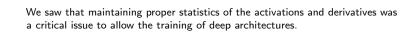
Deep learning

6.4. Batch normalization

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A different approach consists of explicitly forcing the activation statistics during the forward pass by re-normalizing them.

Batch normalization proposed by loffe and Szegedy (2015) was the first method introducing this idea.

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Batch normalization can be done anywhere in a deep architecture, and forces the activations' first and second order moments, so that the following layers do not need to adapt to their drift.

During training batch normalization shifts and rescales according to the mean and variance estimated on the batch.



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During test, it simply shifts and rescales according to the empirical moments estimated during training.

If $x_b \in \mathbb{R}^D$, $b = 1, \dots, B$ are the samples in the batch, we first compute the empirical per-component mean and variance **on the batch**

$$\hat{m}_{batch} = \frac{1}{B} \sum_{b=1}^{B} x_b$$

$$\hat{v}_{batch} = \frac{1}{B} \sum_{b=1}^{B} (x_b - \hat{m}_{batch})^2$$

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from which we compute normalized $z_b \in \mathbb{R}^D$, and outputs $y_b \in \mathbb{R}^D$

$$\forall b = 1, \dots, B, \ z_b = \frac{x_b - \hat{m}_{batch}}{\sqrt{\hat{v}_{batch} + \epsilon}}$$
$$y_b = \gamma \odot z_b + \beta.$$

where \odot is the Hadamard component-wise product, and $\gamma \in \mathbb{R}^D$ and $\beta \in \mathbb{R}^D$ are parameters to optimize.

During inference, batch normalization shifts and rescales independently each component of the input x according to statistics estimated during training:

$$y = \gamma \odot \frac{x - \hat{m}}{\sqrt{\hat{v} + \epsilon}} + \beta.$$

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As for dropout, the model behaves differently during train and test.

As dropout, batch normalization is implemented as separate modules that process input components independently.

```
>>> bn = nn.BatchNorm1d(3)
>>> with torch.no_grad():
... bn.bias.copy_(torch.tensor([2., 4., 8.]))
...
bn.weight.copy_(torch.tensor([1., 2., 3.]))
...
Parameter containing:
tensor([2., 4., 8.], requires_grad=True)
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tensor([2., 4., 8.], requires_grad=True)
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tensor([1., 2., 3.], requires_grad=True)
>>> x = torch.randn(1000, 3)
>>> x = x * torch.tensor([2., 5., 10.]) + torch.tensor([-10., 25., 3.])
>>> x.mean(0)
tensor([-9.9669, 25.0213, 2.4361])
>>> x.std(0)
tensor([1.9063, 5.0764, 9.7474])
>>> v = bn(x)
>>> y.mean(0)
tensor([2.0000, 4.0000, 8.0000], grad fn=<MeanBackward2>)
>>> y.std(0)
tensor([1.0005, 2.0010, 3.0015], grad_fn=<StdBackward1>)
```

As for any other module, we have to compute the derivatives of the loss ${\mathscr L}$ with respect to the inputs values and the parameters. For clarity, since components are processed independently, in what follows we

consider a single dimension and do not index it.

We have

$$\hat{m}_{batch} = \frac{1}{B} \sum_{b=1}^{B} x_b$$

$$\hat{v}_{batch} = \frac{1}{B} \sum_{b=1}^{B} (x_b - \hat{m}_{batch})^2$$

$$\forall b = 1, \dots, B, \ z_b = \frac{x_b - \hat{m}_{batch}}{\sqrt{\hat{v}_{batch} + \epsilon}}$$

$$y_b = \gamma z_b + \beta.$$

From which

$$\forall b = 1, \dots, B, \ \frac{\partial \mathcal{L}}{\partial z_b} = \gamma \frac{\partial \mathcal{L}}{\partial y_b}$$
$$\frac{\partial \mathcal{L}}{\partial \gamma} = \sum_b \frac{\partial \mathcal{L}}{\partial y_b} \frac{\partial y_b}{\partial \gamma} = \sum_b \frac{\partial \mathcal{L}}{\partial y_b} z_b$$
$$\frac{\partial \mathcal{L}}{\partial \beta} = \sum_b \frac{\partial \mathcal{L}}{\partial y_b} \frac{\partial y_b}{\partial \beta} = \sum_b \frac{\partial \mathcal{L}}{\partial y_b}.$$

Every sample in the batch impacts the moment estimates, hence all the outputs, which makes the derivative with respect to an input complicated.

$$\begin{split} \frac{\partial \mathcal{L}}{\partial \hat{v}_{batch}} &= -\frac{1}{2} \left(\hat{v}_{batch} + \epsilon \right)^{-3/2} \sum_{b=1}^{B} \frac{\partial \mathcal{L}}{\partial z_{b}} (x_{b} - \hat{m}_{batch}) \\ \frac{\partial \mathcal{L}}{\partial \hat{m}_{batch}} &= -\frac{1}{\sqrt{\hat{v}_{batch} + \epsilon}} \sum_{b=1}^{B} \frac{\partial \mathcal{L}}{\partial z_{b}} \end{split}$$

$$\forall b = 1, \dots, B, \ \frac{\partial \mathcal{L}}{\partial x_b} = \frac{\partial \mathcal{L}}{\partial z_b} \frac{1}{\sqrt{\hat{v}_{batch} + \epsilon}} + \frac{2}{B} \frac{\partial \mathcal{L}}{\partial \hat{v}_{batch}} \left(x_b - \hat{m}_{batch} \right) + \frac{1}{B} \frac{\partial \mathcal{L}}{\partial \hat{m}_{batch}}$$

In standard implementations, test \hat{m} and \hat{v} are estimated with a moving average during train, to avoid the need for an additional pass through the samples.

Results on ImageNet's LSVRC2012:

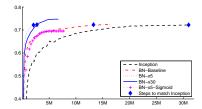


Figure 2: Single crop validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps.

| Model | Steps to 72.2% | Max accuracy |
|---------------|---------------------|--------------|
| Inception | $31.0 \cdot 10^{6}$ | 72.2% |
| BN-Baseline | $13.3 \cdot 10^{6}$ | 72.7% |
| BN-x5 | $2.1 \cdot 10^{6}$ | 73.0% |
| BN-x30 | $2.7 \cdot 10^{6}$ | 74.8% |
| BN-x5-Sigmoid | | 69.8% |

Figure 3: For Inception and the batch-normalized variants, the number of training steps required to reach the maximum accuracy of Inception (72.2%), and the maximum accuracy achieved by the network.

(loffe and Szegedy, 2015)

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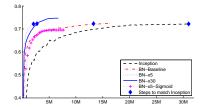


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The authors state that with batch normalization

- · samples have to be shuffled carefully,
- · the learning rate can be greater,
- dropout and local normalization are not necessary,
- L² regularization influence should be reduced.

Deep MLP on a 2d "disc" toy example, with naive Gaussian weight initialization, cross-entropy, standard SGD, $\eta=0.1$.

```
def create_model(with_batchnorm, dimh = 32, nb_layers = 16):
    modules = []

modules.append(nn.Linear(2, dimh))
    if with_batchnorm: modules.append(nn.BatchNorm1d(dimh))
    modules.append(nn.ReLU())

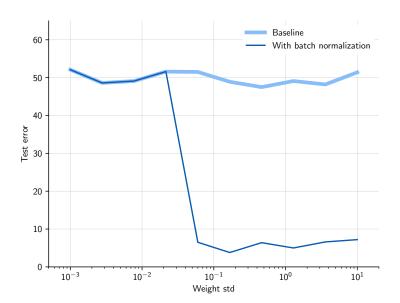
for d in range(nb_layers):
    modules.append(nn.Linear(dimh, dimh))
        if with_batchnorm: modules.append(nn.BatchNorm1d(dimh))
        modules.append(nn.ReLU())

modules.append(nn.ReLU())

return nn.Sequential(*modules)
```

We try different standard deviations for the weights

```
with torch.no_grad():
    for p in model.parameters(): p.normal_(0, std)
```



The position of batch normalization relative to the non-linearity is not clear.

"We add the BN transform immediately before the nonlinearity, by normalizing x = Wu + b. We could have also normalized the layer inputs u, but since u is likely the output of another nonlinearity, the shape of its distribution is likely to change during training, and constraining its first and second moments would not eliminate the covariate shift. In contrast, Wu + b is more likely to have a symmetric, non-sparse distribution, that is 'more Gaussian' (Hyvärinen and Oja, 2000); normalizing it is likely to produce activations with a stable distribution."

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However, this argument goes both ways: activations after the non-linearity are less "naturally normalized" and benefit more from batch normalization. Experiments are generally in favor of this solution, which is the current default.



As for dropout, using properly batch normalization on a convolutional map requires parameter-sharing.

The module torch.BatchNorm2d (respectively torch.BatchNorm3d) processes samples as multi-channels 2d maps (respectively multi-channels 3d maps) and normalizes each channel separately, with a γ and a β for each.

Another normalization in the same spirit is the **layer normalization** proposed by Ba et al. (2016).

Given a single sample $x \in \mathbb{R}^D$, it normalizes the components of x, hence normalizing activations across the layer instead of doing it across the batch

$$\mu = \frac{1}{D} \sum_{d=1}^{D} x_d$$

$$\sigma = \sqrt{\frac{1}{D} \sum_{d=1}^{D} (x_d - \mu)^2}$$

$$\forall d, \ y_d = \frac{x_d - \mu}{\sigma}$$

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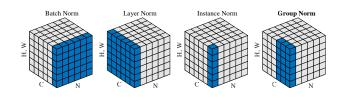
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Although it gives slightly worst improvements than BN it has the advantage of behaving similarly in train and test, and processing samples individually.

These normalization schemes are examples of a larger class of methods.



(Wu and He, 2018)



References

- J. L. Ba, J. R. Kiros, and G. E. Hinton. Layer normalization. CoRR, abs/1607.06450, 2016.
- A. Hyvärinen and E. Oja. Independent component analysis: Algorithms and applications.
- Neural Networks, 13(4-5):411-430, 2000.

 S. loffe and C. Szegedy. Batch normalization: Accelerating deep network training by reducing internal covariate shift. In International Conference on Machine Learning (ICML), 2015.
- Y. Wu and K. He. Group normalization. \underline{CoRR} , abs/1803.08494, 2018.