Quick Introduction of Batch Normalization

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Changing Landscape

w_2

Loss L

smooth

w_1

+Δy   small

$\hat{y}$ ⋯⟶ y ⟵ + ⟵ $w_1 + \Delta w_1$ ⟵ x_1 1, 2 ……   small

e

+Δe   small

b

w_2

$L = \sum e$

+ΔL   small

1

x_2

Changing Landscape

Loss L

w_2 w_1

steep   smooth

Loss L

w_2 w_1

+Δy large

$\hat{y} \longleftrightarrow y \longleftarrow$ w_1

e

+Δe large

$L = \sum e$

+ΔL large

b

1

w_2 +Δw_2

$+$

x_1

x_2

1, 2 ...... small

100, 200 ..... large

same range

3

Feature Normalization

x^1 x^2 x^3 $\quad\quad x^r$ $\quad\quad x^R$

x_1^1 $\quad x_1^2$

x_2^1 $\quad x_2^2$

...... $\quad$ ......
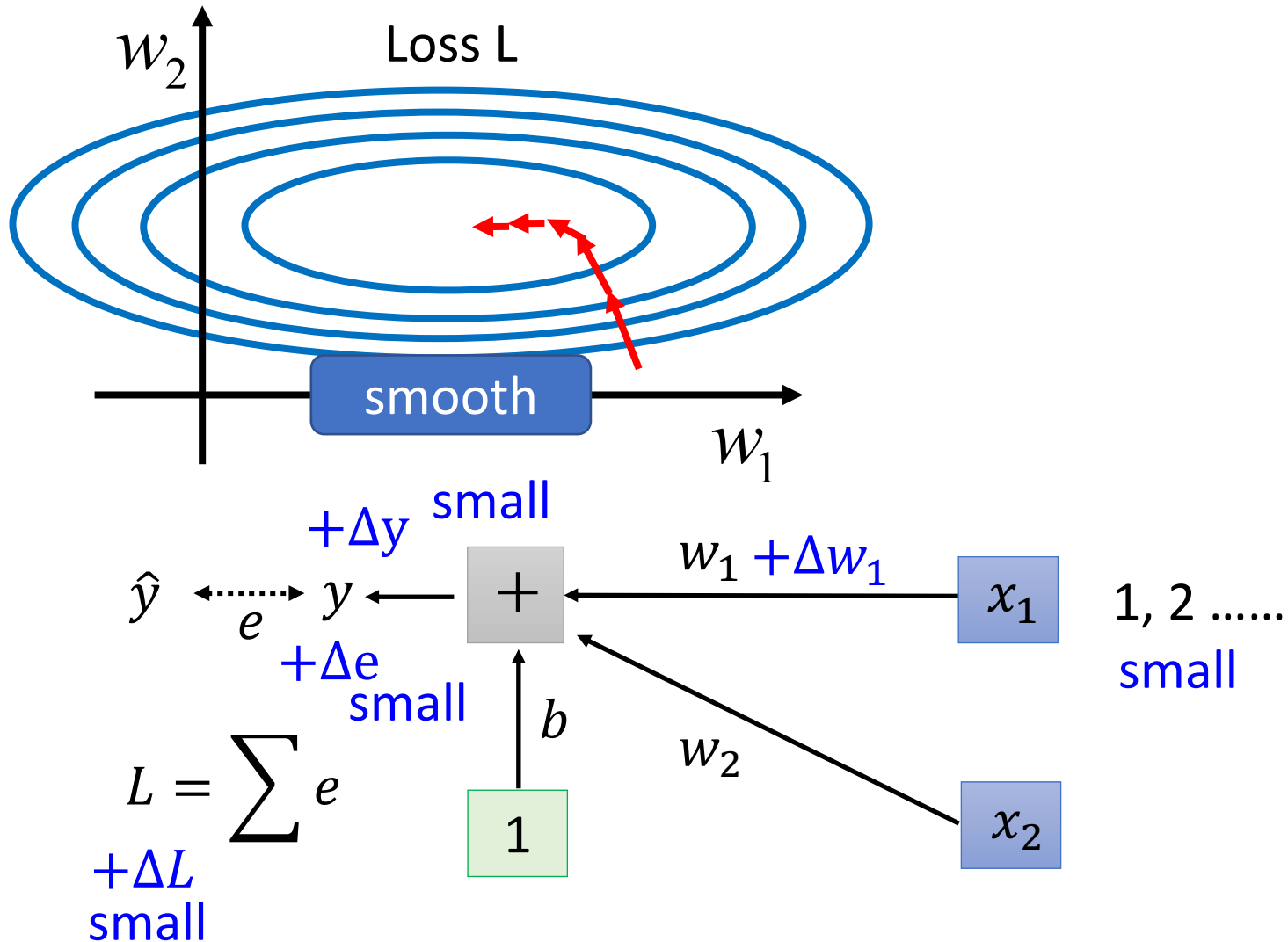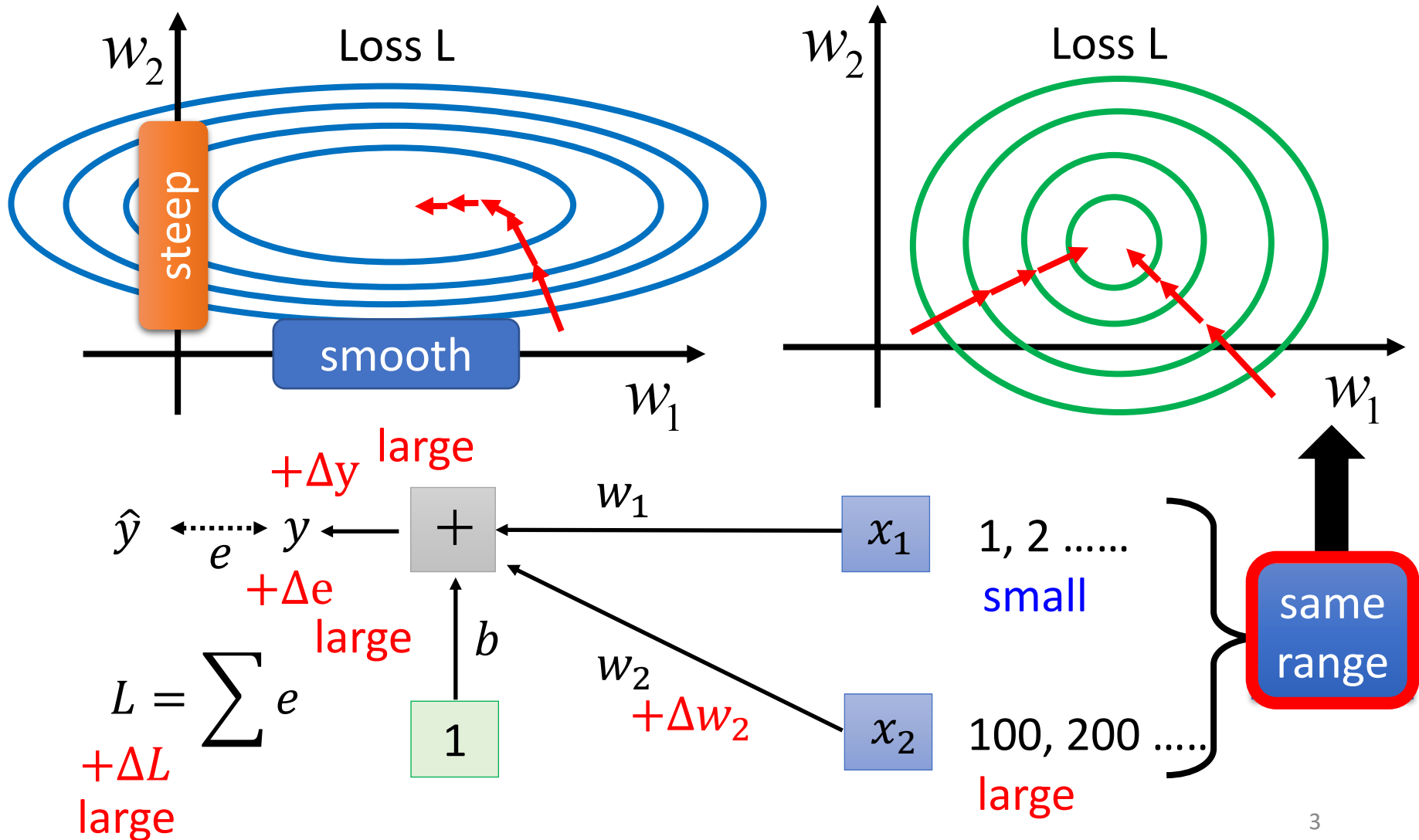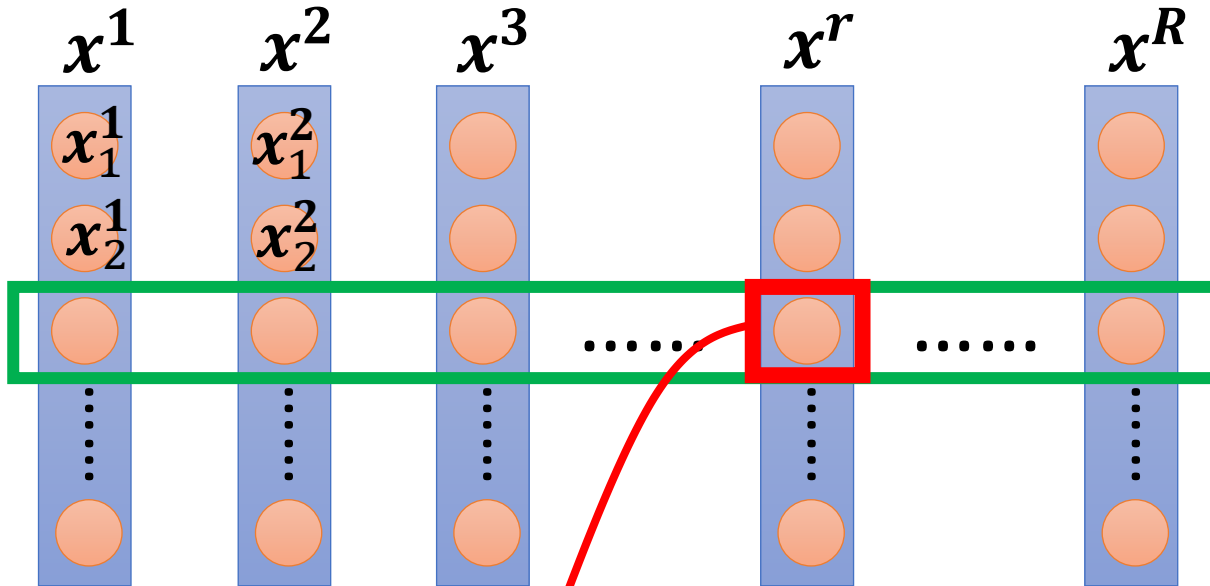
For each dimension i:

mean: m_i

standard deviation: σ_i

$$\widetilde{x}_i^r \leftarrow \frac{x_i^r - m_i}{\sigma_i}$$

The means of all dims are 0, and the variances are all 1

In general, feature normalization makes gradient descent converge faster.

Considering Deep Learning
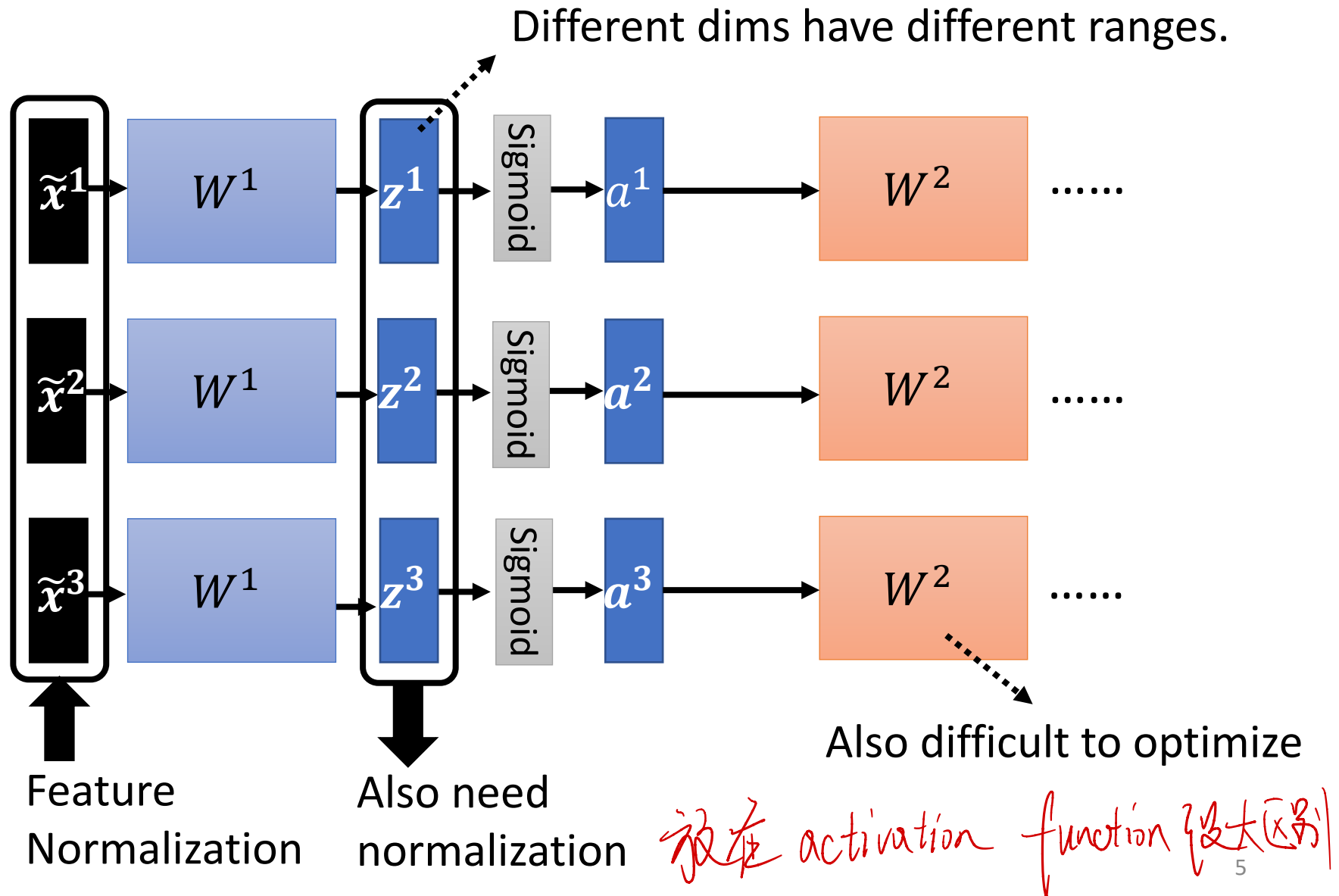
Different dims have different ranges.

Also difficult to optimize

Feature Normalization

Also need normalization

被在 activation function 很大区别

5

Considering Deep Learning

$$\mu = \frac{1}{3}\sum_{i=1}^{3} z^i$$

$$\sigma = \sqrt{\frac{1}{3}\sum_{i=1}^{3}(z^i - \mu)^2}$$

Considering Deep Learning

This is a large network!

$$\tilde{z}^i = \frac{z^i - \mu}{\sigma}$$

μ and σ depends on z^i

Consider a batch

Batch Normalization

7
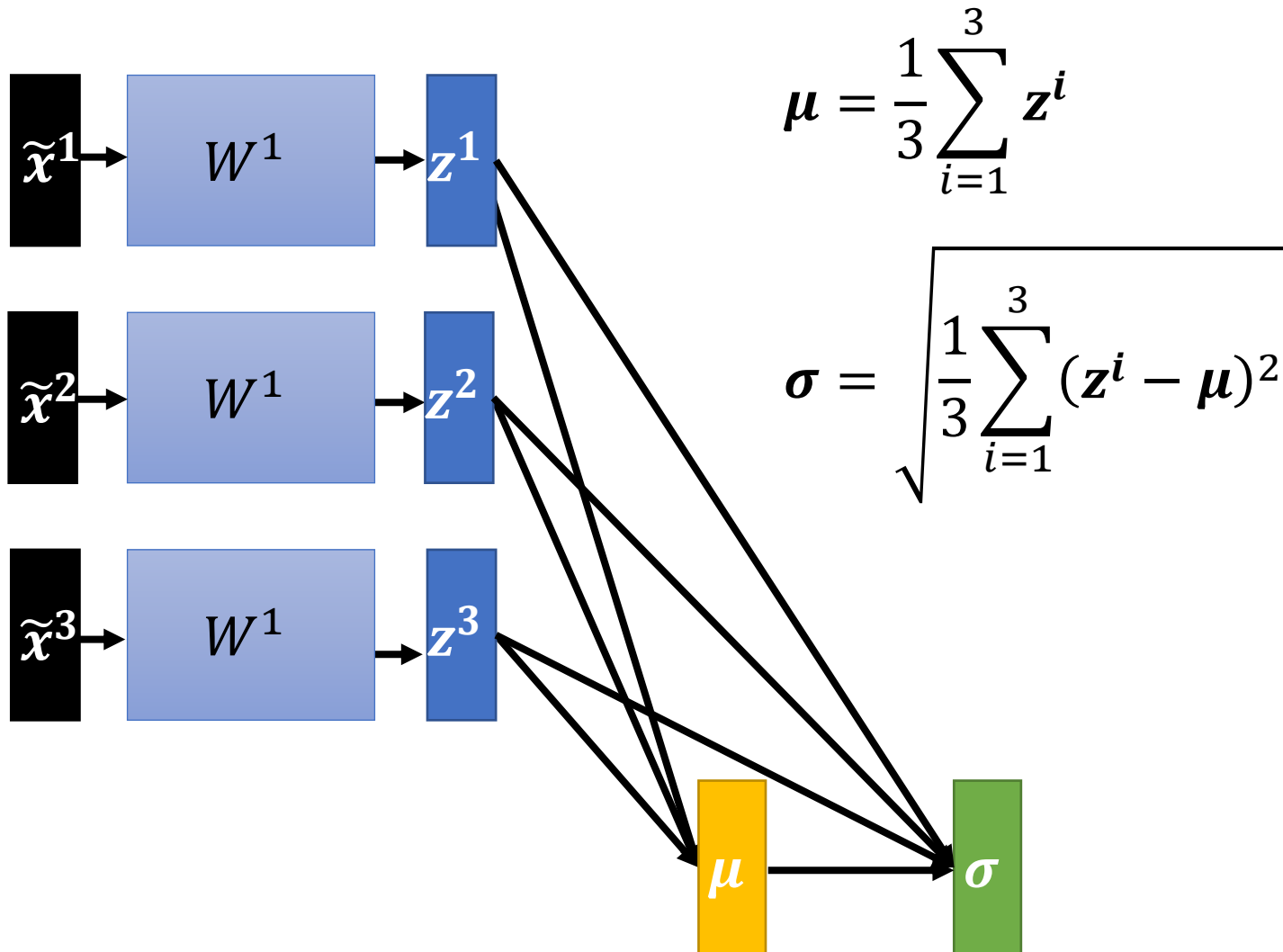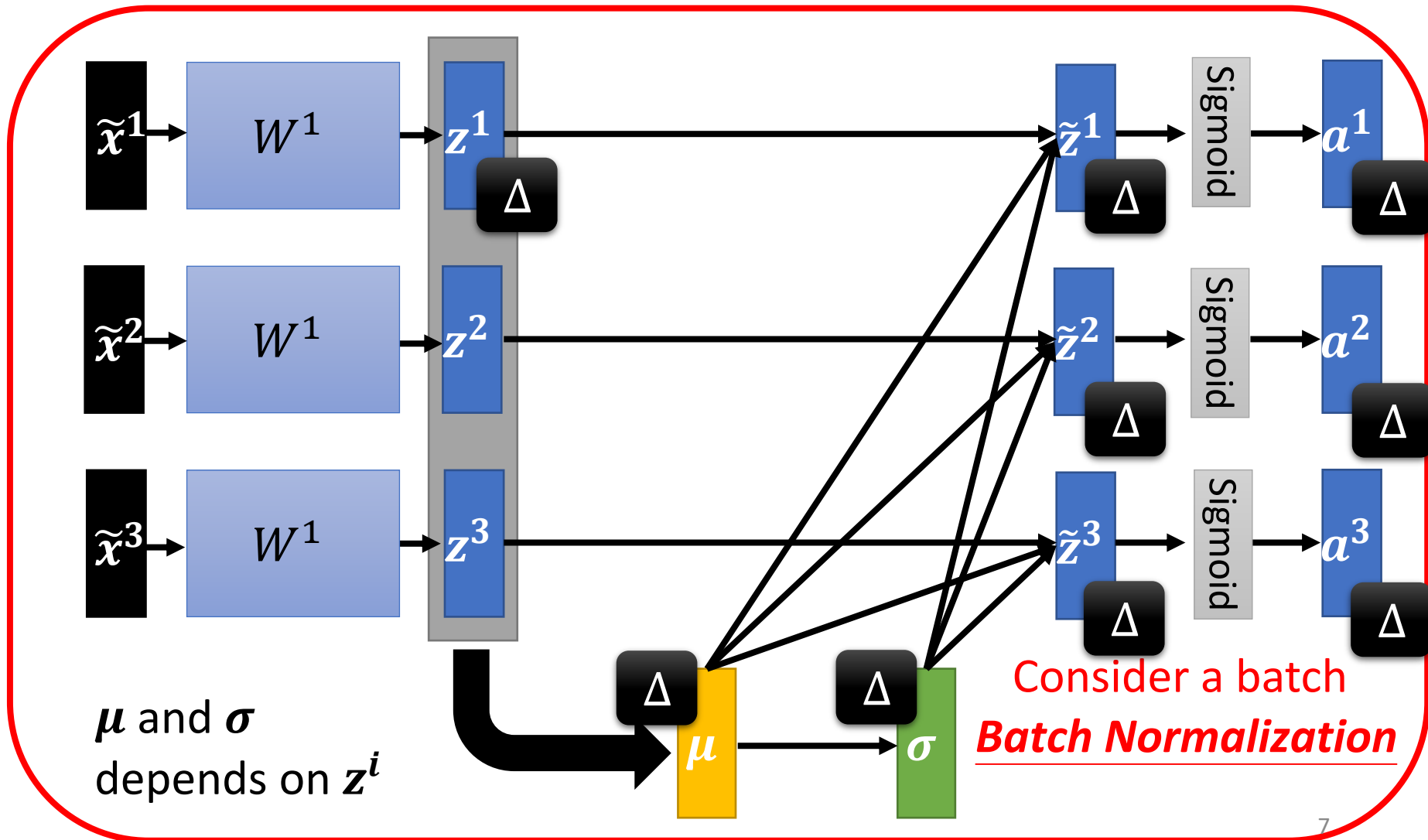
Batch normalization

$$\tilde{z}^i = \frac{z^i - \mu}{\sigma}$$

$$\hat{z}^i = \gamma \odot \tilde{z}^i + \beta$$

μ and σ depends on z^i
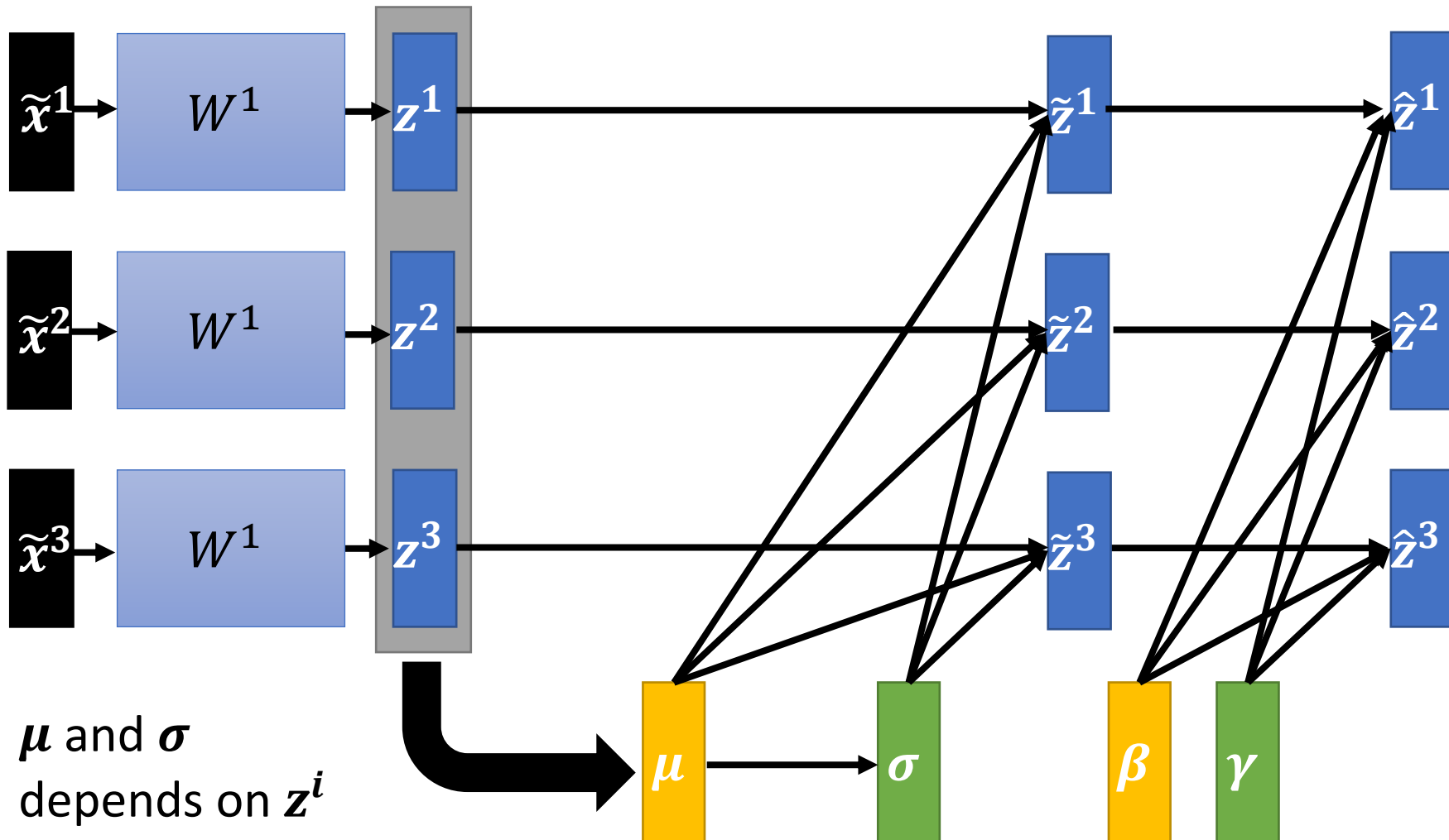
Batch normalization – Testing

$$\tilde{z} = \frac{z - \bar{\mu}}{\bar{\sigma}}$$

μ, σ are from **batch**?
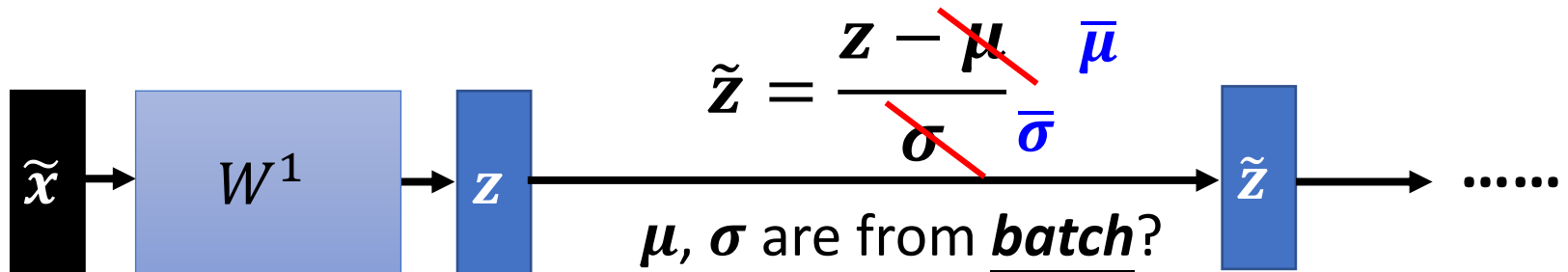
We do not always have **batch** at testing stage.

Computing the moving average of μ and σ of the batches during training.

$$\mu^1 \qquad \mu^2 \qquad \mu^3 \qquad \ldots\ldots \qquad \mu^t$$

$$\bar{\mu} \leftarrow p\bar{\mu} + (1 - p)\mu^t$$

Batch normalization

Original paper: https://arxiv.org/abs/1502.03167
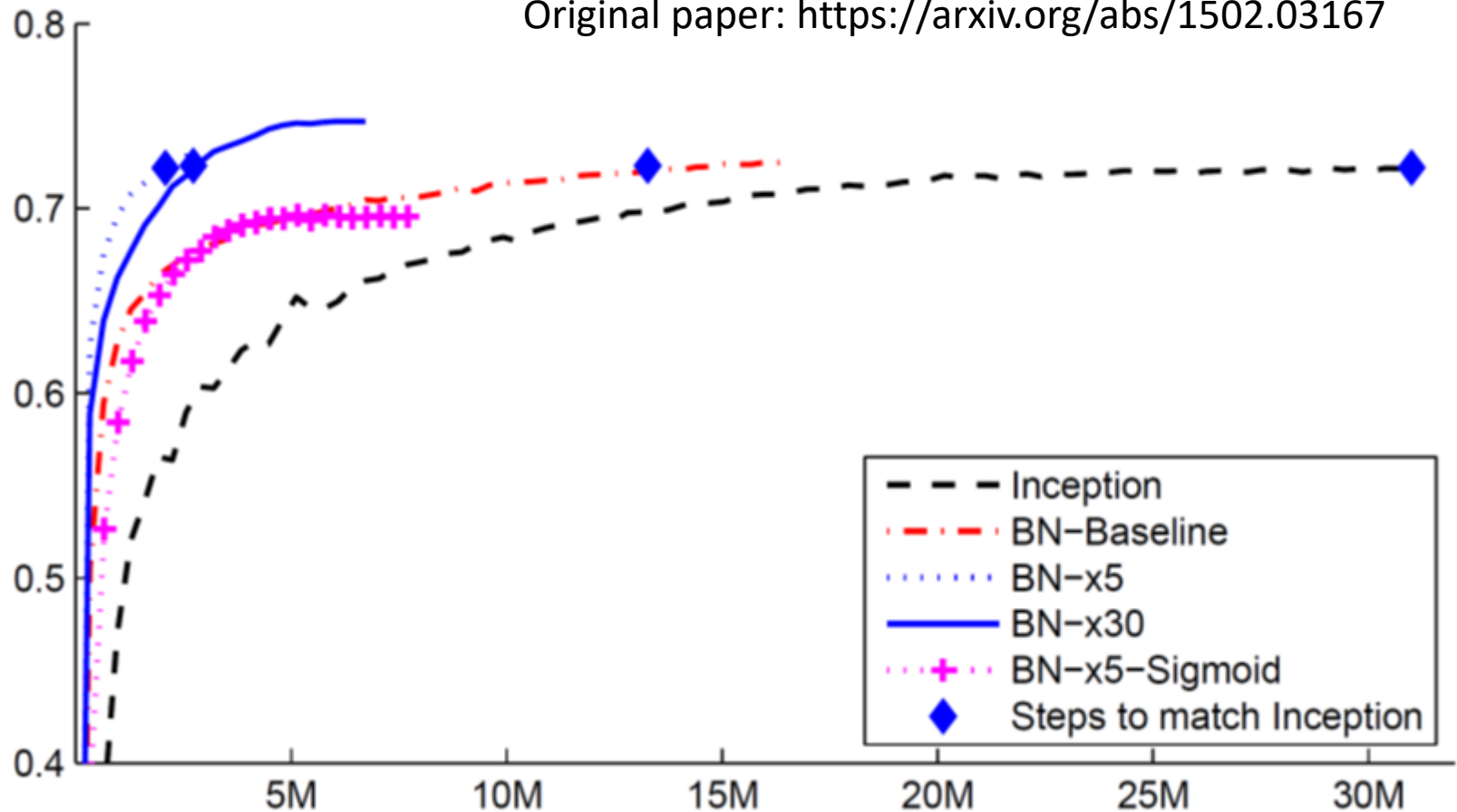
Internal Covariate Shift?

How Does Batch Normalization Help Optimization?

https://arxiv.org/abs/1805.11604
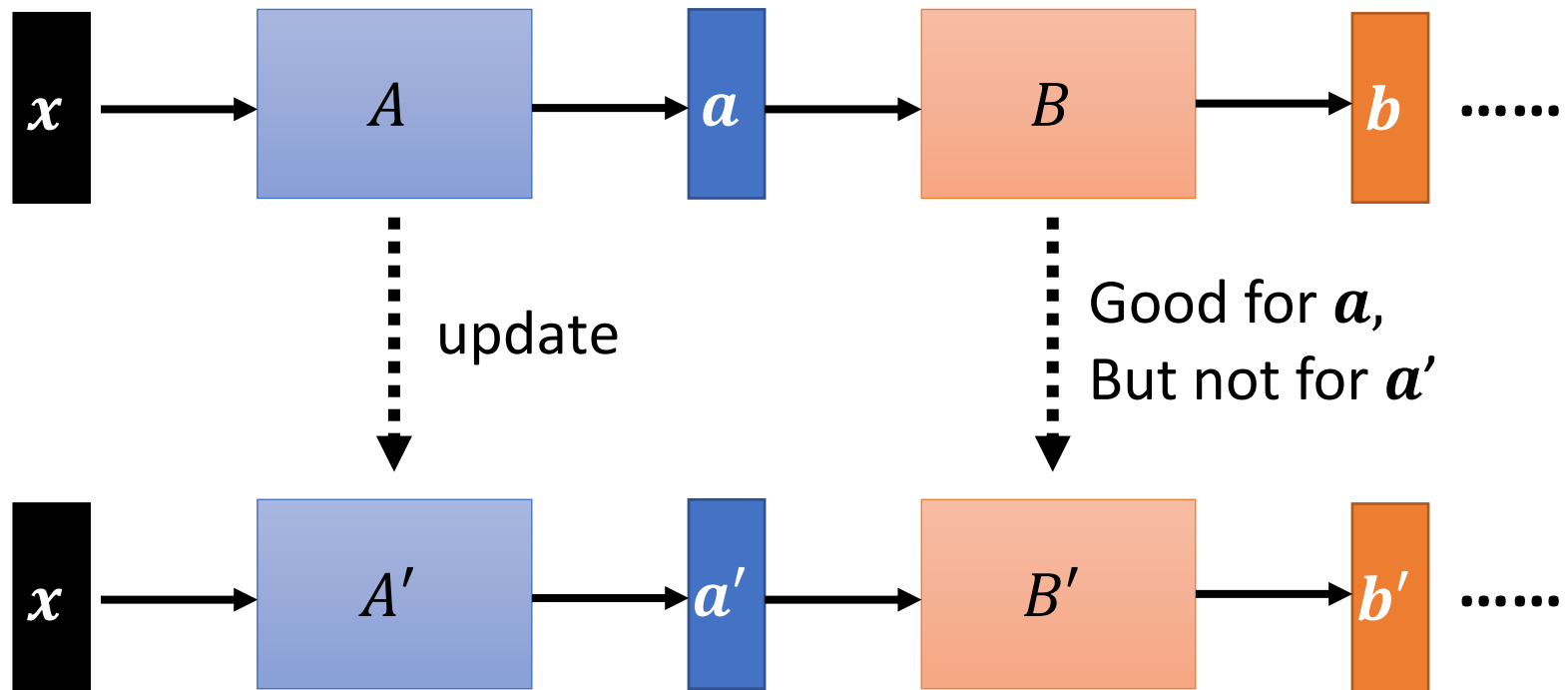
Batch normalization make a and a' have similar statistics.

Experimental results do not support the above idea.

Internal Covariate Shift?

How Does Batch Normalization Help Optimization?

Experimental results (and theoretically analysis) support batch normalization change the landscape of error surface.

and 12 of Appendix B.) This suggests that the positive impact of BatchNorm on training might be somewhat serendipitous. Therefore, it might be valuable to perform a principled exploration of the design space of normalization schemes as it can lead to better performance.

serendipitous （偶然的）

penicillin

To learn more ……

- Batch Renormalization
  - https://arxiv.org/abs/1702.03275

- Layer Normalization
  - https://arxiv.org/abs/1607.06450

- Instance Normalization
  - https://arxiv.org/abs/1607.08022

- Group Normalization
  - https://arxiv.org/abs/1803.08494

- Weight Normalization
  - https://arxiv.org/abs/1602.07868

- Spectrum Normalization
  - https://arxiv.org/abs/1705.10941

有一篇博语写的太好了，所以直接拿来用了，
链接是 ：   https://blog.csdn.net/weixin_44023658/article/details/105844861

Batch Normalization (BN) 超详细解析

单层训练

多层训练

图. 多层前馈Team神经网络。可以看出，当每一层的参数发生变化时，后面每一层接收到的输入数据的分布也会发生变化，所以每一层都需要不断重新适应新的数据分布。[Internal Covariate Shift, 内部协变量偏移]

Batch Normalization原理

Standard Network

Adding a BatchNorm layer (between weights and activation function)

3 Normalization via Mini-Batch Statistics

Since the full whitening of each layer's inputs is costly and not everywhere differentiable, we make two necessary simplifications. The first is that instead of whitening the features in layer inputs and outputs jointly, we will normalize each scalar feature independently, by making it have the mean of zero and the variance of 1. For a layer with d-dimensional input $x = (x^{(1)} \ldots x^{(d)})$, we will normalize each dimension

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1 \ldots m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

For each
dimension i:
mean: μ_i
standard
deviation: σ_i

$$z_i^1 \leftarrow \gamma \cdot \frac{z_i^1 - \mu_i}{\sigma_i} + \beta$$

$$y_i^{(k)} = BN(x_i^{(k)}) = \gamma \cdot \left(\frac{x_i^{(k)} - \mu(x_i)}{\sqrt{\sigma(x_i)^2 + \epsilon}}\right) + \beta$$

Batch Normalization的反向传播

$$\frac{\partial \ell}{\partial \widehat{x}_i} = \frac{\partial \ell}{\partial y_i} \cdot \gamma$$

$$\frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial \widehat{x}_i} \cdot (x_i - \mu_{\mathcal{B}}) \cdot \frac{-1}{2}(\sigma_{\mathcal{B}}^2 + \epsilon)^{-3/2}$$

$$\frac{\partial \ell}{\partial \mu_{\mathcal{B}}} = \left(\sum_{i=1}^{m} \frac{\partial \ell}{\partial \widehat{x}_i} \cdot \frac{-1}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}\right) + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} \cdot \frac{\sum_{i=1}^{m} -2(x_i - \mu_{\mathcal{B}})}{m}$$

$$\frac{\partial \ell}{\partial x_i} = \frac{\partial \ell}{\partial \widehat{x}_i} \cdot \frac{1}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} \cdot \frac{2(x_i - \mu_{\mathcal{B}})}{m} + \frac{\partial \ell}{\partial \mu_{\mathcal{B}}} \cdot \frac{1}{m}$$

$$\frac{\partial \ell}{\partial \gamma} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_i} \cdot \widehat{x}_i$$

$$\frac{\partial \ell}{\partial \beta} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_i}$$

Batch Normalization的预测阶段

在预测阶段，所有参数既已确定，基于测试样本，对BN的处理过程，单条数据x_i、σ_i^2，但都是确定值。

γ和β已经计算好，固有参数状态，两者都已作为模型参数确定下来，预测时这部分只需读取即可，我们也不管它了。

但有个问题，训练过程中，$E[x]$和$Var[x]$的值是分什么得来的，都是以batch为单位的。pBN一般在训练时，输入数据都是以batch喂给网络，这样做，每个bath的各组数据的分布都不一样，在预测时，因为我们只对单条测试数据逐样本的预测(当然你也可以组batch预测，但实际应用很少这样做)，作为预测阶段的数据，训练中计算的$E[x]$和$Var[x]$对当前单条数据就不合适了。

Input: Network N with trainable parameters Θ;
    subset of activations $\{x^{(k)}\}_{k=1}^K$
Output: Batch-normalized network for inference, N_{BN}^{inf}
1: $N_{BN}^{tr} \leftarrow N$ // Training BN network
2: for $k = 1 \ldots K$ do
3:     Add transformation $y^{(k)} = \mathrm{BN}_{\gamma^{(k)}, \beta^{(k)}}(x^{(k)})$ to
        N_{BN}^{tr} (Alg. 1)
4:     Modify each layer in N_{BN}^{tr} with input $x^{(k)}$ to take
        $y^{(k)}$ instead
5: end for
6: Train N_{BN}^{tr} to optimize the parameters $\Theta \cup$
    $\{\gamma^{(k)}, \beta^{(k)}\}_{k=1}^K$
7: $N_{BN}^{inf} \leftarrow N_{BN}^{tr}$ // Inference BN network with frozen
    parameters
8: for $k = 1 \ldots K$ do
9:     // For clarity, $x \equiv x^{(k)}$, $\gamma \equiv \gamma^{(k)}$, $\mu_B \equiv \mu_B^{(k)}$, etc.
10:    Process multiple training mini-batches B, each of
        size m, and average over them:
            $E[x] \leftarrow E_B[\mu_B]$
            $\mathrm{Var}[x] \leftarrow \frac{m}{m-1} E_B[\sigma_B^2]$
11:    In N_{BN}^{inf}, replace the transform $y = \mathrm{BN}_{\gamma, \beta}(x)$ with
        $y = \frac{\gamma}{\sqrt{\mathrm{Var}[x]+\epsilon}} \cdot x + \left(\beta - \frac{\gamma E[x]}{\sqrt{\mathrm{Var}[x]+\epsilon}}\right)$
12: end for

Algorithm 2: Training a Batch-Normalized Network

如第10行所示，测试时，$E[x]$和$Var[x]$用的是基于所有训练数据的无偏估计，使用Random(随机)和cache(缓存)的shift方法得到的。

Batch Normalization的作用

使用Batch Normalization，可以获得如下好处。

- 可以使用更大的学习率，训练过程更加稳定，极大提高了训练速度。
- 可以将bias置0，因为Batch Normalization的Standardization处理会移除直流分量，所以不再需要bias。
- 对权重初始化不再敏感，通常权重采样自0均值单位方差的高斯分布，以往对高斯分布的方差设置十分重要，有了Batch Normalization后，对与同一个方向相对大小将变得稀疏，因为过大或过小的权重经过标准化后不再对结果产生影响。
- 对权重的大小更加的鲁棒，同样也是因为Standardization。
- 可以使用随机梯度下降(Stochastic gradient descent)，缓解过拟合。
- 使用BatchNorm让神经网络的调参更加简单，对于深层网络，各层之间的Scale差异较大, 学习率选择需要谨慎的进行折衷，BatchNorm之后, 每层的Scale相近，参数设置更加友好。

几个常见问题

卷积层如何使用BatchNorm?

1个卷积核产生1个feature map，1个feature map有1对γ和β参数，同一batch中同一个channel的feature map共享同一对γ和β参数，若卷积有n个卷积核，则有n对γ和β参数。

没有scale and shift过程可不可以?

BatchNorm有两个过程，Standardization和scale and shift，看似scale and shift过程是多余的，因为反过来看，Standardization过程将数据转换成标准分布，而scale and shift又将数据给变了回去，这不是没起作用吗?

其实并不是没用，shift过程增加了参数的可调节性，通过scale and shift，数据的均值和方差将不再局限于0和1，可以是任意值，增加了网络的学习能力。

BN层放在ReLU前面还是后面?

原paper建议将BN层放置在ReLU前，因为ReLU激活函数的输出非负，不能近似为高斯分布。

> The goal of Batch Normalization is to achieve a stable distribution of activation values throughout training, and ...

但是，也有人做了对比实验，BN放ReLU后面效果更好。实验结果见下表，放在ReLU后面要更好些。

	Name	Accuracy	LogLoss	Comments
	Before	0.474	2.35	As in paper
	Before + scale&bias layer	0.478	2.33	As in paper
	After	0.499	2.21	
	After + scale&bias layer	0.493	2.24	

实验来源：[caffenet-benchmark-batchnorm](https://github.com/)

放在ReLU过后也能取得一定的效果提升，但大多数BN层还在ReLU前。以上分析来自于Standardization的一致性。

caffenet-benchmark-batchnorm中，还有更多BN的对比实验，感兴趣的可以访问一探究竟。

其实，更好的BatchNorm位置是放在dropout前面，因为BatchNorm会降低模型的方差，dropout同样可以降低方差，两者同时存在会使得方差更低，削弱了模型的学习能力。

BN层为什么有效?

BN层的有效性已有很多实验证明，但具体BN层为什么有效，还需要进一步研究，以下是几个已经有的解释，供参考。

- **BN层让损失函数更平滑**。论文How Does Batch Normalization Help Optimization中，通过分析训练过程中每层参数的变化情况，发现BN层让损失函数更平滑(loss landscape如下图所示)。损失函数的平滑性对于提高网络学习率和收敛速度有很大帮助。

Figure 4: Analysis of the optimization landscape of VGG networks. At a particular training step, we measure the variation (shaded region) in loss (a) and ℓ_2 changes in the gradient (b) as we move in the gradient direction. The "effective" β-smoothness (c) refers to the maximum difference (in ℓ_2-norm) in gradient over distance moved in that direction. There is a clear improvement in all of these measures in networks with BatchNorm, indicating a more well-behaved loss landscape. (Here, we cap the maximum distance to be $\eta = 0.4 \times$ the gradient since for larger steps the standard network just performs worse (see Figure 1)). BatchNorm however continues to provide smoothing for even larger distances.) Note that these results are supported by our theoretical findings (Section 5).

- **BN层让损失函数更平滑**。论文An empirical analysis of the optimization of deep network loss surfaces中，得出了VGG网络有无BN的损失函数图示(参考下图)，BN让损失函数的landscape(loss landscape)曲面更平滑，即BN更容易找到更好的minima(极小值)。

- **BN更有利于梯度下降**。论文An empirical analysis of the optimization of deep network loss surfaces，绘制了VGG和NIN网络在有无BN层的情况下的loss surface差异，见下图。有BN层的(With BN)曲面更平滑，凸性更好，而没有BN层的(Without BN)曲面凹凸不平，深沟纵横，不管权重如何初始化，总能平滑的过渡到minima。

- 这里有篇博文，用二维拟合的例子，实际演示出了BN对于loss landscape的影响，使用BN后loss会更加的平滑，感兴趣的可以访问。同时，对于正则化是否只是BN的一个副作用还是BN的主要作用，也一直存在争议，关于这个问题，推荐阅读How Does Batch Normalization Help Optimization 这篇论文，里面有详细的分析。

参考阅读：
- 原博客：[How Does Batch Normalization Help Optimization中文版](https://)，同名的论文How Does Batch Normalization Help Optimization提供了理论上的分析，推荐阅读。

参考：[1]
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