Seminar: Explainable Machine Learning

Carsten Lüth 5/17/2018

Matrix Capsules with EM routing

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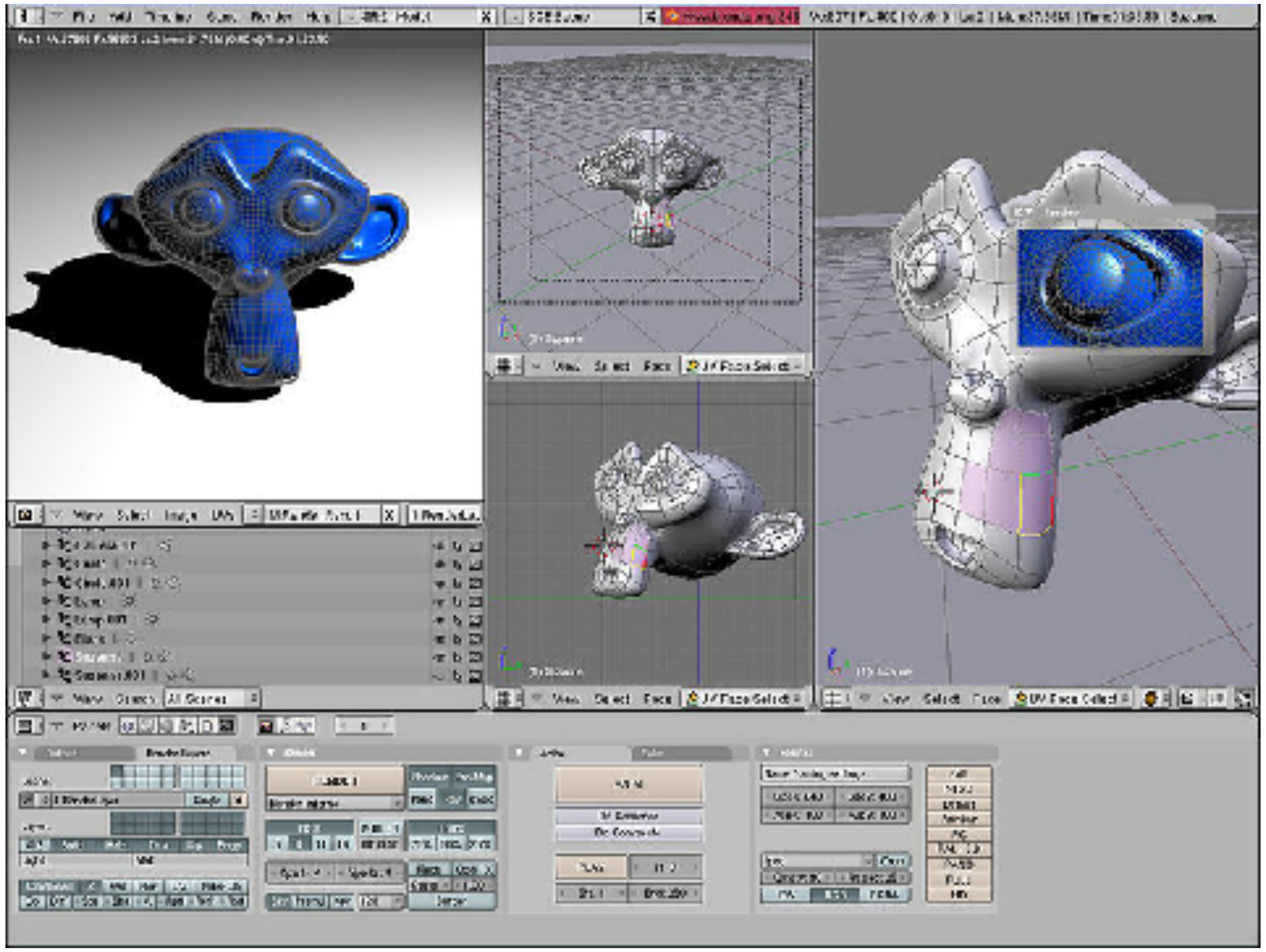
Capsule networks' core idea is to break up the neural net into chunks, or capsules, that work in teams and are assigned a portion of a problem; each capsule is pre-loaded with basic training on its portion of the object or process it will examine. The individual capsules work cooperatively, sharing their findings and contributing to solving the problem as a whole.

–Mike Fitzmaurice

Capsules General

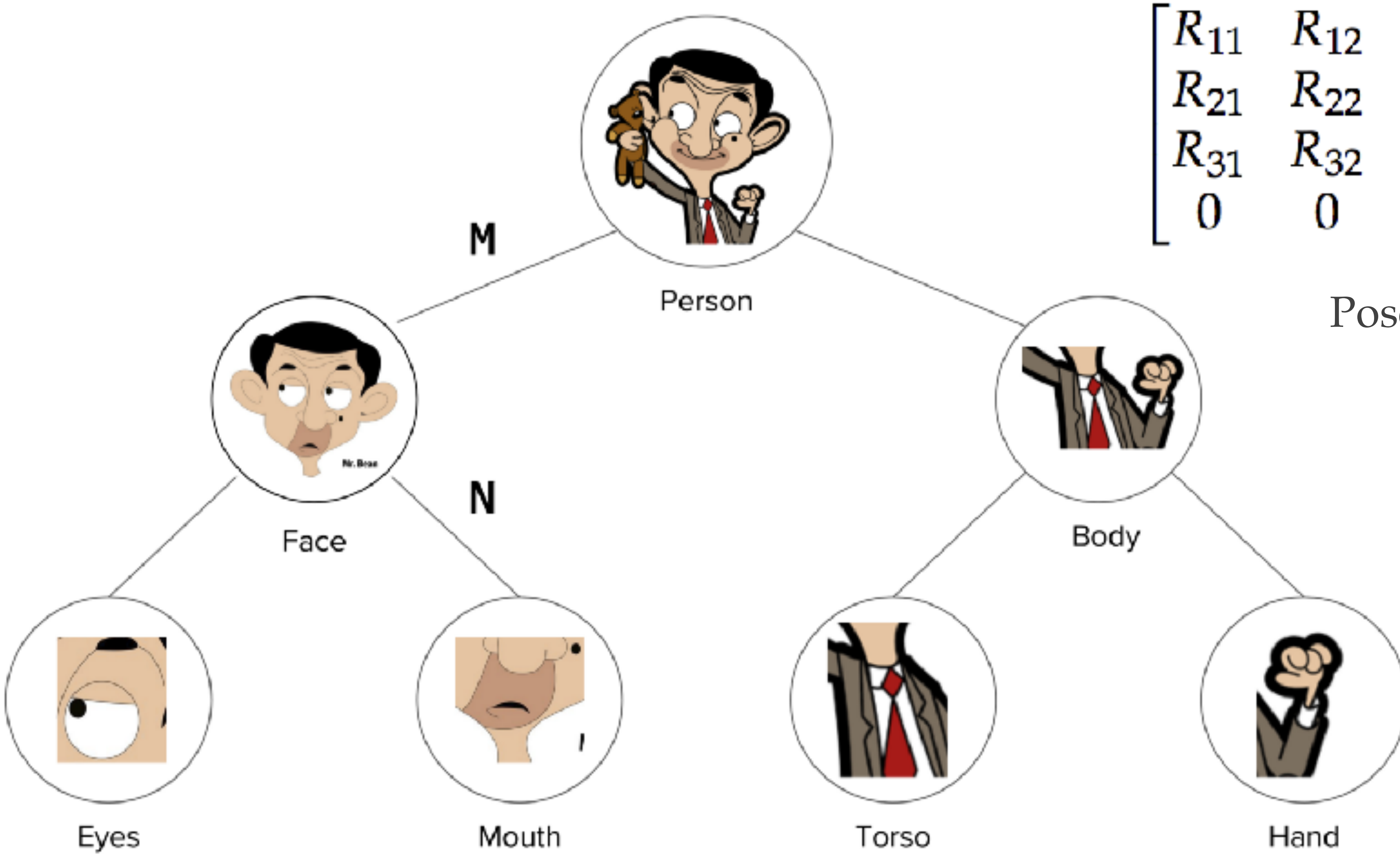
- contains both probability of occurence (activation) and parameters of the specific feature or entity (pose)
- filter out irrelevant information for the task without max-pooling
- works like an inverse graphical rendering program where entity is described by a vector or pose



Difference Capsule and Standard Network

- Activations are based on:
  - Standard Net:
    - compare single incoming activity vector and weight vector
  - Capsule Net:
    - compares multiple incoming pose predictions and their corresponding activations
      - thereby assigns parts to wholes via cluster finding

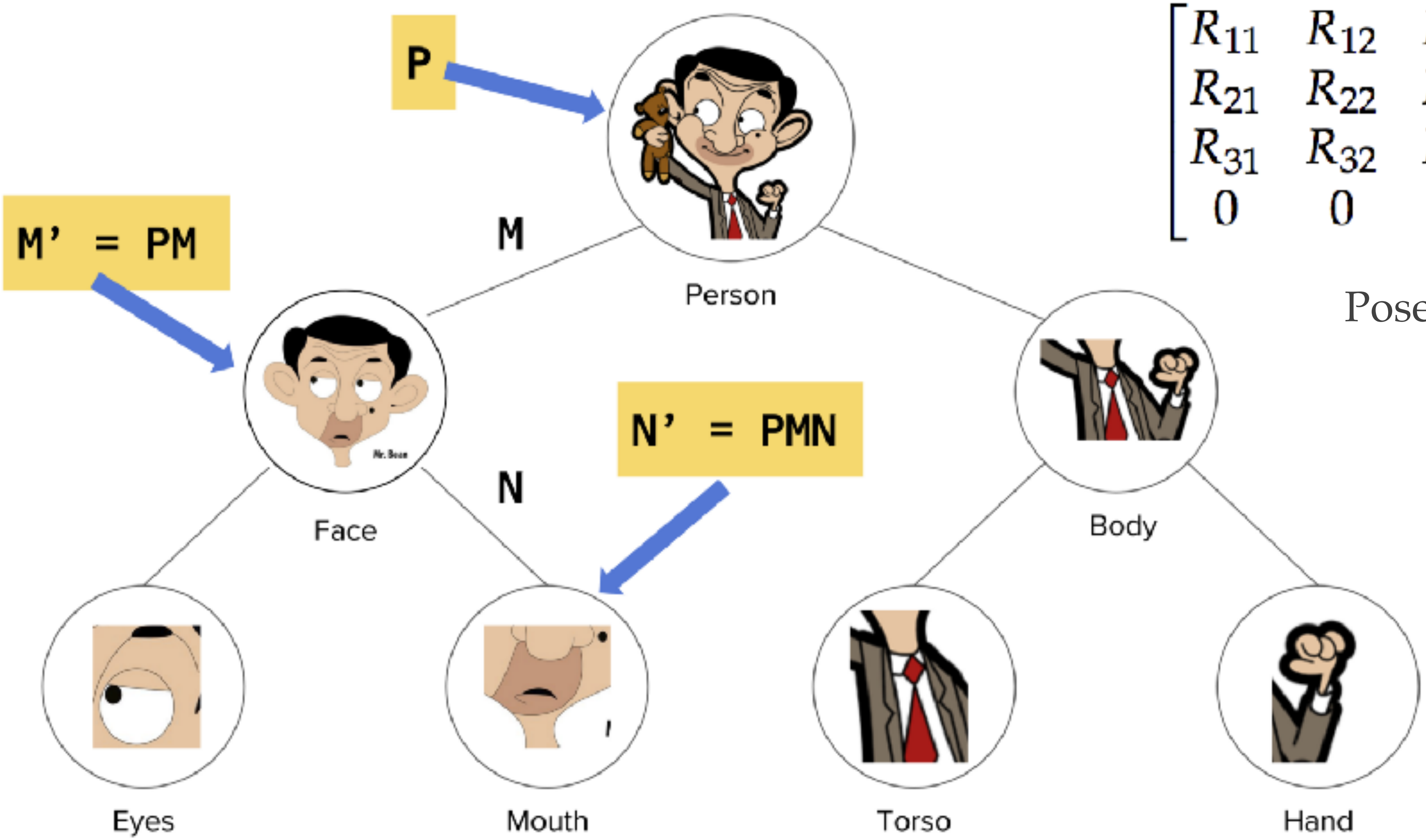
Rendering



$$\begin{bmatrix} R_{11} & R_{12} & R_{13} & T_1 \\ R_{21} & R_{22} & R_{23} & T_2 \\ R_{31} & R_{32} & R_{33} & T_3 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Pose Matrix

Rendering



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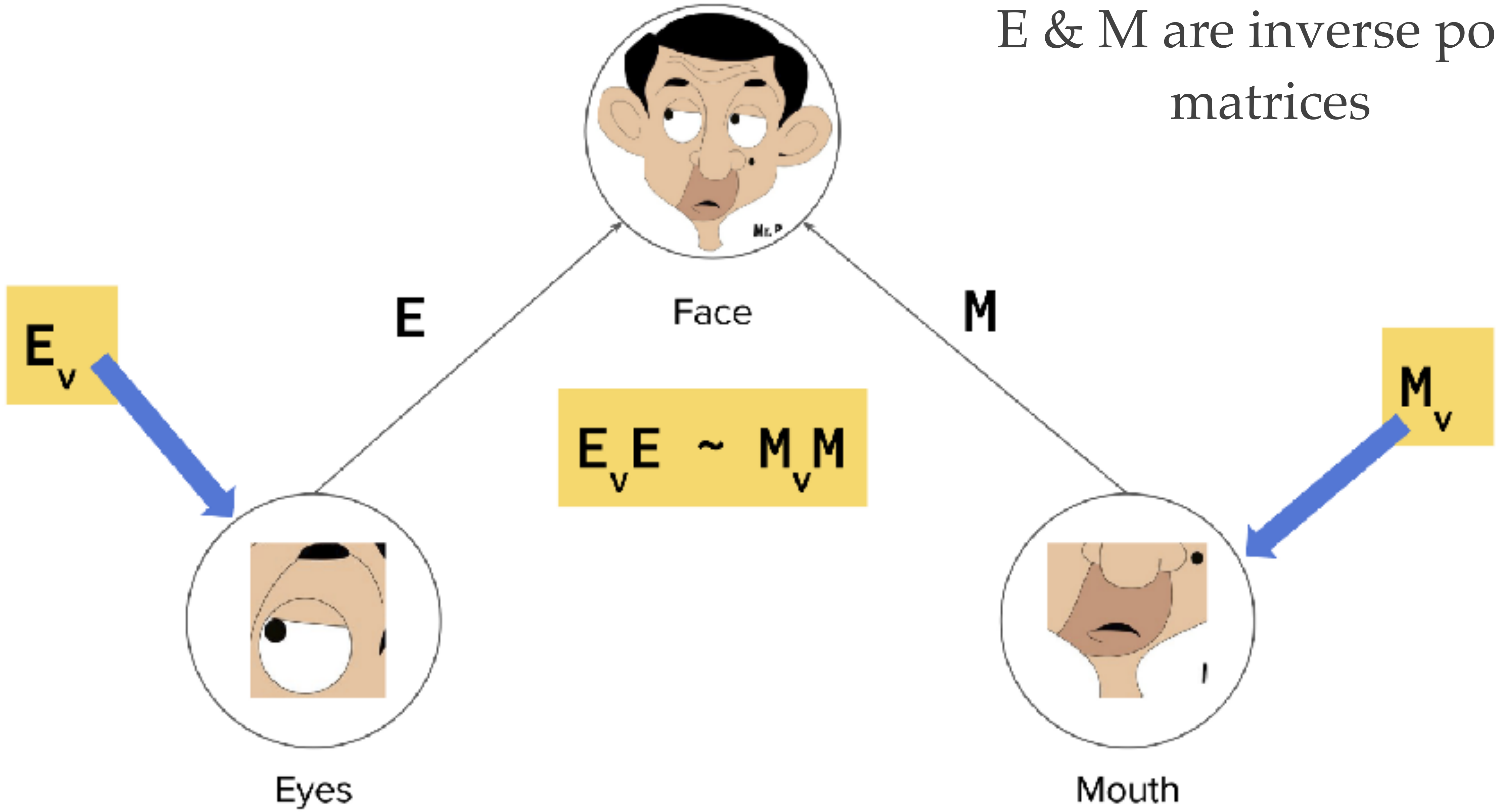
Pose Matrix

Inverse Rendering

E & M are inverse pose matrices



Assigning parts to wholes

- done via routing algorithm between Capsules
  - utilization of high- dim. coincidence filtering: looking for agreement of capsule votes
  - votes produced by a learned linear transformation of the pose of each capsule
  - linear transf. represents viewpoint invariant relationship between part and whole

Improved Explainability

- Likelihood or the activation of the capsules can be interpreted as saliency for specific regions
- Instantiation parameter pose values usable to explain consistency among the layers
    - Capsules describing the same object are in an appropriate relationship with consistence parameters, leading to a parse tree like structure

Difference between dyn. routing and EM routing

- length of pose vector is activation
- Cosine of angle to measure agreement
- pose is vector with length n

- dedicated activation element
- log variance of a Gaussian cluster
- pose is matrix with n x n elements

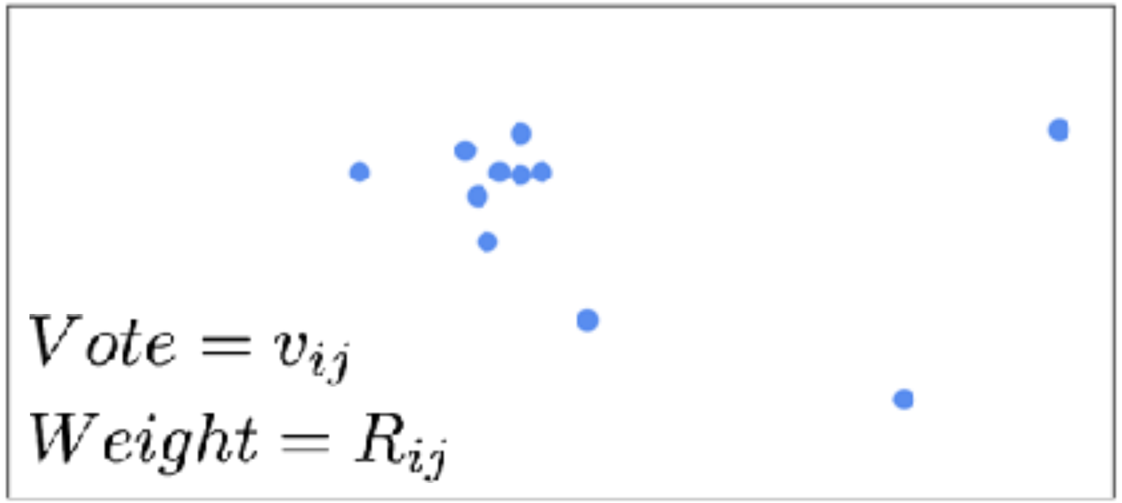
EM routing

- Each Capsule in Layer L+1 corresponds to Gaussian where μ is the pose
- Utilization of the “Minimum Description Length” principle (best hypothesis or regulariser allows strongest compression of data)
  - choice whether to activate capsule in L+1 based on votes from L

Computation of the votes

- Set of Capsules in Layer L : Ω_L
- Each Capsules has "Pose Matrix" $M \in \mathbb{R}^{4\times4}$ and activation $a \in (0,1)$
- Weight matrix connecting capsule i from Ω_L with j from Ω_{L+1} : $V_{ij} \in \mathbb{R}^{4\times4}$
- Vote from Ω_L i to Ω_{L+1} j: $V_{ij} = M_i W_{ij}$

EM - Schematic in 2d-space for one capsule j in Layer L+1

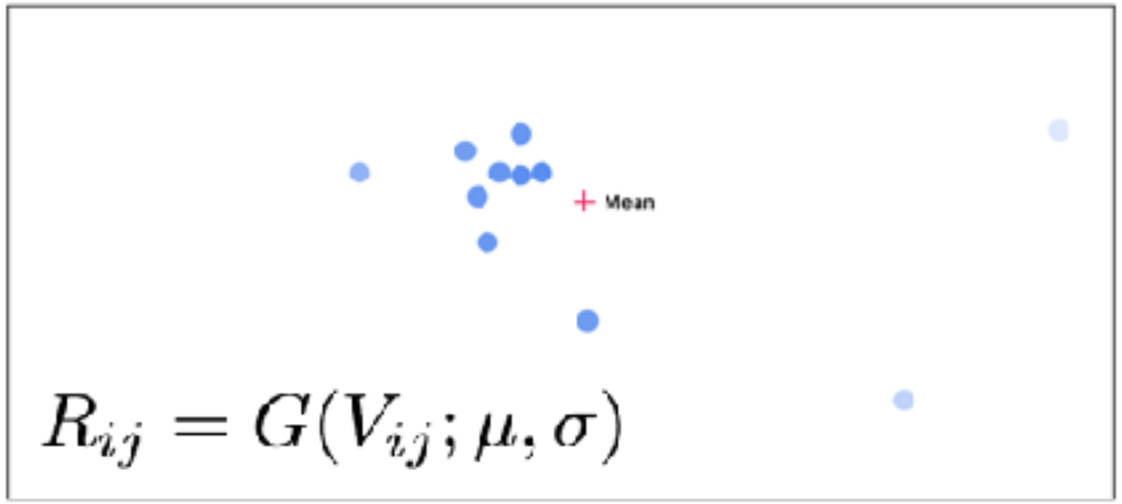


$Vote = v_{ij}$

$Weight = R_{ij}$

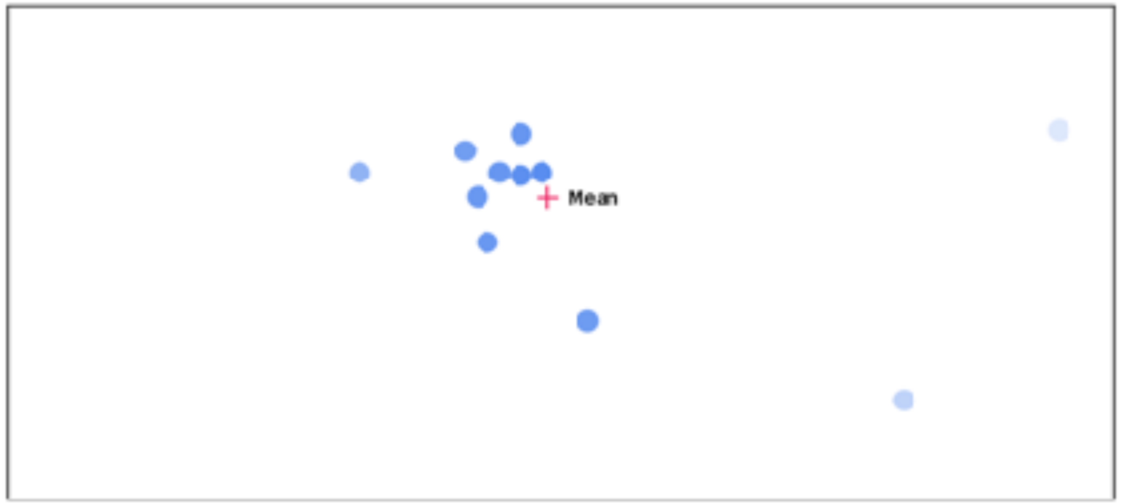
Start

M-Step $\mu = \dfrac{\sum_i R_{ij} V_{ij}}{\sum_i R_{ij}}$ σ



$R_{ij} = G(V_{ij}; \mu, \sigma)$

E-Step



M-Step

Choice of activation

- introduce a cost of explaining data point i by using capsule j: $cost_{j|i} = -ln(G(V_{ij}; \mu_j, \sigma_j))$
- cost for activation of j:

$$cost_j = -\sum_i R_{ij} \cdot ln(G(V_{ij}; \mu_j, \sigma_j)) = \sum_i R_{ij}(ln(\sigma_j) + \beta_v)$$

- activation of capsule j:

$$a_j = logistic(\lambda(\beta_a - cost_j))$$

$\sum_i R_{ij}$: amount of data assigned to j

Algorithm

Procedure 1 Routing algorithm returns **activation** and **pose** of the capsules in layer $L+1$ given the **activations** and **votes** of capsules in layer L. V_{ij}^h is the h^{th} dimension of the vote from capsule i with activation a_i in layer L to capsule j in layer $L+1$. β_a, β_v are learned discriminatively and the inverse temperature λ increases at each iteration with a fixed schedule.

procedure EM ROUTING($\boldsymbol{a}$, V)
    $\forall i \in \Omega_L, j \in \Omega_{L+1}$: $R_{ij} \leftarrow 1/|\Omega_{L+1}|$
    for t iterations **do**
        $\forall j \in \Omega_{L+1}$: M-STEP($\boldsymbol{a}$, R, V, j)
        $\forall i \in \Omega_L$: E-STEP(μ, σ, $\boldsymbol{a}$, V, i)
    return $\boldsymbol{a}$, M

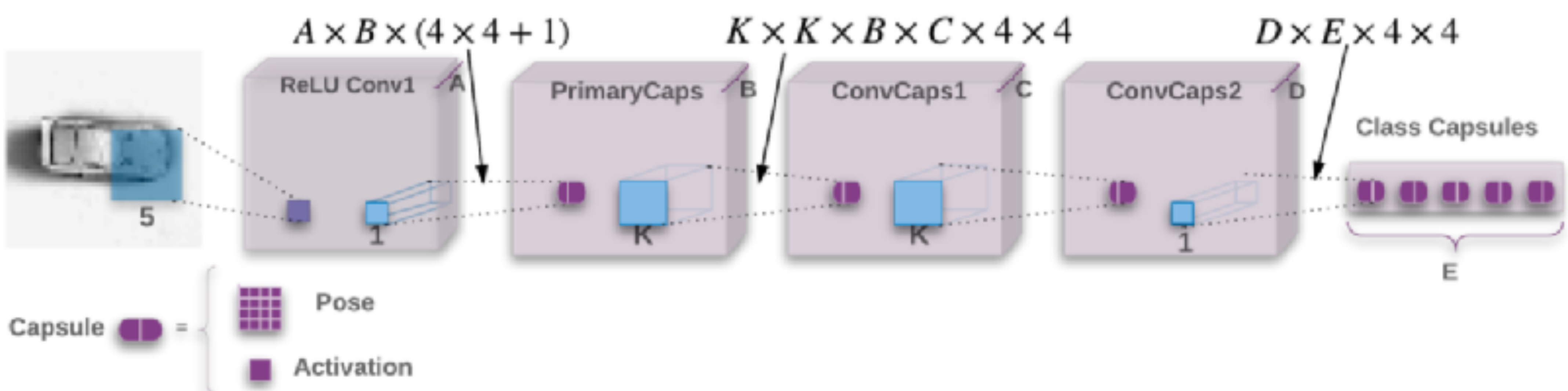
procedure M-STEP($\boldsymbol{a}$, R, V, j) ▷ for one higher-level capsule
    $\forall i \in \Omega_L$: $R_{ij} \leftarrow R_{ij} * \boldsymbol{a}_i$
    $\forall h$: $\mu_j^h \leftarrow \frac{\sum_i R_{ij} V_{ij}^h}{\sum_i R_{ij}}$
    $\forall h$: $(\sigma_j^h)^2 \leftarrow \frac{\sum_i R_{ij}(V_{ij}^h - \mu_j^h)^2}{\sum_i R_{ij}}$
    $cost^h \leftarrow (\beta_v + log(\sigma_j^h)) \sum_i R_{ij}$
    $a_j \leftarrow sigmoid(\lambda(\beta_a - \sum_h cost^h))$

$$\sum_j R_{ij} = a_i$$

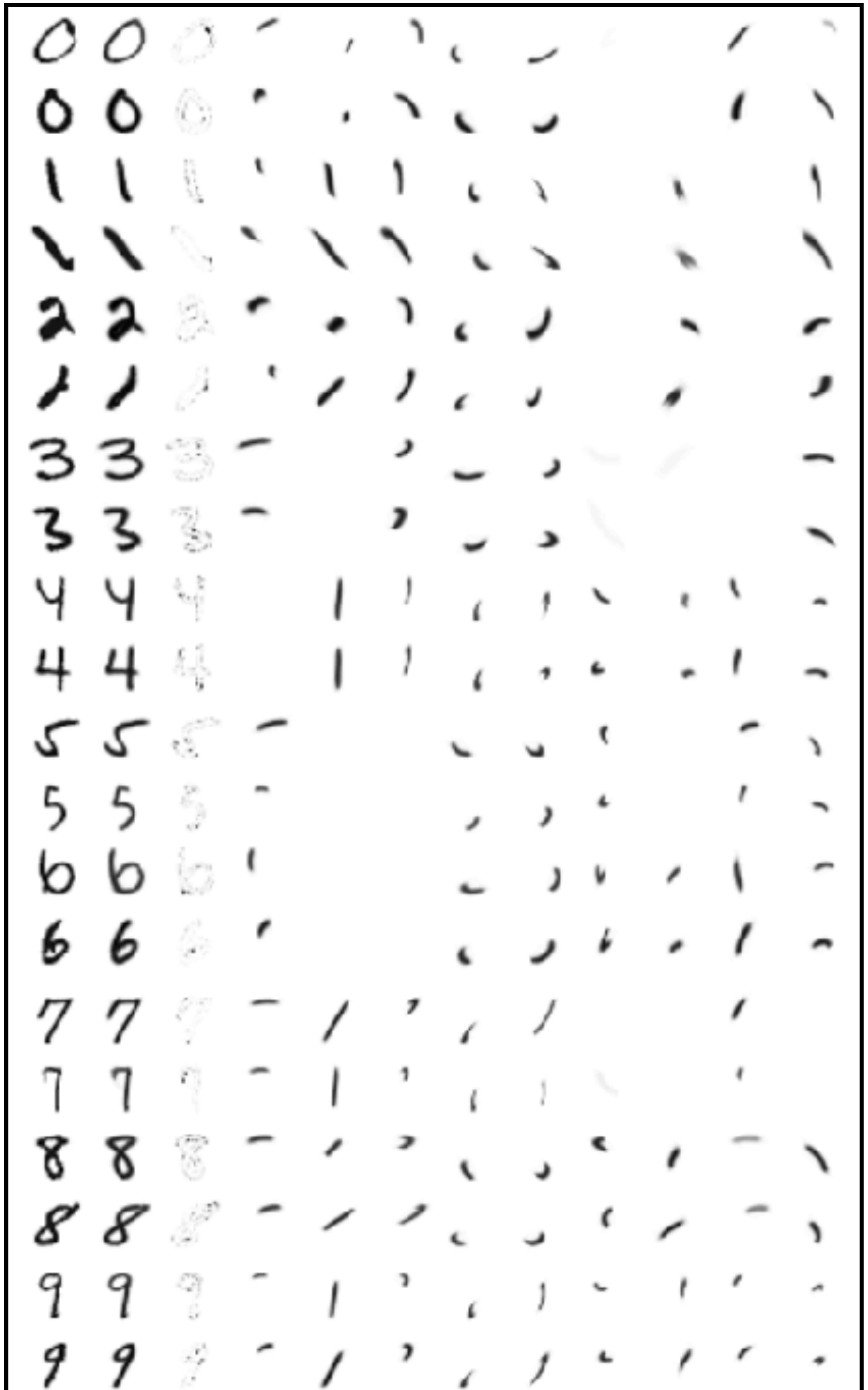
procedure E-STEP(μ, σ, $\boldsymbol{a}$, V, i) ▷ for one lower-level capsule
    $\forall j \in \Omega_{L+1}$: $\boldsymbol{p}_j \leftarrow \frac{1}{\sqrt{\prod_h^H 2\pi(\sigma_j^h)^2}} e^{-\sum_h^H \frac{(V_{ij}^h - \boldsymbol{\mu}_j^h)^2}{2(\sigma_j^h)^2}}$
    $\forall j \in \Omega_{L+1}$: $\boldsymbol{R}_{ij} \leftarrow \frac{\boldsymbol{a}_j p_j}{\sum_{u \in \Omega_{L+1}} \boldsymbol{a}_u p_u}$

$$\sum_j R_{ij} = 1$$

Architecture

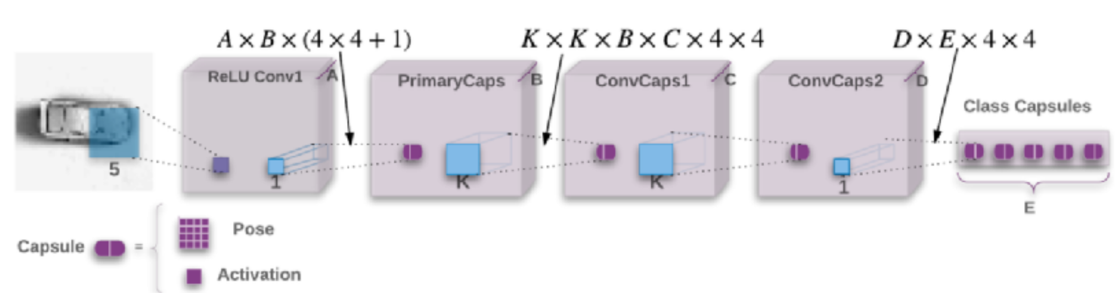


- Convolution + ReLU to filter low level features
- Primary Capsules with B different capsule types
- Convolutional Capsules with C/D different capsule types
- Class capsules detecting E different classes



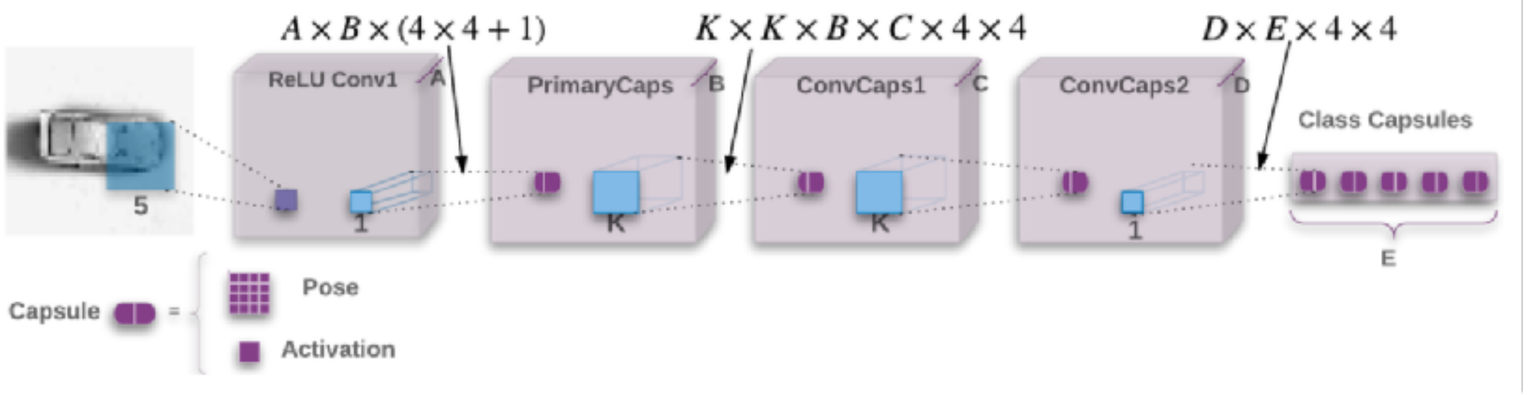
Primary Capsule

- detects specific low level features
- Domain Specific Auto Encoder
- keep spatial information
- learns task specific features



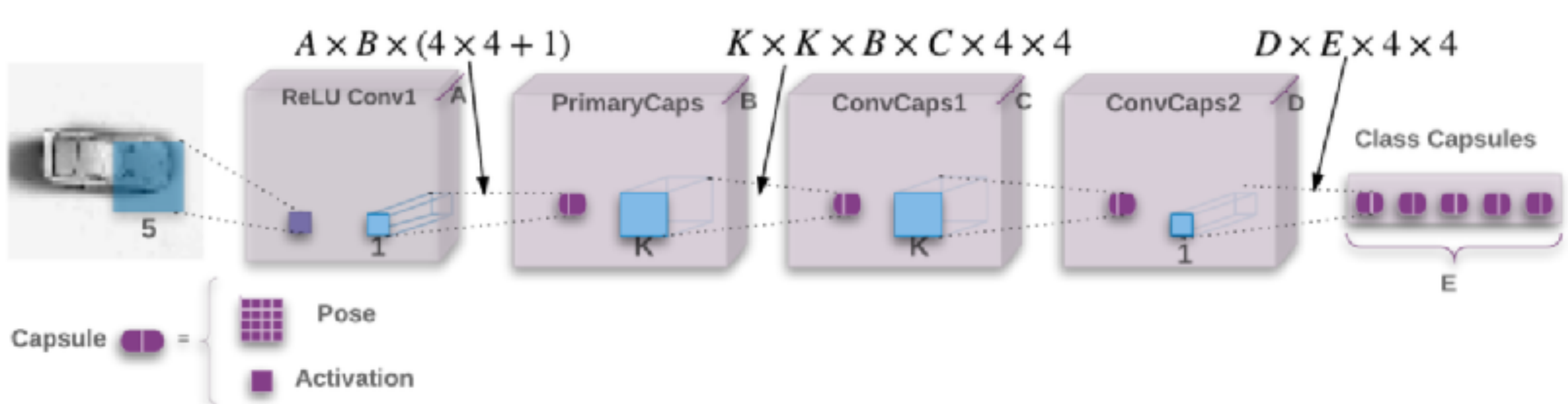
Convolutional Capsule

- routing procedure only for lower capsules in the receptive field of higher level capsules (kernel)
- divide the task of detecting high level features or classes into small steps
- speed up the model



Class Capsules

- use fact: all capsules of the same type detect same entity in different positions
- share transformation matrix between different positions of the same capsule type
- possible addition of receptive field of the lower layer capsules in the computation (coordinate addition)



Spread Loss

$$L_i = (max(0, m - (a_t - a_i))^2, \quad L = \sum_{i \neq t} L_i$$

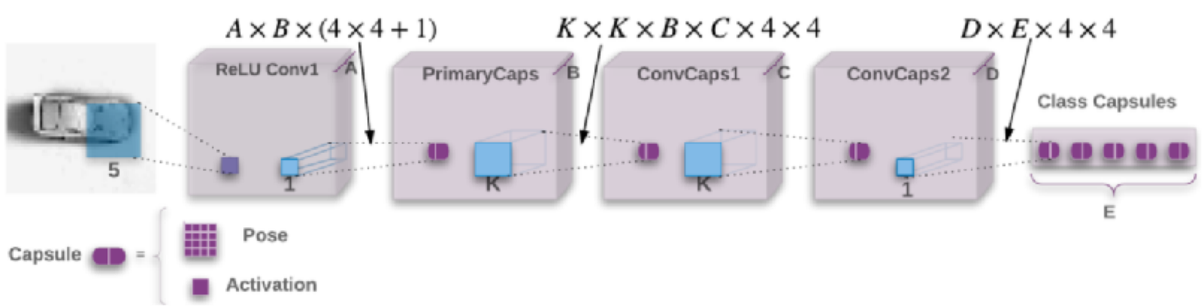
a_t: target class activation $\qquad$ a_i: wrong class activation

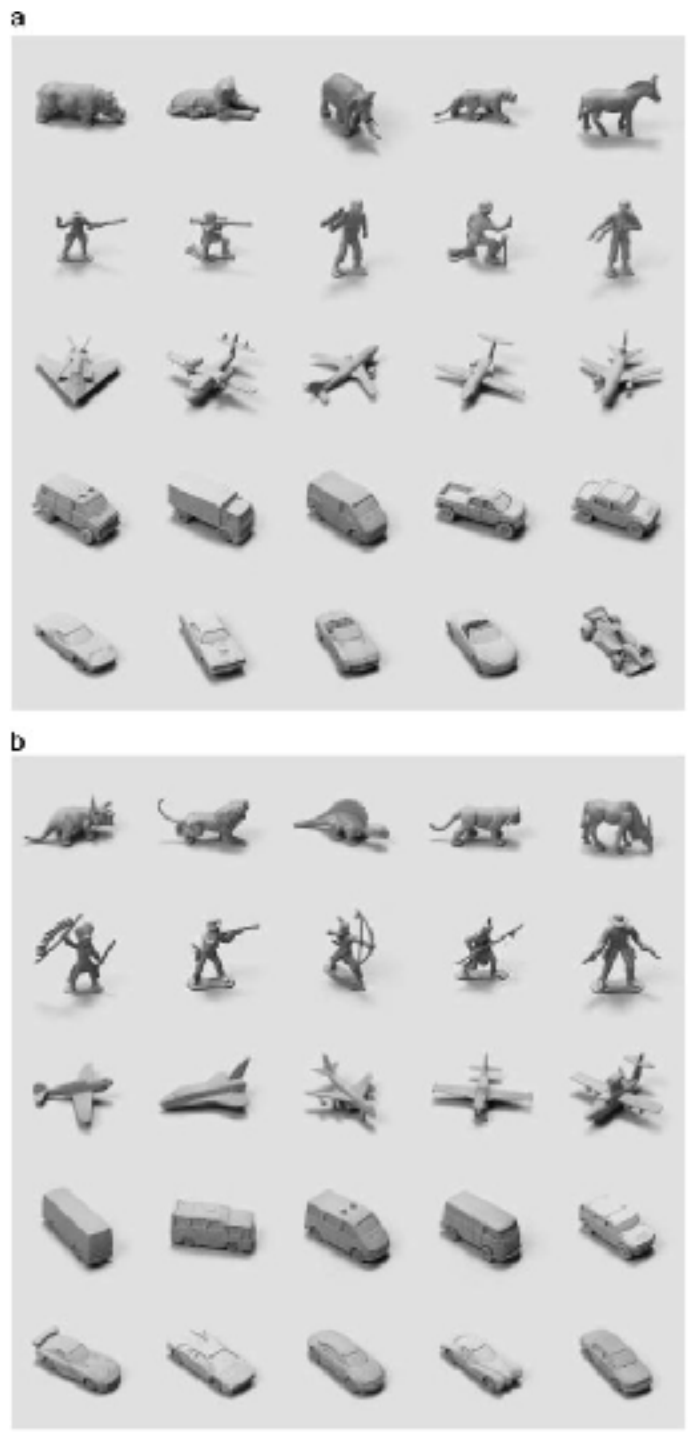
m: margin

- margin is linearly increased during training
- avoids dead capsules and makes training less sensitive

Experiment on smallNORB

- Dataset:
  - 5 classes of toys
  - same entity photographed in different positions
  - pure shape recognition task
  - no disturbing background
  - downsampled to 48x48 pixels
  - training: randomly cropped 32x32
  - test: center cropped 32x32
- Model:





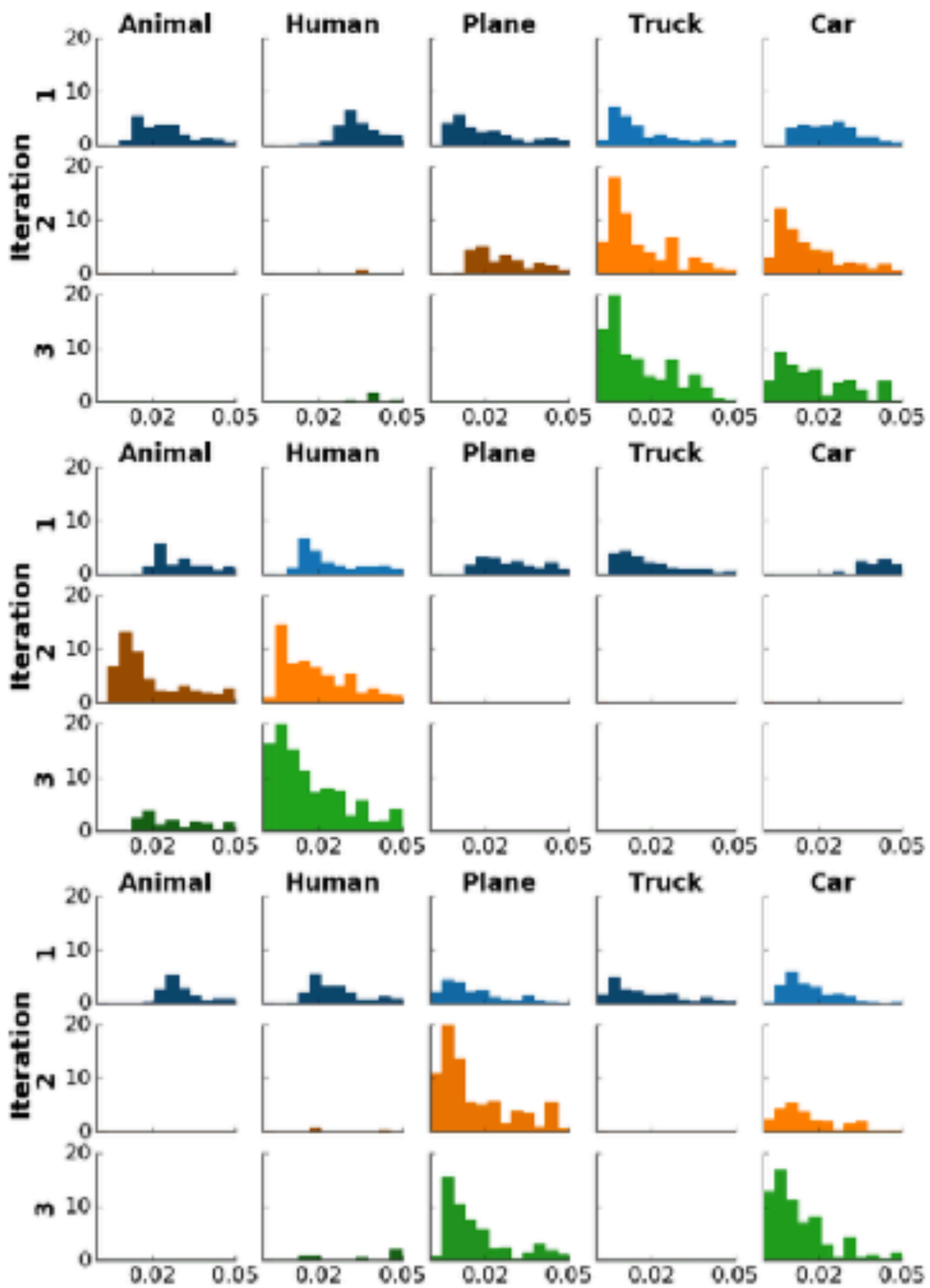
Results

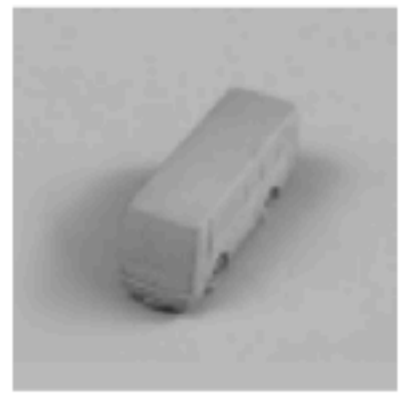
Routing iterations	Pose structure	Loss	Coordinate Addition	Test error rate
1	Matrix	Spread	Yes	9.7%
2	Matrix	Spread	Yes	2.2%
3	Matrix	Spread	Yes	**1.8%**
5	Matrix	Spread	Yes	3.9%
3	Vector	Spread	Yes	2.9%
3	Matrix	Spread	No	2.6%
3	Vector	Spread	No	3.2%
3	Matrix	Margin[1]	Yes	3.2%
3	Matrix	CrossEnt	Yes	5.8%
Baseline CNN with 4.2M parameters				5.2%
CNN of Cireşan et al. (2011) with extra input images & deformations				2.56%
Our Best model (third row), with multiple crops during testing				**1.4%**

- Sabour et al. Capsules achieve 2.7% test error rate
- Ciresan et al. CNN used classical methods to create additional input

- Baseline CNN fine-tuned for this task and trained like Capsule Net
- Matrix Capsule Net has 310k Parameters but smaller model with 68k Parameters achieved 2.2% test error rate

Routing





- Histogram of distances of votes to the main in the last layer
  - x-axis distance of the vote
  - y-axis amount of data

Generalization to novel viewpoints

Test set	Azimuth		Elevation	
	CNN	Capsules	CNN	Capsules
Novel viewpoints	20%	13.5%	17.8%	12.3%
Familiar viewpoints	3.7%	3.7%	4.3%	4.3%

- Trained on 1/3 of training data with specific azimuths/elevation levels
- Capsule Net is trained to match accuracy on familiar viewpoints

Results on other datasets

- NORB:
  MCN: 2.6% TE
  State of the Art: 2.7% TE

- MNIST:
  MCNet: 0.44% TE
  Sabour et. AL.: 0.25% TE
- CIFAR10:
  Matrix Capsule Net: 11.9%TE
  Convolutional Deep Belief Networks(2010): 21.9%

Disadvantages

- computational expensive routing
- models take a massive amount of RAM
- has a problem with backgrounds
- cannot detect two objects of the same class very near to each other
- difficult to scale to datasets with more classes & higher dimensions

Advantages

- design similar to a parse tree and thereby more understandable
- requires less training data
- smaller amount of parameters
- model learns to a degree generative properties
- capsules activation in lower levels works similary to saliency or Region Proposal Networks
- more robust against adversarial examples than standard CNN

Sources

- Slide 15: https://www.cs.toronto.edu/~tijmen/tijmen_thesis.pdf
- Slide 12: https://medium.freecodecamp.org/understanding-capsule-networks-ais-alluring-new-architecture-bdb228173ddc
- Slide 5 to 7: https://hackernoon.com/uncovering-the-intuition-behind-capsule-networks-and-inverse-graphics-part-i-7412d121798d
- Slide 2: https://www.enterprisetech.com/2017/11/22/ais-cool-new-thing-capsule-networks-explained/
- Paper: https://openreview.net/pdf?id=HJWLfGWRb
- Other Resources:
  http://web.cse.ohio-state.edu/~wang.3602/courses/cse5542-2013-spring/6-Transformation_II.pdf
  https://arxiv.org/abs/1802.10204v1

THANK YOU FOR YOUR ATTENTION!