Network Regularization

Weight initialization, dropout, batch normalization

Machine Learning and Data Mining, 2024

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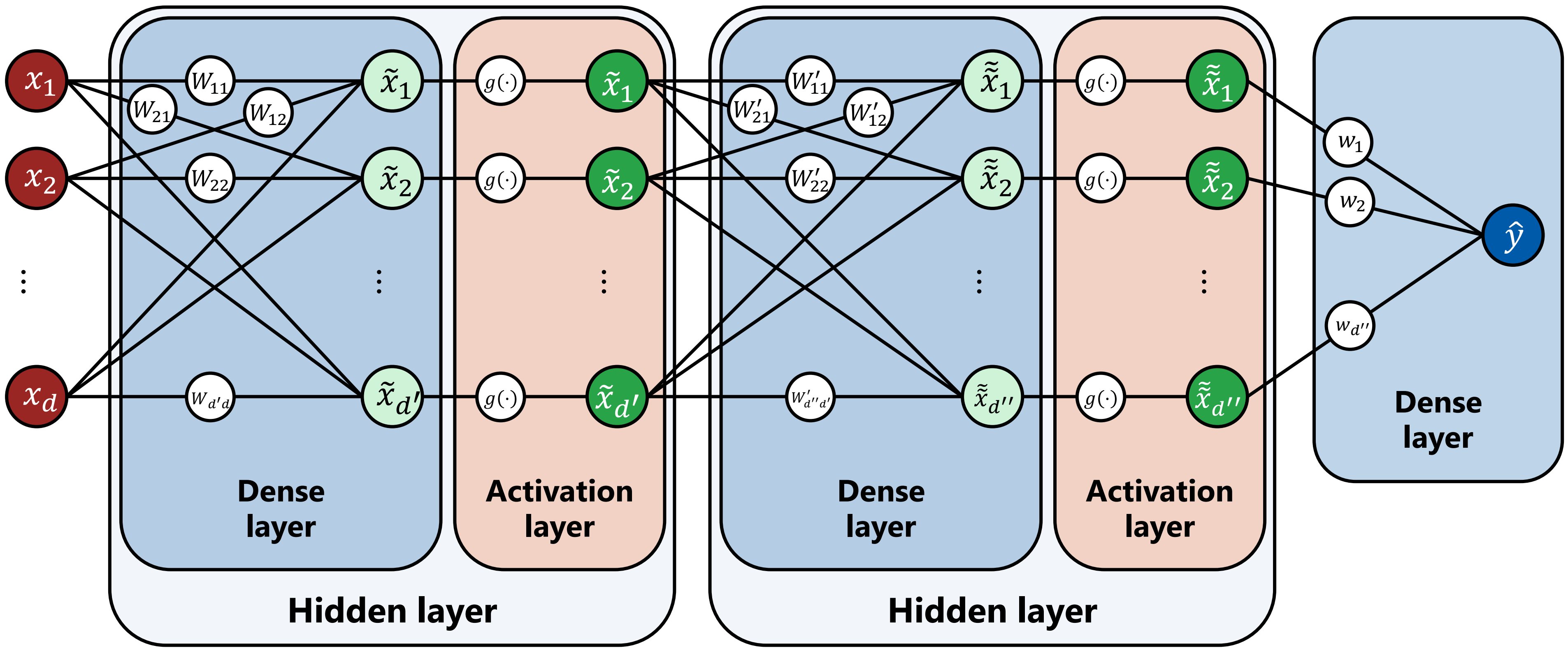
Why care about weight initialization?

Initialization with a constant (?)



What happens if we initialize all weights with the same value?

Majid Sohrabi, NRU HSE

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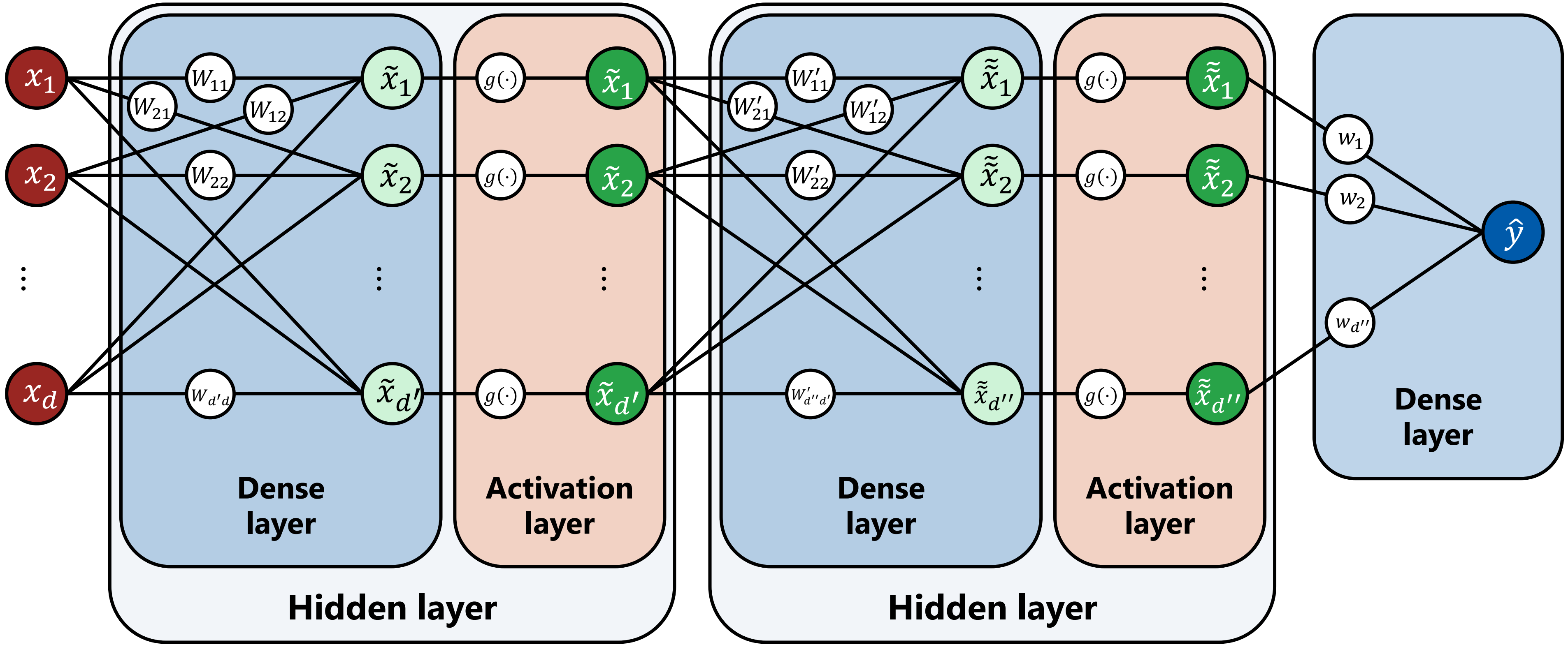

What happens if we initialize all weights with the same value?

Within each layer, the gradients for each of the weights will be the same as well ⇒ **updates will be the same** ⇒ network degrades!

Initialization with a constant (?)

Ok, so constant initialization is a bad idea

So, any random initialization should be fine, right?

Some intuition

For simplicity, let's omit the activation functions for now

Then, the output of a neural network composed of dense layers only is:

$$\hat{y} = W_{out} \cdot \dots \cdot W_{h2} \cdot W_{h1} x$$

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$$g \sim S^{m-1}$$

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For S too large, the gradients will **explode**; for S too small, they will **vanish**

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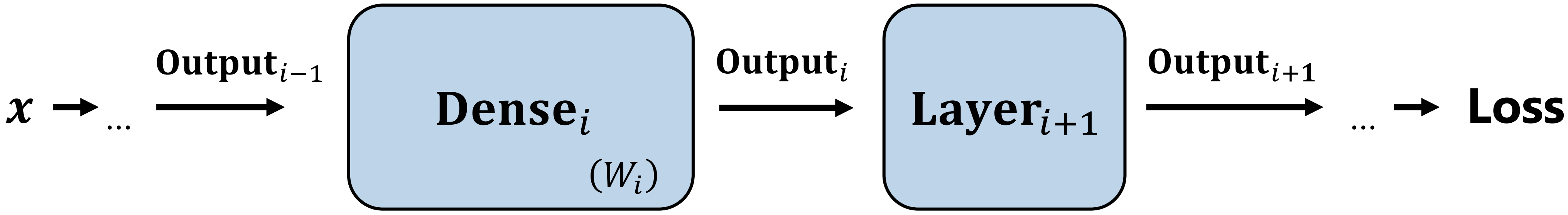

More generally:

$$\frac{\partial \mathbf{Loss}}{\partial W_i} = \frac{\partial \mathbf{Loss}}{\partial \mathbf{Output}_i} \cdot \frac{\partial \mathbf{Dense}_i}{\partial W_i} = \frac{\partial \mathbf{Loss}}{\partial \mathbf{Output}_{i+1}} \cdot \frac{\partial \mathbf{Layer}_{i+1}}{\partial \mathbf{Output}_i} \cdot \mathbf{Output}_{i-1}$$

Some intuition

$$x \to \dots \xrightarrow{\mathbf{Output}_{i-1}} \boxed{\mathbf{Dense}_i \; (W_i)} \xrightarrow{\mathbf{Output}_i} \boxed{\mathbf{Layer}_{i+1}} \xrightarrow{\mathbf{Output}_{i+1}} \dots \to \mathbf{Loss}$$

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This will accumulate the product of the gradients for the subsequent layers

Idea: for stable learning we would like to “keep” the scale of the gradients at each step:

$$\mathrm{Var}\left(\frac{\partial \textbf{Layer}_{i+1}}{\partial \textbf{Output}_i} \cdot \frac{\partial \textbf{Layer}_i}{\partial \textbf{Output}_{i-1}}\right) \approx \mathrm{Var}\left(\frac{\partial \textbf{Layer}_{i+1}}{\partial \textbf{Output}_i}\right)$$

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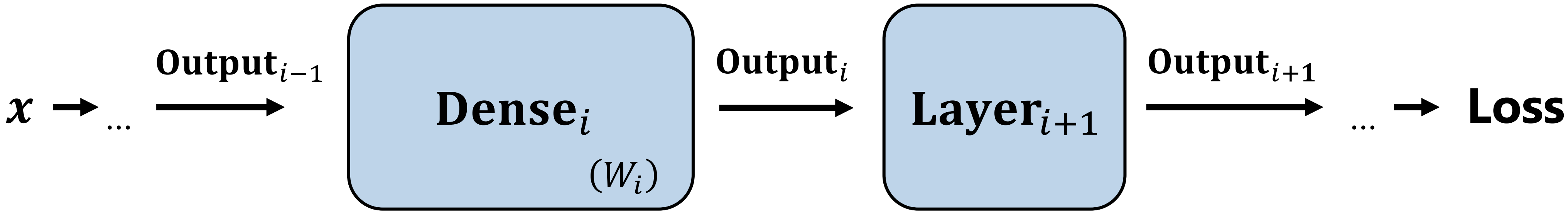

Similarly, we would also like to not scale the outputs at each step of the forward pass:

$$\mathrm{Var}\left(\mathbf{Layer}_{i+1}(\mathbf{Layer}_i(\mathbf{Output}_{i-1}))\right) \approx \mathrm{Var}(\mathbf{Layer}_i(\mathbf{Output}_{i-1}))$$

Random initialization

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Generally, these two requirements may contradict each other

E.g. for ReLU activation they result in initialization requirements, respectively:

$$Var(W_{ij}) = \frac{2}{(\#\ \text{outgoing connections})}$$

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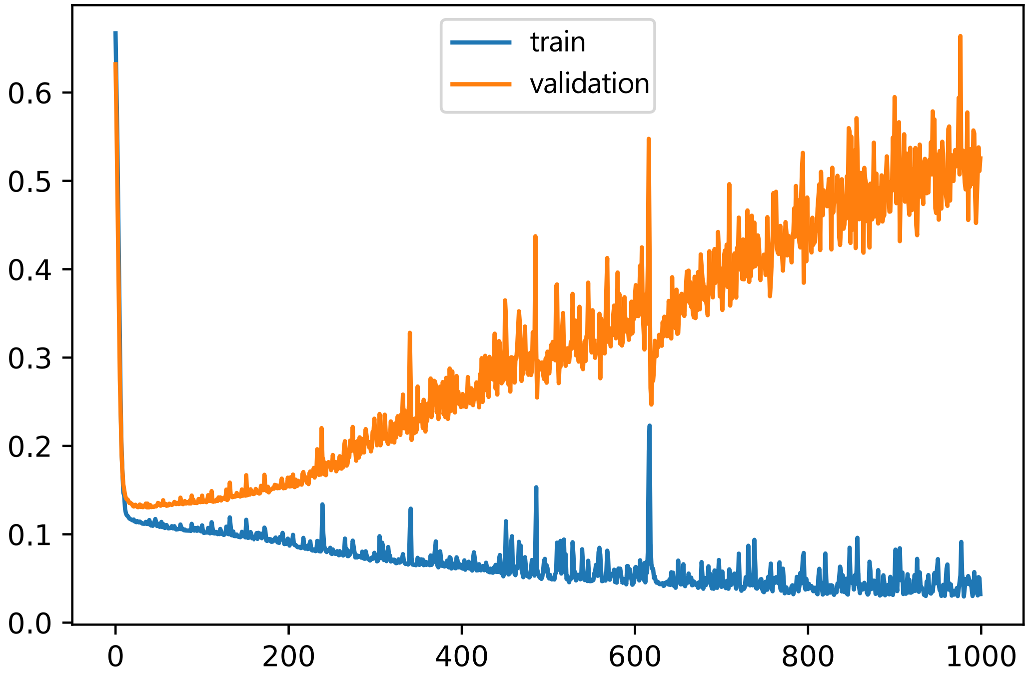
Typically you can just choose one of them, or alternatively average them out:

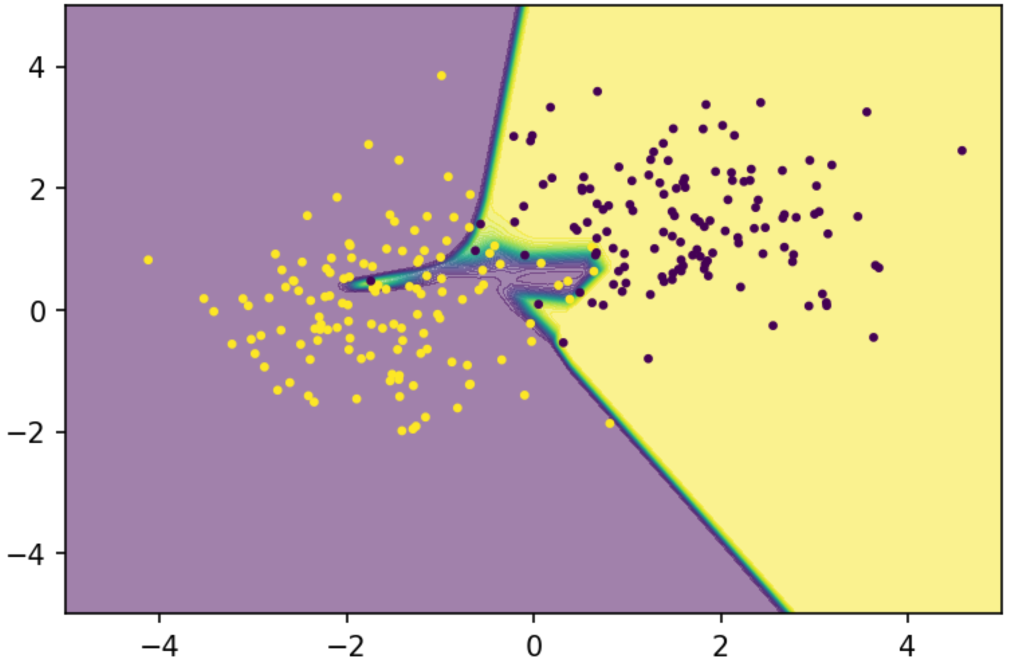
$$Var(W_{ij}) = \frac{4}{(\#\ \text{outgoing connections}) + (\#\ \text{incoming connections})}$$

Overfitting with neural networks

The problem of overfitting

Being highly complex models, neural networks are prone to overfitting





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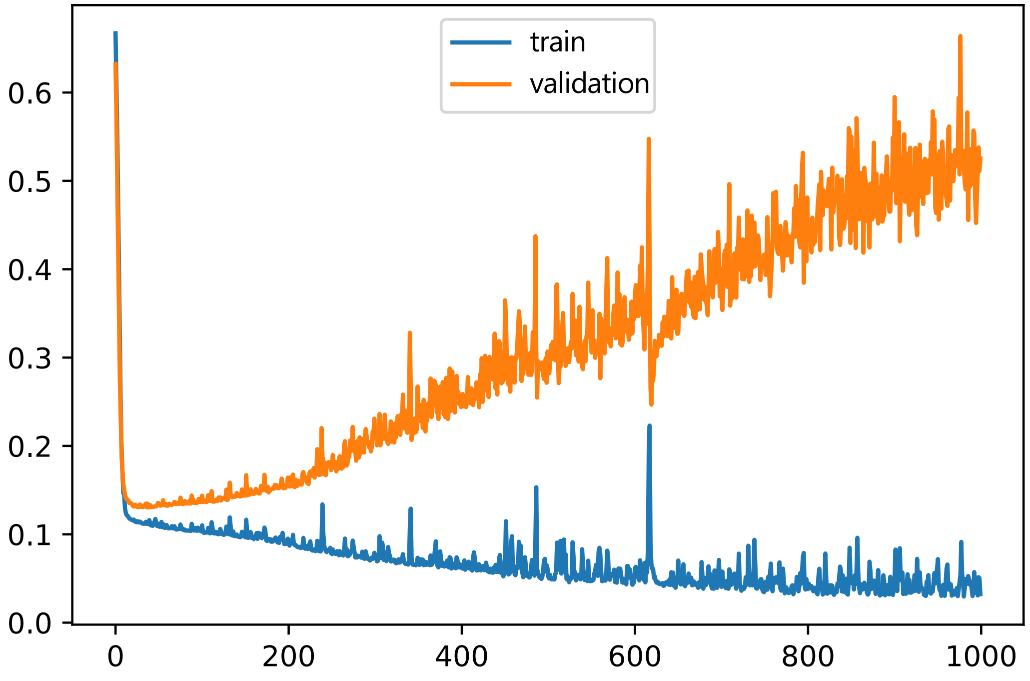
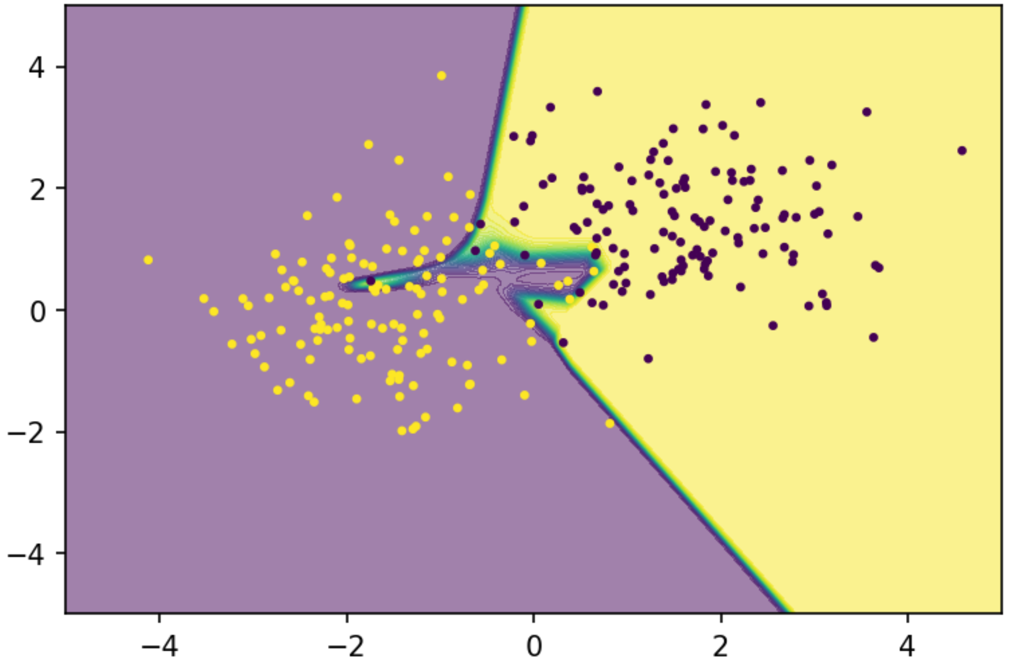




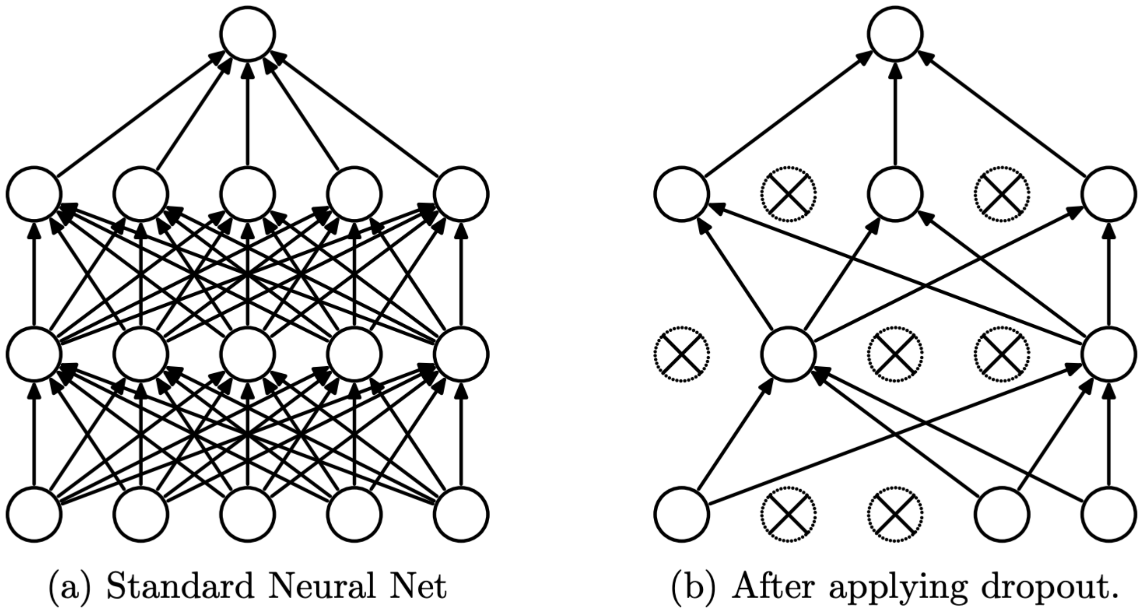
Regularization techniques like L1/L2 regularization are also available for neural networks

We also discussed **early stopping** (i.e. stop the training before validation error grows)

Dropout

At train time – sets neuron activations to 0 with a given probability p

Image from:
http://jmlr.org/papers/v15/srivastava14a.html



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- i.e. sets it to the **expected value**

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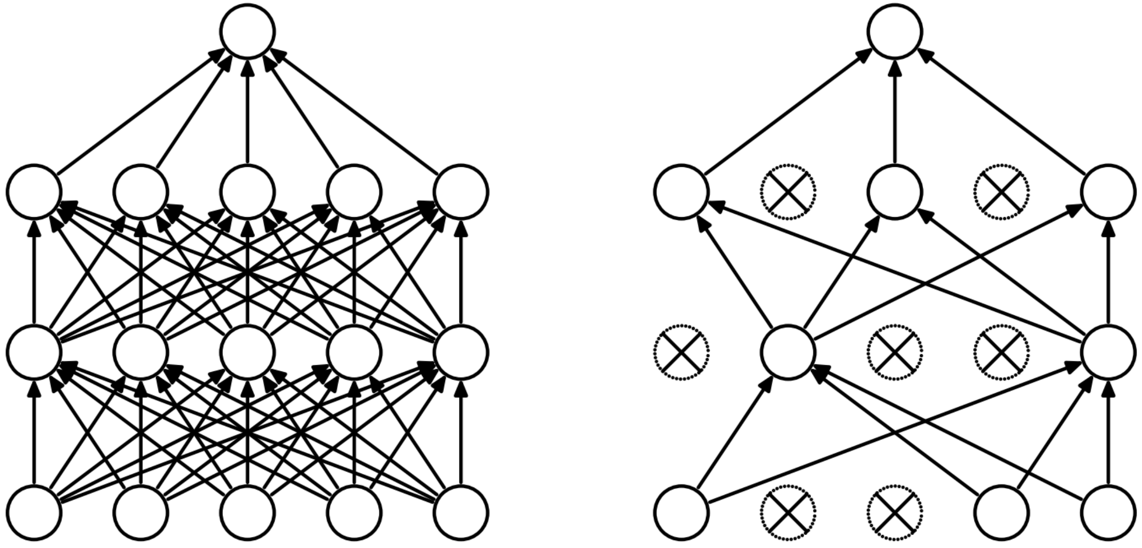
(a) Standard Neural Net (b) After applying dropout.

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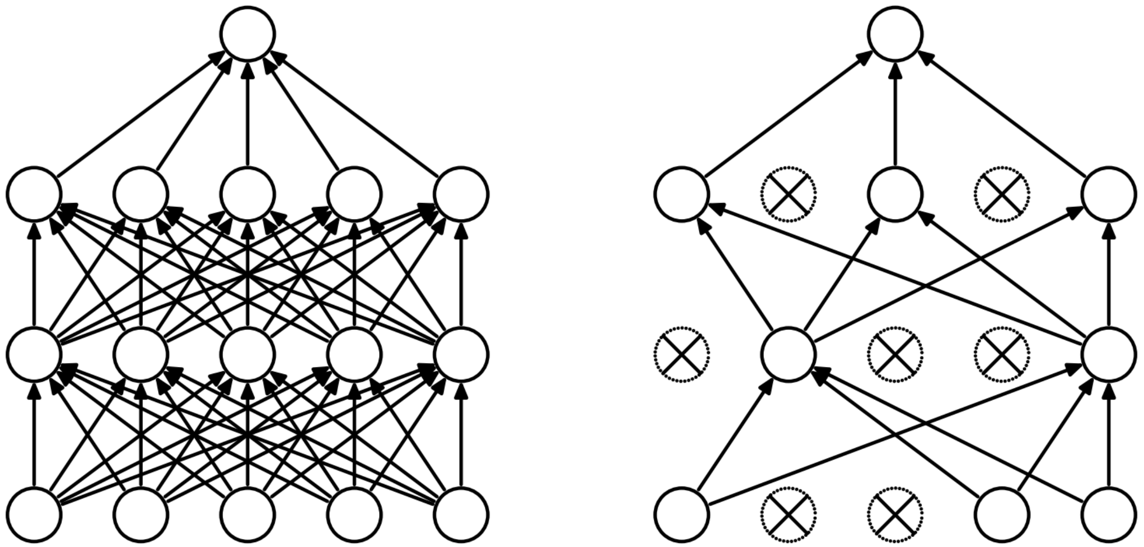

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Makes neuron learn to work with a **randomly chosen sample** of other neurons

Drives it towards **creating useful features** rather than relying on other neurons to correct its mistakes

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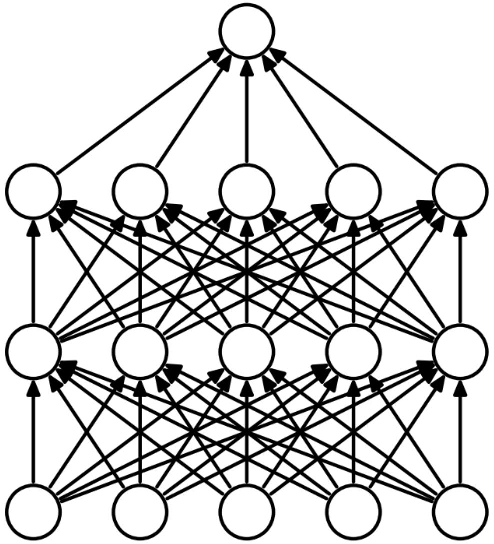
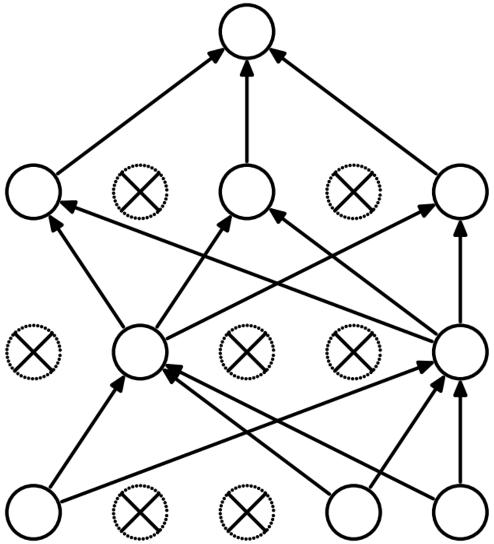
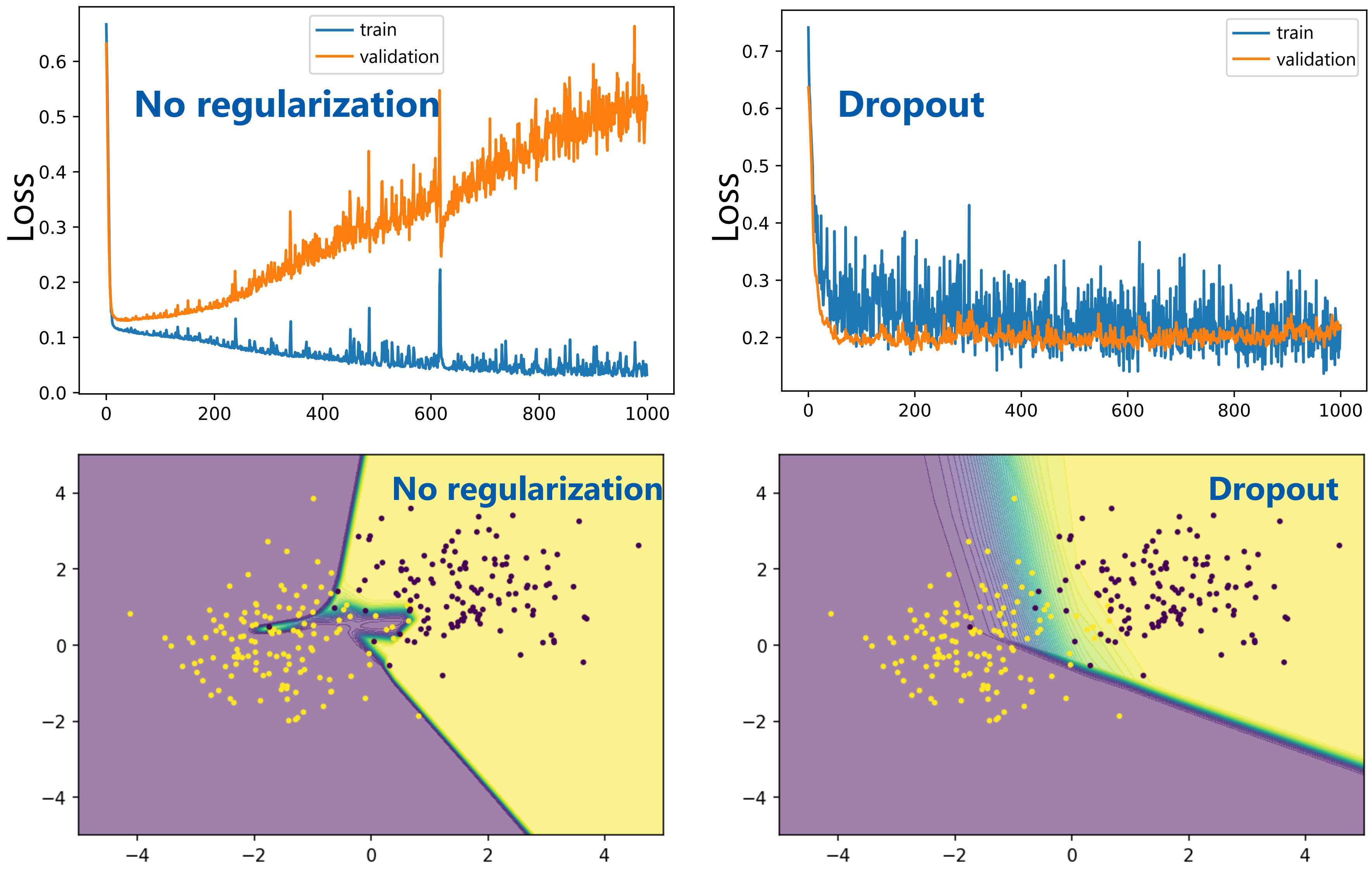


(a) Standard Neural Net



(b) After applying dropout.

Example from before



In this example, dropout results in a much better (though still not perfect) fit with lower test error

Normalization layers

Batch normalization

This technique was originally proposed to mitigate the "internal covariate shift"

internal covariate shift

the updates in one layer change the input distributions of the subsequent layers

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Works as follows (layer inputs x_i, outputs y_i):

- calculate sample **mean** and **variance** of the input on a single batch B

$$\mu_B = \frac{1}{|B|}\sum_{i \in B} x_i \qquad \sigma_B^2 = \frac{1}{|B|}\sum_{i \in B} (x_i - \mu_B)^2$$

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- **normalize** the input, then **scale and shift** (with the trainable parameters γ, β):

$$y_i = \gamma \cdot \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}} + \beta$$

Batch normalization

Turned out to be **extremely powerful** in many cases

- Faster and more stable convergence

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internal covariate shift

the updates in one layer change the input distributions of the subsequent layers

Effectively **removes** the 'shift' and 'scale' degrees of freedom from the previous layer

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Batch normalization

Which dimension to normalize over? Typically, like this:

- Batch of 1D vectors [Batch_dim x Features_dim]
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Batch normalization

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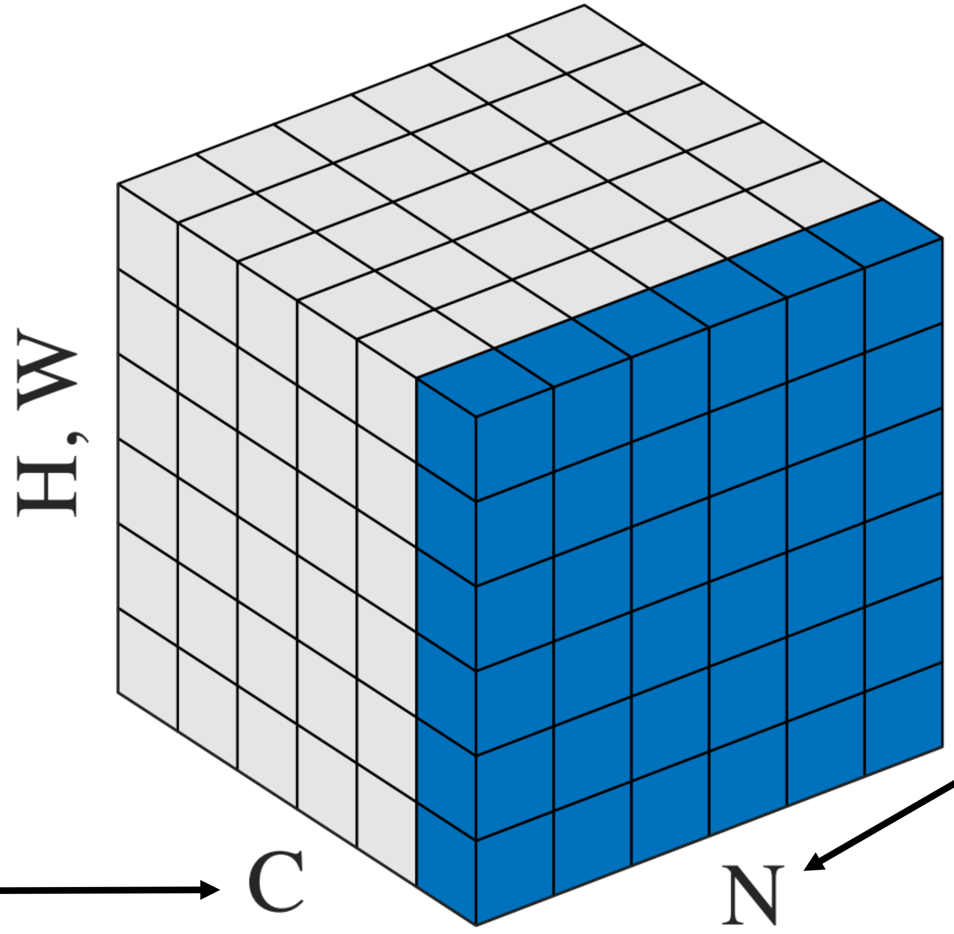
- Batch of ND objects [Batch_dim x Spacial_dim1 x … x Channel_dim]
  - separately for each component in Channel_dim, i.e., over Batch_dim x Spacial_dim1 x …

Batch normalization

Image from
https://arxiv.org/pdf/1803.08494.pdf

Spatial dimensions



Batch dimension

Channels

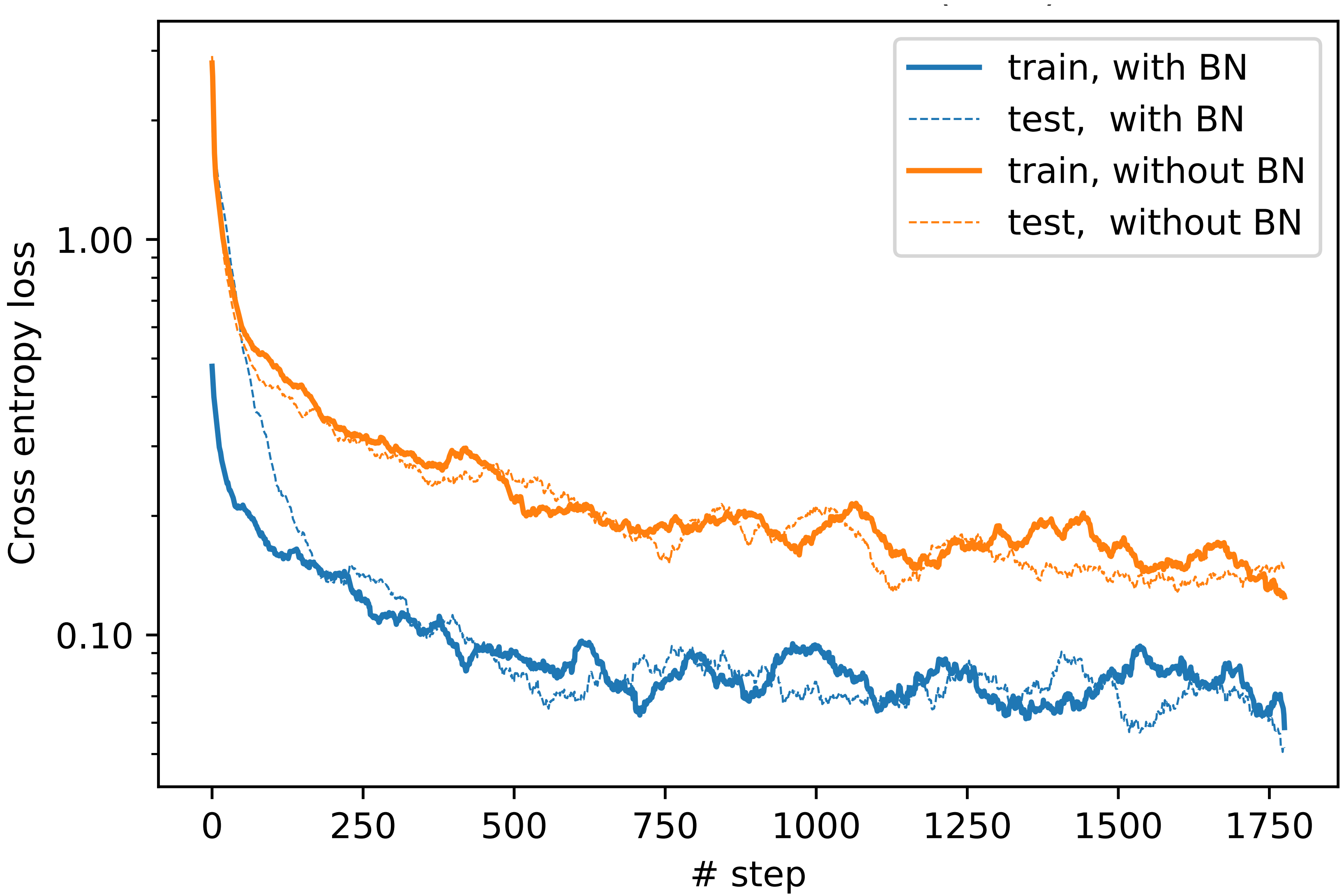
Batch normalization at inference time

Calculating batch statistics at test time may be problematic

- e.g. when there’s a single object to predict

Instead: calculate running mean and variance during training, apply at test time

Example: CNN on MNIST



(shown: moving average loss)

Layer Normalization

Batch normalization imposes limits on the batch size

- if too small, the variance of the sample statistics will be too high

Problematic to use in recurrent networks

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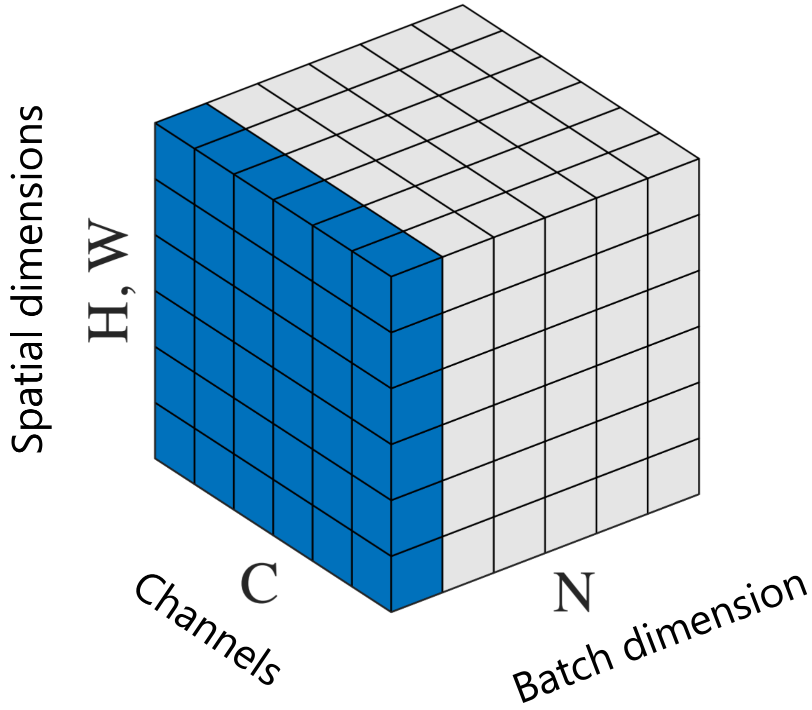
Alternative: **Layer Normalization**

- the math is same, except statistics is calculated over channels rather than batch elements



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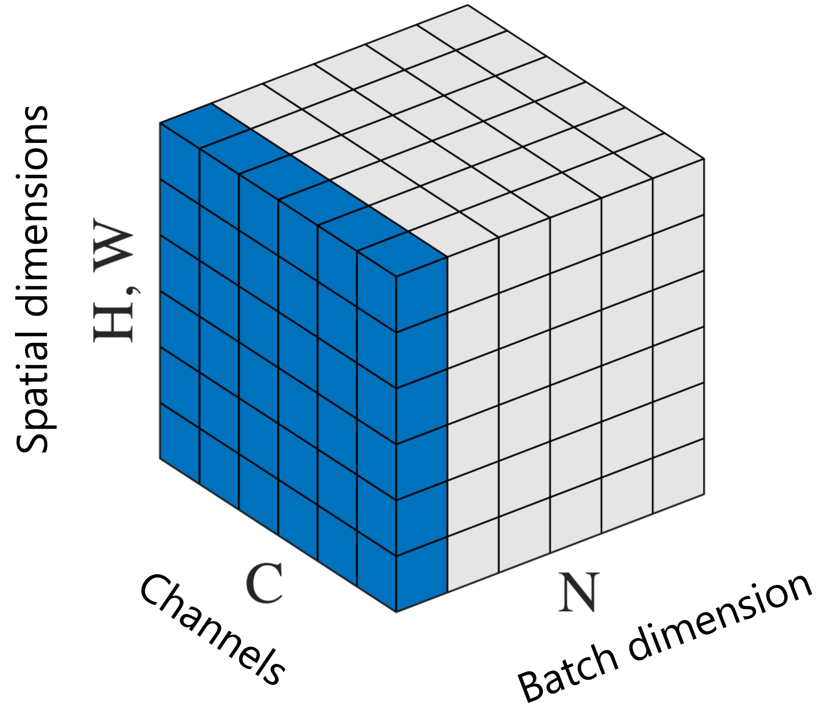

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Alternative: **Layer Normalization**

- the math is same, except statistics is calculated over channels rather than batch elements
- the effect is quite different though
  - e.g. Layer Normalization "entangles" different neurons within a layer

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Batch normalization is an **extremely powerful** regularization technique, though the reason for that is not entirely clear

Food for thought: how exactly would you implement an early stopping rule?

Thank you!

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