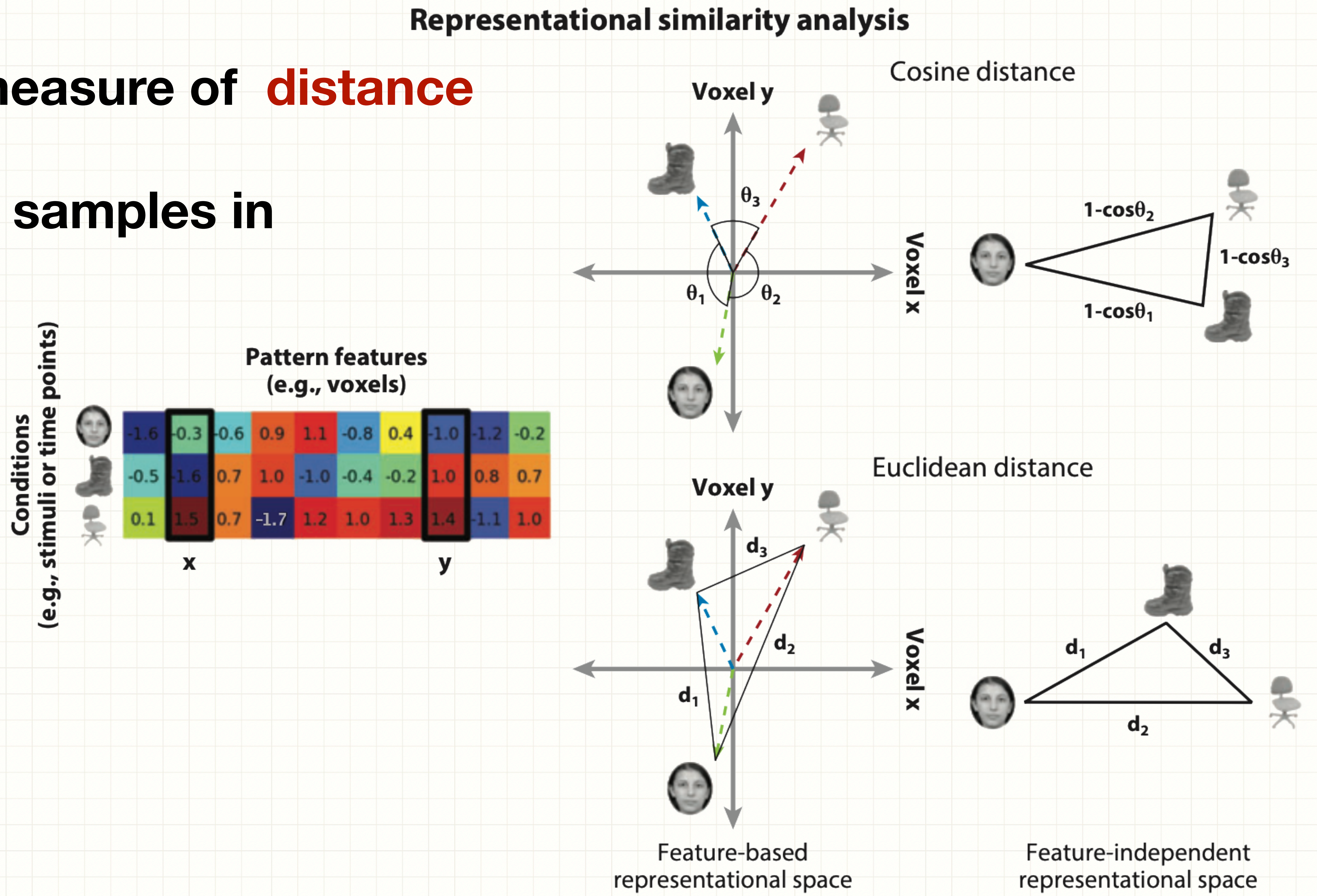
- **Q3 - Which categories are misidentified as what?**
- **Confuse Matrix (error pattern) reveals the discriminability between any two categories**
- **Two subcategories of objects are confused in all areas**
- **Discriminability as a measure of distance**

```
[pred, acc, ~] = svmpredict(test_label', test_data,model);
acc_save(rr,bb)= acc(1); % save accuracy
% save confuse matrix
for sample_now = 1:length(test_label)
    confuse_matrix(bb, rr ,test_label(sample_now), pred(sample_now))=confuse_matrix(bb, rr
end
```



Multivariate Analysis - Distance

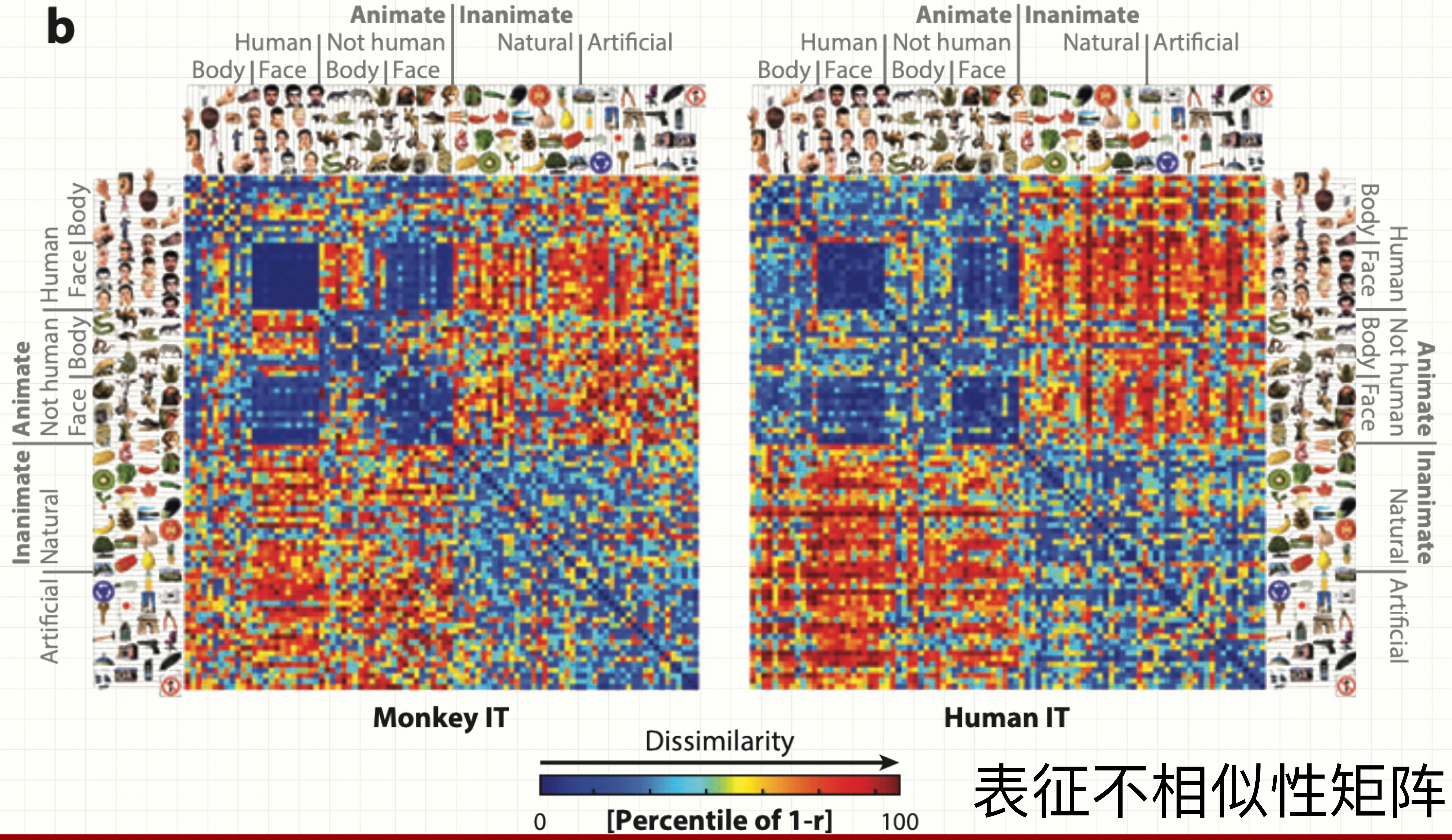
- **Discriminability as a measure of distance**
- **Distance between any samples in representation space.**



Multivariate Analysis - RSA

REPRESENTATIONAL SIMILARITY ANALYSIS

- **RSA examines the structure of representations within a representational space in terms of distances between response vectors**



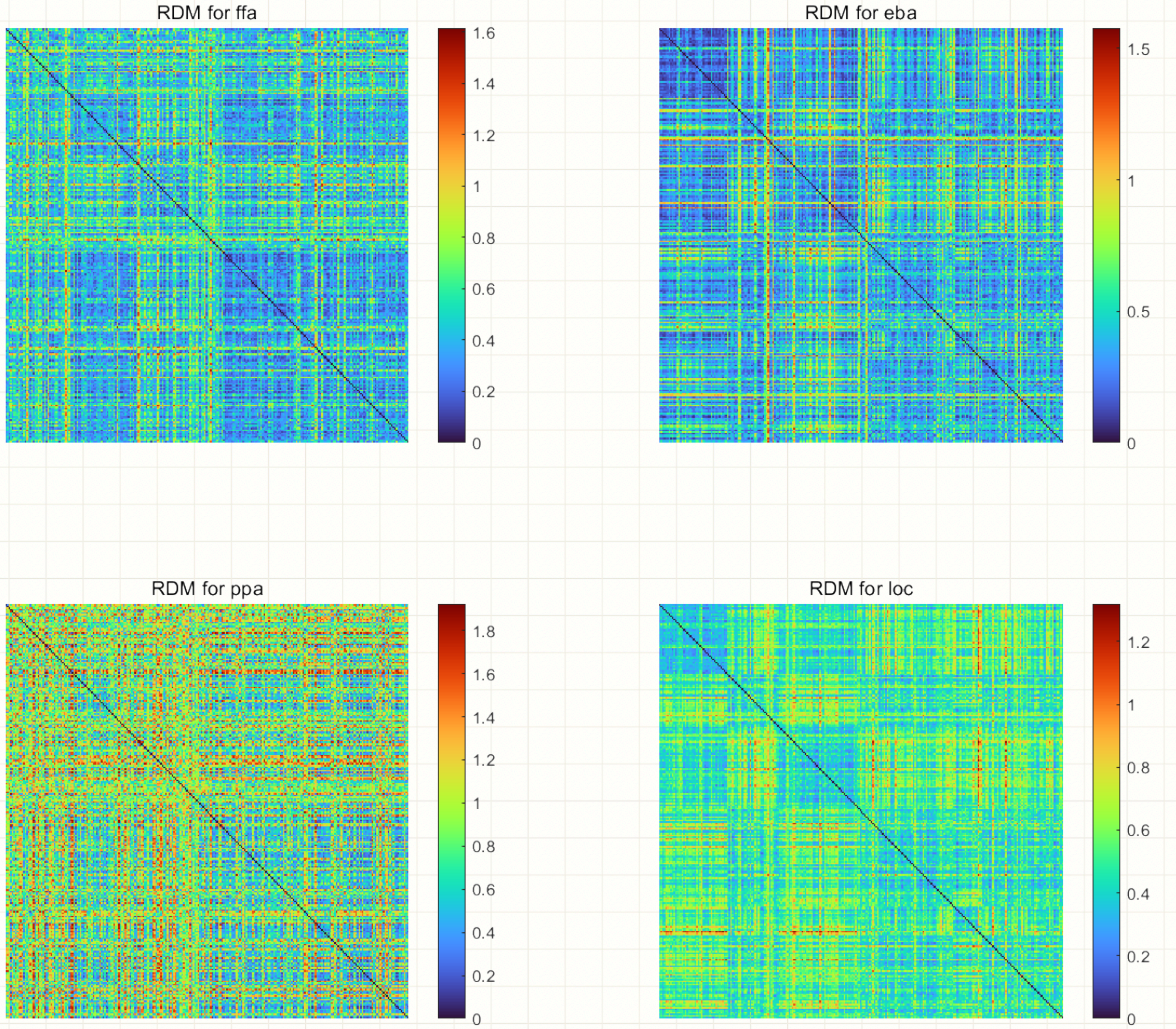
表征不相似性矩阵

Multivariate Analysis - RSA

REPRESENTATIONAL SIMILARITY ANALYSIS

Draw RDM

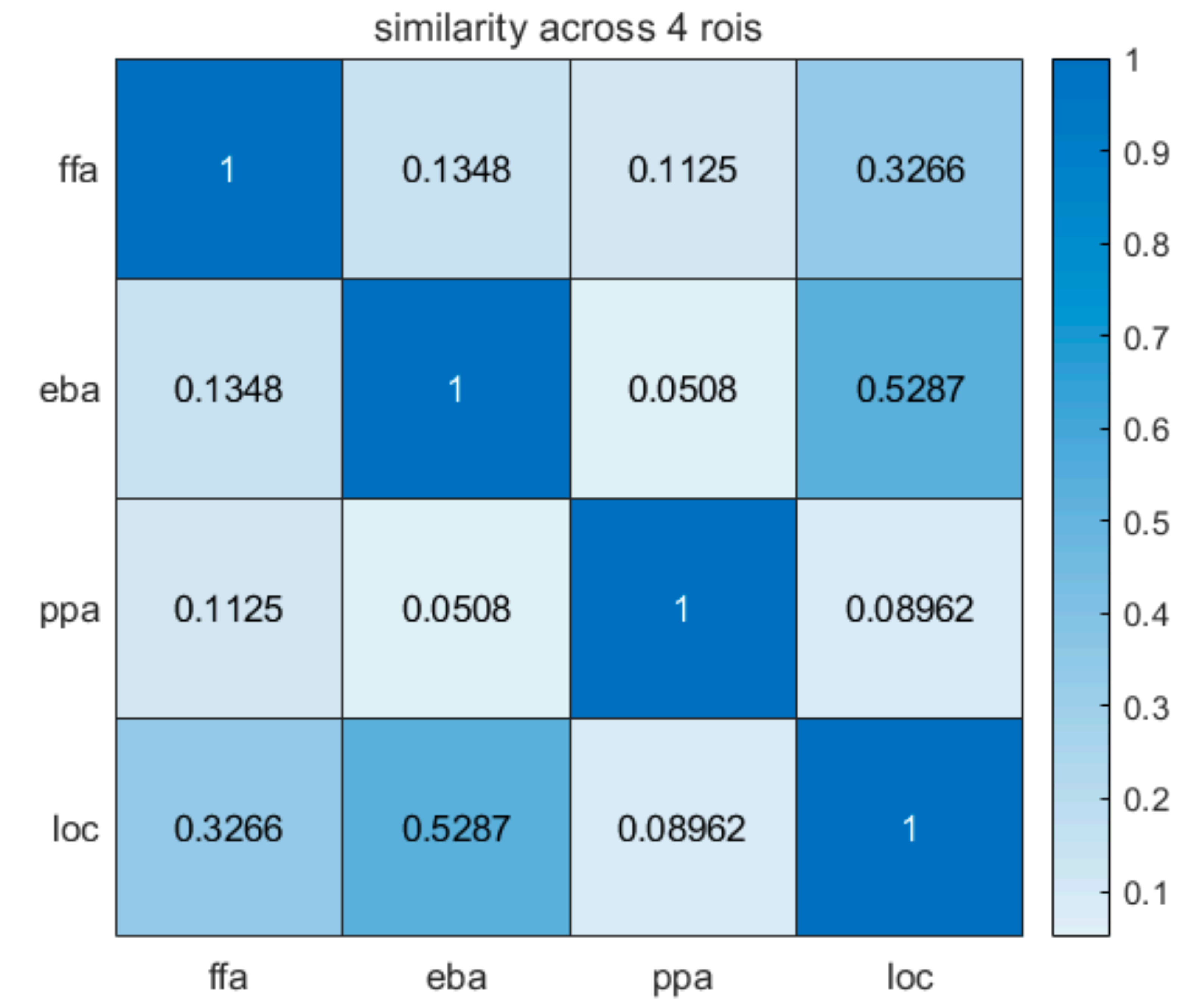
```
load('average_roi_beta.mat')
load("category_label.mat")
% sort categories
image_idx = [];
for cc = 1:length(image_category)
    image_idx = [image_idx image_category(cc).picset];
end
image_idx = image_idx(1:2:500);
figure
for rr = 1:length(average_beta)
    subplot(2,2,rr)
    beta_now = average_beta{rr,1};
    beta_now = beta_now(image_idx, :);
    pd = squareform(pdist(beta_now,'correlation'));

    imagesc(pd)
    title(['RDM for ' roi_legend{rr}])
    axis off
    colorbar
    pd_save{rr}=pd;
end
```



Multivariate Analysis - RSA

REPRESENTATIONAL SIMILARITY ANALYSIS

- **Compare across systems**
- **PPA shows a geometry inconsistent with other areas**




```
figure
for rx = 1:length(average_beta)
    for ry = 1:length(average_beta)
        rs(rx, ry) = corr(pd_save{rx}(find(tril(ones(size(pd)), -1))) , pd_save{ry}(find(tril(ones(size(pd)), -1))));
    end
end
heatmap(roi_legend,roi_legend,rs)
title('similarity across 4 rois')
set(gcf, 'position',[744,653,473,396])
toc
```

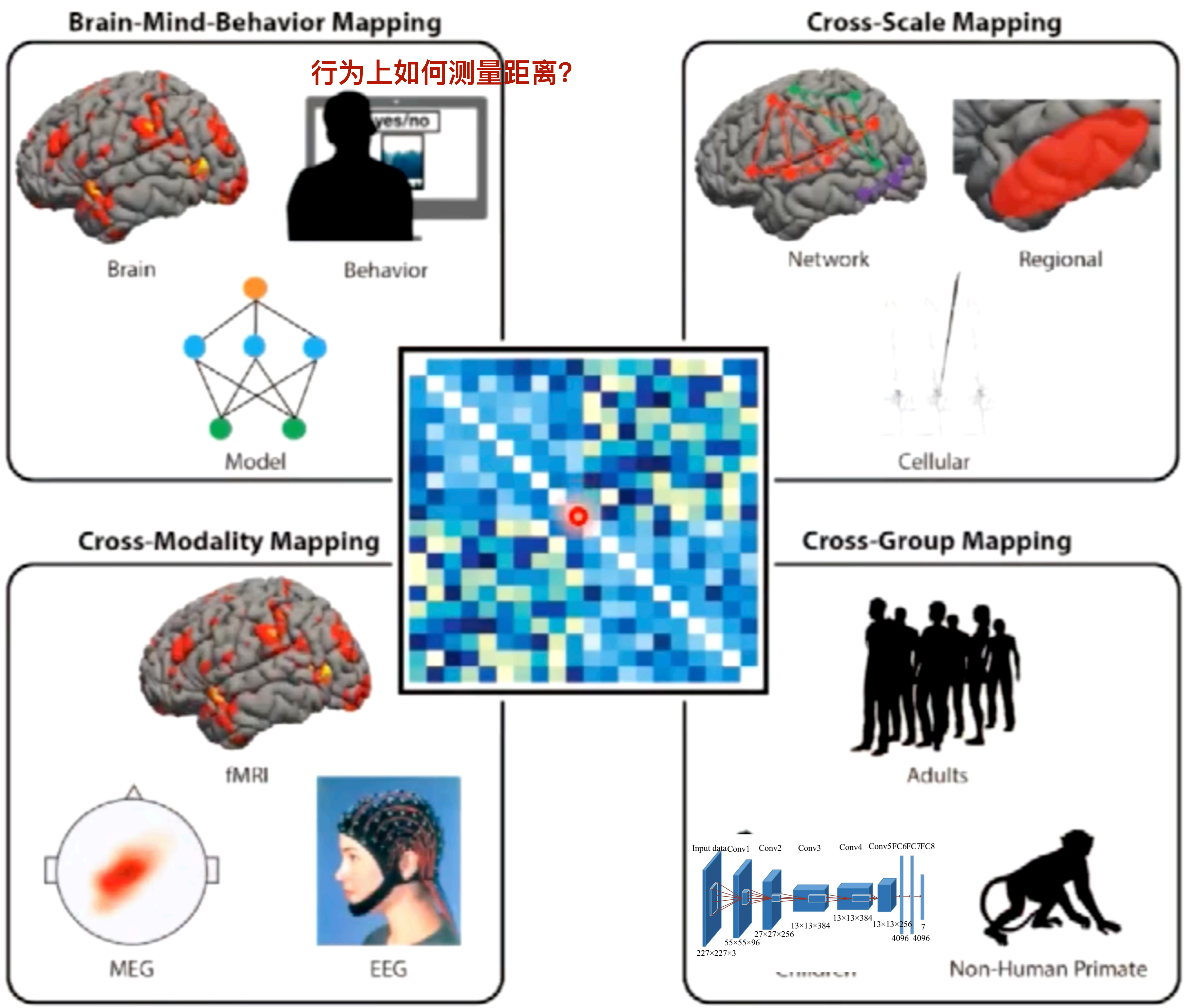
Multivariate Analysis - RSA

REPRESENTATIONAL SIMILARITY ANALYSIS

Pros

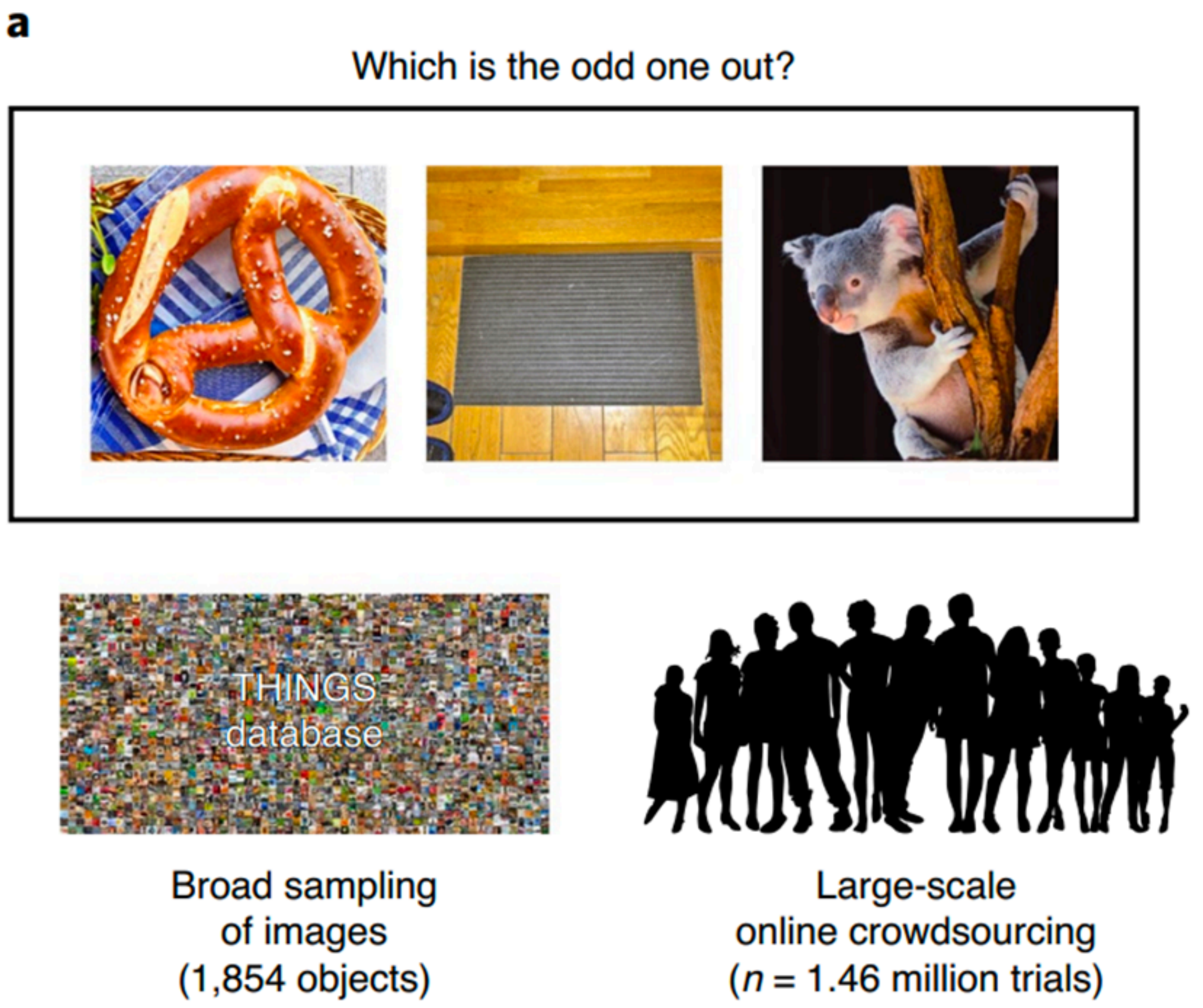
1. RSA can reveal that representations in different brain areas differ even if MVP classification is equivalent in those areas

2. By converting the locations of response vectors from a set of feature coordinates to a set of distances between vectors, the geometry of the representational space is now in a format that is not dependent on the feature coordinate axes



Multivariate Analysis - RSA

行为上测量RSA



Multivariate Analysis - RSA

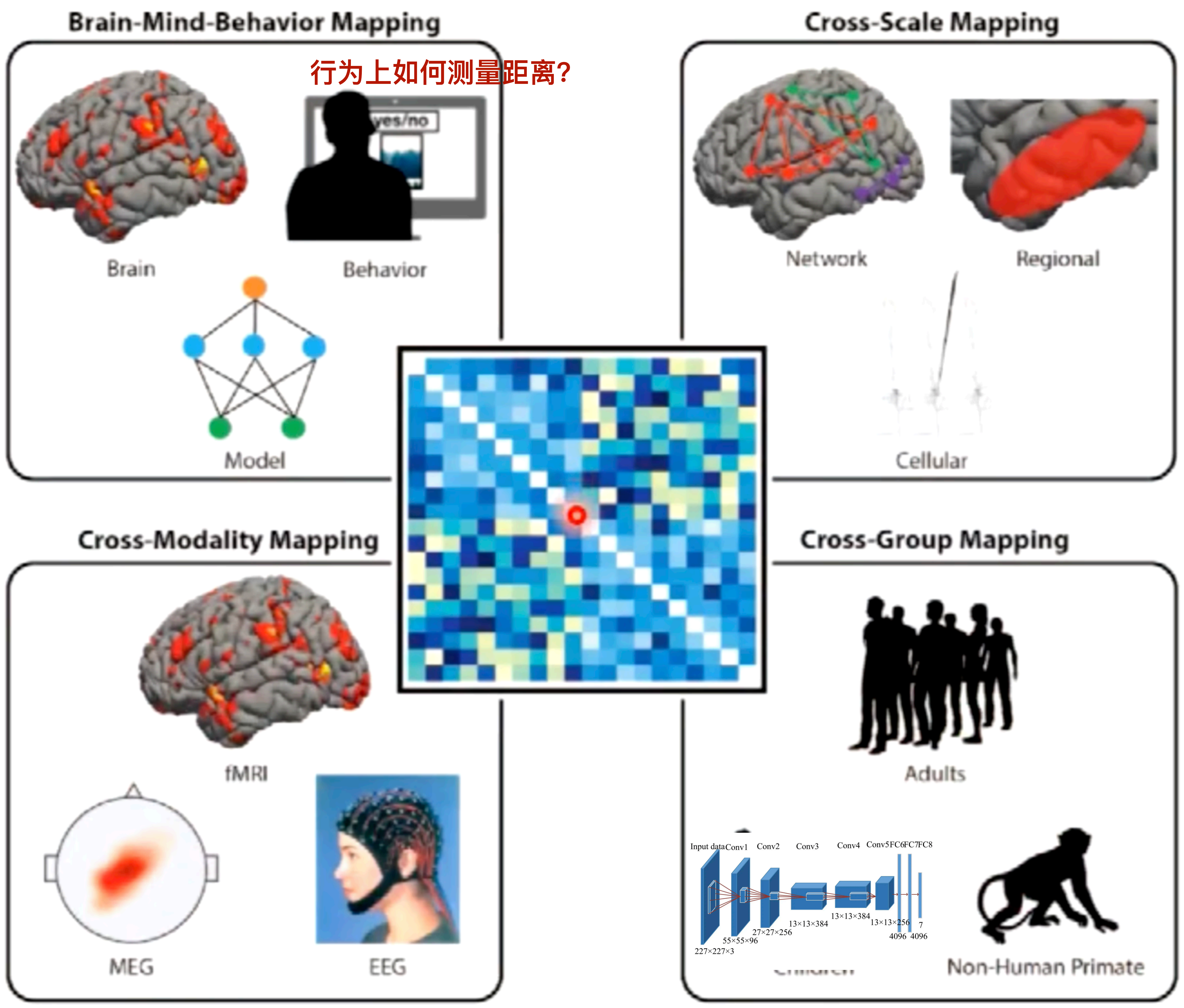
REPRESENTATIONAL SIMILARITY ANALYSIS

Cons

1）RSA忽略了物理空间的差异，fMRI 的voxel位置已经不再重要了

2）RSA强调了表征差异，而忽略了表征强度的区别

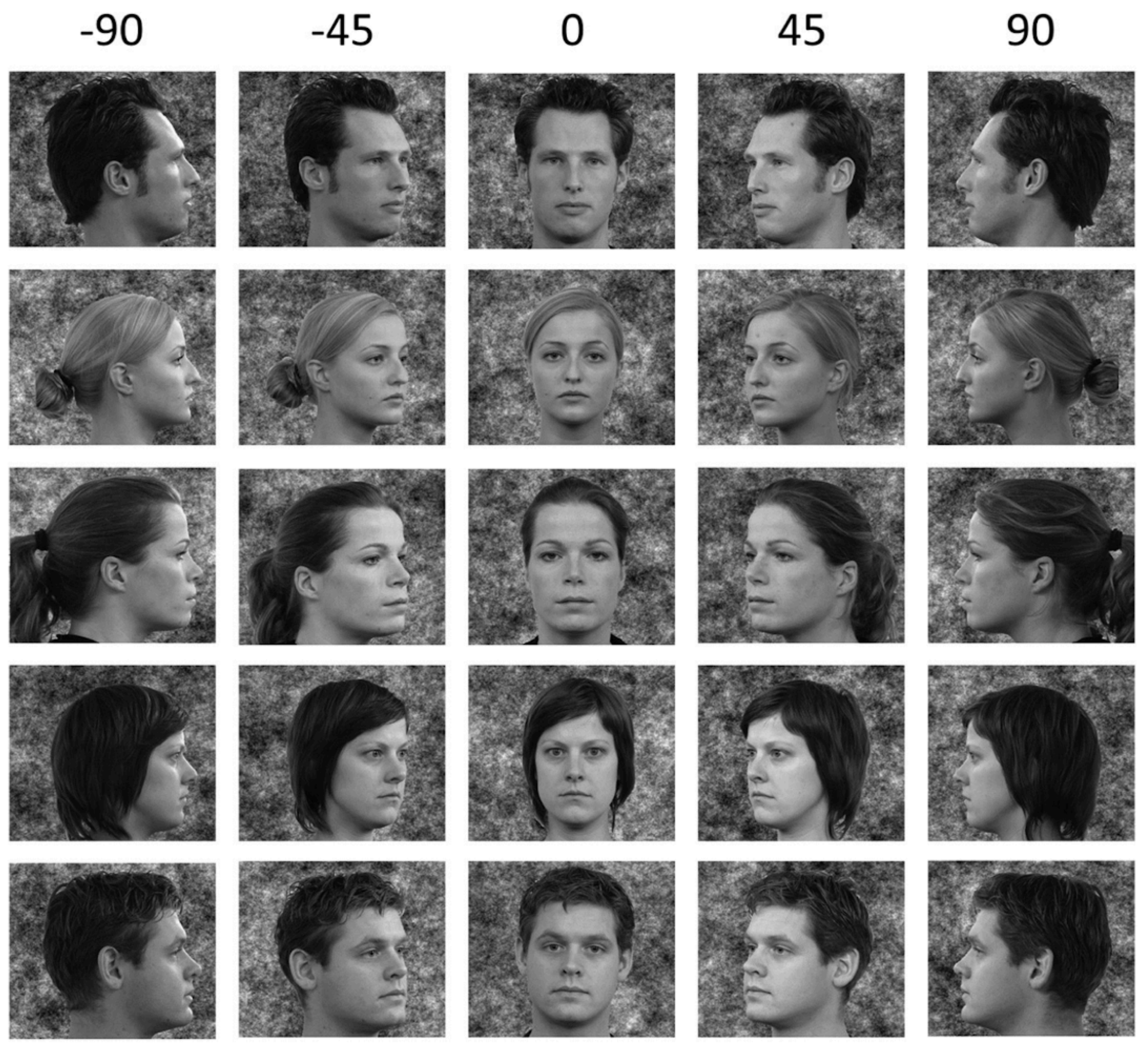
3）基于Correlation的RSA过分关注所有channel(Voxel, Neuron, etc.)的反应，可能忽略了少部分channel 的特有表征。

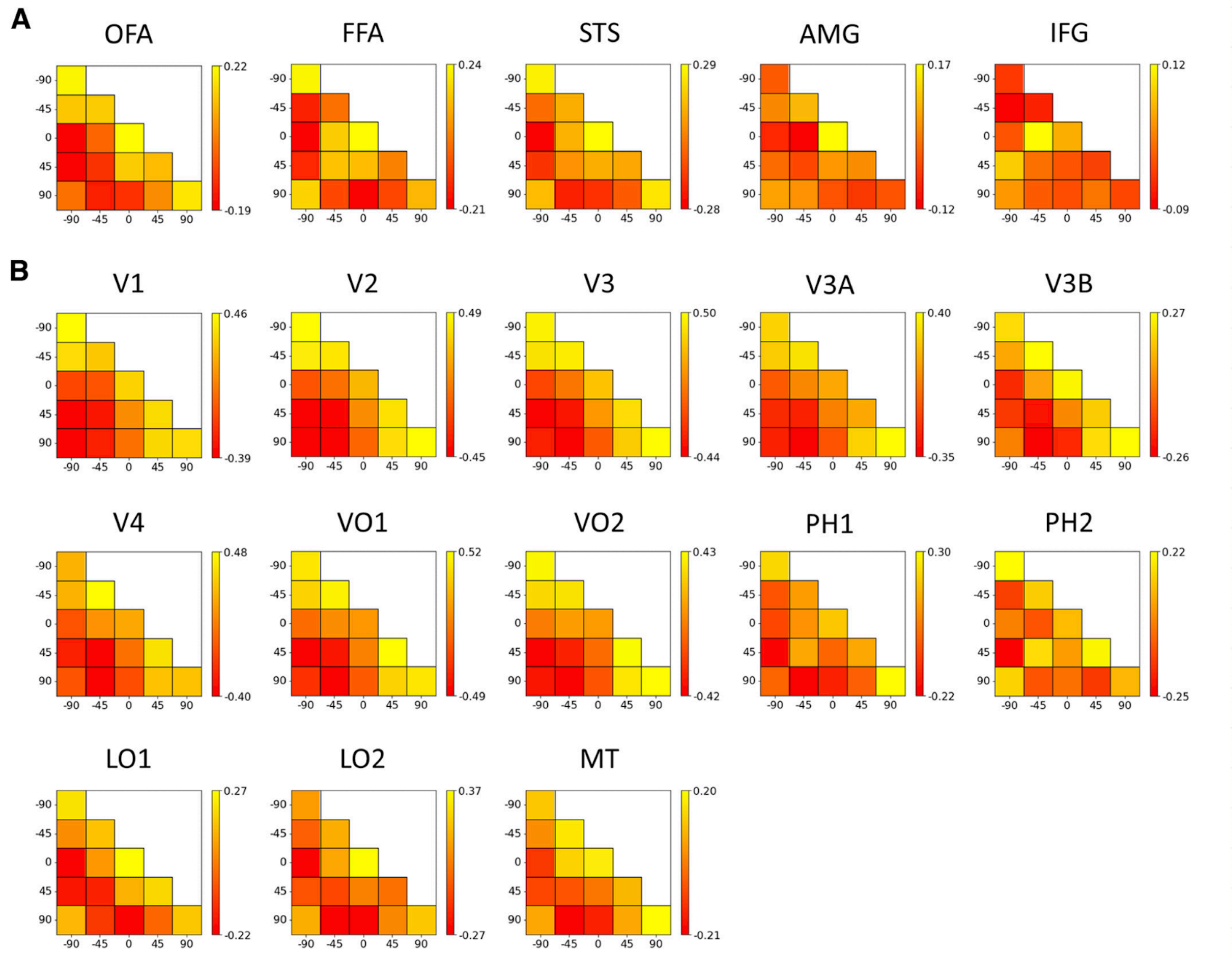


Multivariate Analysis - RSA

REPRESENTATIONAL SIMILARITY ANALYSIS

Example - Use RSA to determine whether the representation of symmetrical viewpoints in face-selective regions is directly linked to the perception and recognition of face identity





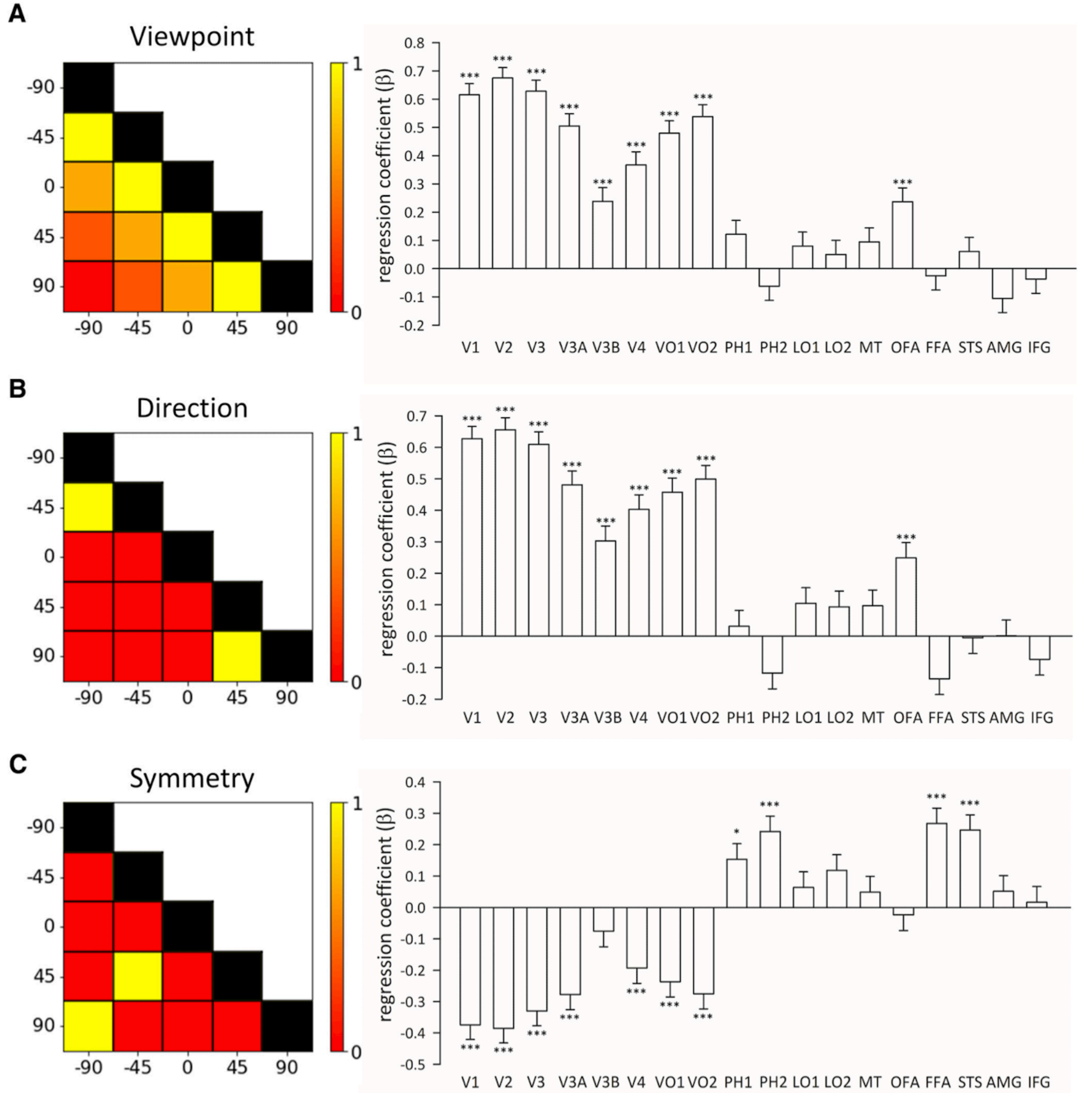
Symmetrical Viewpoint Representations in Face-Selective Regions Convey an Advantage in the Perception and Recognition of Faces

Multivariate Analysis - RSA

REPRESENTATIONAL SIMILARITY ANALYSIS

Example - Use RSA to determine whether the representation of symmetrical viewpoints in face-selective regions is directly linked to the perception and recognition of face identity

fMRI - model



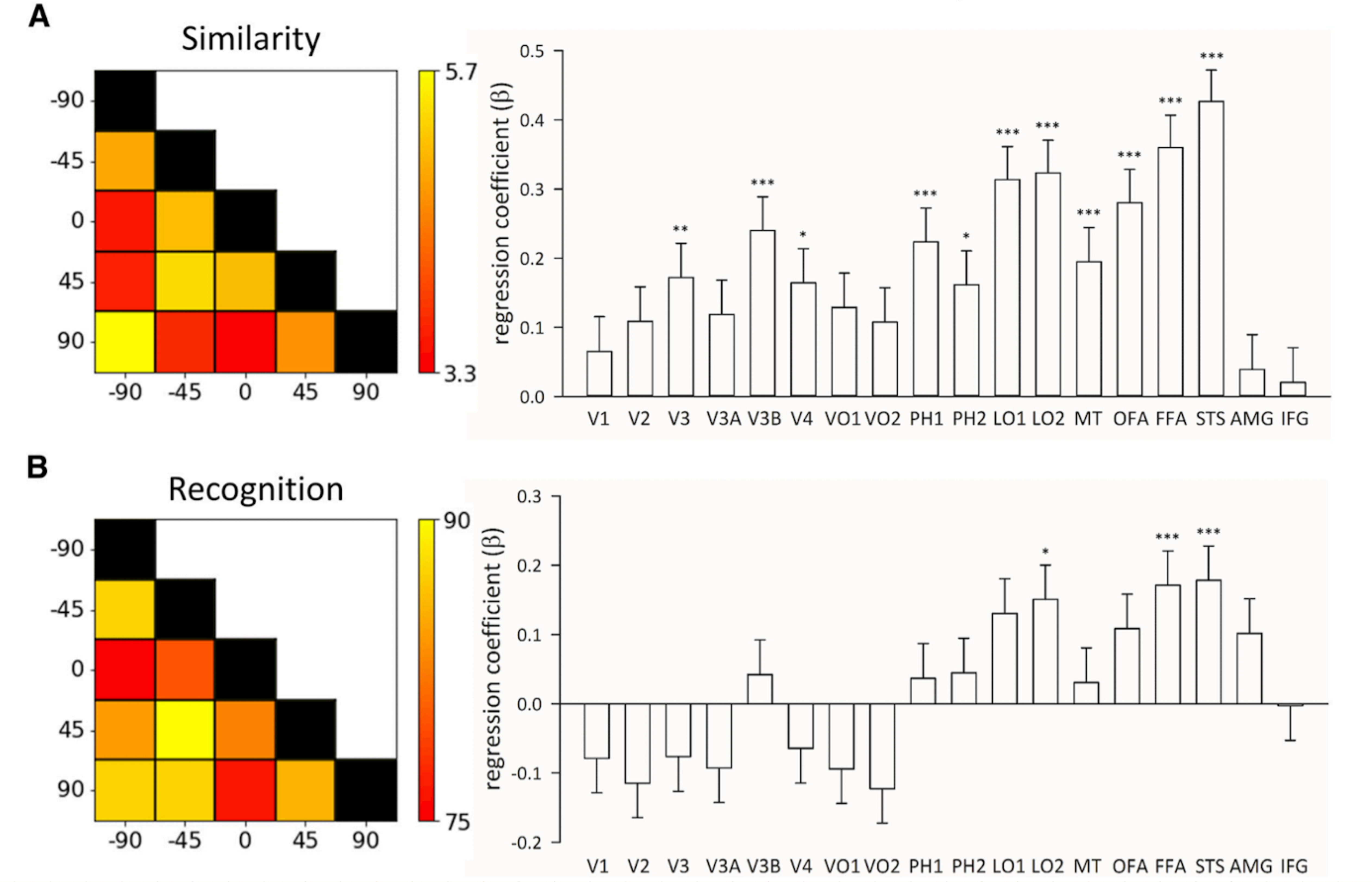
Symmetrical Viewpoint Representations in Face-Selective Regions Convey an Advantage in the Perception and Recognition of Faces

Multivariate Analysis - RSA

REPRESENTATIONAL SIMILARITY ANALYSIS

Example - Use RSA to determine whether the representation of symmetrical viewpoints in face-selective regions is directly linked to the perception and recognition of face identity

fMRI - behavior



Symmetrical Viewpoint Representations in Face-Selective Regions Convey an Advantage in the Perception and Recognition of Faces

Recommended Reading

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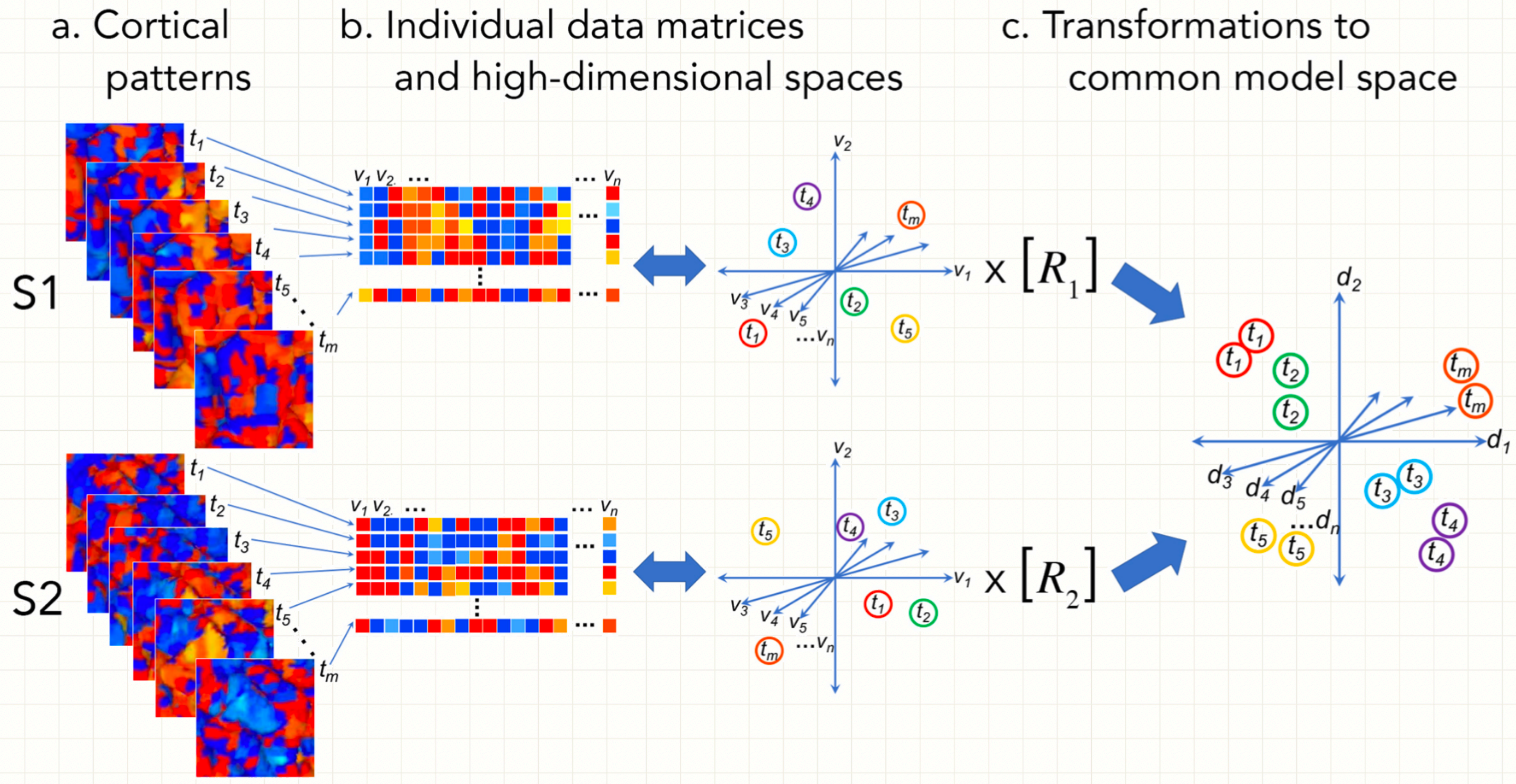
Decoding Neural Representational Spaces Using Multivariate Pattern Analysis

James V. Haxby,[1,2] Andrew C. Connolly,[1] and J. Swaroop Guntupalli[1]

[1]Department of Psychological and Brain Sciences, Center for Cognitive Neuroscience, Dartmouth College, Hanover, New Hampshire 03755;
email: james.v.haxby@dartmouth.edu, andrew.c.connolly@dartmouth.edu, swaroopgj@gmail.com

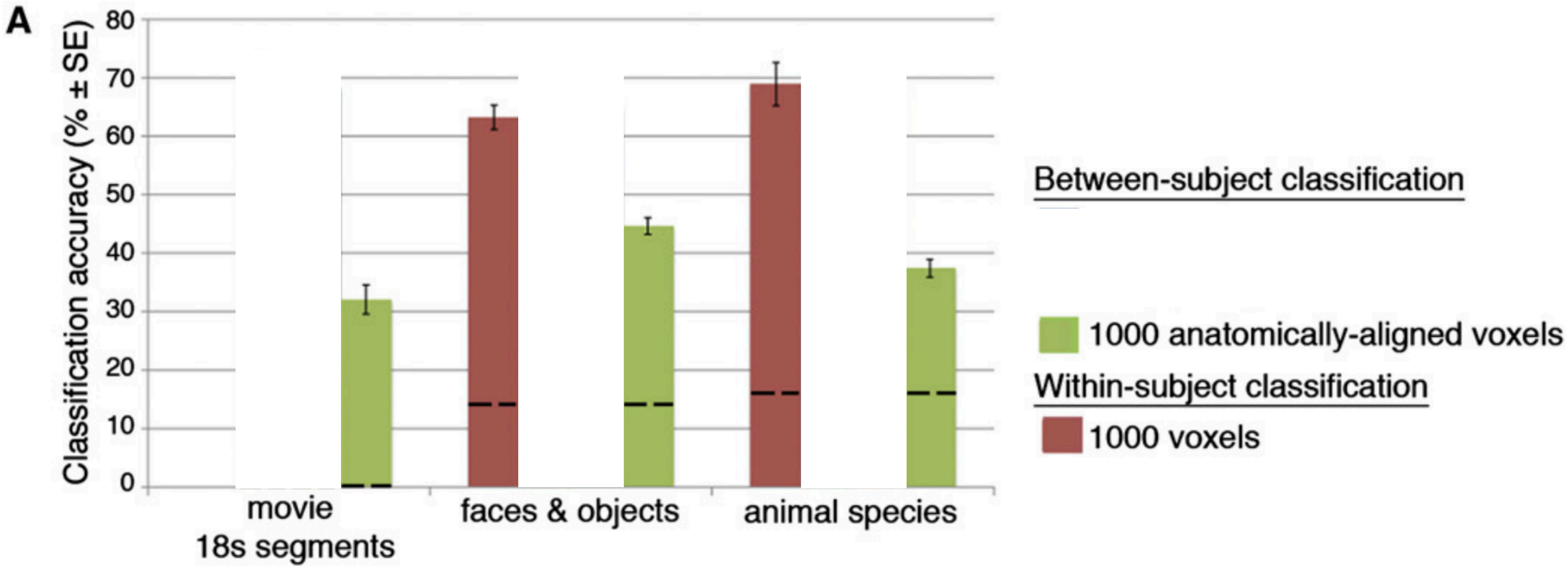
[2]Center for Mind/Brain Sciences (CIMeC), University of Trento, Rovereto, Trentino 38068, Italy

功能磁共振中的大脑超配准
Cortical Hyper-alignment in fMRI



Cross-Subject MVPA

MVPA performs poorly in cross-subject decoding



Haxby, J. V., Guntupalli, J. S., Connolly, A. C., Halchenko, Y. O., Conroy, B. R., Gobbini, M. I., ... & Ramadge, P. J. (2011). A common, high-dimensional model of the representational space in human ventral temporal cortex. *Neuron*, *72*(2), 404-416.

Cross-Subject MVPA

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Neural mind-reading technique performs poorly in cross-subject decoding

Actual stimulus

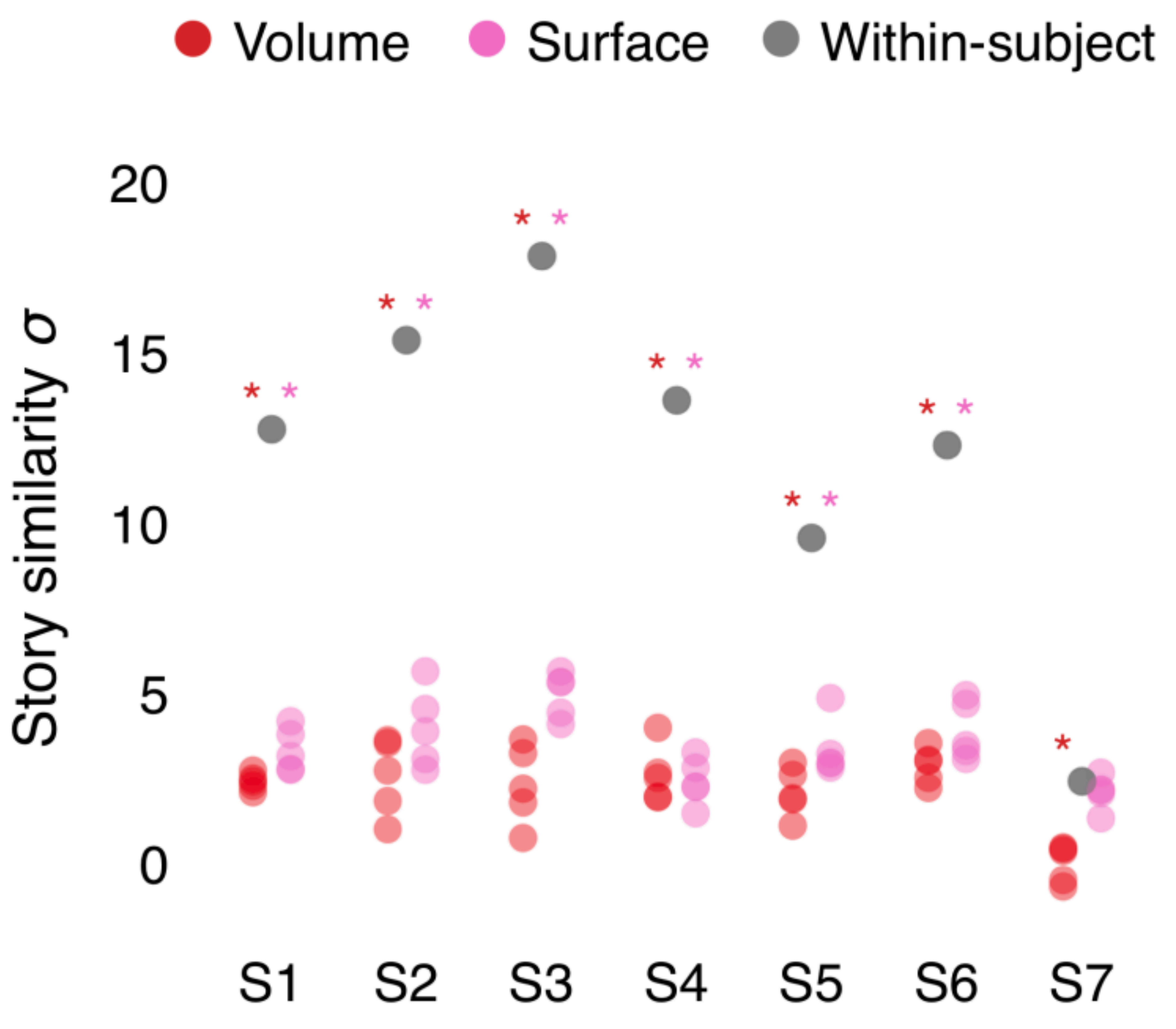
i got up from the air mattress and pressed my face against the glass of the bedroom window expecting to see eyes staring back at me but instead finding only darkness

i didn't know whether to scream cry or run away instead i said leave me alone i don't need your help adam disappeared and i cleaned up alone crying

Decoded stimulus

i just continued to walk up to the window and open the glass i stood on my toes and peered out i didn’t see anything and looked up again i saw nothing

started to scream and cry and then she just said i told you to leave me alone you can't hurt me i'm sorry and then he stormed off i thought he had left i started to cry



J Tang, A LeBel, S Jain, AG Huth - Nature Neuroscience, 2023

Cortical registration - Anatomical

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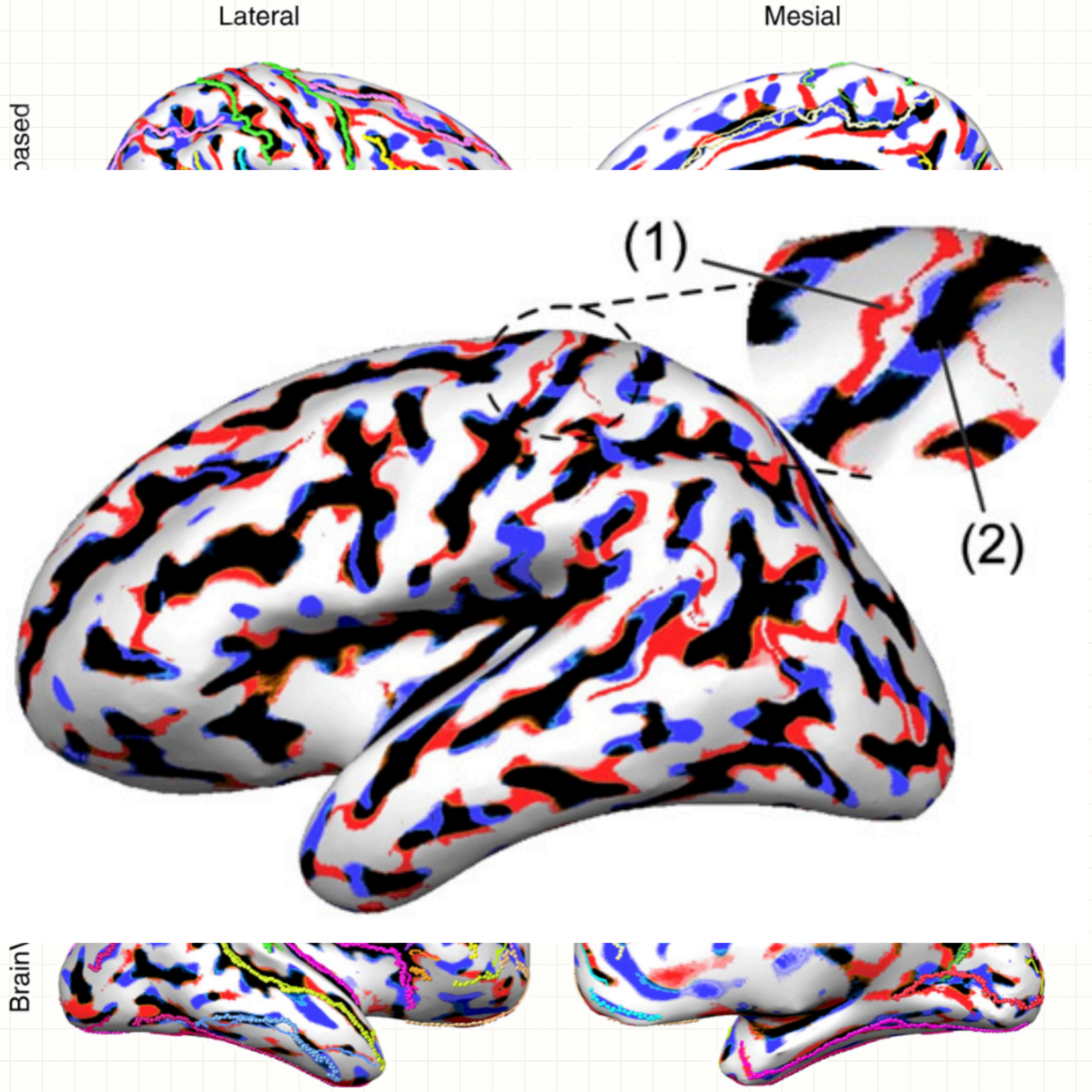
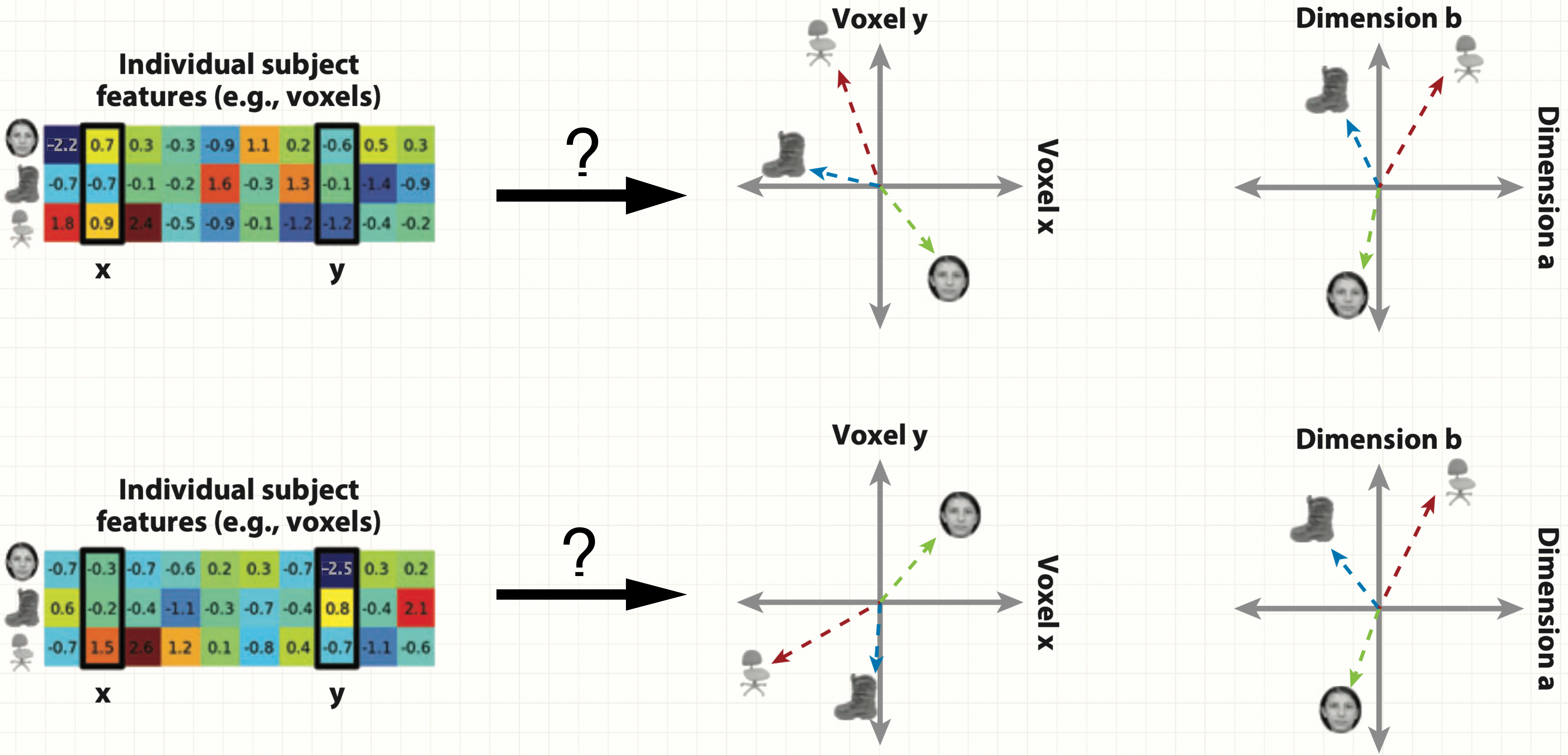
- Between subjects registration of the brain is am important issue for group-level analysis in fMRI study.
- Voxel-based method
  - Talairach Space
  - MNI Space
- Surface-based method—————————>
- Anatomical registration methods can not accurately delineate individual differences in fine-grained cortical architecture



(Pantazis et al., 2010)

Functional registration: Hyperalignment

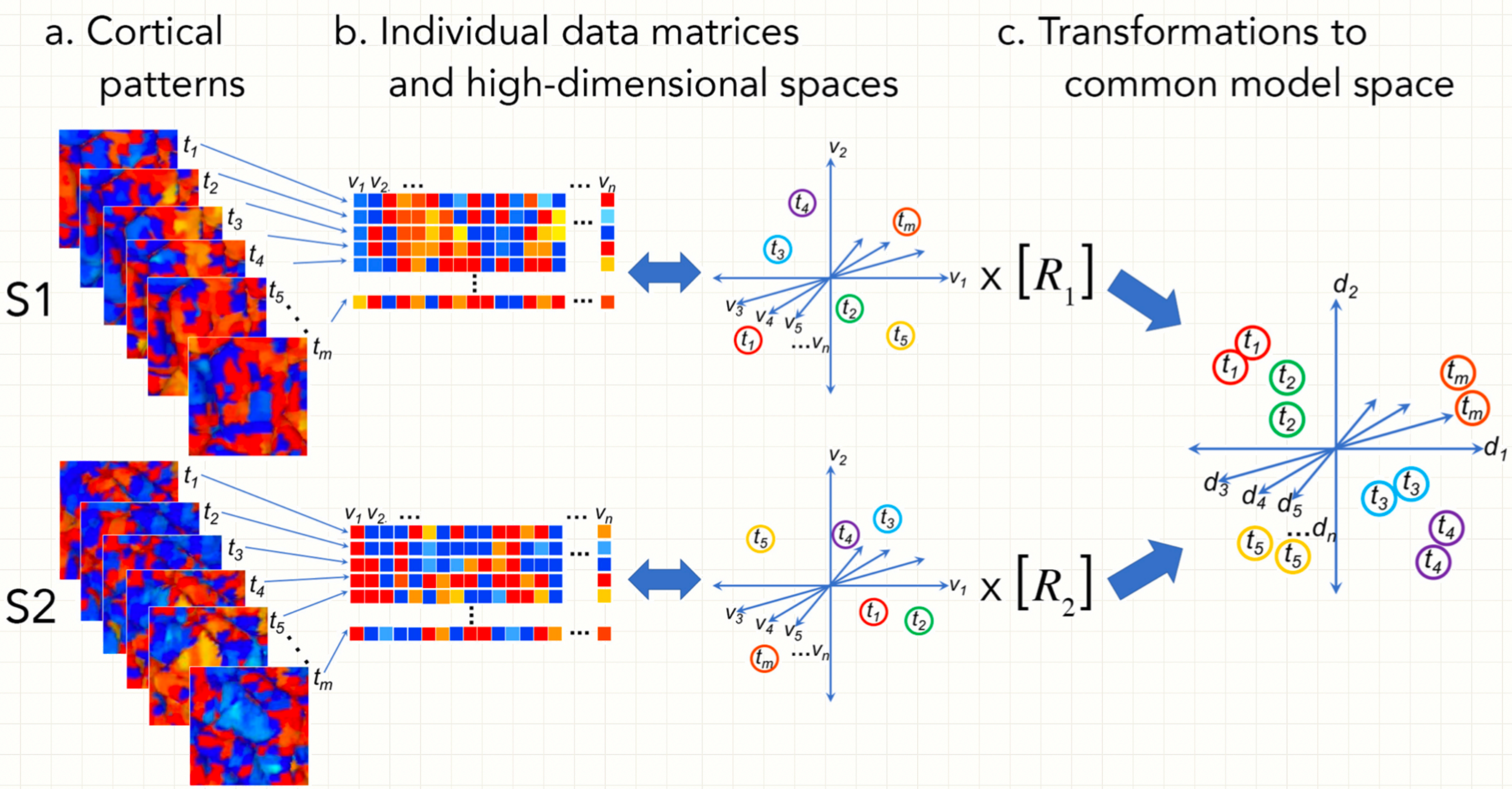
- **Cortical response patterns: high-dimensional features**
- **Multiple subjects: rotate axis based on the shared tuning properties**



(Haxby et al., 2014)

Functional registration: Hyperalignment

- Cortical response patterns: high-dimensional features
- Multiple subjects: rotate axis based on the shared tuning properties
- **Hyperalignment: find the orthogonal matrix for high-dimensional axis rotating**



(Haxby et al., 2020)

Cross-Subject MVPA

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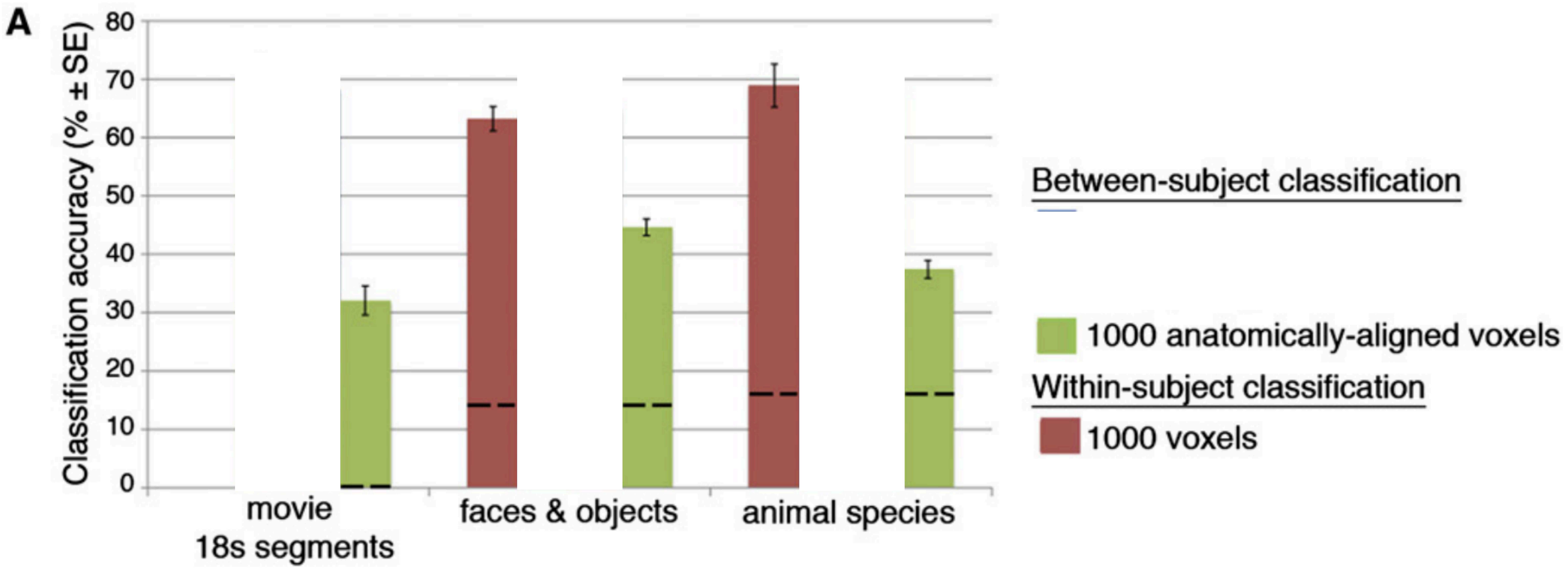
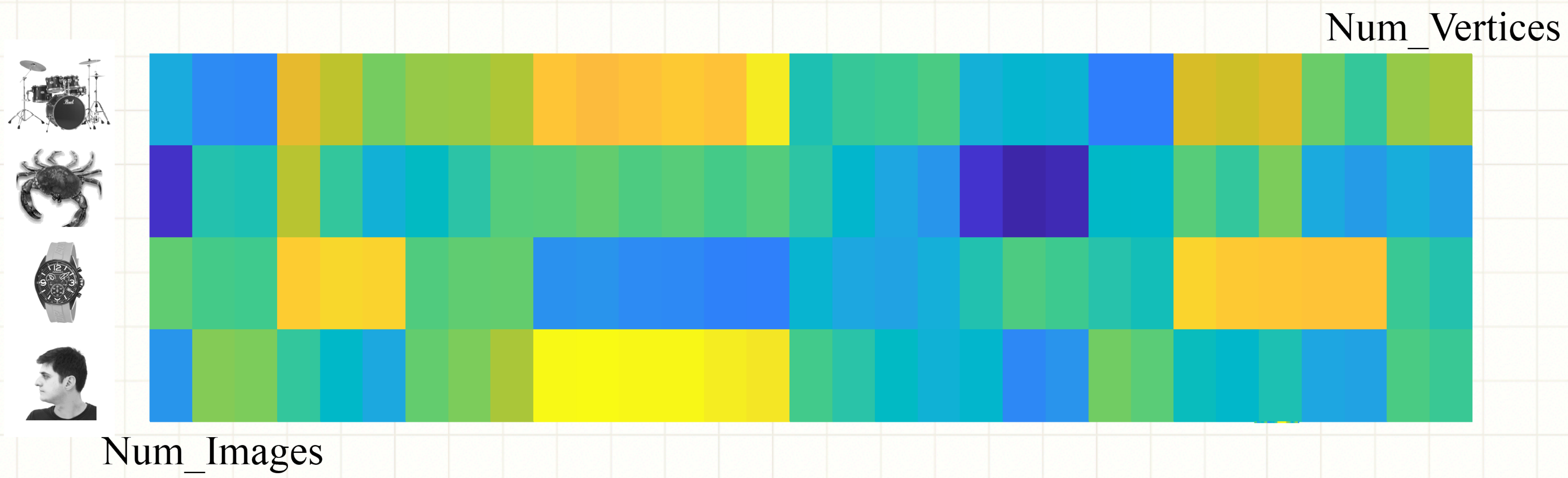
Improve cross subject mvpa by hyperalignment

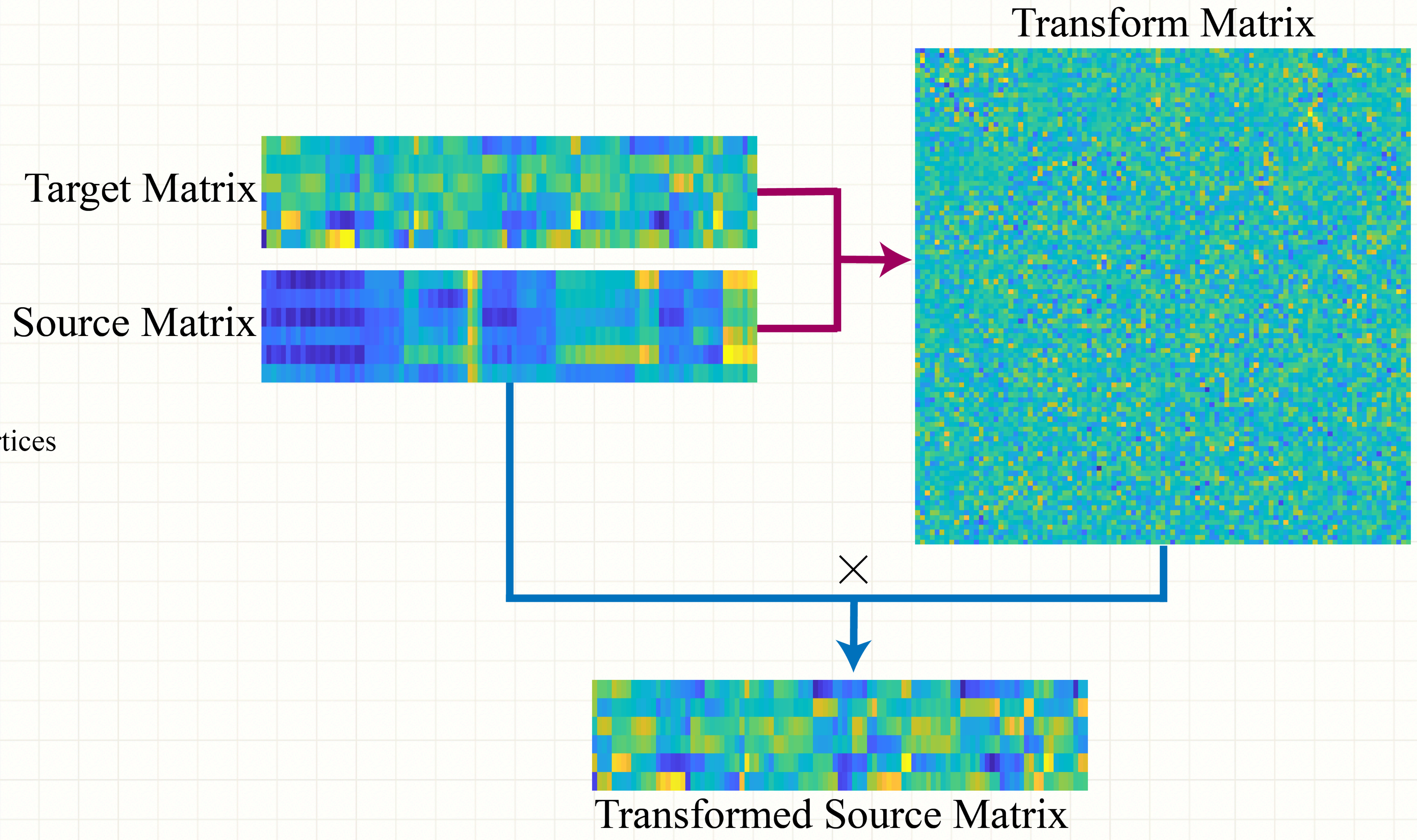


Haxby, J. V., Guntupalli, J. S., Connolly, A. C., Halchenko, Y. O., Conroy, B. R., Gobbini, M. I., ... & Ramadge, P. J. (2011). A common, high-dimensional model of the representational space in human ventral temporal cortex. *Neuron*, *72*(2), 404-416.

Mechanism of HyperAlignment

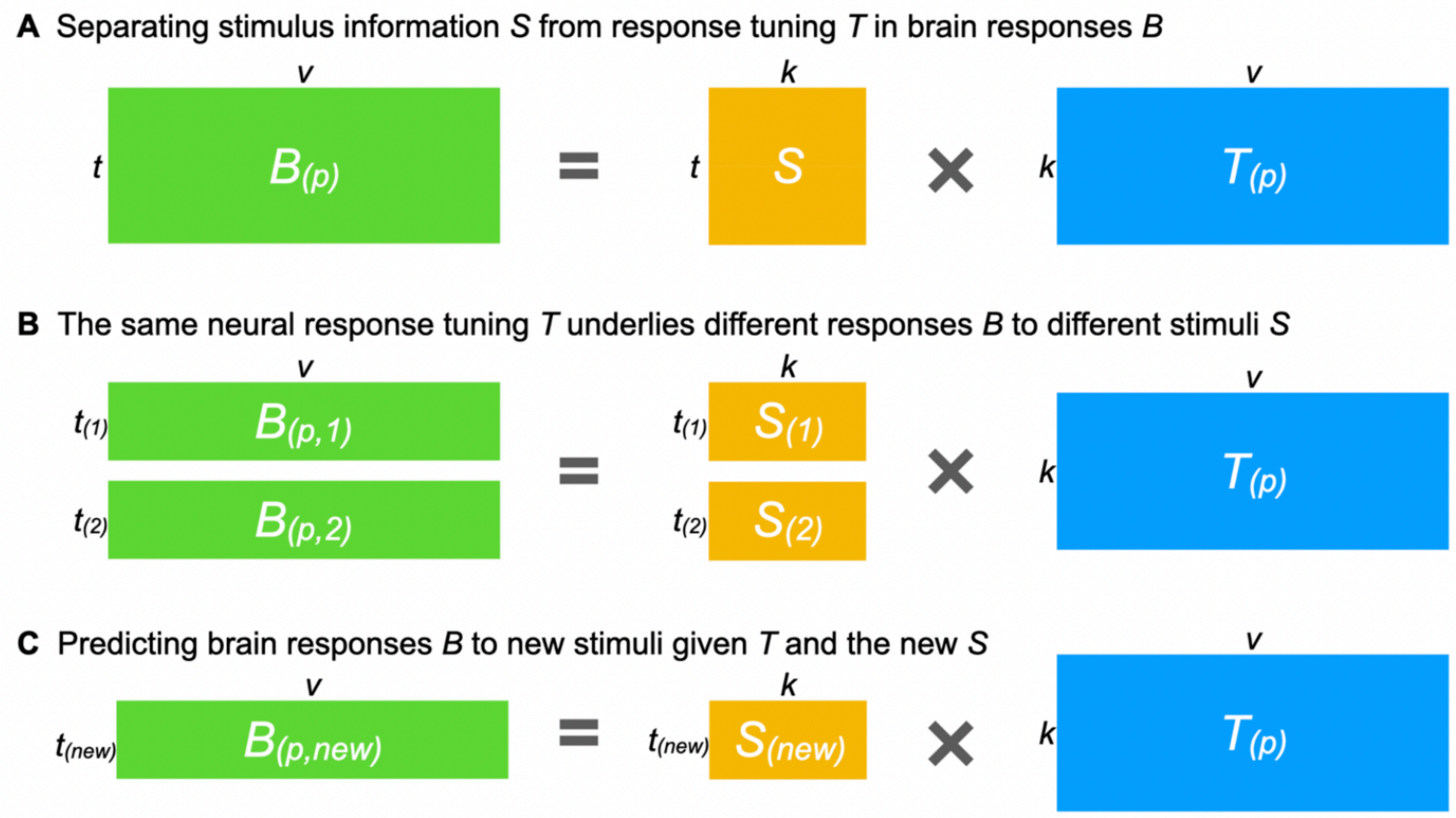
- Representation Geometry differs for 3 image sets
- The representation of the near-image is the most inconsistent, resulting in the poorest generalization performance.
- **Why?**
- **procrustes(X,Y) determines a linear transformation (orthogonal rotation) of the points in matrix Y to best conform them to the points in matrix X**
- **The assumption behind procrustes: two systems share the same representation geometry.**

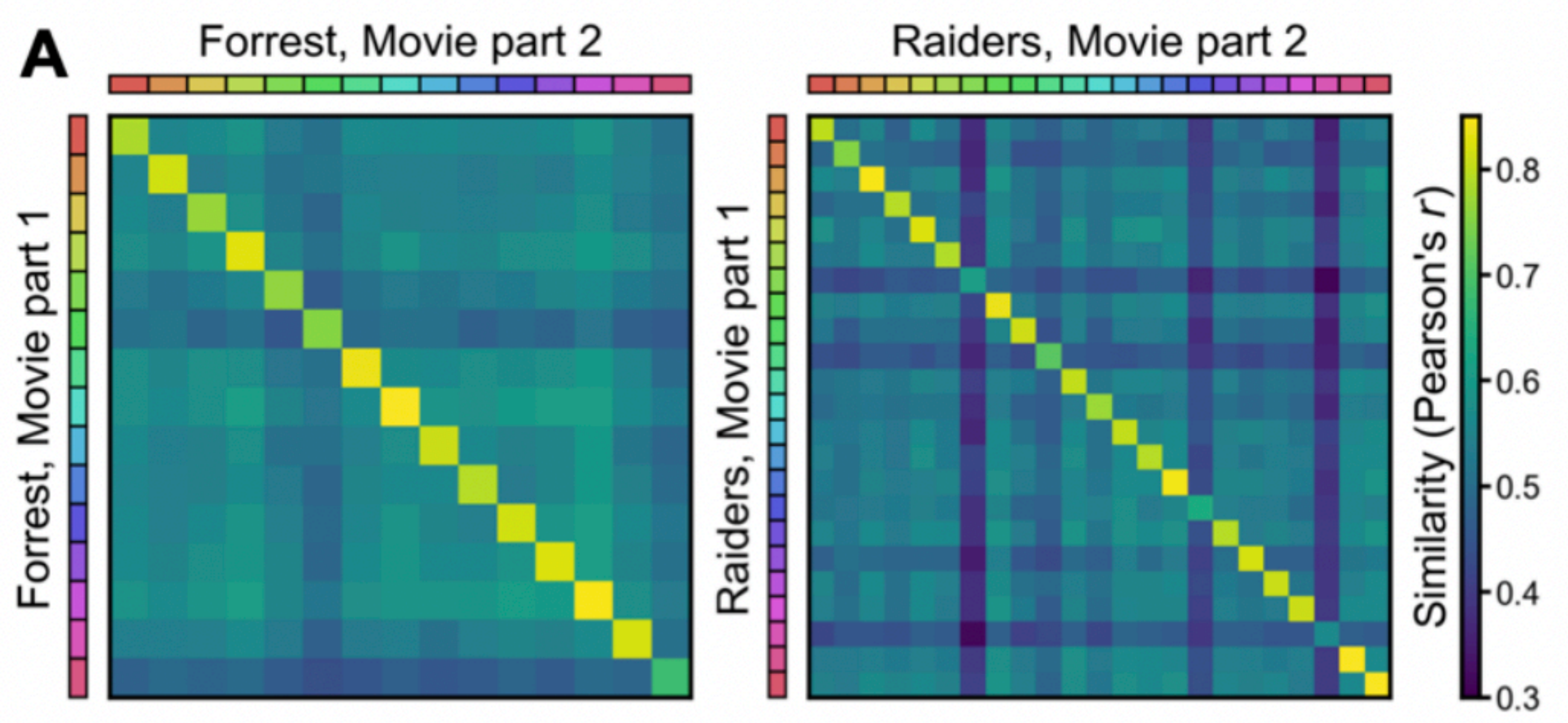




Progress of HyperAlignment

- **Modeling both functional differences and topographic differences by Individualized Neural Tuning (INT) model.**

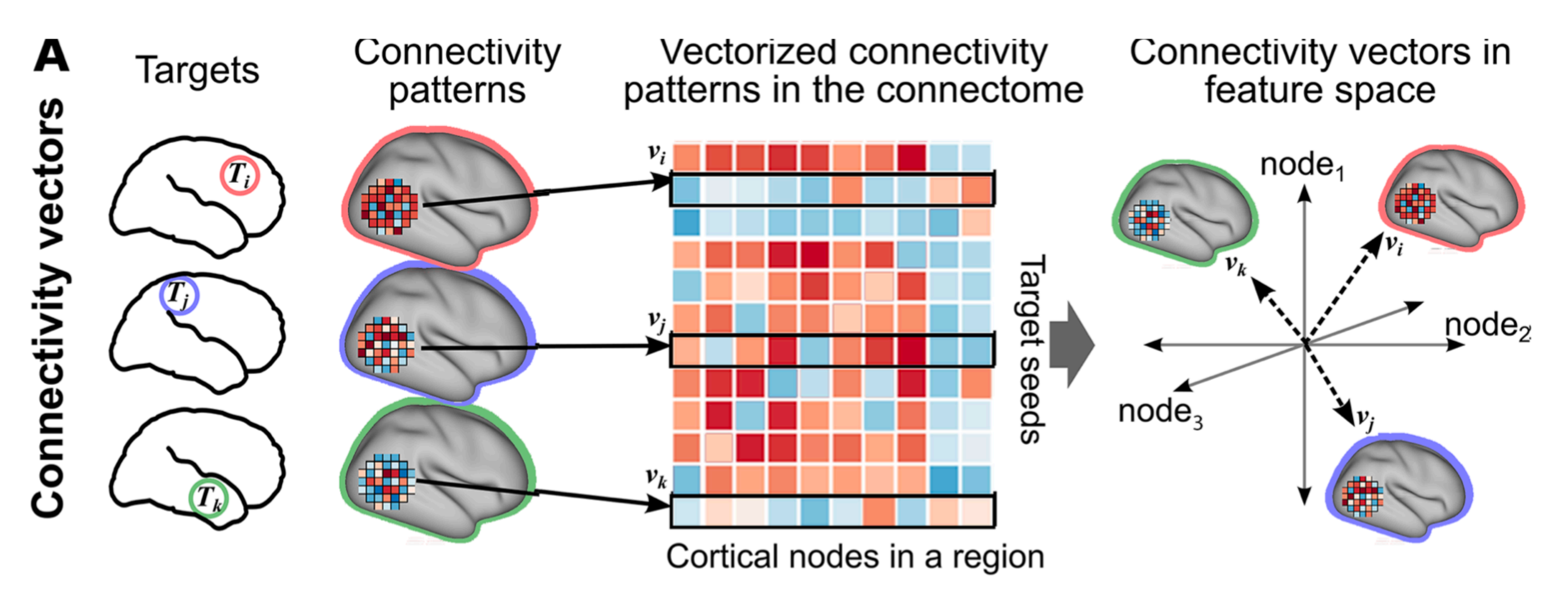




(Ma et al,. 2022, bioRxiv)

Progress of HyperAlignment

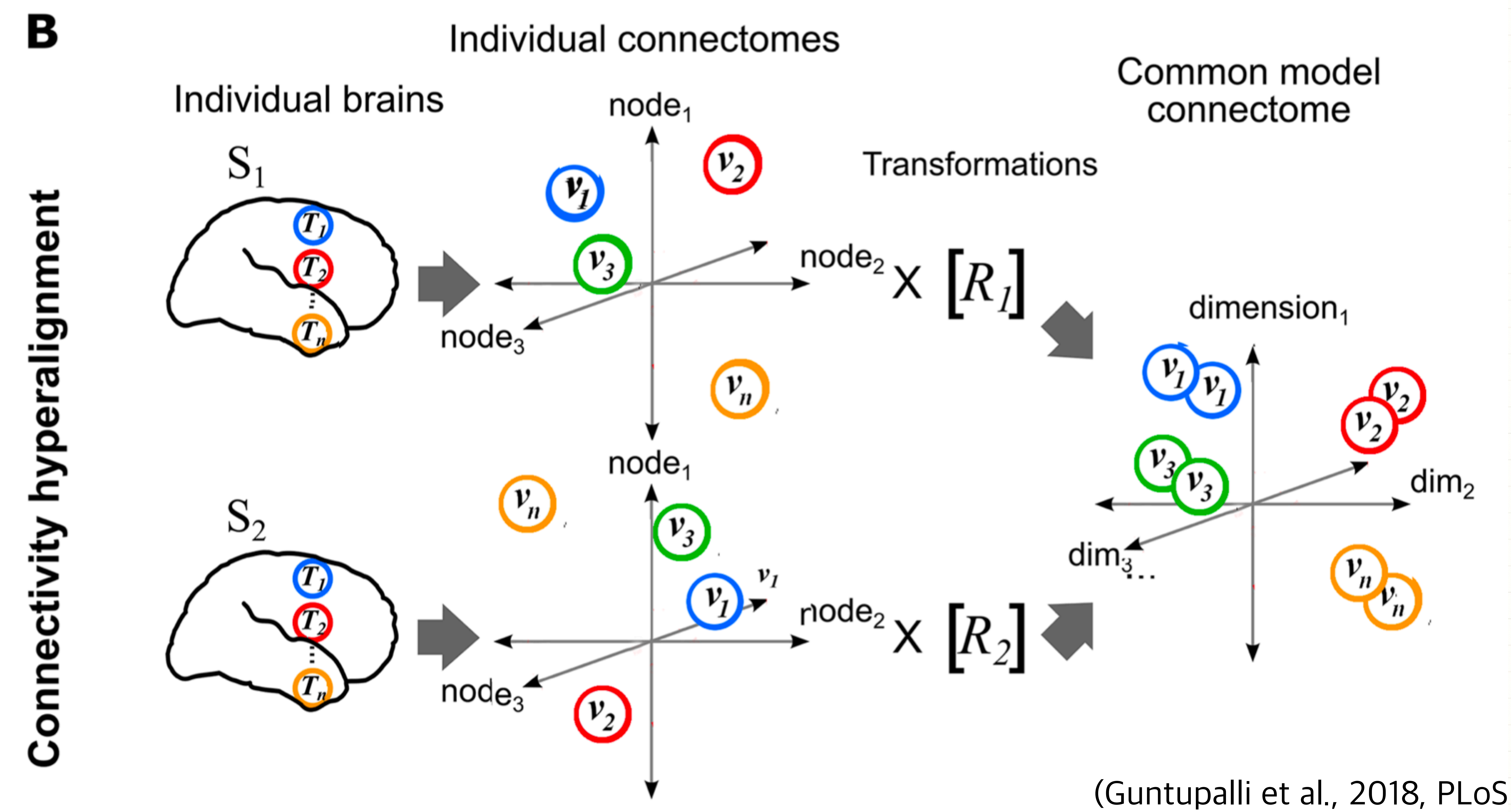
- **Fine scale connectome hyperalignment**



(Guntupalli et al., 2018, PLoS computational biology)

Progress of HyperAlignment

- **Fine scale connectome hyperalignment**



(Guntupalli et al., 2018, PLoS computational biology)

Progress of HyperAlignment

Cross-movie prediction of individualized functional topography

Guo Jiahui, Ma Feilong, Samuel A. Nastase, James V. Haxby, M. Ida Gobbini

doi: https://doi.org/10.1101/2022.11.21.517253