About

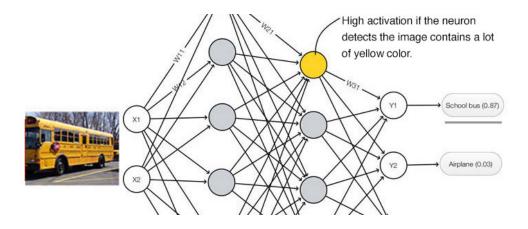
"Understanding Dynamic Routing between Capsules (Capsule Networks)"

Nov 3, 2017

This article covers the technical paper by Sara Sabour, Nicholas Frosst and Geoffrey Hinton on Dynamic Routing between Capsules. In this article, we will describe the basic Capsule concept and apply it with the Capsule network *CapsNet* to detect digits in MNist. In the last third of the article, we go through a detail implementation. The source code implementation is originated from XifengGuo using Keras with Tensorflow.

CNN challenges

In deep learning, the activation level of a neuron is often interpreted as the likelihood of detecting a specific feature.



If we pass the Picasso's "Portrait of woman in d'hermine pass" into a CNN classifier, how likely that the classifier may mistaken it as a real human face?

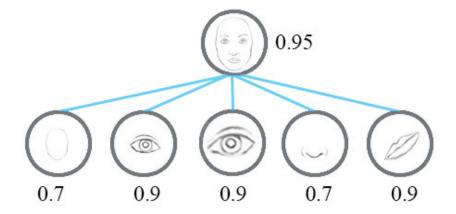


CNN is good at detecting features but less effective at exploring the spatial relationships among features (perspective, size, orientation). For example, the following picture may fool a *simple* CNN model in believing that this a good sketch of a human face.

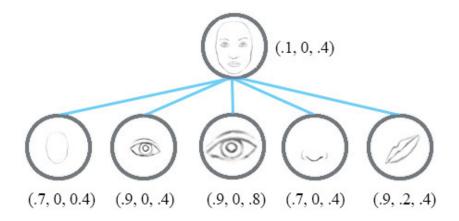


(image source)

A simple CNN model can extract the features for nose, eyes and mouth correctly but will wrongly activate the neuron for the face detection. Without realize the mis-match in spatial orientation and size, the activation for the face detection will be too high.



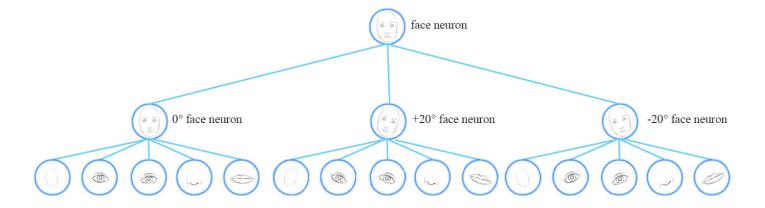
Now, we imagine that each neuron contains the likelihood as well as properties of the features. For example, it outputs a vector containing [likelihood, orientation, size]. With this spatial information, we can detect the in-consistence in the orientation and size among the nose, eyes and ear features and therefore output a much lower activation for the face detection.



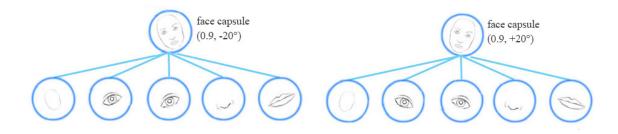
Instead of using the term neurons, the technical paper uses the term **capsules** to indicate that capsules output a vector instead of a single scaler value.

Equivariance

Conceptually, a CNN model uses multiple neurons and layers in capturing different feature's variants:



A capsule network share the same capsule to detect multiple variants in a simpler network.



Equivariance is the detection of objects that can transform to each other. Intuitively, a capsule detects the face is rotated right 20° (or rotated left 20°) rather than realizes the face matched a variant that is rotated right 20°. By forcing the model to learn the feature variant in a capsule, we *may* extrapolate possible variants more effectively with less training data.

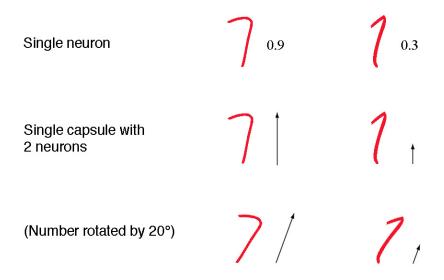
MNist dataset contains 55,000 training data. i.e. 5,500 samples per digits. However, it is unlikely that children need to read this large amount of samples to learn digits. Our existing deep learning models including CNN seem inefficient in utilizing datapoints.

With feature property as part of the information extracted by capsules, we may generalize the model better without an over extensive amount of labeled data.

Capsule

A capsule is a group of neurons that not only capture the likelihood but also the parameters of the specific feature.

For example, the first row below indicates the probabilities of detecting the number "7" by a neuron. A 2-D capsule is formed by combining 2 neurons. This capsule outputs a 2-D vector in detecting the number "7". For the first image in the second row, it outputs a vector v = (0, 0.9). The magnitude of the vector $||v|| = \sqrt{0^2 + 0.9^2} = 0.9$ corresponds to the probability of detecting "7". The second image of each row looks more like a "1" than a "7". Therefore its corresponding likelihood as "7" is smaller (smaller scaler value or smaller vector's magnitude but with the same orientation).



In the third row, we rotate the image by 20°. The capsule will generate vectors with the same magnitude but different orientations. Here, the angle of the vector represents the angle of rotation for the number "7". As we can image, we can add 2 more neurons to a capsule to capture the size and stroke width.



We call the output vector of a capsule as the **activity vector** with magnitude represents the probability of detecting a feature and its orientation represents its parameters (properties).

Dynamic routing

Dynamic routing groups capsules to form a parent capsule, and it calculates the capsule's output.

Intuition

We collect 3 similar sketches with different scale and orientation, and we measures the horizontal width of the mouth and the eye in pixels. They are $s^{(1)} = (100, 66), s^{(2)} = (200, 131)$ and $s^{(3)} = (50, 33)$.

(Image modified from)

Let's assume $W_m=2,\,W_e=3$, and we calculate a vote from the mouth and the eye for $s^{(1)}$ as:

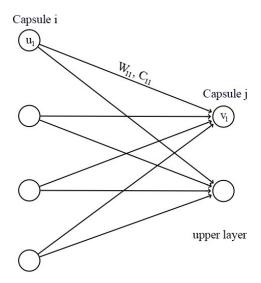
$$v_m^{(1)} = W_m \times width_m = 2 \times 100 = 200$$

 $v_e^{(1)} = W_e \times width_e = 3 \times 66 = 198$

We realize both $v_m^{(1)}$ and $v_e^{(1)}$ are very similar. When we repeat it with other sketches, we get the same findings. So the mouth capsule and the eye capsule can be strongly related to a parent capsule with width approximate 200 pixels. From our experience, a face is 2 times ($W_m=2$) the width of a mouth and 3 times the width ($W_e=3$) of an eye. So the parent capsule we detected is a face capsule. Of course, we can make it more accurate by adding more properties like height or color. In dynamic routing, we transform the vectors of an input capsules with a transformation matrix W to form a vote, and group capsules with similar votes. Those votes eventually becomes the output vector of the parent capsule. So how can we know W? Just do it in the deep learning way: backpropagation with a cost function.

Calculating a capsule output

For a capsule, the input u_i and the output v_i of a capsule are vectors.



We apply a **transformation matrix** W_{ij} to the capsule output u_i of the pervious layer. For example, with a $p \times k$ matrix, we transform u_i to $u_{j|i}$ from k-dimension to p-dimension. ($(p \times k) \times (k \times 1) \implies p \times 1$) Then we compute a weighted sum s_i with weights c_{ij} .

$$\hat{u_{j|i}} = W_{ij}u_i$$

$$s_j = \sum_i c_{ij}\hat{u_{j|i}}$$

 c_{ij} are **coupling coefficients** that are calculated by the iterative dynamic routing process (discussed next) and $\sum_j c_{ij}$ are designed to sum to one. Conceptually, c_{ij} measures how likely capsule i may activate capsule j.

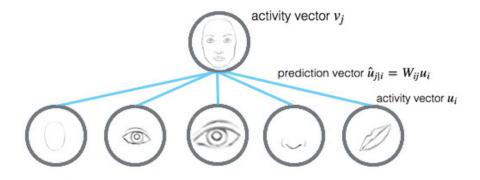
Instead of applying a ReLU function, we apply a squashing function to s_j so the final output vector v_j of the capsule has length between 0 and 1. This function shrinks small vectors to zero and large vectors to unit vectors.

$$v_j = \frac{\|s_j\|^2}{1 + \|s_i\|^2} \frac{s_j}{\|s_i\|}$$

$$v_j \approx ||s_j||s_j$$
 for s_j is small.
 $v_j \approx \frac{s_j}{||s_i||}$ for s_j is large.

Iterative dynamic Routing

In capsule, we use iterative dynamic routing to compute the capsule output by calculating an intermediate value c_{ij} (coupling coefficient).



Recall that the **prediction vector** $\hat{u_{j|i}}$ is computed as:

$$\hat{u_{j|i}} = W_{ij}u_i$$

and the **activity vector** v_j (the capsule j output) is:

$$s_j = \sum_{i} c_{ij} \hat{u_{j|i}}$$

$$v_j = \frac{\|s_j\|^2}{1 + \|s_i\|^2} \frac{s_j}{\|s_i\|}$$

Intuitively, prediction vector $\hat{u_{j|i}}$ is the prediction (**vote**) from the capsule i on the output of the capsule j above. If the activity vector has close similarity with the prediction vector, we conclude that both capsules are highly related. Such similarity is measured using the scalar product of the prediction and the activity vector.

$$b_{ij} \leftarrow \hat{u_{j|i}} \cdot v_j$$

Therefore, the similarity score b_{ij} takes into account on both likeliness and the feature properties, instead of just likeliness in neurons. Also, b_{ij} remains low if the activation u_i of capsule i is low since $u_{\hat{j}|i}$ length is proportional to u_i . i.e. b_{ij} should remain low between the mouth capsule and the face capsule if the mouth capsule is not activated.

The coupling coefficients c_{ij} is computed as the softmax of b_{ij} :

$$c_{ij} = \frac{\exp b_{ij}}{\sum_{k} \exp b_{ik}}$$

To make b_{ij} more accurate, it is updated iteratively in multiple iterations (typically in 3 iterations).

$$b_{ij} \leftarrow b_{ij} + \hat{u_{i|i}} \cdot v_j$$

Here is the final pseudo code for the dynamic routing:

```
Procedure 1 Routing algorithm.
```

```
1: procedure ROUTING(\hat{\mathbf{u}}_{j|i}, r, l)
2: for all capsule i in layer l and capsule j in layer (l+1): b_{ij} \leftarrow 0.
3: for r iterations do
4: for all capsule i in layer l: \mathbf{c}_i \leftarrow \mathtt{softmax}(\mathbf{b}_i)
5: for all capsule j in layer (l+1): \mathbf{s}_j \leftarrow \sum_i c_{ij} \hat{\mathbf{u}}_{j|i}
6: for all capsule j in layer (l+1): \mathbf{v}_j \leftarrow \mathtt{squash}(\mathbf{s}_j)
7: for all capsule i in layer i and capsule i and capsule
```

Source Sara Sabour, Nicholas Frosst, Geoffrey Hinton

Routing a capsule to the capsule in the layer above based on relevancy is called **Routing-by-agreement**.

The dynamic routing is not a complete replacement of the backpropagation. The transformation matrix W is still trained with the backpropagation using a cost function. However, we use dynamic routing to compute the output of a capsule. We compute c_{ij} to quantify the connection between a capsule and its parent capsules. This value is important but short lived. We re-initialize it to 0 for every datapoint before the dynamic routing

calculation. To calculate a capsule output, training or testing, we always redo the dynamic routing calculation.

Max pooling shortcoming

The max pooling in a CNN handles translational variance. Even a feature is slightly moved, if it is still within the pooling window, it can still be detected. Nevertheless, this approach keeps only the max feature (the most dominating) and throws away the others. Capsules maintain a weighted sum of features from the previous layer. Hence, it is more suitable in detecting overlapping features. For example detecting multiple overlapping digits in the handwriting:

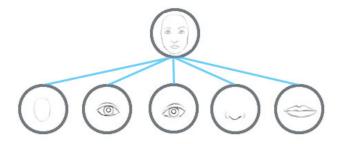


Significant of routing-by-agreement with capsules

In a fully connected network, we calculate the neuron with

$$y_j = ReLU(\sum_i W_{ij}x_i + b_j),$$

and W is trained by the backpropagation with a global cost function. Iterative dynamic routing provides an alternative of calculating how a capsule is activated by using local features' properties. Theoretically, we can group capsules better and simpler to form a **parse tree** with reduced risk of adversaries.



The iterative dynamic routing with capsules is just one showcase in demonstrating the

routing-by-agreement. In a second paper on capsules *Matrix capsules with EM routing*, a matrix capsule [likeliness, 4x4 pose matrix] is proposed with a new Expectation-maximization (EM) routing. The pose matrices are designed to capture different viewpoints so a capsule can capture objects with different azimuths and elevations.



(Source from the paper Matrix capsules with EM routing)

Matrix capsules apply a clustering technique, the EM routing, to cluster related capsules to form a parent capsule. Even the viewpoint may change, the votes will change in a coordinate way from the red dots to the pink dots below. So the EM routing can still cluster the same children capsules together.



The first paper opens a new approach in the deep learning, and the second paper explores deeper into its potential. For those interested, there are more details in my second article on Matrix capsule.

CapsNet architecture

Finally, we apply capsules to build the CapsNet to classify the MNist digits. The following is the architecture using CapsNet.

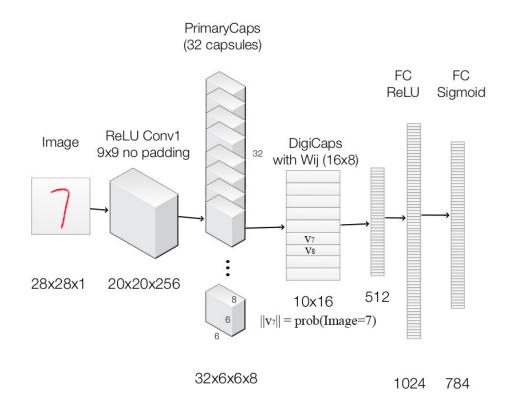


Image is feed into the ReLU Conv1 which is a standard convolution layer. It applies 256 9x9 kernels to generate an output with 256 channels (feature maps). With stride 1 and no padding, the spatial dimension is reduced to 20x20. (28-9+1=20)

It is then feed into PrimaryCapsules which is a modified convolution layer supporting capsules. It generates a 8-D vector instead of a scalar. PrimaryCapsules used 8x32 kernels to generate 32 8-D capsules. (i.e. 8 output neurons are grouped together to form a capsule) PrimaryCapsules uses 9x9 kernels with stride 2 and no padding to reduce the spatial dimension from 20x20 to 6x6 ($\lfloor \frac{20-9}{2} \rfloor + 1 = 6$). In PrimaryCapsules, we have 32x6x6 capsules.

It is then feed into DigiCaps which apply a transformation matrix W_{ij} with shape 16x8 to convert the 8-D capsule to a 16-D capsule for each class j (from 1 to 10).

$$\hat{u_{j|i}} = W_{ij}u_i$$

The final output v_i for class j is computed as:

$$s_j = \sum_{i} c_{ij} u_{j|i}^2$$

$$v_j = \frac{\|s_j\|^2}{1 + \|s_j\|^2} \frac{s_j}{\|s_j\|}$$

Because there are 10 classes, the shape of DigiCaps is 10x16 (10 16-D vector.) Each vector v_j acts as the capsule for class j. The probability of the image to be classify as j is computed by $||v_j||$. In our example, the true label is 7 and v_7 is the latent representation of our input. With a 2 hidden fully connected layers, we can reconstruct the 28x28 image from v_7 .

Here is the summary of each layers:

Layer Name	Apply	Output shape
Image	Raw image array	28x28x1
ReLU Conv1	Convolution layer with 9x9 kernels output 256 channels, stride 1, no padding with ReLU	20x20x256
PrimaryCapsules	Convolution capsule layer with 9x9 kernel output 32x6x6 8-D capsule, stride 2, no padding	6x6x32x8
DigiCaps	Capsule output computed from a W_{ij} (16x8 matrix) between u_i and v_j (i from 1 to 32x6x6 and j from 1 to 10).	10x16
FC1	Fully connected with ReLU	512
FC2	Fully connected with ReLU	1024
Output image	Fully connected with sigmoid	784 (28x28)

Our capsule layers use convolution kernels to explore locality information.

Loss function (Margin loss)

In our example, we want to detect multiple digits in a picture. Capsules use a separate margin loss L_c for each category c digit present in the picture:

$$L_c = T_c \max(0, m^+ - ||v_c||)^2 + \lambda (1 - T_c) \max(0, ||v_c|| - m^-)^2$$

which $T_c=1$ if an object of class c is present. $m^+=0.9$ and $m^-=0.1$. The λ downweighting (default 0.5) stops the initial learning from shrinking the activity vectors of all classes. The total loss is just the sum of the losses of all classes.

Computing the margin loss in Keras

CapsNet model

Here is the Keras code in creating the CapsNet model:

```
def CapsNet(input_shape, n_class, num_routing):
    """
    :param input_shape: (None, width, height, channels)
    :param n_class: number of classes
    :param num_routing: number of routing iterations
```

```
:return: A Keras Model with 2 inputs (image, label) and
         2 outputs (capsule output and reconstruct image)
0.00
# Image
x = layers.Input(shape=input_shape)
# ReLU Conv1
conv1 = layers.Conv2D(filters=256, kernel size=9, strides=1,
                 padding='valid', activation='relu', name='conv1')(x
# PrimaryCapsules: Conv2D layer with `squash` activation,
# reshape to [None, num capsule, dim vector]
primarycaps = PrimaryCap(conv1, dim vector=8, n channels=32,
                        kernel size=9, strides=2, padding='valid')
# DigiCap: Capsule layer. Routing algorithm works here.
digitcaps = DigiCaps(num capsule=n class, dim vector=16,
            num routing=num routing, name='digitcaps')(primarycaps)
# The length of the capsule's output vector
out caps = Length(name='out caps')(digitcaps)
# Decoder network.
y = layers.Input(shape=(n class,))
# The true label is used to extract the corresponding vj
masked = Mask()([digitcaps, y])
x recon = layers.Dense(512, activation='relu')(masked)
x recon = layers.Dense(1024, activation='relu')(x recon)
x recon = layers.Dense(784, activation='sigmoid')(x recon)
x recon = layers.Reshape(target shape=[28, 28, 1], name='out recon')
# two-input-two-output keras Model
return models.Model([x, y], [out_caps, x_recon])
```

The length of the capsule's output vector $||v_j||$ corresponds to the probability that it belong to the class j. For example, $||v_7||$ is the probability of the input image belongs to 7.

```
class Length(layers.Layer):
    def call(self, inputs, **kwargs):
        # L2 length which is the square root
        # of the sum of square of the capsule element
        return K.sqrt(K.sum(K.square(inputs), -1))
```

PrimaryCapsules

PrimaryCapsules converts 20x20 256 channels into 32x6x6 8-D capsules.

```
def PrimaryCap(inputs, dim_vector, n_channels, kernel_size, strides, pad
    """

Apply Conv2D `n_channels` times and concatenate all capsules
    :param inputs: 4D tensor, shape=[None, width, height, channels]
    :param dim_vector: the dim of the output vector of capsule
    :param n_channels: the number of types of capsules
    :return: output tensor, shape=[None, num_capsule, dim_vector]
    """

    output = layers.Conv2D(filters=dim_vector*n_channels, kernel_size=ke
    outputs = layers.Reshape(target_shape=[-1, dim_vector])(output)
    return layers.Lambda(squash)(outputs)
```

Squash function

Squash function behaves like a sigmoid function to squash a vector such that its length falls between 0 and 1.

$$v_j = \frac{\|s_j\|^2}{1 + \|s_i\|^2} \frac{s_j}{\|s_i\|}$$

```
def squash(vectors, axis=-1):
    """

The non-linear activation used in Capsule. It drives the length of a
    :param vectors: some vectors to be squashed, N-dim tensor
    :param axis: the axis to squash
```

```
:return: a Tensor with same shape as input vectors
"""

s_squared_norm = K.sum(K.square(vectors), axis, keepdims=True)
scale = s_squared_norm / (1 + s_squared_norm) / K.sqrt(s_squared_nor
return scale * vectors
```

DigiCaps with dynamic routing

DigiCaps converts the capsules in PrimaryCapsules to 10 capsules each making a prediction for class j. The following is the code in creating 10 (n_class) 16-D (dim_vector) capsules:

DigiCap is just a simple extension of a dense layer. Instead of taking a scalar and output a scalar, it takes a vector and output a vector:

- input shape = (None, input_num_capsule (32), input_dim_vector(8))
- output shape = (None, num_capsule (10), dim_vector(16))

Here is the DigiCaps and we will detail some part of the code for explanation later.

```
super(DigiCap, self). init (**kwargs)
    self.num capsule = num_capsule # 10
    self.dim vector = dim vector
                                     # 16
    self.num routing = num routing
                                     # 3
    self.kernel initializer = initializers.get(kernel_initializer)
    self.b initializer = initializers.get(b initializer)
def build(self, input shape):
    "The input Tensor should have shape=[None, input num capsule, in
    assert len(input shape) >= 3,
    self.input num capsule = input shape[1]
    self.input dim vector = input shape[2]
    # Transform matrix W
    self.W = self.add_weight(shape=[self.input_num_capsule, self.num
                             self.input dim vector, self.dim vector
                             initializer=self.kernel initializer,
                             name='W')
    # Coupling coefficient.
    # The redundant dimensions are just to facilitate subsequent mat
    self.b = self.add weight(shape=[1, self.input num capsule, self.
                                initializer=self.b initializer,
                                name='b',
                                trainable=False)
    self.built = True
def call(self, inputs, training=None):
    # inputs.shape = (None, input num capsule, input dim vector)
    # Expand dims to (None, input num capsule, 1, 1, input dim vecto
    inputs expand = K.expand dims(K.expand dims(inputs, 2), 2)
    # Replicate num capsule dimension to prepare being multiplied by
    # Now shape = [None, input num capsule, num capsule, 1, input di
    inputs tiled = K.tile(inputs expand, [1, 1, self.num capsule, 1,
    # Compute `inputs * W` by scanning inputs tiled on dimension 0.
    # inputs hat.shape = [None, input num capsule, num capsule, 1, c
```

build declares the self.W parameters representing the transform matrix W and self.b representing the b_{ij} .

```
def build(self, input shape):
    "The input Tensor should have shape=[None, input num capsule, in
    assert len(input shape) >= 3,
    self.input num capsule = input shape[1]
    self.input_dim_vector = input_shape[2]
    # Transform matrix W
    self.W = self.add weight(shape=[self.input num capsule, self.num
                             self.input dim vector, self.dim vector
                             initializer=self.kernel initializer,
                             name='W')
    # Coupling coefficient.
    # The redundant dimensions are just to facilitate subsequent mat
    self.b = self.add weight(shape=[1, self.input num capsule, self.
                                initializer=self.b initializer,
                                name='b',
                                trainable=False)
    self.built = True
```

To compute:

$$u_{j|i} = W_{ij}u_i$$

The code first expand the dimension of u_i and then multiple it with w. Nevertheless, the simple dot product implementation of $W_{ij}u_i$ (commet out below) is replaced by tf.scan for better speed performance.

```
class DigiCap(layers.Layer):
    def call(self, inputs, training=None):
        # inputs.shape = (None, input num capsule, input dim vector)
        # Expand dims to (None, input num capsule, 1, 1, input dim vecto
        inputs expand = K.expand dims(K.expand dims(inputs, 2), 2)
        # Replicate num capsule dimension to prepare being multiplied by
        # Now shape = [None, input num capsule, num capsule, 1, input di
        inputs tiled = K.tile(inputs expand, [1, 1, self.num capsule, 1,
        0.00
        # Compute `inputs * W`
        # By expanding the first dim of W.
        # W has shape (batch size, input num capsule, num capsule, input
        w tiled = K.tile(K.expand dims(self.W, 0), [self.batch size, 1,
        # Transformed vectors,
        inputs hat.shape = (None, input num capsule, num capsule, 1, dim
        inputs_hat = K.batch_dot(inputs_tiled, w_tiled, [4, 3])
        0.00
        # However, we will implement the same code with a faster impleme
        # Compute `inputs * W` by scanning inputs tiled on dimension 0.
        # inputs hat.shape = [None, input num capsule, num capsule, 1, c
        inputs hat = tf.scan(lambda ac, x: K.batch dot(x, self.W, [3, 2]
                             elems=inputs tiled,
                             initializer=K.zeros([self.input num capsule
```

5:

Here is the code to implement the following Iterative dynamic Routing pseudo code.

Procedure 1 Routing algorithm. 1: procedure ROUTING($\hat{\boldsymbol{u}}_{j|i}, r, l$) 2: for all capsule i in layer l and capsule j in layer (l+1): $b_{ij} \leftarrow 0$. 3: for r iterations do 4: for all capsule i in layer l: $\mathbf{c}_i \leftarrow \mathtt{softmax}(\mathbf{b}_i)$

6: for all capsule j in layer (l + 1): v_j ← squash(s_j)
7: for all capsule i in layer l and capsule j in layer (l + 1): b_{ij} ← b_{ij} + û_{j|i}.v_j
return v_i

for all capsule j in layer (l+1): $\mathbf{s}_{i} \leftarrow \sum_{i} c_{ij} \hat{\mathbf{u}}_{i|i}$

```
class DigiCap(layers.Layer):
    ...
    def call(self, inputs, training=None):
        ...
        # Routing algorithm
        assert self.num_routing > 0, 'The num_routing should be > 0.'

for i in range(self.num_routing): # Default: loop 3 times
        c = tf.nn.softmax(self.b, dim=2) # dim=2 is the num_capsule

        # outputs.shape=[None, 1, num_capsule, 1, dim_vector]
        outputs = squash(K.sum(c * inputs_hat, 1, keepdims=True))

# last iteration needs not compute b which will not be passe
    if i != self.num_routing - 1:
            self.b += K.sum(inputs_hat * outputs, -1, keepdims=True)
    return K.reshape(outputs, [-1, self.num_capsule, self.dim_vector)
```

Image reconstruction

We use the true label to select v_j to reconstruct the image during training. Then we feed v_j through 3 fully connected layers to re-generate the original image.

Select v_i in training with Mask

```
class Mask(layers.Layer):
    Mask a Tensor with shape=[None, d1, d2] by the max value in axis=1.
    Output shape: [None, d2]
    . . . .
    def call(self, inputs, **kwargs):
        # use true label to select target capsule, shape=[batch size, nu
        if type(inputs) is list: # true label is provided with shape =
            assert len(inputs) == 2
            inputs, mask = inputs
        else: # if no true label, mask by the max length of vectors of
            x = inputs
            # Enlarge the range of values in x to make max(new x)=1 and
            x = (x - K.max(x, 1, True)) / K.epsilon() + 1
            mask = K.clip(x, 0, 1) # the max value in x clipped to 1 and
        # masked inputs, shape = [batch size, dim vector]
        inputs masked = K.batch dot(inputs, mask, [1, 1])
        return inputs masked
```

Reconstruction loss

A reconstruction loss ||image - reconstructed image|| is added to the loss function. It trains the network to capture the critical properties into the capsule. However, the reconstruction loss is multiple by a regularization factor (0.0005) so it does not dominate over the marginal loss.

What capsule is learning?

Each capsule in DigiCaps is a 16-D vector. By slightly varying one dimension by holding other constant, we can learn what property for each dimension is capturing. Each row below is the reconstructed image (using the decoder) of changing only one dimension.

Scale and thickness	000000000000000000000000000000000000000
Localized part	066666666666
Stroke thickness	<i>555</i> 55555555
Localized skew	99999999444
Width and translation	111333333333
Localized part	2222222222

Sabour implementation

Sara Sabour released an implementation on Capsule at Github Sara Sabour. Since this is an ongoing research, do expect the implementation may be different from the paper.

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