Training Neural Networks: Normalization, Regularization etc.

Intro to Deep Learning, Spring 2021

Recap

- We train a network by minimizing a "loss"

$$L(W) = \frac{1}{N_X} \sum_X div(f(X;W), D(X))$$

  - Average divergence between true and desired outputs over "training" inputs
  - Approximation to "true" risk – *expected* divergence between desired and true outputs

- We minimize it through gradient descent
  - Iterative updates against the gradient of the loss w.r.t. W

- Batch updates must process the entire training data before each update
  - Incremental update algorithms, like SGD and minibatch update, speed it up by updating using random individual inputs or subsets of the input
  - Faster to converge, but greater variance may result in worse estimates

- Trend algorithms smooth out the variations in incremental update methods by considering long-term trends in gradients.
  - This can lead to faster, and better convergence

Quick Recap: Training a network

Total loss

Average over all training instances

Divergence between desired output and actual output of net for a given input X

Output of net in response to input X

Desired output in response to input X

$$L(W) = \frac{1}{N_X} \sum_X div(f(X; W), D(X))$$

$$\widehat{W} = \arg\min_W L(W)$$

- Define a total "loss" over all training instances
  - Quantifies the difference between desired output and the actual output, as a function of weights
- Find the weights that minimize the loss

Quick Recap: Training networks by gradient descent

$$L(W) = \frac{1}{N_X} \sum_X div(f(X;W), D(X))$$

$$\nabla_W L(W) = \frac{1}{N_X} \sum_X \underbrace{\nabla_W div(f(X;W), D(X))}$$

Computed using backpropagation

Solved through gradient descent as

$$\widehat{W} = \underset{W}{\arg\min}\, L(W) \quad \Rightarrow \quad W_k = W_{k-1} - \eta \nabla_W L(W)^T$$

Recap: Incremental methods

- Batch methods that consider *all* training points before making an update to the parameters can be terribly inefficient

- Online methods that present training instances incrementally make quicker updates
  - "Stochastic Gradient Descent" updates parameters after individual randomly-chosen instances
  - "Mini batch descent" updates them after minibatches of randomly-chosen instances
  - Require shrinking learning rates to converge
    - Not absolute summable
    - But square summable

- Online methods have greater variance than batch methods
  - Potentially leading to worse model estimates

Recap: Trend Algorithms

- Trend algorithms smooth out the variations in incremental update methods by considering long-term trends in gradients
  - Leading to faster and more assured convergence

- Momentum and Nestorov's method improve convergence by smoothing updates with the *mean* (first moment) of the sequence of derivatives

- Second-moment methods consider the variation (*second moment*) of the derivatives
  - RMS Prop only considers the second moment of the derivatives
  - ADAM and its siblings consider both the first and second moments
  - All of them typically provide considerably faster than simple gradient descent

Moving on: Topics for the day

- Incremental updates
- Revisiting “trend” algorithms
- Generalization
- Tricks of the trade
  - Divergences..
  - Activations
  - Normalizations

Tricks of the trade..

- To make the network converge better
  - The Divergence
  - Batch normalization
  - Dropout
  - Other tricks
    - Gradient clipping
    - Data augmentation
    - Other hacks..

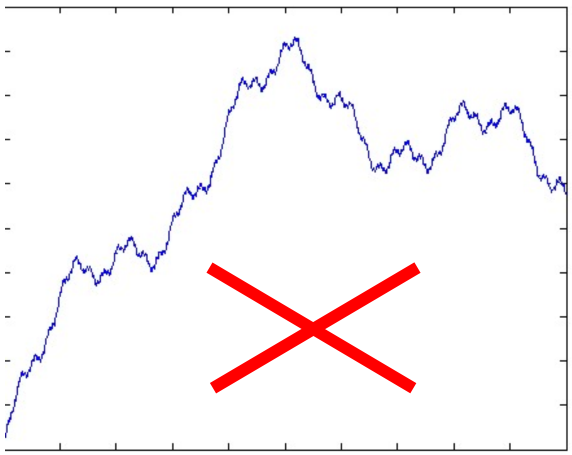
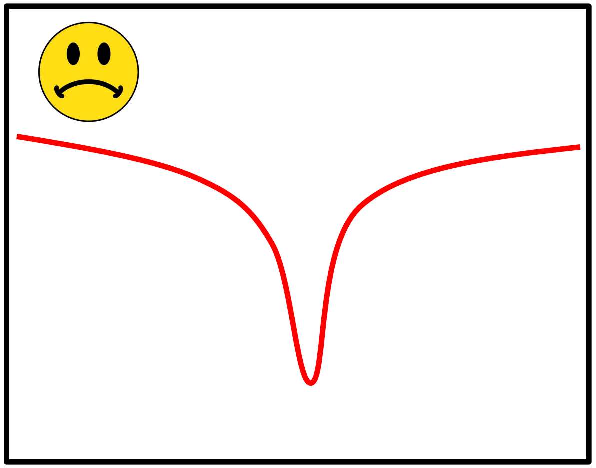
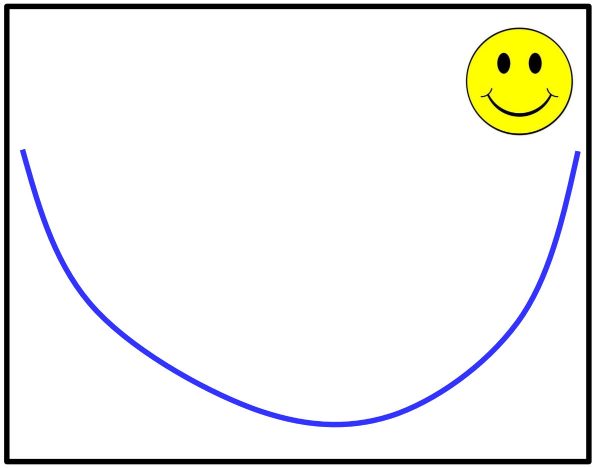
Training Neural Nets by Gradient Descent: The Divergence

Total training loss:

$$Loss = \frac{1}{T}\sum_{t} Div(\boldsymbol{Y_t}, \boldsymbol{d_t}; \mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_K)$$

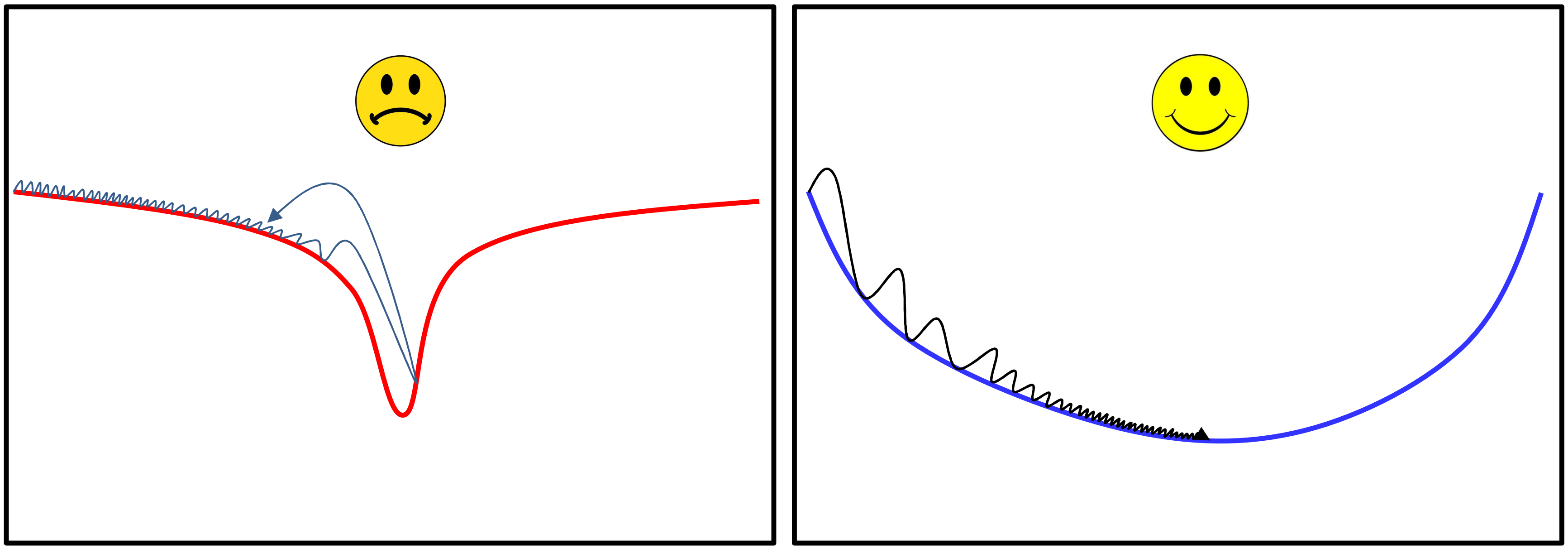
- The convergence of the gradient descent depends on the divergence
  - Ideally, must have a shape that results in a significant gradient in the right direction outside the optimum
    - To "guide" the algorithm to the right solution

Desiderata for a good divergence

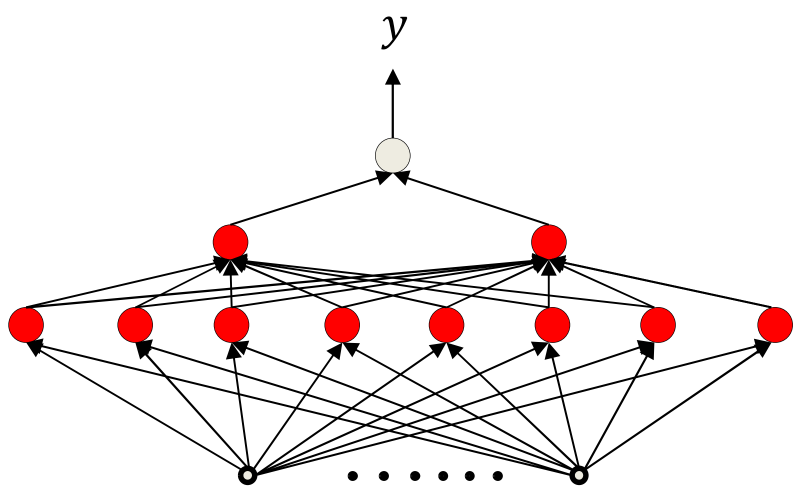
- Must be smooth and not have many poor local optima
- Low slopes far from the optimum == bad
  - Initial estimates far from the optimum will take forever to converge
- High slopes near the optimum == bad
  - Steep gradients

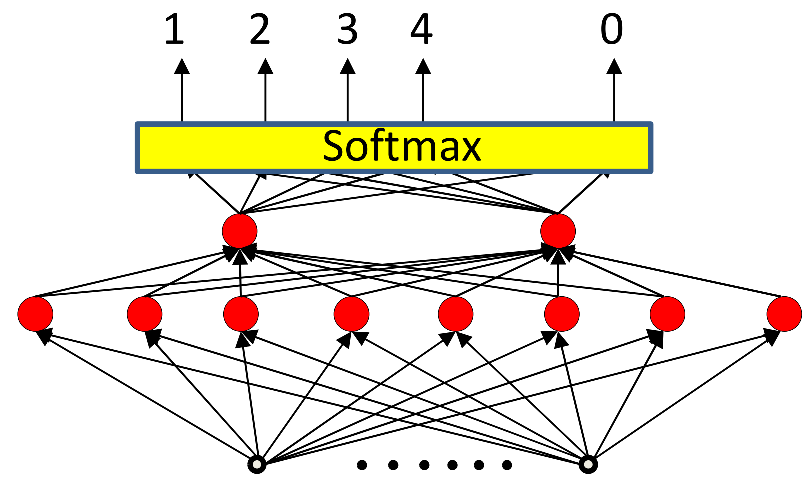
Desiderata for a good divergence



- Functions that are shallow far from the optimum will result in very small steps during optimization
  - Slow convergence of gradient descent
- Functions that are steep near the optimum will result in large steps and overshoot during optimization
  - Gradient descent will not converge easily
- The best type of divergence is steep far from the optimum, but shallow at the optimum
  - But not *too* shallow: ideally quadratic in nature

Choices for divergence





Desired output:	d	Desired output: $[0,0, \ldots, 1, \ldots, 0]$
L2	$Div = \frac{1}{2}(y-d)^2$	$Div = \frac{1}{2}\sum_i (y_i - d_i)^2$
KL	$Div = -d\log(y) - (1-d)\log(1-y)$	$Div = \sum_i d_i \log(d_i) - \sum_i d_i \log(y_i)$

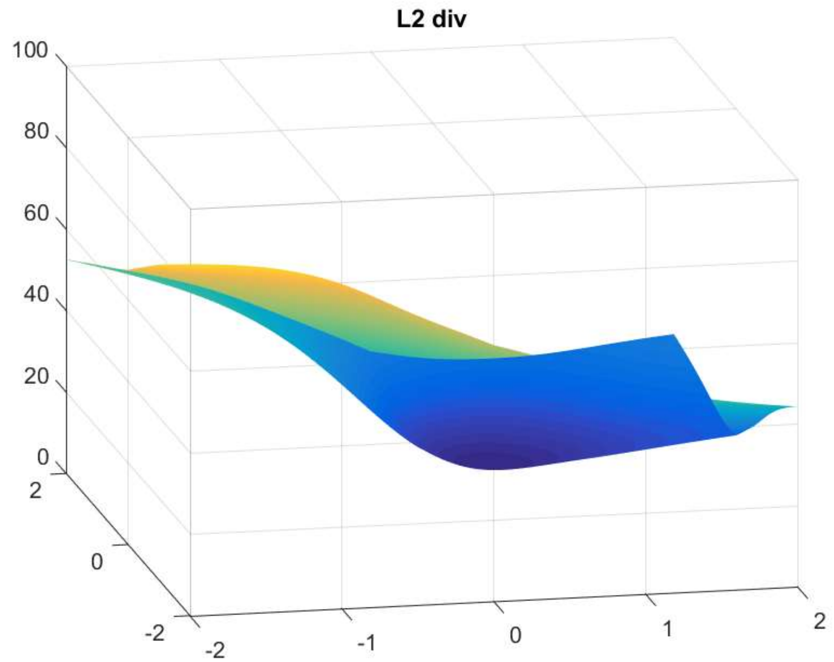
- Most common choices: The L2 divergence and the KL divergence
- L2 is popular for networks that perform numeric prediction/regression
- KL is popular for networks that perform classification

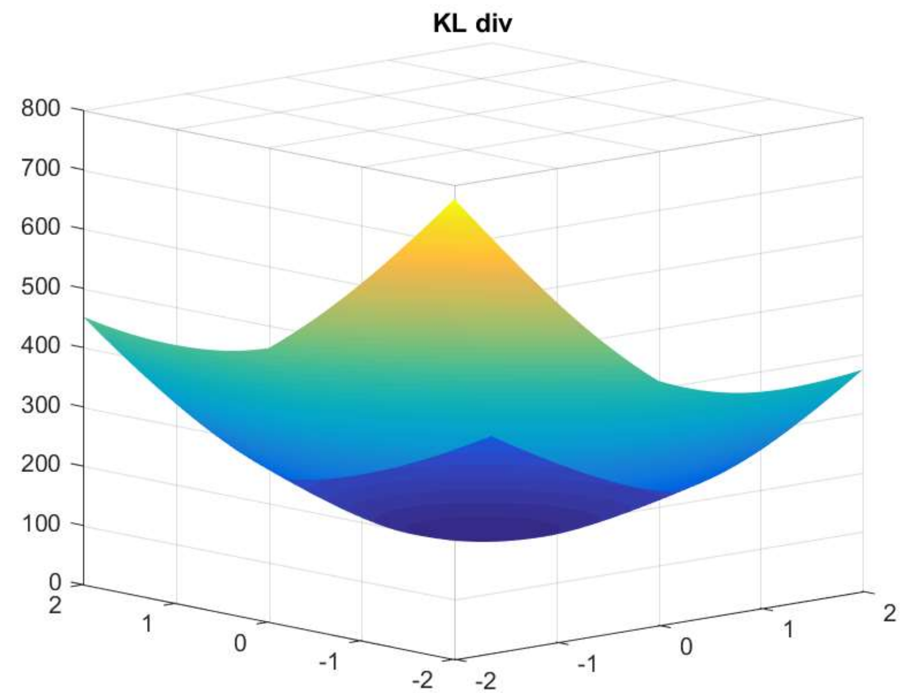
L2 or KL?

- The L2 divergence has long been favored in most applications
- It is particularly appropriate when attempting to perform *regression*
  - Numeric prediction

- The KL divergence is better when the intent is classification
  - The output is a probability vector

L2 or KL



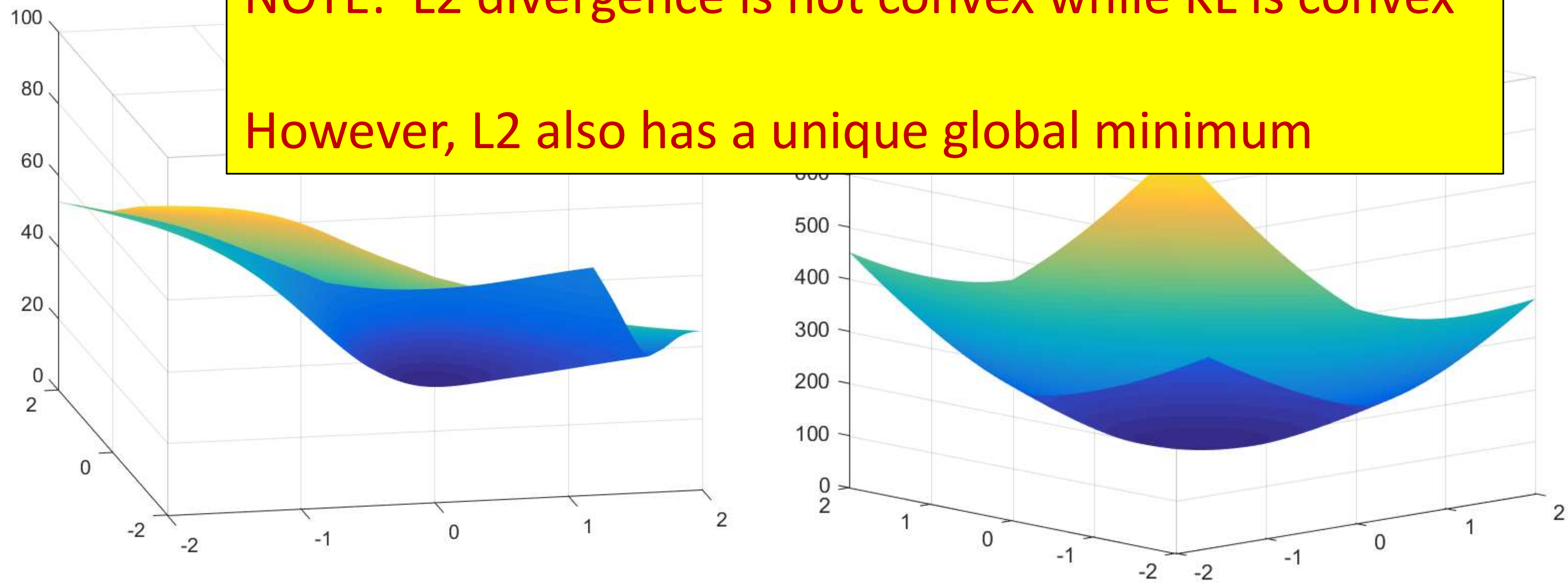


- Plot of L2 and KL divergences for a *single* perceptron, as function of weights
  - Setup: 2-dimensional input
  - 100 training examples randomly generated

L2 or KL

NOTE: L2 divergence is not convex while KL is convex

However, L2 also has a unique global minimum



- Plot of L2 and KL divergences for a *single* perceptron, as function of weights
  - Setup: 2-dimensional input
  - 100 training examples randomly generated

A note on derivatives

- Note: For L2 divergence the derivative w.r.t. the output of the network is:

$$\nabla_{\boldsymbol{y}} \frac{1}{2} \|\boldsymbol{y} - \boldsymbol{d}\|^2 = (\boldsymbol{y} - \boldsymbol{d})$$

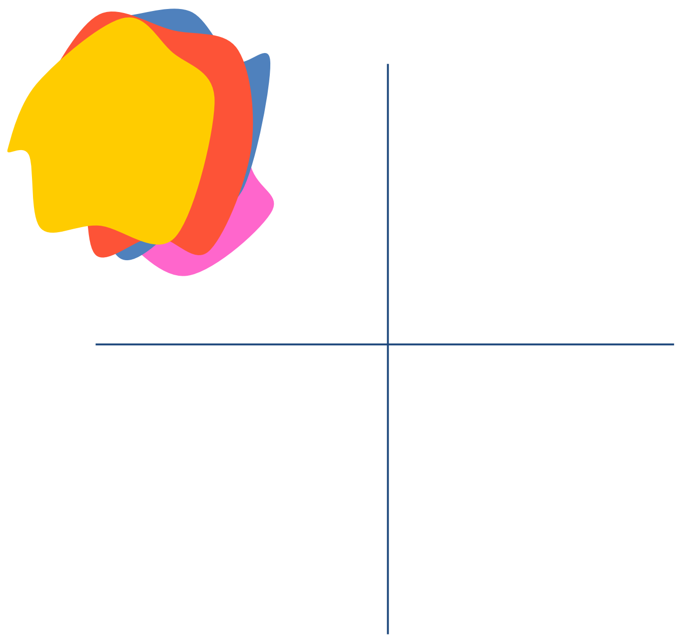
- We literally "propagate" the error $(\boldsymbol{y} - \boldsymbol{d})$ backward
  - Which is why the method is sometimes called "error backpropagation"

Story so far

- Gradient descent can be sped up by incremental updates
- Convergence can be improved using smoothed updates

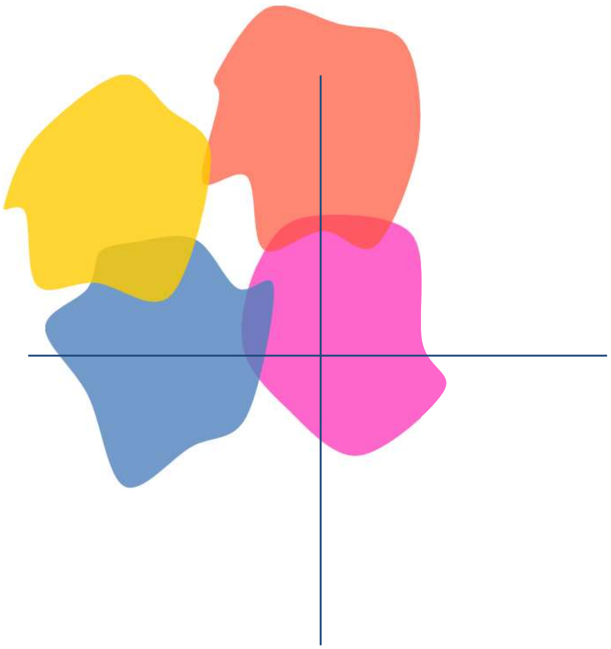
- The choice of divergence affects both the learned network and results

The problem of covariate shifts



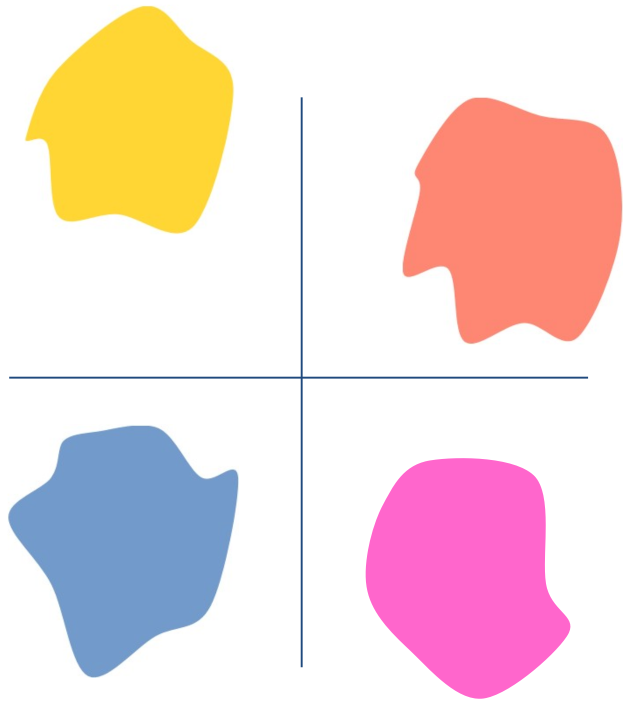
- Training assumes the training data are all similarly distributed
  - Minibatches have similar distribution

The problem of covariate shifts



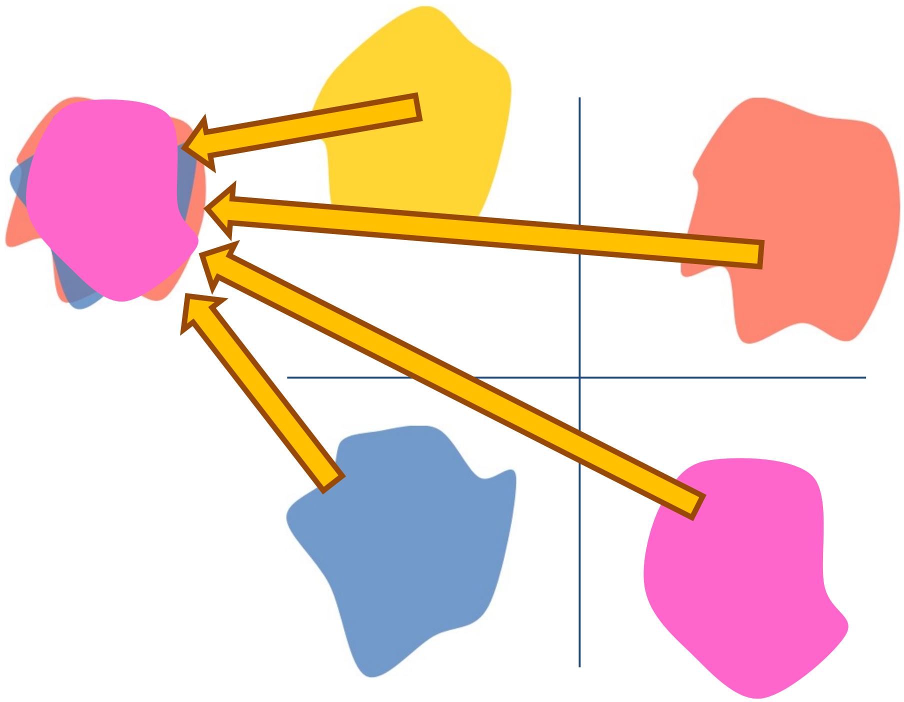
- Training assumes the training data are all similarly distributed
  - Minibatches have similar distribution
- In practice, each minibatch may have a different distribution
  - A “covariate shift”
  - Which may occur in *each* layer of the network

The problem of covariate shifts



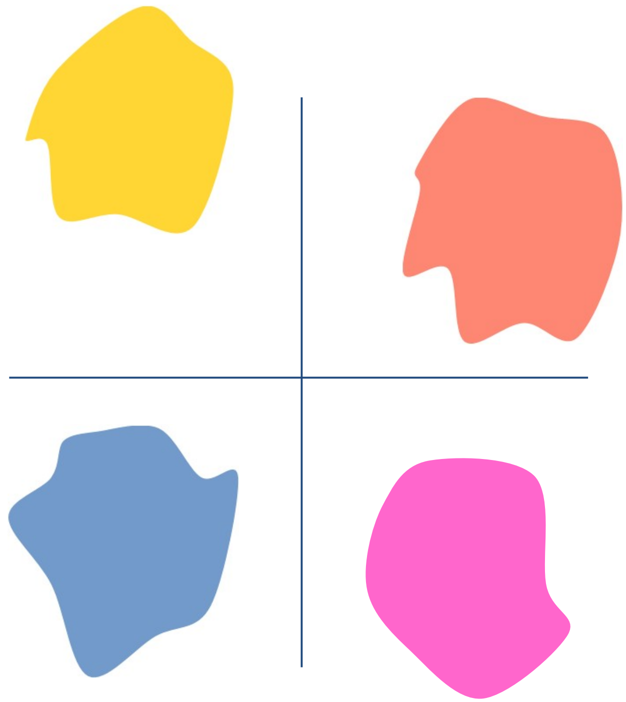
- Training assumes the training data are all similarly distributed
  - Minibatches have similar distribution
- In practice, each minibatch may have a different distribution
  - A “covariate shift”
- Covariate shifts can be large!
  - All covariate shifts can affect training badly

Solution: Move all minibatches to a "standard" location



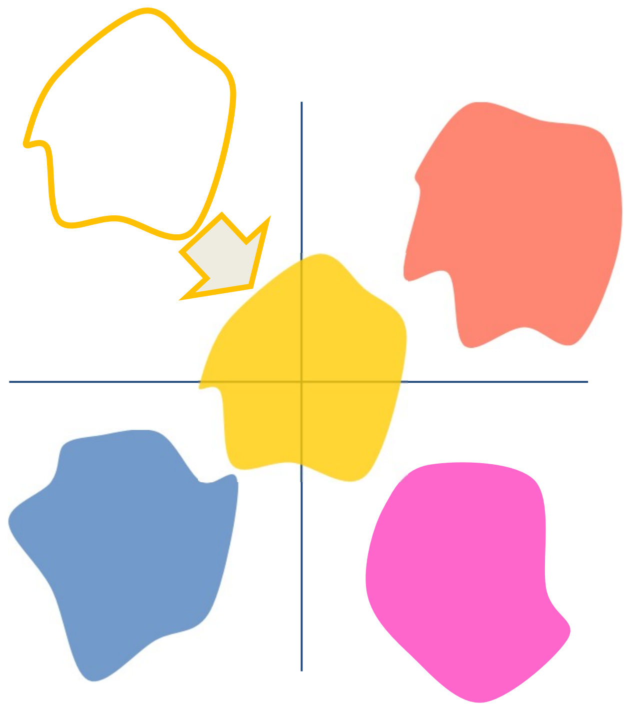
- "Move" all batches to a "standard" location of the space
  - But where?
  - To determine, we will follow a two-step process

Move all minibatches to a “standard” location



- “Move” all batches to have a mean of 0 and unit standard deviation
  - Eliminates covariate shift between batches

Move all minibatches to a “standard” location



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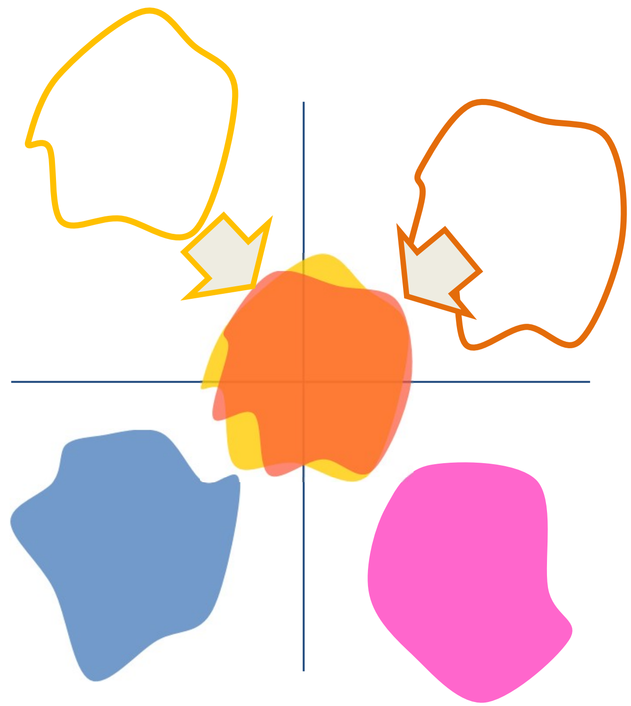

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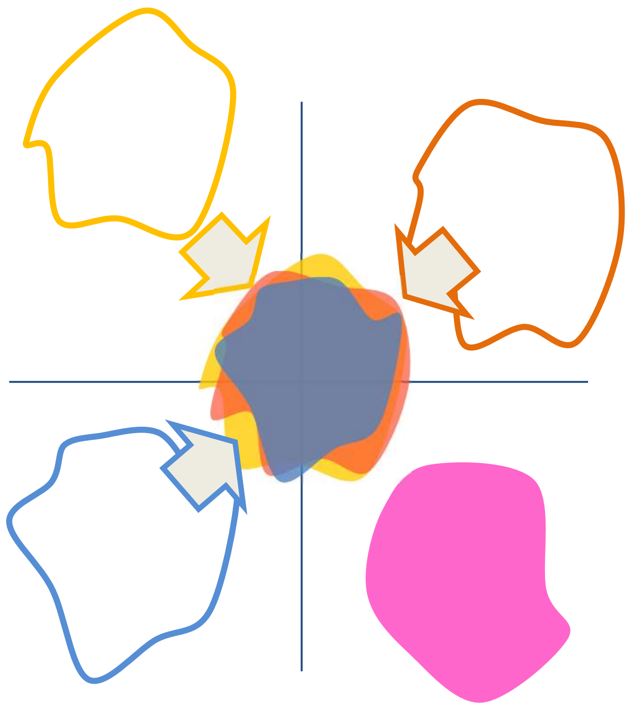
Move all minibatches to a "standard" location



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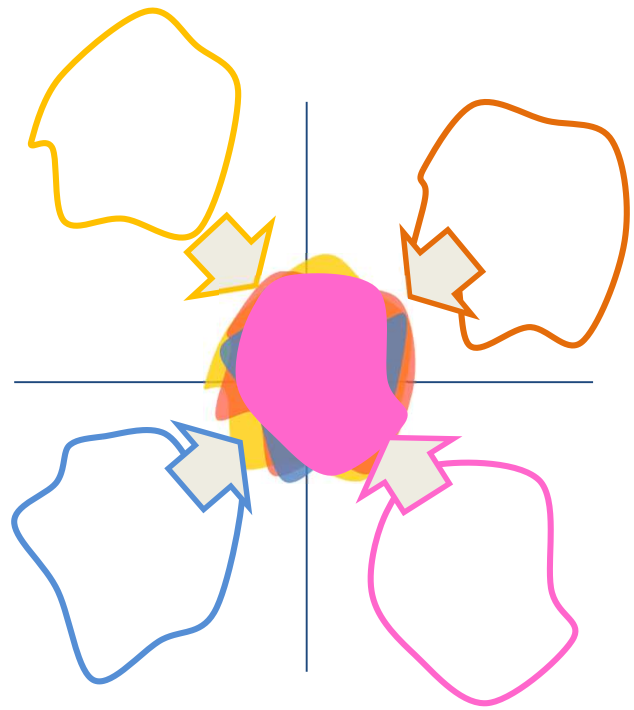
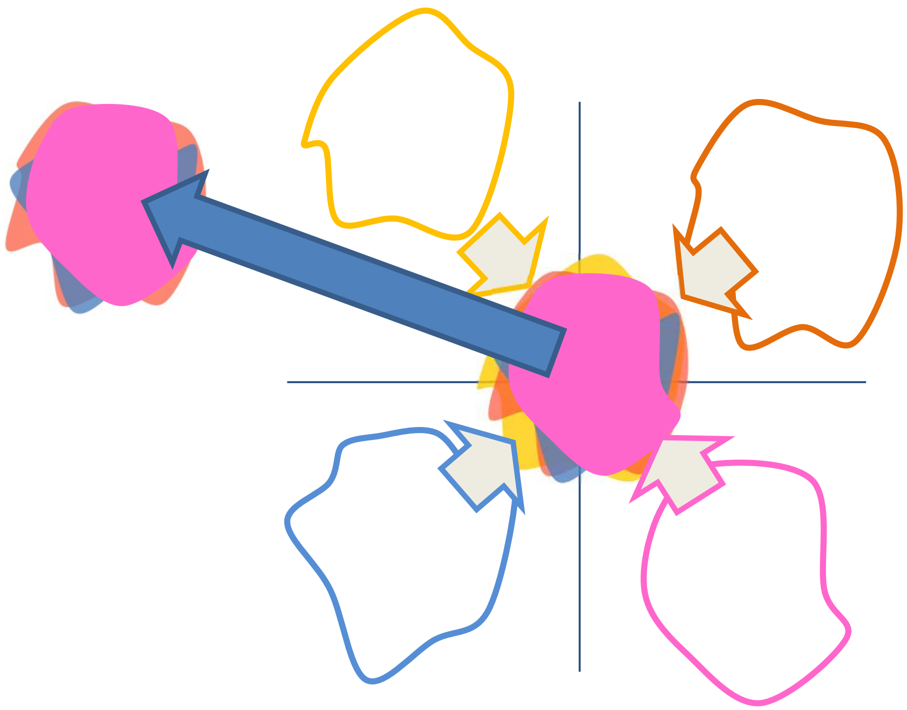
Move all minibatches to a "standard" location



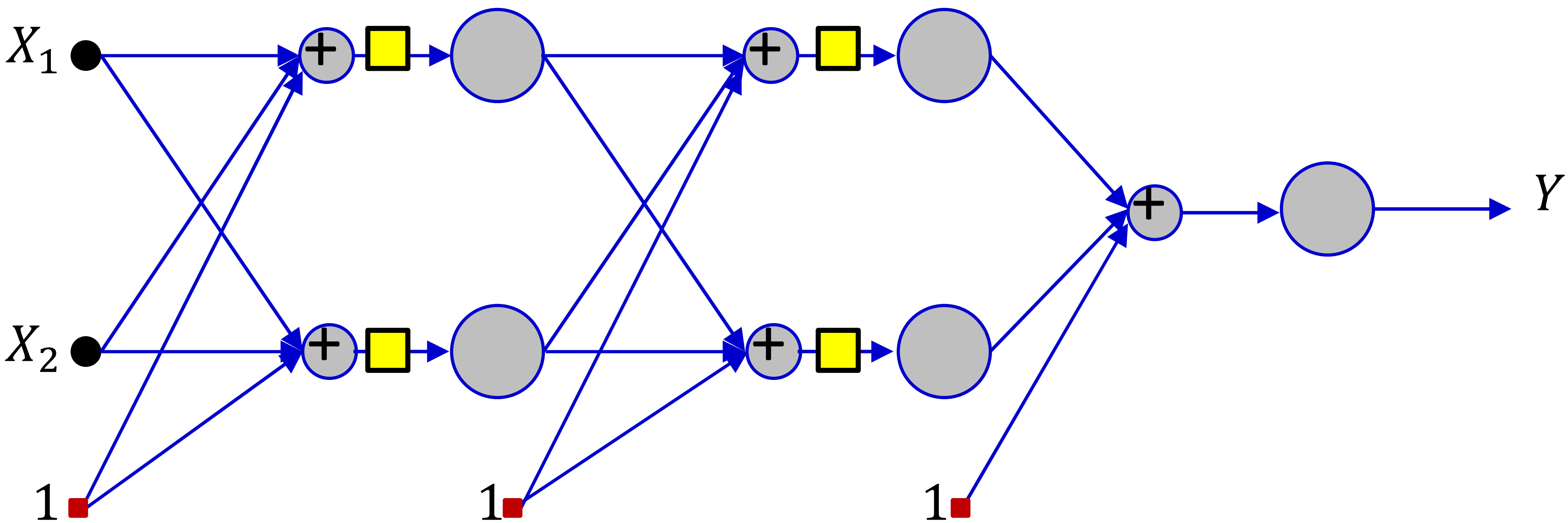
- "Move" all batches to have a mean of 0 and unit standard deviation
  - Eliminates covariate shift between batches

(Mini)Batch Normalization



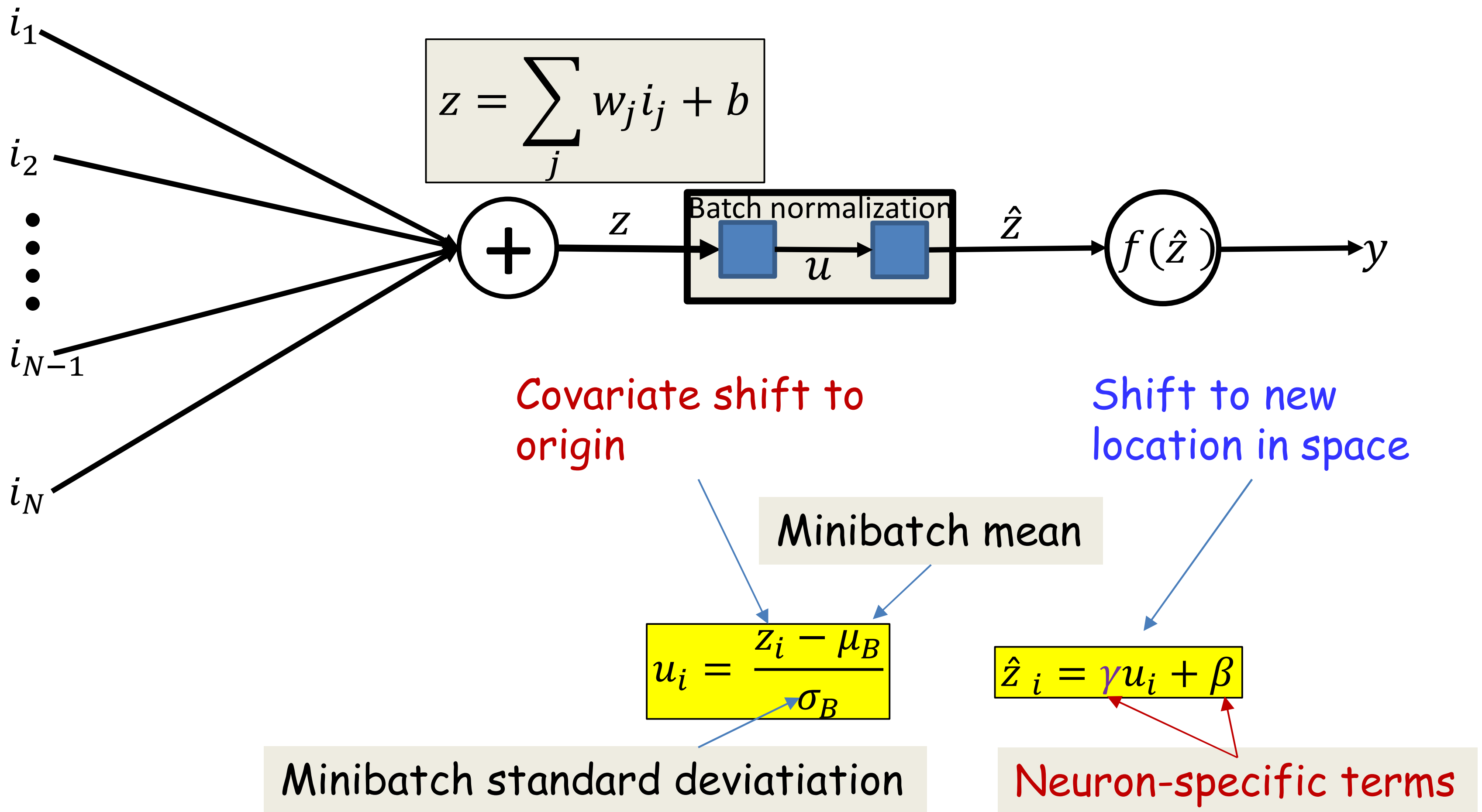
- “Move” all batches to have a mean of 0 and unit standard deviation
  - Eliminates covariate shift between batches
- **Then move the entire collection to the appropriate location**

Batch normalization



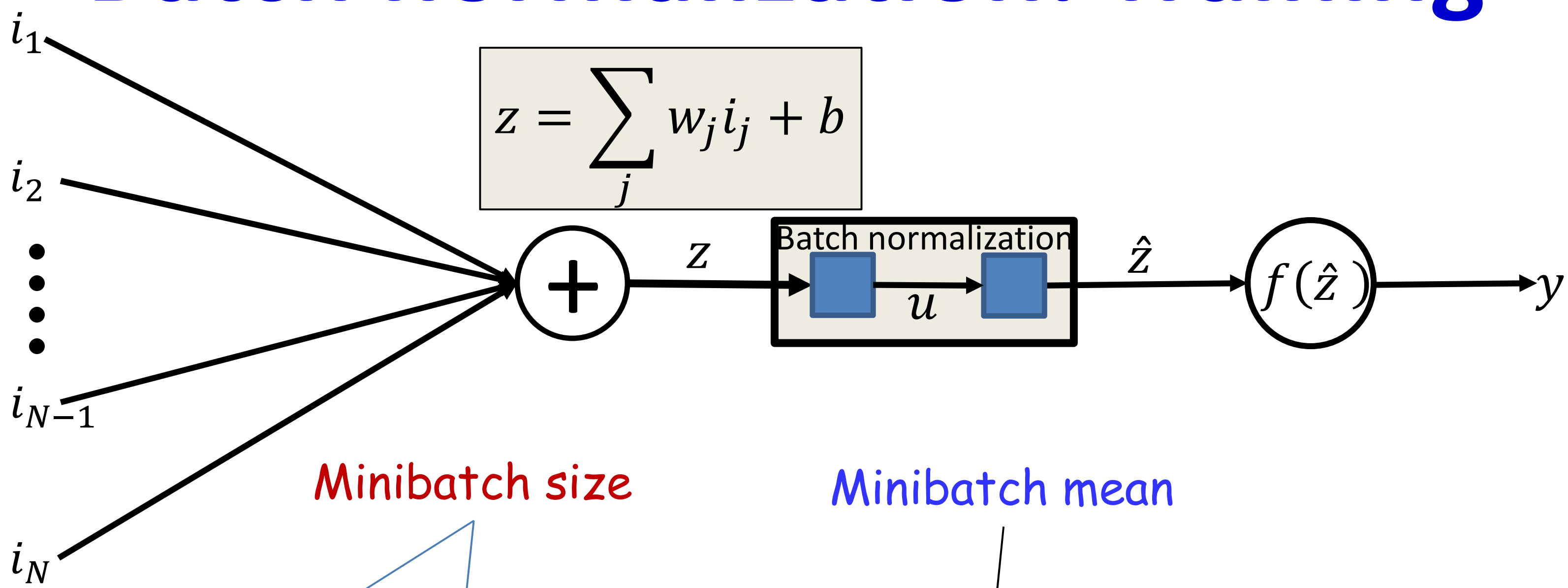
- Batch normalization is a covariate adjustment unit that happens after the weighted addition of inputs but before the application of activation
  - Is done independently for each unit, to simplify computation
- **Training: The adjustment occurs over individual minibatches**

Batch normalization



- BN aggregates the statistics over a minibatch and normalizes the batch by them
- Normalized instances are "shifted" to a *unit-specific* location

Batch normalization: Training



Minibatch size

Minibatch mean

Minibatch standard deviation

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B} (z_i - \mu_B)^2$$

$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\hat{z}_i = \gamma u_i + \beta$$

- BN aggregates the statistics over a minibatch and normalizes the batch by them
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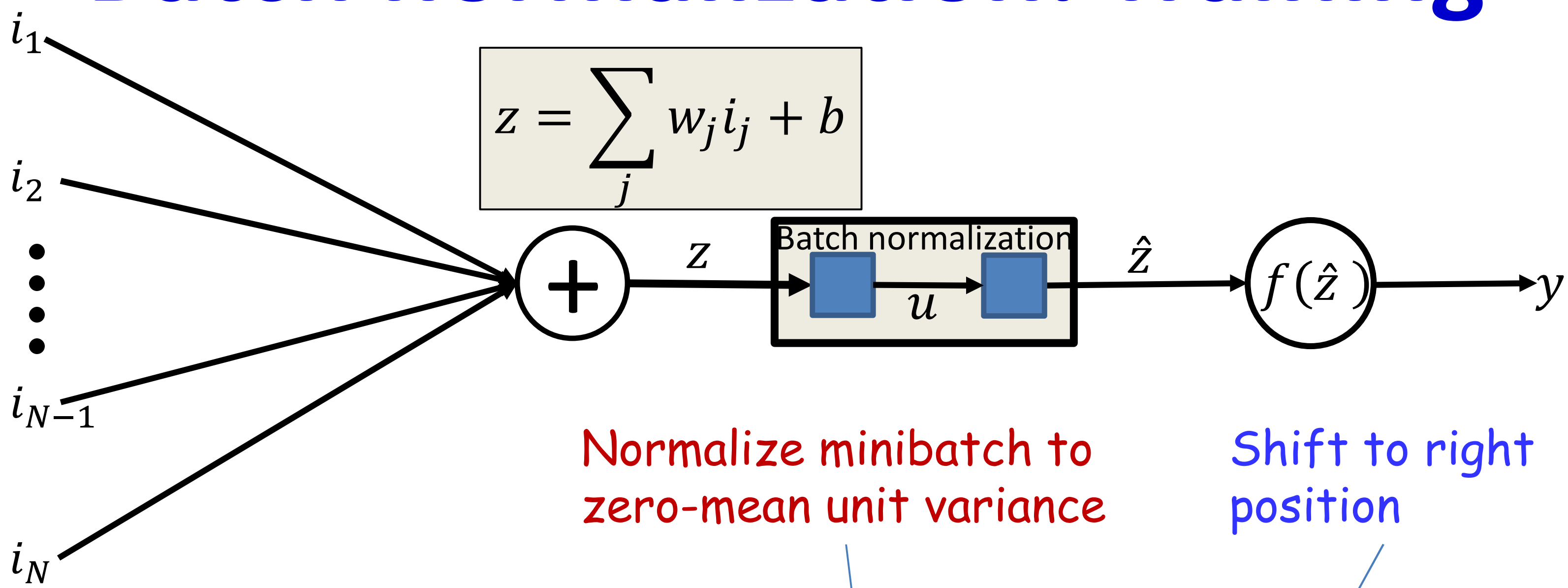
Batch normalization: Training



Normalize minibatch to zero-mean unit variance

Shift to right position

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

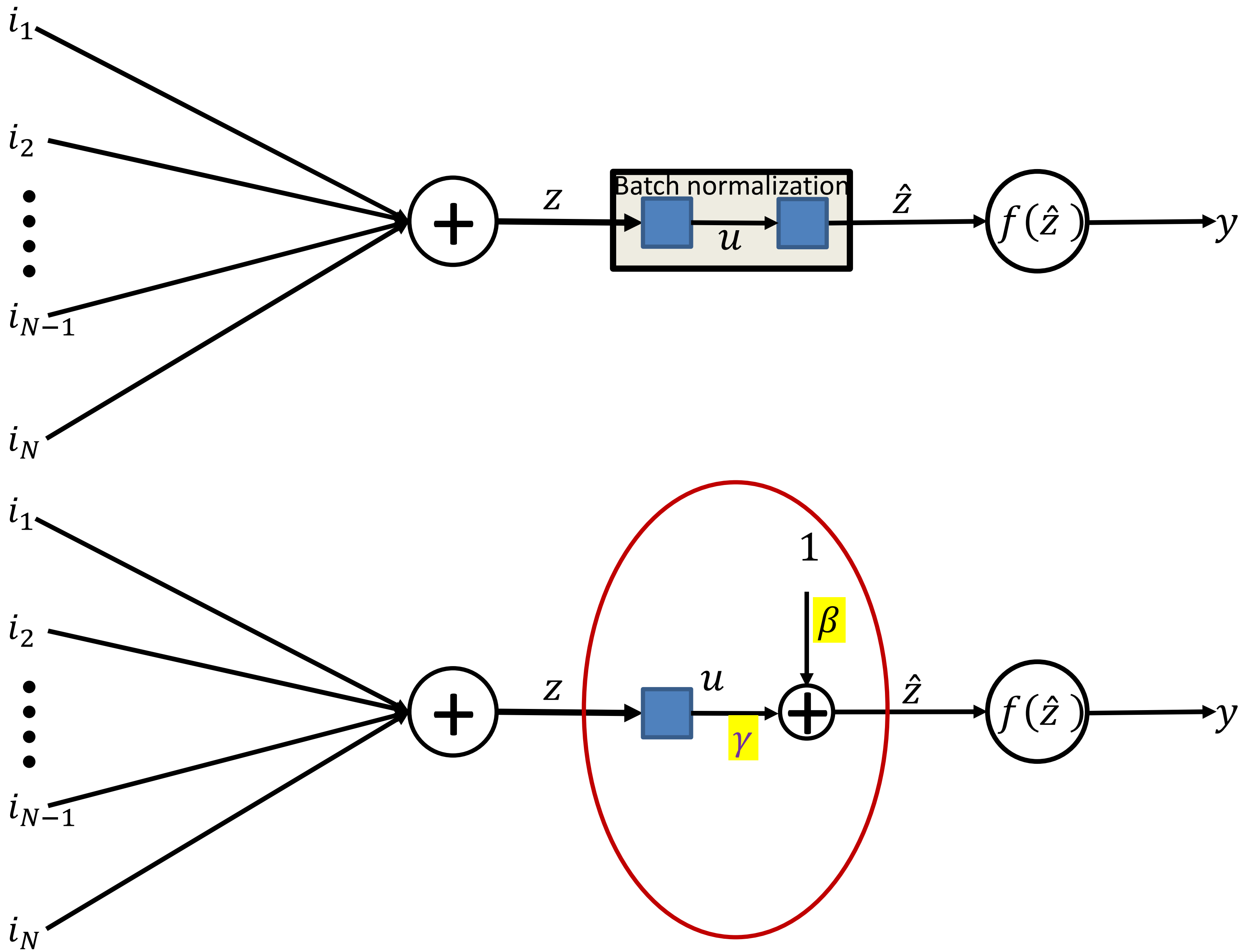
$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B} (z_i - \mu_B)^2$$

$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\hat{z}_i = \gamma u_i + \beta$$

- BN aggregates the statistics over a minibatch and normalizes the batch by them
- Normalized instances are “shifted” to a *unit-specific* location

A better picture for batch norm



A note on derivatives

- The minibatch loss is the average of the divergence between the actual and desired outputs of the network for all inputs in the minibatch

$$Loss(minibatch) = \frac{1}{B} \sum_t Div(Y_t(X_t), d_t(X_t))$$

- The derivative of the minibatch loss w.r.t. network parameters is the average of the derivatives of the divergences for the *individual* training instances w.r.t. parameters

$$\frac{dLoss(minibatch)}{dw_{i,j}^{(k)}} = \frac{1}{B} \sum_t \frac{dDiv(Y_t(X_t), d_t(X_t))}{dw_{i,j}^{(k)}}$$

- In conventional training, both, the output of the network in response to an input, and the derivative of the divergence for any input are independent of other inputs in the minibatch

- If we use Batch Norm, the above relation gets a little complicated

A note on derivatives

- The outputs are now functions of μ_B and σ_B^2 which are functions of the entire minibatch

$$Loss(minibatch)$$

$$= \frac{1}{B} \sum_t Div(Y_t(X_t, \mu_B, \sigma_B^2), d_t(X_t))$$

- The Divergence for each Y_t depends on *all* the X_t within the minibatch
  - Training instances within the minibatch are no longer independent

The actual divergence with BN

- The actual divergence for any minibatch with terms explicity written

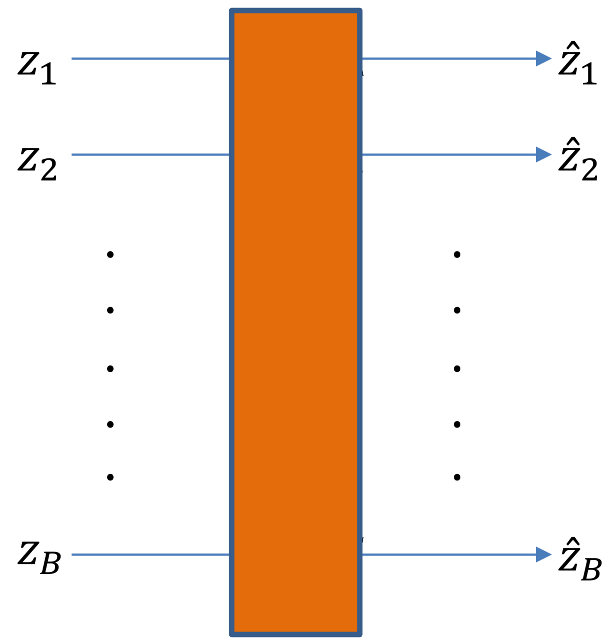
$$Loss(minibatch)$$

$$= \frac{1}{B}\sum_t Div\left(Y_t\left(X_t, \mu_B(X_t, X_{t'\neq t}), \sigma_B^2\left(X_t, X_{t'\neq t}, \mu_B(X_t, X_{t'\neq t})\right)\right), d_t(X_t)\right)$$

- We need the derivative for this function

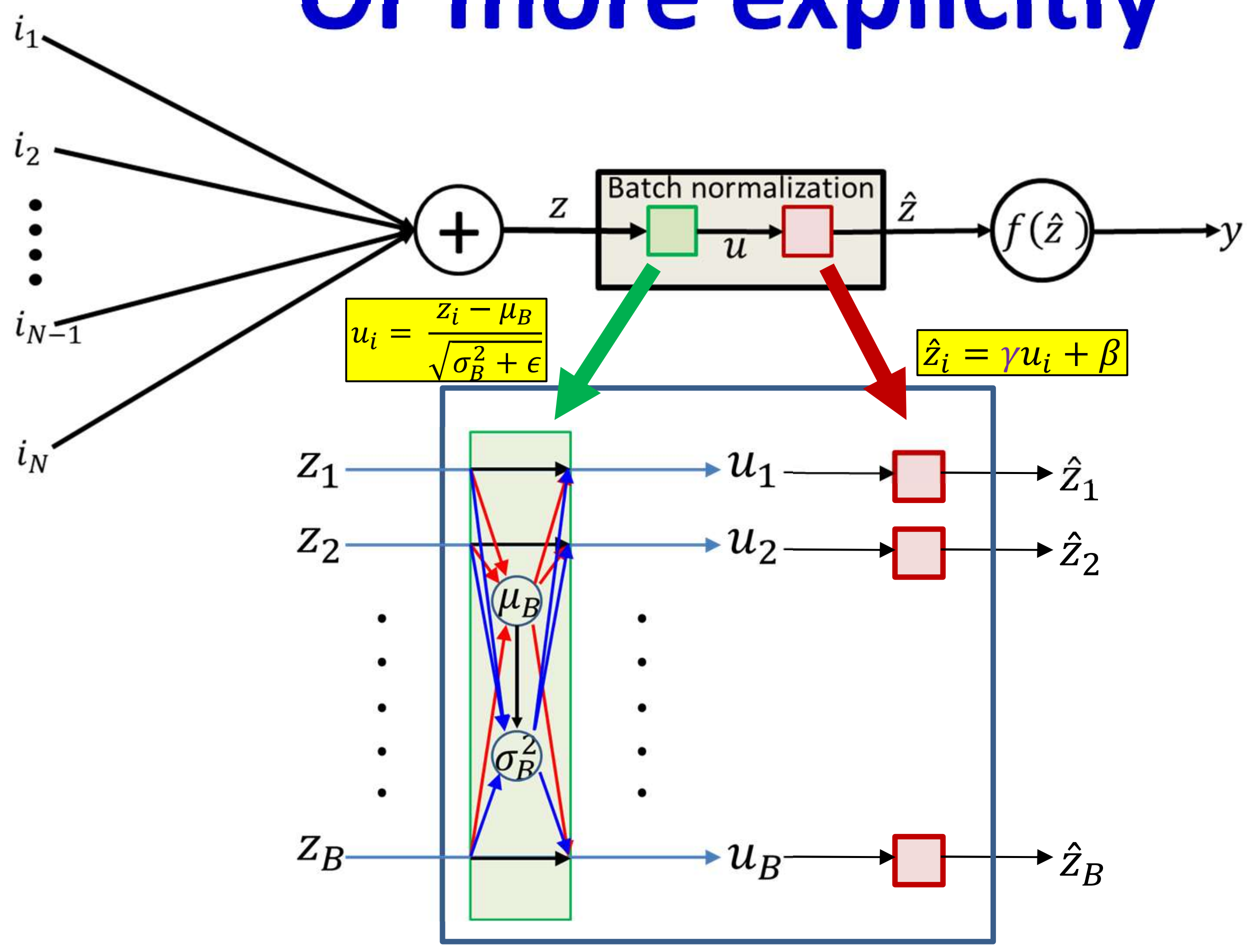
- To derive the derivative lets consider the dependencies at a *single* neuron
  – Shown pictorially in the following slide

Batchnorm is a vector function over the minibatch



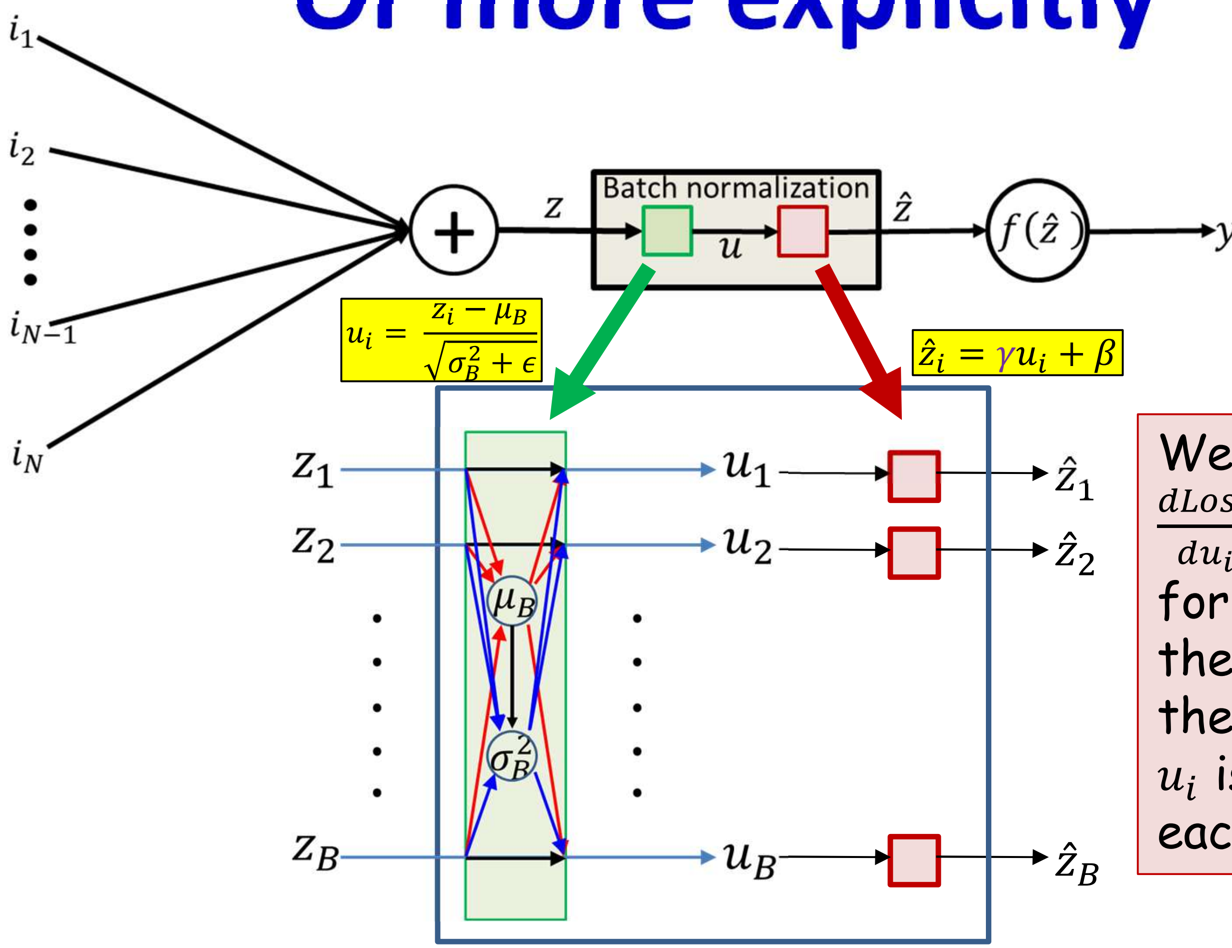
- Batch normalization is really a *vector* function applied over all the inputs from a minibatch
  - Every z_i affects every $\hat{z}_j$
  - Shown on the next slide
- To compute the derivative of the minibatch loss w.r.t any z_i, we must consider all $\hat{z}_j s$ in the batch

Or more explicitly



- The computation of mini-batch normalized u's is a vector function
  - Invoking mean and variance statistics across the minibatch
- The subsequent shift and scaling is individually applied to each u to compute the corresponding $\hat{z}$

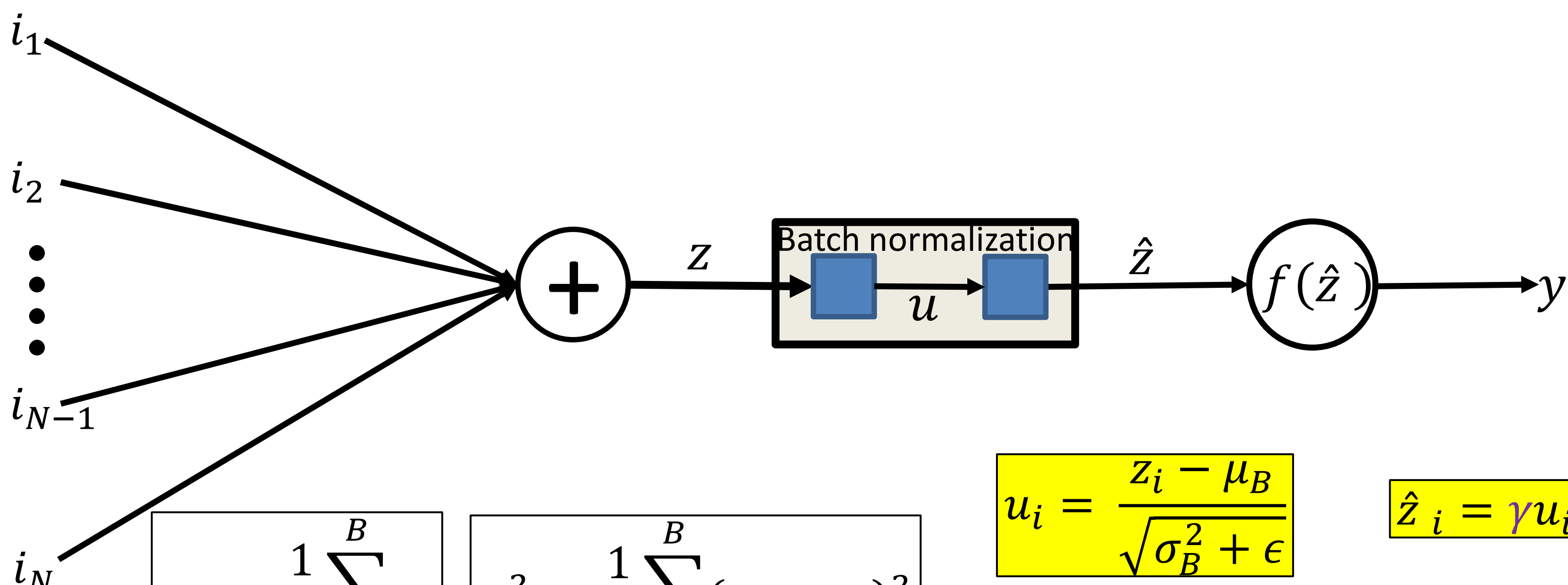
Or more explicitly



We can compute $\frac{dLoss}{du_i}$ individually for each u_i because the processing *after* the computation of u_i is independent for each u_i

- The computation of mini-batch normalized u's is a vector function
  - Invoking mean and variance statistics across the minibatch
- The subsequent shift and scaling is individually applied to each u to compute the corresponding $\hat{z}$

Batch normalization: Forward pass



$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

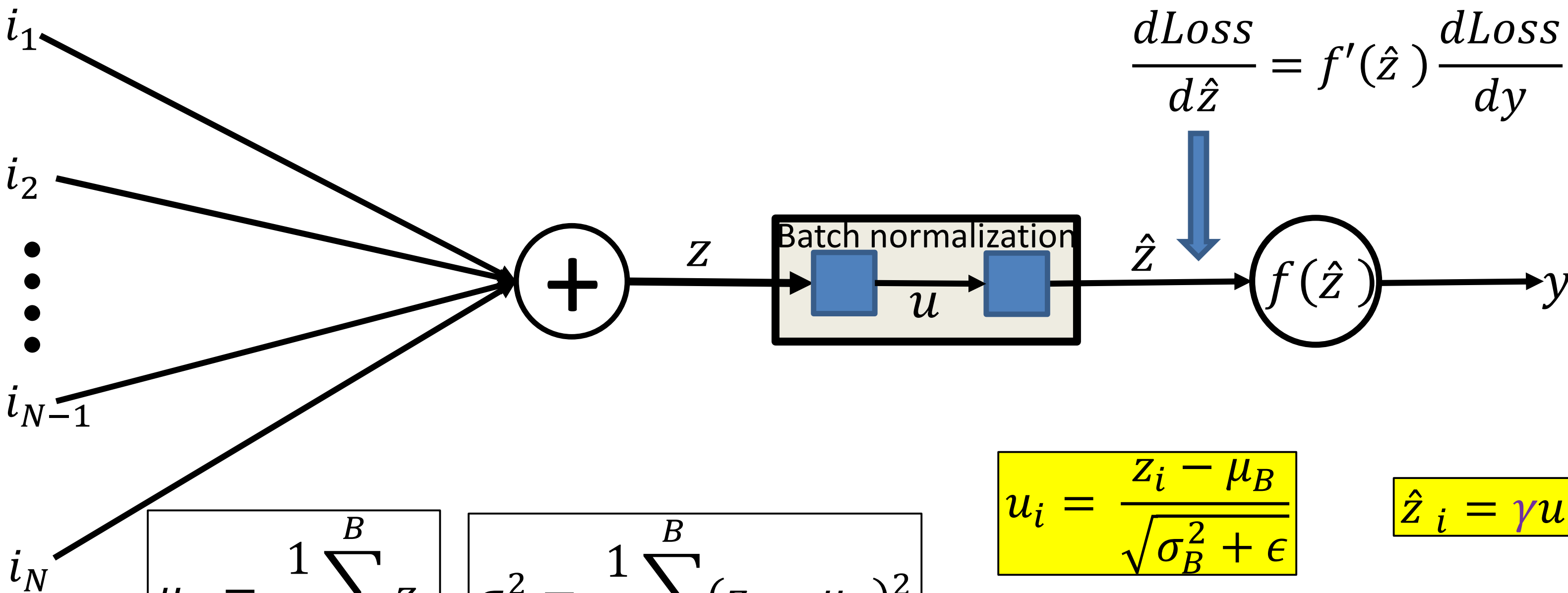
$$\hat{z}_i = \gamma u_i + \beta$$

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B} (z_i - \mu_B)^2$$

Batch normalization: Backpropagation

$$\frac{dLoss}{d\hat{z}} = f'(\hat{z})\frac{dLoss}{dy}$$



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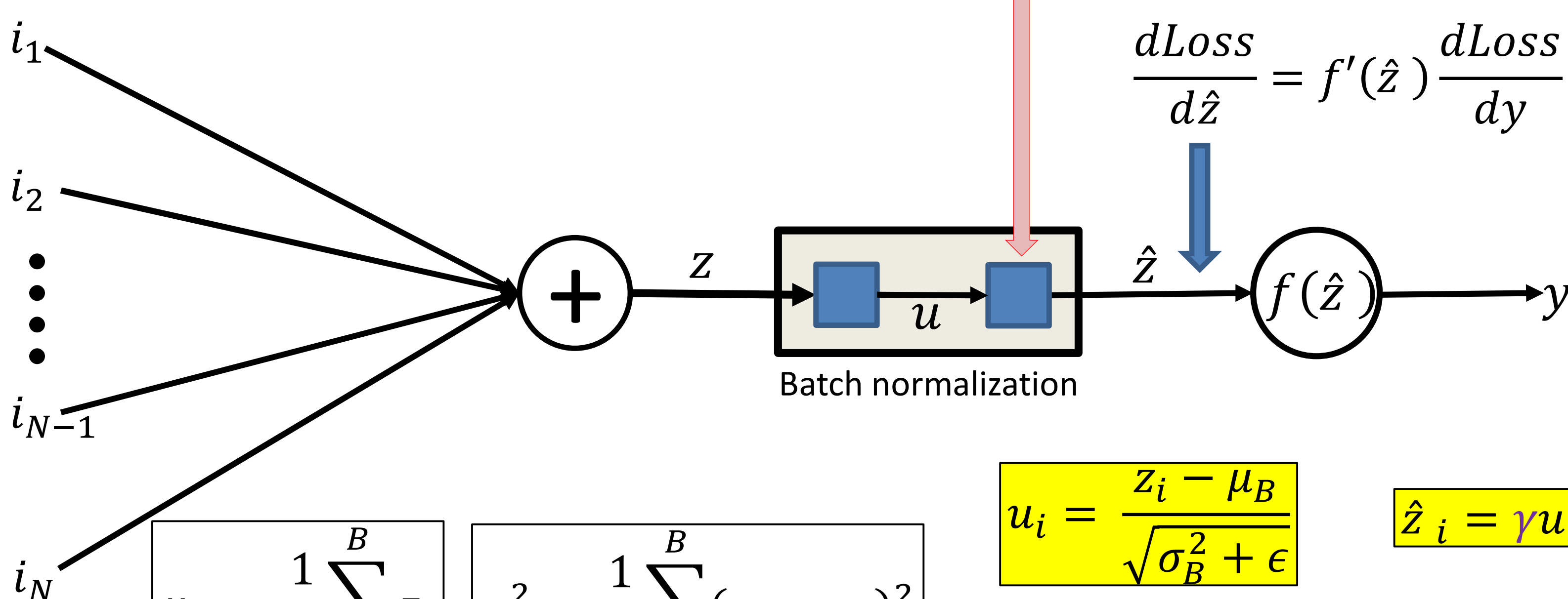
Batch normalization: Backpropagation

$$\frac{dLoss}{d\beta} = \frac{dLoss}{d\hat{z}}$$

$$\frac{dLoss}{d\gamma} = u\frac{dLoss}{d\hat{z}}$$

Parameters to be learned

$$\frac{dLoss}{d\hat{z}} = f'(\hat{z})\frac{dLoss}{dy}$$



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Batch normalization: Backpropagation

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Parameters to be learned

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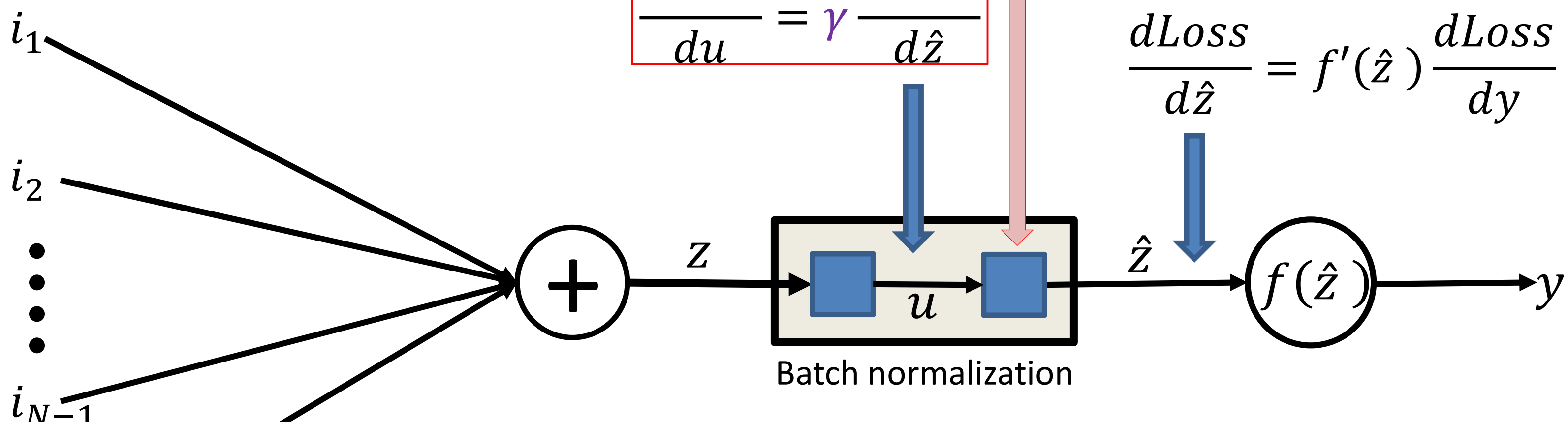
$$\frac{dLoss}{d\hat{z}} = f'(\hat{z}\,)\frac{dLoss}{dy}$$



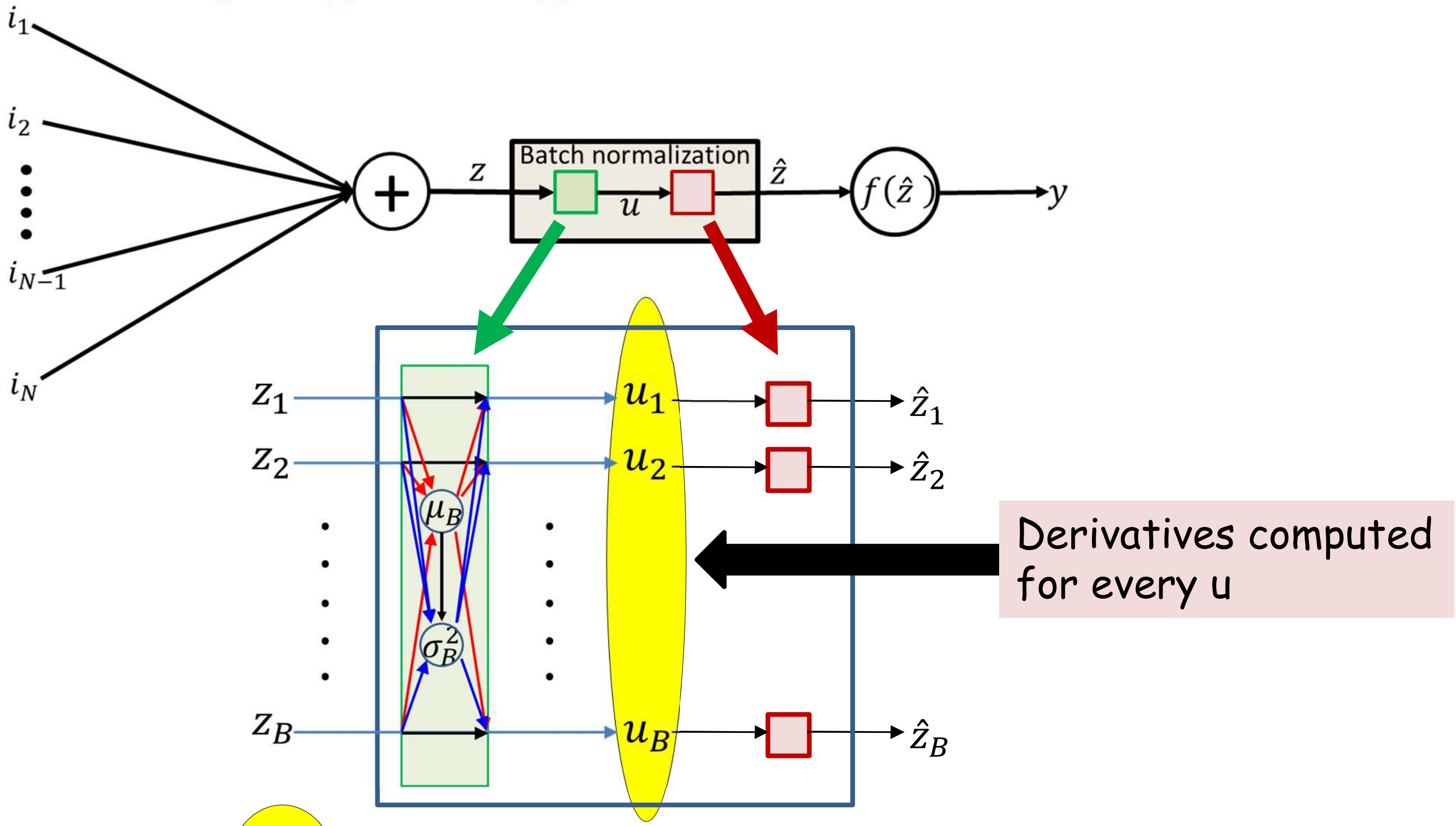
$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\hat{z}_{\,i} = \gamma u_i + \beta$$

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

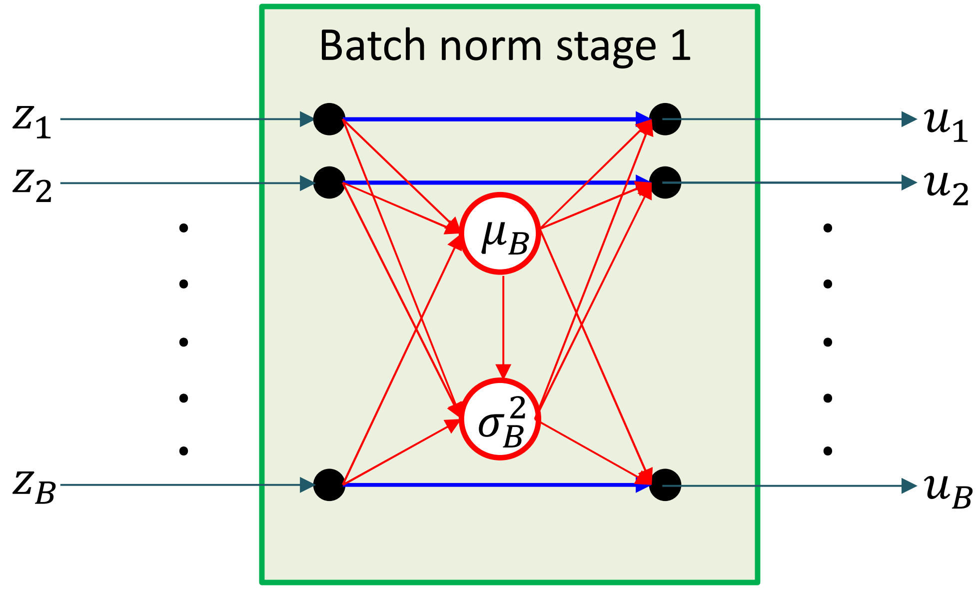
$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B}(z_i - \mu_B)^2$$

Propogating the derivative



- We now have $\frac{dLoss}{du_i}$ for every u_i
- We must propagate the derivative through the first stage of BN
  - Which is a vector operation over the minibatch

The first stage of batchnorm

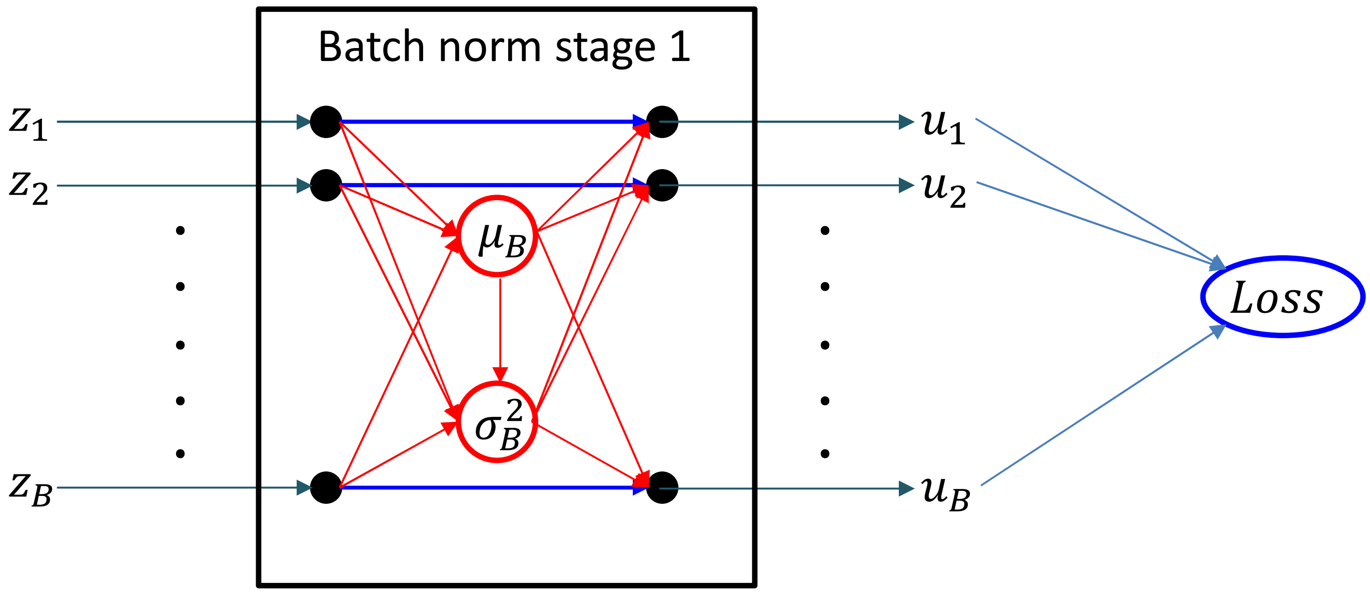


- The complete dependency figure for the first “normalization” stage of Batchnorm
  - Which computes the centered “u”s from the “z”s for the minibatch

- Note : inputs and outputs are different *instances* in a minibatch
  - The diagram represents BN occurring at a *single neuron*

- Let’s complete the figure and work out the derivatives

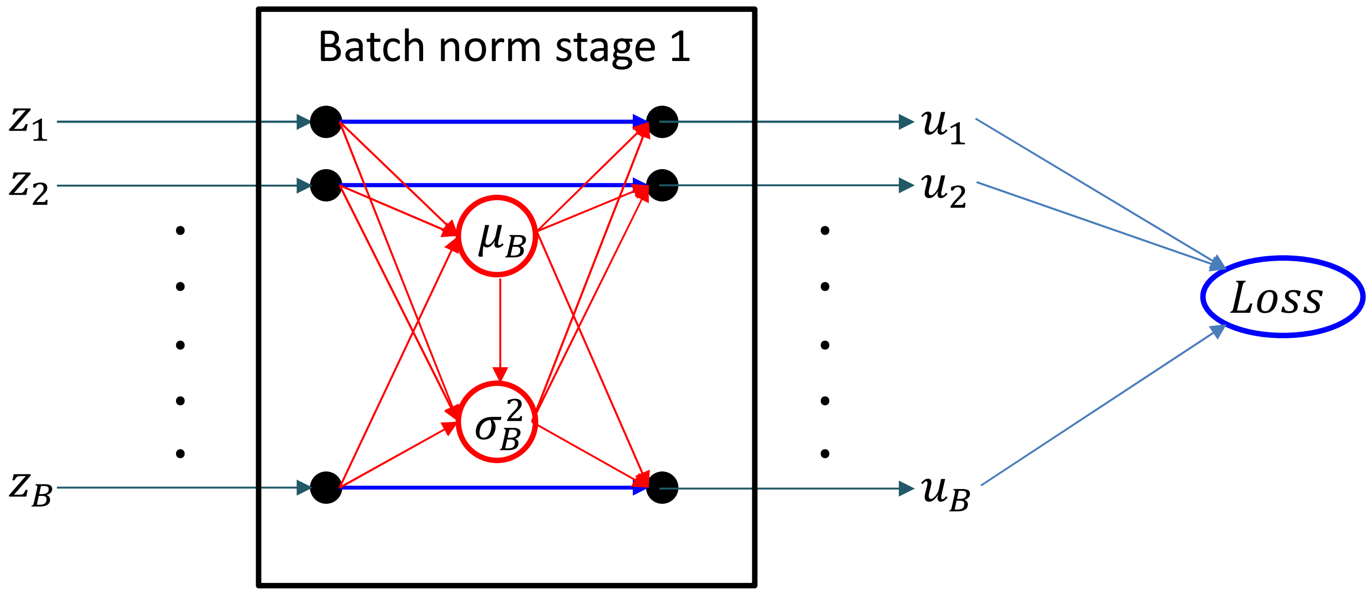
The first stage of Batchnorm



- The complete derivative of the mini-batch loss w.r.t. z_i

$$\frac{dLoss}{dz_i} = \sum_j \frac{dLoss}{du_j} \frac{du_j}{dz_i}$$

The first stage of Batchnorm

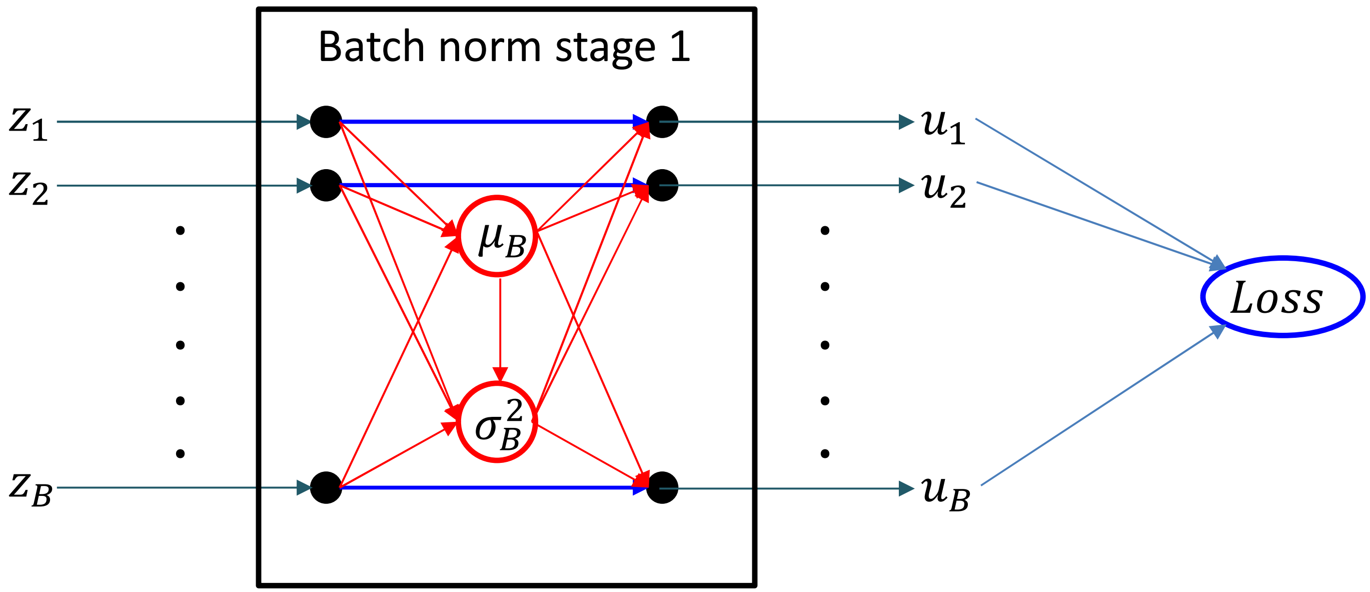


- The complete derivative of the mini-batch loss w.r.t. z_i

$$\frac{dLoss}{dz_i} = \sum_j \frac{dLoss}{du_j}\frac{du_j}{dz_i}$$

Already computed

The first stage of Batchnorm



- The complete derivative of the mini-batch loss w.r.t. z_i

$$\frac{dLoss}{dz_i} = \sum_j \frac{dLoss}{du_j} \frac{du_j}{dz_i}$$

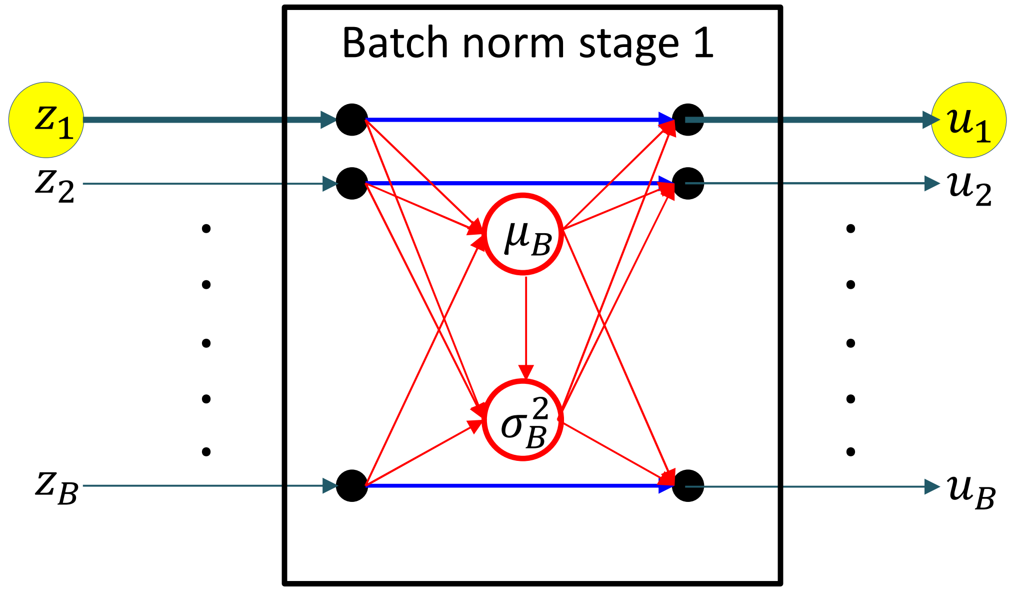
Must compute for every i,j pair

The first stage of Batchnorm

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B}(z_i - \mu_B)^2$$

$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$



- The derivative for the "through" line ($i = j$)

$$\frac{du_i}{dz_i} =$$

The first stage of Batchnorm

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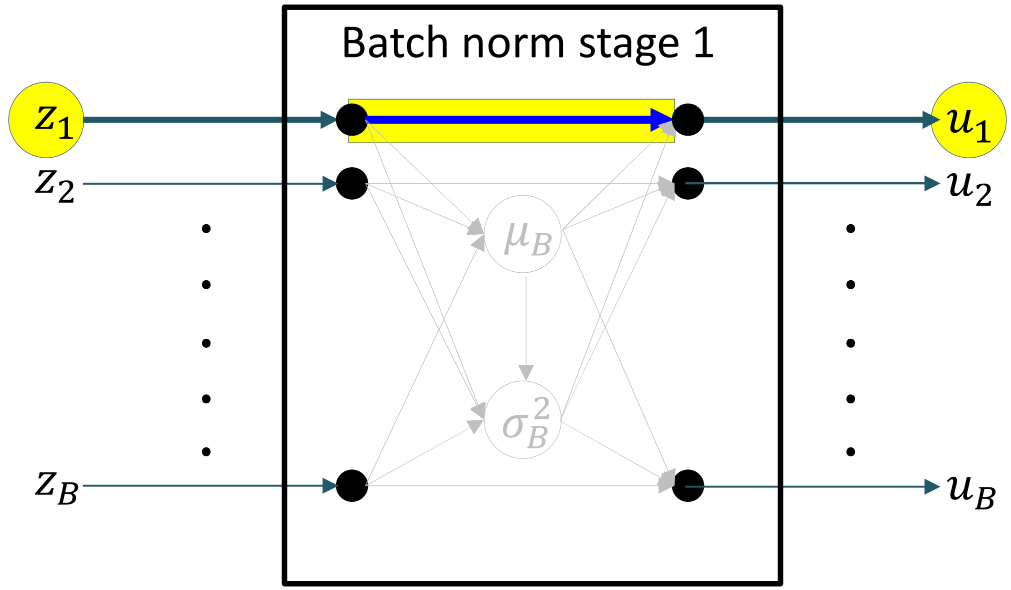

- The derivative for the “through” line ($i = j$)

$$\frac{du_i}{dz_i} = \frac{\partial u_i}{\partial z_i} +$$

The first stage of Batchnorm

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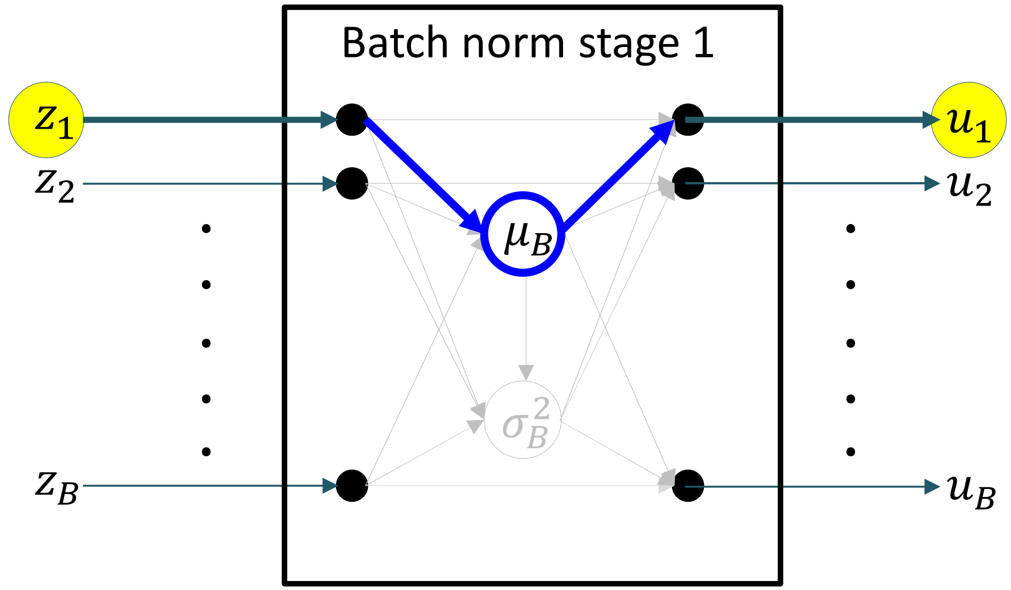

- The derivative for the "through" line ($i = j$)

$$\frac{du_i}{dz_i} = \frac{\partial u_i}{\partial z_i} + \frac{\partial u_i}{\partial \mu_B}\frac{d\mu_B}{dz_i} +$$

The first stage of Batchnorm

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

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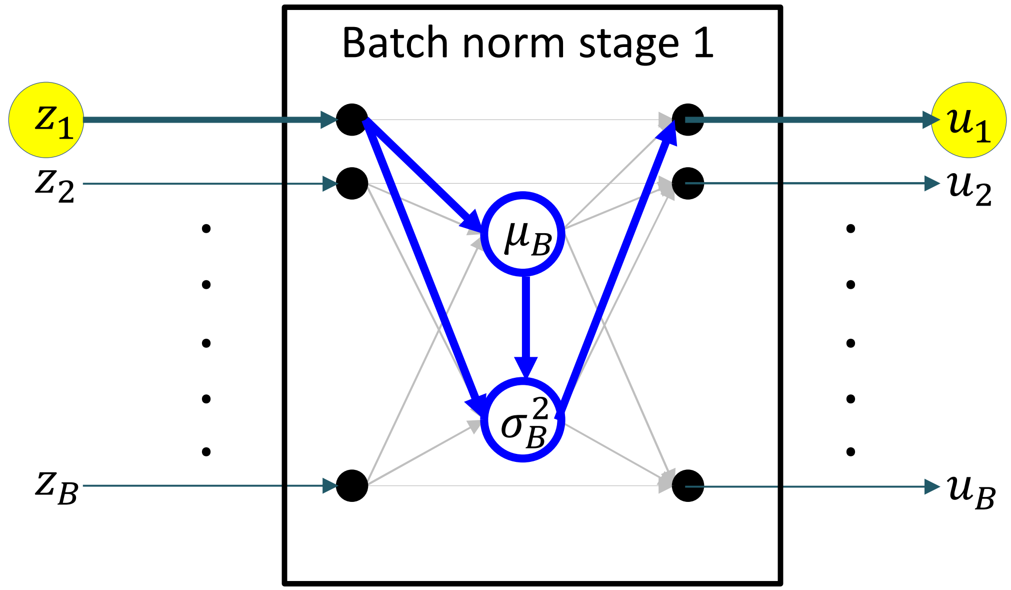

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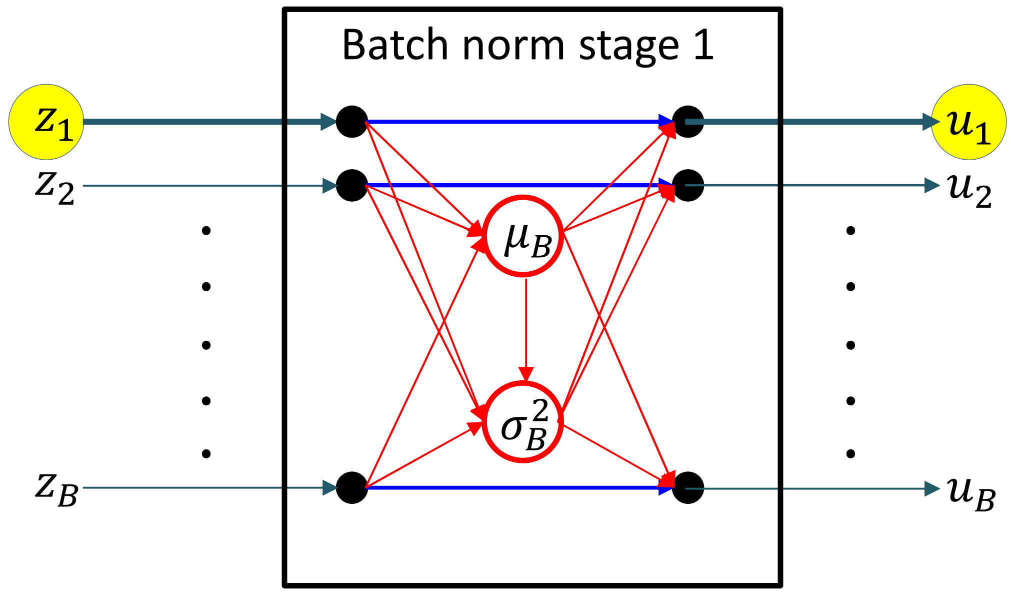

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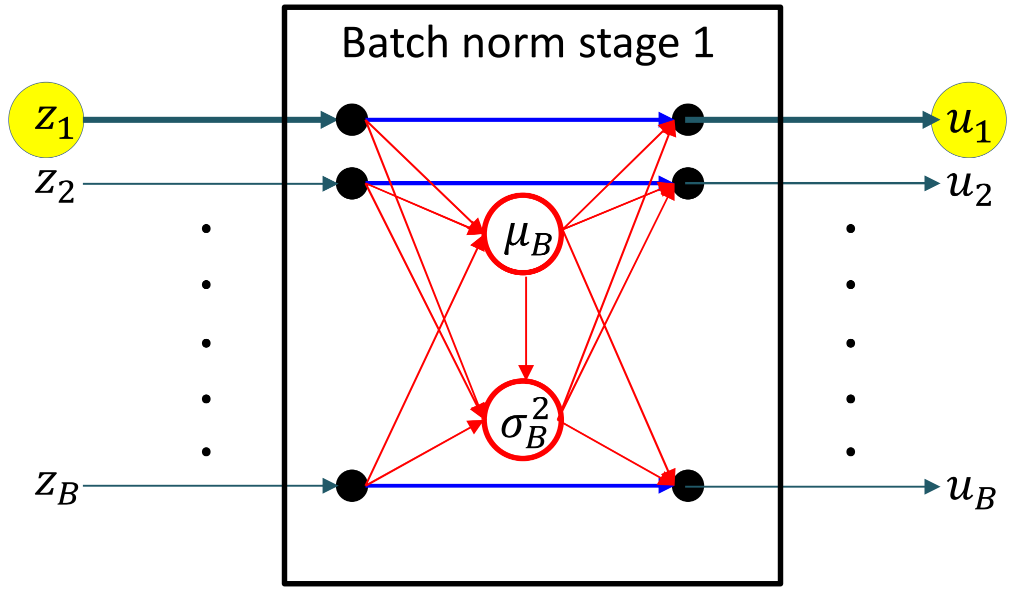

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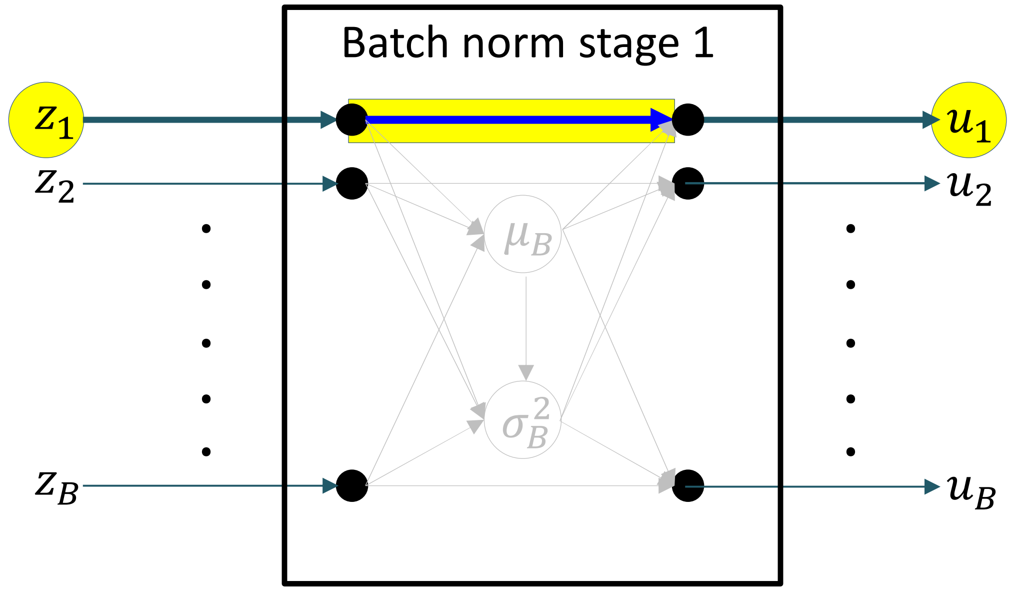

- From the highlighted relation

$$\frac{\partial u_i}{\partial z_i} = \frac{1}{\sqrt{\sigma_B^2 + \epsilon}}$$

The first stage of Batchnorm

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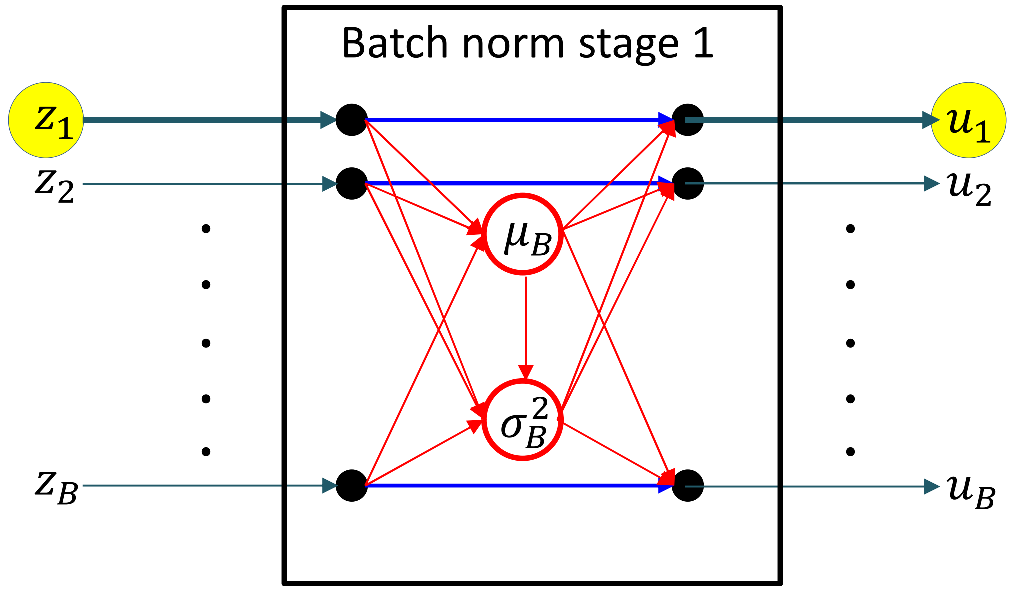

- The derivative for the "through" line ($i = j$)

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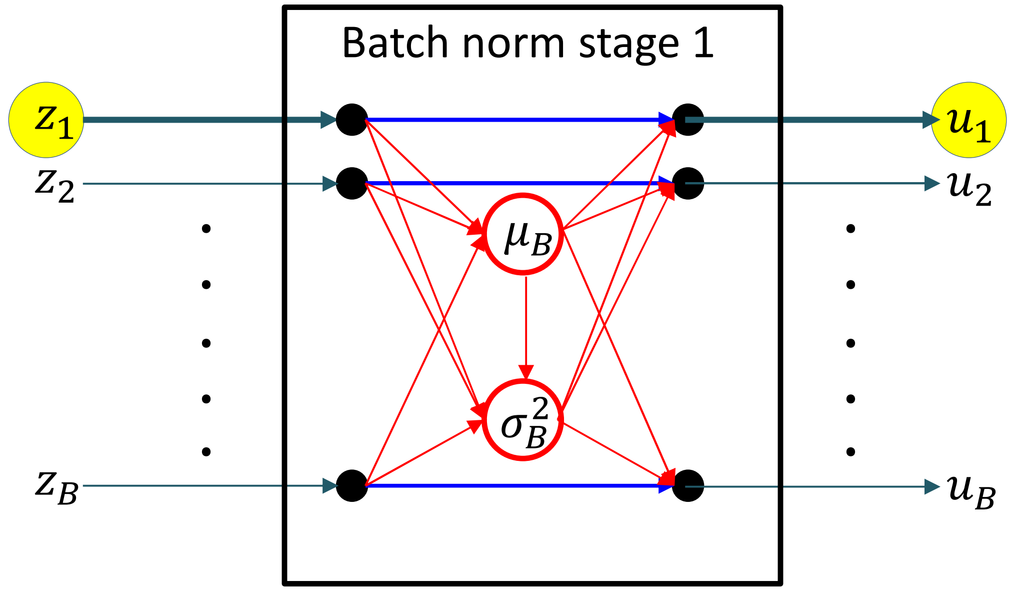

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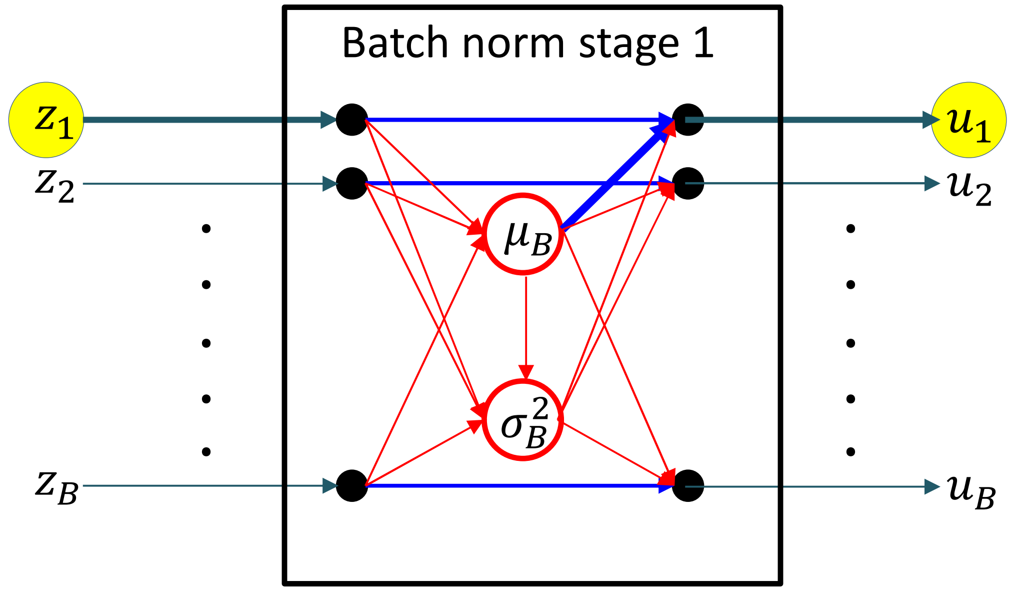

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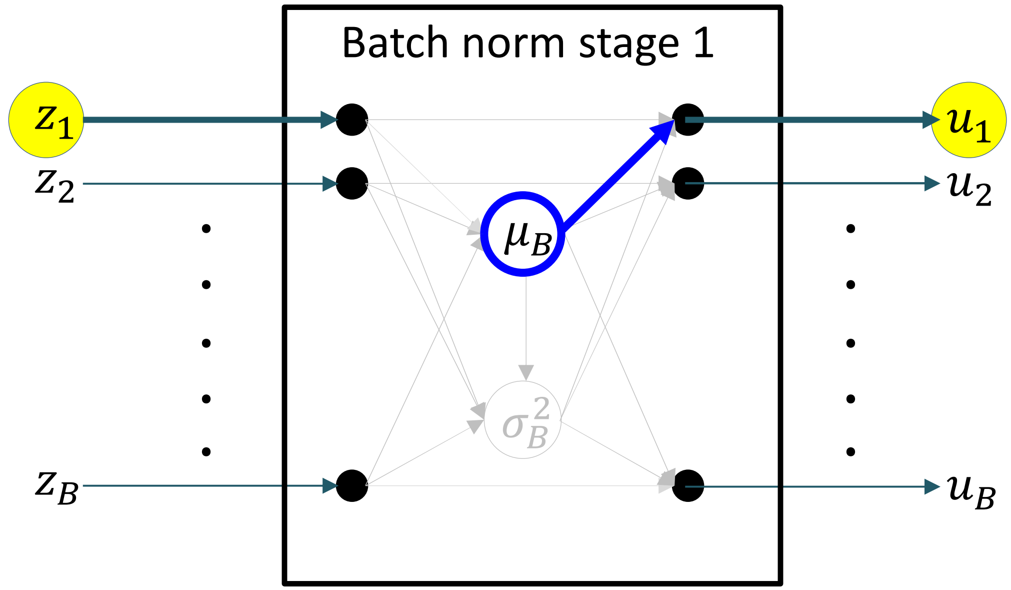

- From the highlighted relation

$$\frac{\partial u_i}{\partial \mu_B} = \frac{-1}{\sqrt{\sigma_B^2 + \epsilon}}$$

The first stage of Batchnorm

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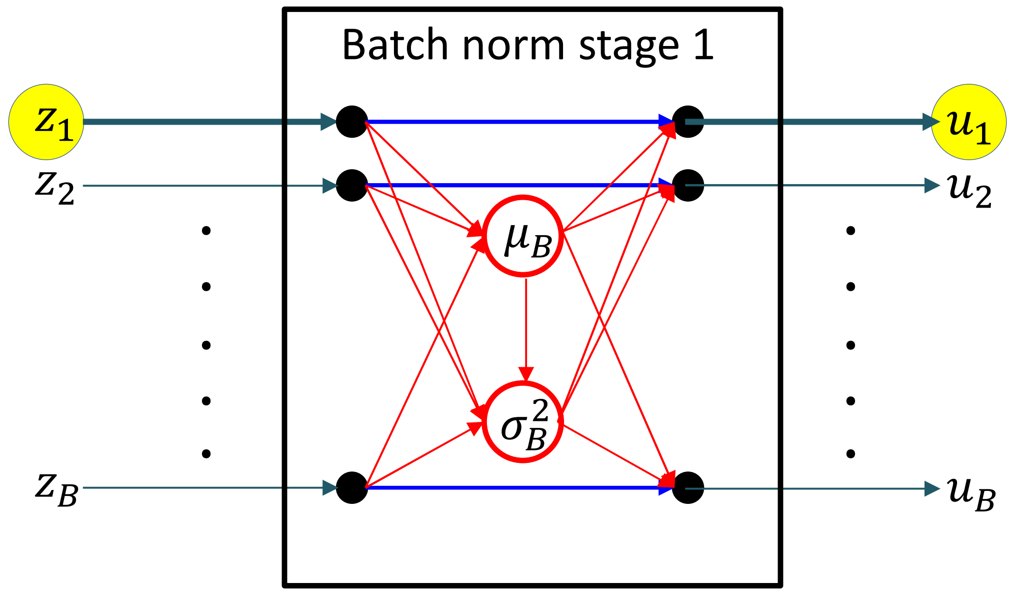

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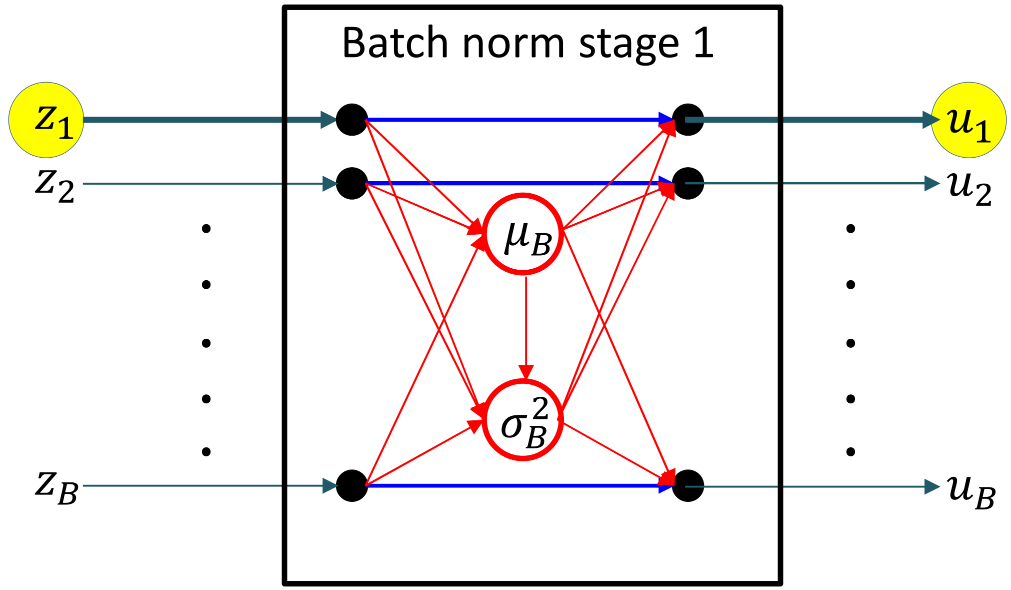

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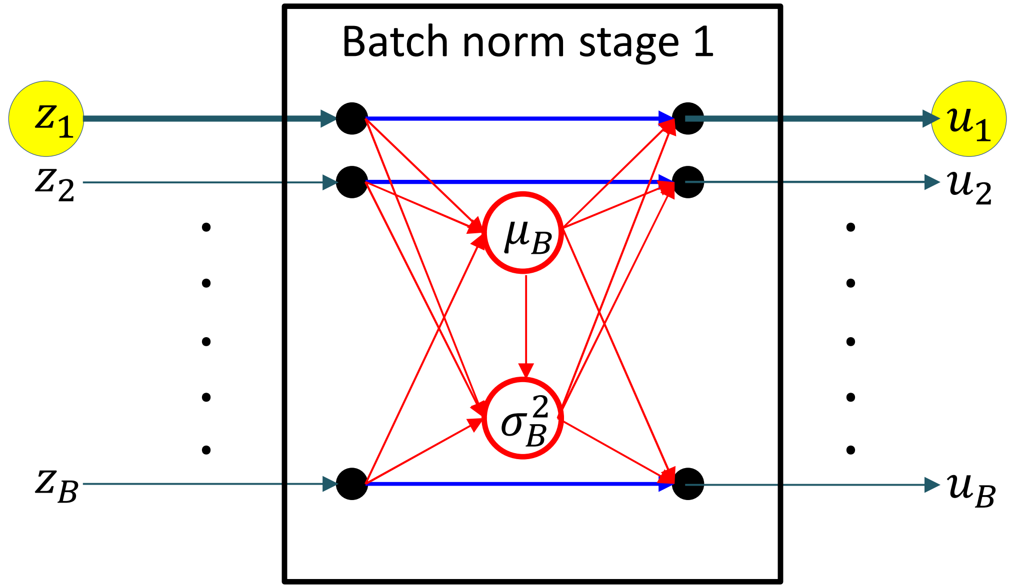

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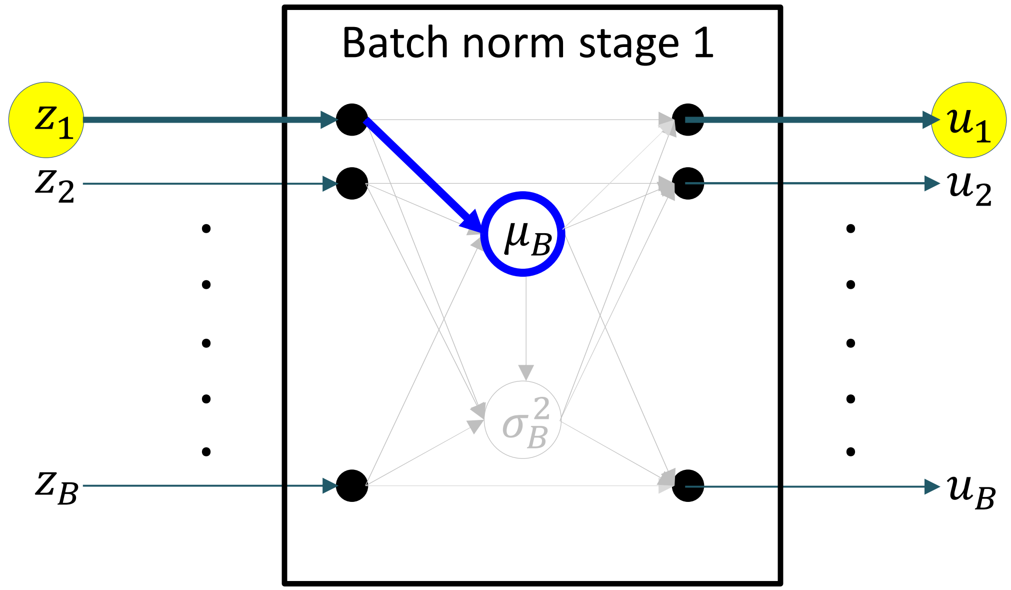

- From the highlighted relation

$$\frac{\partial \mu_B}{\partial z_i} = \frac{1}{B}$$

The first stage of Batchnorm

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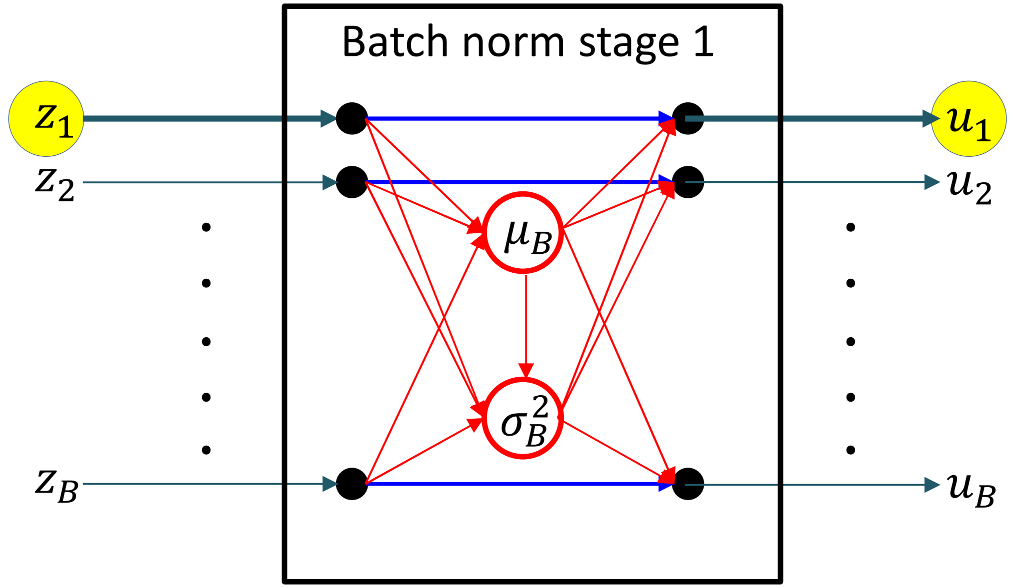

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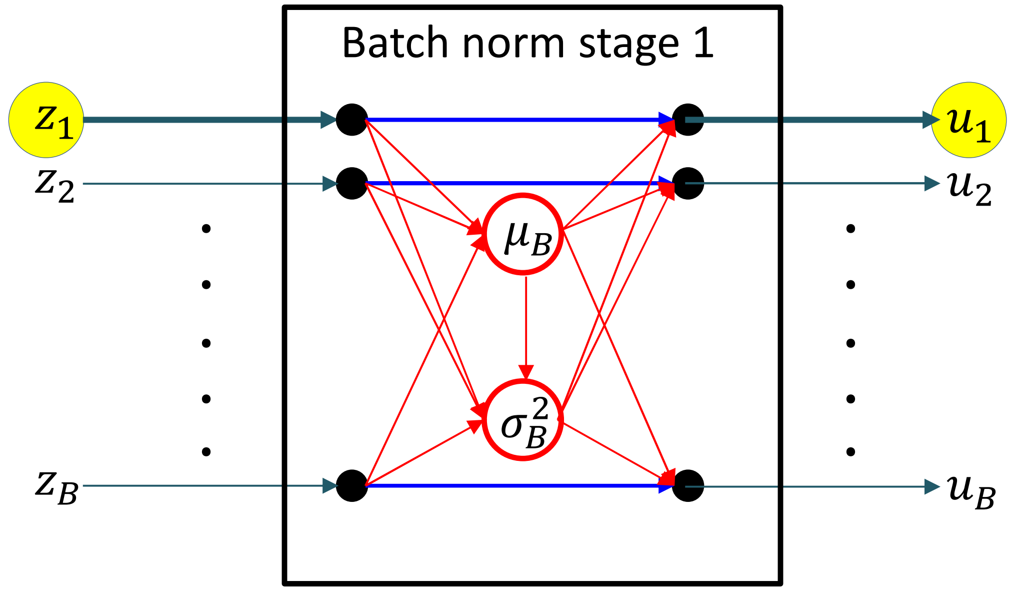

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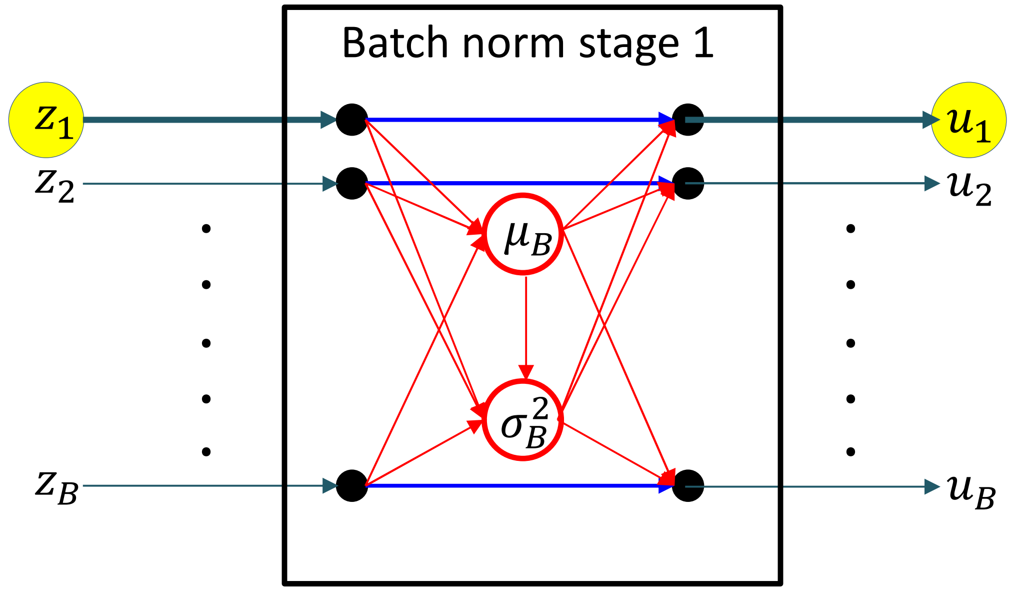

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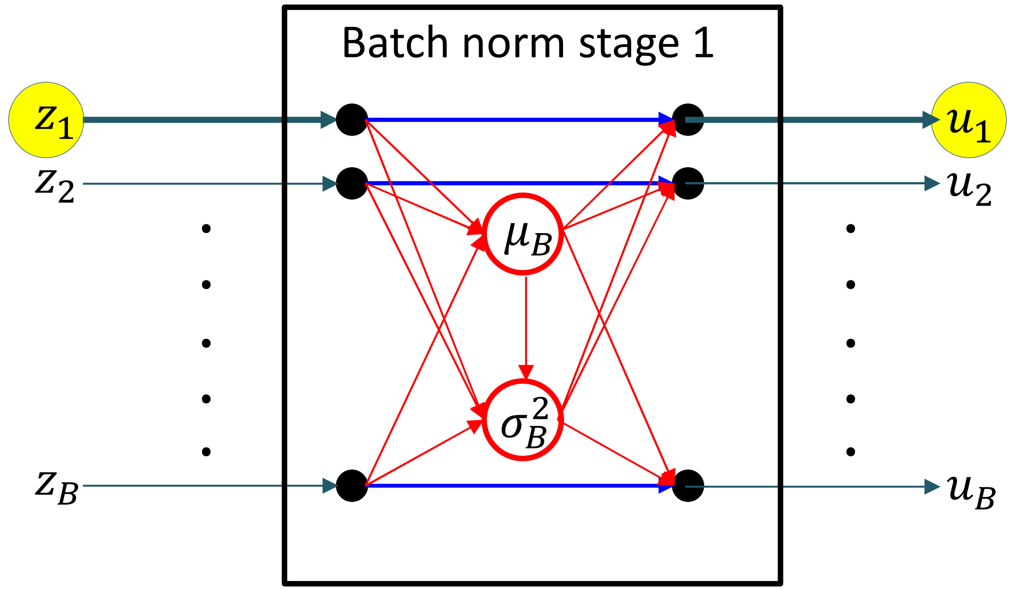

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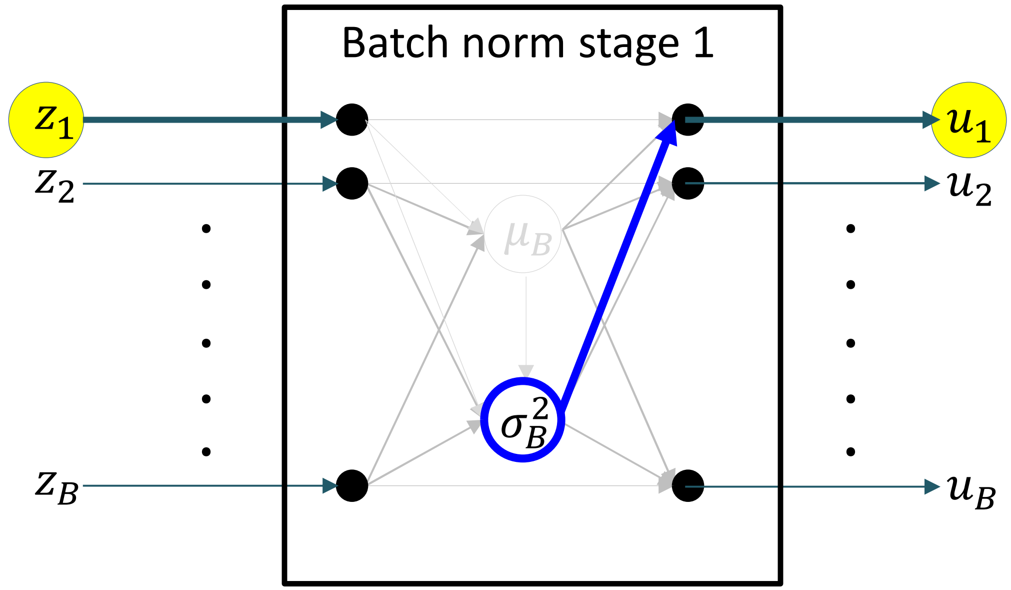

- From the highlighted equation

$$\frac{\partial u_i}{\partial \sigma_B^2} = \frac{-(z_i - \mu_B)}{2}\left(\sigma_B^2 + \epsilon\right)^{-3/2}$$

The first stage of Batchnorm

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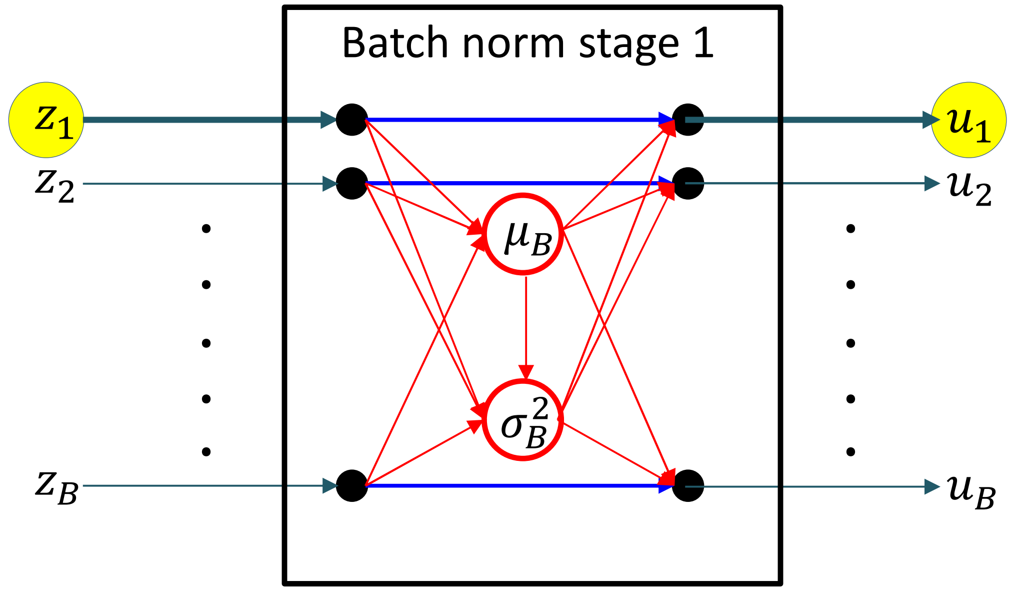

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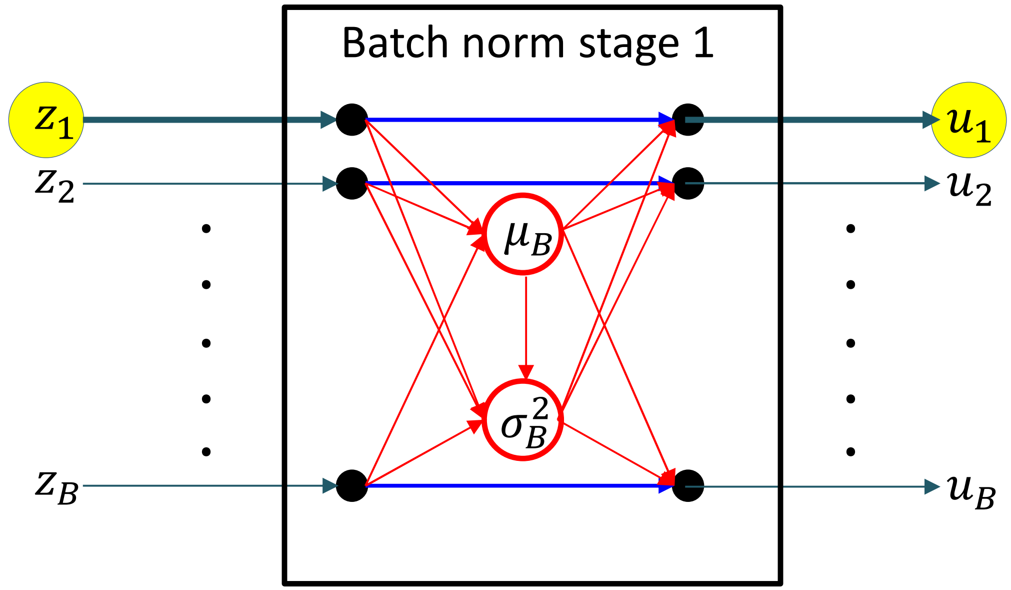

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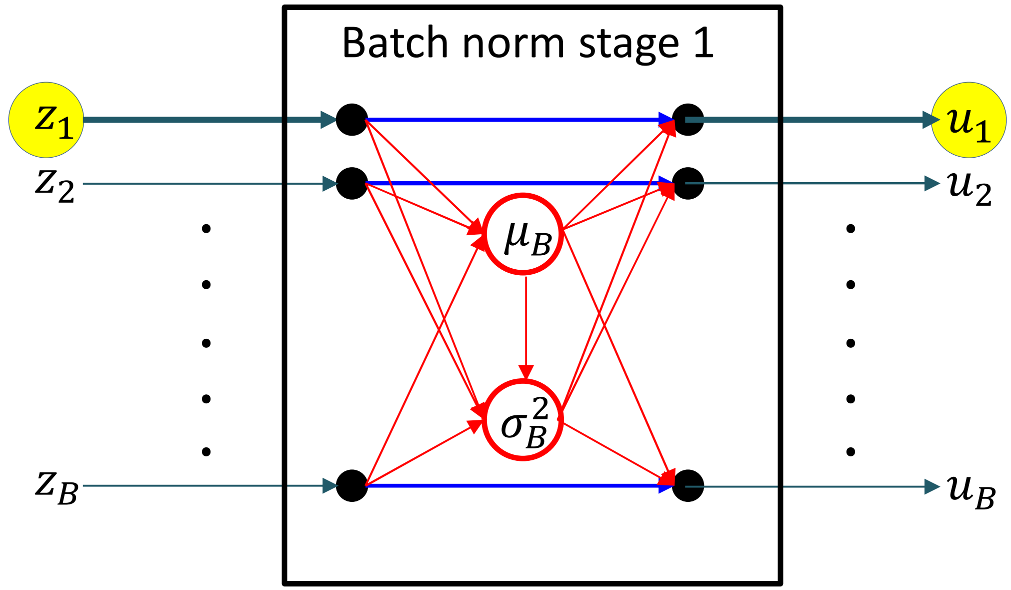

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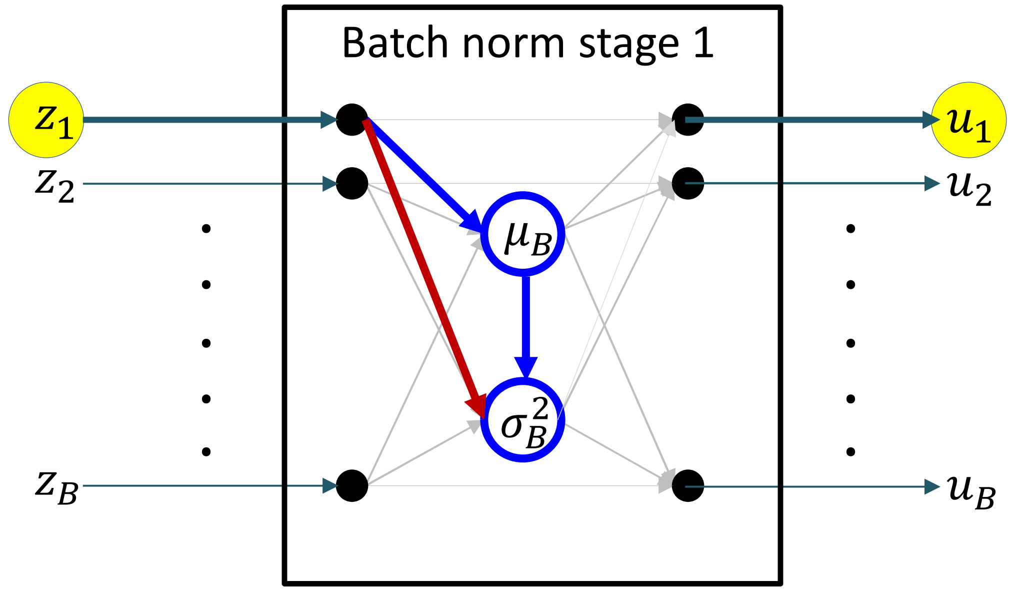

- From the highlighted equations

$$\frac{d\sigma_B^2}{dz_i} = \frac{\partial \sigma_B^2}{\partial z_i} + \frac{\partial \sigma_B^2}{\partial \mu_B}\frac{d\mu_B}{dz_i}$$

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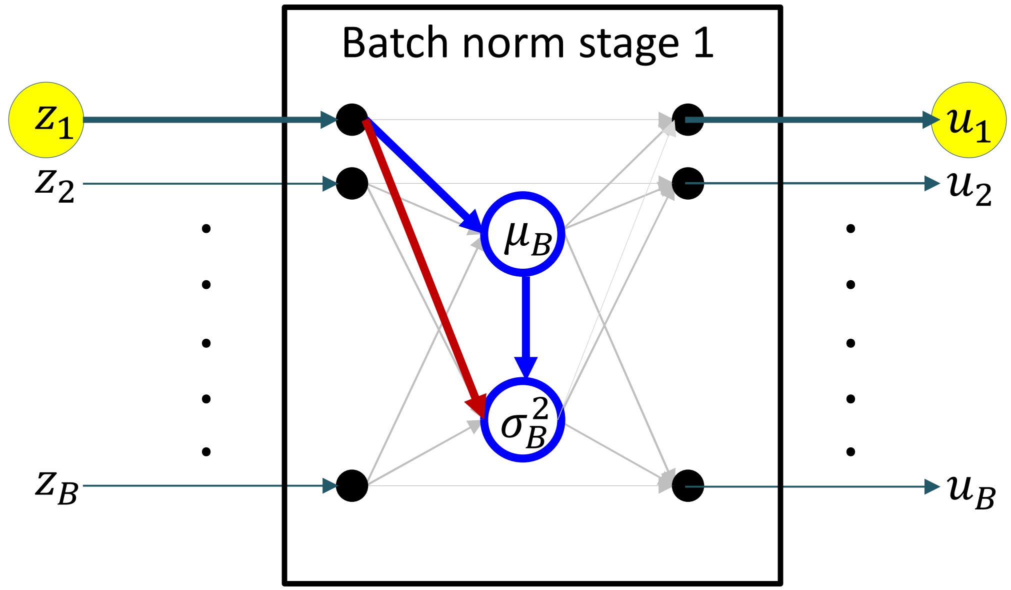

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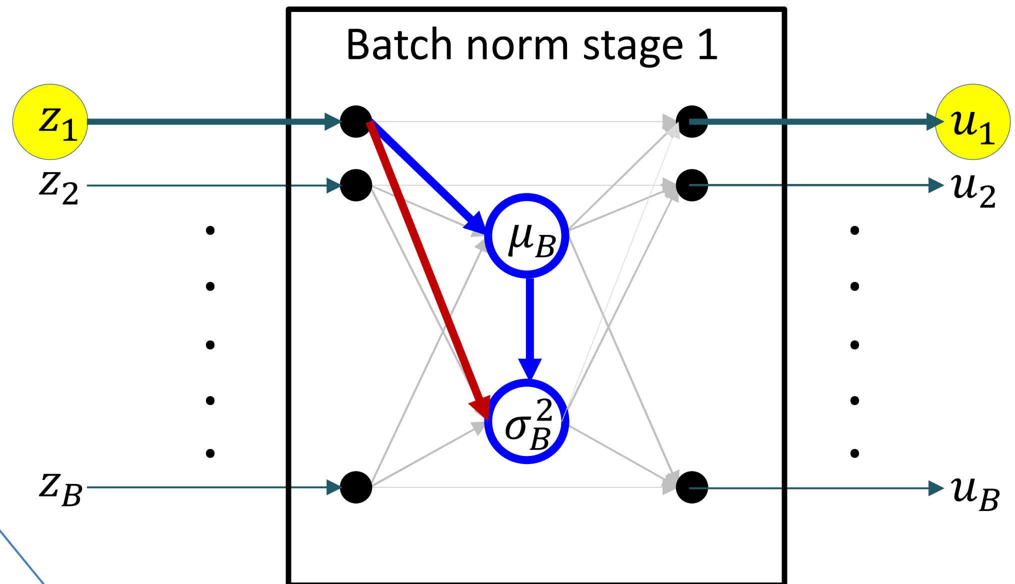

- From the highlighted equations

$$\frac{\partial \sigma_B^2}{\partial z_i} = \frac{2(z_i - \mu_B)}{B}$$

The first stage of Batchnorm

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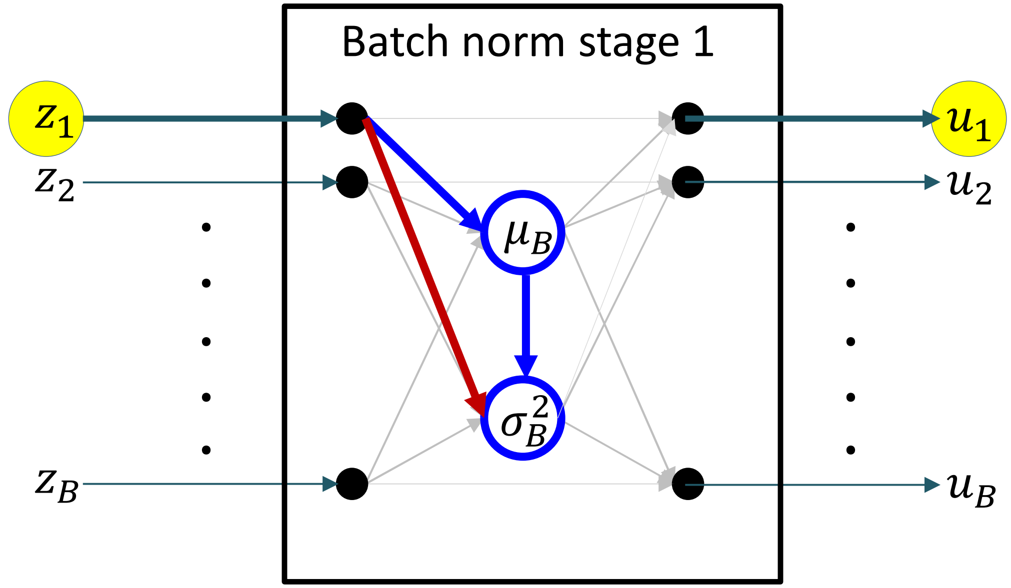

- From the highlighted equations

$$\frac{d\sigma_B^2}{dz_i} = \frac{\partial \sigma_B^2}{\partial z_i} + \frac{\partial \sigma_B^2}{\partial \mu_B}\frac{d\mu_B}{dz_i}$$

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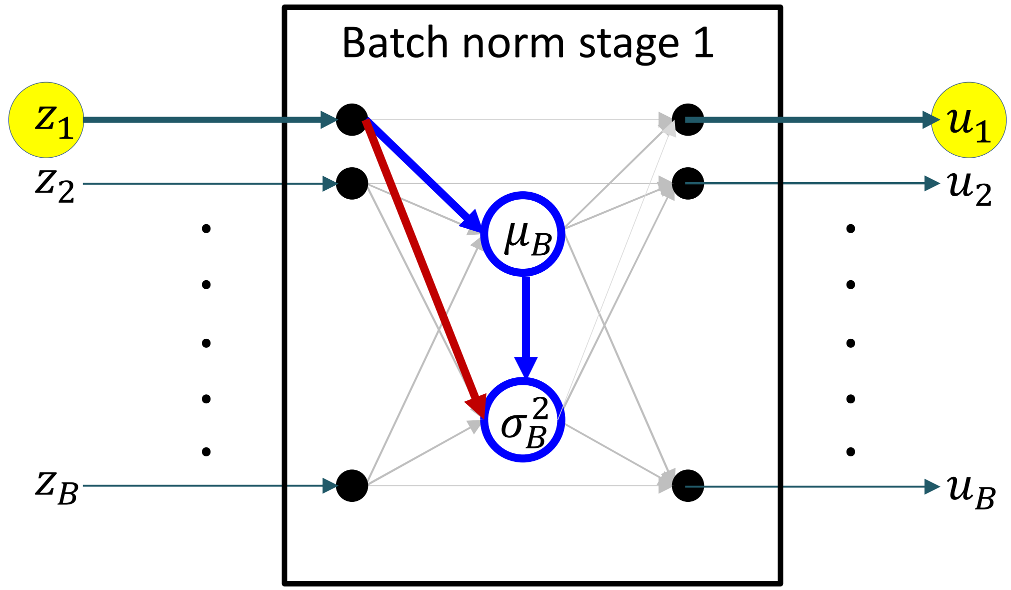


- From the highlighted equations

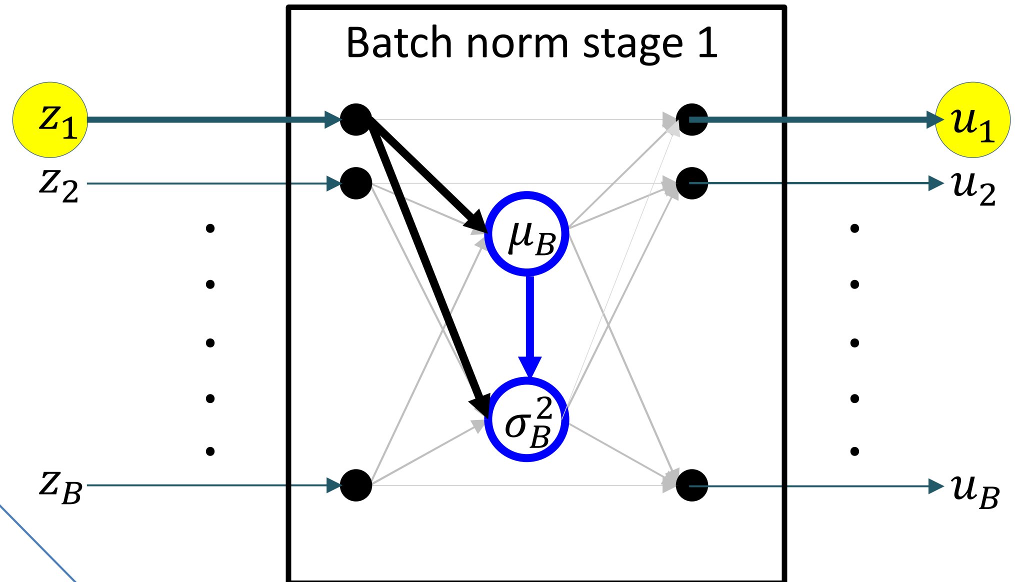
$$\frac{d\sigma_B^2}{dz_i} = \frac{2(z_i - \mu_B)}{B} + \frac{\partial \sigma_B^2}{\partial \mu_B}\frac{d\mu_B}{dz_i}$$

The first stage of Batchnorm

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B} (z_i - \mu_B)^2$$

$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$



$$\frac{\partial \sigma_B^2}{\partial \mu_B} = \frac{1}{B}\sum_{i=1}^{B} -2(z_i - \mu_B) = -2\left(\frac{1}{B}\sum_{i=1}^{B} z_i - \frac{1}{B}\sum_{i=1}^{B} \mu_B\right)$$

$$= -2\left(\mu_B - \frac{1}{B}B\mu_B\right) = -2(\mu_B - \mu_B) = 0$$

The first stage of Batchnorm

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

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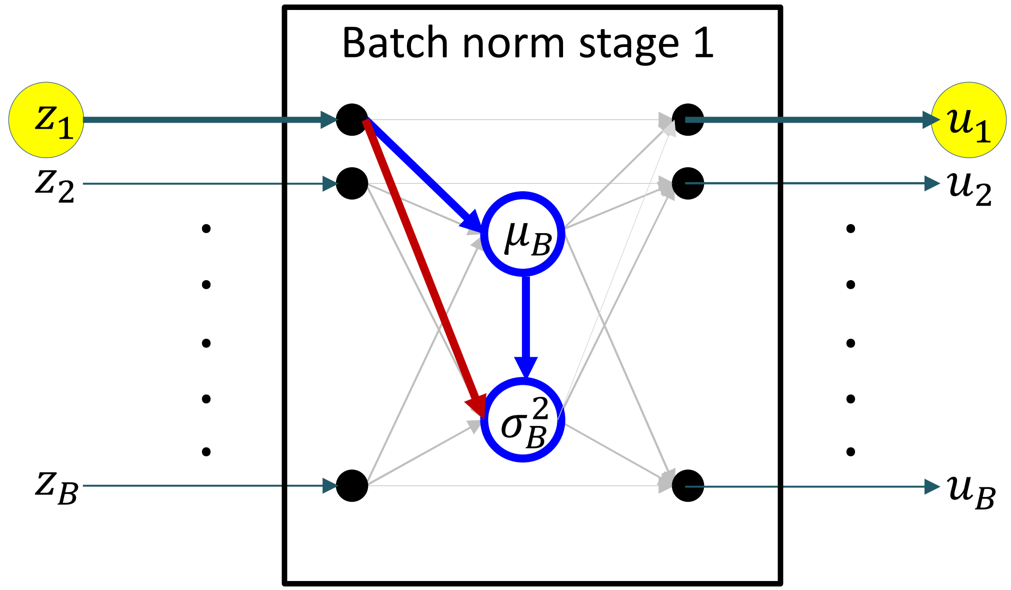

- From the highlighted equations

$$\frac{d\sigma_B^2}{dz_i} = \frac{2(z_i - \mu_B)}{B} + \frac{\partial \sigma_B^2}{\partial \mu_B}\frac{d\mu_B}{dz_i}$$

0

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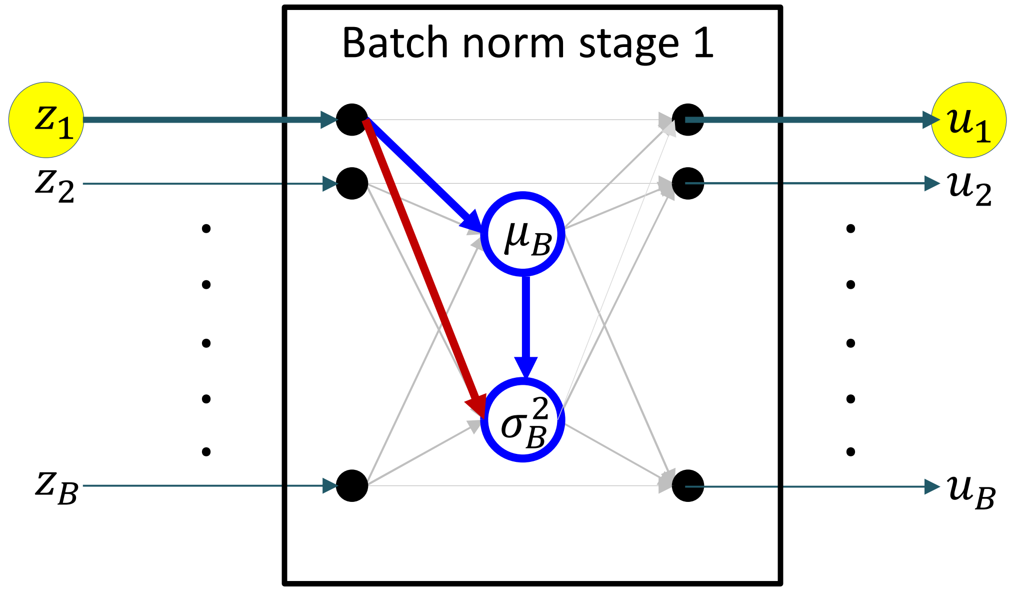

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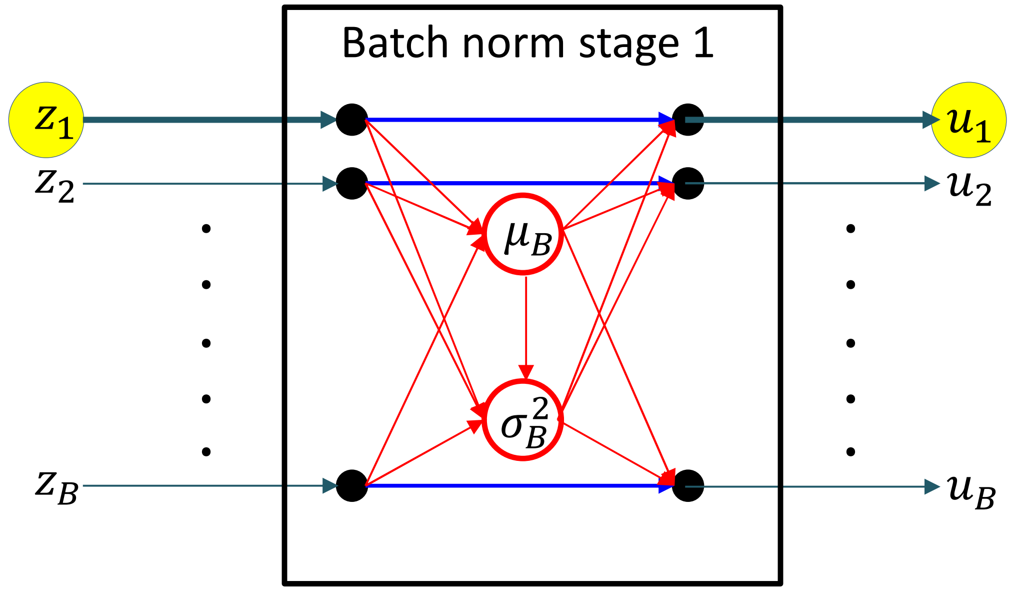

- The derivative for the "through" line ($i = j$)

$$\frac{du_i}{dz_i} = \frac{1}{\sqrt{\sigma_B^2 + \epsilon}} + \frac{-1}{B\sqrt{\sigma_B^2 + \epsilon}} + \frac{-(z_i - \mu_B)}{2(\sigma_B^2 + \epsilon)^{3/2}}\frac{d\sigma_B^2}{dz_i}$$

The first stage of Batchnorm

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

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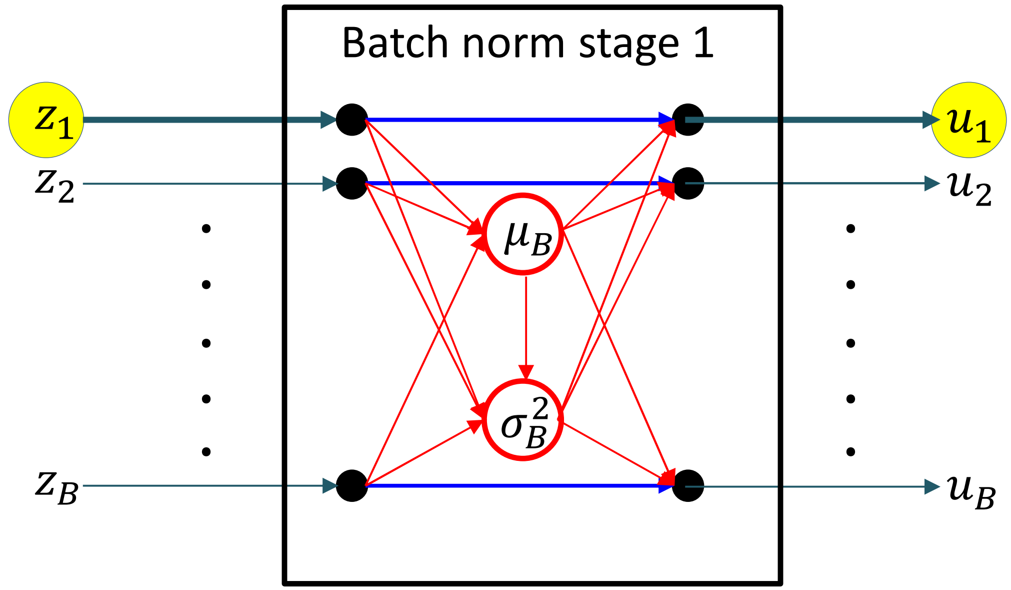

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The first stage of Batchnorm

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

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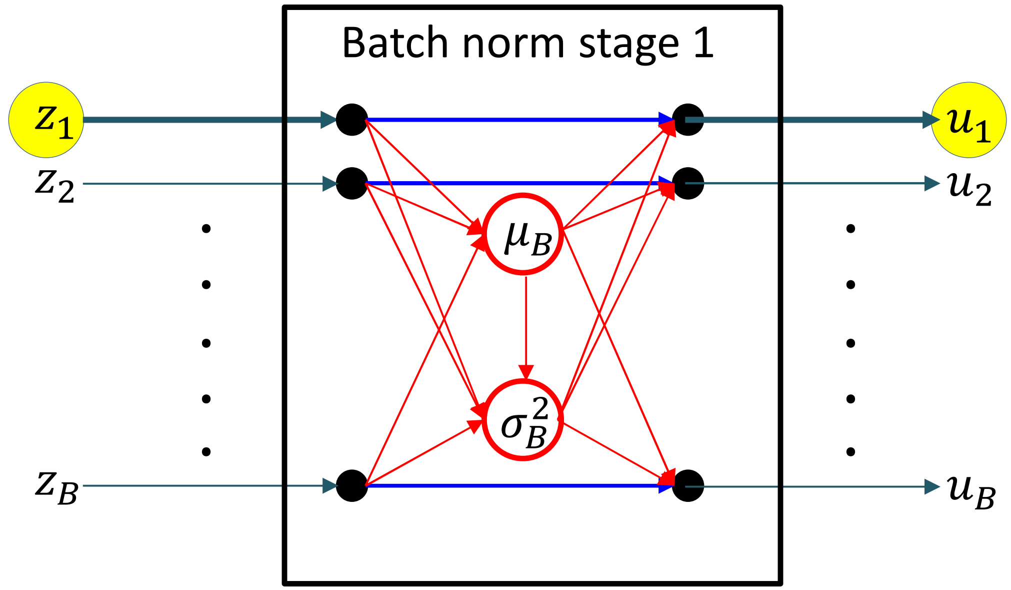

- **The derivative for the "through" line ($i = j$)**

$$\frac{du_i}{dz_i} = \frac{1}{\sqrt{\sigma_B^2 + \epsilon}} + \frac{-1}{B\sqrt{\sigma_B^2 + \epsilon}} + \frac{-(z_i - \mu_B)^2}{B(\sigma_B^2 + \epsilon)^{3/2}}$$

The first stage of Batchnorm

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

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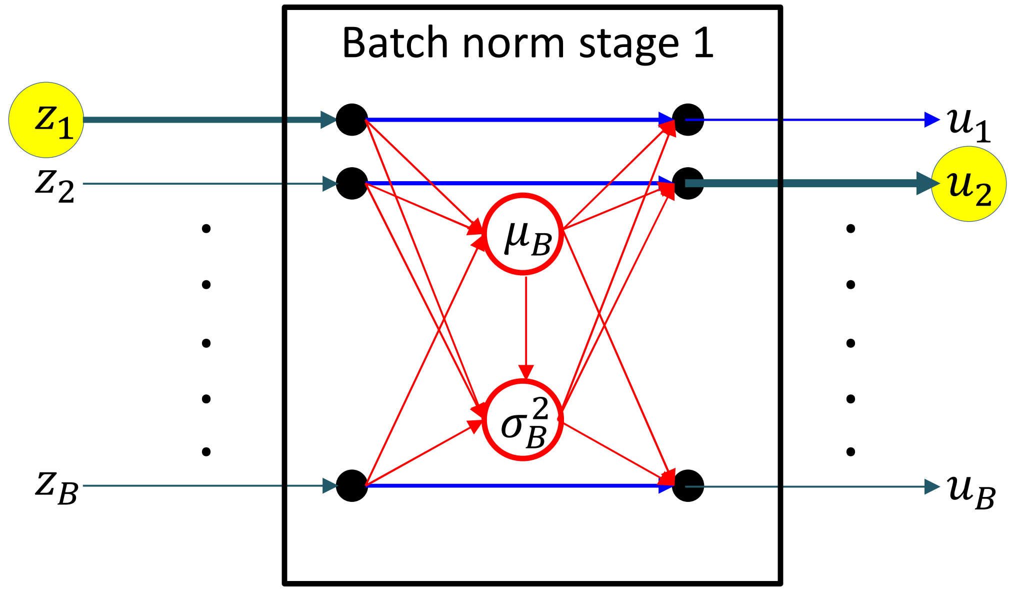


- The derivative for the "cross" lines ($i \neq j$)

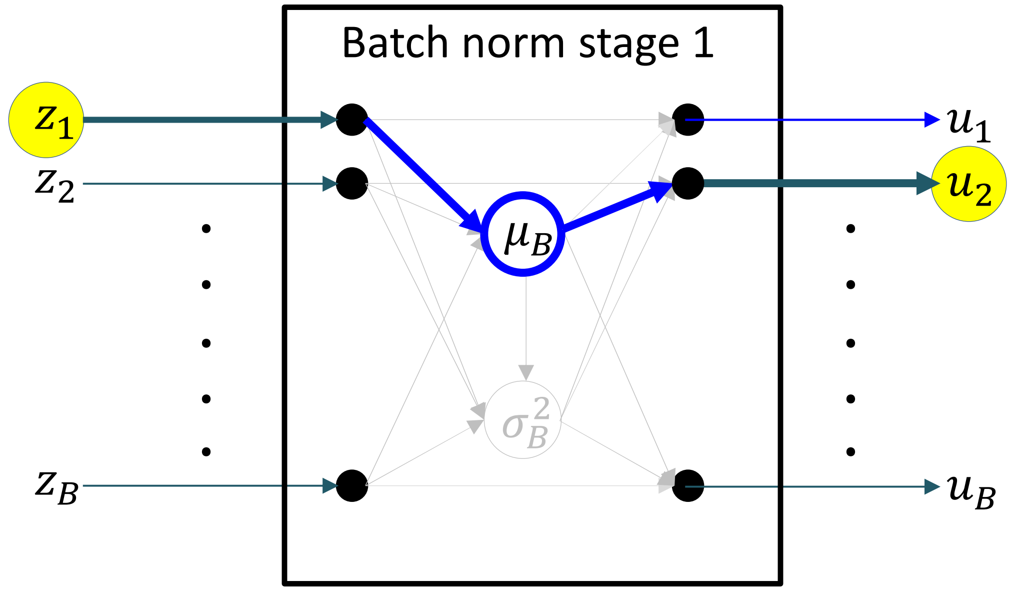
$$\frac{du_j}{dz_i} =$$

The first stage of Batchnorm

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B}(z_i - \mu_B)^2$$

$$u_i = \frac{z_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$



- The derivative for the "cross" lines ($i \neq j$)

$$\frac{du_j}{dz_i} = \frac{\partial u_j}{\partial \mu_B}\frac{d\mu_B}{dz_i} +$$

The first stage of Batchnorm

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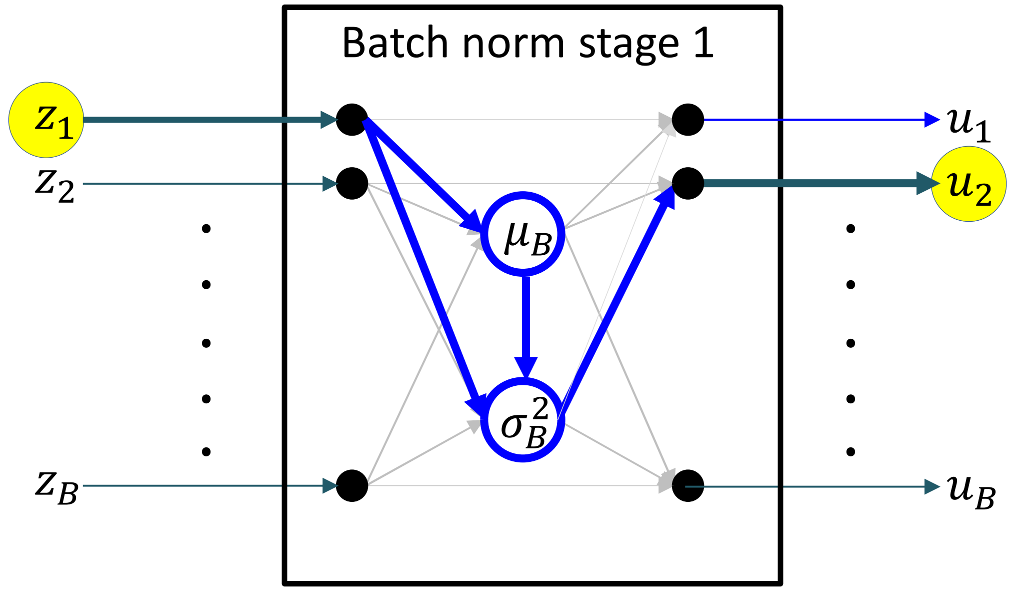

- The derivative for the "cross" lines ($i \neq j$)

$$\frac{du_j}{dz_i} = \frac{\partial u_j}{\partial \mu_B}\frac{d\mu_B}{dz_i} + \frac{\partial u_j}{\partial \sigma_B^2}\frac{d\sigma_B^2}{dz_i}$$

The first stage of Batchnorm

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

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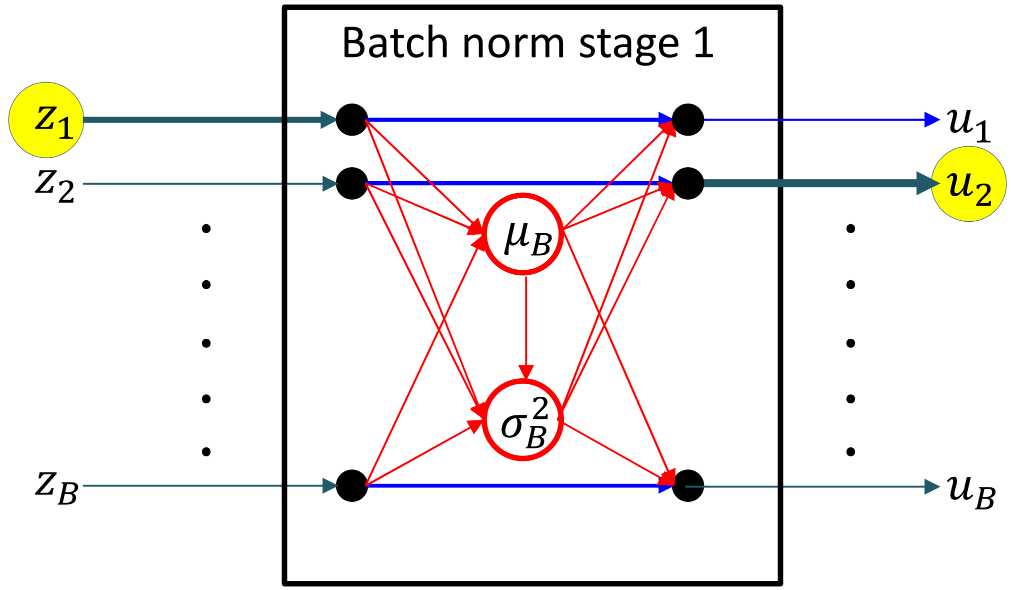

- The derivative for the "cross" lines ($i \neq j$)

$$\frac{du_j}{dz_i} = \frac{\partial u_j}{\partial \mu_B}\frac{d\mu_B}{dz_i} + \frac{\partial u_j}{\partial \sigma_B^2}\frac{d\sigma_B^2}{dz_i}$$

This is identical to the equation for $i = j$, without the first "through" term

The first stage of Batchnorm

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} z_i$$

$$\sigma_B^2 = \frac{1}{B}\sum_{i=1}^{B} (z_i - \mu_B)^2$$

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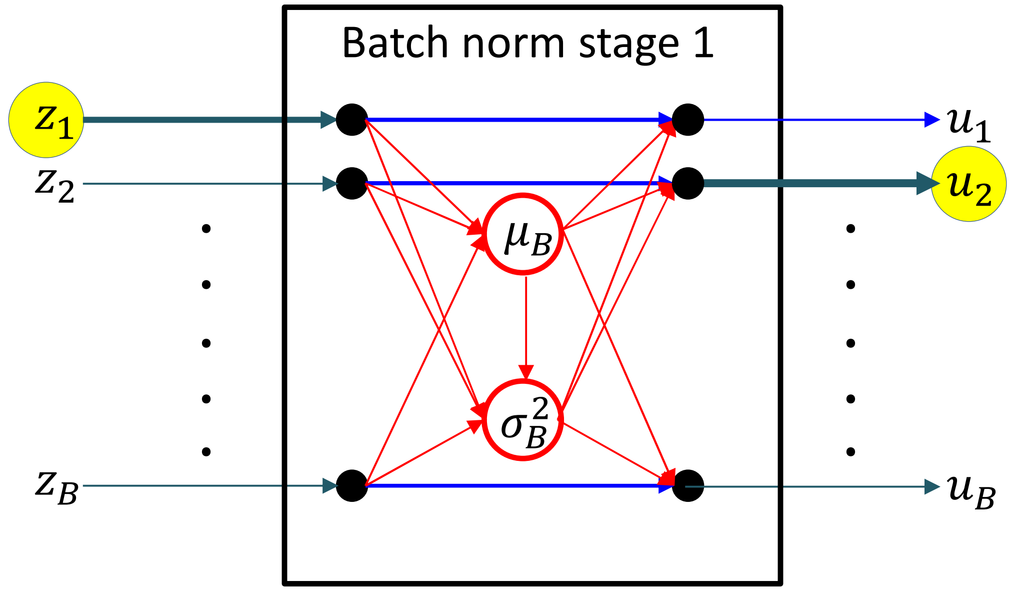
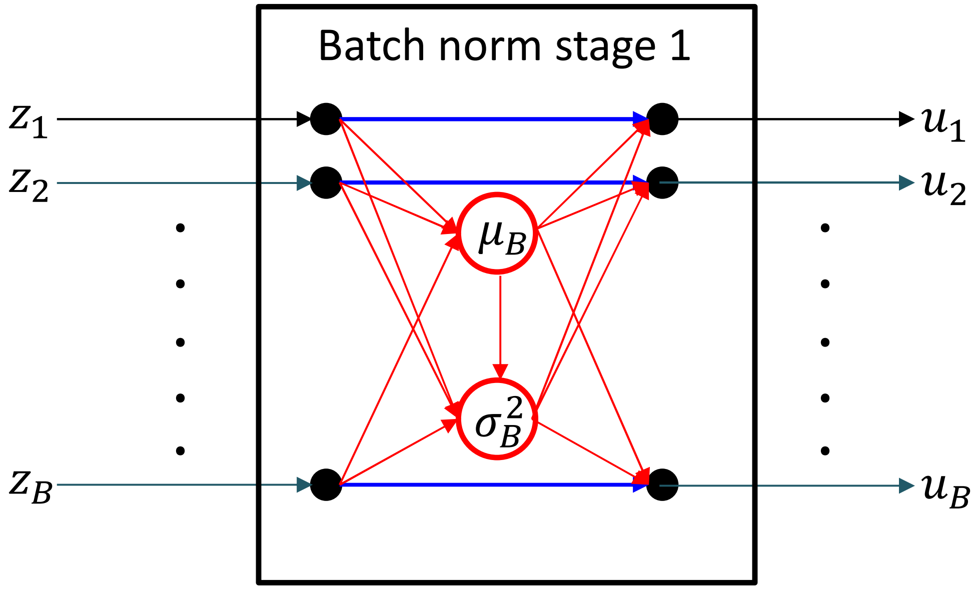


- The derivative for the "cross" lines ($i \neq j$)

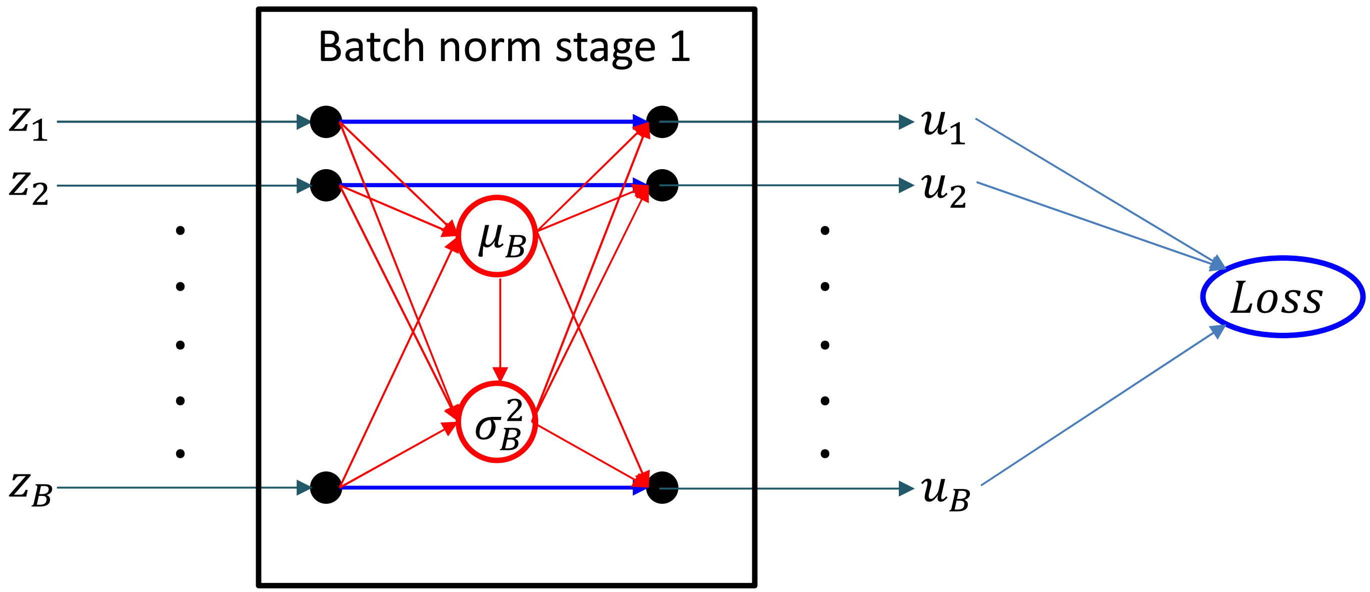
$$\frac{du_j}{dz_i} = \frac{-1}{B\sqrt{\sigma_B^2 + \epsilon}} + \frac{-(z_i - \mu_B)^2}{B(\sigma_B^2 + \epsilon)^{3/2}}$$

The first stage of Batchnorm



$$\frac{du_j}{dz_i} = \begin{cases} \frac{1}{\sqrt{\sigma_B^2+\epsilon}} + \frac{-1}{B\sqrt{\sigma_B^2+\epsilon}} + \frac{-(z_i-\mu_B)^2}{B(\sigma_B^2+\epsilon)^{3/2}} & \text{if } j = i \\ \frac{-1}{B\sqrt{\sigma_B^2+\epsilon}} + \frac{-(z_i-\mu_B)^2}{B(\sigma_B^2+\epsilon)^{3/2}} & \text{if } j \neq i \end{cases}$$

The first stage of Batchnorm



- The complete derivative of the mini-batch loss w.r.t. z_i

$$\frac{dLoss}{dz_i} = \sum_j \frac{dLoss}{du_j} \frac{du_j}{dz_i}$$

The first stage of Batchnorm

$$\frac{du_j}{dz_i} = \begin{cases} \frac{1}{\sqrt{\sigma_B^2 + \epsilon}} + \frac{-1}{B\sqrt{\sigma_B^2 + \epsilon}} + \frac{-(z_i - \mu_B)^2}{B(\sigma_B^2 + \epsilon)^{3/2}} & \text{if } j = i \\ \frac{-1}{B\sqrt{\sigma_B^2 + \epsilon}} + \frac{-(z_i - \mu_B)^2}{B(\sigma_B^2 + \epsilon)^{3/2}} & \text{if } j \neq i \end{cases}$$

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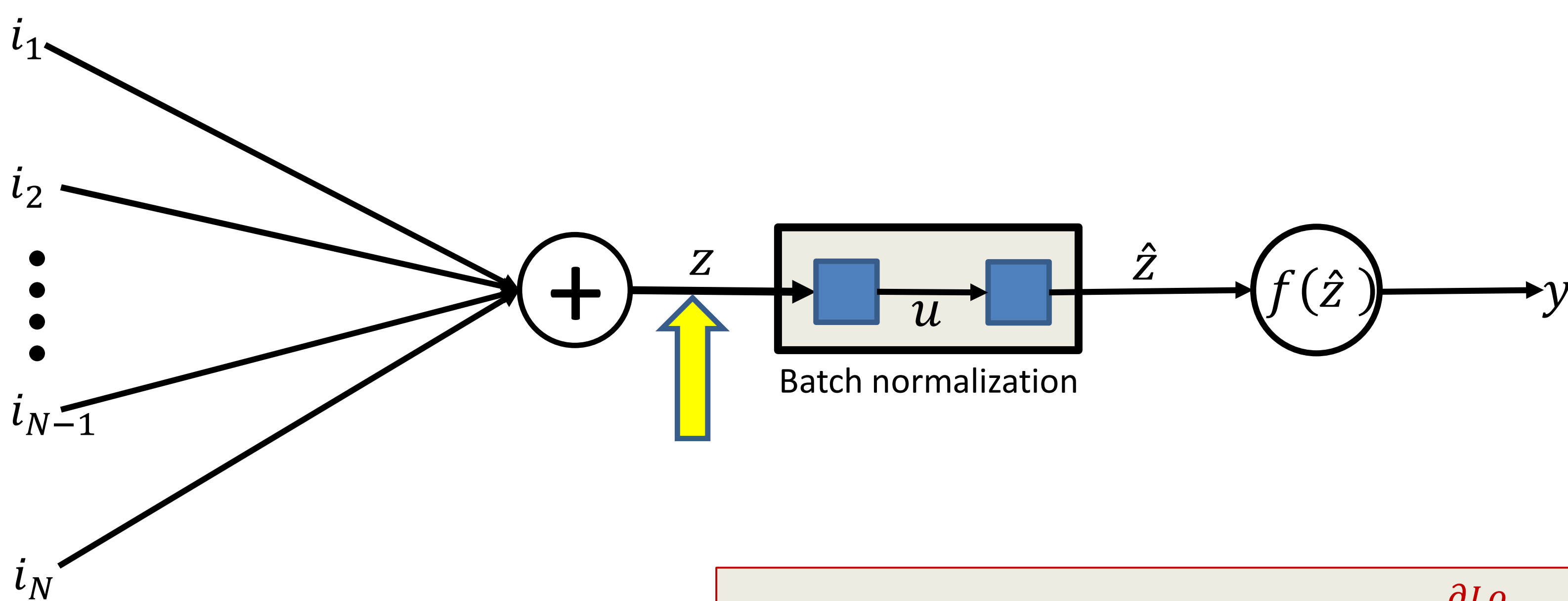
- The complete derivative of the mini-batch loss w.r.t. z_i

$$\frac{dLoss}{dz_i} = \frac{1}{\sqrt{\sigma_B^2 + \epsilon}} \frac{dLoss}{du_i} - \frac{1}{B\sqrt{\sigma_B^2 + \epsilon}} \sum_j \frac{dLoss}{du_j} - \frac{1}{B(\sigma_B^2 + \epsilon)^{3/2}} \sum_j \frac{dLoss}{du_j} (z_i - \mu_B)^2$$

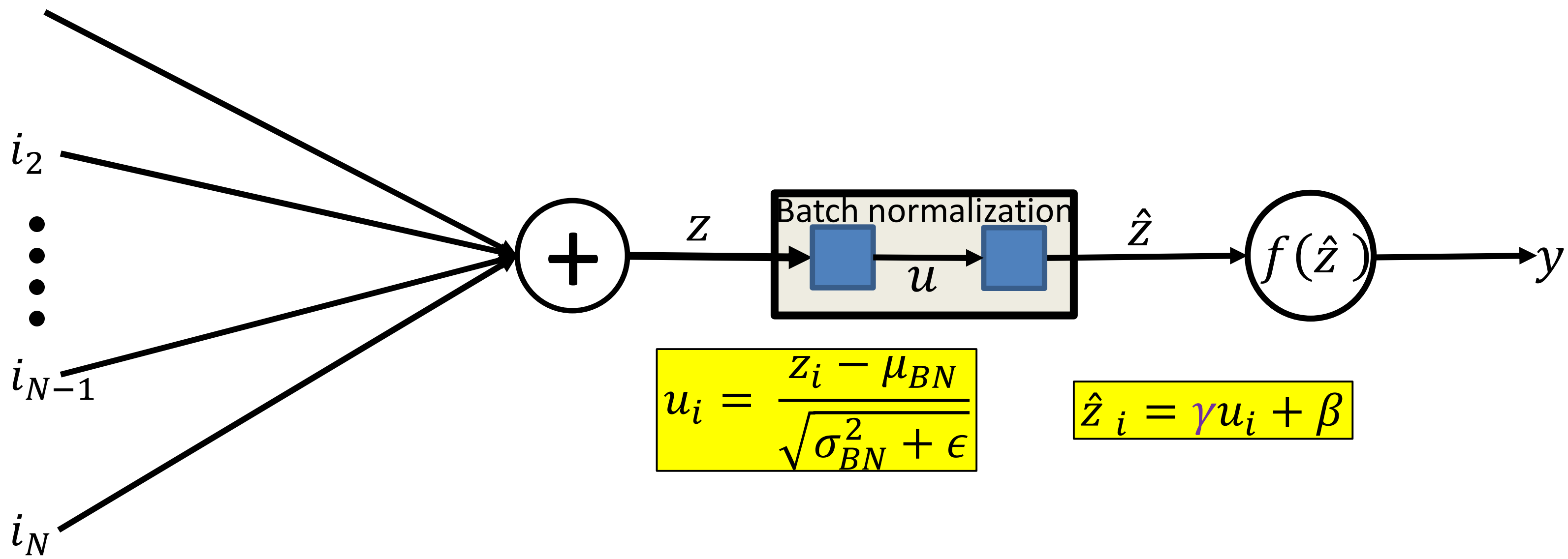
Batch normalization: Backpropagation

$$\frac{dLoss}{dz_i} = \frac{1}{\sqrt{\sigma_B^2 + \epsilon}} \frac{dLoss}{du_i} - \frac{1}{B\sqrt{\sigma_B^2 + \epsilon}} \sum_j \frac{dLoss}{du_j} - \frac{1}{B(\sigma_B^2 + \epsilon)^{3/2}} \sum_j \frac{dLoss}{du_j} (z_i - \mu_B)^2$$



The rest of backprop continues from $\frac{\partial Lo}{\partial z_i}$

Batch normalization: Inference



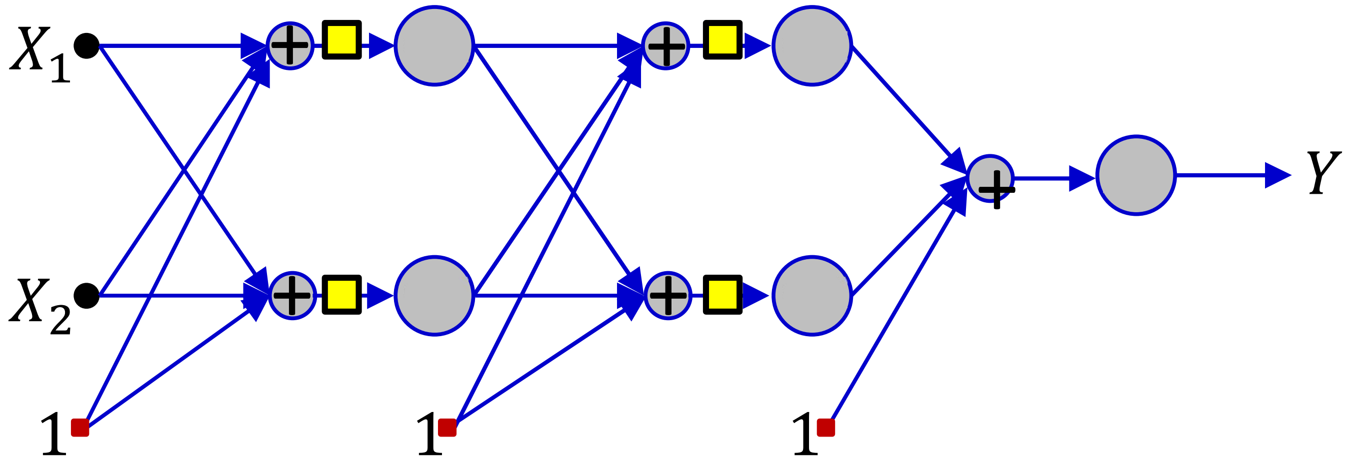
- On test data, BN requires μ_B and σ_B^2.
- We will use the *average over all training minibatches*

$$\mu_{BN} = \frac{1}{Nbatches} \sum_{batch} \mu_B(batch)$$

$$\sigma_{BN}^2 = \frac{B}{(B-1)Nbatches} \sum_{bat} \sigma_B^2(batch)$$

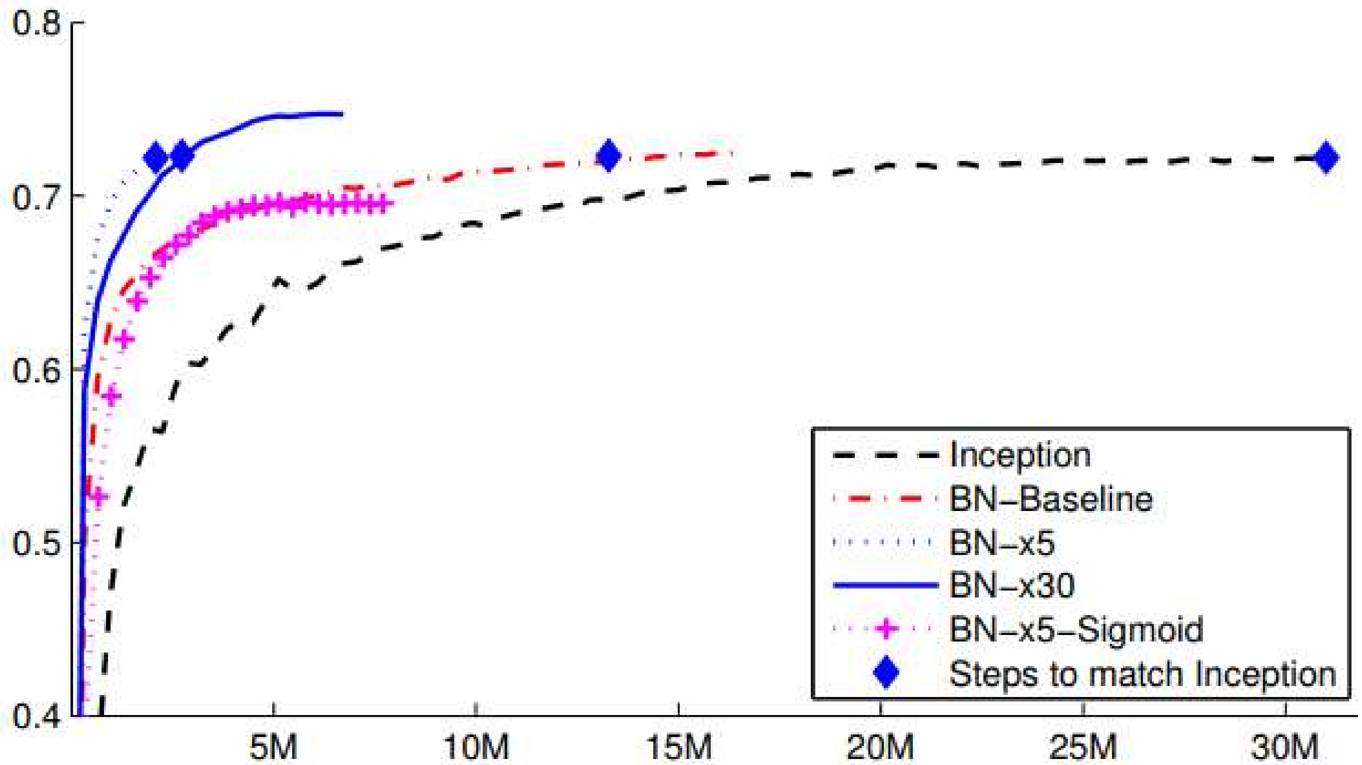
- Note: these are *neuron-specific*
  - $\mu_B(batch)$ and $\sigma_B^2(batch)$ here are obtained from the *final converged network*
  - The $B/(B-1)$ term gives us an unbiased estimator for the variance

Batch normalization



- Batch normalization may only be applied to *some* layers
  - Or even only selected neurons in the layer
- Improves both convergence rate and neural network performance
  - Anecdotal evidence that BN eliminates the need for dropout
  - To get maximum benefit from BN, learning rates must be increased and learning rate decay can be faster
    - Since the data generally remain in the high-gradient regions of the activations
  - Also needs better randomization of training data order

Batch Normalization: Typical result



- Performance on Imagenet, from Ioffe and Szegedy, JMLR 2015

Story so far

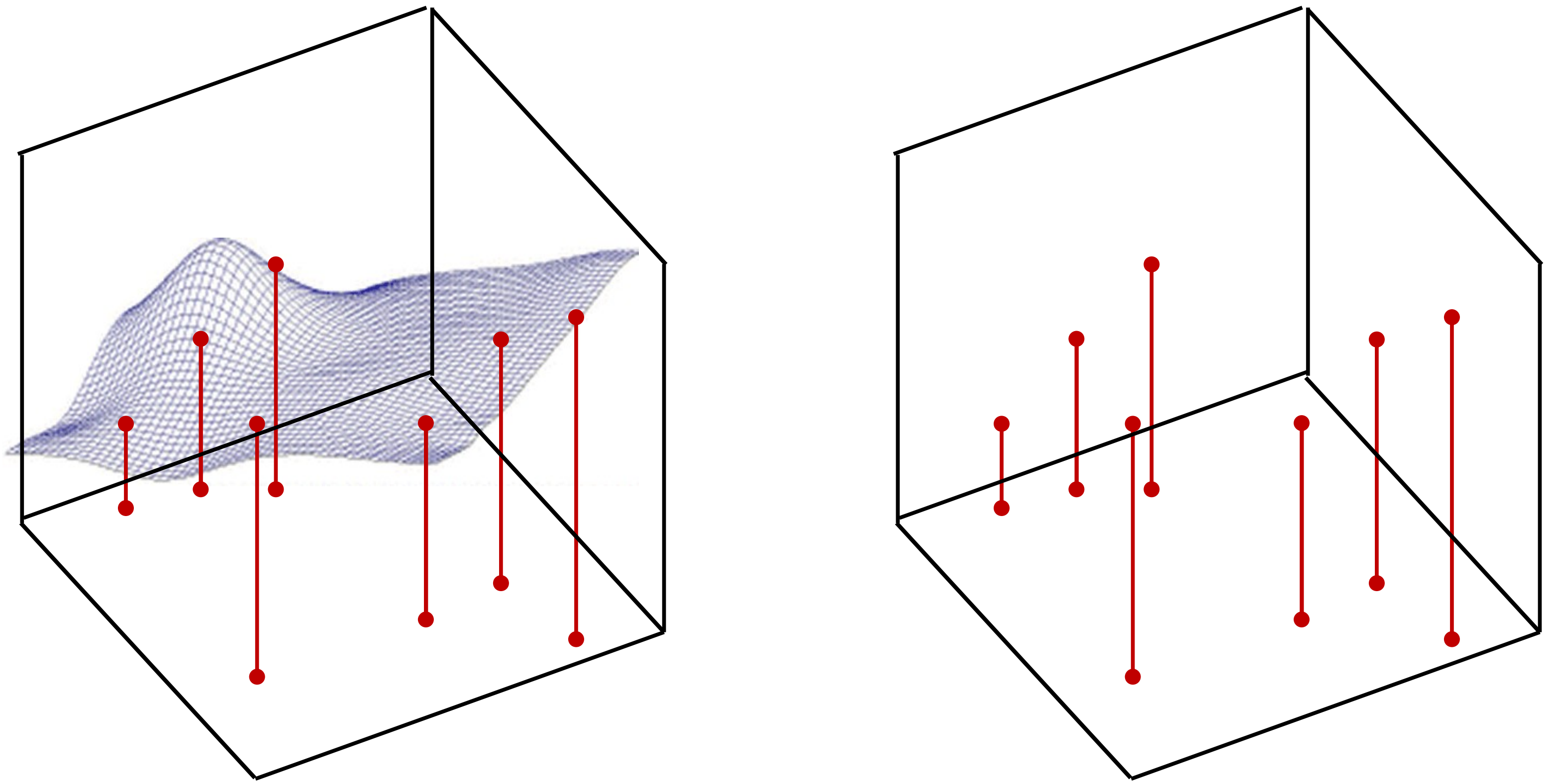
- Gradient descent can be sped up by incremental updates
- Convergence can be improved using smoothed updates

- The choice of divergence affects both the learned network and results
- Covariate shift between training and test may cause problems and may be handled by batch normalization

The problem of data underspecification

- The figures shown to illustrate the learning problem so far were *fake news*..

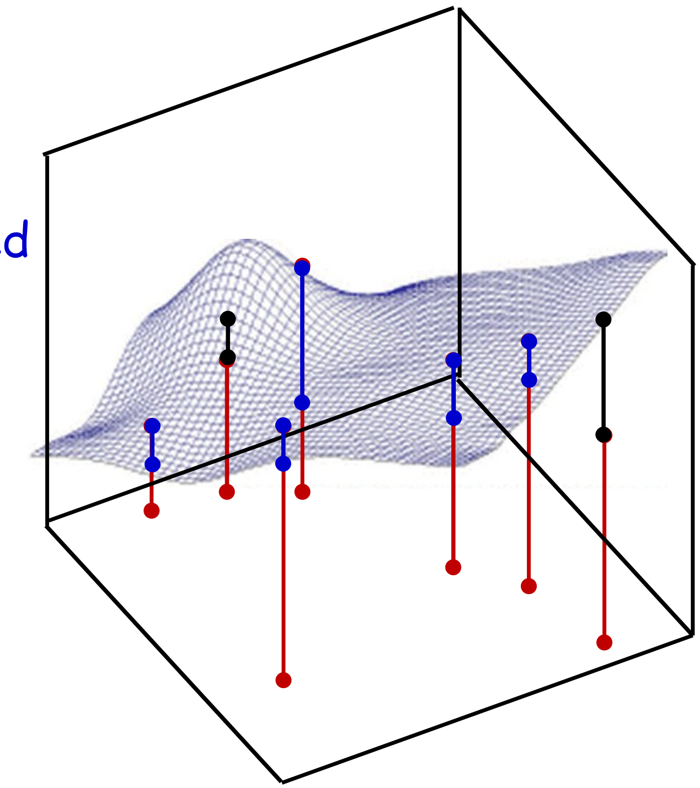
Learning the network



- We attempt to learn an entire function from just a few *snapshots* of it

General approach to training

Blue lines: error when function is *below* desired output

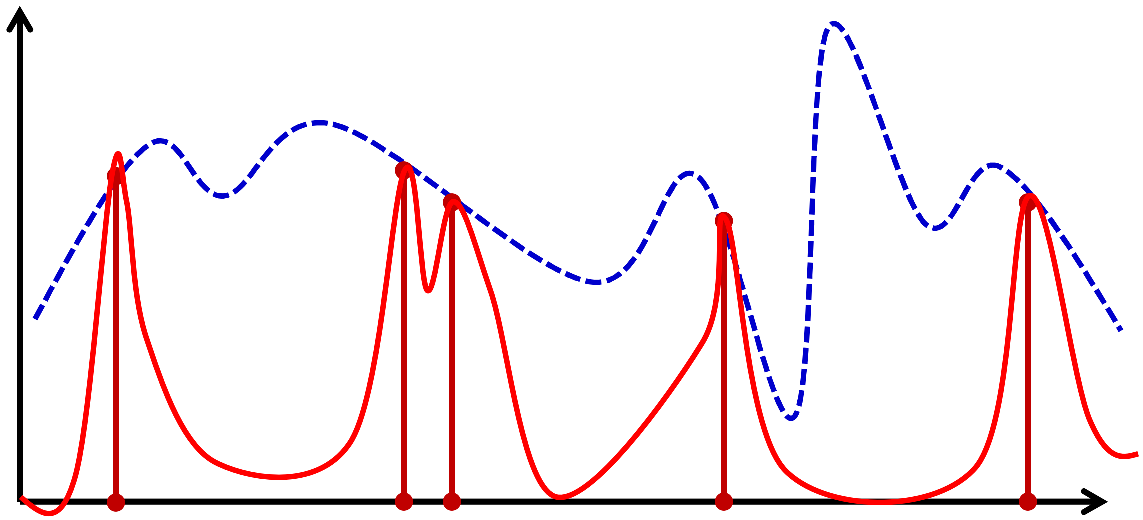


Black lines: error when function is *above* desired output

$$E = \sum_i (d_i - f(\mathbf{x}_i, \mathbf{W}))^2$$

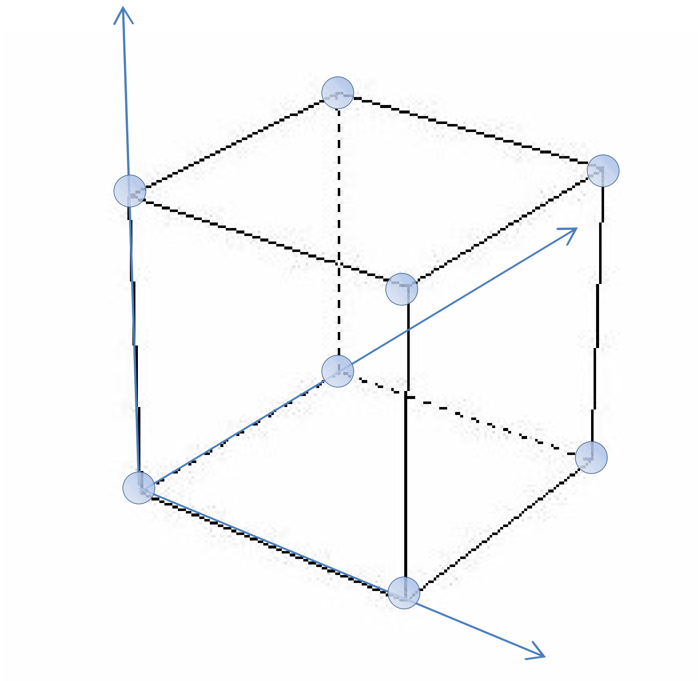
- Define a *divergence* between the ***actual*** network output for any parameter value and the *desired* output
  - Typically L2 divergence or KL divergence

Overfitting



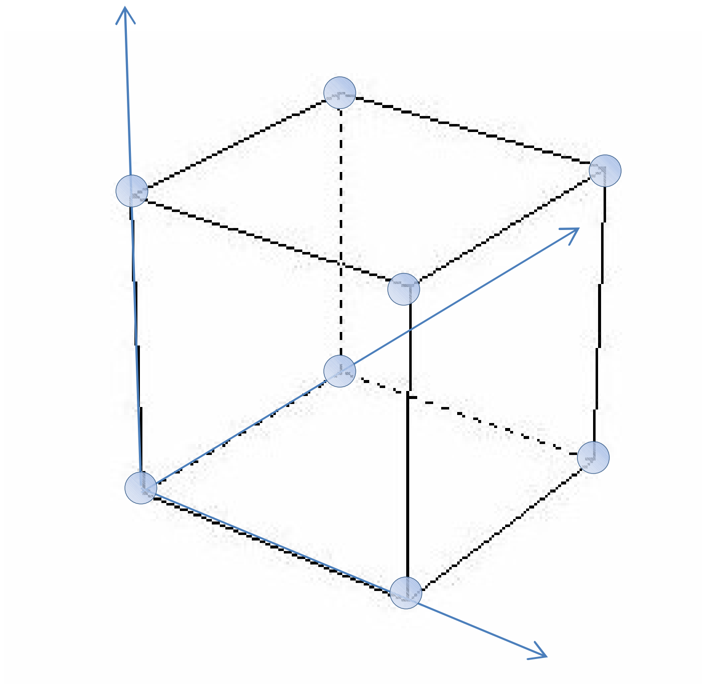
- Problem: Network may just learn the values at the inputs
  - Learn the red curve instead of the dotted blue one
    - Given only the red vertical bars as inputs

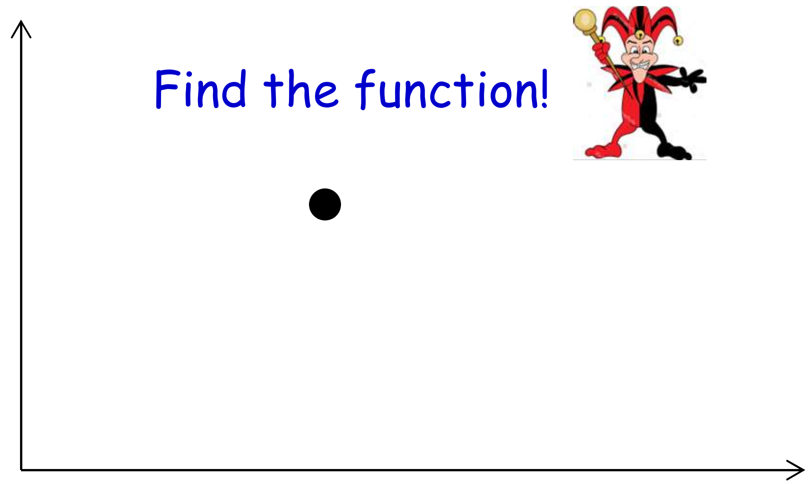
Data under-specification



- Consider a binary 100-dimensional input
- There are $2^{100}=10^{30}$ possible inputs
- Complete specification of the function will require specification of 10^{30} output values
- A training set with only 10^{15} training instances will be off by a factor of 10^{15}

Data under-specification in learning





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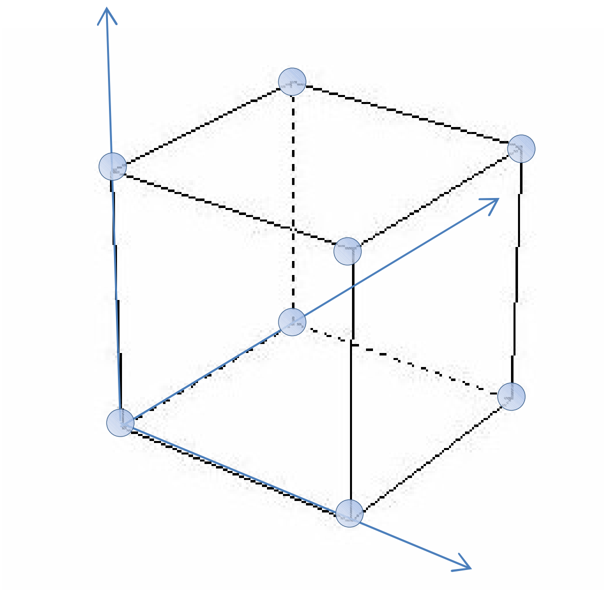
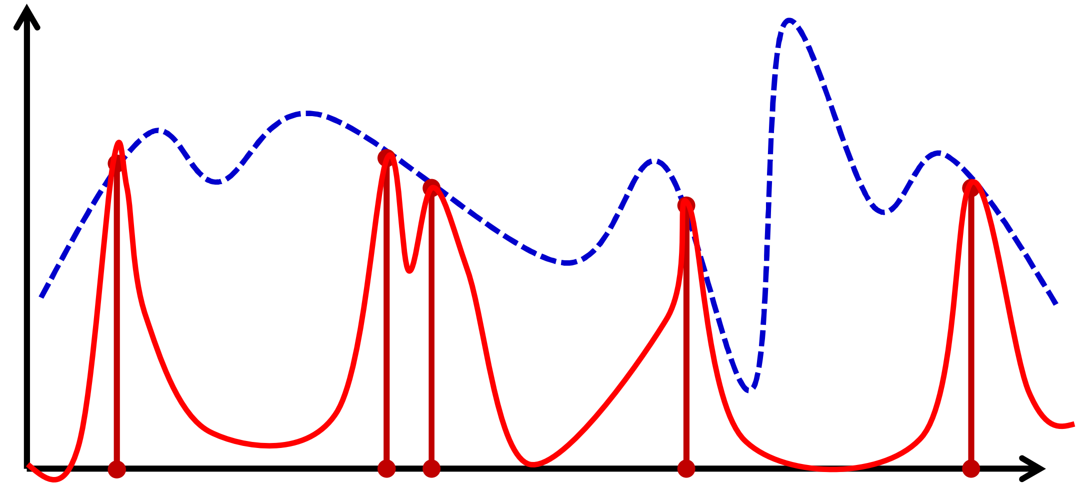
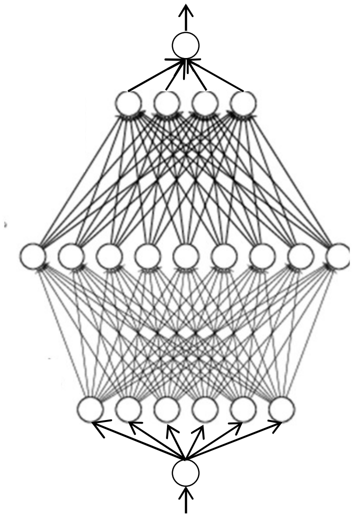
Need "smoothing" constraints

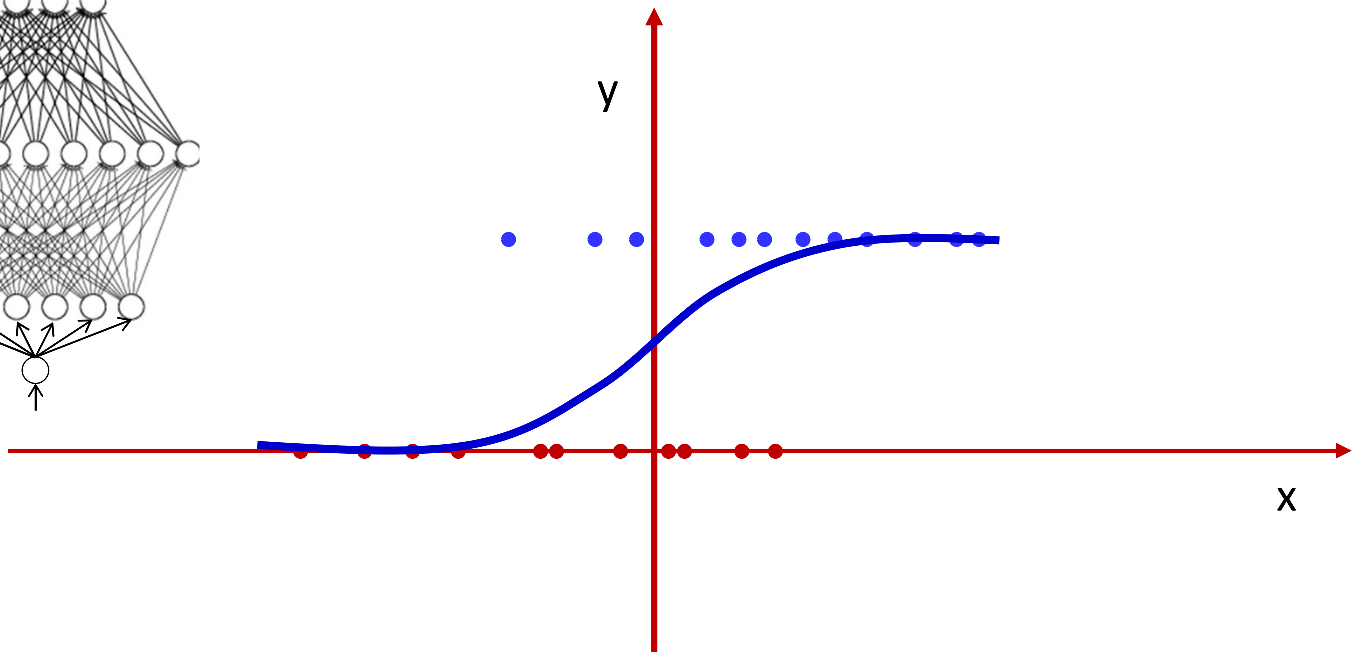




- Need additional constraints that will "fill in" the missing regions acceptably
  - Generalization

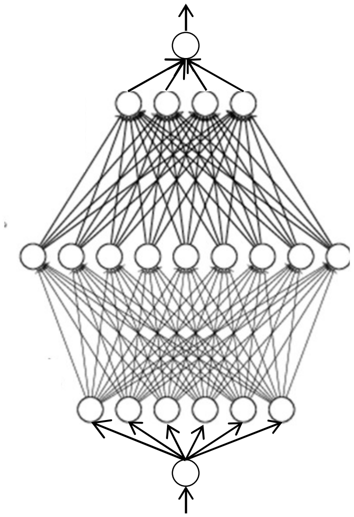
Smoothness through weight manipulation

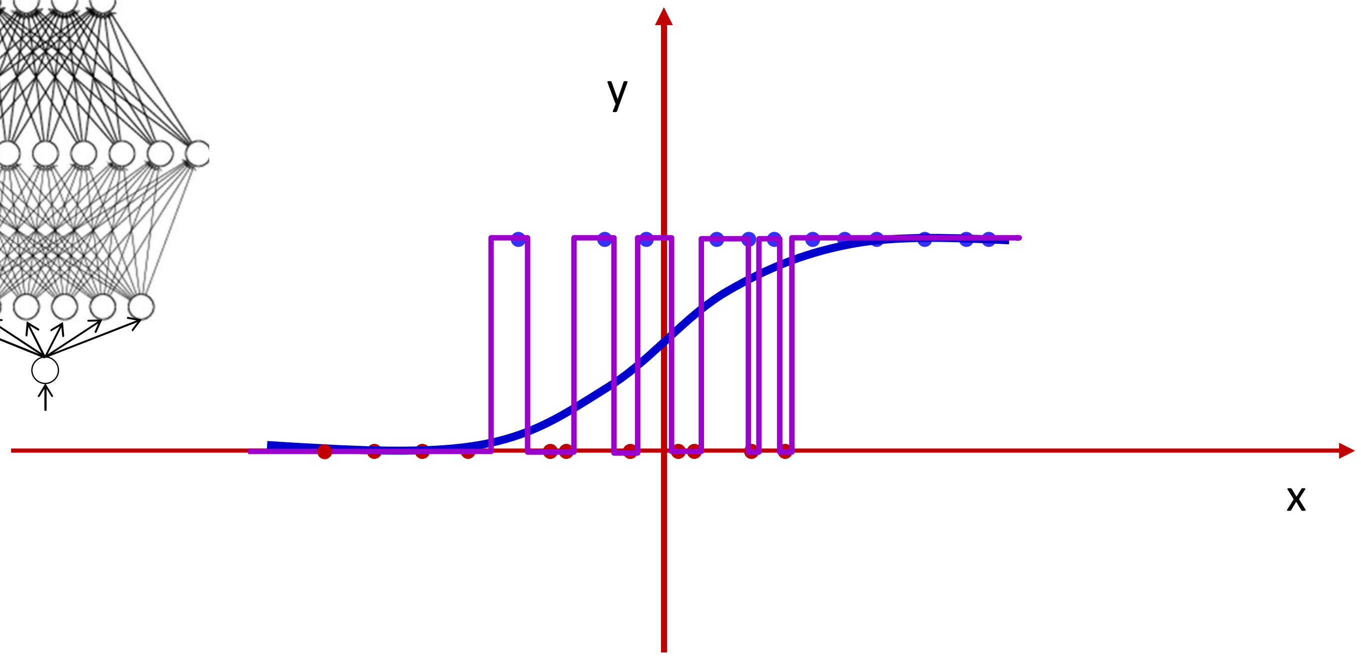




- Illustrative example: Simple binary classifier
  - The "desired" output is generally smooth

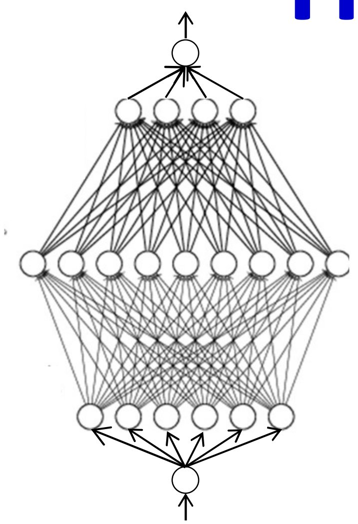
Smoothness through weight manipulation

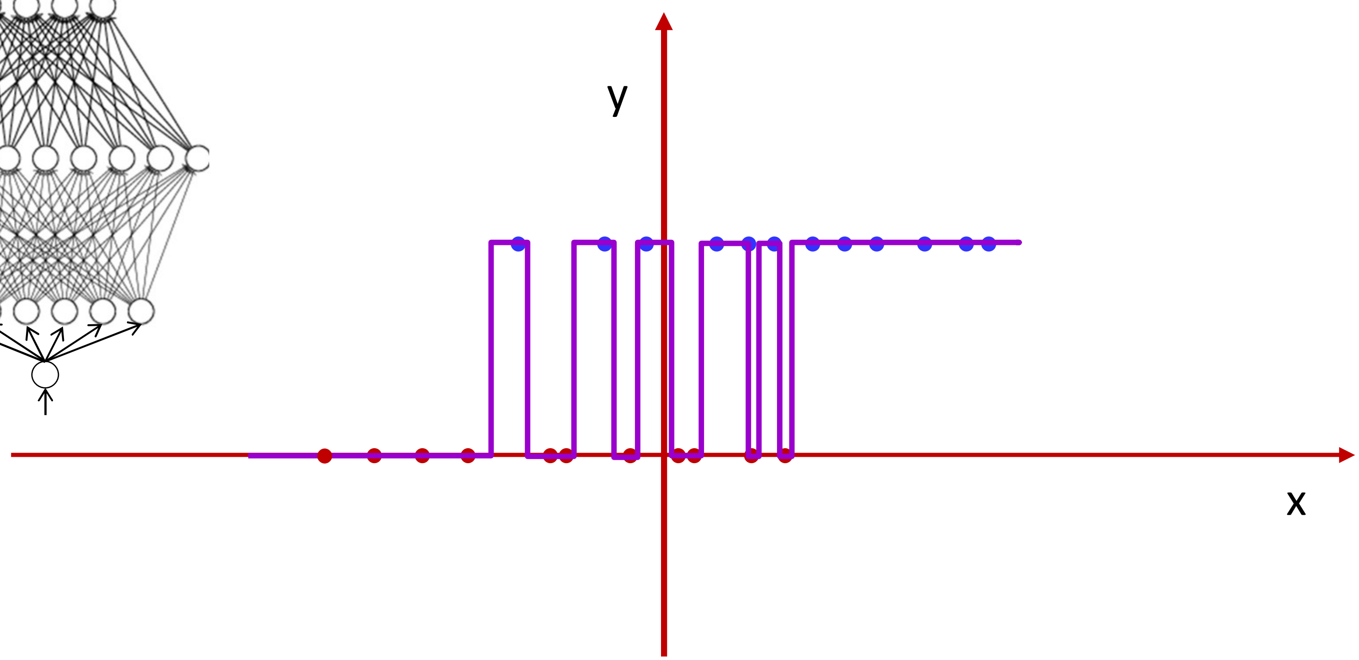




- Illustrative example: Simple binary classifier
  - The "desired" output is generally smooth
    - Capture statistical or average trends
  - An unconstrained model will model individual instances instead

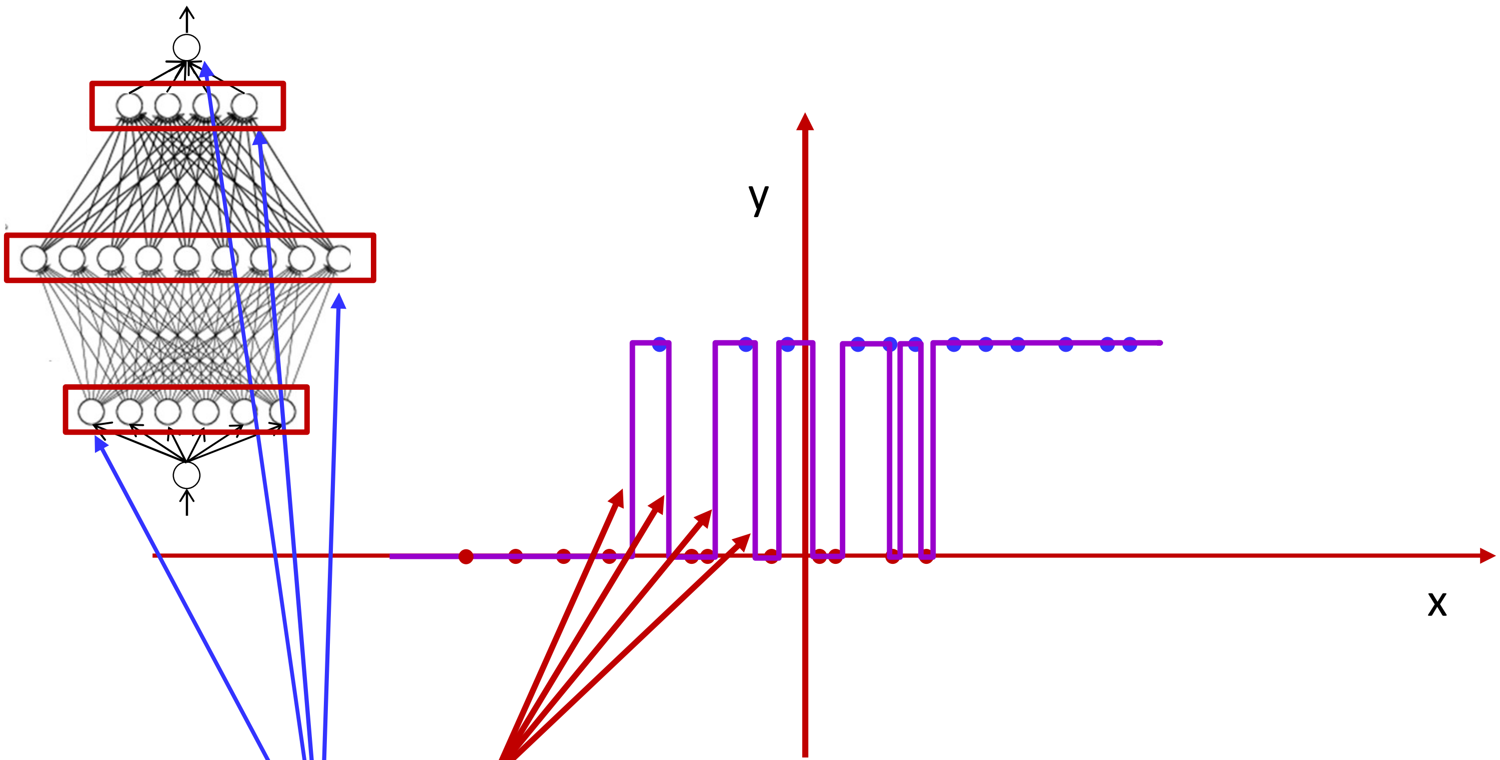
The unconstrained model





- Illustrative example: Simple binary classifier
  - The “desired” output is generally smooth
    - Capture statistical or average trends
  - An unconstrained model will model individual instances instead

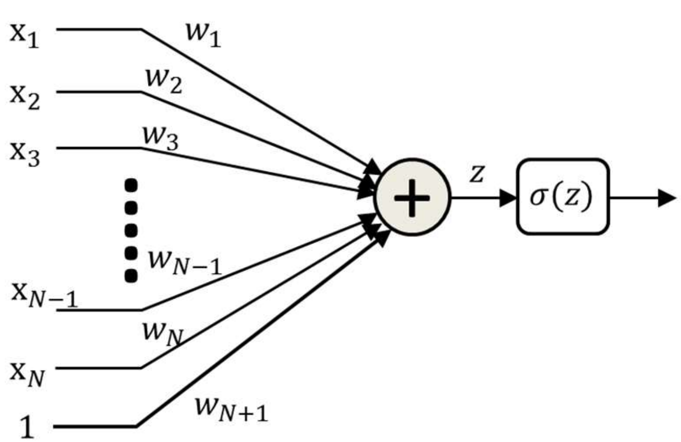
Why overfitting

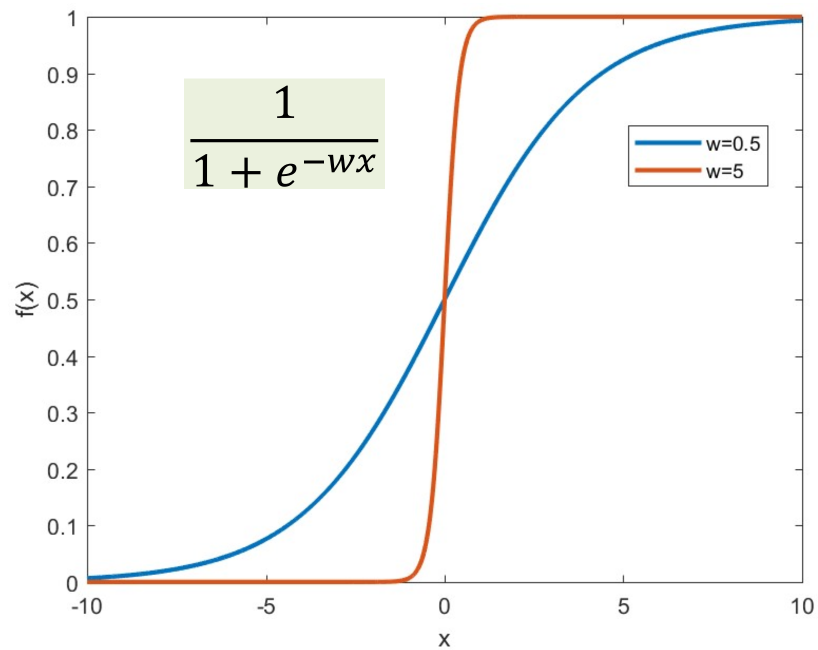


These sharp changes happen because ..

..the perceptrons in the network are individually capable of sharp changes in output

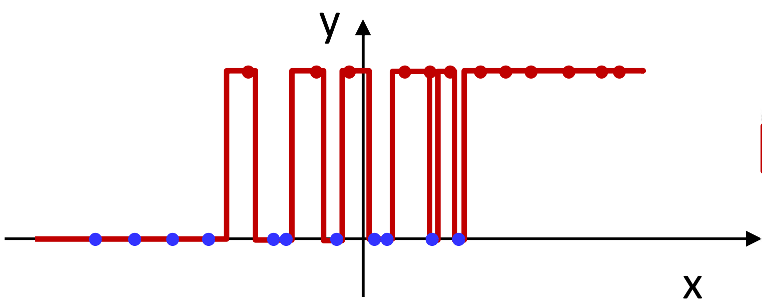
The individual perceptron

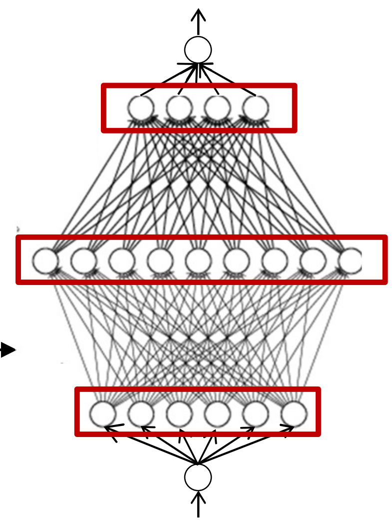


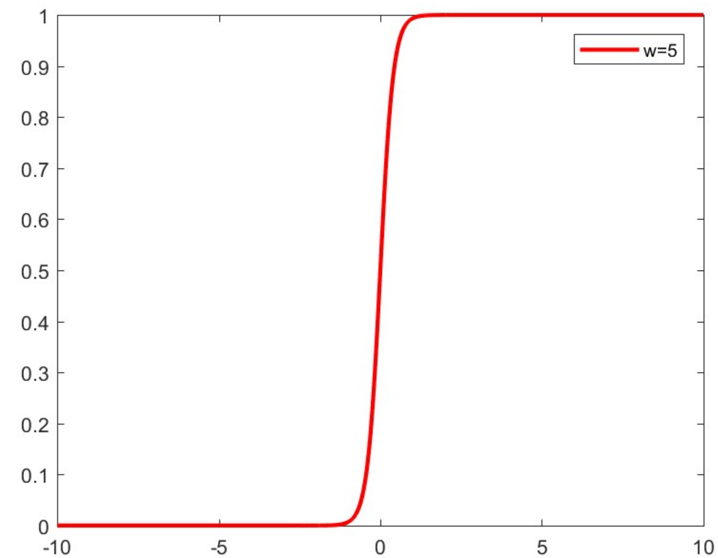


- Using a sigmoid activation
  - As $|w|$ increases, the response becomes steeper

Smoothness through weight manipulation

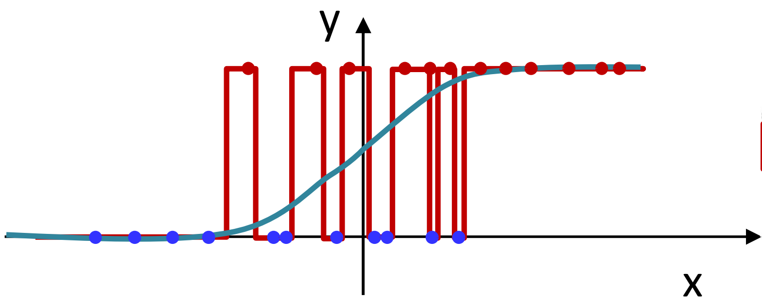


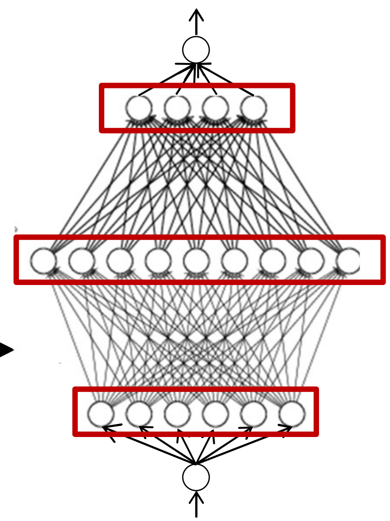


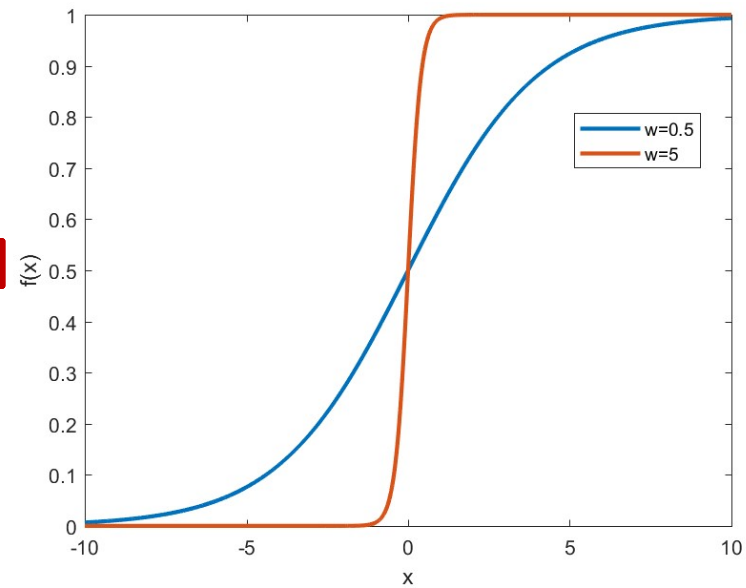


- Steep changes that enable overfitted responses are facilitated by perceptrons with large *w*

Smoothness through weight manipulation



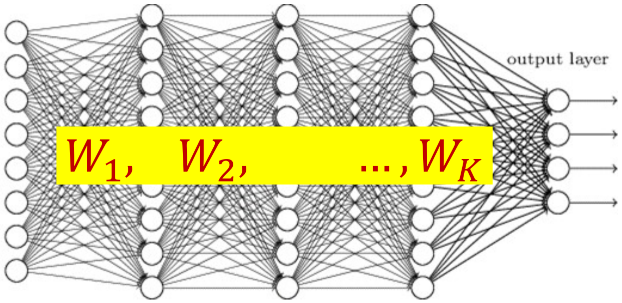




- Steep changes that enable overfitted responses are facilitated by perceptrons with large w

- Constraining the weights w to be low will force slower perceptrons and smoother output response

Objective function for neural networks



Y_t

Desired output of network: d_t

Error on i-th training input: $Div(Y_t, d_t; W_1, W_2, \ldots, W_K)$

Training loss:

$$Loss(W_1, W_2, \ldots, W_K) = \frac{1}{T}\sum_t Div(Y_t, d_t; W_1, W_2, \ldots, W_K)$$

- Conventional training: minimize the loss:

$$\widehat{W}_1, \widehat{W}_2, \ldots, \widehat{W}_K = \underset{W_1, W_2, \ldots, W_K}{\operatorname{argmin}} Loss(W_1, W_2, \ldots, W_K)$$

Smoothness through weight constraints

- Regularized training: minimize the loss while also minimizing the weights

$$L(W_1, W_2, \ldots, W_K) = \frac{1}{T}\sum_t Div(Y_t, d_t; W_1, W_2, \ldots, W_K) + \frac{1}{2}\lambda \sum_k \|W_k\|_F^2$$

$$\widehat{W}_1, \widehat{W}_2, \ldots, \widehat{W}_K = \underset{W_1, W_2, \ldots, W_K}{\operatorname{argmin}} \; L(W_1, W_2, \ldots, W_K)$$

- λ is the regularization parameter whose value depends on how important it is for us to want to minimize the weights

- Increasing λ assigns greater importance to shrinking the weights
  - Make greater error on training data, to obtain a more acceptable network

Regularizing the weights

$$L(W_1, W_2, \dots, W_K) = \frac{1}{T}\sum_t Div(Y_t, d_t) + \frac{1}{2}\lambda \sum_k \|W_k\|_F^2$$

- Batch mode:

$$\Delta W_k = \frac{1}{T}\sum_t \nabla_{W_k} Div(Y_t, d_t)^T + \lambda W_k$$

- SGD:

$$\Delta W_k = \nabla_{W_k} Div(Y_t, d_t)^T + \lambda W_k$$

- Minibatch:

$$\Delta W_k = \frac{1}{b}\sum_{\tau=t}^{t+b-1} \nabla_{W_k} Div(Y_\tau, d_\tau)^T + \lambda W_k$$

- Update rule:

$$W_k \leftarrow W_k - \eta \Delta W_k$$

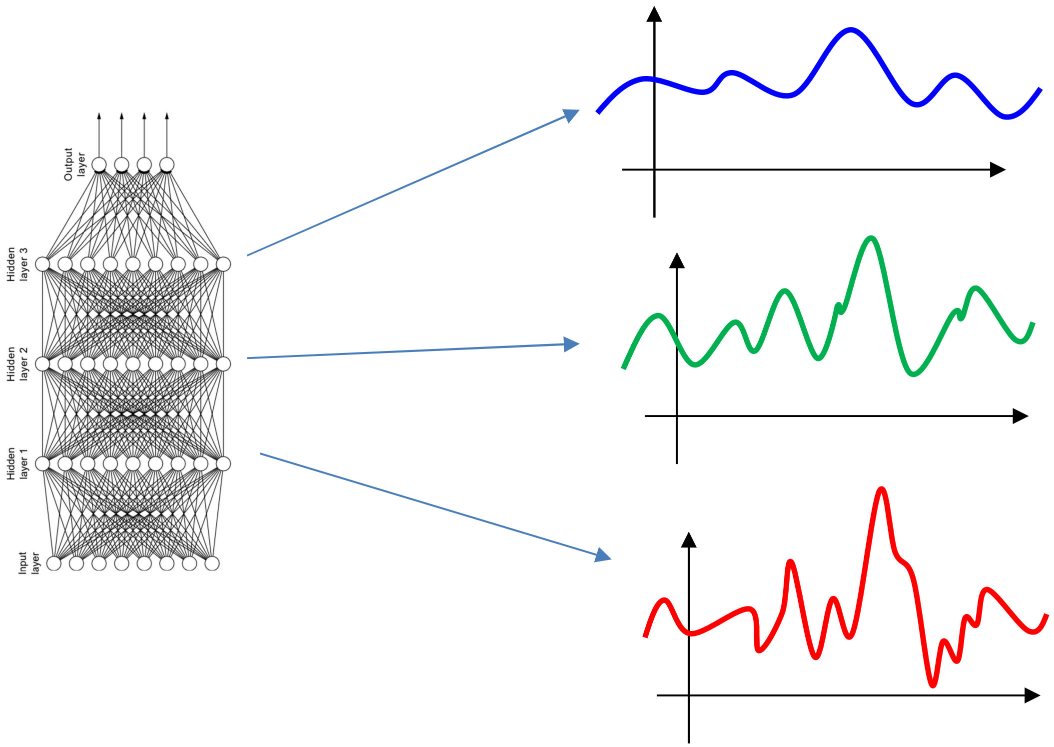
Incremental Update: Mini-batch update

- Given (X_1, d_1), (X_2, d_2),…, (X_T, d_T)
- Initialize all weights $W_1, W_2, \dots, W_K$; $j = 0$
- Do:
  - Randomly permute (X_1, d_1), (X_2, d_2),…, (X_T, d_T)
  - For $t = 1: b: T$
    - $j = j + 1$
    - For every layer k:
      - $\Delta W_k = 0$
    - For t' = t : t+b-1
      - For every layer k:
        - » Compute $\nabla_{W_k} Div(Y_t, d_t)$
        - » $\Delta W_k = \Delta W_k + \nabla_{W_k} Div(Y_t, d_t)^T$
    - Update
      - For every layer k:

$$W_k = W_k - \eta_j (\Delta W_k + \lambda W_k)$$

- Until $Loss$ has converged

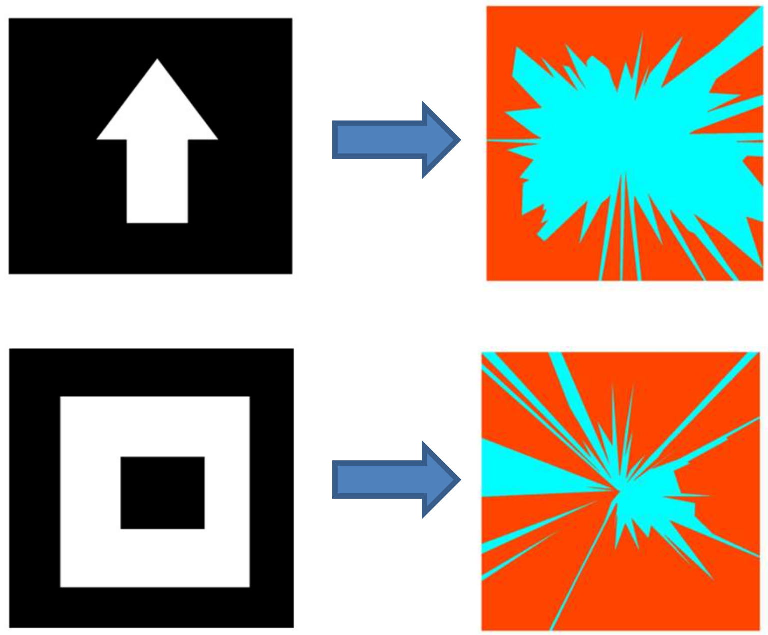
Smoothness through network structure



- Smoothness constraints can also be imposed through the network *structure*

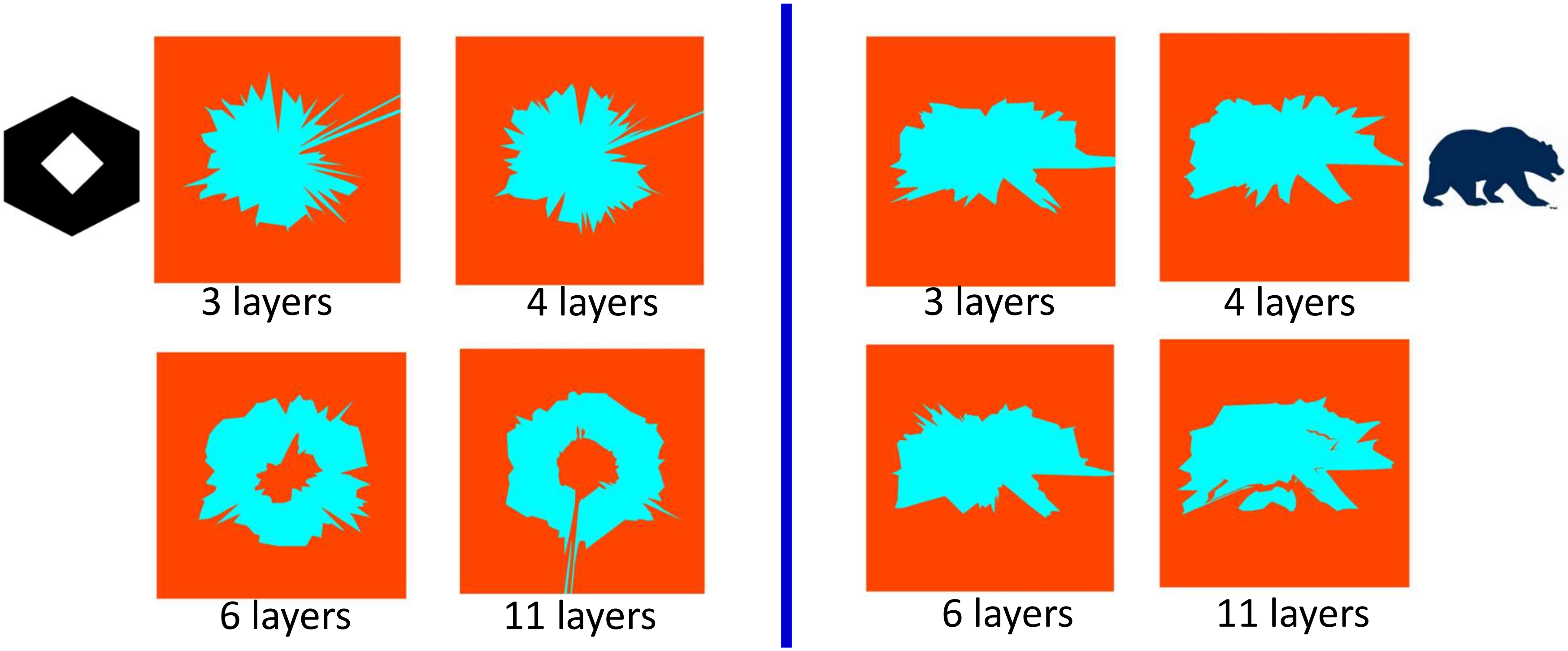
- *For a given number of parameters deeper networks impose more smoothness than shallow ones*
  - Each layer works on the already smooth surface output by the previous layer

Minimal correct architectures are hard to train



- Typical results (varies with initialization)
- 1000 training points – orders of magnitude more than you usually get
- All the training tricks known to mankind

But depth and training data help



- Deeper networks seem to learn better, for the same number of total neurons
  - ***Implicit smoothness constraints***
    - ***As opposed to explicit constraints from more conventional regularization methods***
- Training with more data is also better ☺

10000 training instances

Story so far

- Gradient descent can be sped up by incremental updates
- Convergence can be improved using smoothed updates

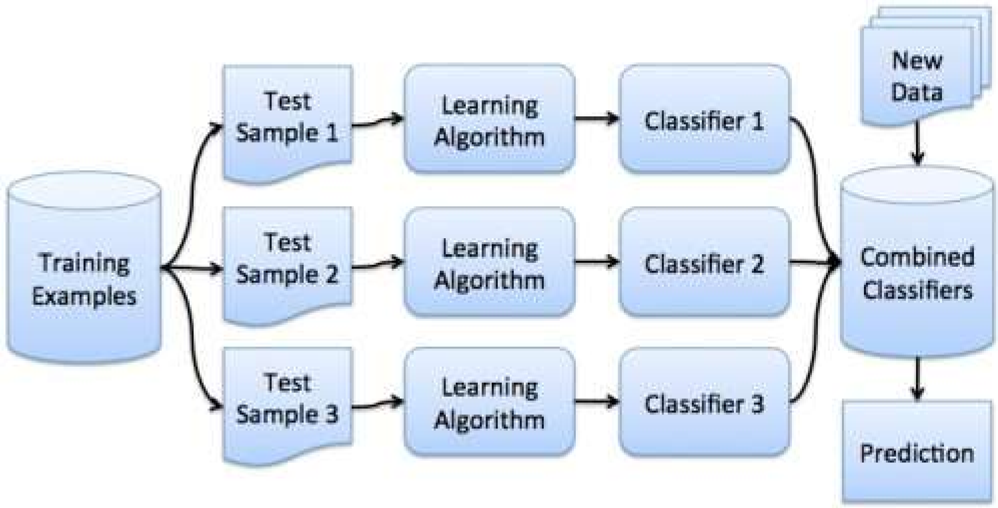
- The choice of divergence affects both the learned network and results
- Covariate shift between training and test may cause problems and may be handled by batch normalization
- Data underspecification can result in overfitted models and must be handled by regularization and more constrained (generally deeper) network architectures

Regularization..

- Other techniques have been proposed to improve the smoothness of the learned function
  - L_1 regularization of network activations
  - Regularizing with added noise..

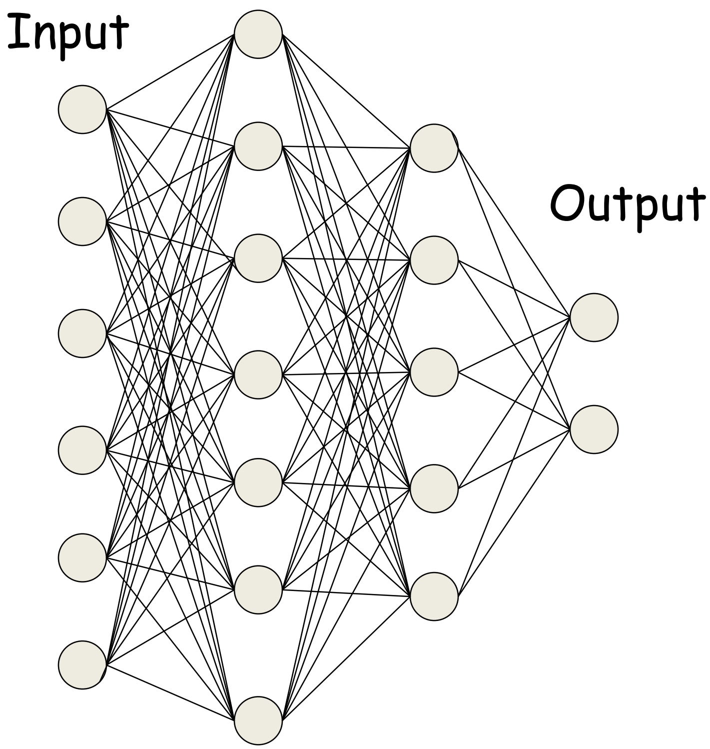
- Possibly the most influential method has been "dropout"

A brief detour.. Bagging



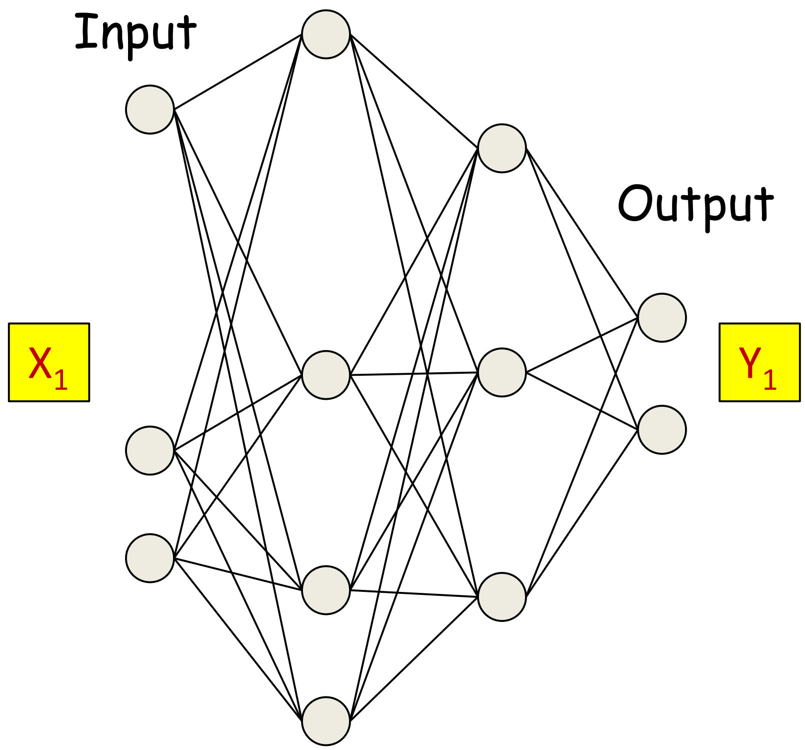
- Popular method proposed by Leo Breiman:
  - Sample training data and train several different classifiers
  - Classify test instance with entire ensemble of classifiers
  - Vote across classifiers for final decision
  - Empirically shown to improve significantly over training a single classifier from combined data
- Returning to our problem….

Dropout



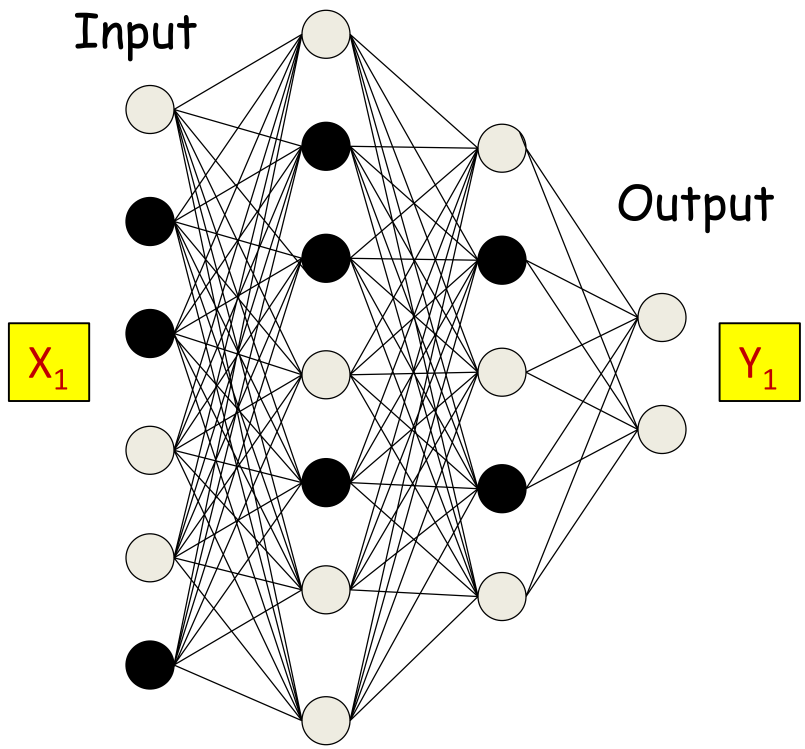
- **During training:** For each input, at each iteration, "turn off" each neuron with a probability 1-α

Dropout



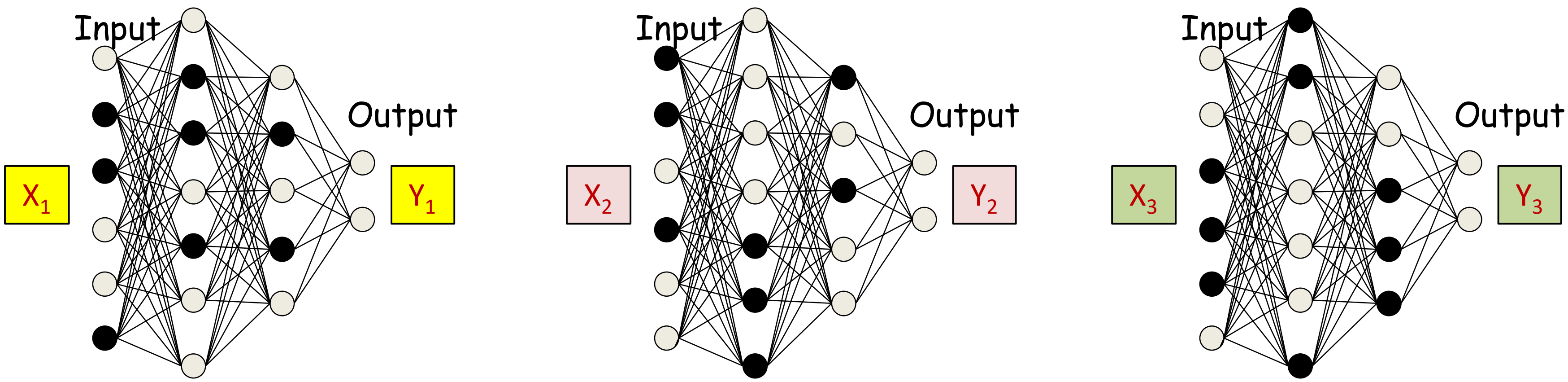
- **During training:** For each input, at each iteration, "turn off" each neuron with a probability 1-α
  - Also turn off inputs similarly

Dropout



- **During training:** For each input, at each iteration, "turn off" each neuron (including inputs) with a probability $1-\alpha$
  - In practice, set them to 0 according to the failure of a Bernoulli random number generator with success probability α

Dropout



The pattern of dropped nodes changes for *each input*
i.e. in every pass through the net

- **During training:** For each input, at each iteration, "turn off" each neuron (including inputs) with a probability 1-α
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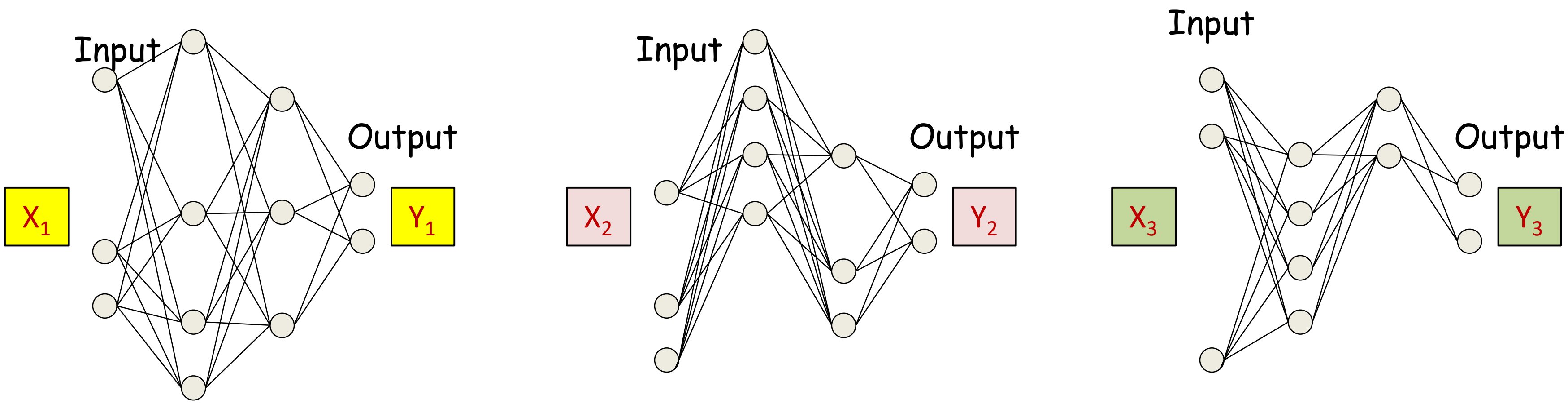
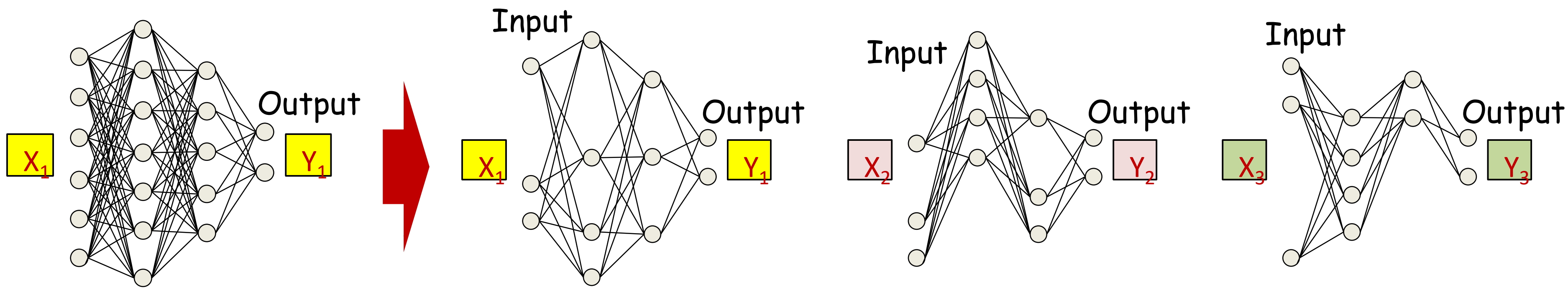
Dropout



The pattern of dropped nodes changes for *each input*
i.e. in every pass through the net

- **During training:** Backpropagation is effectively performed only over the remaining network
  - The effective network is different for different inputs
  - Gradients are obtained only for the weights and biases *from* "On" nodes *to* "On" nodes
    - For the remaining, the gradient is just 0

Statistical Interpretation



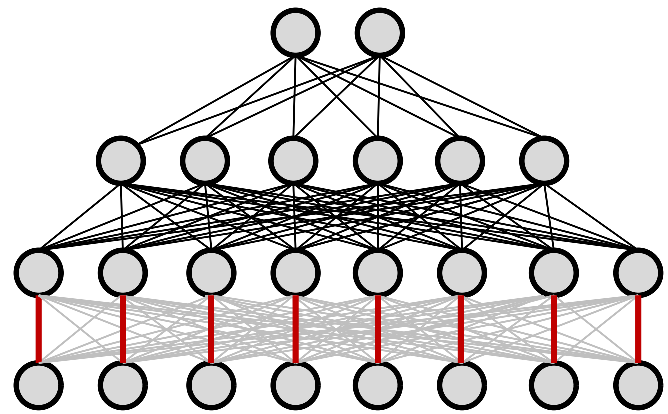
- For a network with a total of N neurons, there are 2^N possible sub-networks
  - Obtained by choosing different subsets of nodes
  - Dropout *samples* over all 2^N possible networks
  - Effectively learns a network that *averages* over all possible networks
    - Bagging

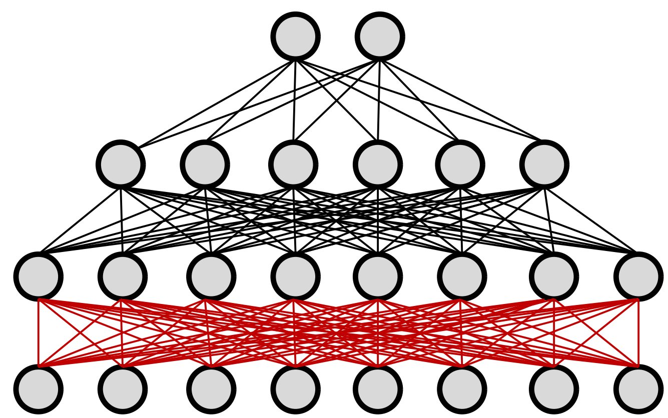
Dropout as a mechanism to increase pattern density

- Dropout forces the neurons to learn "rich" and redundant patterns

- E.g. without dropout, a non-compressive layer may just "clone" its input to its output
  - Transferring the task of learning to the rest of the network upstream

- Dropout forces the neurons to learn denser patterns
  - With redundancy





The forward pass

- Input: D dimensional vector $\mathbf{x} = [x_j,\ j = 1 \dots D]$
- Set:
  - $D_0 = D,$ is the width of the 0th (input) layer
  - $y_j^{(0)} = x_j,\ j = 1 \dots D; \qquad y_0^{(k=1\dots N)} = x_0 = 1$
- For layer $k = 1 \dots N$

  # Mask takes value 1 with prob. α, 0 with prob $1 - \alpha$
  - $mask(k-1, j) = \ Bernoulli(\alpha)\ ,\ j = 1 \dots D_{k-1}$
  - $y_j^{(k-1)} = y_j^{(k-1)}.mask(k-1, j),\ j = 1 \dots D_{k-1}$
  - For $j = 1 \dots D_k$
    - $z_j^{(k)} = \sum_{i=0}^{N_k} w_{i,j}^{(k)} y_i^{(k-1)} + b_j^{(k)}$
    - $y_j^{(k)} = f_k\left(z_j^{(k)}\right)$
- Output:
  - $Y = y_j^{(N)}, j = 1..D_N$

Backward Pass

- Output layer (N) :
  - $\frac{\partial Div}{\partial Y_i} = \frac{\partial Div(Y,d)}{\partial y_i^{(N)}}$
  - $\frac{\partial Div}{\partial z_i^{(k)}} = f_k'\left(z_i^{(k)}\right)\frac{\partial Div}{\partial y_i^{(k)}}$
- For layer $k = N - 1\ downto\ 0$
  - For $i = 1 \dots D_k$
    - $\frac{\partial Div}{\partial y_i^{(k)}} = mask(k,i)\sum_j w_{ij}^{(k+1)} \frac{\partial Div}{\partial z_j^{(k+1)}}$
    - $\frac{\partial Div}{\partial z_i^{(k)}} = f_k'\left(z_i^{(k)}\right)\frac{\partial Div}{\partial y_i^{(k)}}$
    - $\frac{\partial Div}{\partial w_{ij}^{(k+1)}} = y_i^{(k)} \frac{\partial Div}{\partial z_j^{(k+1)}}$ for $j = 1 \dots D_{k+1}$

Testing with Dropout

- Dropout effectively trains 2^N networks
- On test data the "Bagged" output, in principle, is the ensemble average over all 2^N networks and is thus the statistical expectation of the output over all networks

$$Y = E\left[network\left(y_j^{(k)}, j = 1 \dots D_k, k = 1 \dots K\right)\right]$$

  - Explicitly showing the network as a function of the outputs of individual neurons in the net

- We cannot explicitly compute this expectation

- Instead we will use the following approximation

$$E\left[network\left(y_j^{(k)}, \forall k, j\right)\right] = network\left(E[y_j^{(k)}] \forall k, j\right)$$

  - Where $E[y_j^{(k)}]$ is the expected output of the jth neuron in the kth layer over all networks in the ensemble
  - I.e. approximate the expectation of a function as the function of expectations

- We require $E[y_j^{(k)}]$ to compute this

What each neuron computes

- Each neuron actually has the following activation:

$$y_i^{(k)} = D\sigma\left(\sum_j w_{ji}^{(k)} y_j^{(k-1)} + b_i^{(k)}\right)$$

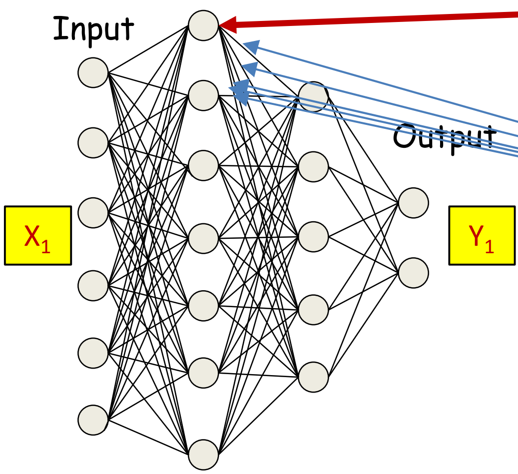
  – Where D is a Bernoulli variable that takes a value 1 with probability α

- D may be switched on or off for individual sub networks, but over the ensemble, the *expected output* of the neuron is

$$\mathrm{E}[y_i^{(k)}] = \alpha\sigma\left(\sum_j w_{ji}^{(k)} y_j^{(k-1)} + b_i^{(k)}\right)$$

- During *test* time, we will use the *expected* output of the neuron
  – Consists of simply scaling the output of each neuron by α

Dropout during test: implementation



apply α here (to the output of the neuron) OR..

Push the α to all outgoing weights

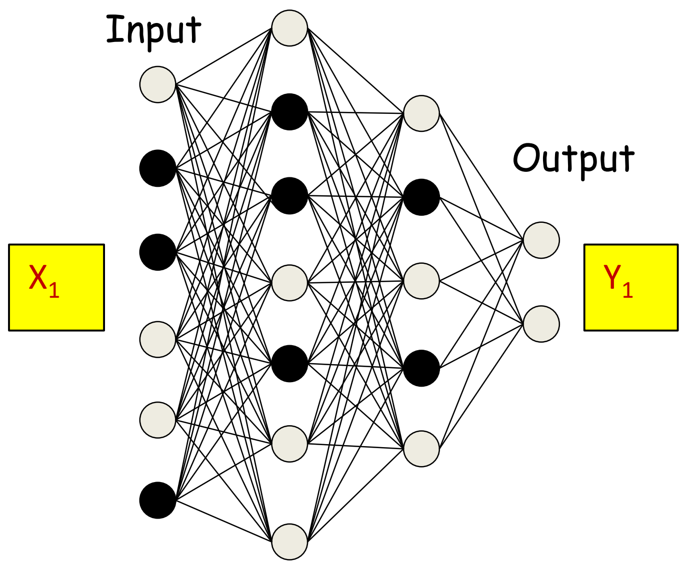
$$y_i^{(k)} = \alpha\sigma\left(z_i^{(k)}\right)$$

$$z_i^{(k)} = \sum_j w_{ji}^{(k)} y_j^{(k-1)} + b_i^{(k)}$$
$$= \sum_j w_{ji}^{(k)} \alpha\sigma\left(z_j^{(k-1)}\right) + b_i^{(k)}$$
$$= \sum_j \left(\alpha w_{ji}^{(k)}\right) \sigma\left(z_j^{(k-1)}\right) + b_i^{(k)}$$

$$W_{test} = \alpha W_{trained}$$

- Instead of multiplying every output by α, multiply all weights by α

Dropout : alternate implementation

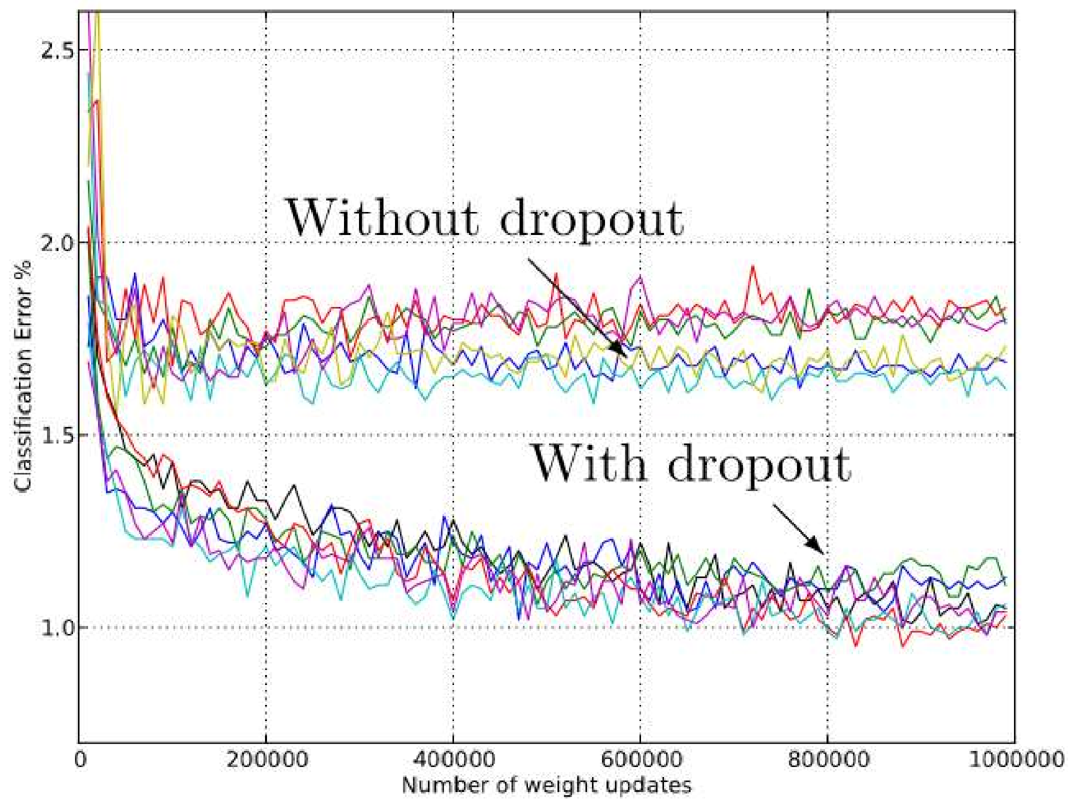


- Alternately, during *training,* replace the activation of all neurons in the network by $\alpha^{-1}\sigma(.)$
  - This does not affect the dropout procedure itself
  - We will use $\sigma(.)$ as the activation during testing, and not modify the weights

Inference with dropout (testing)

- Input: D dimensional vector $\mathbf{x} = [x_j,\ j = 1 \ldots D]$
- Set:
  - $D_0 = D,$ is the width of the 0th (input) layer
  - $y_j^{(0)} = x_j,\ j = 1 \ldots D; \qquad y_0^{(k=1 \ldots N)} = x_0 = 1$
- For layer $k = 1 \ldots N$
  - For $j = 1 \ldots D_k$
    - $z_j^{(k)} = \sum_{i=0}^{N_k} w_{i,j}^{(k)} y_i^{(k-1)} + b_j^{(k)}$
    - $y_j^{(k)} = \alpha f_k\left(z_j^{(k)}\right)$
- Output:
  - $Y = y_j^{(N)}, j = 1..D_N$

Dropout: Typical results



- From Srivastava et al., 2013. Test error for different architectures on MNIST with and without dropout
  - 2-4 hidden layers with 1024-2048 units

Variations on dropout

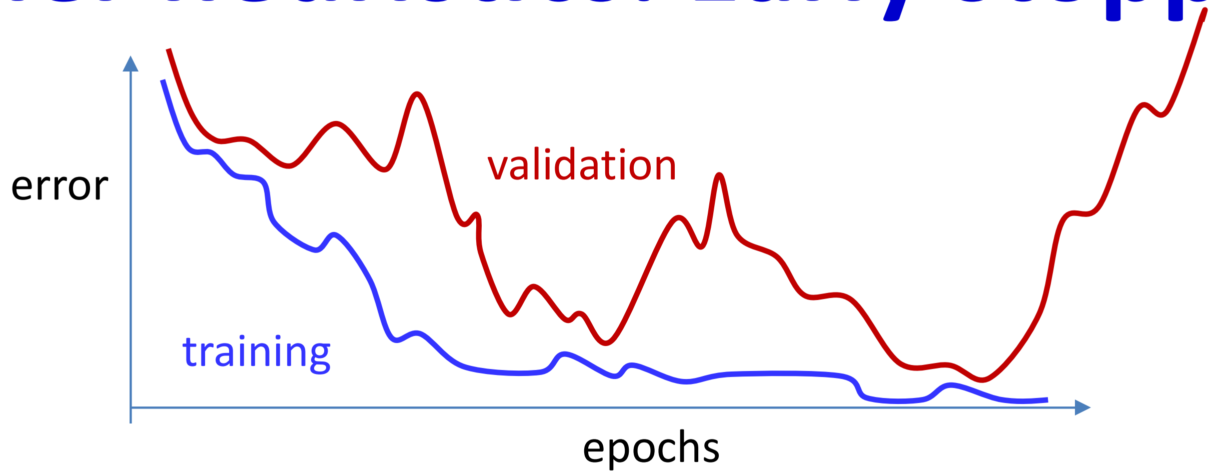
- Zoneout: For RNNs
  - Randomly chosen units remain unchanged across a time transition
- Dropconnect
  - Drop individual connections, instead of nodes
- Shakeout
  - Scale *up* the weights of randomly selected weights
    - $|w| \rightarrow \alpha|w| + (1-\alpha)c$
  - Fix remaining weights to a negative constant
    - $w \rightarrow -c$
- Whiteout
  - Add or multiply weight-dependent Gaussian noise to the signal on each connection

Story so far

- Gradient descent can be sped up by incremental updates
- Convergence can be improved using smoothed updates

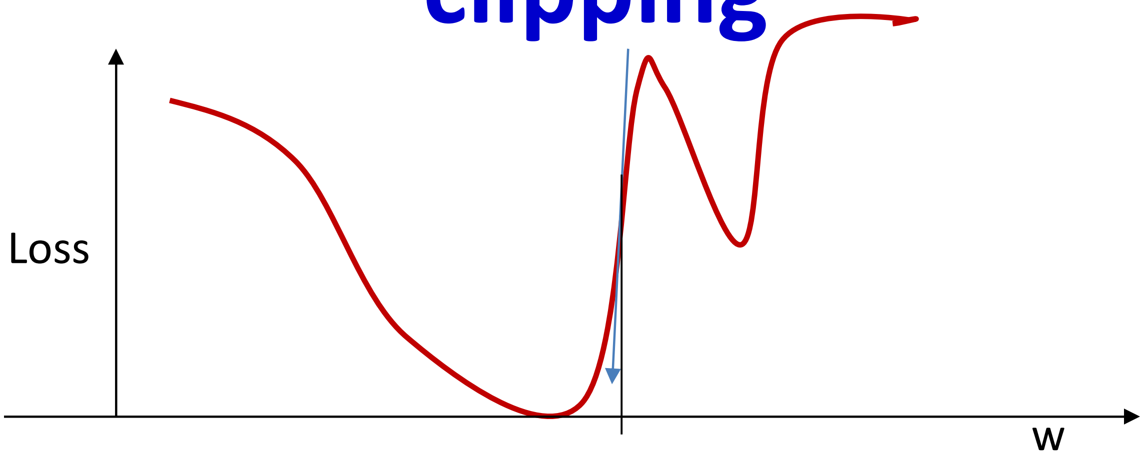
- The choice of divergence affects both the learned network and results
- Covariate shift between training and test may cause problems and may be handled by batch normalization
- Data underspecification can result in overfitted models and must be handled by regularization and more constrained (generally deeper) network architectures
- “Dropout” is a stochastic data/model erasure method that sometimes forces the network to learn more robust models

Other heuristics: Early stopping



- Continued training can result in over fitting to training data
  - Track performance on a held-out validation set
  - Apply one of several early-stopping criterion to terminate training when performance on validation set degrades significantly

Additional heuristics: Gradient clipping

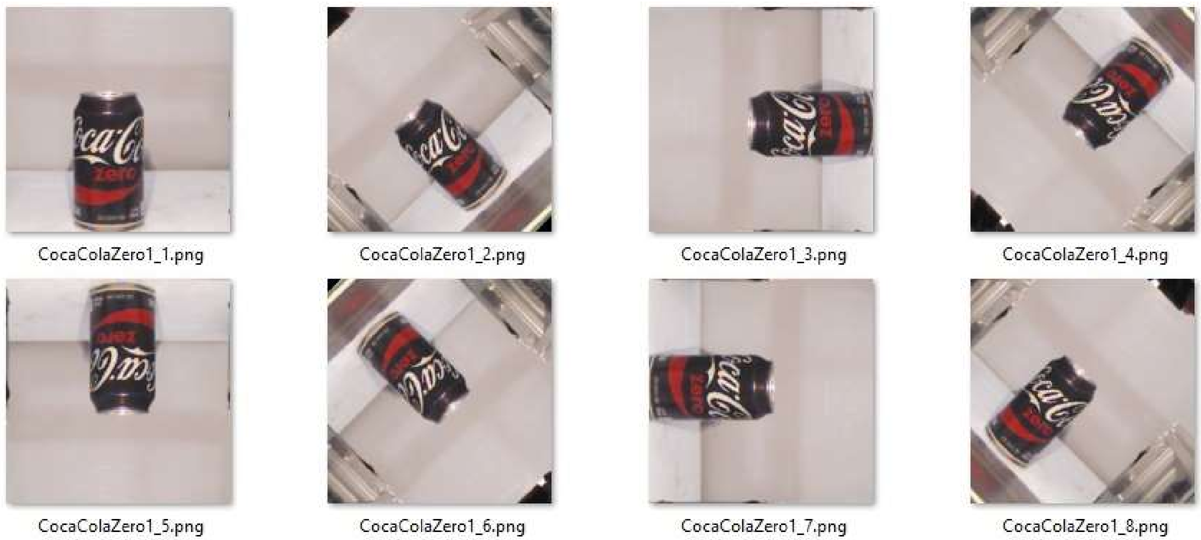


- Often the derivative will be too high
  - When the divergence has a steep slope
  - This can result in instability
- **Gradient clipping**: set a ceiling on derivative value

$$if\ \partial_w D > \theta\ then\ \partial_w D = \theta$$

  - Typical θ value is 5

Additional heuristics: Data Augmentation



- Available training data will often be small
- “Extend” it by distorting examples in a variety of ways to generate synthetic labelled examples
  - E.g. rotation, stretching, adding noise, other distortion

Other tricks

- Normalize the input:
  - Normalize entire training data to make it 0 mean, unit variance
  - Equivalent of batch norm on input

- A variety of other tricks are applied
  - Initialization techniques
    - Xavier, Kaiming, SVD, etc.
    - Key point: neurons with identical connections that are identically initialized will never diverge
  - Practice makes man perfect

Setting up a problem

- Obtain training data
  - Use appropriate representation for inputs and outputs
- Choose network architecture
  - More neurons need more data
  - Deep is better, but harder to train
- Choose the appropriate divergence function
  - Choose regularization
- Choose heuristics (batch norm, dropout, etc.)
- Choose optimization algorithm
  - E.g. ADAM
- Perform a grid search for hyper parameters (learning rate, regularization parameter, …) on held-out data
- Train
  - Evaluate periodically on validation data, for early stopping if required

In closing

- Have outlined the process of training neural networks
  - Some history
  - A variety of algorithms
  - Gradient-descent based techniques
  - Regularization for generalization
  - Algorithms for convergence
  - Heuristics
- Practice makes perfect..