

Applied Deep Learning

Chapter 3: Advancing Our Toolbox

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Standardization

If you implement **forward and backward pass** of an **FNN** for **MNIST classification from scratch**: giving **image pixels** to NN can return **huge features!**

Feature

Outputs of **hidden layers**, i.e., \mathbf{y}_ℓ

This is a **typical observation in practice**; however, it does **not make trouble only in forward pass**: it **can also impact** severely the **training**, i.e., **backward pass**

The solution to this issue is to **standardize** the **inputs** and **features**

Standardization means making variables **look the same** in **all directions**

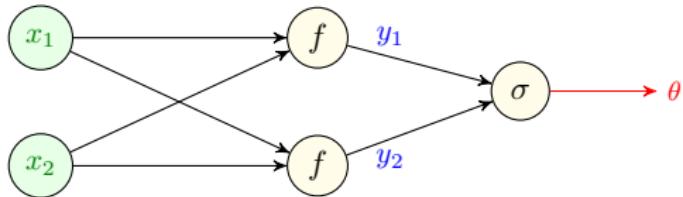
This is done by two particular techniques **in practice**

- **input standardization**
- **batch normalization**

Let's understand them through **an easy example**

Standardization: Example

Consider the following simple NN: here we have a **two-dimensional input**, one hidden layer with a **two-dimensional feature** and a **single output**



The inputs could be anything, for instance

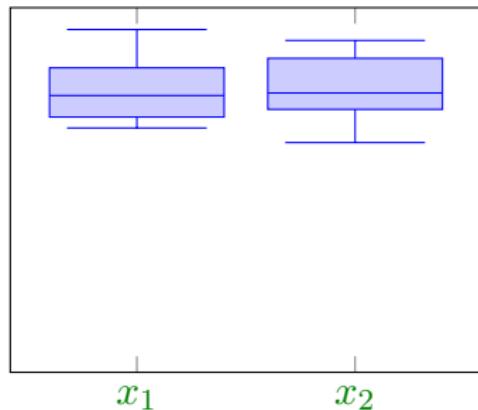
- **Example A:** both are heights in centimeters
 - ↳ they are in the same range
 - ↳ distributions of variables have close means and variances
- **Example B:** x_1 is height centimeters and x_2 is number of children
 - ↳ they are in the widely-different range
 - ↳ distributions of variables have strongly-different means and variances

Standardization: Example

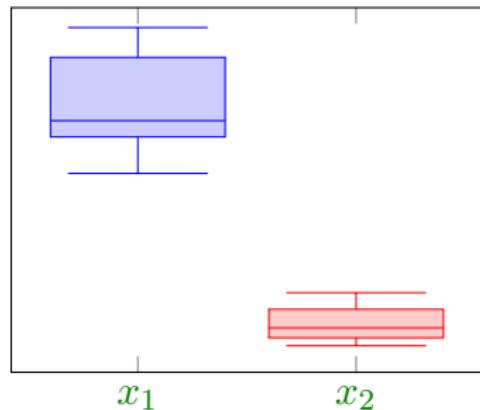
We expect **different** behavior in **forward pass**:

- in **Example A** all variables are in the **same scale**
- in **Example B** each variable is in **different scale**

Example A



Example B



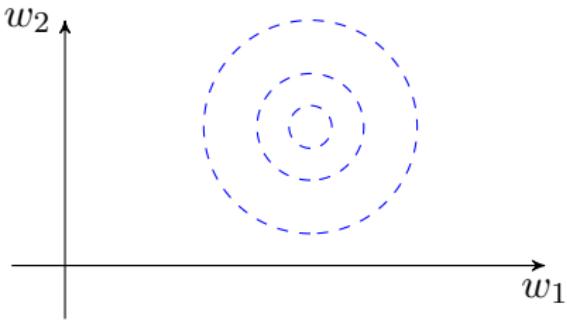
Standardization: Example

It also leads to **different** behavior in **backward pass**:

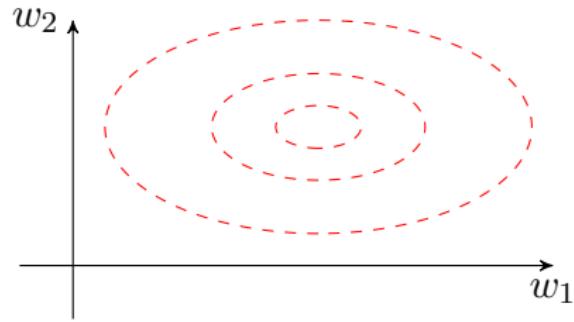
- in **Example A** empirical risk's curvature is similar in all directions
- in **Example B** empirical risk's curvature **varies** from one direction to another

For instance, if we assume NN has only two weights to train, **the counters of empirical loss** can look as below

Example A

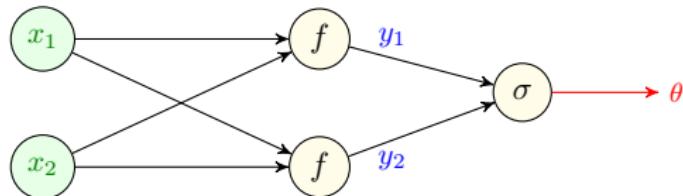


Example B

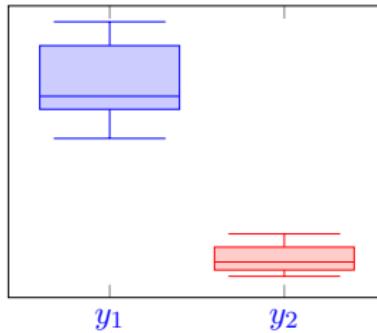


Standardization: Different Layers

Such behavior is **not specific** to the **input layer**: we could also see **the same behavior** at hidden layers



For instance in our **example**, even with **properly-scaled inputs**, **features** may evolve **differently** through **training**: after **multiple iterations** we end up with



Standardization via Normalization

The solution for *any layer* is to *shift* and *scale* every sample *input* such that it becomes *zero-mean* and *unit-variance*

Then, we work with the *standardized input*

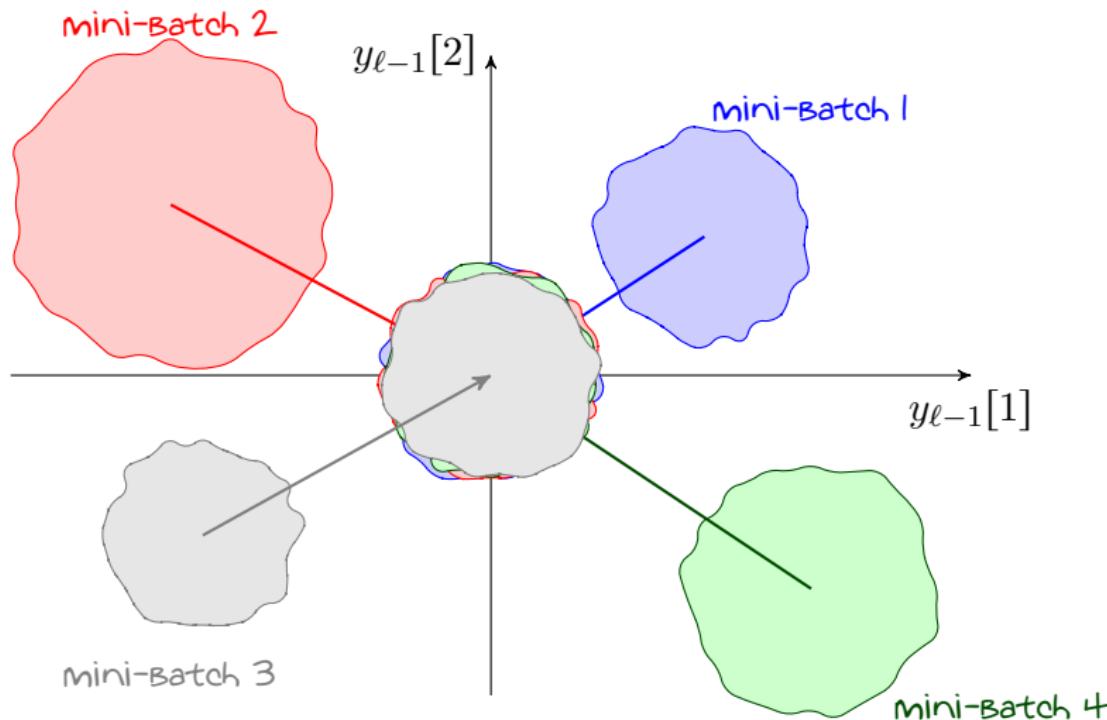
Say we are at layer ℓ : a sample input is $\mathbf{y}_{\ell-1,b}$, so we compute

$$\bar{\mathbf{y}}_{\ell-1,b} = \frac{\mathbf{y}_{\ell-1,b} - \mathbb{E}\{\mathbf{y}_{\ell-1}\}}{\sqrt{\text{Var}\{\mathbf{y}_{\ell-1}\}}}$$

and then perform all further operations on $\bar{\mathbf{y}}_{\ell-1,b}$

Visualizing Normalization

We can visualize *normalization* as below for two-dimensional inputs



Standardization via Normalization

$$\bar{\mathbf{y}}_{\ell-1,b} = \frac{\mathbf{y}_{\ell-1,b} - \mathbb{E}\{\mathbf{y}_{\ell-1}\}}{\sqrt{\text{Var}\{\mathbf{y}_{\ell-1}\}}}$$

- + How do we compute mean and variance? We don't know data distribution!
- Well, as always: we can approximate them from the dataset

Say our dataset has B data-points: we approximate mean and variance as

$$\mathbb{E}\{\mathbf{y}_{\ell-1}\} \approx \frac{1}{B} \sum_{b=1}^B \mathbf{y}_{\ell-1,b} \equiv \boldsymbol{\mu}_{\ell-1}$$

$$\text{Var}\{\mathbf{y}_{\ell-1}\} \approx \frac{1}{B} \sum_{b=1}^B (\mathbf{y}_{\ell-1,b} - \boldsymbol{\mu}_{\ell-1})^2 \equiv \sigma_{\ell-1}^2$$

Let's check this idea for each layer!

Normalization: Input Layer

With input layer, i.e., $\ell = 1$, this **approximation** works well: we *apply normalization just once* and **work with normalized data** from then on, i.e.,

$$\bar{\mathbf{x}}_b = \frac{\mathbf{x}_b - \mu_0}{\sigma_0}$$

for μ_0 and σ_0 that are computed from the **dataset** as

$$\mu_0 = \frac{1}{B} \sum_{b=1}^B \mathbf{x}_b \quad \sigma_0 = \sqrt{\frac{1}{B} \sum_{b=1}^B (\mathbf{x}_b - \mu_0)^2}$$

Let's define the operator $\mathcal{U}(\cdot)$ as the **standardizer**, i.e.,

$$\bar{\mathbf{x}}_b = \mathcal{U}(\mathbf{x}_b | \mathbb{D})$$

where \mathbb{D} is the training dataset

Forward Propagation with Input Normalization

`ForwardProp()`:

```
1: Initiate with  $\mathbf{y}_0 = \mathcal{U}(\mathbf{x}_b | \mathbb{D})$ 
2: for  $\ell = 0, \dots, L$  do
3:   Add  $\mathbf{y}_\ell[0] = 1$  and determine  $\mathbf{z}_{\ell+1} = \mathbf{W}_{\ell+1}\mathbf{y}_\ell$           # forward affine
4:   Determine  $\mathbf{y}_{\ell+1} = f_{\ell+1}(\mathbf{z}_{\ell+1})$                       # forward activation
5: end for
6: for  $\ell = 1, \dots, L + 1$  do
7:   Return  $\mathbf{y}_\ell$  and  $\mathbf{z}_\ell$ 
8: end for
```

- + Shall we do the same for every layer?
- Well, we could try, but we end up with computation complexity close to full-batch training!

Normalization: Hidden Layers

At hidden layers, i.e., $\ell > 1$, the input depends on the weights and biases of previous layer: for instance, after normalizing input we compute

$$\mathbf{z}_1 = \mathbf{W}_1 \bar{\mathbf{x}} \rightsquigarrow \mathbf{y}_1 = f_1(\mathbf{z}_1)$$

if we approximate mean and variance with same approach, we should compute

$$\boldsymbol{\mu}_1 = \frac{1}{B} \sum_{b=1}^B \mathbf{y}_{1,b} \quad \sigma_1 = \sqrt{\frac{1}{B} \sum_{b=1}^B (\mathbf{y}_{1,b} - \boldsymbol{\mu}_1)^2}$$

These parameters depend on \mathbf{W}_1 ! This means after each update of weights at the end of each mini-batch, we should repeat this for the entire training dataset!

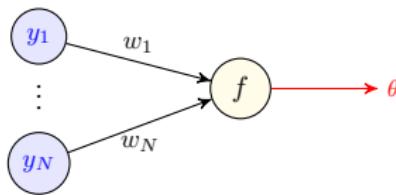
This is not the only issue: since the normalization of these layers depends on weights, the gradient of loss with respect to weights also changes

Batch Normalization: Training with Normalization

Batch normalization extends the training loop of **mini-batch SGD** to incorporate also **normalization** of **hidden layers**: the idea is simple

- approximate mean and variance using the **mini-batch**
- compute derivatives by taking **normalization** into account

Let's focus first on a **single neuron** in a **hidden layer**



Say the output neuron has no bias, i.e., θ is given by

$$z = \sum_{n=1}^N w_n y_n = \mathbf{w}^\top \mathbf{y} \quad \rightsquigarrow \quad \theta = f(z)$$

Also assume we train via **mini-batches** with **batch size** Ω

Recap: Basic Forward and Backward Pass

Without batch normalization, we pass forward \mathbf{y}_ω for every $\omega = 1, \dots, \Omega$

- by first computing the affine transform

$$\mathbf{z}_\omega = \mathbf{w}^\top \mathbf{y}_\omega$$

- then activating as $\theta_\omega = f(\mathbf{z}_\omega)$

Once we get to the **output**: we backpropagate by

- first computing derivative with respect to \mathbf{z}_ω , i.e.,

$$\frac{d}{d\mathbf{z}_\omega} \mathcal{L} = \left(\frac{d}{d\theta_\omega} \mathcal{L} \right) \dot{f}(\mathbf{z}_\omega)$$

- and then tracking back to \mathbf{y}_ω , i.e.,

$$\nabla_{\mathbf{y}_\omega} \mathcal{L} = \mathbf{w} \left(\frac{d}{d\mathbf{z}_\omega} \mathcal{L} \right)$$

Batch Normalization: Forward Pass

With batch normalization *in forward pass*, we wait till the whole mini-batch is over: **wait** till we have \mathbf{y}_ω for $\omega = 1, \dots, \Omega$. We then

- approximate mean and variance as

$$\boldsymbol{\mu} = \frac{1}{\Omega} \sum_{\omega=1}^{\Omega} \mathbf{y}_\omega \quad \sigma = \sqrt{\frac{1}{\Omega} \sum_{\omega=1}^{\Omega} (\mathbf{y}_\omega - \boldsymbol{\mu})^2}$$

- normalize \mathbf{y}_ω for $\omega = 1, \dots, \Omega$ as

$$\mathbf{u}_\omega = \frac{\mathbf{y}_\omega - \boldsymbol{\mu}}{\sigma}$$

→ *scale and shift* to a *common place*

$$\bar{\mathbf{y}}_\omega = \gamma \odot \mathbf{u}_\omega + \beta$$

- compute the affine transforms $\mathbf{z}_\omega = \mathbf{w}^\top \bar{\mathbf{y}}_\omega$ and activate as $\theta_\omega = f(\mathbf{z}_\omega)$

Batch Normalization: Learnable Shift and Scale

- + Why do we **scale** and **shift** after normalization?
- This is not guaranteed that center with unit variance is the best place:
we can learn the best place through training!

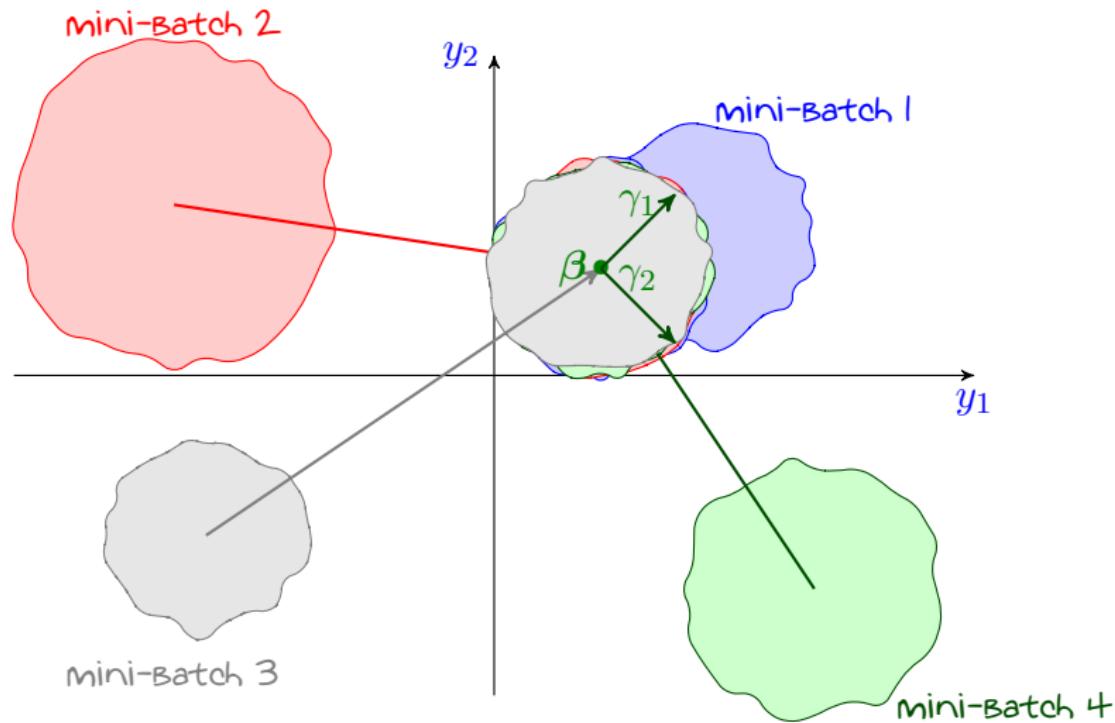
Depending on **activation**, it might be better to **center** all features at **another place** with some **different variances**

- It seems hard to **engineer this point and the variance**
- We hence introduce a **general point** $\beta, \gamma \in \mathbb{R}^N$
 - ↳ We treat these vectors as **learnable parameters**
 - ↳ We **update them** in addition to weight matrices \mathbf{W}_ℓ in **backward pass**

We denote this operation by

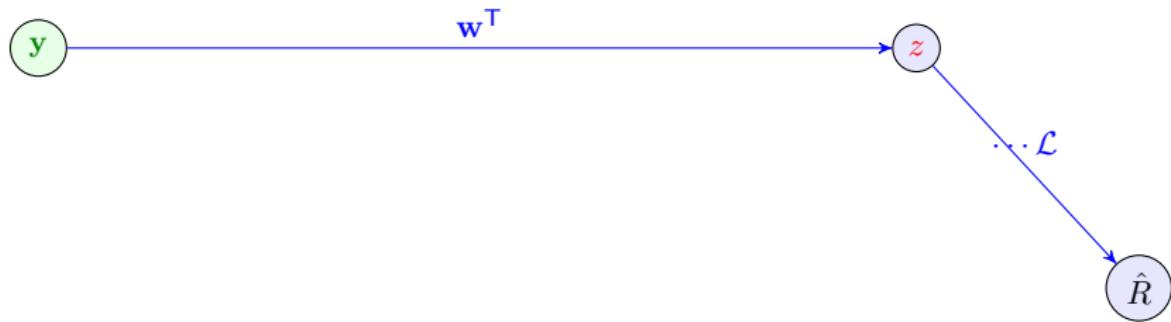
$$\mathcal{B}_N(\mathbf{u} | \gamma, \beta) = \gamma \odot \mathbf{u} + \beta$$

Batch Normalization: Learnable Shift and Scale



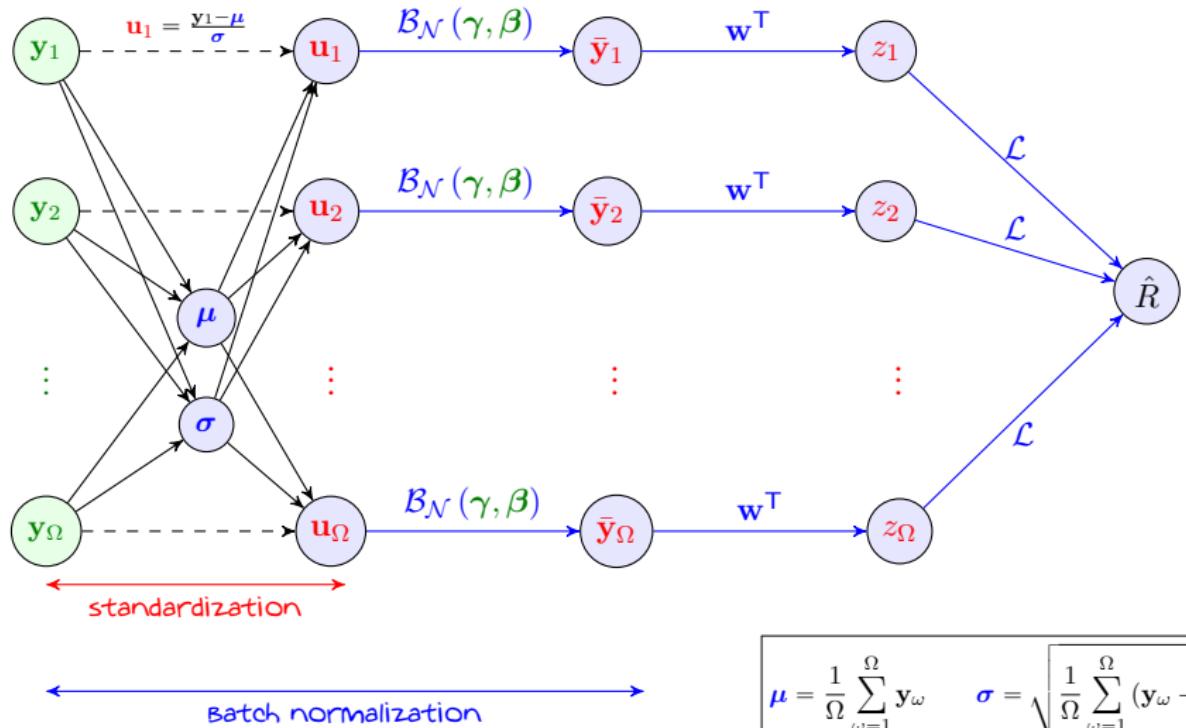
Batch Normalization: Computation Graph

In good old days **without batch-normalization**, we had



But, it gets more complicated now!

Batch Normalization: Computation Graph



Batch Normalization: Backpropagation

Now assume that *forward pass is over for the complete mini-batch*
we could easily get back to normalized variables, i.e., $\bar{\mathbf{y}}_\omega$

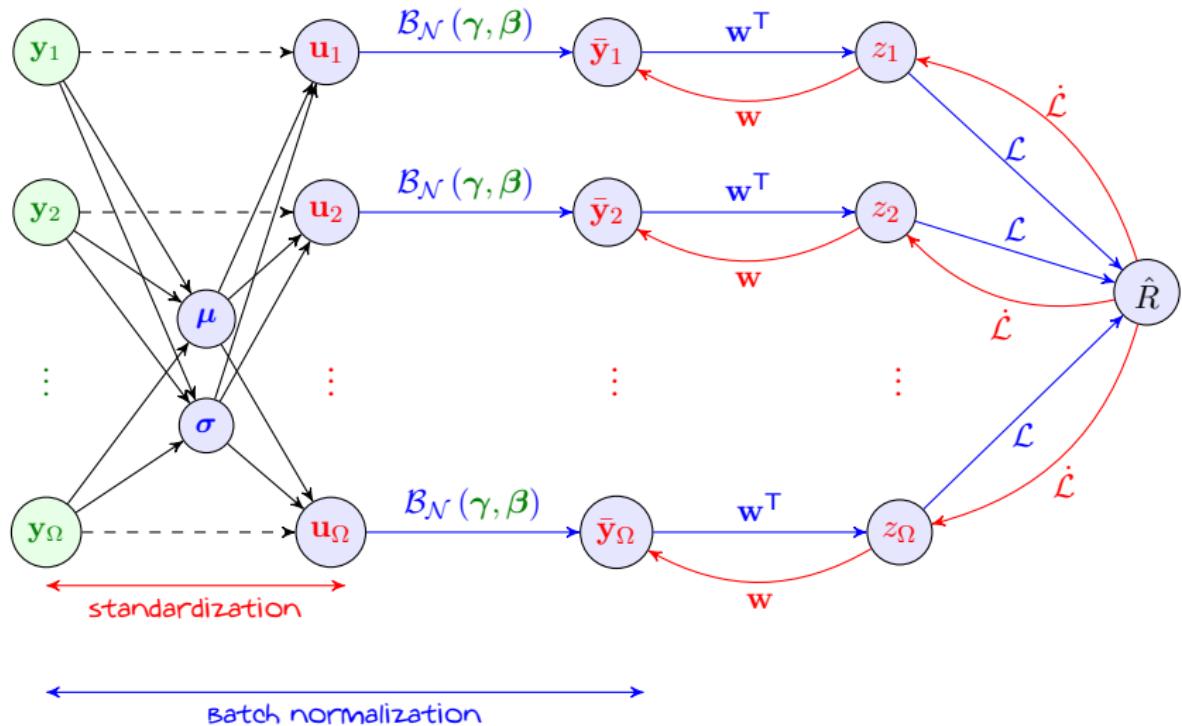
First, we note that our *empirical risk* reads

$$\hat{R} = \frac{1}{\Omega} \sum_{\omega=1}^{\Omega} \underbrace{\mathcal{L}(\theta_\omega, v_\omega)}_{\hat{R}_\omega} = \frac{1}{\Omega} \sum_{\omega=1}^{\Omega} \hat{R}_\omega$$

- We compute $\nabla_{z_\omega} \hat{R}_\omega$ using $\dot{\mathcal{L}}(\cdot)$ and $\dot{f}(\cdot)$
- We compute $\nabla_{\bar{\mathbf{y}}_\omega} \hat{R}_\omega$ from $\nabla_{z_\omega} \hat{R}_\omega$
 - ↳ We just need to apply standard backward pass of linear transforms

$$\nabla_{\bar{\mathbf{y}}_\omega} \hat{R}_\omega = \left(\nabla_{z_\omega} \hat{R}_\omega \right) \mathbf{w} = \left(\frac{d}{dz_\omega} \hat{R}_\omega \right) \mathbf{w}$$

Batch Normalization: Backpropagation



Batch Normalization: Backpropagation

By now, we have $\nabla_{\bar{y}_\omega} \hat{R}_\omega$ for $\omega = 1, \dots, \Omega$; next, we move **backward** from *scaled* and *shifted* variables to standard ones

$\mathcal{B}_N(\gamma, \beta)$ scales and shifts **entry-wise**

$$\begin{bmatrix} \bar{y}_{1,\omega} \\ \vdots \\ \bar{y}_{N,\omega} \end{bmatrix} = \begin{bmatrix} \gamma_1 u_{1,\omega} + \beta_1 \\ \vdots \\ \gamma_N u_{N,\omega} + \beta_N \end{bmatrix}$$

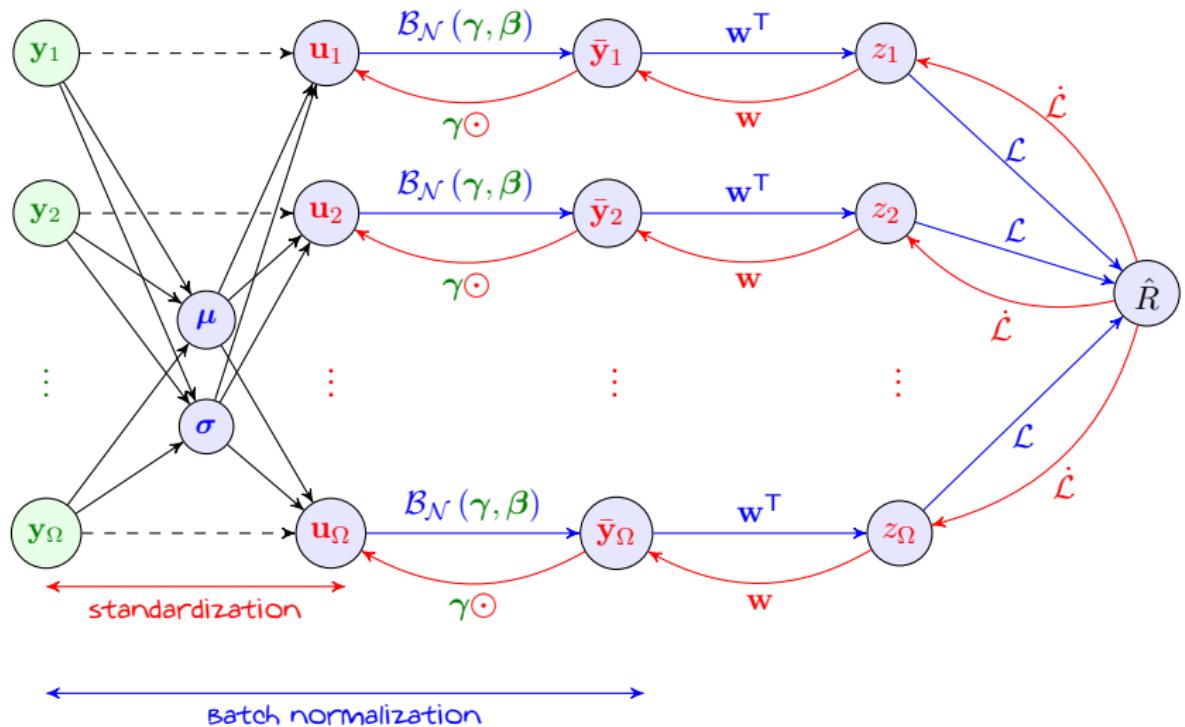
So, we can say

$$\frac{\partial}{\partial u_{i,\omega}} \hat{R}_\omega = \gamma_i \frac{\partial}{\partial \bar{y}_{i,\omega}} \hat{R}_\omega$$

The **backward pass** is hence for $\omega = 1, \dots, \Omega$ is

$$\nabla_{\mathbf{u}_\omega} \hat{R}_\omega = \gamma \odot \nabla_{\bar{\mathbf{y}}_\omega} \hat{R}_\omega$$

Batch Normalization: Backpropagation



Batch Normalization: Backpropagation

At this point, we can also compute the *gradients* with respect to γ and β

For $\omega = 1, \dots, \Omega$, we have

$$\begin{aligned}\nabla_{\gamma} \hat{R}_{\omega} &= \mathbf{u}_{\omega} \odot \nabla_{\bar{\mathbf{y}}_{\omega}} \hat{R}_{\omega} \\ \nabla_{\beta} \hat{R}_{\omega} &= \nabla_{\bar{\mathbf{y}}_{\omega}} \hat{R}_{\omega}\end{aligned}$$

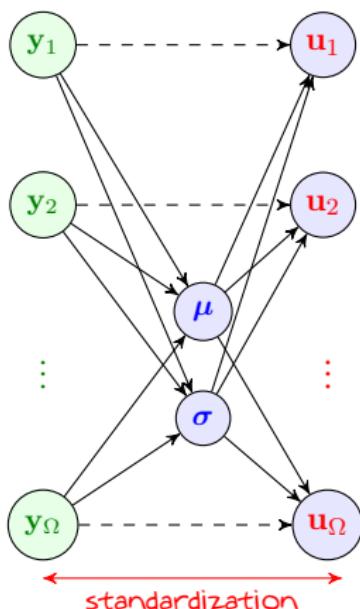
In our **optimizer**, we then update γ and β using $\nabla_{\gamma} \hat{R}_{\omega}$ and $\nabla_{\beta} \hat{R}_{\omega}$: for instance with **standard SGD** we have

$$\gamma^{(t+1)} = \gamma^{(t)} - \frac{\eta}{\Omega} \sum_{\omega=1}^{\Omega} \nabla_{\gamma} \hat{R}_{\omega}$$

$$\beta^{(t+1)} = \beta^{(t)} - \frac{\eta}{\Omega} \sum_{\omega=1}^{\Omega} \nabla_{\beta} \hat{R}_{\omega}$$

Batch Normalization: Backpropagation

The most challenging block is **standardization**: we open expand everything



Let's write again forward pass

$$\mathbf{u}_\omega = \frac{\mathbf{y}_\omega - \mu(\mathbf{y}_1, \dots, \mathbf{y}_\Omega)}{\sigma(\mathbf{y}_1, \dots, \mathbf{y}_\Omega)}$$

Here, \hat{R}_ω depends on all branches, i.e.,

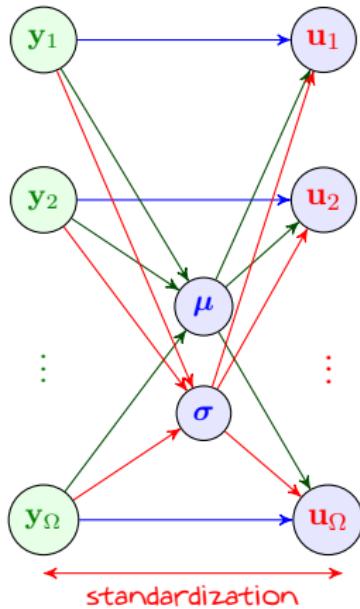
$$\hat{R}_\omega(\mathbf{y}_1, \dots, \mathbf{y}_\Omega)$$

We know how to use chain rule

$$\begin{aligned} \nabla_{\mathbf{y}_\tau} \hat{R}_\omega &= \sum_{\lambda=1}^{\Omega} \nabla_{\mathbf{u}_\lambda} \hat{R}_\omega \circ \nabla_{\mathbf{y}_\tau} \mathbf{u}_\lambda \\ &= \nabla_{\mathbf{u}_\omega} \hat{R}_\omega \circ \nabla_{\mathbf{y}_\tau} \mathbf{u}_\omega \end{aligned}$$

Batch Normalization: Backpropagation

All operations are entry-wise, i.e.,



$$u_{i,\omega} = \frac{y_{i,\omega} - \mu_i(y_{i,1}, \dots, y_{i,\Omega})}{\sigma_i(y_{i,1}, \dots, y_{i,\Omega})}$$

So, it's safe to think of u_ω and y_τ as scalars

$$\frac{\partial \hat{R}_\omega}{\partial y_{i,\tau}} = \frac{\partial \hat{R}_\omega}{\partial u_{i,\omega}} \frac{\partial u_{i,\omega}}{\partial y_{i,\tau}}$$

If we set $\tau = \omega$; then, we have

$$\begin{aligned} \frac{\partial u_{i,\omega}}{\partial y_{i,\omega}} &= \frac{1}{\sigma_i} + \frac{\partial u_{i,\omega}}{\partial \mu_i} \frac{\partial \mu_i}{\partial y_{i,\omega}} + \frac{\partial u_{i,\omega}}{\partial \sigma_i} \frac{\partial \sigma_i}{\partial y_{i,\omega}} \\ &= \frac{1}{\sigma_i} - \frac{1}{\sigma_i} \frac{\partial \mu_i}{\partial y_{i,\omega}} - \frac{y_{i,\omega} - \mu_i}{\sigma_i^2} \frac{\partial \sigma_i}{\partial y_{i,\omega}} \end{aligned}$$

Batch Normalization: Backpropagation

Now, let us determine partial derivatives

$$\mu_i = \frac{1}{\Omega} \sum_{\omega=1}^{\Omega} y_{i,\omega}$$

$$\sigma_i = \sqrt{\frac{1}{\Omega} \sum_{\omega=1}^{\Omega} (y_{i,\omega} - \mu_i)^2}$$

So, we can write

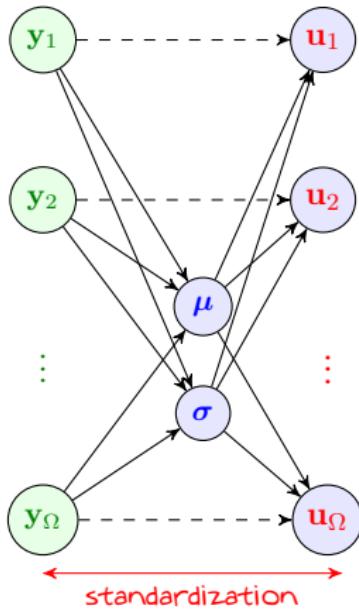
$$\frac{\partial \mu_i}{\partial y_{i,\omega}} = \frac{1}{\Omega}$$

Here, we should do it in two steps

$$\begin{aligned}\frac{\partial \sigma_i}{\partial y_{i,\omega}} &= \frac{1}{2\sigma_i} \left(\frac{2}{\Omega} (y_{i,\omega} - \mu_i) \right) + \frac{\partial \sigma_i}{\partial \mu_i} \frac{\partial \mu_i}{\partial y_{i,\omega}} \\ &= \frac{1}{\Omega \sigma_i} (y_{i,\omega} - \mu_i) + \underbrace{\frac{\partial \sigma_i}{\partial \mu_i}}_0 \frac{\partial \mu_i}{\partial y_{i,\omega}} \\ &= \frac{1}{\Omega \sigma_i} (y_{i,\omega} - \mu_i)\end{aligned}$$

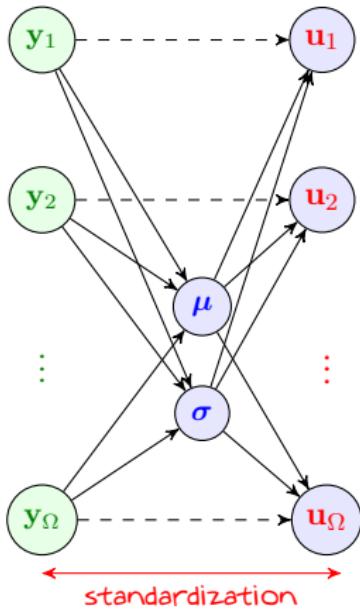
Batch Normalization: Backpropagation

Let's replace for the case $\tau = \omega$



$$\begin{aligned}\frac{\partial u_{i,\tau}}{\partial y_{i,\omega}} &= \frac{1}{\sigma_i} + \frac{\partial u_{i,\omega}}{\partial \mu_i} \frac{\partial \mu_i}{\partial y_{i,\omega}} + \frac{\partial u_{i,\omega}}{\partial \sigma_i} \frac{\partial \sigma_i}{\partial y_{i,\omega}} \\ &= \frac{1}{\sigma_i} - \frac{1}{\sigma_i} \frac{\partial \mu_i}{\partial y_{i,\omega}} - \frac{y_{i,\omega} - \mu_i}{\sigma_i^2} \frac{\partial \sigma_i}{\partial y_{i,\omega}} \\ &= \frac{1}{\sigma_i} - \frac{1}{\Omega \sigma_i} - \frac{(y_{i,\omega} - \mu_i)^2}{\Omega \sigma_i^3}\end{aligned}$$

Batch Normalization: Backpropagation



$$u_{i,\omega} = \frac{y_{i,\omega} - \mu_i(y_{i,1}, \dots, y_{i,\Omega})}{\sigma_i(y_{i,1}, \dots, y_{i,\Omega})}$$

If we set $\tau \neq \omega$; then, we have

$$\begin{aligned}\frac{\partial u_{i,\omega}}{\partial y_{i,\tau}} &= 0 + \frac{\partial u_{i,\omega}}{\partial \mu_i} \frac{\partial \mu_i}{\partial y_{i,\tau}} + \frac{\partial u_{i,\omega}}{\partial \sigma_i} \frac{\partial \sigma_i}{\partial y_{i,\tau}} \\ &= -\frac{1}{\sigma_i} \frac{\partial \mu_i}{\partial y_{i,\tau}} - \frac{y_{i,\omega} - \mu_i}{\sigma_i^2} \frac{\partial \sigma_i}{\partial y_{i,\tau}} \\ &= -\frac{1}{\Omega \sigma_i} - \frac{(y_{i,\tau} - \mu_i)^2}{\Omega \sigma_i^3}\end{aligned}$$

Everything as before

↳ Just the *first term drops*

Batch Normalization: Backpropagation

The last piece of derivation is to relate these partial derivatives to gradient of empirical risk determined over the whole mini-batch

$$\nabla_{\mathbf{y}_\tau} \hat{R} = \nabla_{\mathbf{y}_\tau} \frac{1}{\Omega} \sum_{\omega=1}^{\Omega} \hat{R}_\omega = \frac{1}{\Omega} \sum_{\omega=1}^{\Omega} \nabla_{\mathbf{y}_\tau} \hat{R}_\omega$$

From above derivation we have

$$\nabla_{\mathbf{y}_\tau} \hat{R}_\omega = \frac{\mathbb{1}\{\tau = \omega\}}{\sigma} - \frac{1}{\Omega\sigma} - \frac{(\mathbf{y}_\tau - \mu)^2}{\Omega\sigma^3}$$

with all operations being entry-wise! We then derive $\nabla_{\mathbf{W}_\ell} \hat{R}$ exactly as in sample-wise backpropagation

Suggestion

Try to write the complete backpropagation with batch normalization

Batch Normalization: Testing

- + Say we trained our NN! Now how we test it for **single** new point? We do not have any mini-batch anymore!
- Good point! In practice, we use **moving average**

Throughout training, we compute moving averages $\bar{\mu}_\ell$ and $\bar{\sigma}_\ell$

At each layer ℓ , we start with some initial $\bar{\mu}_\ell$ and $\bar{\sigma}_\ell$ and compute

$$\bar{\mu}_\ell = \alpha \bar{\mu}_\ell + (1 - \alpha) \mu_\ell$$

$$\bar{\sigma}_\ell = \alpha \bar{\sigma}_\ell + (1 - \alpha) \sigma_\ell$$

after each iteration for some $0 < \alpha < 1$: typically close to 1

We use these values for **normalization** after we are over with training

Batch Normalization: Final Points

Few points that you may observe in **implementation** of **batch normalization**

- We usually **perturb variance** with a **small constant** for numerical stability

$$\sigma = \sqrt{\frac{1}{\Omega} \sum_{\omega=1}^{\Omega} (y_{\omega} - \mu)^2 + \epsilon}$$

- We could normalize **before** or **after** activation
 - ↳ Here, we did it **after** activation
 - ↳ In the **original proposal** is was **before** activation
 - ↳ In general, it is **not fully known** which one is better
 - ~~~ We may **try both** and see which one gives better result
- With batch-normalization, we should distinguish **training** from **evaluation**
 - ↳ We use `model.train()` for **training**
 - ~~~ Here, we **update** the moving averages
 - ↳ We use `model.eval()` for **evaluation**
 - ~~~ Here, we **only use** the moving averages