Deep learning

9.3. Visualizing the processing in the input

François Fleuret
https://fleuret.org/dlc/
Occlusion sensitivity
Another approach to understanding the functioning of a network is to look at the behavior of the network “around” an image.

For instance, we can get a simple estimate of the importance of a part of the input image for a given output by computing the difference between:

1. the value of that output on the original image, and
2. the value of the same output with that part occluded.

This is computationally intensive since it requires as many forward passes as there are locations of the occlusion mask, ideally the number of pixels.
Notes

A small $32 \times 32$ square will be moved at every single location in the images. The first row shows the original images, while the second shows the perturbed images at a given location.
Notes

At every location in a given image,

- we occlude a $32 \times 32$ square by filling it with the mean pixel value,
- we compute the response of the classifier for the predicted class of the image (labrador for instance),
- we compute the difference between the score of the predicted class on the original, and the score of this same class when the image is occluded at that location.

At each location, we have a score showing how the response of the true class evolves, and we represent it as an heat map:

- red pixels when the score of the true class on the perturbed image is lower than on the original image,
- blue values when the true class is predicted with a greater confidence on the perturbed image.

We see that when hiding the head of the dog, the network is less confident in predicting class “labrador”. This shows that the head of the dog is a very important queue, because when it is hidden, the response goes down strongly.

For the elephant, it seems that its ears are the important cues.

For the penguin, surprisingly, the ice matters a lot and not the penguin itself.

For the car, the back and the front are the important parts.
Saliency maps
An alternative is to compute the gradient of an output with respect to the input (Erhan et al., 2009; Simonyan et al., 2013), e.g.

\[ \nabla_{|x} f_c(x; w) \]

where \( |x \) stresses that the gradient is computed with respect to the input \( x \) and not as usual with respect to the parameters \( w \).
This can be implemented by specifying that we need the gradient with respect to the input.

Using `torch.autograd.grad` to compute the gradient w.r.t. the input image instead of `torch.autograd.backward` has the advantage of not changing the model’s parameter gradients.

```python
input.requires_grad_()
output = model(input)
grad_input, = torch.autograd.grad(output[0, c], input)
```

Note that since `torch.autograd.grad` computes the gradient of a function with possibly multiple inputs, the returned result is a tuple.

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**Notes**

Remember that PyTorch models take as input a batch of samples. So the output of one classification network is of size $N \times C$, where $N$ is the number of samples in the batch to process, and $C$ the number of classes.

Here, we input a batch of one sample, so we access the prediction of the true class with `output[0, c]`.  

The resulting maps are quite noisy. For instance with AlexNet:

![Images of a dog, an elephant, a penguin, and a truck with their corresponding gradient maps.]

**Notes**

The images at the bottom were generated by computing the gradient of the most responsive unit w.r.t. the input image, and summing the gradient over the three input channels red, green, and blue to produce a gray-scale image.

We have the same behavior as with the occlusion sensitivity. For instance, pixels around the dog head have a high gradient: perturbing the pixels of the head will have more impact on the output class prediction than perturbing its body.

These results are more noisy because we are at the pixel level.
This is due to the local irregularity of the network’s response as a function of the input.

Figure 2. The partial derivative of $S_c$ with respect to the RGB values of a single pixel as a fraction of the maximum entry in the gradient vector, $\max_i \frac{\partial S_c}{\partial x_i}(t)$, (middle plot) as one slowly moves away from a baseline image $x$ (left plot) to a fixed location $x + \epsilon$ (right plot). $\epsilon$ is a random sample from $\mathcal{N}(0, 0.01^2)$. The final image $(x + \epsilon)$ is indistinguishable to a human from the origin image $x$.

(Smilkov et al., 2017)
Smilkov et al. (2017) proposed to smooth the gradient with respect to the input image by averaging over slightly perturbed versions of the latter.

\[
\hat{\nabla}_{|x} f_y(x; w) = \frac{1}{N} \sum_{n=1}^{N} \nabla_{|x} f_y(x + \epsilon_n; w)
\]

where \(\epsilon_1, \ldots, \epsilon_N\) are i.i.d of distribution \(\mathcal{N}(0, \sigma^2 I)\), and \(\sigma\) is a fraction of the gap \(\Delta\) between the maximum and the minimum of the pixel values.
A simple version of this “SmoothGrad” approach can be implemented as follows:

```python
std = std_fraction * (img.max() - img.min())
acc_grad = img.new_zeros(img.size())
for q in range(nb_smooth):  # This should be done with mini-batches ...
    noisy_input = img + img.new(img.size()).normal_(0, std)
    noisy_input.requires_grad_()
    output = model(noisy_input)
    grad_input, = torch.autograd.grad(output[0, c], noisy_input)
    acc_grad += grad_input

acc_grad = acc_grad.abs().sum(1)  # sum across channels
```

**Notes**

`std_fraction` is typically between 0.1 and 0.25.

Remember that `new_*` initialize tensors with the same type and same device as the input tensor. Here, `acc_grad` will be on the GPU if `img` already is, on the CPU otherwise.

At then end, `.sum(1)` sums across RGB channels, so we go from a tensor of size $1 \times 3 \times 224 \times 224$ to a tensor of size $1 \times 224 \times 224$, which can be represented as a gray-scale image. Here, the 1 is for a mini-batch of one sample.

This code could be made more efficient by processing the perturbed images in mini-batches.
Notes

The middle row is the original version by computing the derivative w.r.t. the original input only.

The bottom row is when averaging over a hundred perturbed images.

The smooth version exhibit more details such as the ears of the dog, the legs of the elephant, the head of the penguin the wheels of the car.

Overall, we get a sense of what the important parts of the image are, and which of them are carrying information for the prediction.
Deconvolution and guided back-propagation
Zeiler and Fergus (2014) proposed to invert the processing flow of a convolutional network by constructing a corresponding **deconvolutional network** to compute the “activating pattern” of a sample.

As they point out, the resulting processing is identical to a standard backward pass, except when going through the ReLU layers.
Remember that if $s$ is one of the input to a ReLU layer, and $x$ the corresponding output, we have for the forward pass

$$x = \max(0, s),$$

and for the backward

$$\frac{\partial \ell}{\partial s} = 1_{\{s > 0\}} \frac{\partial \ell}{\partial x}.$$
Zeiler and Fergus’s deconvolution can be seen as a backward pass where we propagate back through ReLU layers the quantity

\[
\max \left( 0, \frac{\partial \ell}{\partial x} \right) = 1\{ \frac{\partial \ell}{\partial x} > 0 \} \frac{\partial \ell}{\partial x},
\]

instead of the usual

\[
\frac{\partial \ell}{\partial s} = 1\{ s > 0 \} \frac{\partial \ell}{\partial x}.
\]

This quantity is positive for units whose output has a positive contribution to the response, kills the others, and is not modulated by the pre-layer activation \( s \).
Springenberg et al. (2014) improved upon the deconvolution with the **guided back-propagation**, which aims at the best of both worlds: Discarding structures which would not contribute positively to the final response, and discarding structures which are not already present.

It back-propagates through the ReLU layers the quantity

\[ 1_{\{s > 0\}} 1_{\{\frac{\partial r}{\partial x} > 0\}} \frac{\partial \ell}{\partial x} \]

which keeps only units which have a positive contribution and activation.
So these three visualization methods differ only in the quantities propagated through ReLU layers during the back-pass:

- back-propagation (Erhan et al., 2009; Simonyan et al., 2013):
  \[ 1_{\{s > 0\}} \frac{\partial \ell}{\partial x}, \]

- deconvolution (Zeiler and Fergus, 2014):
  \[ 1_{\{\frac{\partial \ell}{\partial x} > 0\}} \frac{\partial \ell}{\partial x}, \]

- guided back-propagation (Springenberg et al., 2014):
  \[ 1_{\{s > 0\}} 1_{\{\frac{\partial \ell}{\partial x} > 0\}} \frac{\partial \ell}{\partial x}, \]
These procedures can be implemented simply in PyTorch by changing the `nn.ReLU`'s backward pass.

The class `nn.Module` provides methods to register “hook” functions that are called during the forward or the backward pass, and can implement a different computation for the latter.
For instance

```python
>>> x = torch.tensor([ 1.23, -4.56 ])
>>> m = nn.ReLU()
>>> m(x)
tensor([ 1.2300, 0.0000])

>>> def my_hook(m, input, output):
...     print(str(m) + ' got ' + str(input[0].size()))
...
>>> handle = m.register_forward_hook(my_hook)
>>> m(x)
ReLU() got torch.Size([2])
tensor([ 1.2300, 0.0000])

>>> handle.remove()
>>> m(x)
tensor([ 1.2300, 0.0000])
```

Notes

The top example shows the default behavior of `nn.ReLU()` which simply set to zero negative coefficients of the input and returns the new tensor.

We define a hook `my_hook` which simply prints the name of the module and the size of the input. Then we attach the hook to the forward pass of our model `m`. Attaching the hook returns a handle useful for removing the hook later.

PyTorch provides:

- “forward pre-hooks” through `register_module_forward_pre_hook`. This hook is called before `forward` is invoked.
- “forward hooks” through `register_module_forward_hook`. This hook is called after `forward` has computed the output.
- “backward hooks” through `register_module_backward_hook`. This hook is called after the module has computed the gradient w.r.t. its input.
Using hooks, we can implement the deconvolution as follows:

```python
def relu_backward_deconv_hook(module, grad_input, grad_output):
    return F.relu(grad_output[0]),

def equip_model_deconv(model):
    for m in model.modules():
        if isinstance(m, nn.ReLU):
            m.register_backward_hook(relu_backward_deconv_hook)
```
def grad_view(model, image_name):
    to_tensor = transforms.ToTensor()
    img = to_tensor(PIL.Image.open(image_name))
    img = 0.5 + 0.5 * (img - img.mean()) / img.std()

    model.to(device)
    img = img.to(device)

    input = img.view(1, img.size(0), img.size(1), img.size(2)).requires_grad()
    output = model(input)
    result, = torch.autograd.grad(output.max(), input)

    result = result / result.max() + 0.5

    return result

model = models.vgg16(pretrained = True)
model.eval()
model = model.features
equip_model_deconv(model)
result = grad_view(model, 'blacklab.jpg')
utils.save_image(result, 'blacklab-vgg16-deconv.png')
The code is the same for the guided back-propagation, except the hooks themselves:

def relu_forward_gbackprop_hook(module, input, output):
    module.input_kept = input[0]

def relu_backward_gbackprop_hook(module, grad_input, grad_output):
    return F.relu(grad_output[0]) * F.relu(module.input_kept).sign(),

def equip_model_gbackprop(model):
    for m in model.modules():
        if isinstance(m, nn.ReLU):
            m.register_forward_hook(relu_forward_gbackprop_hook)
            m.register_backward_hook(relu_backward_gbackprop_hook)
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Experiments with an AlexNet-like network. Original images + deconvolution (or filters) for the top-9 activations for channels picked randomly.

(Zeiler and Fergus, 2014)
(Zeiler and Fergus, 2014)
Grad-CAM
Gradient-weighted Class Activation Mapping (Grad-CAM) proposed by Selvaraju et al. (2016) visualizes the importance of the input sub-parts according to the activations in a specific layer.

It computes a sum of the activations weighted by the average gradient of the output of interest w.r.t. individual channels.
Formally, let $k \in \{1, \ldots, C\}$ be a channel number, $A^k \in \mathbb{R}^{H \times W}$ the output feature map $k$ of the selected layer, $c$ a class number, and $y^c$ the network’s logit for that class.

The channel weights are

$$\alpha^c_k = \frac{1}{HW} \sum_{i=1}^{H} \sum_{j=1}^{W} \frac{\partial y^c}{\partial A^k_{i,j}}.$$ 

And the final localization map is

$$L^{c}_{\text{Grad-CAM}} = \text{ReLU} \left( \sum_{k=1}^{C} \alpha^c_k A^k \right).$$
We are going to test it with VGG19.

VGG(
    (features): Sequential(
        (0): Conv2d(3, 64, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
        (1): ReLU(inplace=True)
        /.../
        (34): Conv2d(512, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
        (35): ReLU(inplace=True)
        (36): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)
    )
    (avgpool): AdaptiveAvgPool2d(output_size=(7, 7))
    (classifier): Sequential(
        (0): Linear(in_features=25088, out_features=4096, bias=True)
        (1): ReLU(inplace=True)
        (2): Dropout(p=0.5, inplace=False)
        (3): Linear(in_features=4096, out_features=4096, bias=True)
        (4): ReLU(inplace=True)
        (5): Dropout(p=0.5, inplace=False)
        (6): Linear(in_features=4096, out_features=1000, bias=True)
    )
)
To implement Grad-CAM, first define hooks to store the feature maps in the forward pass, and the gradient w.r.t. them in the backward:

```python
def hook_store_A(module, input, output):
    module.A = output[0]

def hook_store_dydA(module, grad_input, grad_output):
    module.dydA = grad_output[0]
```

Then, load a pre-trained VGG19, and install the hooks in the last ReLU layer of the convolutional part:

```python
model = torchvision.models.vgg19(pretrained = True)
model.eval()

layer = model.features[35]  # Last ReLU of the conv layers

layer.register_forward_hook(hook_store_A)
layer.register_backward_hook(hook_store_dydA)
```
Load an image and make it a one sample batch:

```python
to_tensor = torchvision.transforms.ToTensor()
input = to_tensor(PIL.Image.open('example_images/elephant_hippo.png')).unsqueeze(0)
```

Compute the network’s output, the gradient, and $L_{\text{Grad-CAM}}$:

```python
output = model(input)
c = 386 # African elephant
output[0, c].backward()
alpha = layer.dydA.mean((2, 3), keepdim = True)
L = torch.relu((alpha * layer.A).sum(1, keepdim = True))

Save it as a resized colored heat-map:

```python
L = L / L.max()
L = F.interpolate(L, size = (input.size(2), input.size(3)),
    mode = 'bilinear', align_corners = False)

l = L.view(L.size(2), L.size(3)).detach().numpy()
PIL.Image.fromarray(numpy.uint8(cm.gist_earth(l) * 255)).save('result.png')
```

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**Notes**

`unsqueeze(0)` turns the input tensor of size $3 \times H \times W$ into a batch of a single tensor of size $1 \times 3 \times H \times W$.

`mean((2, 3), keepdim = True)` computes the mean over the height and width of the image. So we go from a tensor of size $1 \times 3 \times H \times W$ to a tensor of size $1 \times 3 \times 1 \times 1$. The last two “1” are preserved by `keepdim = True`.

`gist_earth` is a color map with orange color for high values, blue for low ones, and green for intermediate ones.
African elephant  Hippopotamus

Ox  Fountain
Coffee mug

Bagel

Bee

Daisy
References


