Network Regularization

Weight initialization, dropout, batch normalization

Machine Learning and Data Mining, 2021

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LAMBDA • HSE

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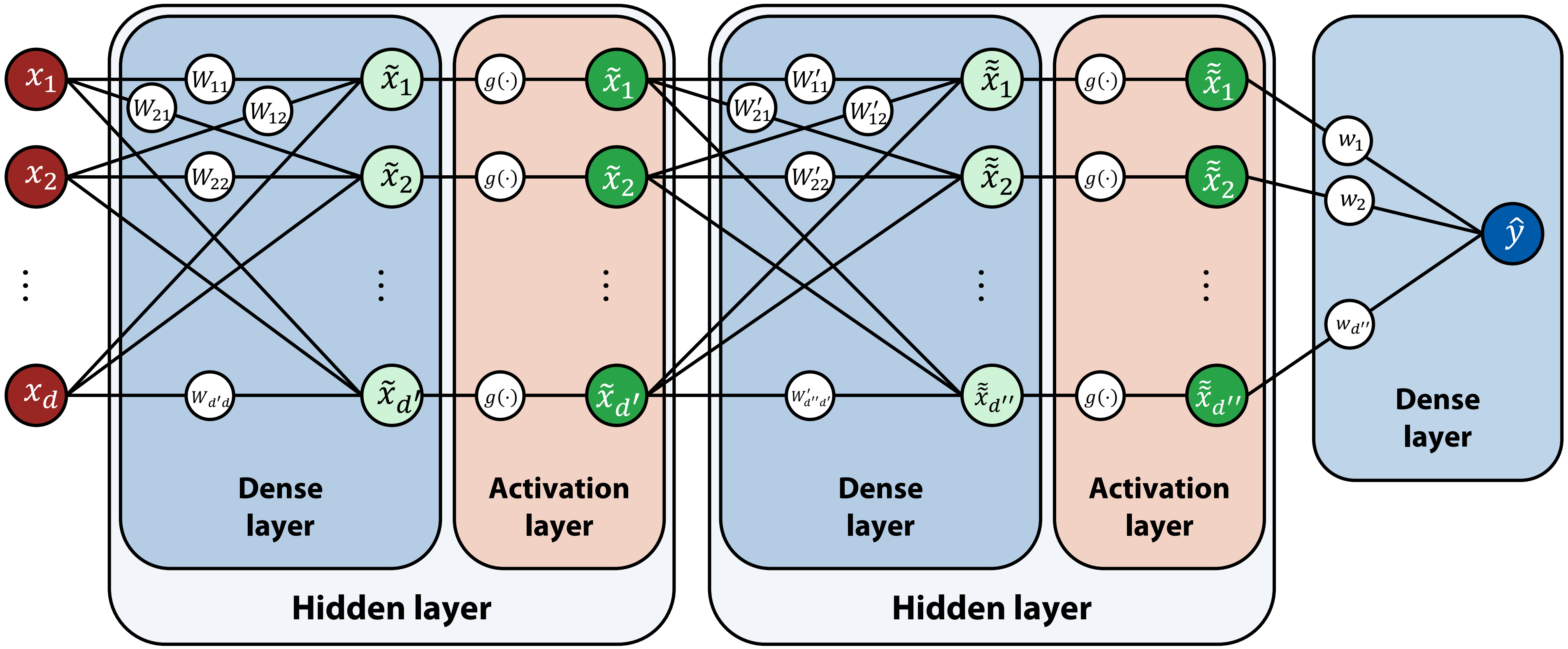
Why care about weight initialization?

Initialization with a constant (?)



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

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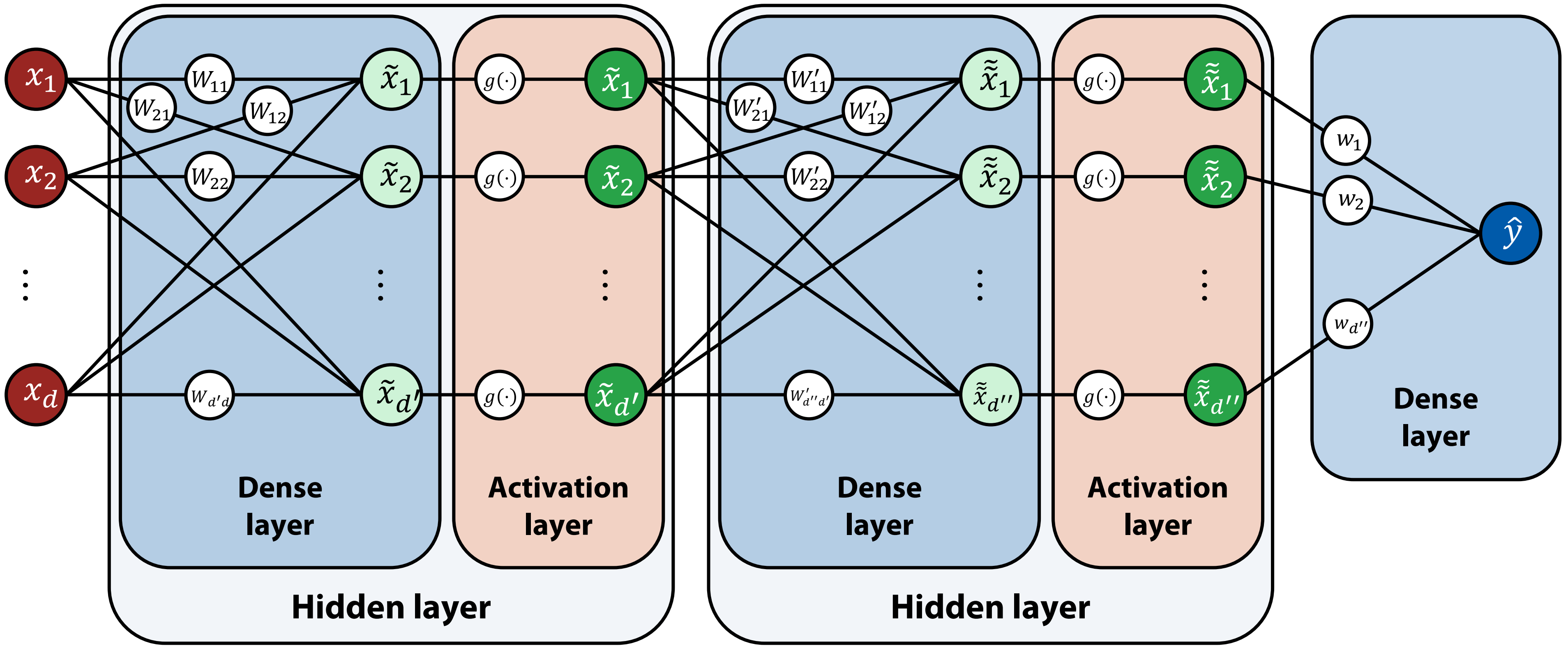

- What happens if we initialize all weights with the same value?
- Within each layer, the gradients for each of the weights will be the same as well $\Rightarrow$ **updates will be the same** $\Rightarrow$ network degrades!

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:

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

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  where m is the **depth** of the network
- For S too large, the gradients will **explode**; for S too small, they will **vanish**

Some intuition

$$\begin{tikzcd}
\boldsymbol{x} \arrow[r] & \ldots \arrow[r, "\mathbf{Output}_{i-1}"] & \boxed{\mathbf{Dense}_i \;\; (W_i)} \arrow[r, "\mathbf{Output}_{i}"] & \boxed{\mathbf{Layer}_{i+1}} \arrow[r, "\mathbf{Output}_{i+1}"] & \ldots \arrow[r] & \mathbf{Loss}
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- More generally:

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

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

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

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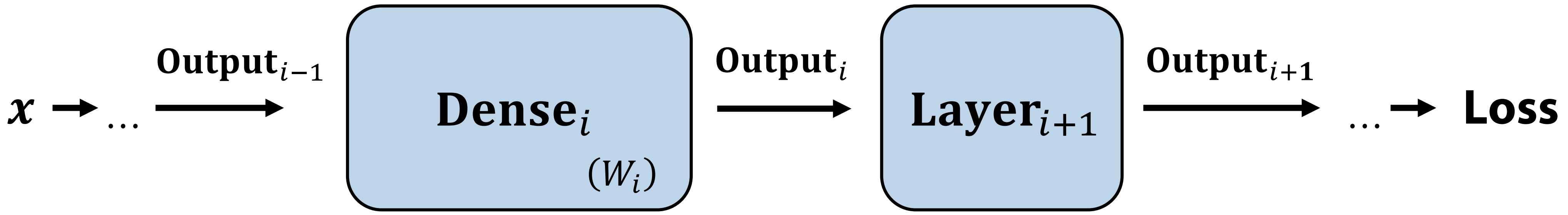

- Similarly, we would also like to not scale the outputs at each step of the forward pass:

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

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:

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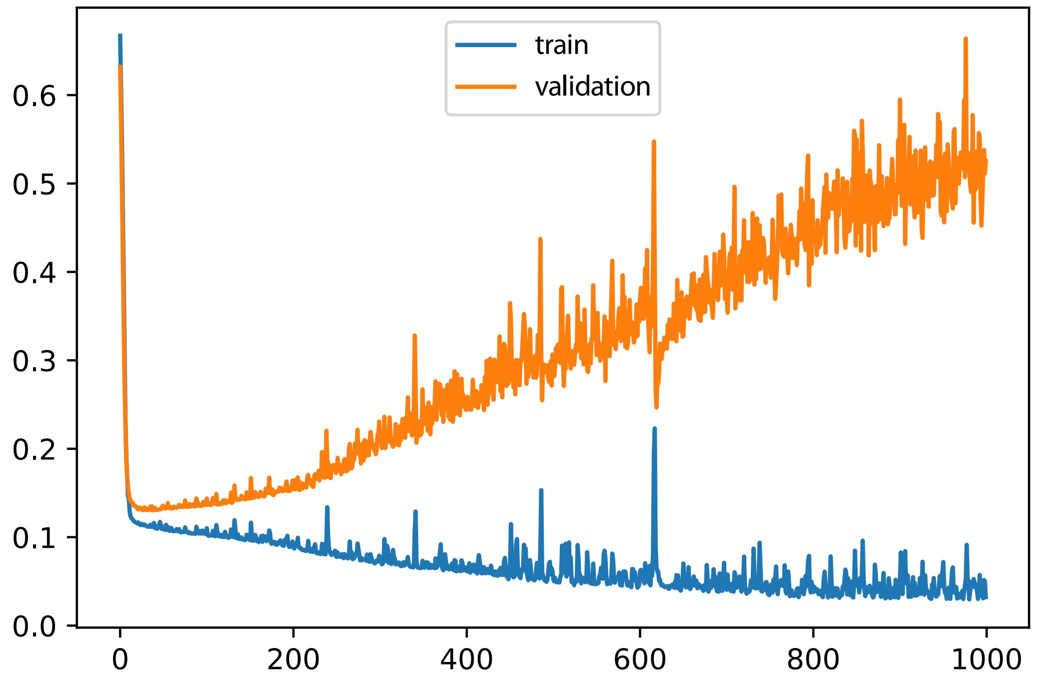
- Typically you can just choose one of them, or alternatively average them out:

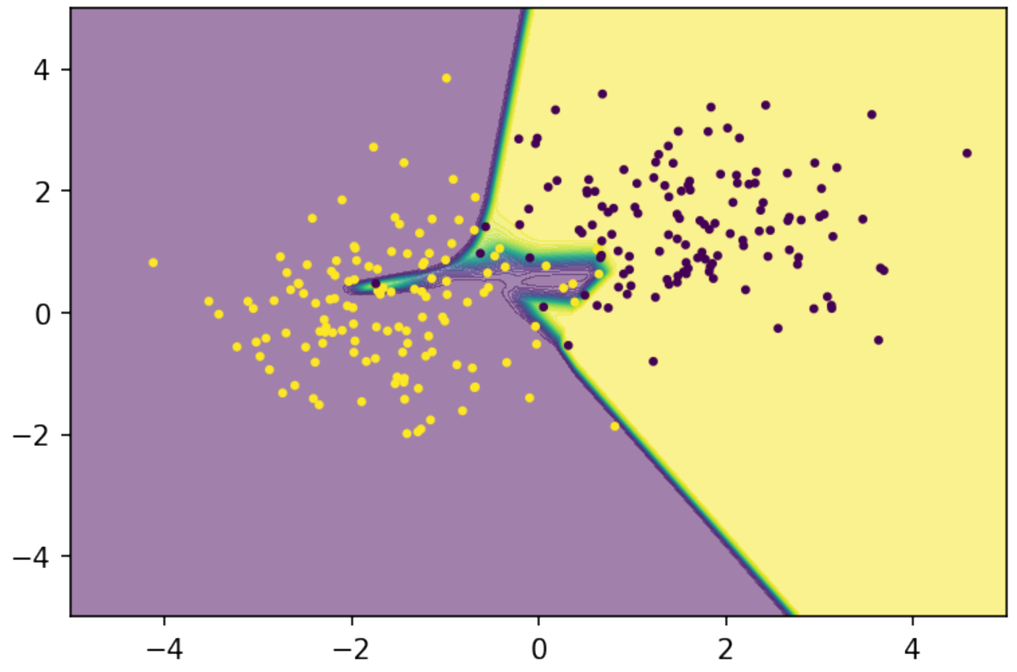
$$Var(W_{ij})=\frac{4}{(\#\text{ outgoing connections})+(\#\text{ incoming connections})}$$

Overfitting with neural networks

The problem of overfitting

- Being highly complex models, neural networks are prone to overfitting





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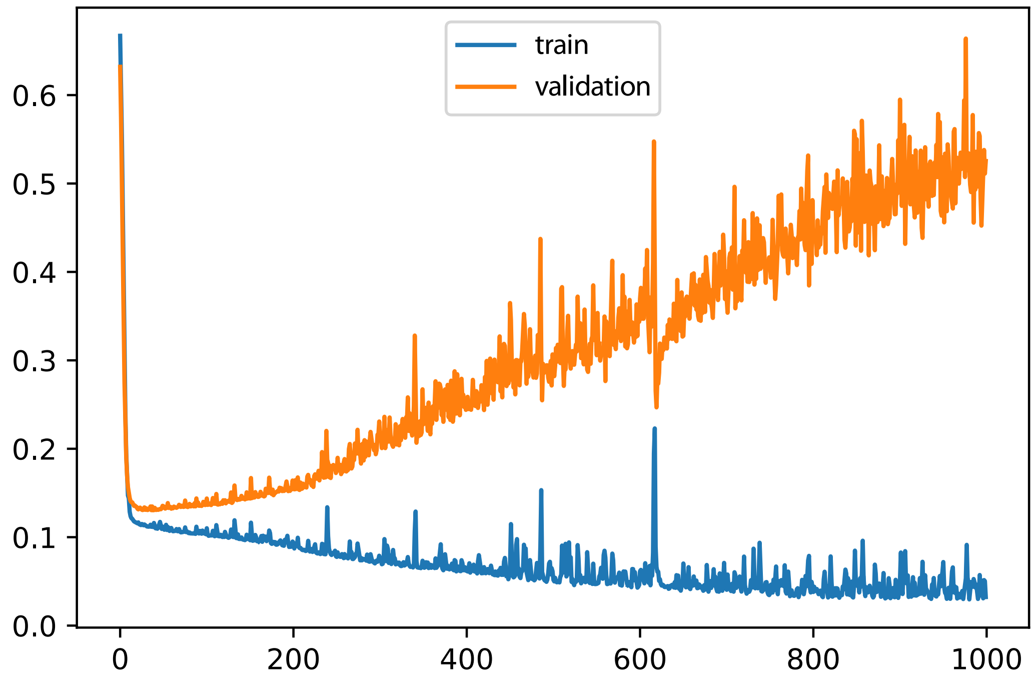
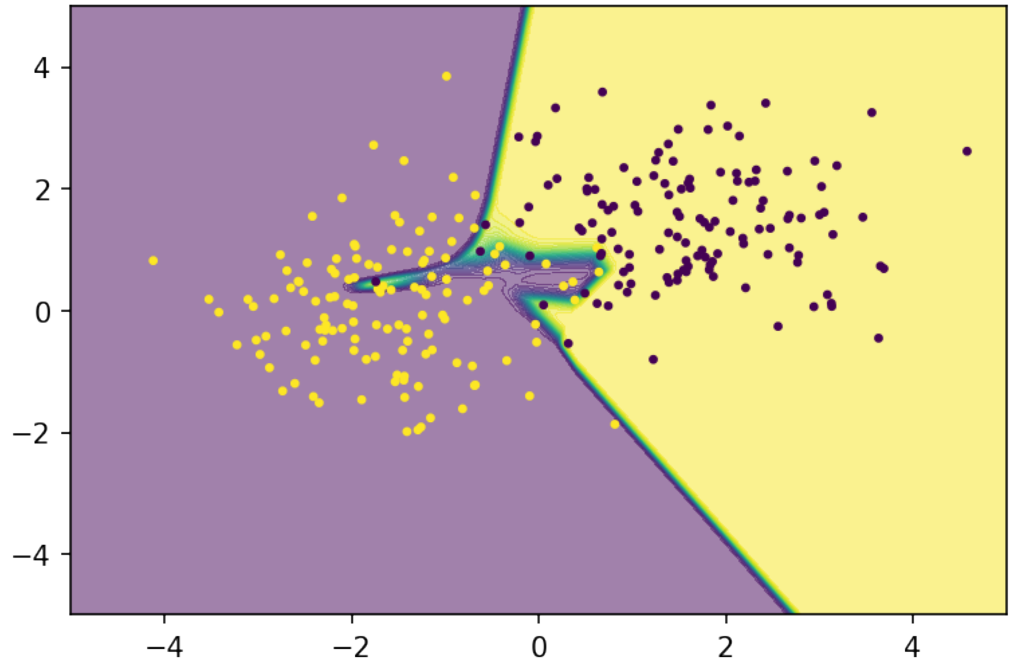


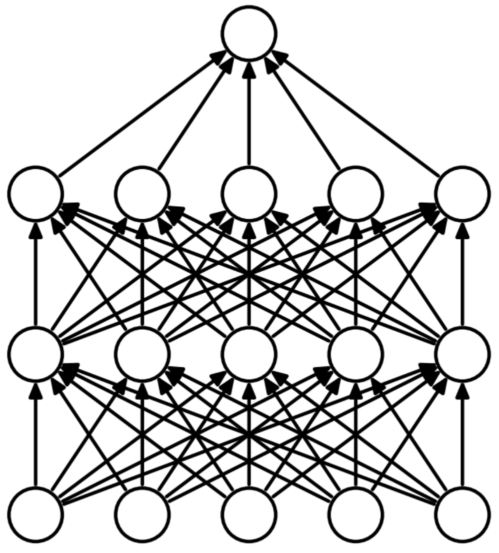


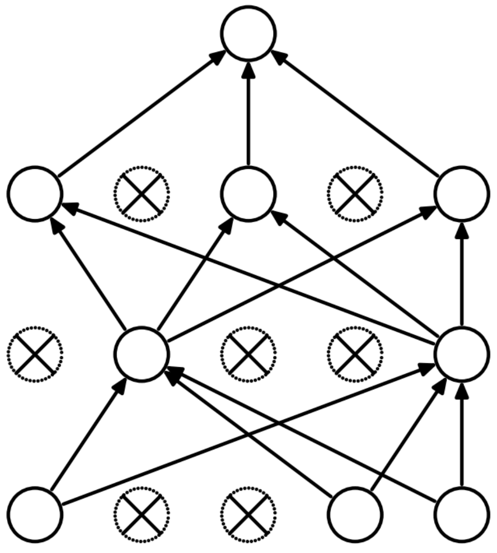
- Regularization techniques like L1/L2 regularization are also available for neural networks
- We also discussed **early stopping** (i.e. stop the training before validation error grows)

Dropout

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

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


(a) Standard Neural Net


(b) After applying dropout.

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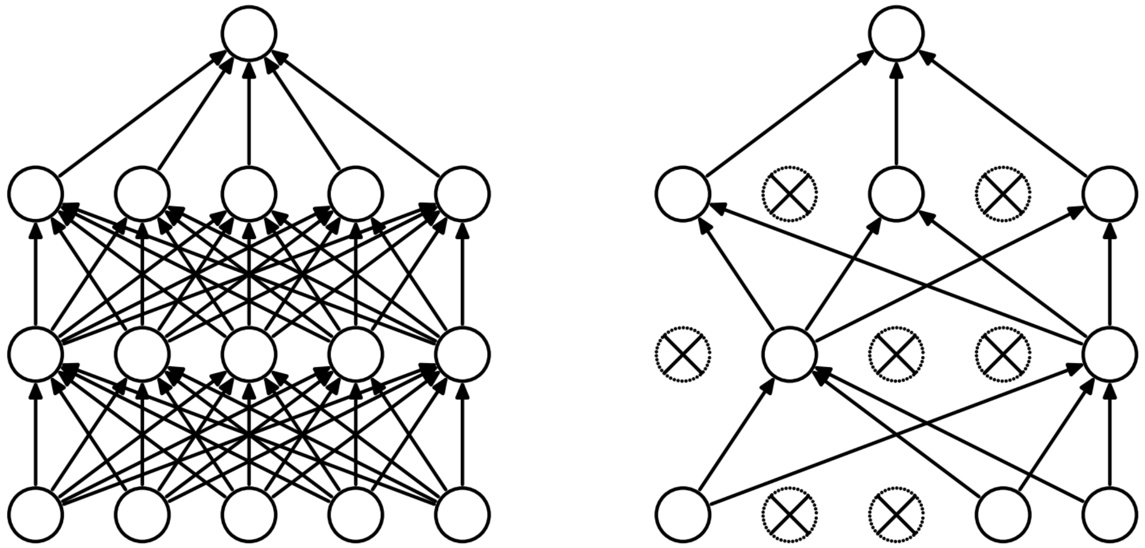
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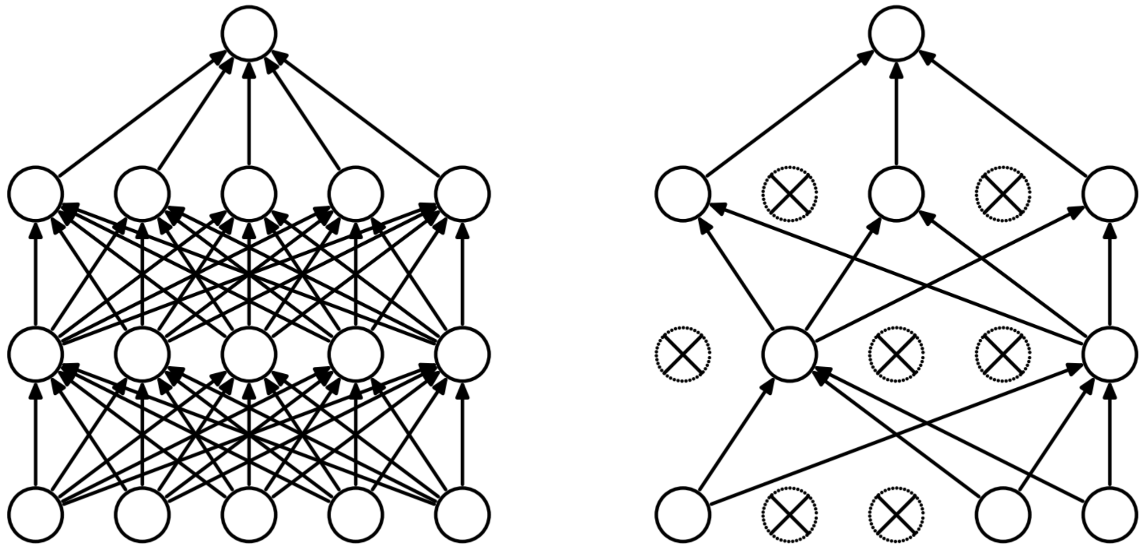

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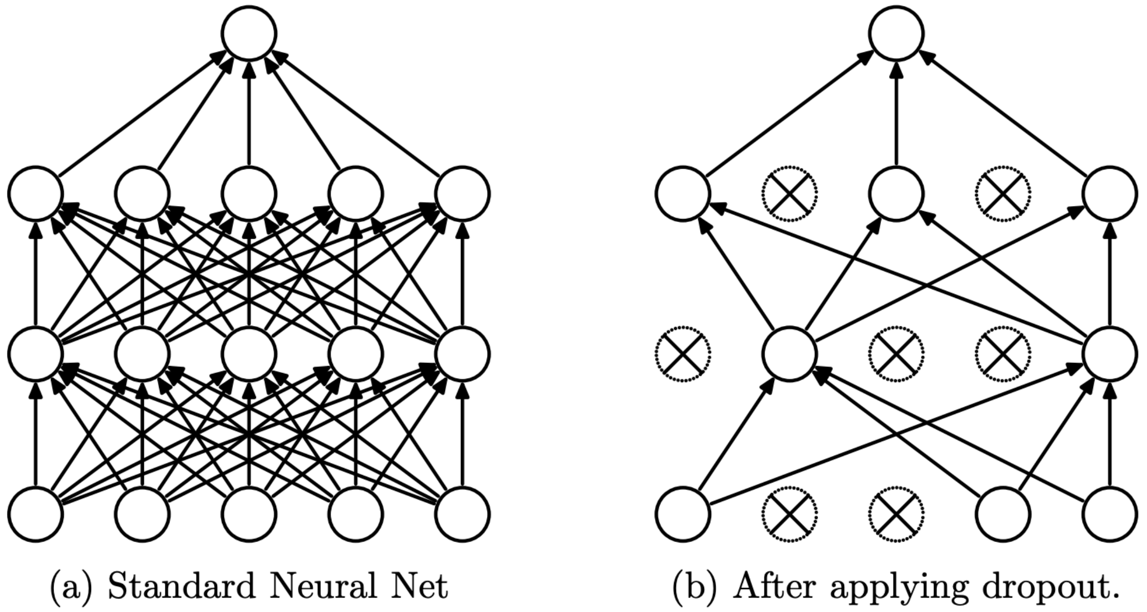
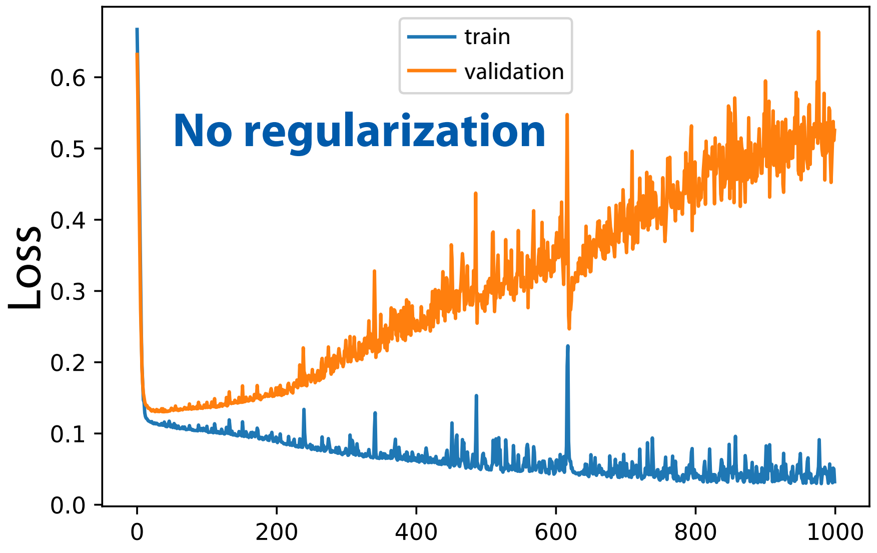
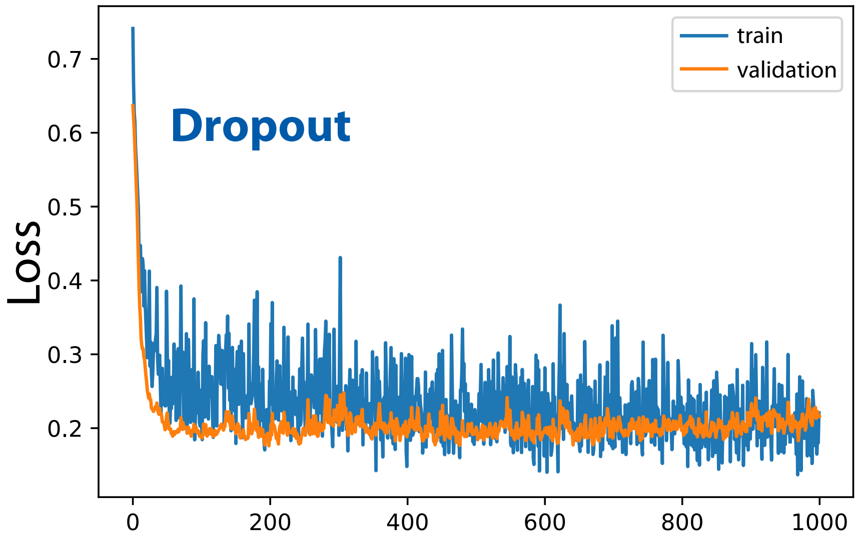
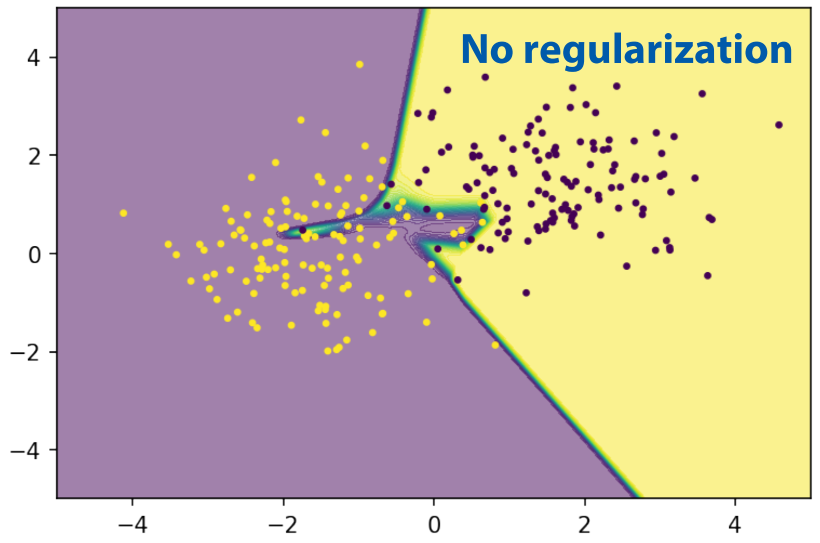


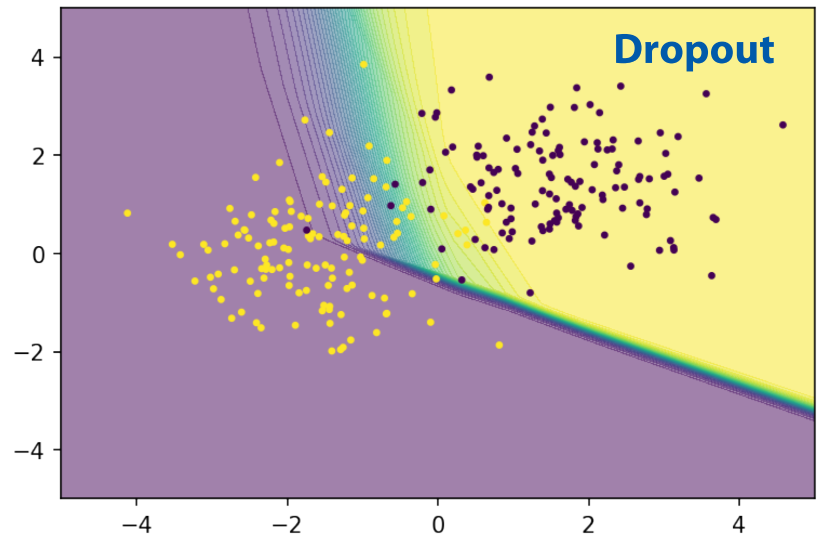
- Drives it towards **creating useful features** rather than relying on other neurons to correct its mistakes

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

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

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

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Batch normalization

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- Effectively **removes** the ‘shift’ and ‘scale’ degrees of freedom from the previous layer

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- Which dimension to normalize over? Typically, like this:
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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

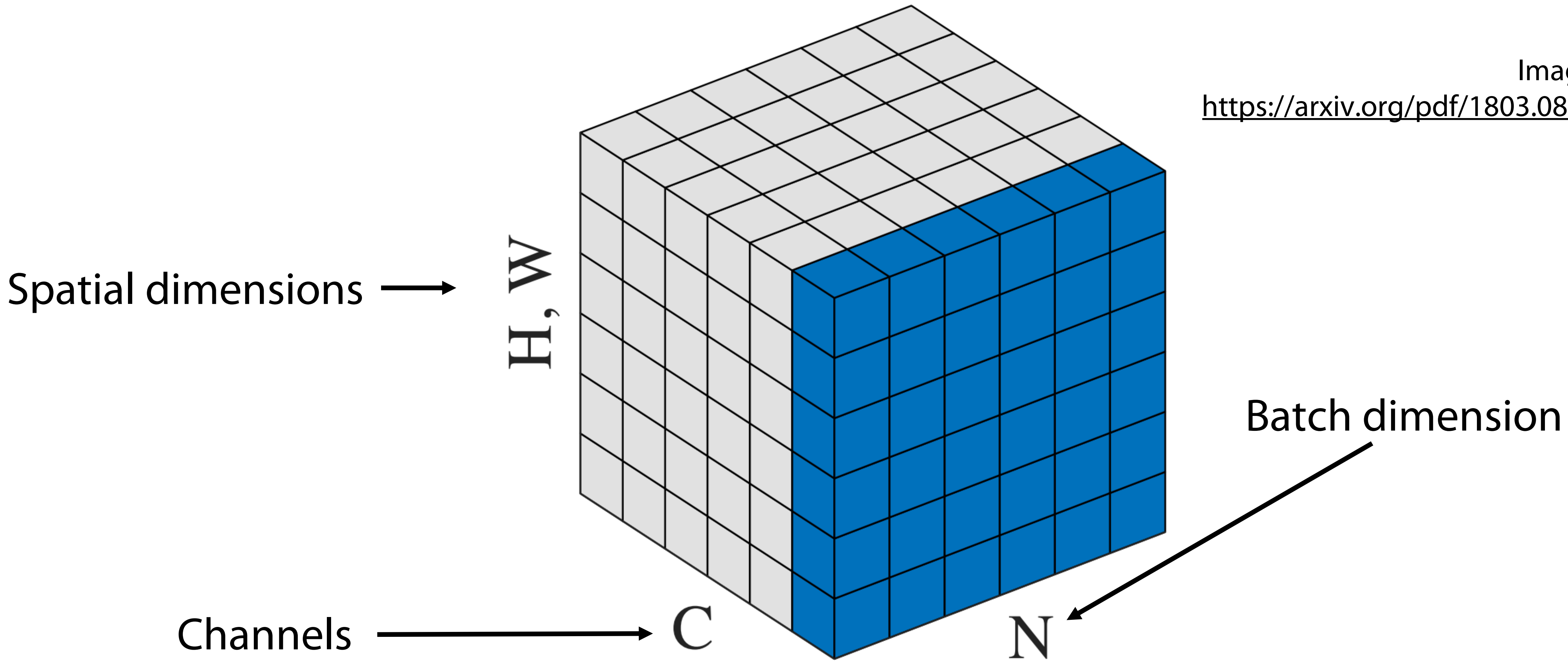
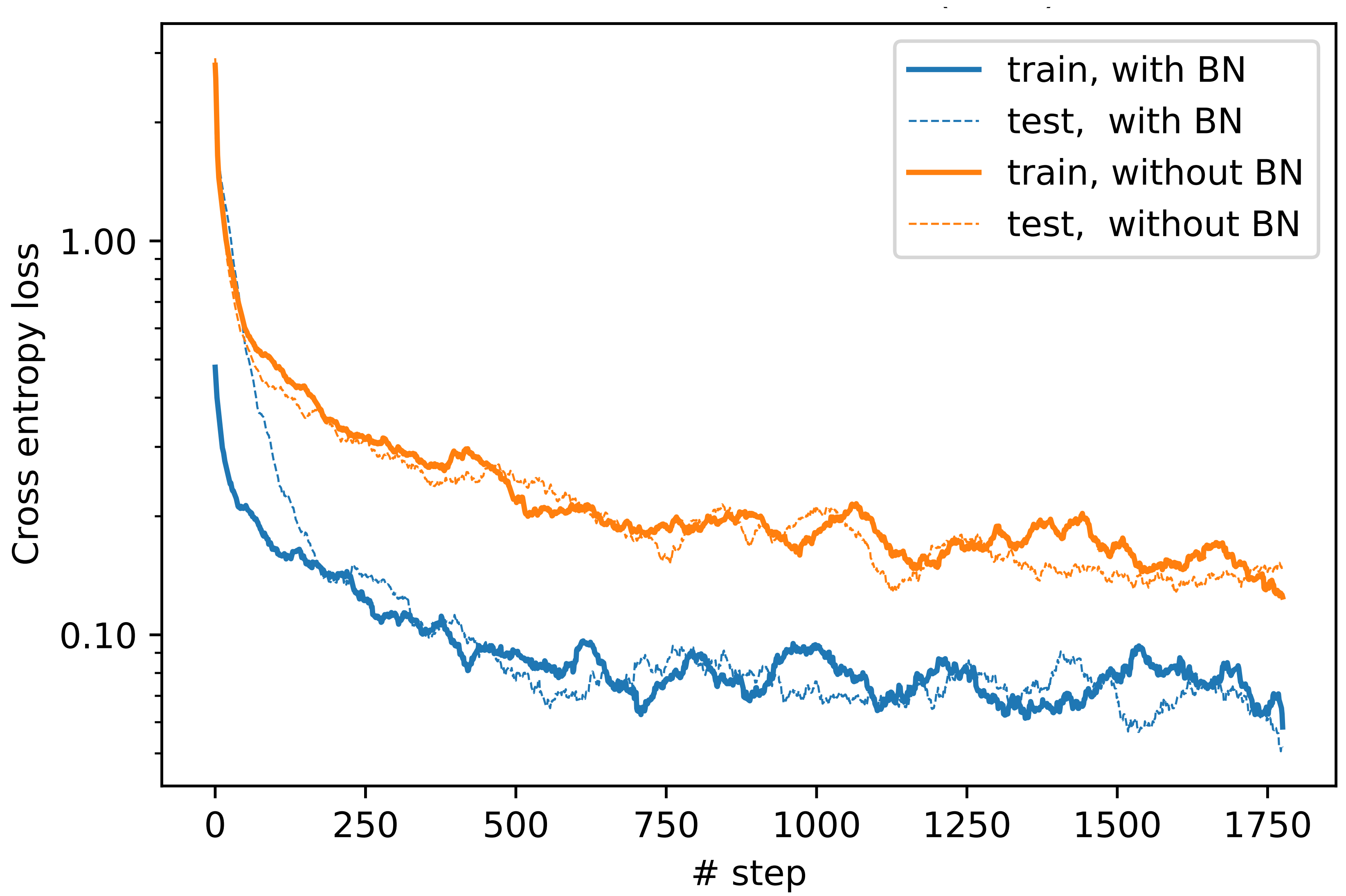


Image from
https://arxiv.org/pdf/1803.08494.pdf

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)

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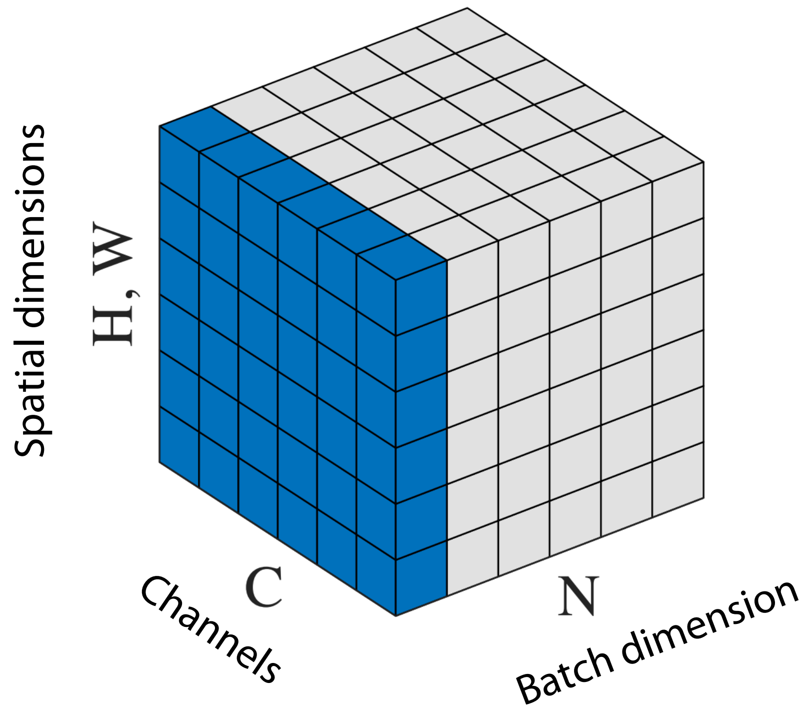

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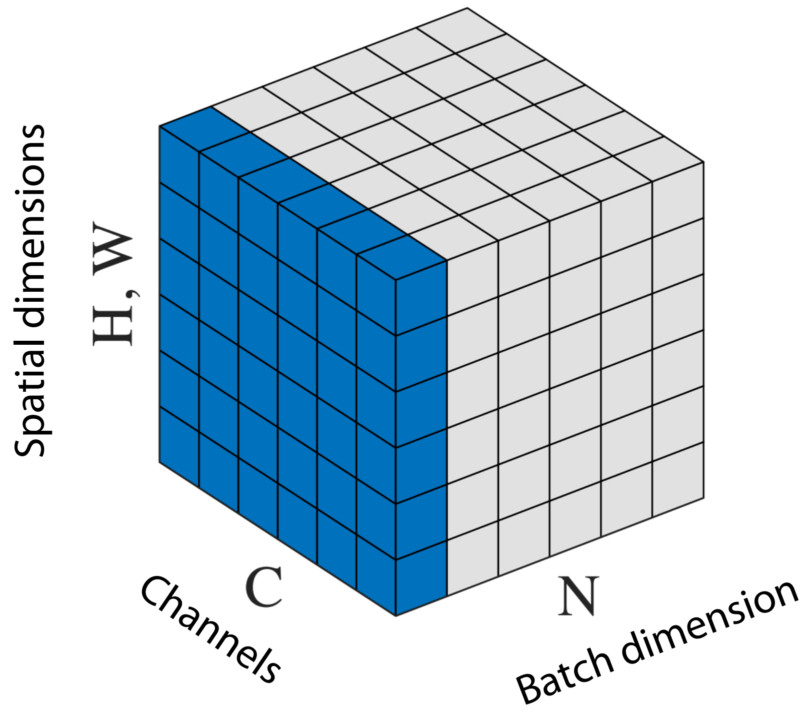
  - the effect is quite different though
    - e.g. Layer Normalization “entangles” different neurons within a layer



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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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