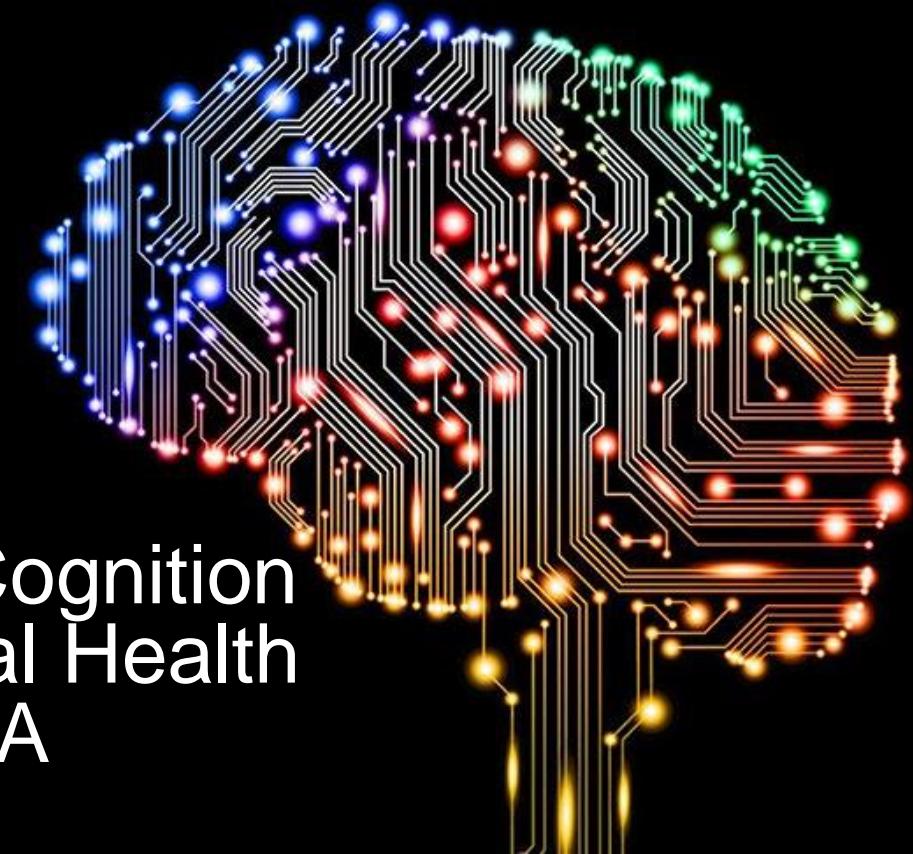


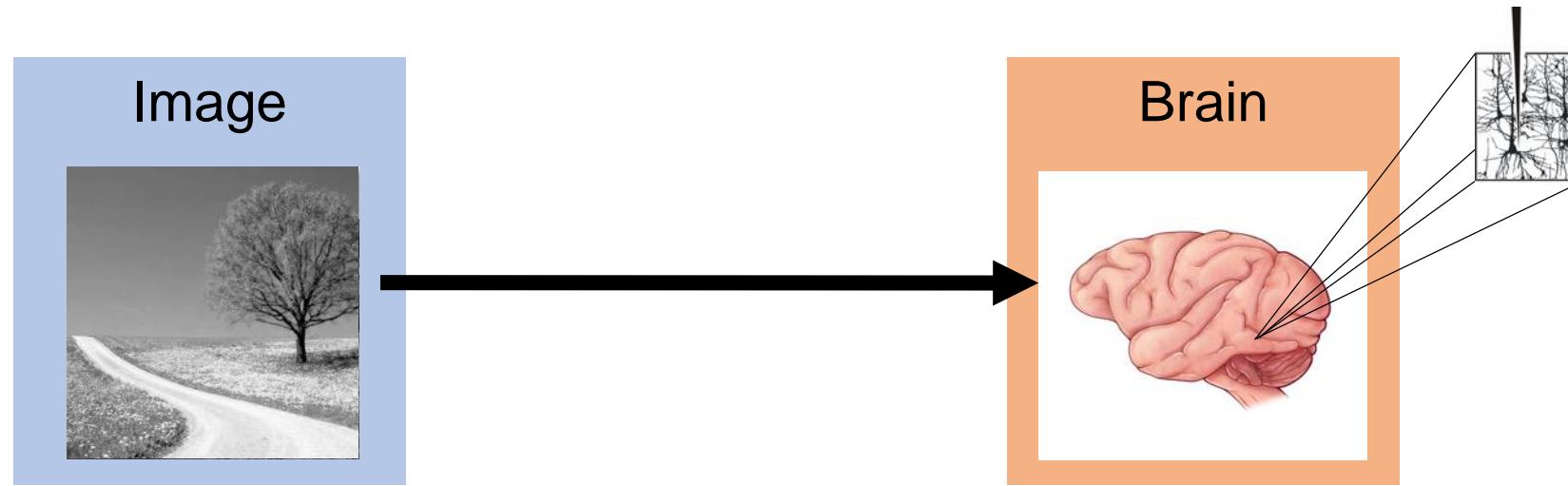
# Comparing brains and DNNs: Methods and findings

Martin Hebart

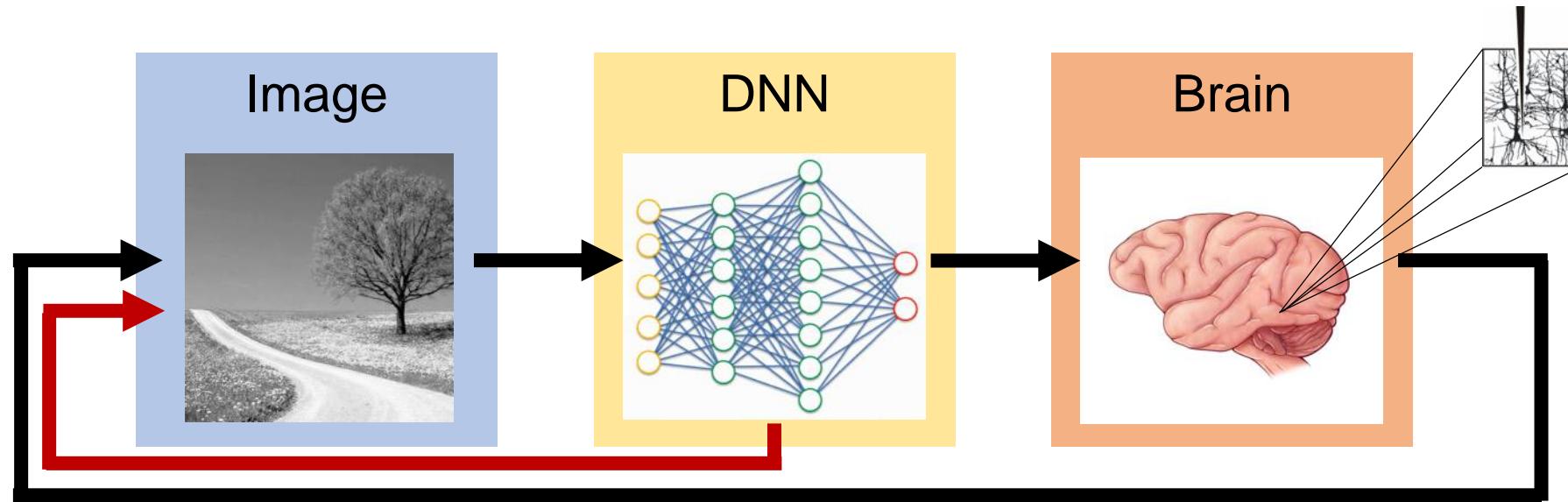
Laboratory of Brain and Cognition  
National Institute of Mental Health  
Bethesda, MD, USA



# What information does a neuron represent?



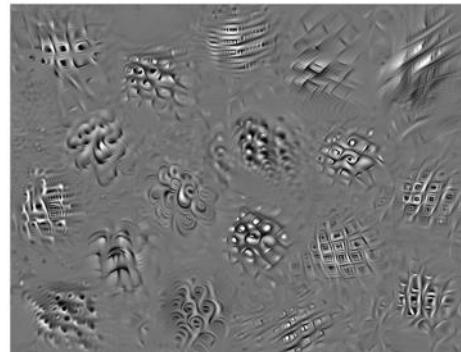
# What information does a neuron represent?



**Mouse V1**



**Monkey V4**



**Monkey IT**



Walker et al, 2018, *bioRxiv*

Bashivan et al, 2019, *Science*

Ponce et al, 2019, *Neuron*

# Overview

**Comparing brains and DNNs: Overview**

**Methods and findings for comparing brains and DNNs**

**Practical considerations**

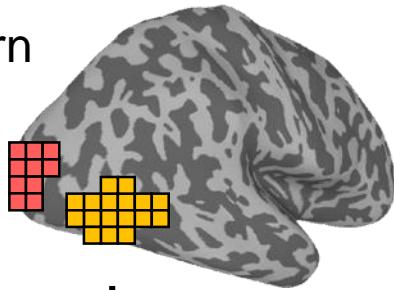
# Disclaimer / comments

- Presentation offers only incomplete overview
- Focus on methods and results, less interpretation
- More human data, more similarity-based methods
- Strong focus on vision

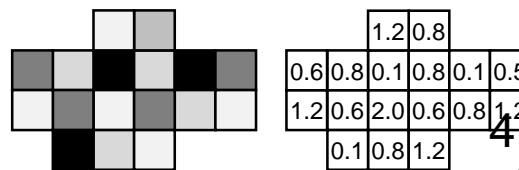
# Comparing brains and DNNs: Overview

## Brain (e.g. fMRI)

1. Identify pattern  
(e.g. region of interest)



2. Extract activation estimate for condition



4. Get pattern for all conditions



3. Vectorize (i.e. flatten) pattern

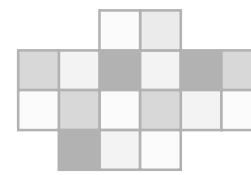
# Comparing brains and DNNs: Overview

## Brain (e.g. fMRI)

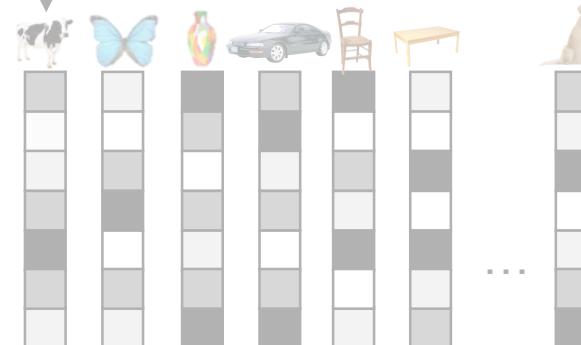
1. Identify pattern  
(e.g. region of interest)



2. Extract activation estimate for condition



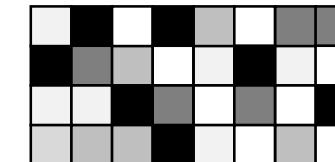
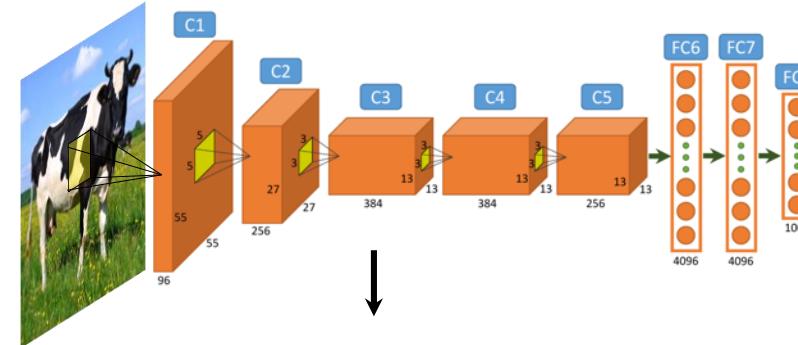
4. Get pattern for all conditions



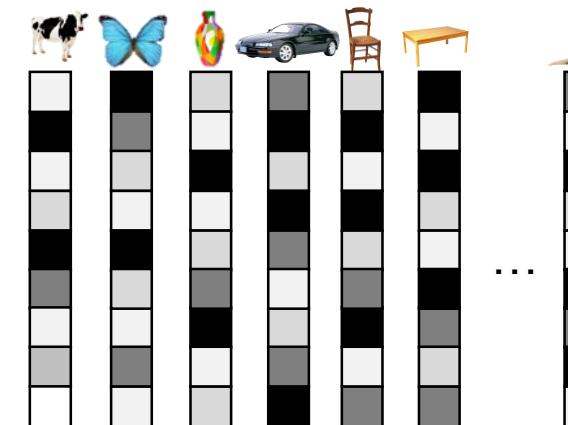
3. Vectorize (i.e. flatten) pattern

## DNN

1. Choose DNN architecture and layer



2. Push image through DNN and extract activation at layer

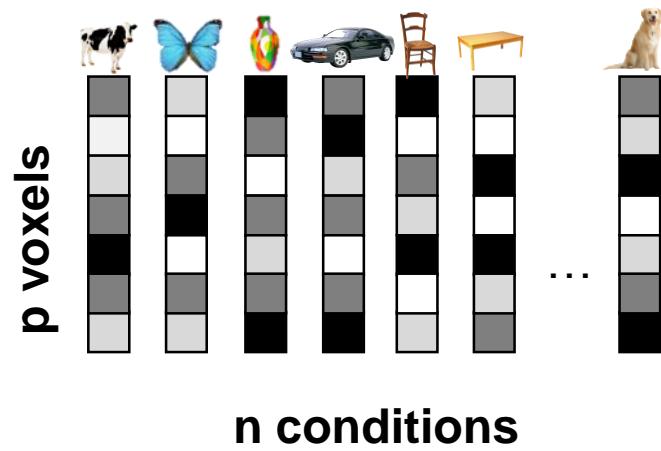


3. Vectorize (i.e. flatten) pattern

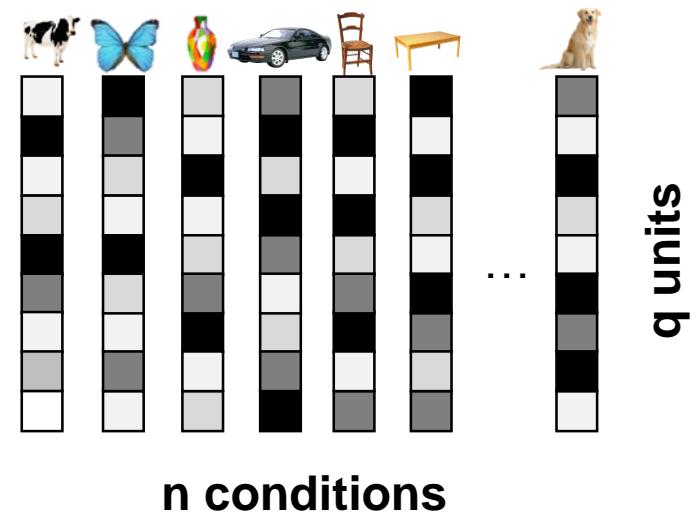
4. Get pattern for all conditions

# Comparing brains and DNNs: Overview

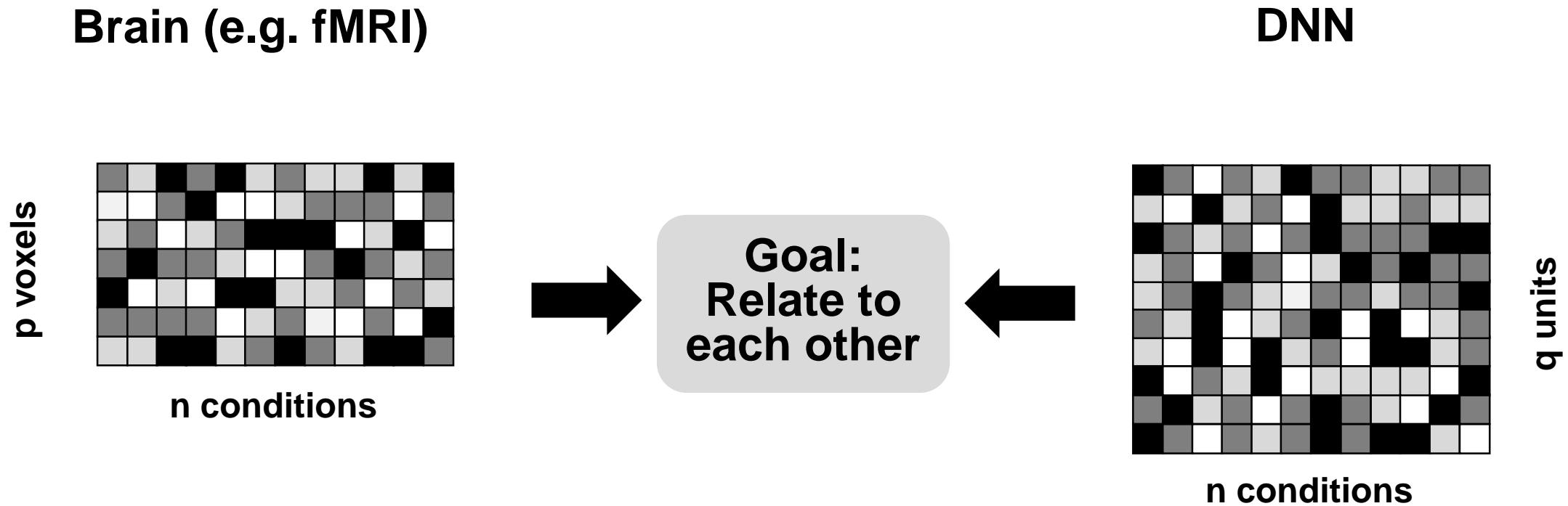
**Brain (e.g. fMRI)**



**DNN**



# Comparing brains and DNNs: Overview

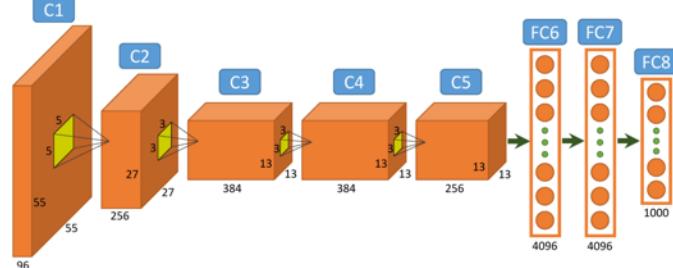


# Overview of methods relating DNNs and brains

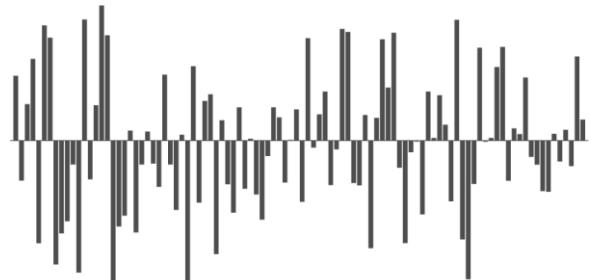
S: Stimuli



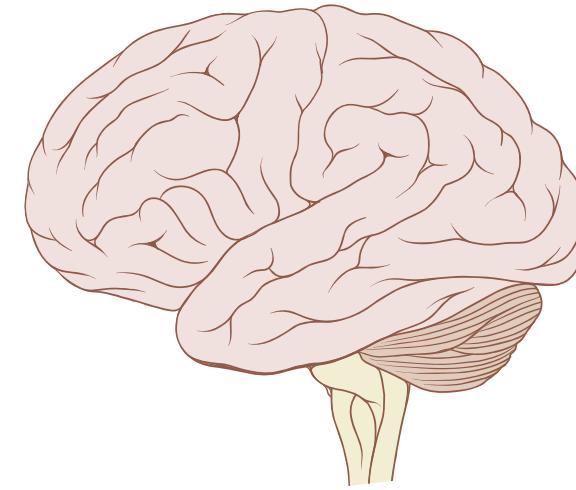
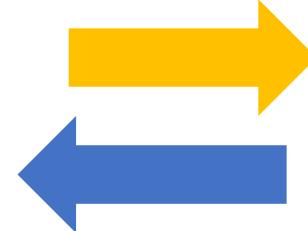
$$X = f(S)$$



X: Model (stimulus feature representation)

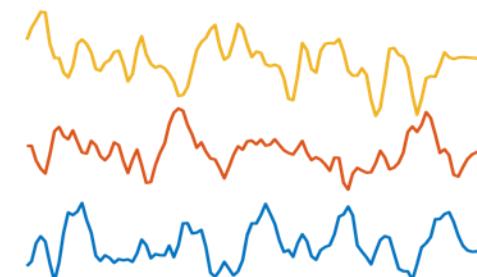


Encoding:  $g: X \rightarrow Y$



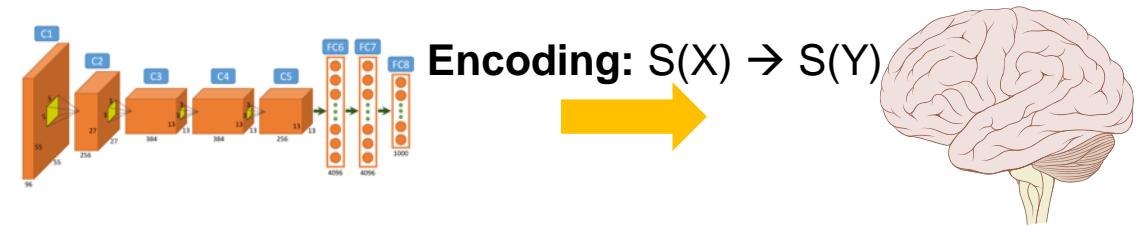
Decoding:  $h: Y \rightarrow X$

Y: Measurement (brain data)



# Overview of methods relating DNNs and brains

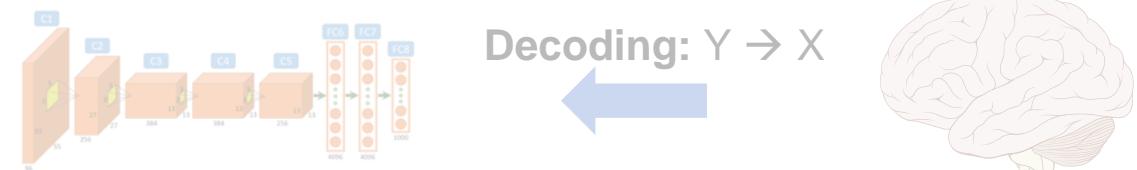
## Similarity-based encoding methods (RSA)



## Regression-based encoding methods

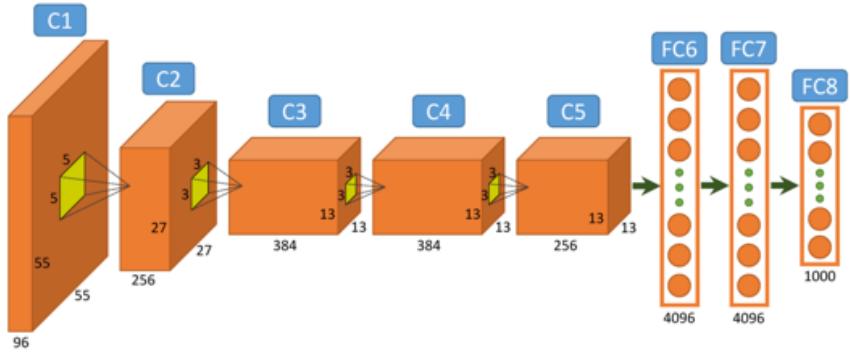


## Regression- and classification-based decoding methods



Horikawa & Kamitani, 2017, Nat Commun

# Similarity-based encoding methods

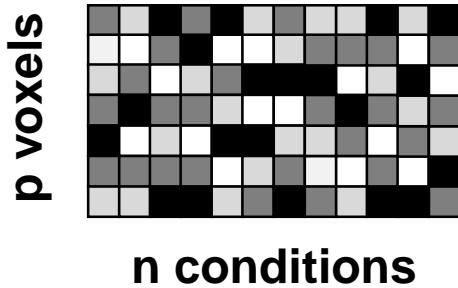


Encoding:  $S(X) \rightarrow S(Y)$



# Vanilla representational similarity analysis

Brain (e.g. fMRI betas)

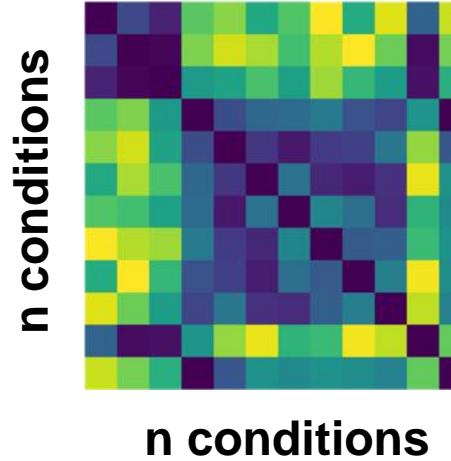


$n$  conditions



$1 - \text{Pearson } R$

Brain RDM



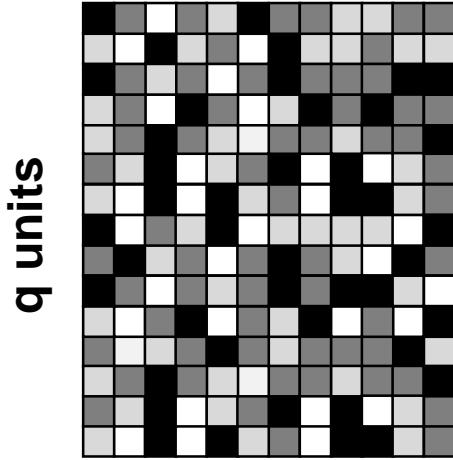
$n$  conditions

Brain RDV



*Extract lower  
triangular part  
and flatten*

DNN layer activations



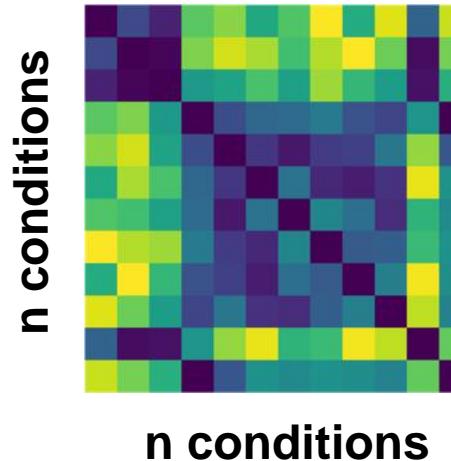
$q$  units

$n$  conditions



$1 - \text{Pearson } R$

DNN layer RDM



$n$  conditions

DNN layer RDV

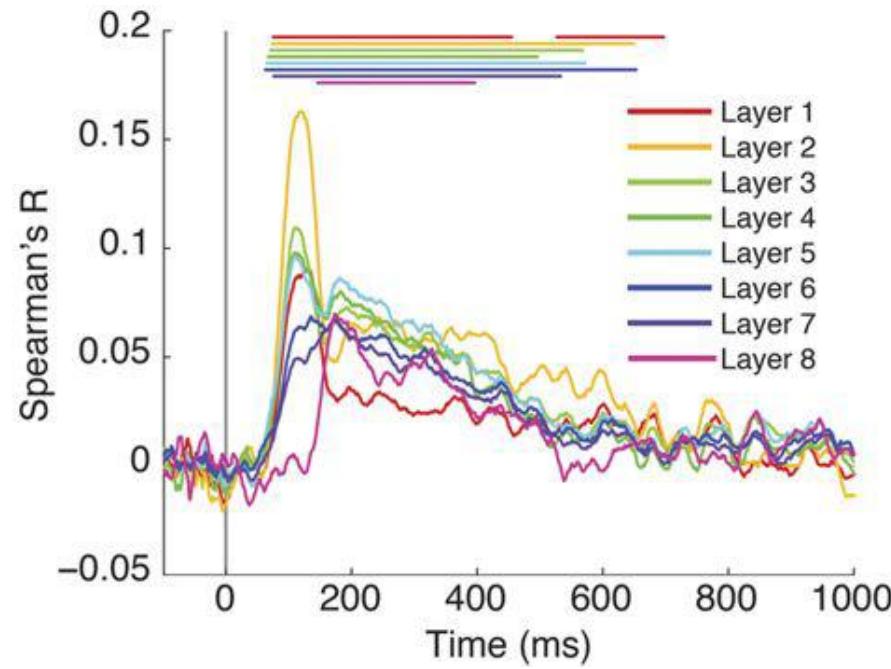


*Extract lower  
triangular part  
and flatten*

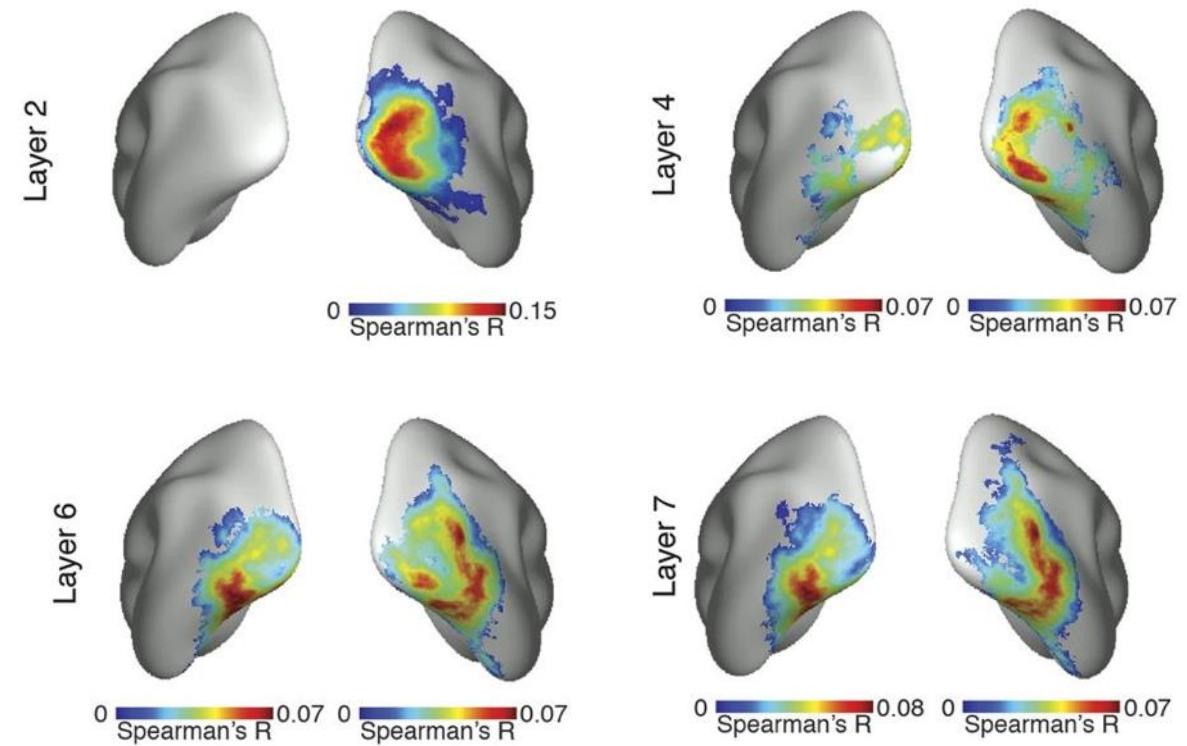
*Spearman  $R$*  → **Brain-DNN  
similarity**

# Results: Comparing DNN with MEG and fMRI

**MEG (time-resolved)**



**fMRI (searchlight)**

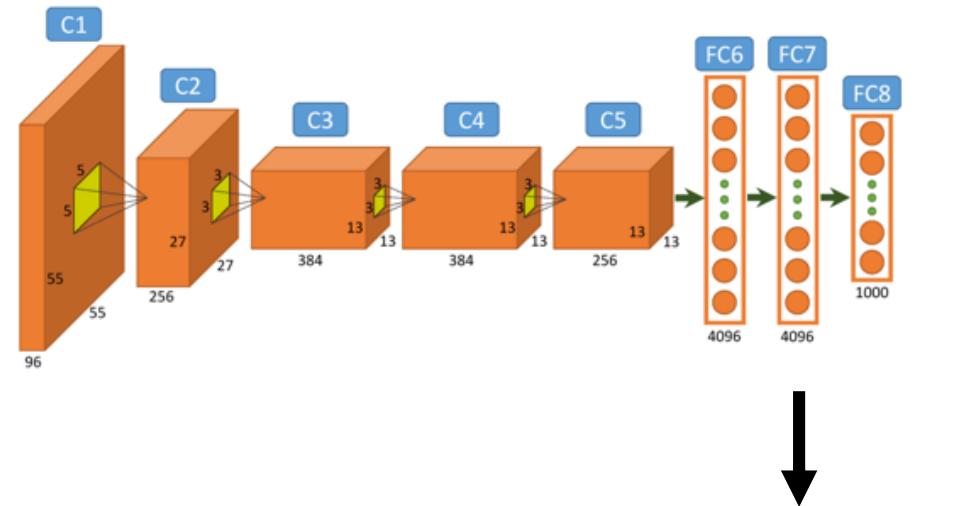


- 118 natural objects with background
- custom-trained AlexNet

# Advanced RSA: remixing and reweighting

**Remixing:** Does the layer contain a representation of the category that can be linearly read out?

1. Train classifier on layer for relevant categories using new images (e.g. >10 / category)
2. Apply classifier to original images and take output of classifier (e.g. decision values)
3. Construct RDM from output

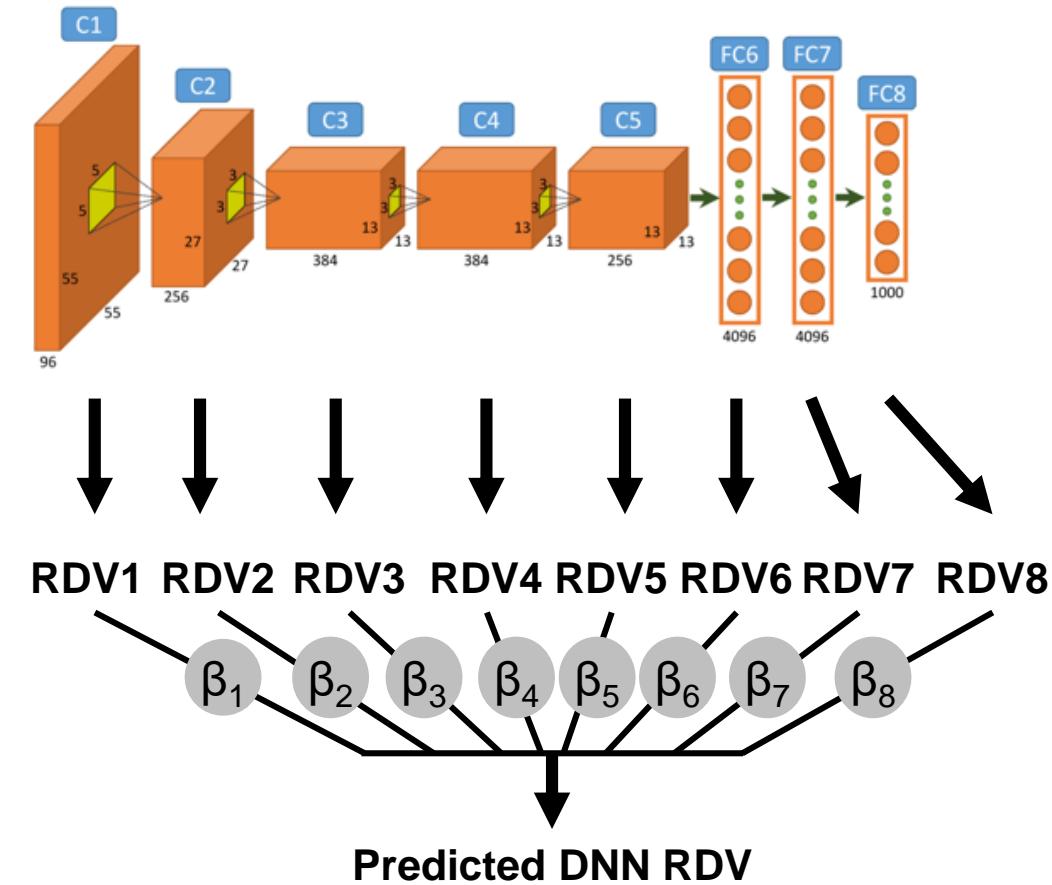


**Classifier**

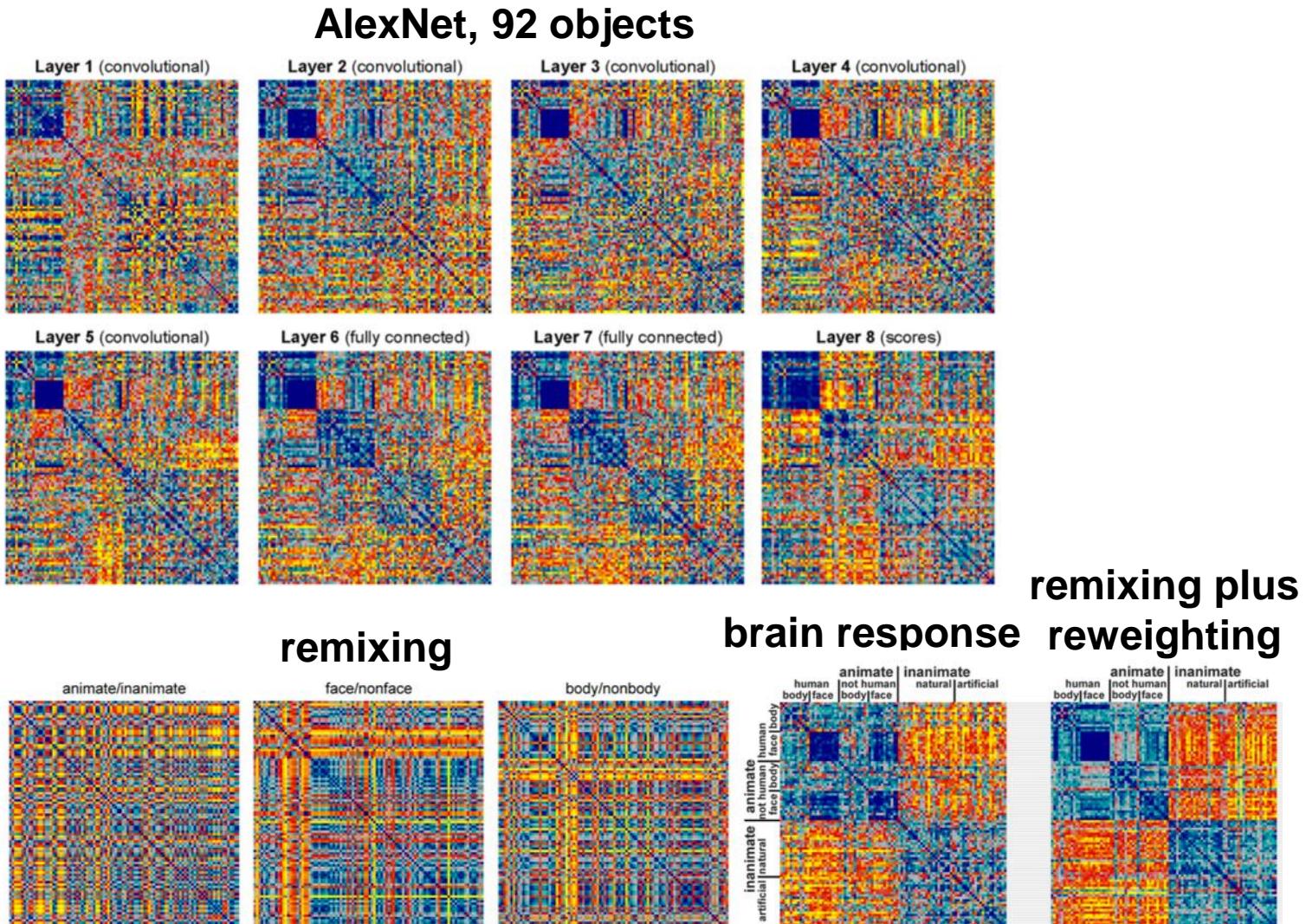
# Advanced RSA: remixing and reweighting

**Reweighting:** Can the measured brain representational geometry be explained as a linear combination of feature representations at different layers?

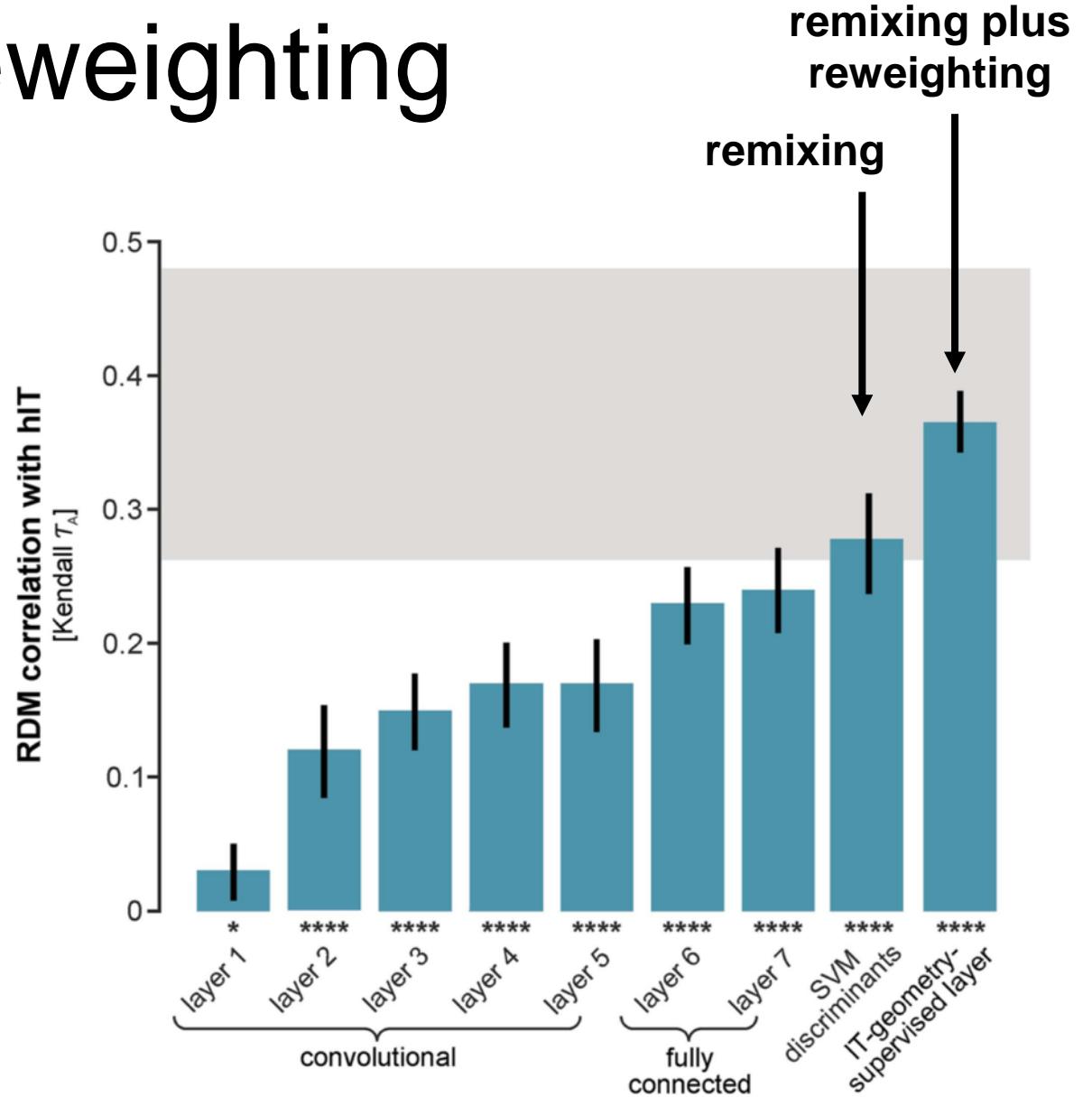
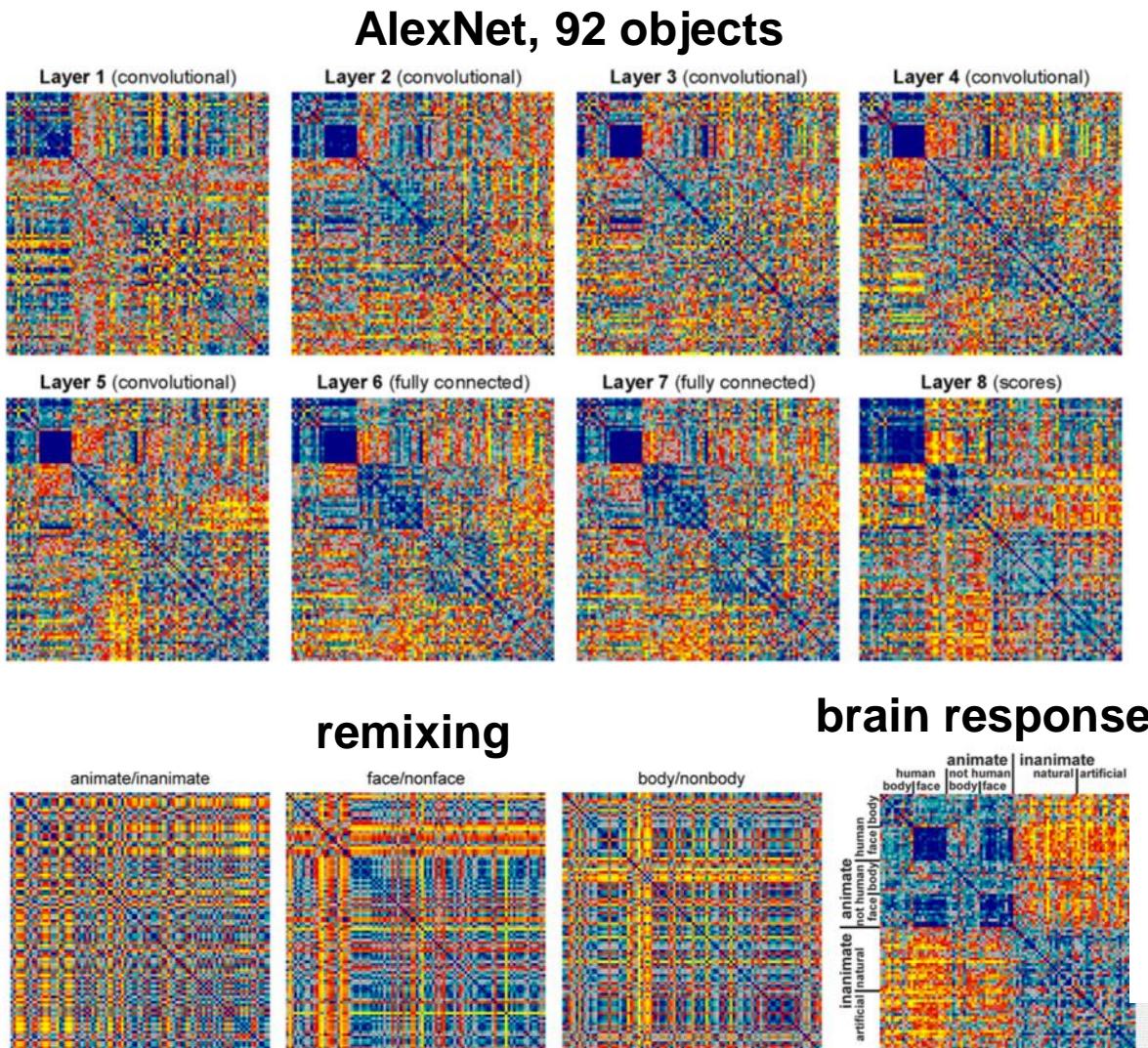
1. Create RDV for each layer
2. Carry-out cross-validated non-negative multiple regression
3. Compare predicted DNN RDV to measured brain RDV



# Results: Remixing & reweighting

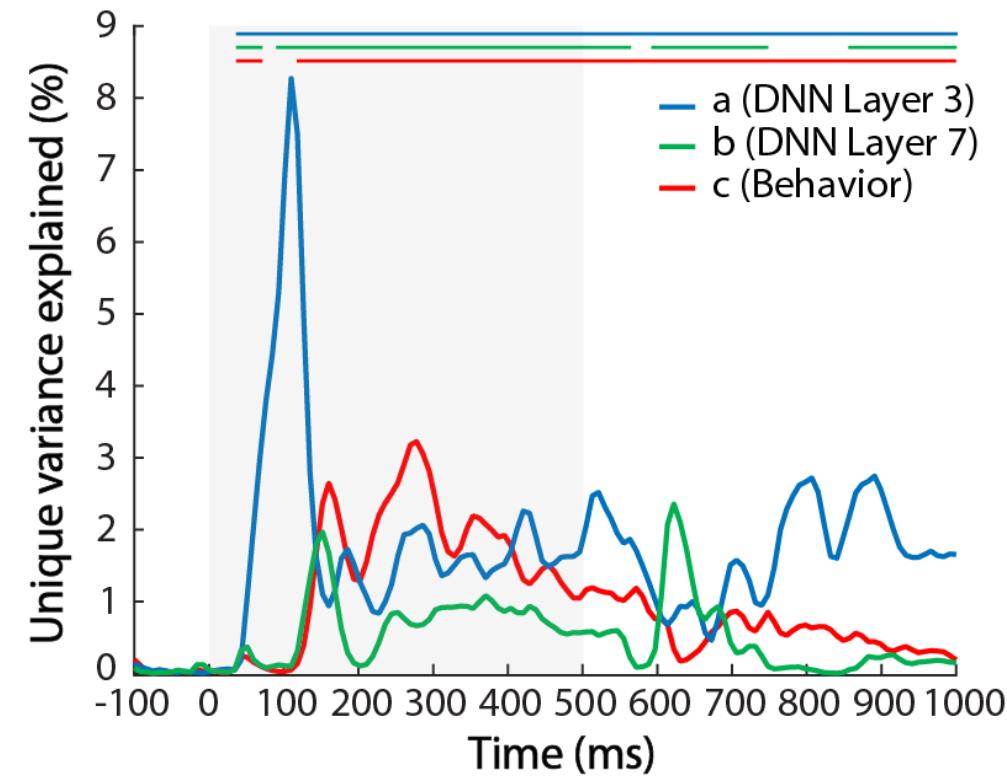
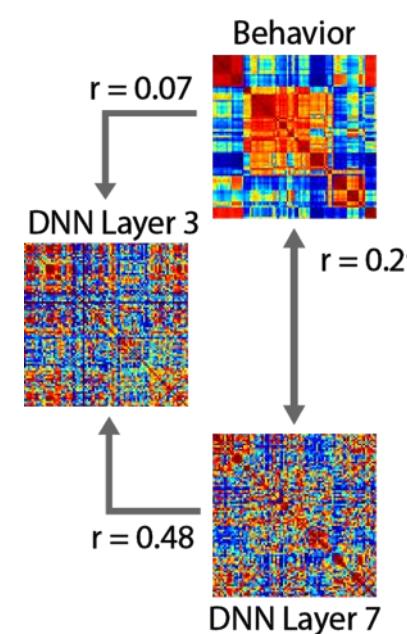
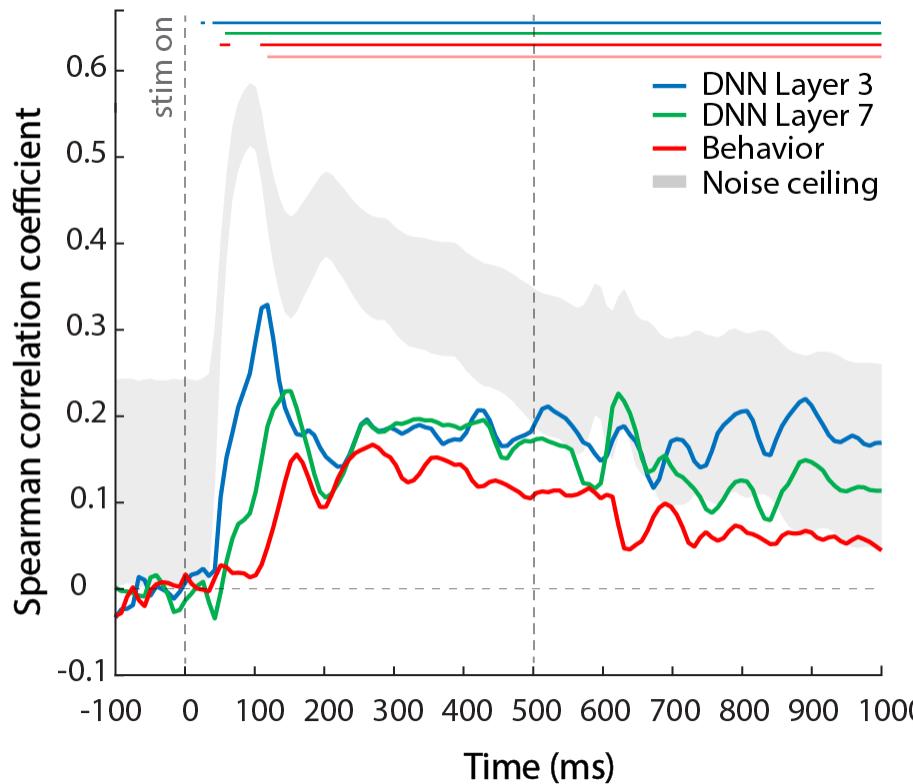


# Results: Remixing & reweighting



# Advanced RSA: variance partitioning to control for low-level features

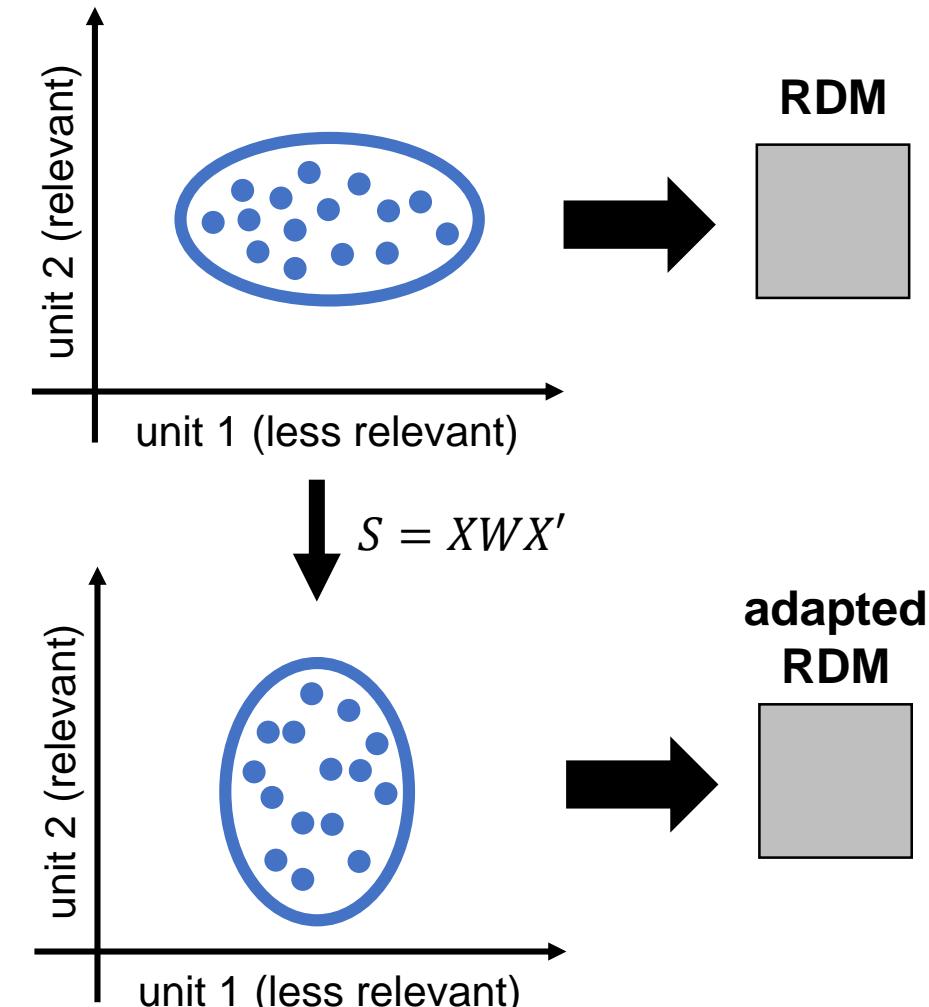
Can we tease apart low-level and high-level representations?



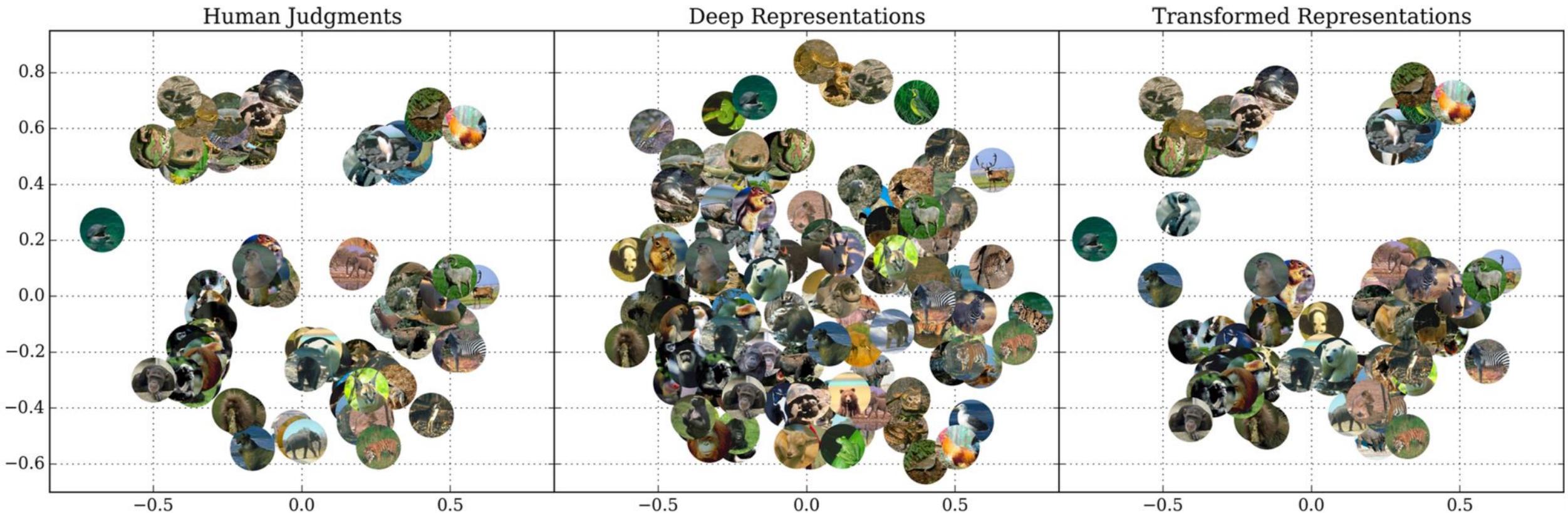
- 84 natural objects without background
- DNN: AlexNet

# Optimal linear weighting of individual DNN units to maximize similarity

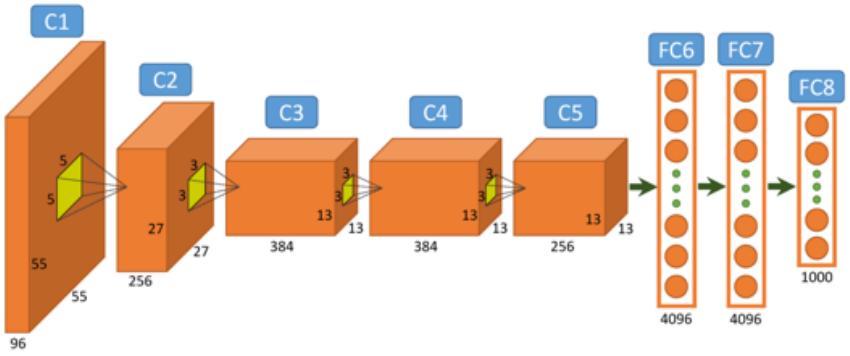
- In standard similarity analysis, all dimensions of the data (e.g. DNN units) contribute the same
- But: Some dimensions may matter more than others
- It is possible to optimize the weighting of each dimension to maximize the fit
- This can be done using cross-validated regression



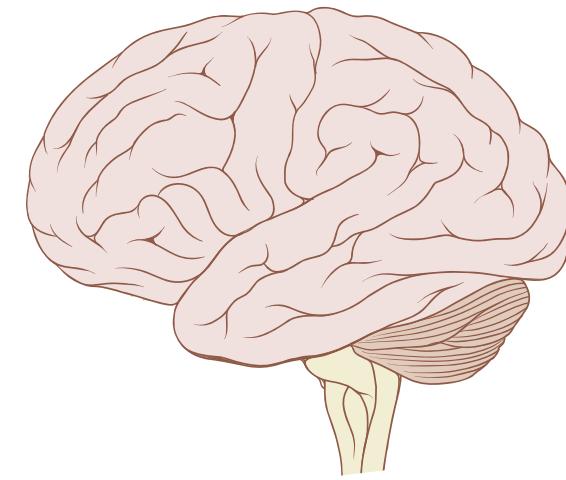
# Optimal linear weighting of individual DNN units to maximize similarity



# Regression-based encoding methods

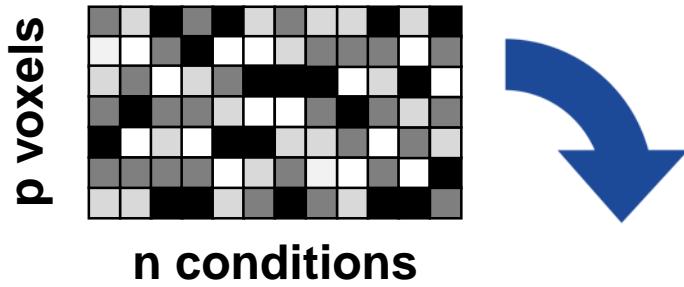


Encoding:  $X \rightarrow Y$

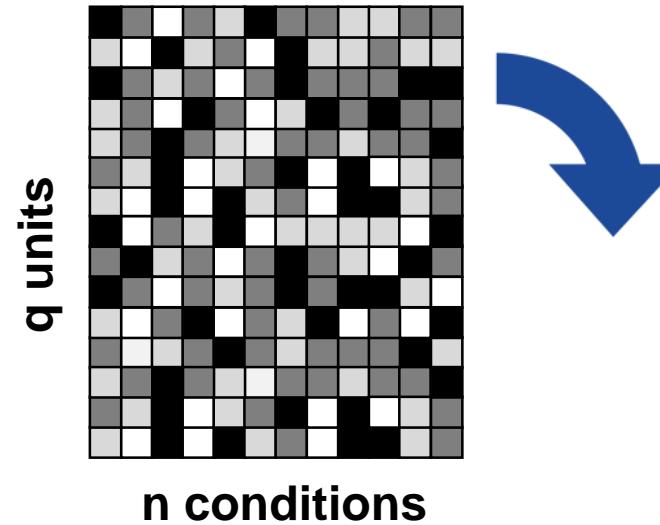


# Simple multiple linear regression

Brain (e.g. fMRI betas)

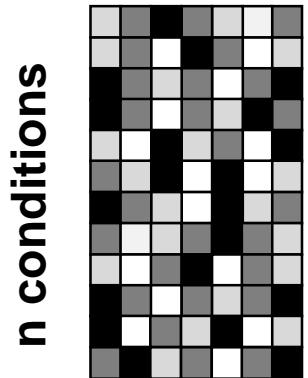


DNN layer activations



# Simple multiple linear regression

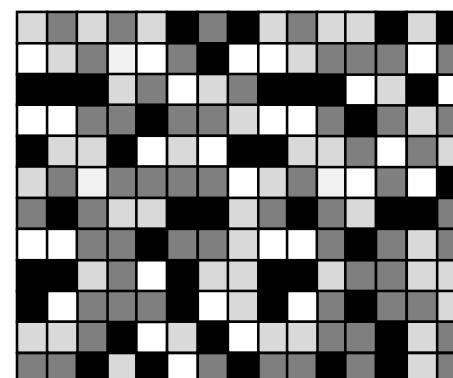
**Brain (e.g. fMRI betas)**



**n conditions**

**p voxels**

**DNN layer activations**

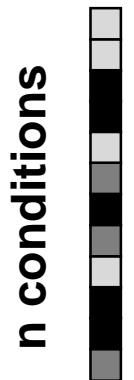


**n conditions**

**q units**

# Simple multiple linear regression

Brain (e.g. fMRI betas)

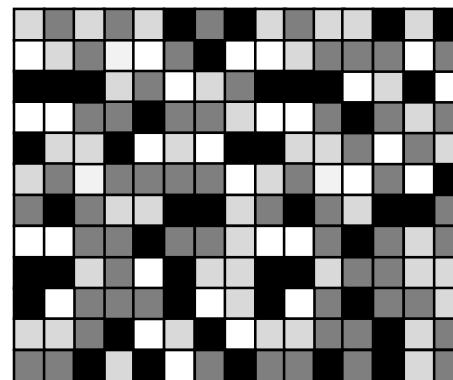


voxel  $i$

$y$

DNN layer activations

$n$  conditions



$q$  units



$$y = X \cdot \beta + \epsilon$$

→ Repeat for each voxel (i.e. univariate method)

# Simple multiple linear regression

**Brain** **Problem:** Often more variables ( $q$  units) than measurements ( $n$  conditions)  
→ no unique solution, unstable parameter estimates and overfitting

**One solution:** Regularization, i.e. adding constraints on the range of values  $\beta$  can take (e.g. Ridge regression, LASSO regression)

**Another solution:** Dimensionality reduction, i.e. projecting data to a subspace (e.g. Principal Component regression, Partial Least Squares)

# Regularization in multiple linear regression

Formula for regression:  $y = X\beta + \varepsilon$

Constrains range  
of beta

Error minimized for OLS regression:

$$\sum (y - X\beta)^2$$

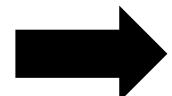


Error minimized for ridge regression:

$$\sum (y - X\beta)^2 + \lambda_r \|\beta\|^2$$

Error minimized for LASSO regression:

$$\sum (y - X\beta)^2 + \lambda_l \|\beta\|$$



Requires optimization of regularization parameter  $\lambda$  (e.g. using cross-validation)



Advanced regularization: explicit assumptions on covariance matrix structure

# Regularization in multiple linear regression

Formula for regression:  $y = X\beta + \varepsilon$

Constrains range  
of beta

Error minimized for OLS regression:

$$\sum (y - X\beta)^2$$

**Presence of many variables leads to potential for overfitting**

Error minimized for ridge regression:

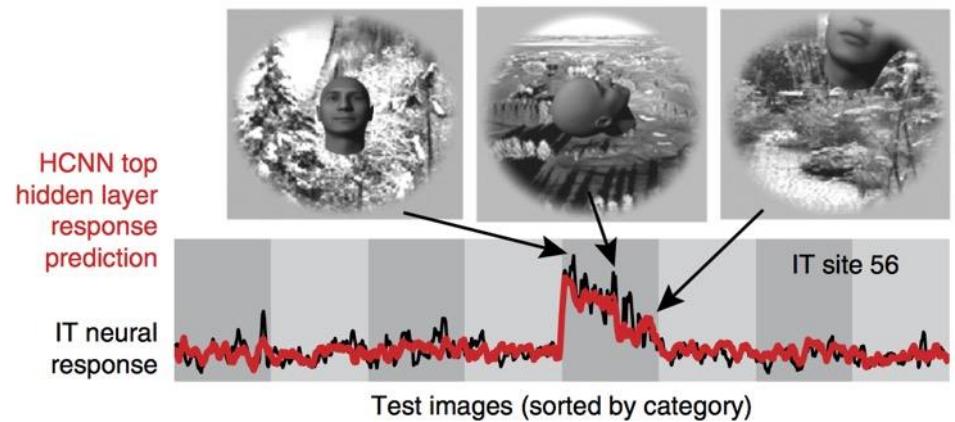
$$\sum (y - X\beta)^2 + \lambda_l \|\beta\|^2$$

→ quality of fit can be estimated using cross-validation  
(e.g. split-half or 90%-10% split)

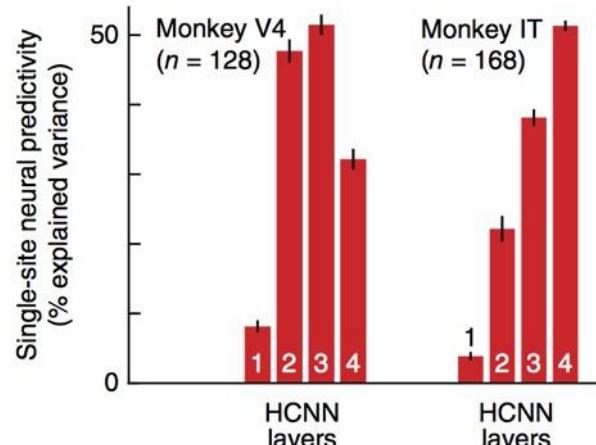
- Requires optimization of regularization parameter  $\lambda$  (e.g. using cross-validation)
- Advanced regularization: explicit assumptions on covariance matrix structure

# Results: Regression-based encoding methods

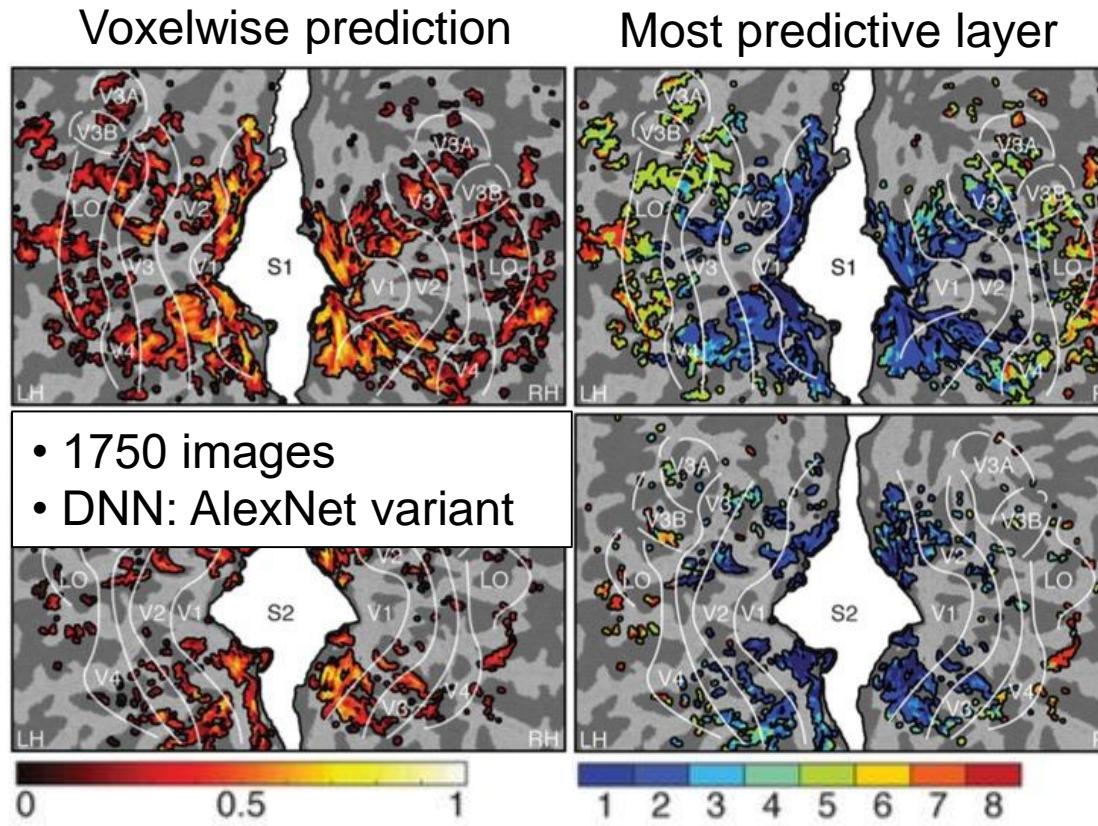
## Monkey V4 and IT



- 5760 images of 64 objects (8 categories)
- custom DNN “HMO”



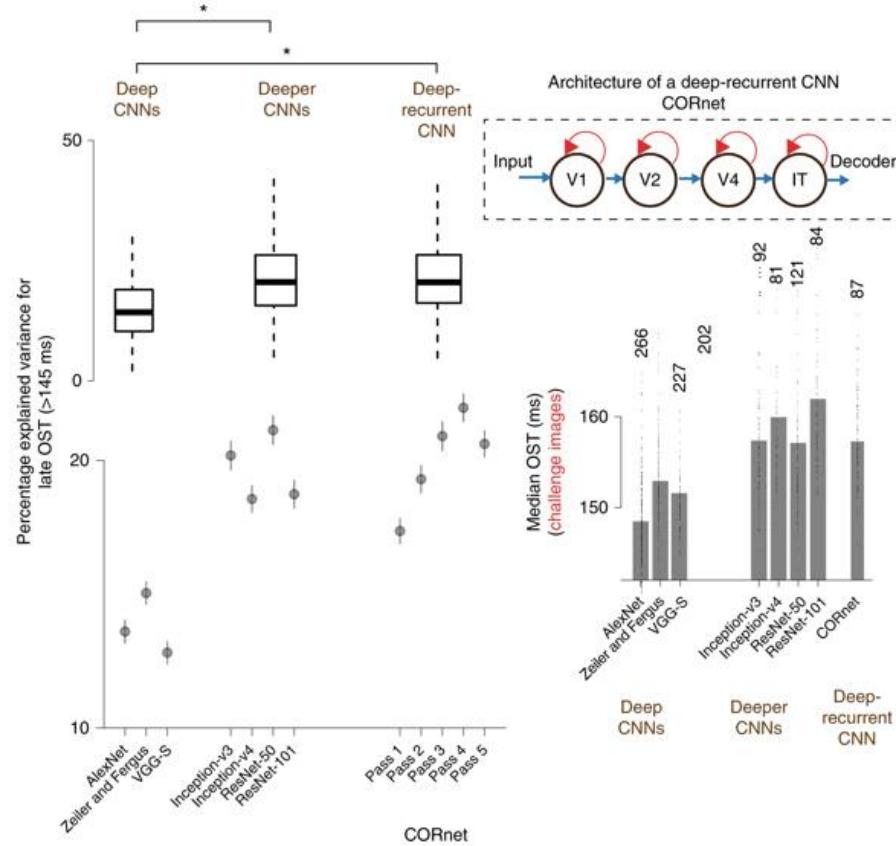
## Human visual cortex



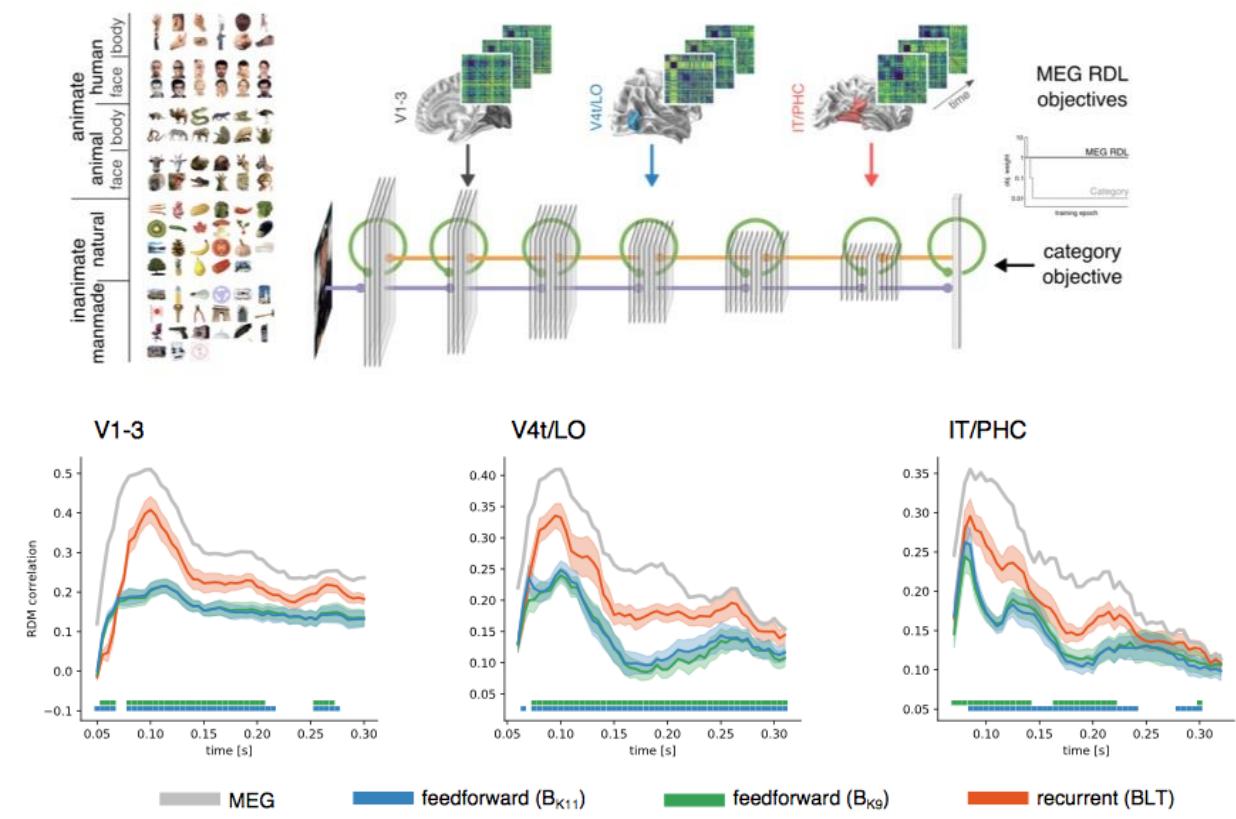
# Building networks to model the brain

# Recurrent models better capture core object recognition in ventral visual cortex

in both monkey recordings...



... and humans (MEG sources)



# Practical considerations

# Matlab users: Using MatConvNet

- Downloading pretrained models:

<http://www.vlfeat.org/matconvnet/pretrained/>

- Quick guide to getting started:

<http://www.vlfeat.org/matconvnet/quick/>

- Function for getting layer activations:

[http://martin-hebart.de/code/get\\_dnnres.m](http://martin-hebart.de/code/get_dnnres.m)

# Python users: Using Keras

- Keras is very easy, but classic TensorFlow or PyTorch also work
- Running images through pretrained models:  
<https://engmrk.com/kerasapplication-pre-trained-model/>
- Getting layer activations (still requires preprocessing images):  
<https://github.com/philipperemy/keract>

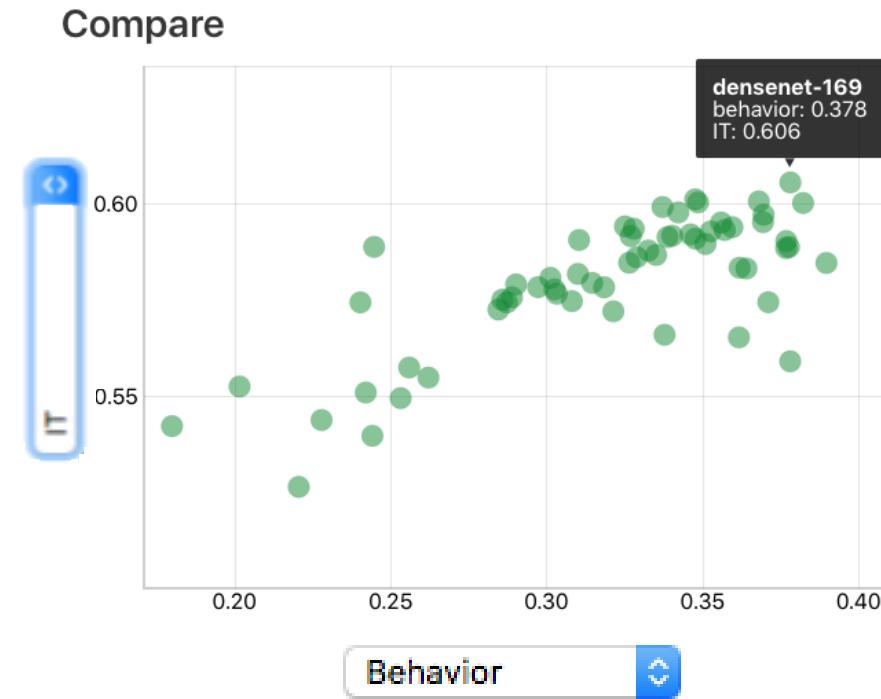
# What architecture should we pick?

**If goal is maximizing brain prediction:**

- Pick network with most predictive layer(s)
- Brain score?

**If goal is using plausible model:**

- Very common / better understood architectures: AlexNet and VGG-16
- Other architectures (e.g. ResNet, DenseNet) less common



Schrimpf, Kubilius et al., 2018, bioRxiv

# Which layers should we pick?

**If goal is to maximize brain prediction**

→ Try all layers

**If goal is using entire DNN as model of brain**

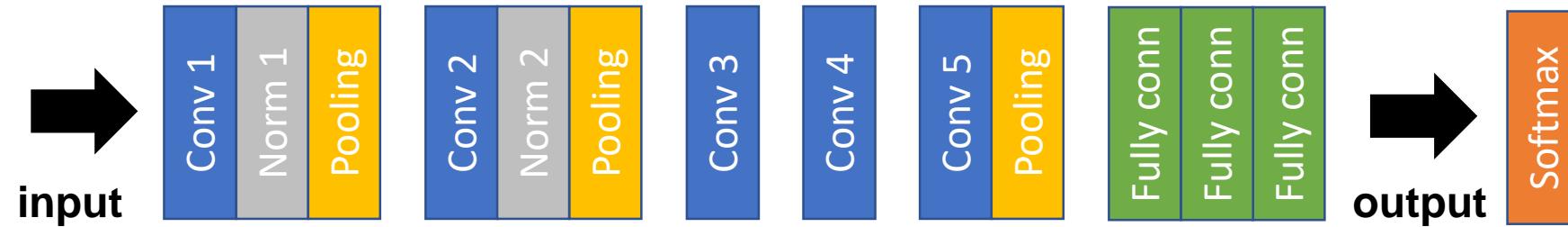
→ Try all or some layers

**If goal is using plausible model where layer progression  
mirrors progression in brain: some layers**

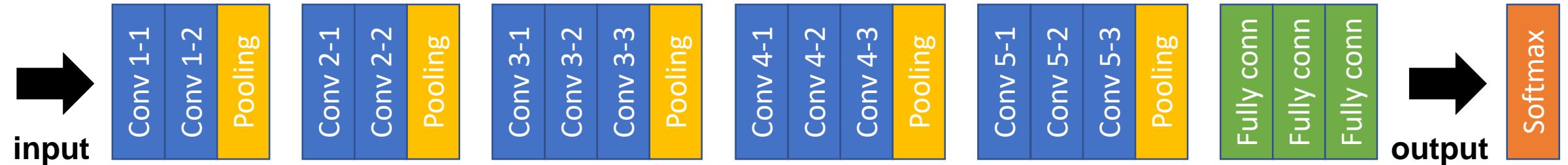
→ Pick plausible layers

# Which layers should we pick?

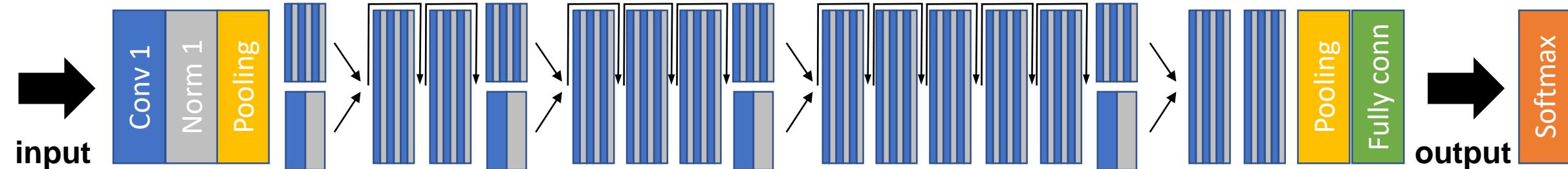
AlexNet architecture (8+ layers)



VGG-16 architecture (16+ layers)

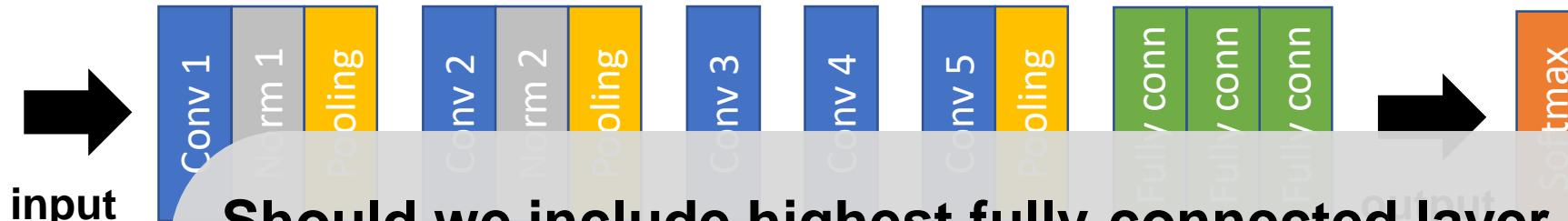


ResNet-50 architecture (50+ layers)



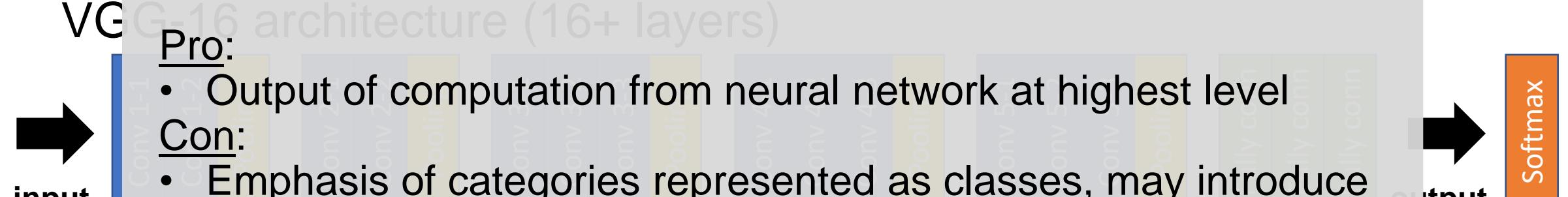
# Which layers should we pick?

AlexNet architecture (8+ layers)



Should we include highest fully-connected layer (1000-D)?

VGG-16 architecture (16+ layers)



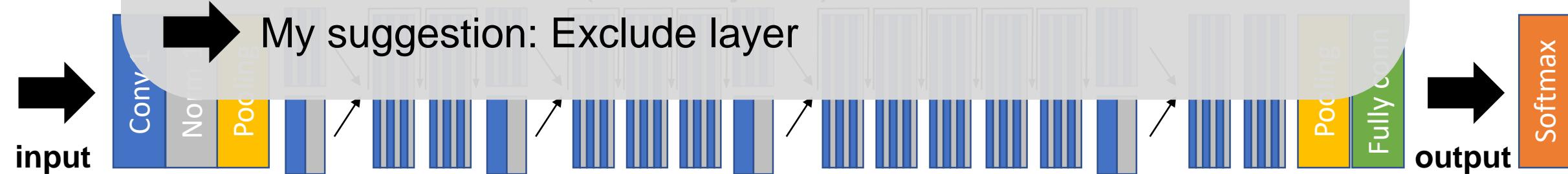
Pro:

- Output of computation from neural network at highest level

Con:

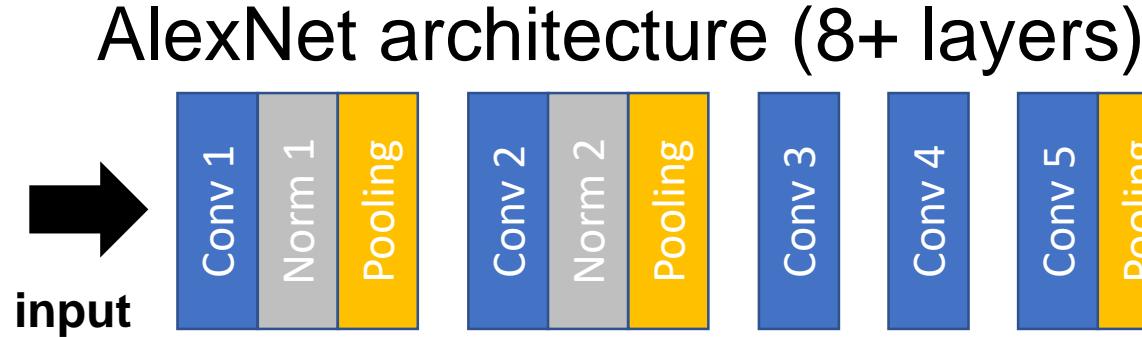
- Emphasis of categories represented as classes, may introduce positive or negative bias in results

ResNet-50 architecture (50+ layers)

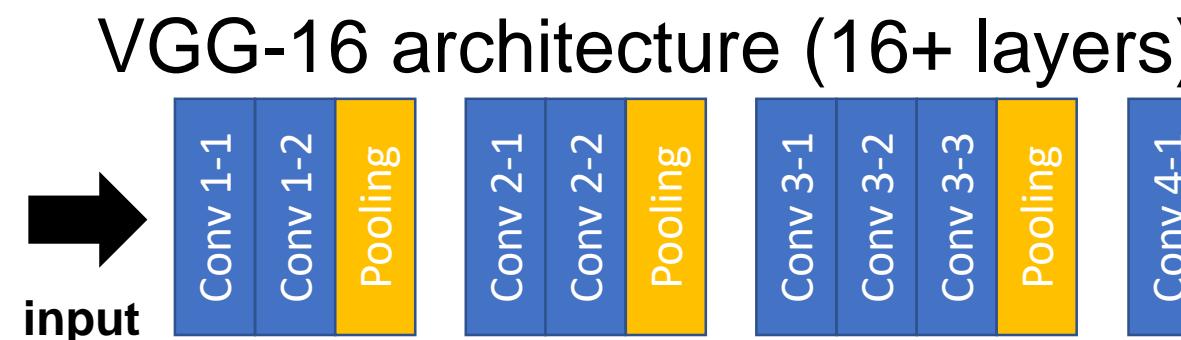


My suggestion: Exclude layer

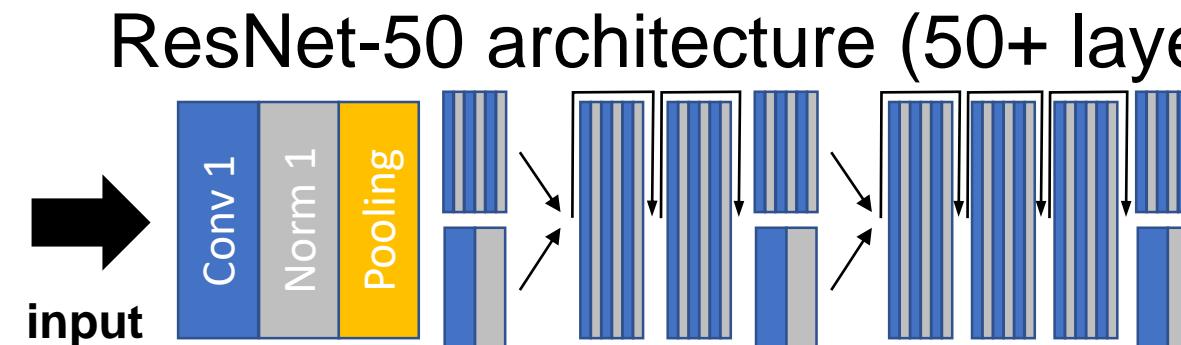
# Which layers should we pick?



AlexNet: Convolutional and fully connected -1 (i.e. 7 layers)



VGG-16: highest conv + fully conn - 1  
pooling + fully connected - 1 (i.e. 7 layers)  
or



ResNet-50: conv1 + summation  
or  
conv1 + first ReLu after summation  
(i.e. 17 layers)

# Common preprocessing of images

**Original image**



**1. Resize**



**2. Crop to square  
and keep 7/8th**



**3. Normalize (e.g. z-score or subtract mean image during training)**



## My advice:

- Run studies on participants / animals using square images
- Resize and crop images to correct size before running toolbox function → provides maximal control
- Make sure image normalization is implemented and correct

# Reduction of model size

- Useful when predicting brain data from layers with many units
  - Makes more complex models possible at all
  - increases computational speed
  - can reduce overfitting
- Examples:
  - AlexNet Layer 1:  $55 \times 55 \times 96 = 290,400$  units
  - VGG-16 / ResNet Layer 1:  $112 \times 112 \times 64 = 802,816$  units

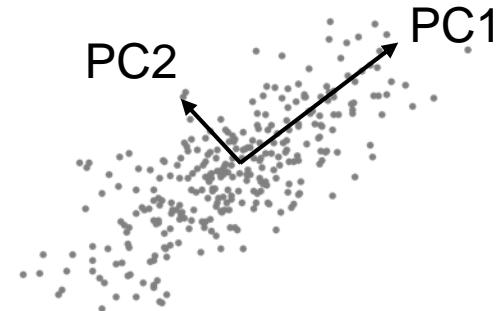
→ Common approach: PCA compression

# PCA compression of DNN layer

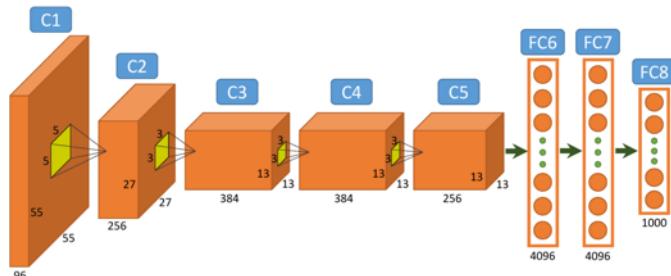
**Step 1:** Get ImageNet validation set of 50,000 images (possibly include test set of 150,000 images)



**Step 3:** Run incremental PCA or random projection (e.g. in scikit-learn), set number of PCs to a reasonable number (e.g. 1000)



**Step 2:** Push images through network in batches, extract layer activation, flatten and store on hard drive



**Step 4:** Save PCA model, push new images through network, extract layer activation, flatten and apply transformation from PCA

# Take-home messages

**Comparing brains and DNNs is easy, but what to do with it is harder**

**Common methods to map DNNs and brains are regression-based and similarity-based encoding methods**

**DNNs often treated only loosely as brain model (e.g. taking all layers to predict activity in V1)**

**Even older models (e.g. AlexNet) perform well and are still common**