EN.601.482/682 Deep Learning

Training Part I

Activation, Initialization, Preprocessing, Dropout, Batch Norm

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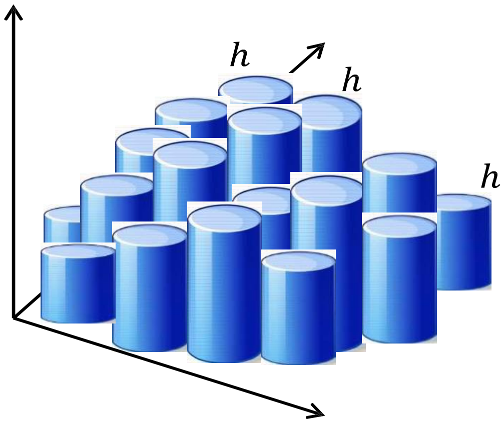
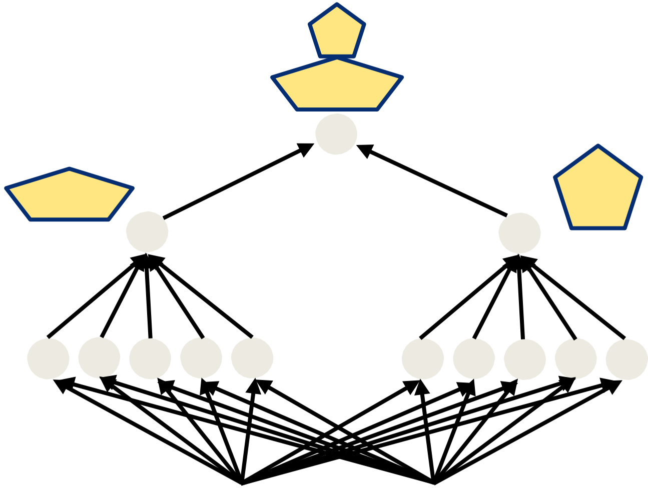
Reminder

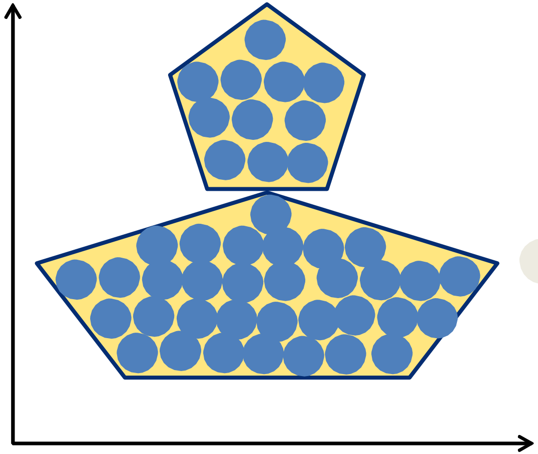


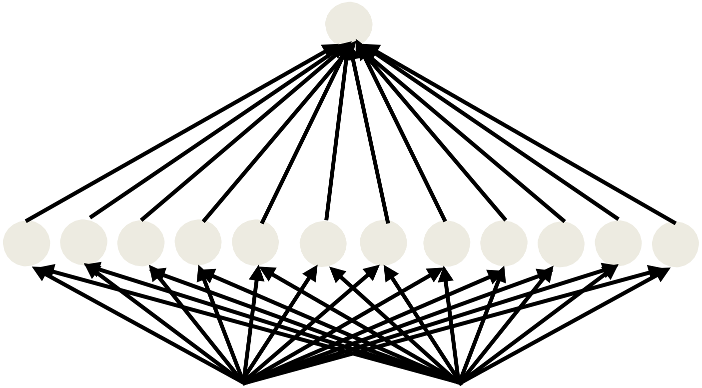
Multi-layer perceptrons are

- Universal Boolean functions
- Universal Classifiers
- Universal approximators

… but may require infinitely many neurons





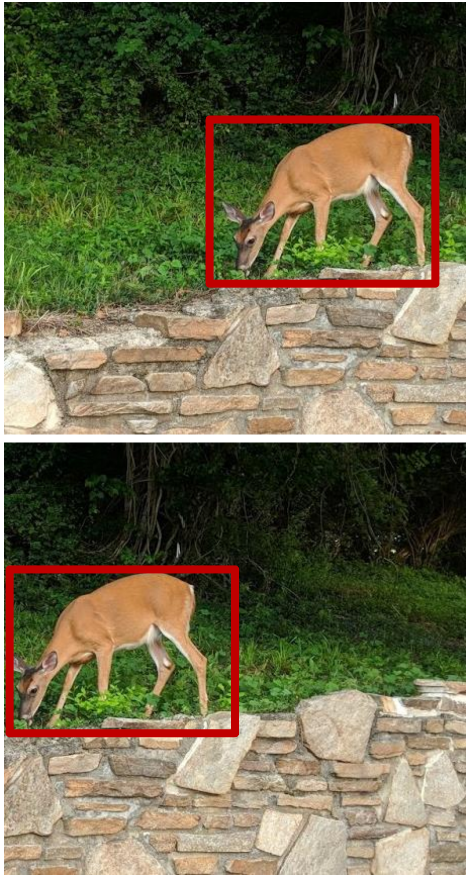


Reminder

- MLPs to recognize patterns:
  Weights act as **templates**

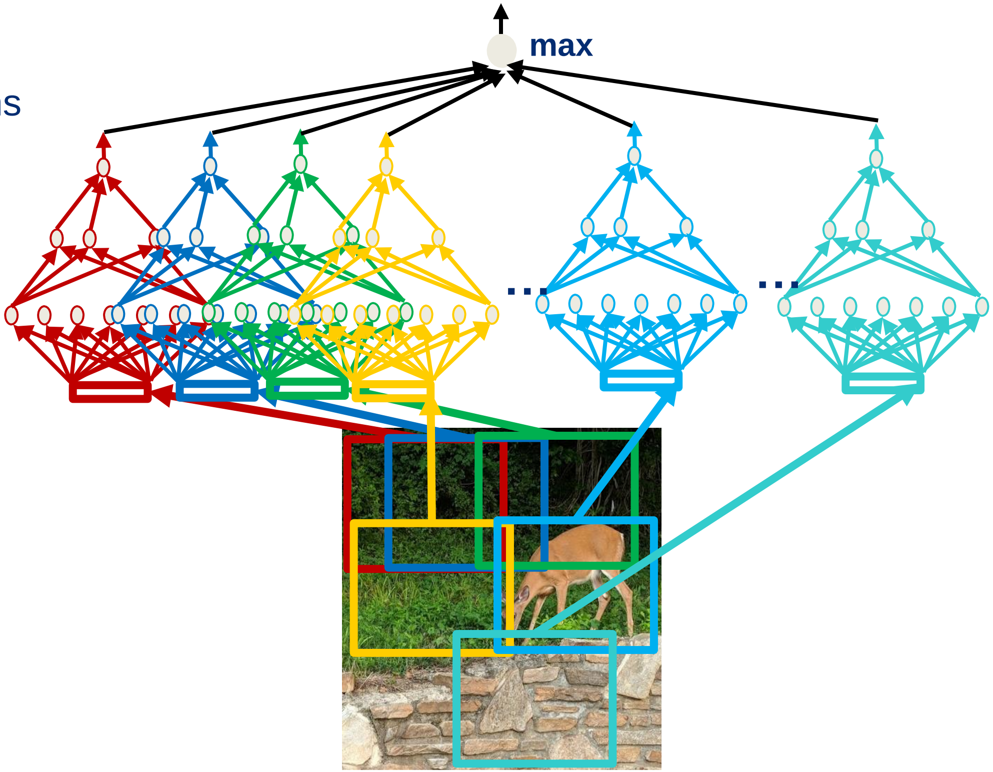
- MLPs are **not shift invariant**

- For many problems, however:
  → Location of pattern does not matter



Reminder

- First idea
  - Apply multiple MLPs at different locations
  - Max over outputs
  - Large number of parameters

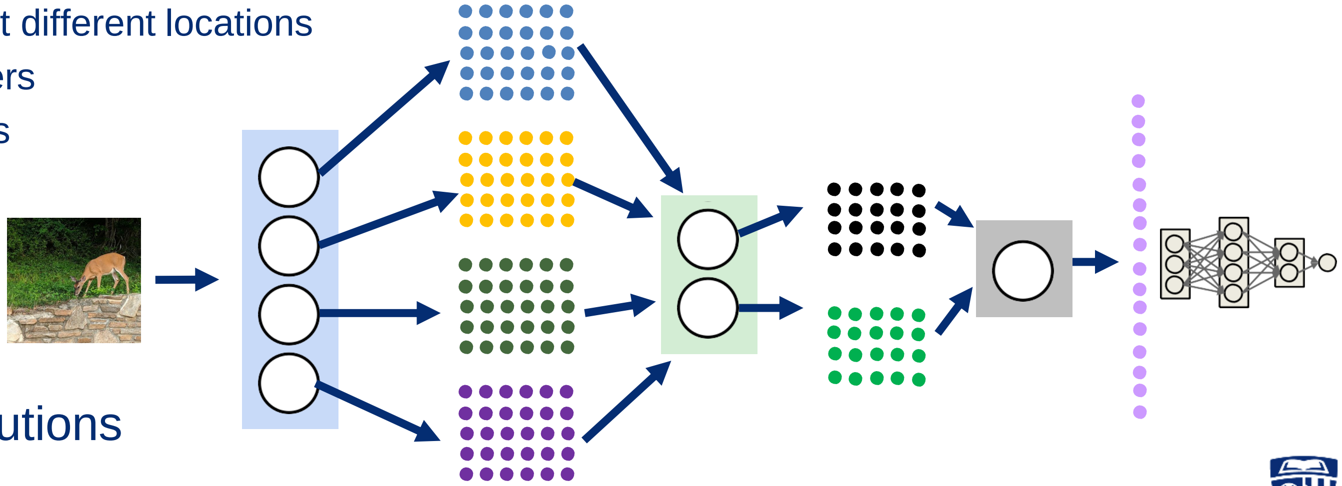


Reminder

- First idea
  - Apply multiple MLPs at different locations
  - Max over outputs
  - Large number of parameters

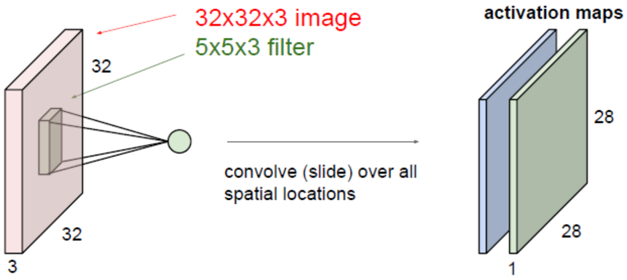
- Second idea
  - Apply same MLP at different locations
  - Reduced parameters
  - Distributed analysis

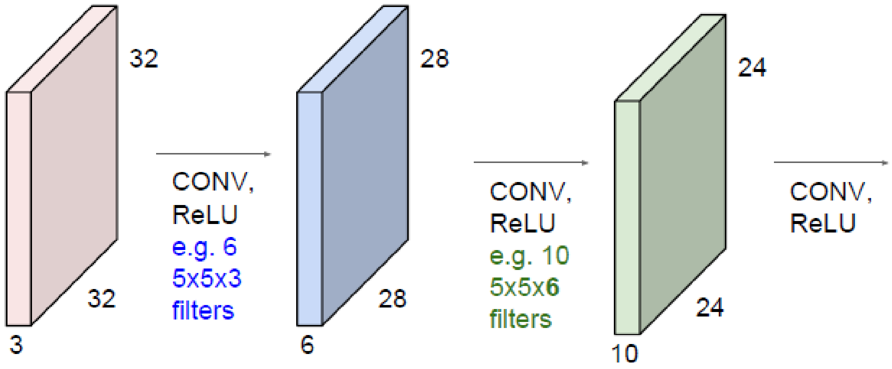
Lower layers learn local features
Deeper layers learn abstract features



→ Realized as convolutions

Reminder





Input volume: **32x32x3**
10 5x5 filters with stride 1, pad 2

Output volume size:
(32+2*2-5)/1+1 = 32 spatially, so
32x32x10

Number of parameters in this layer?
each filter has 5*5*3 + 1 = 76 params (+1 for bias)
=> 76*10 = **760**

Reminder

- Convolutional Neural Networks (ConvNets) stack
  - Convolutional layers
  - Pooling layers
  - Fully connected (FC) layers

- Typical architecture:
  [(Conv→Activation)*N → Pool]*M → (FC→Activation)*F, Softmax

Today (and next time): **Considerations important for training**

- Design choices
- Potential pitfalls

Today’s Lecture

Connecting the Dots

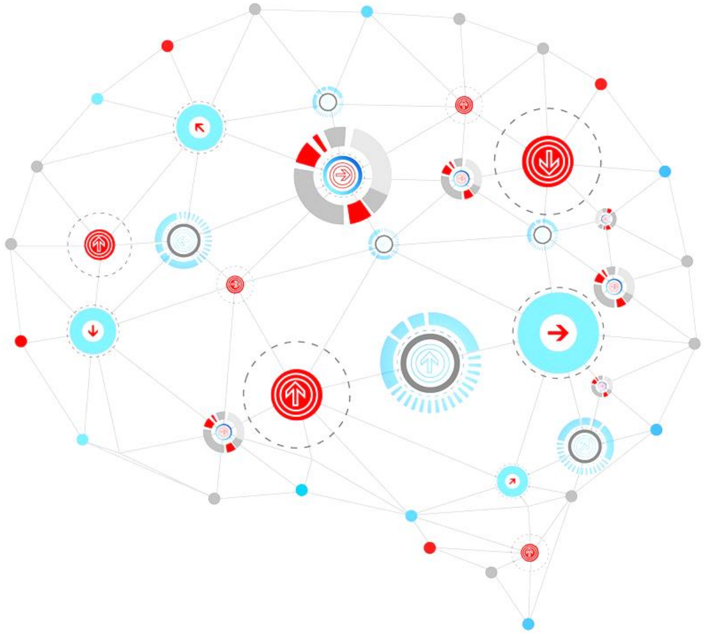
Activation

Initialization

Preprocessing

Dropout

Batch norm



Activation, Initialization, Preprocessing, Dropout, Batch Norm

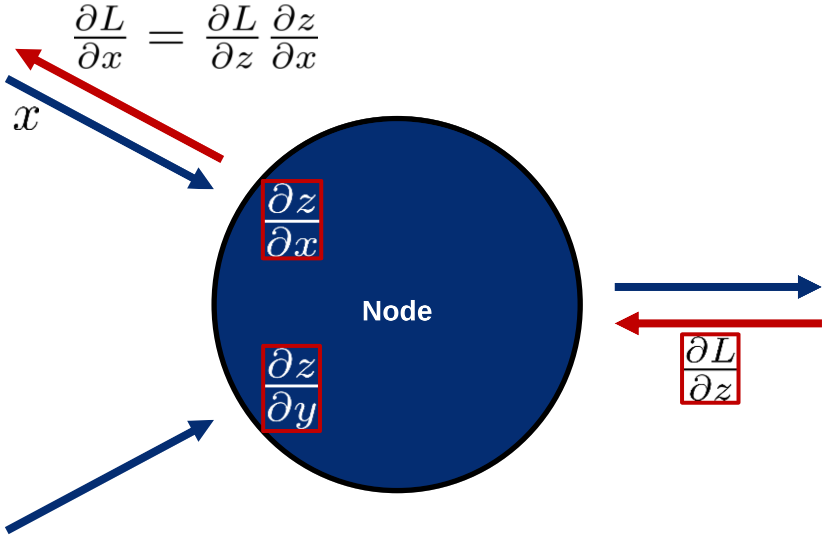
Connecting the Dots

Training MLPs and ConvNets

- Neural networks are universal approximators
  → **But we must train them to approximate a function!**

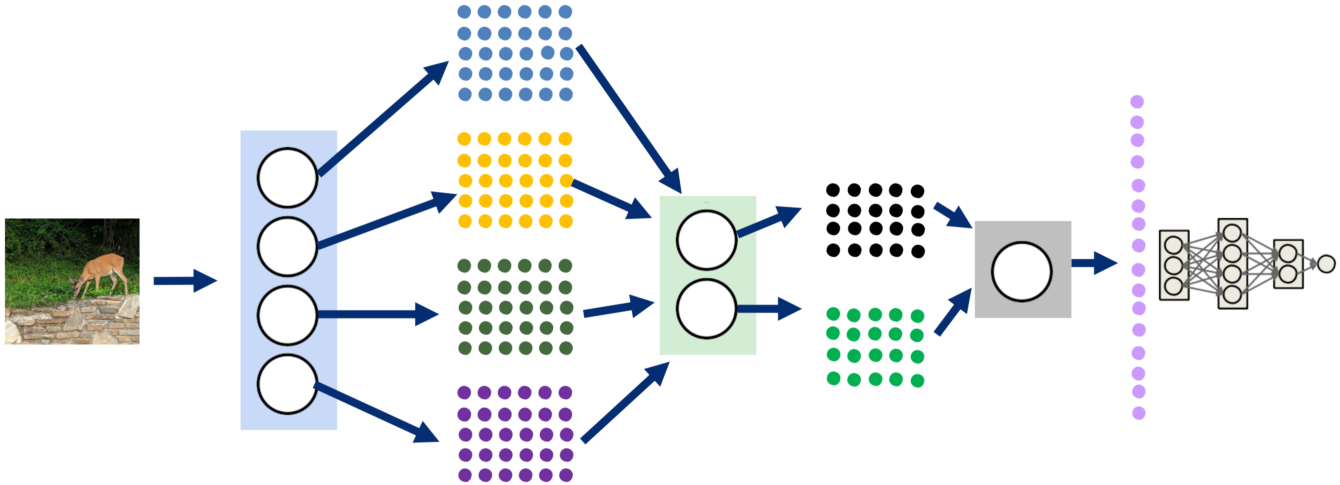
- Computational graphs
  - Consecutively apply chain rule
  - Analytic gradient computation for arbitrarily complex functions

- Convolutional neural networks
  - Same concept still applies!
  - More complicated with shared weights



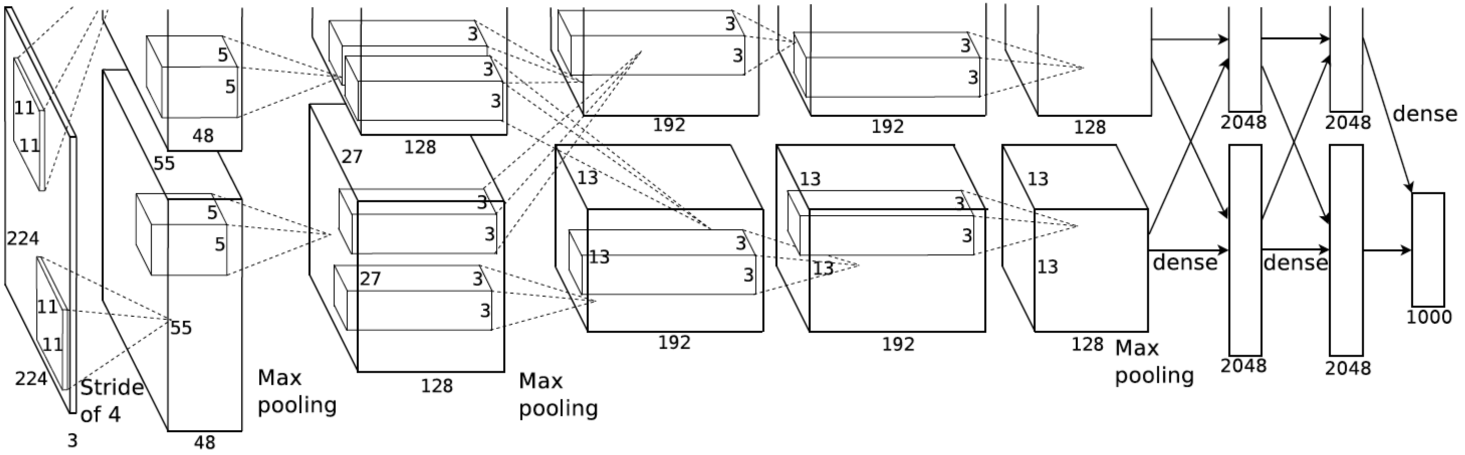
Training MLPs and ConvNets

- This is just a computational graph



Training MLPs and ConvNets

- And so is this



Training MLPs and ConvNets

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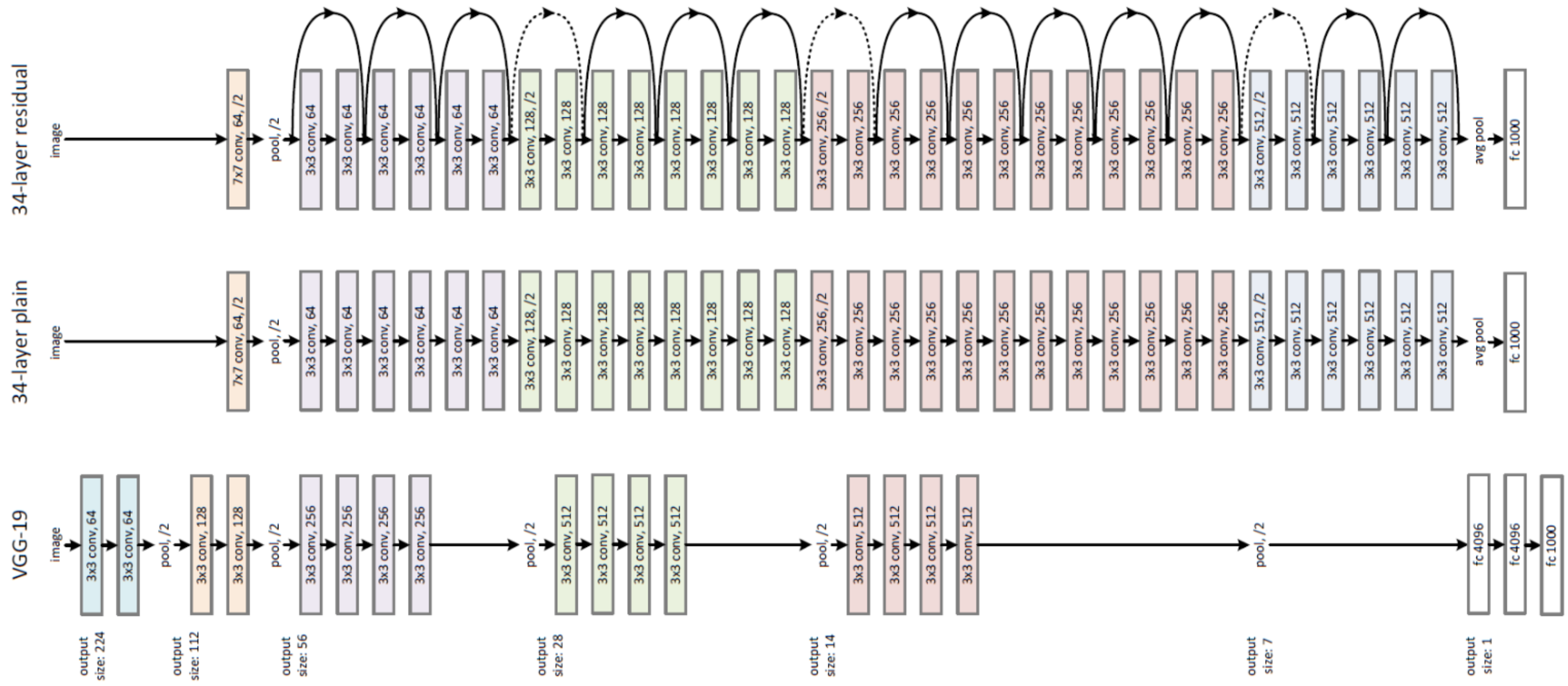
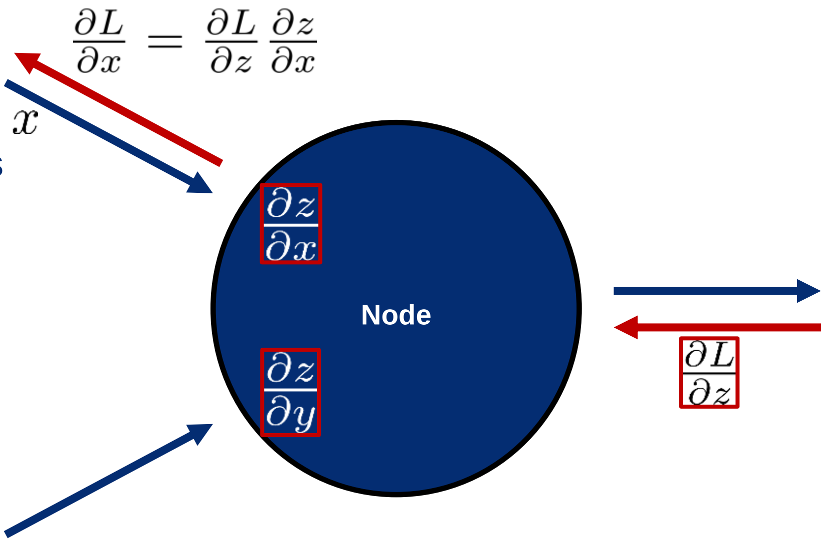


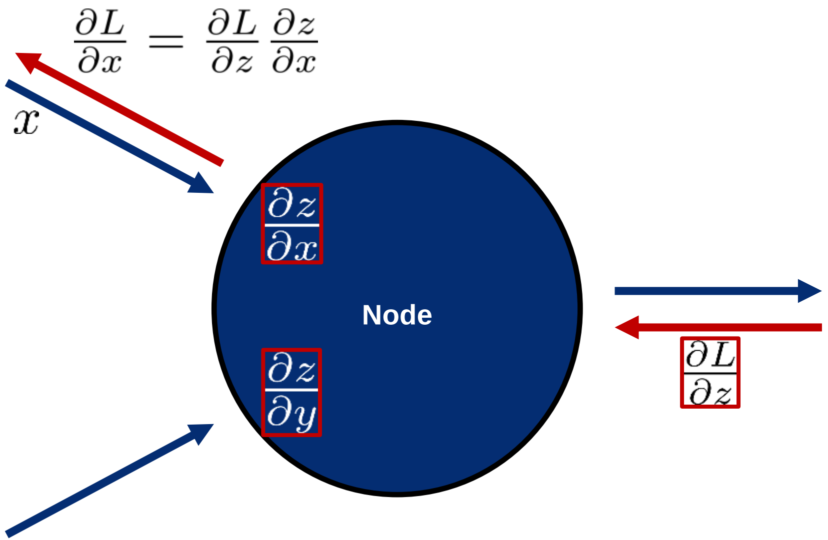
Training MLPs and ConvNets

- **One time setup:** Architecture, Loss, etc.
  - Define forward/backward for every node
  - Setup computational graph by connecting nodes
  - Obtain training/validation/test data

- Apply batched SGD
  → Until not converged, do:
  - **Sample** batch of data
  - **Forward prop** through graph, compute loss
  - **Backward prop** to compute gradients
  - **Update** parameters using gradient



Training MLPs and ConvNets



Today

→ Focus on components relevant for setup

→ Design considerations

→ We will assume the perfect architecture has been found
Selecting it will be discussed a bit later…

Activation, Initialization, Preprocessing, Dropout, Batch Norm

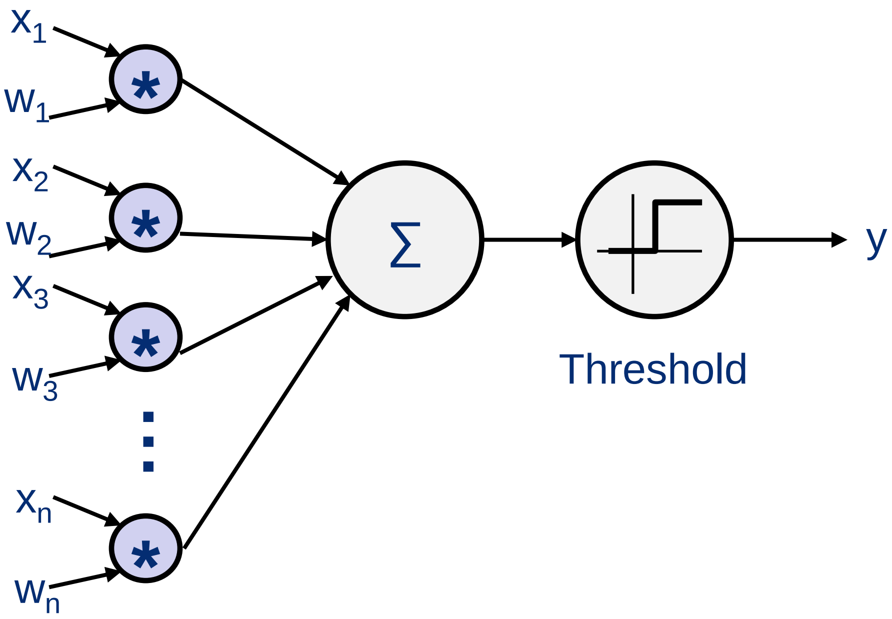
Activation

The Neural View of Perceptrons

The perceptron

- Weighted sum of inputs
- Non-linearity: If exceeds threshold

→ Unit fires!



Recap from 3 slides ago:

How do we train neural networks or even perceptrons in practice?

The Neural View of Perceptrons

The perceptron

- Weighted sum of inputs
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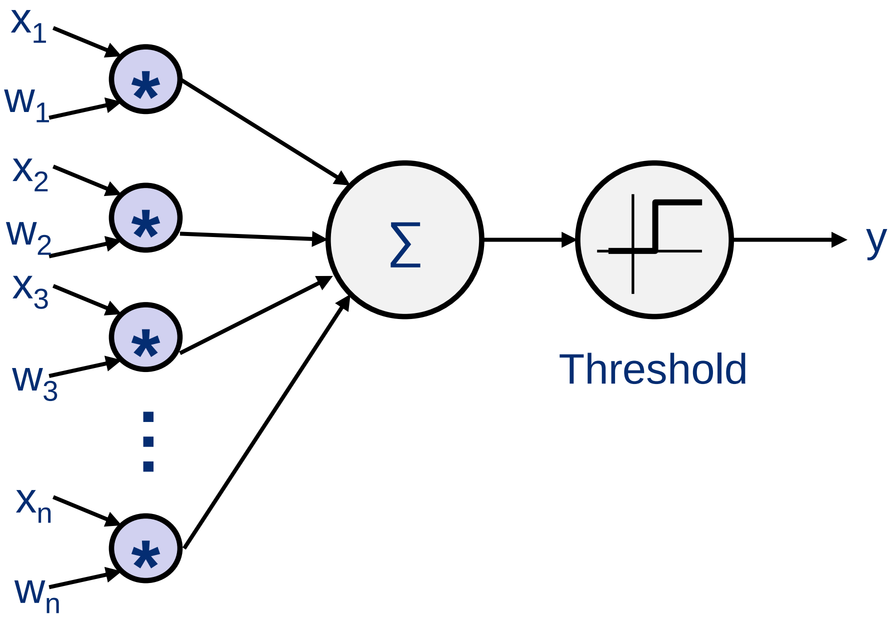

Recap from 3 slides ago:

How do we train neural networks or even perceptrons in practice?

→ Gradient descent

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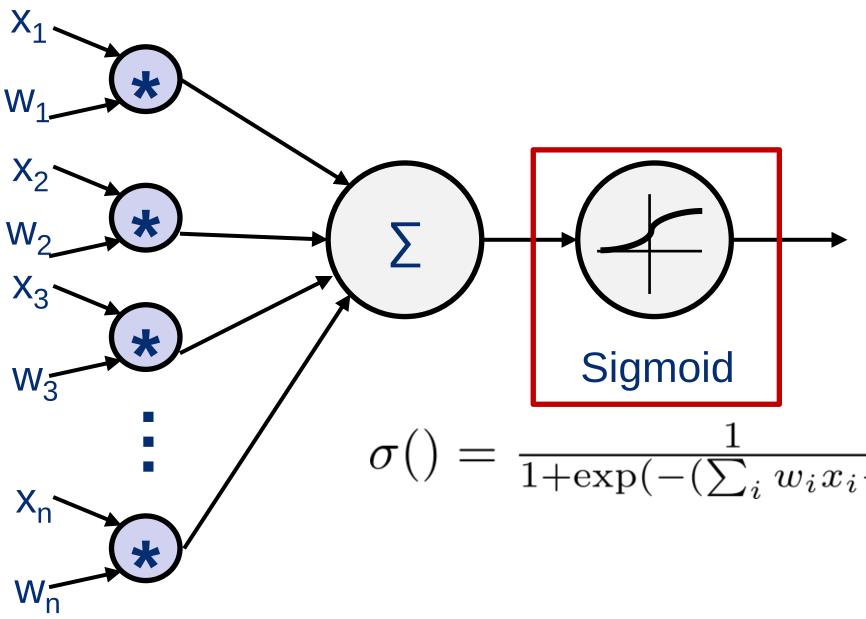


$$\sigma() = \frac{1}{1+\exp(-(\sum_i w_i x_i + b))}$$

Recap from 3 slides ago:

How do we train neural networks or even perceptrons in practice?

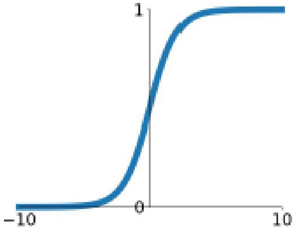
→ Gradient descent

→ Introduce differentiable functions

The Zoo of Common Activation Functions

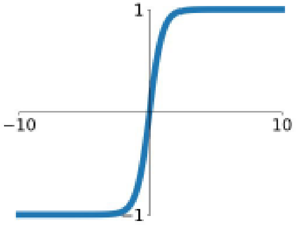
Sigmoid

$\sigma(x) = \frac{1}{1+e^{-x}}$



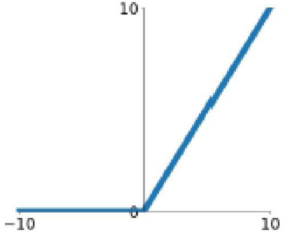
tanh

$\tanh(x)$



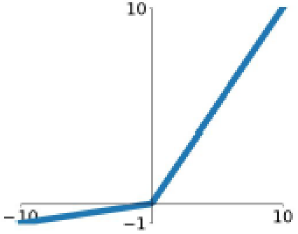
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

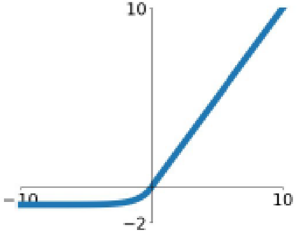


Maxout

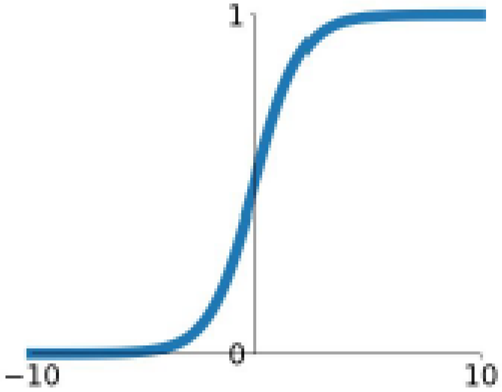
$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



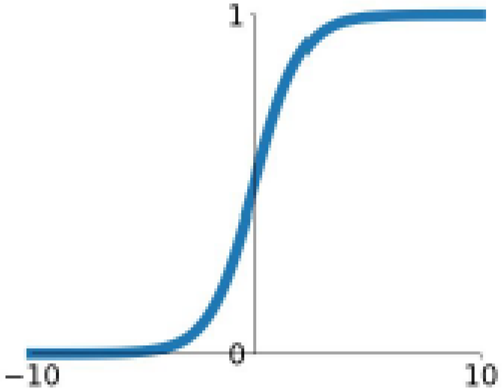
Sigmoid



Sigmoid $\sigma(x) = \frac{1}{1+e^{-x}}$

- Squashes input to [0,1]
- Historically popular:
  Saturating firing rate of a neuron

Sigmoid



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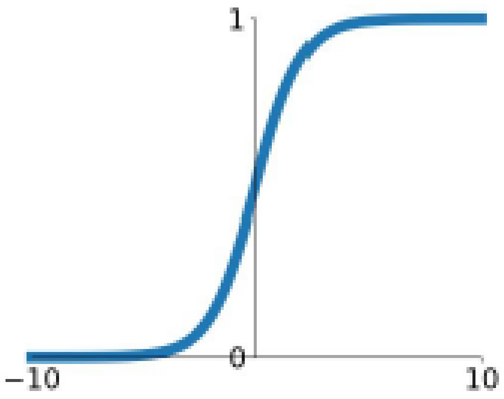
Problems

- Gradient: $\frac{\partial \sigma(x)}{\partial x} = (1 - \sigma(x))\sigma(x)$
  → Gradient vanishes for saturated neurons

As an example: What is the gradient at x = -10, x = 0, x = 10?

Sigmoid



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Sigmoid

What happens if all inputs are positive?

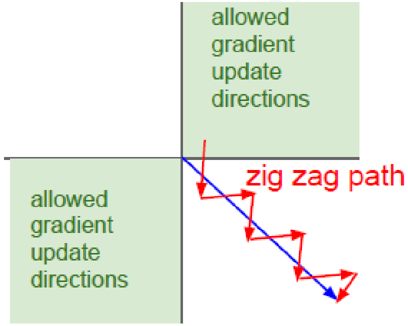
$$f(\sum_i w_i x_i + b)$$

Gradients on w?

Local gradient is x → all positive!

Upstream gradient is pos. or neg.

→ Gradient is either all pos. or all neg.!



→ Ineffective gradient updates!

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Sigmoid

This is also why we want zero-mean data!

What happens if all inputs are positive?

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Gradients on w?

Local gradient is *x* → all positive!

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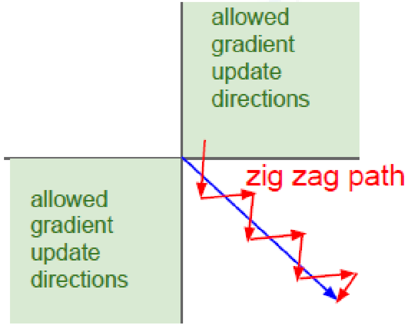

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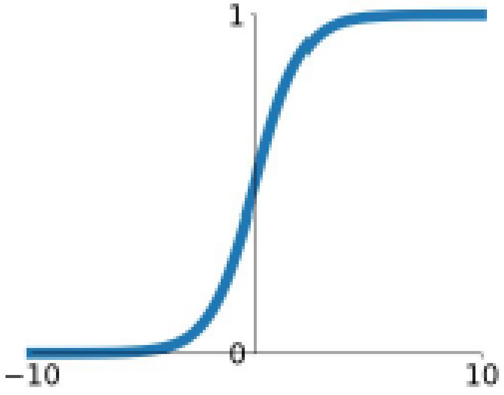

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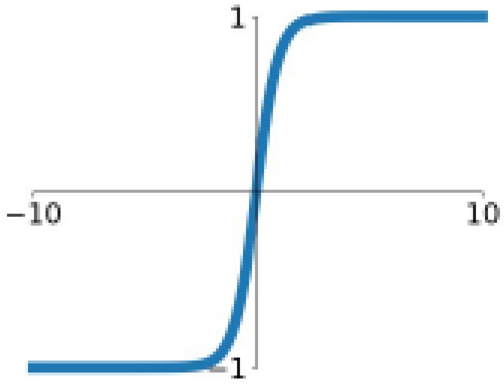
- Outputs are not zero-centered
- exp() computation is a bit expensive

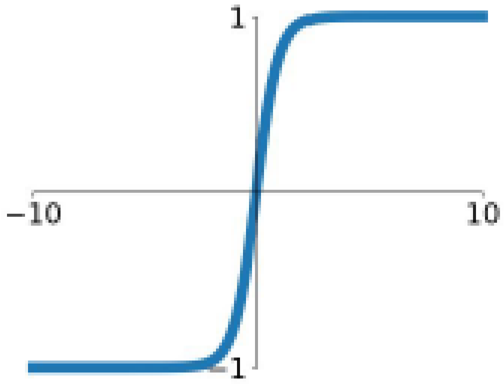
Tanh



Tanh

- Squashes input to [-1,1]
- Zero-centered output

Hyperbolic Tangent



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“Recommended tanh”: $f(x) = 1.7159 \tanh(2/3\ x)$ (LeCun 1991)

LeCun, Y. A., Bottou, L., Orr, G. B., & Müller, K. R. (2012). Efficient backprop. In Neural networks: Tricks of the trade (pp. 9-48). Springer, Berlin, Heidelberg.

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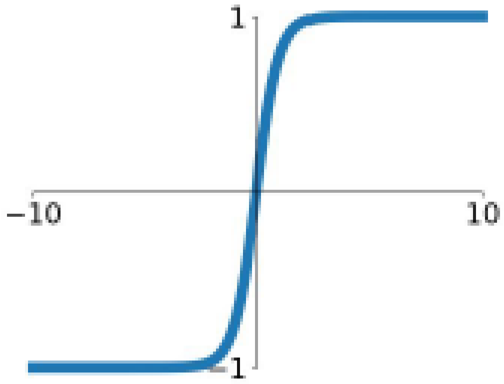

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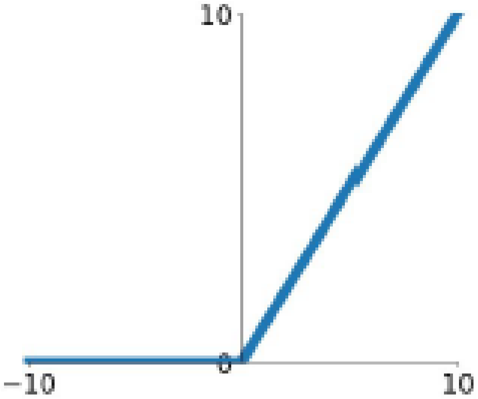
Read this! If not now, then when starting projects at the latest!

LeCun, Y. A., Bottou, L., Orr, G. B., & Müller, K. R. (2012). Efficient backprop. In Neural networks: Tricks of the trade (pp. 9-48). Springer, Berlin, Heidelberg.

Rectified Linear Unit



ReLU $\mathrm{ReLU}(x) = \max(0, x)$

- No saturation in positive regime
- Computationally efficient
- Converges much faster than previous func.s
- Closer to biological neuron activation

Krizhevsky, A., Sutskever, I., & Hinton, G. E. (2012). Imagenet classification with deep convolutional neural networks. NeurIPS (pp. 1097-1105).

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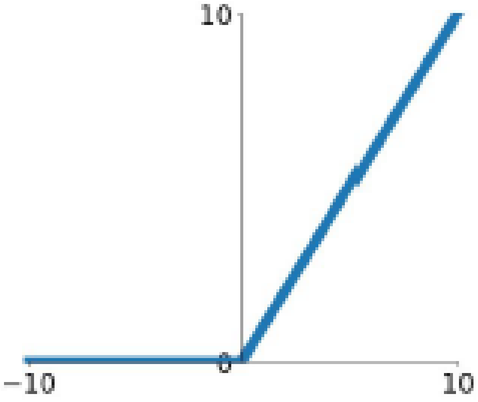

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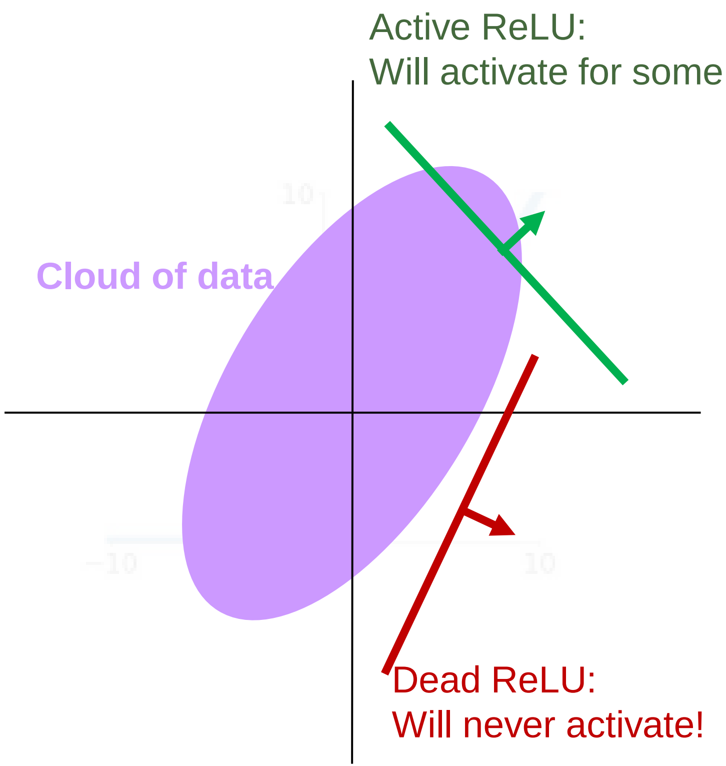

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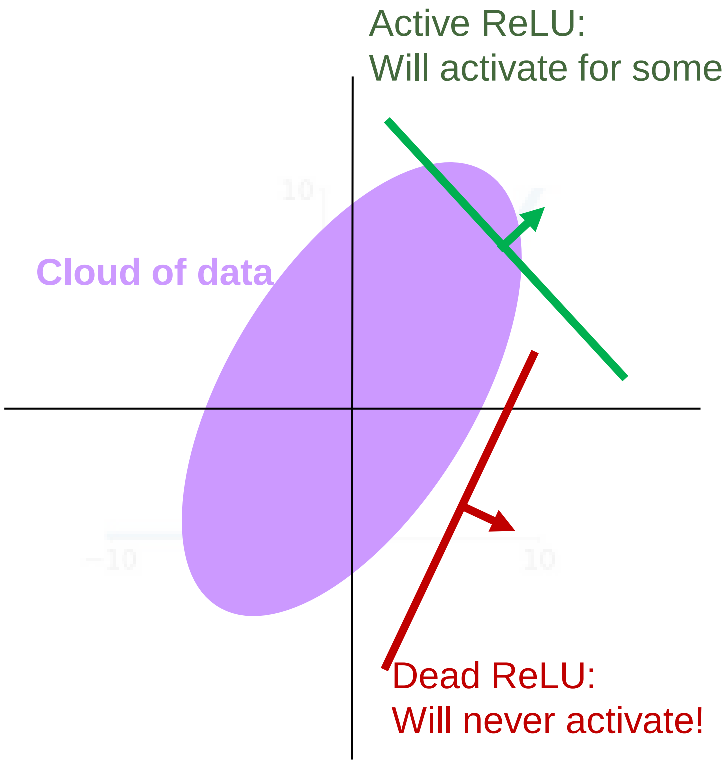

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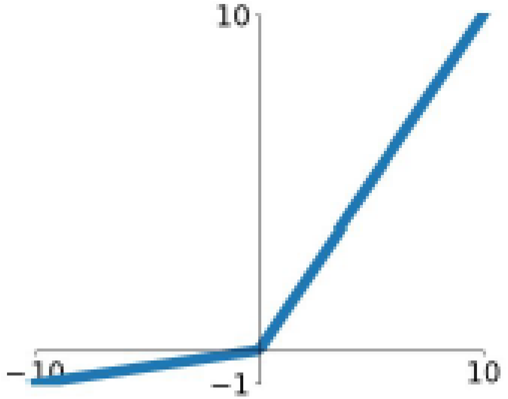
Problems

- Again not zero-centered!

→ Bias term to the rescue!
Initialize with small positive bias

Krizhevsky, A., Sutskever, I., & Hinton, G. E. (2012). Imagenet classification with deep convolutional neural networks. NeurIPS (pp. 1097-1105).

Leaky Rectified Linear Unit

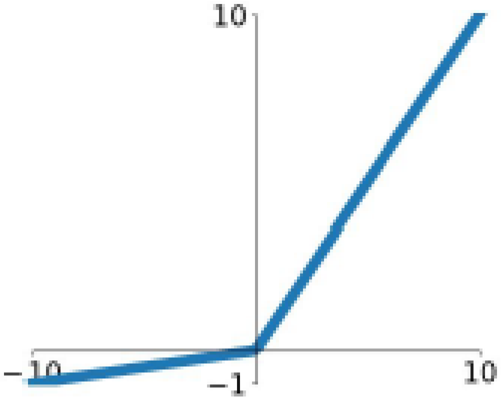


Leaky ReLU $\mathrm{ReLU}(x) = \max(\alpha x, x)$

- No saturation
- Computationally efficient
- Converges much faster than previous func.s
- Will **not die**

He, K., Zhang, X., Ren, S., & Sun, J. (2015). Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. CVPR.

Leaky Rectified Linear Unit



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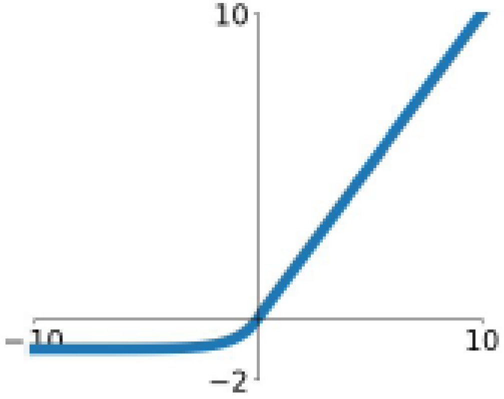
Leaky ReLU:
α is constant and small, e.g. 0.01

Parametric Rectifier PReLU:
Backpropagation into α!

He, K., Zhang, X., Ren, S., & Sun, J. (2015). Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. CVPR.

Exponential Linear Unit



ELU

$$\mathrm{ELU}(x) = \begin{cases} x, & \text{if } x > 0 \\ \alpha(e^x - 1), & \text{if } x < 0 \end{cases}$$

- Benefits of ReLU
- Closer to zero mean
- Saturates in negative regime
  → "Noise-robust deactivation state"

Problems

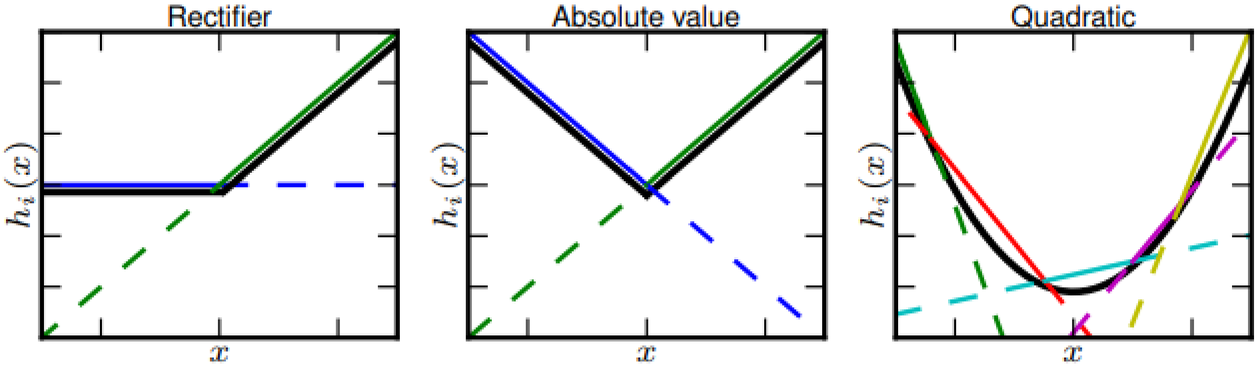
- exp() is a bit expensive to compute

Clevert, D. A., Unterthiner, T., & Hochreiter, S. (2015). Fast and accurate deep network learning by exponential linear units (elus). arXiv:1511.07289.

Maxout

$$\max(W_1 x + b_1, W_2 x + b_2)$$

- Does not follow the conventional “dot product/convolution → activation”
- Generalizes ReLU etc.
- Linear regime: Does not die!



Goodfellow, I. J., Warde-Farley, D., Mirza, M., Courville, A., & Bengio, Y. (2013). Maxout networks. arXiv preprint arXiv:1302.4389.

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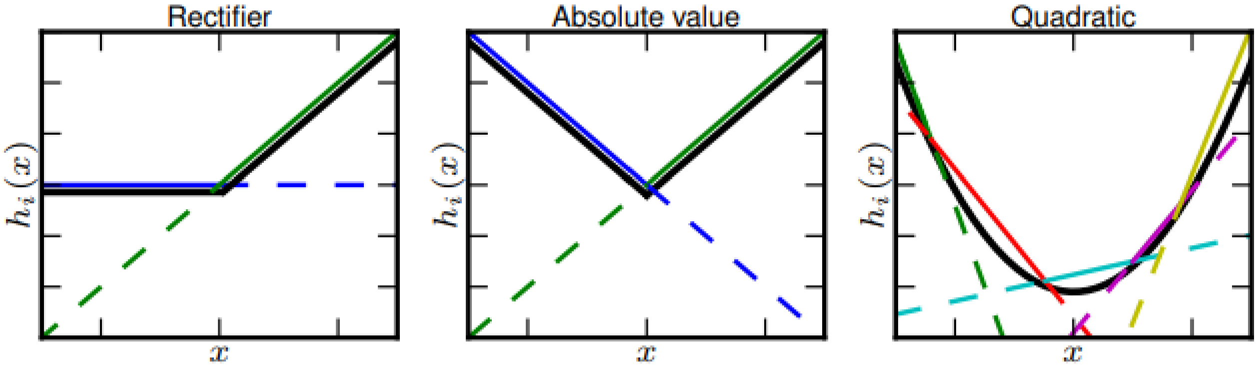
- Generalizes ReLU etc.
- Linear regime: Does not die!

- **Doubles the number of parameters per maxout neuron**



Goodfellow, I. J., Warde-Farley, D., Mirza, M., Courville, A., & Bengio, Y. (2013). Maxout networks. arXiv preprint arXiv:1302.4389.

Recap and Take Away (if nothing else)

- Use ReLU!
- Try Leaky ReLU, PReLU, ELU, maybe even maxout

- Try tanh if you have time
- Do **not** use sigmoid

→ Be careful with learning rates!

Activation, Initialization, Preprocessing, Dropout, Batch Norm

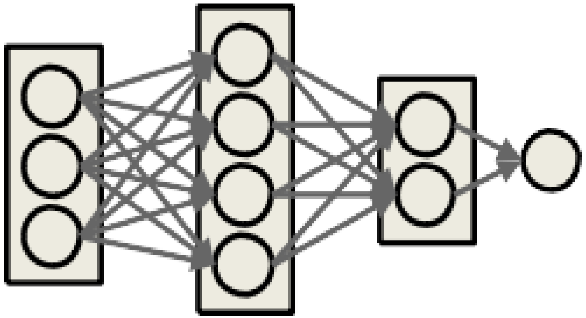
Initialization

Weight Initialization

Where are we now?

- Architecture is decided (number of neurons, activation functions)
- Close to start training!

But: Where should we start? How do we initialize our weights/parameters?



Weight Initialization

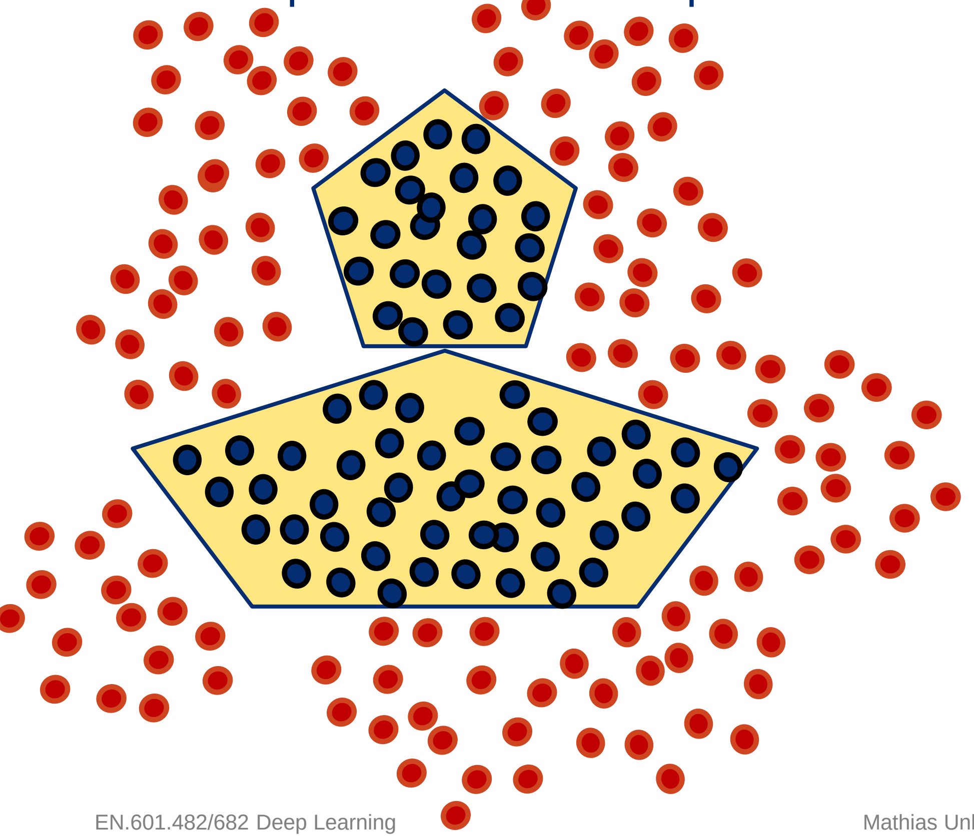
First Idea:

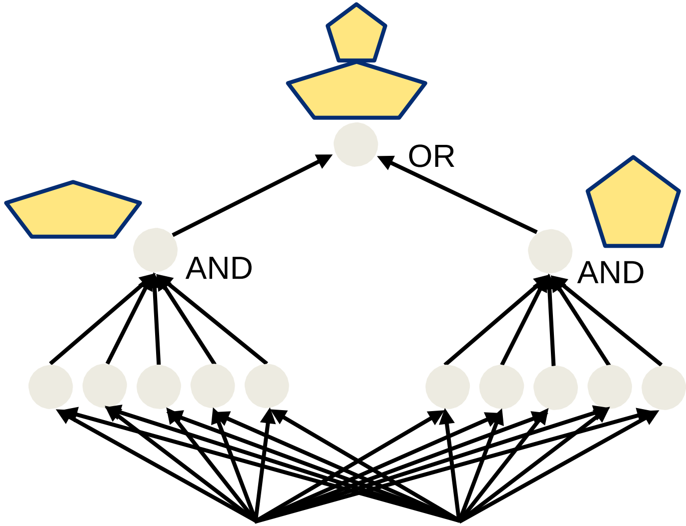
To make training more reproducible, initialize every weight with a constant.
Because 0 is a nice number (and zero-centering is a thing) we use 0.

Q: Why is this a bad idea?

Weight Initialization

An attempt at a visual example

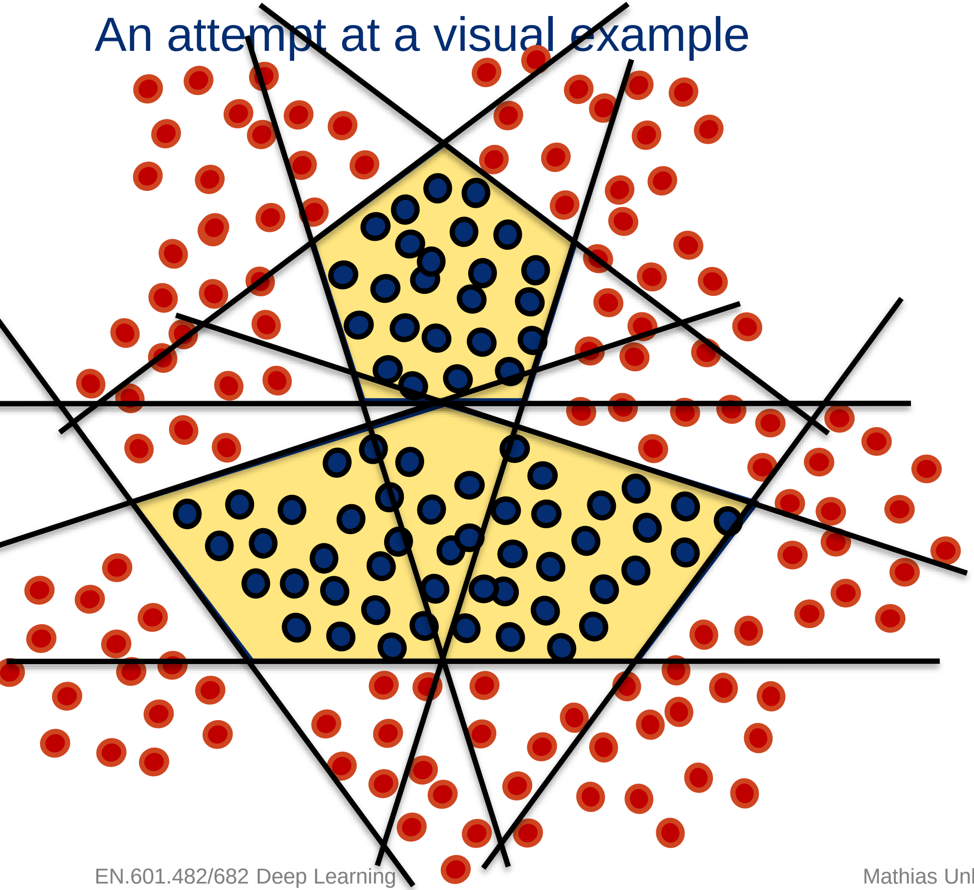


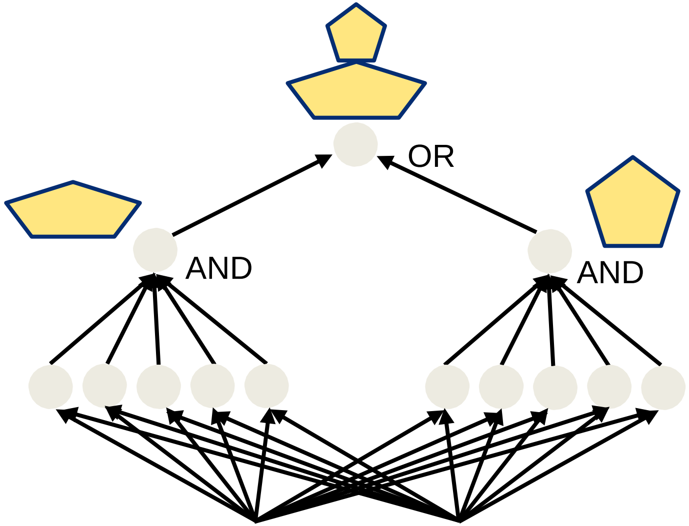


This network can perfectly describe the required decision boundary!

Weight Initialization

An attempt at a visual example



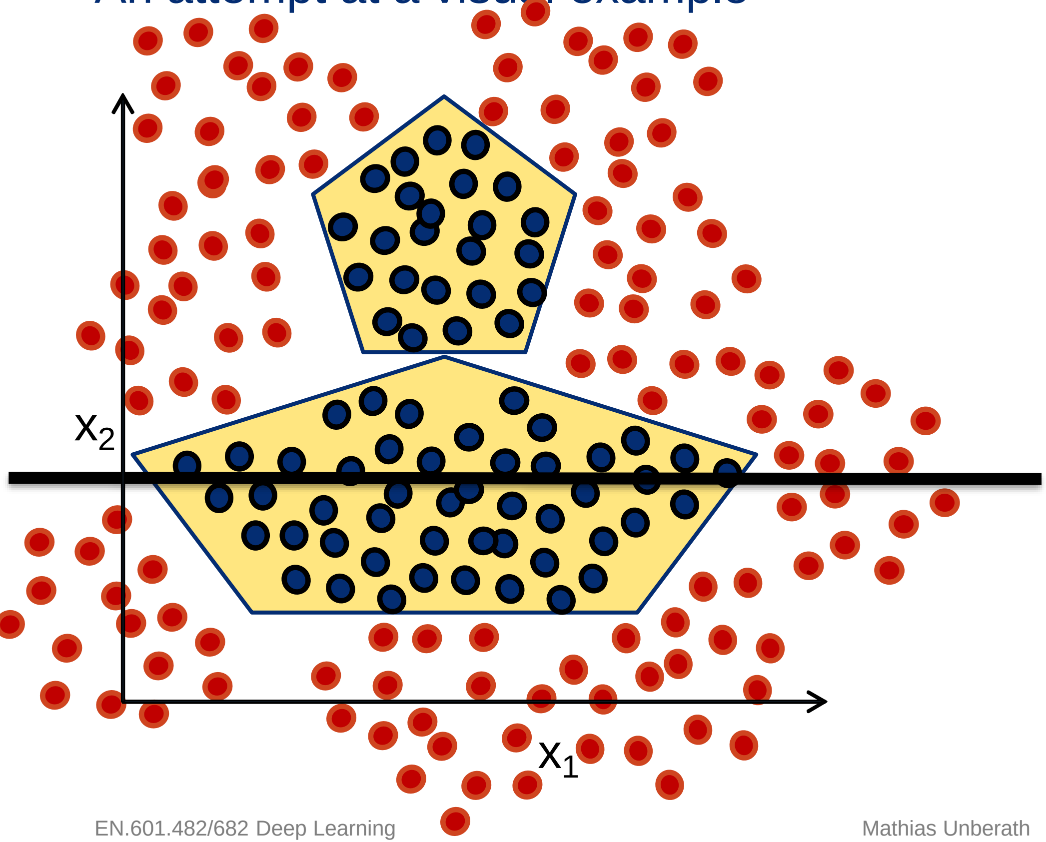


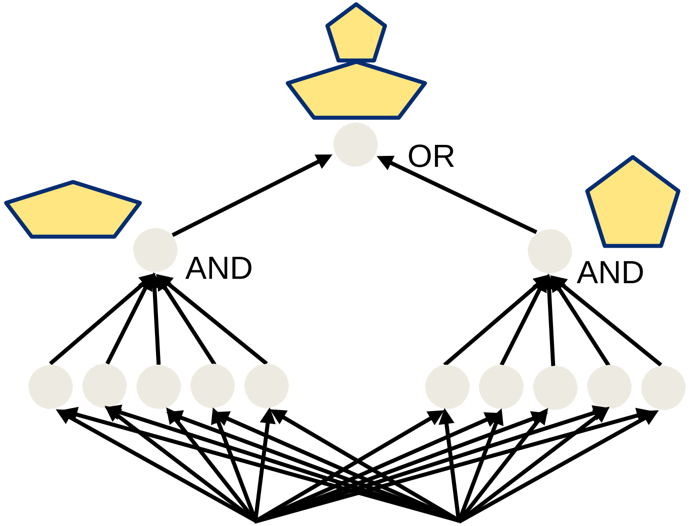
This network can perfectly describe the required decision boundary!

These are the lines a network must discover during training

Weight Initialization

An attempt at a visual example



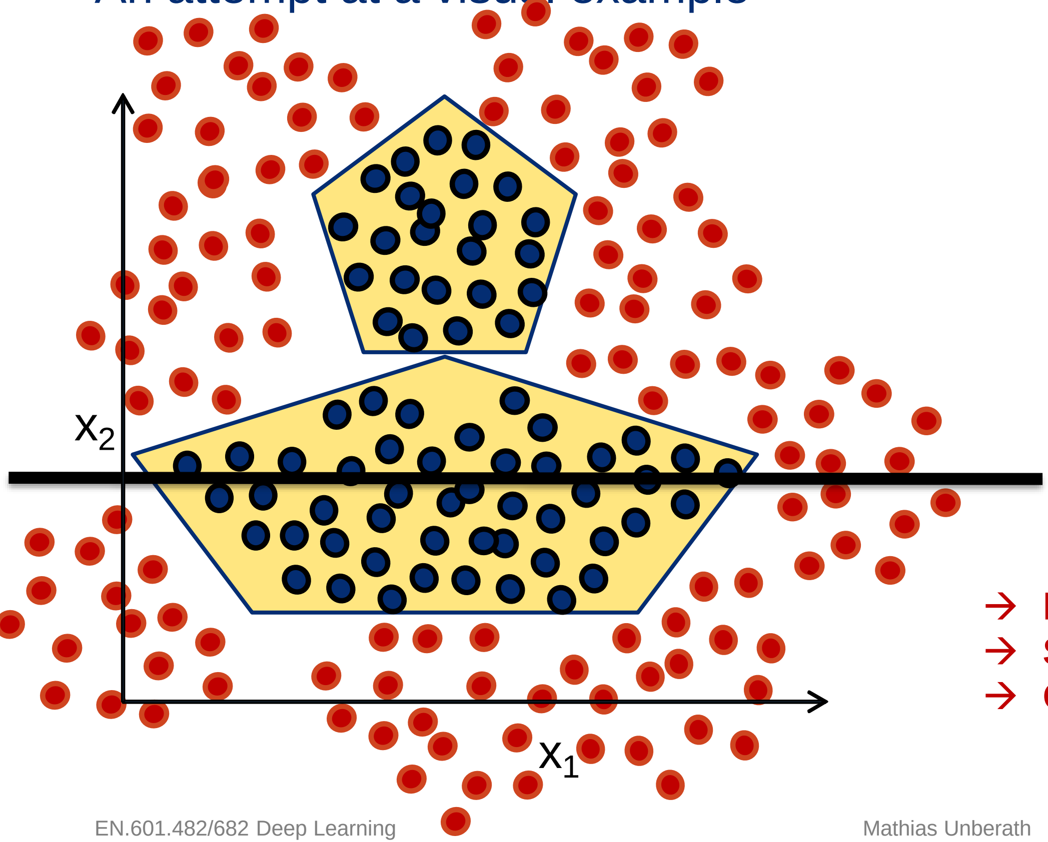


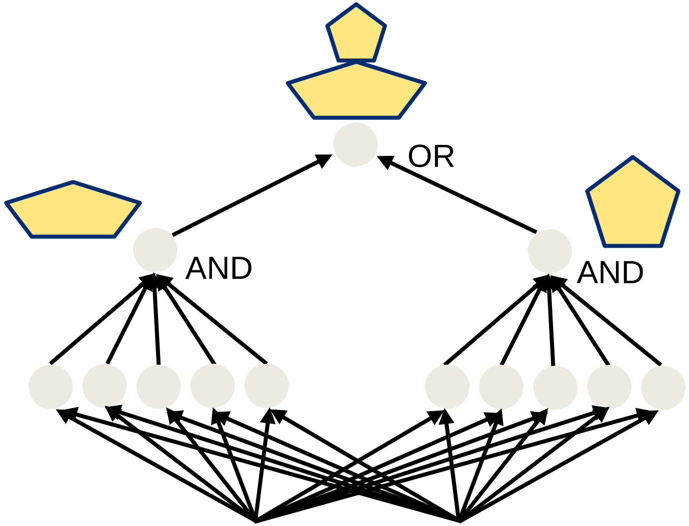
This network can perfectly describe the required decision boundary!

Constant initialization:
e.g. $\mathbf{(0,c)^T(x1,x2) + 0}$

Weight Initialization

An attempt at a visual example



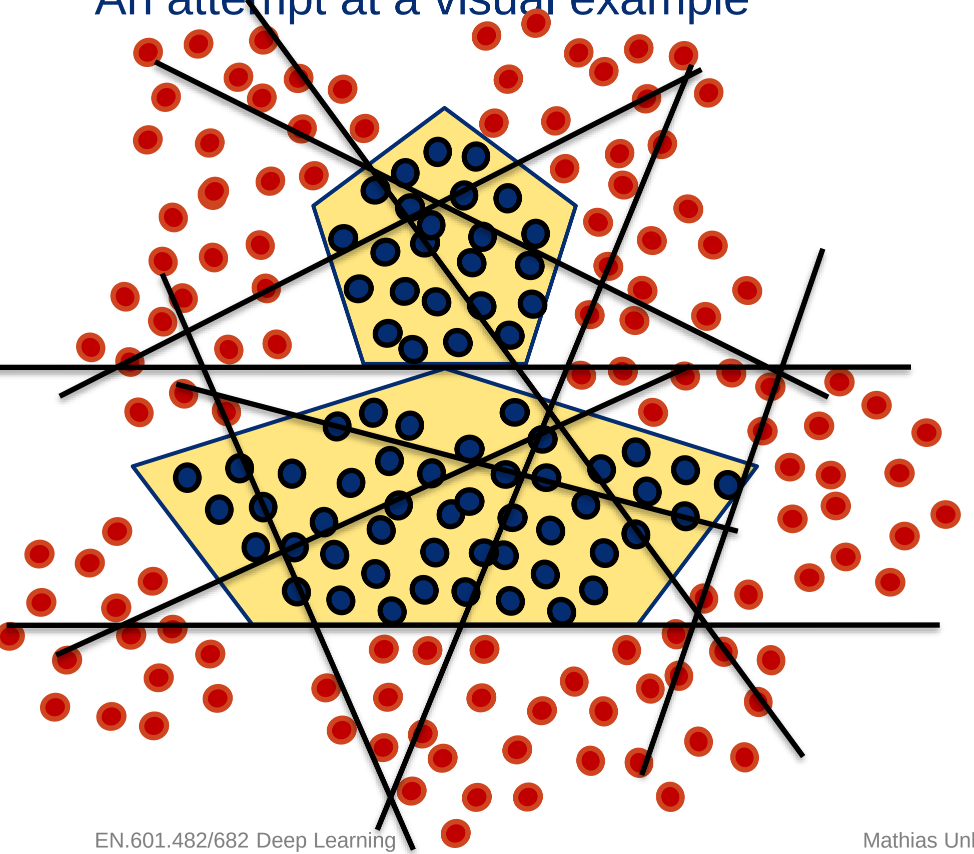


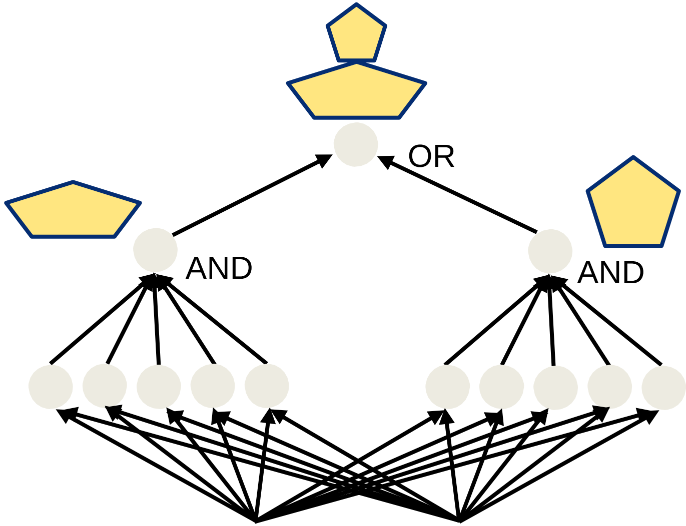
This network can perfectly describe the required decision boundary!

- → **Every neuron "sees" the same situation!**
- → **System is entirely symmetric**
- → **Gradient/updates are the same for every neuron!**

Weight Initialization

An attempt at a visual example



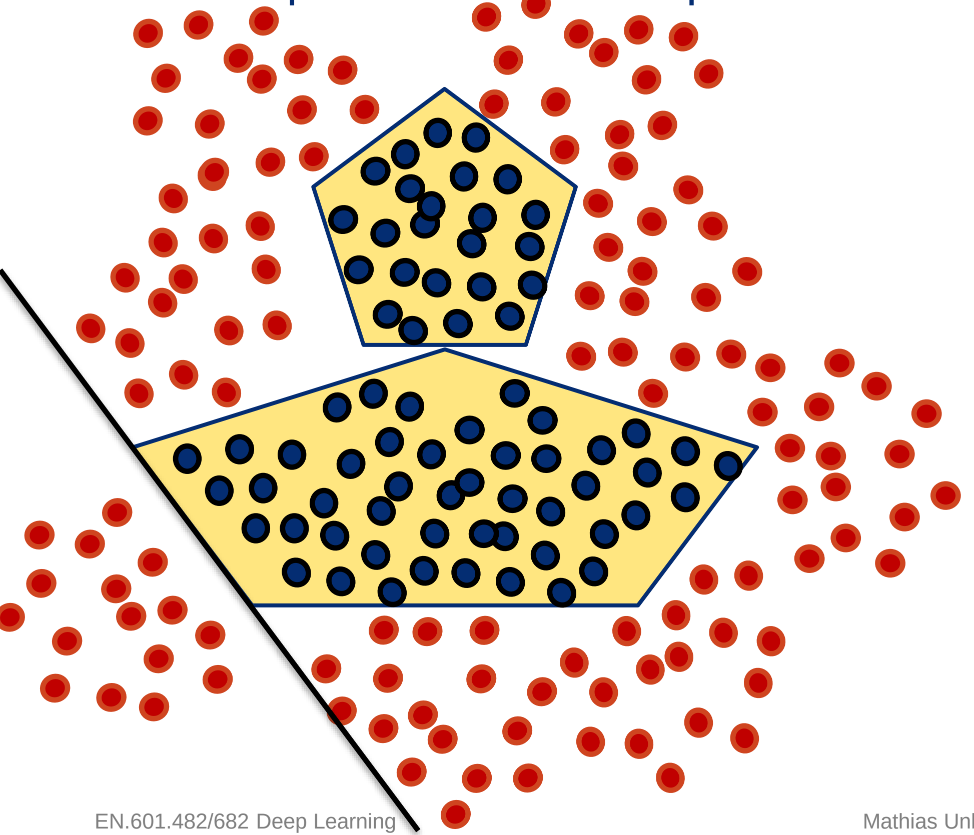


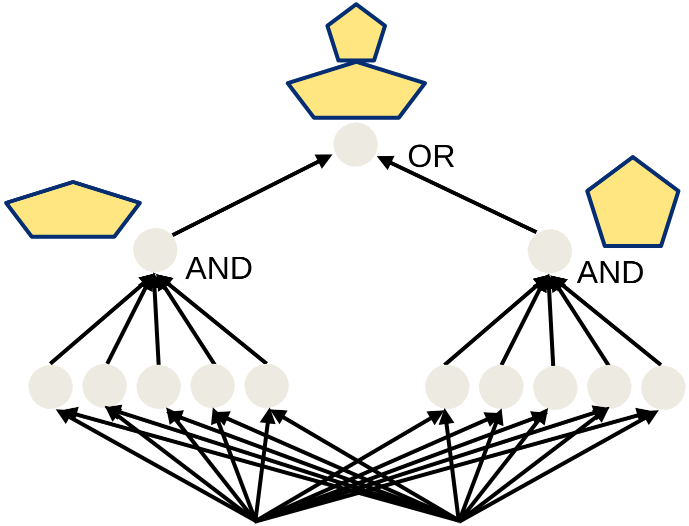
This network can perfectly describe the required decision boundary!

→ **Random initialization**

Another Aside

An attempt at a visual example



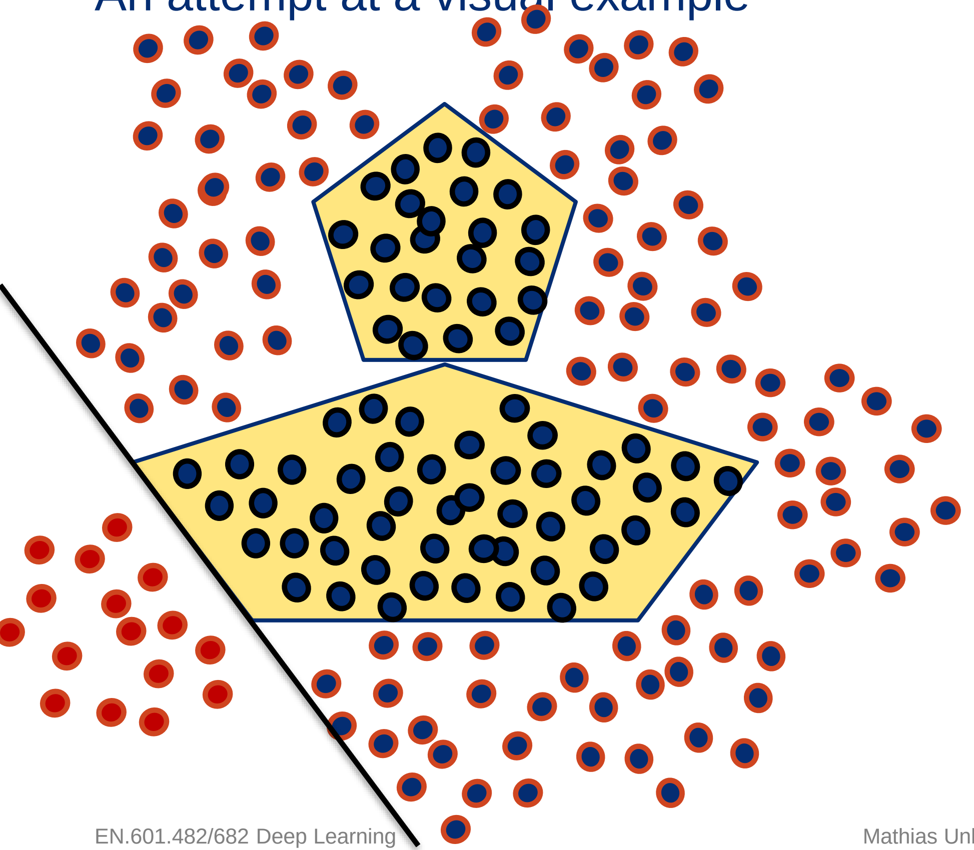


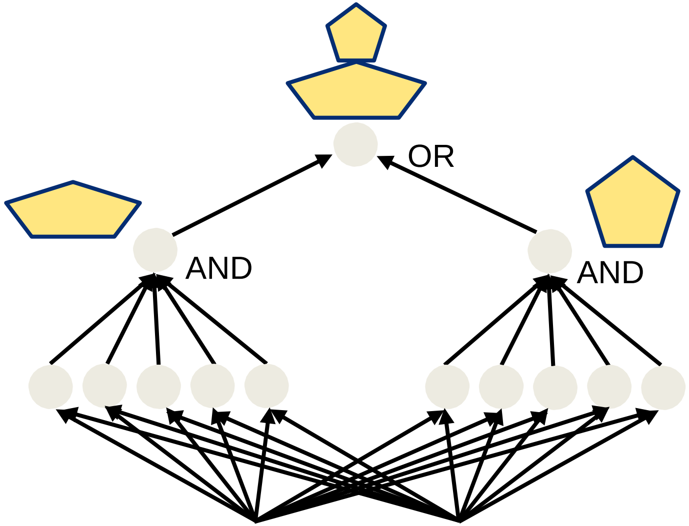
This network can perfectly describe the required decision boundary!

Q: During training, we want to find this line in one of the shallow layers.
Why is it difficult to find this line?

Another Aside

An attempt at a visual example





~~This network can perfectly describe the required decision boundary!~~

Only in theory, because in practice it is very unlikely to converge to this solution.
Network must have larger capacity!

Weight Initialization

Second Idea:
Small random numbers with zero mean and some standard deviation

```
W = 0.01* np.random.randn(D,H)
```

Works OK with shallow networks but is problematic with deeper ones.

Weight Initialization

Third Idea: Xavier initialization
Small random numbers with zero mean and well-defined standard deviation

```
W = np.random.randn(fan_in, fan_out) * np.sqrt(fan_in) # layer initialization
```

Works well, but breaks with ReLU. Why?

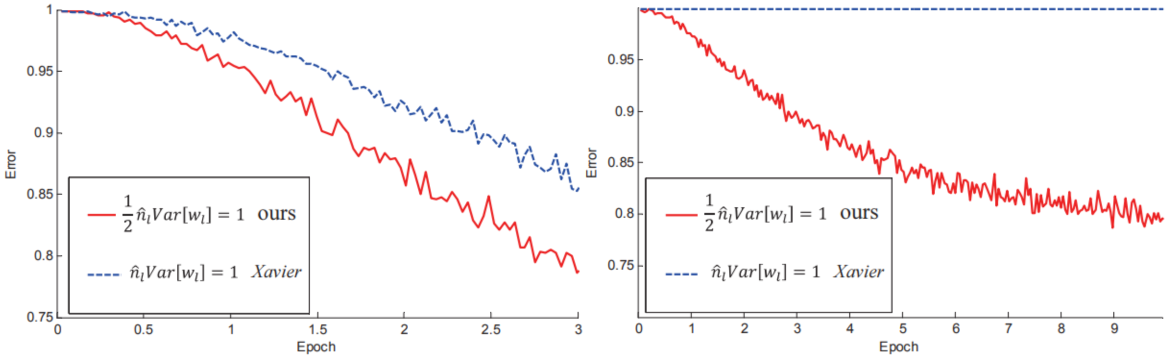
Because derivation is based on linear neuron assumption. After Xavier initialization, outputs will be in the ~linear regime for tanh and sigmoid, but obviously not for ReLU.

Glorot, X., & Bengio, Y. (2010). Understanding the difficulty of training deep feedforward neural networks. Artificial intelligence and statistics (pp. 249-256).

Weight Initialization

Fourth Idea: He initialization
Small random numbers with zero mean and well-defined standard deviation

```
W = np.random.randn(fan_in, fan_out) * np.sqrt(2/fan_in) # layer initialization
```



He, K., Zhang, X., Ren, S., & Sun, J. (2015). Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. ICCV (pp. 1026-1034).

Recap and Take Away (if nothing else)

- Initialization is an active field of research
  (in neural networks and beyond, e.g. image registration)

- Xavier and He initialization played an important role in the success of DL

- If you are using ReLU as recommended: He initialization is your friend!

Activation, Initialization, Preprocessing, Dropout, Batch Norm

Preprocessing

Reminder: The Sigmoid or ReLU Problem

What happens if all inputs are positive?

$f(\sum_i w_i x_i + b)$

Q: Why is this a problem again?

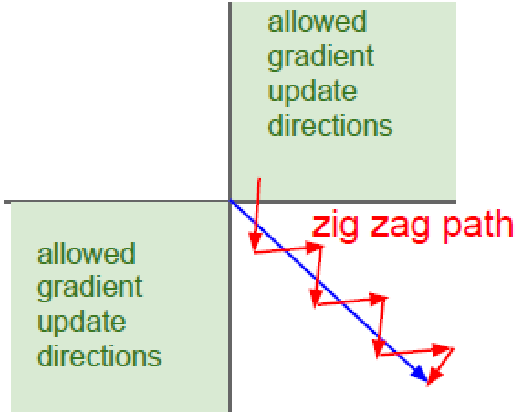
Gradients on w?

Local gradient is x → all positive!

Upstream gradient is positive or negative

→ Gradient is either all positive or all negative!

→ Ineffective updates!



Reminder: The Sigmoid or ReLU Problem

What happens if all inputs are positive?

$f(\sum_i w_i x_i + b)$

Q: Why is this a problem again?

A: Because “normal” images are in [0,255].

Gradients on w?

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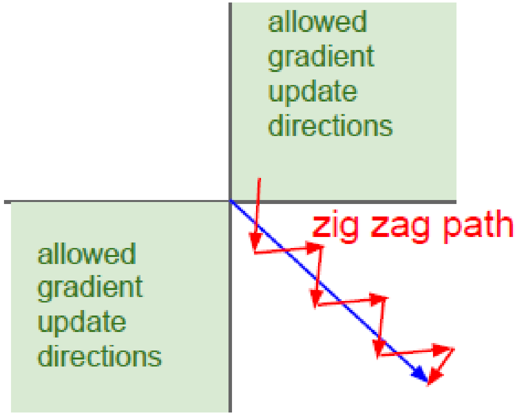
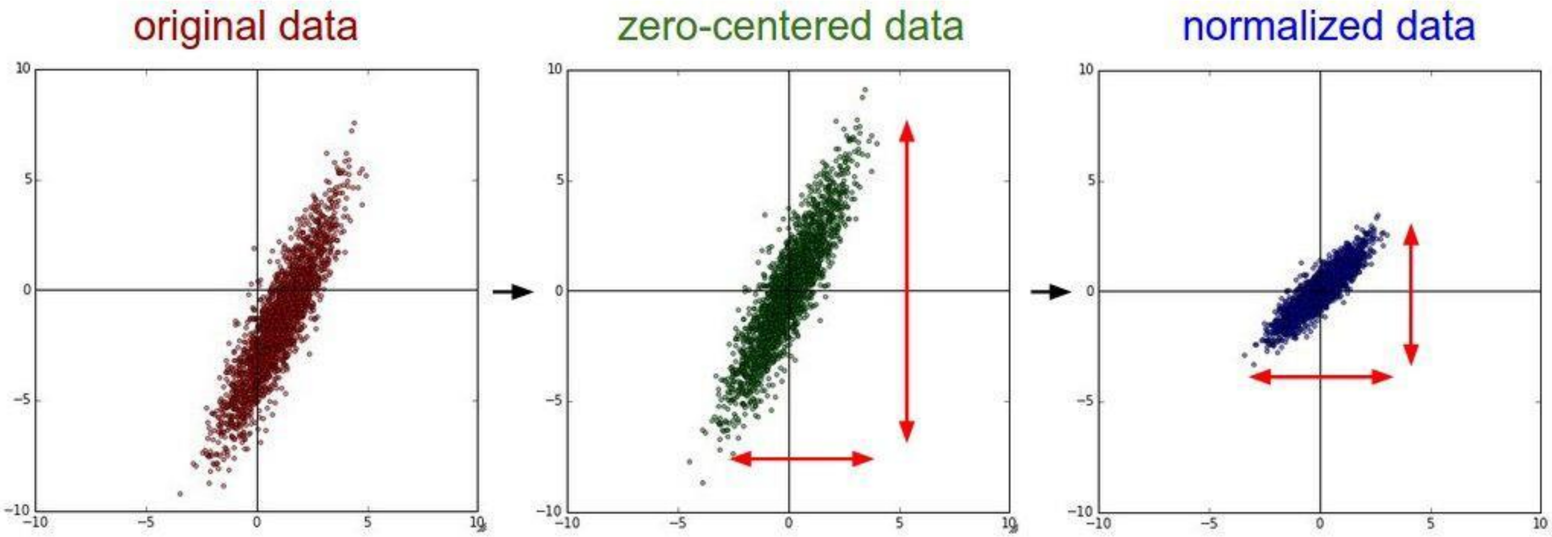


Preprocessing

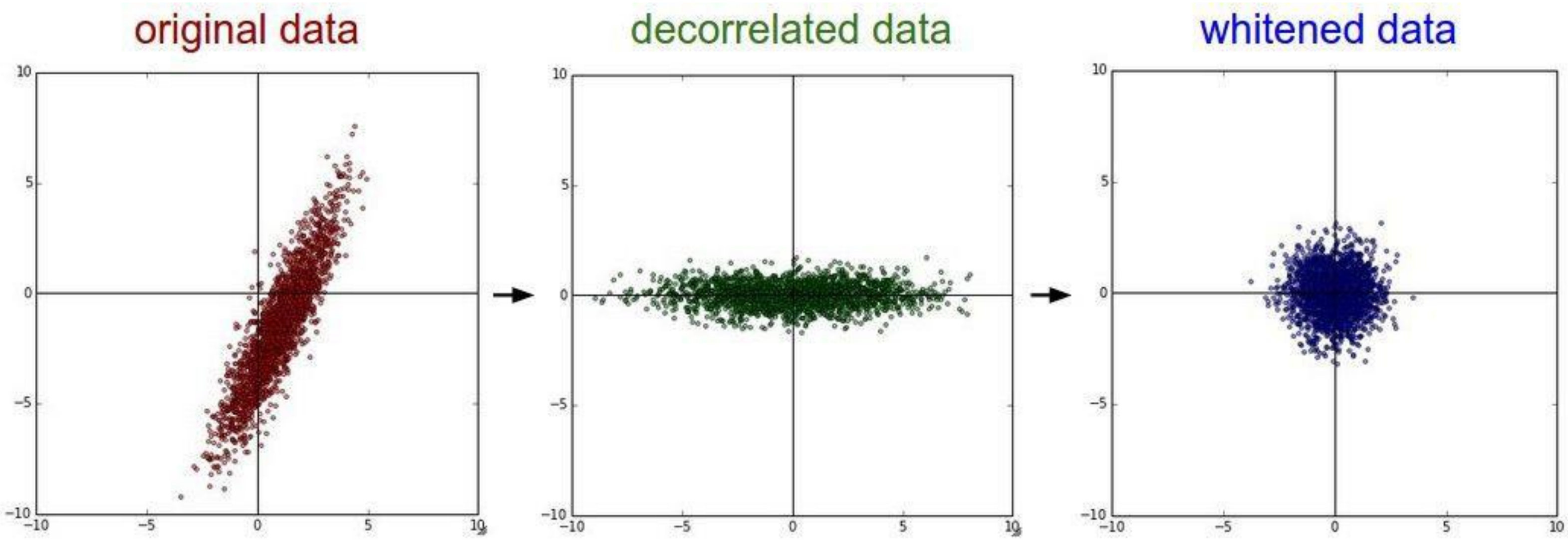


Input data | Mean subtracted | Divided by standard dev

For images, mean centering can be sufficient → Normalization not necessary

Image from Stanford's cs231n.

Preprocessing



Input data

Projected onto PCA

Divided by variance

Whitening: Projection onto axes of highest variation, then normalization
→ Not usually done for images

Image from Stanford's cs231n.

Recap and Take Away (if nothing else)

- Zero-center data
- Try normalizing images

- Do not (necessarily) consider decorrelation, whitening or other techniques for images, but this may be different for other input data

At inference time:

Apply the same transformation (e.g. mean subtraction) with values extracted from the training data.

A Brief (but Important?) Aside

The dynamic range of images

- Natural images (e.g. CIFAR10, ImageNet) are usually 8-bit per channel
  Why? Tradeoff between human perception / storage (8-bit → 255 is nice)

Too coarse quantization is not nice!

A Brief (but Important?) Aside

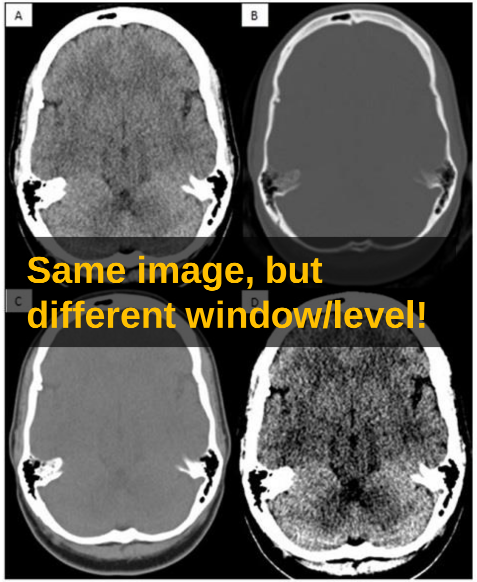
The dynamic range of images

- Natural images (e.g. CIFAR10, ImageNet) are usually 8-bit per channel
  Why? Tradeoff between human perception / storage (8-bit → 255 is nice)

- Medical images **are usually not 8-bit**!
  Depending on protocol, they can be 14,16,32-bit

→ Dynamic range: The span between darkest and brightest value

A Brief **(but Important?)** Aside



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  Why? Tradeoff between human perception / storage (8-bit -

- Medical images **are usually not 8-bit**!
  Depending on protocol, they can be 14,16,32-bit

→ Dynamic range: The span between darkest and brightest value

→ For dynamic ranges >>8-bit, we usually use window/leveling

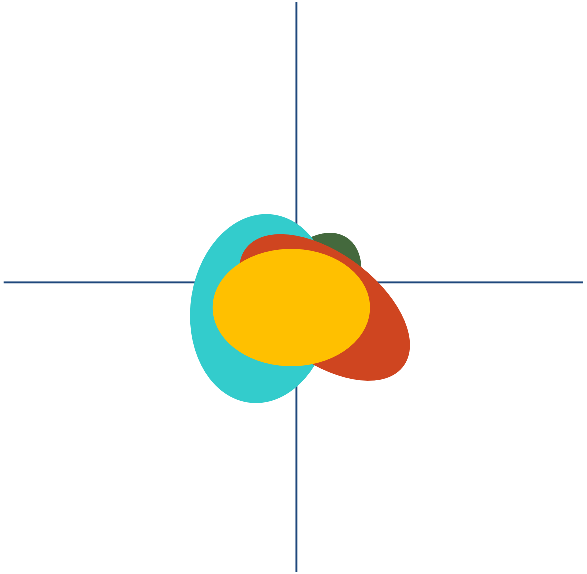
→ When working with such images, do not artificially squash the dynamic range!

Activation, Initialization, Preprocessing, Dropout, Batch Norm

Covariate Shift and Batch Norm

Covariate Shifts

Randomly sampling mini-batches: Training assumes similar distribution!

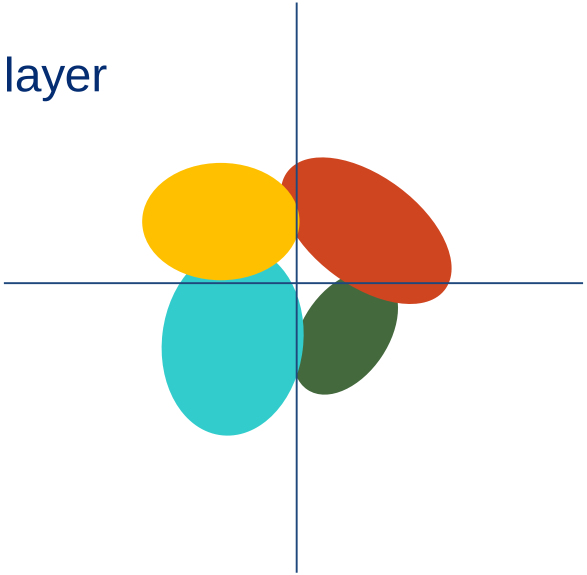


Covariate Shifts

Randomly sampling mini-batches: Training assumes similar distribution!

In practice (and although random), each mini-batch will have different distribution
→ Covariate shift

→ Can happen in **each** layer



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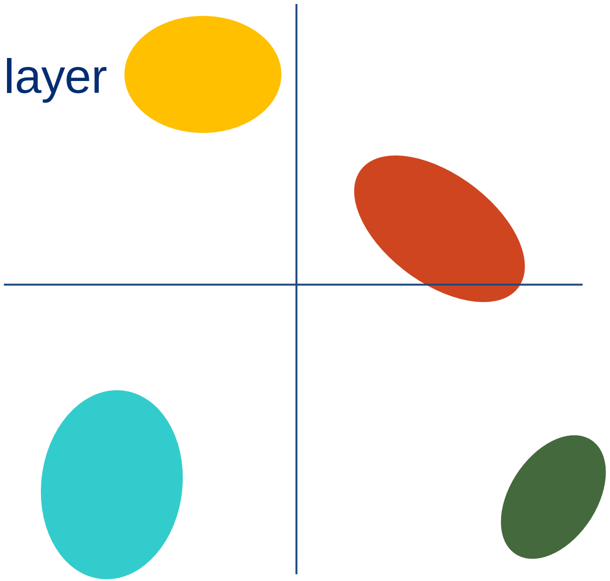
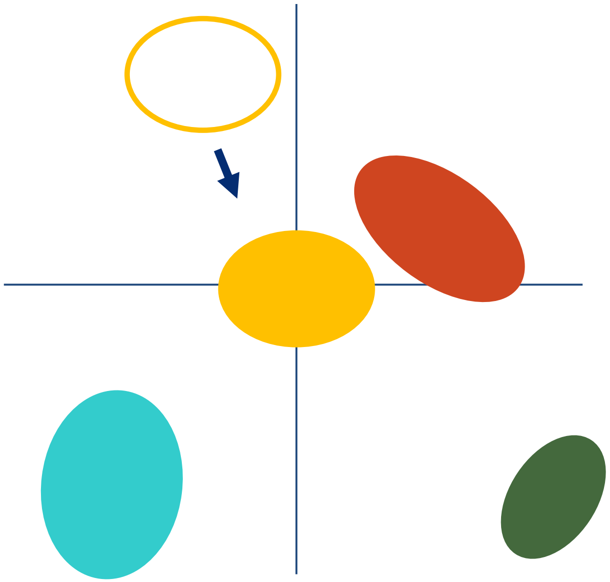


→ Shifts can be large and can negatively affect training!

Move Batches to Standard Location

Eliminate covariate shift by “moving” batches to zero mean and unit standard dev



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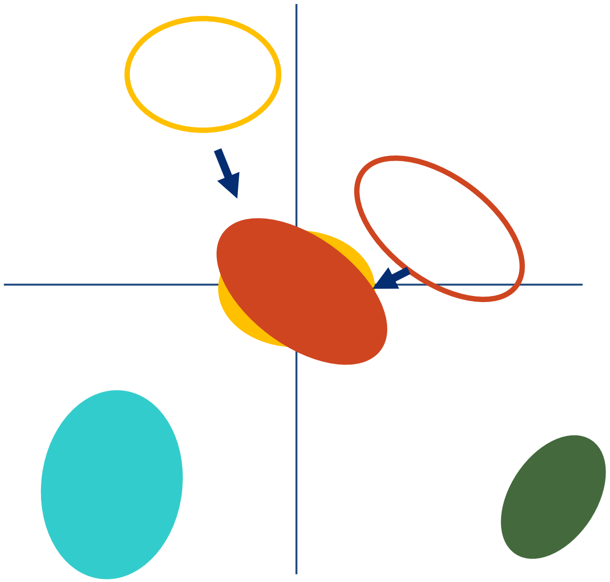

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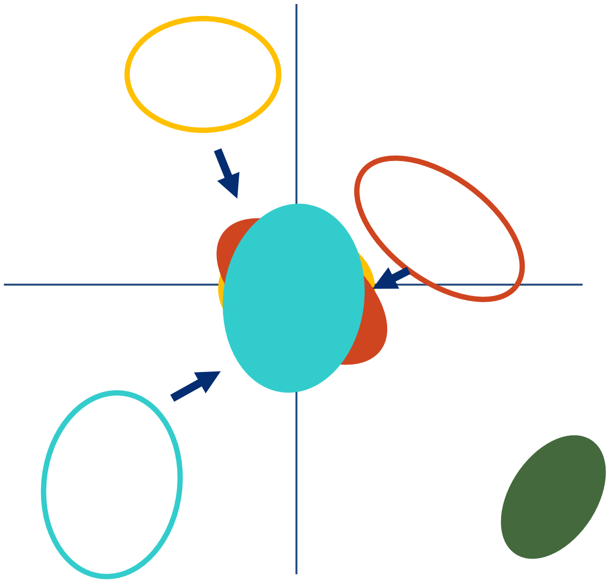

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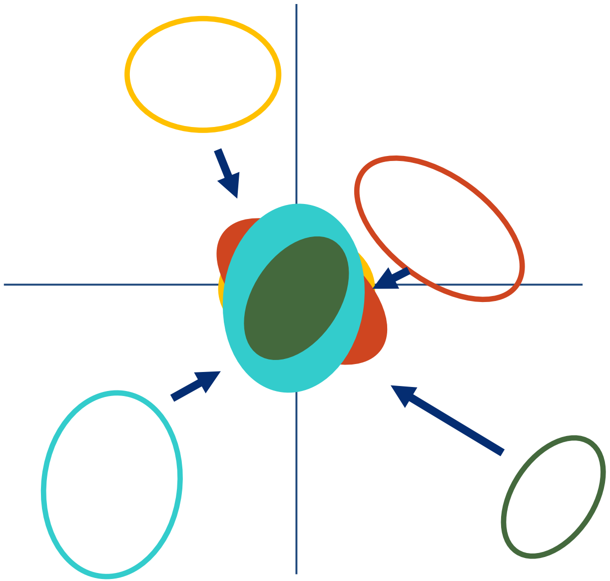

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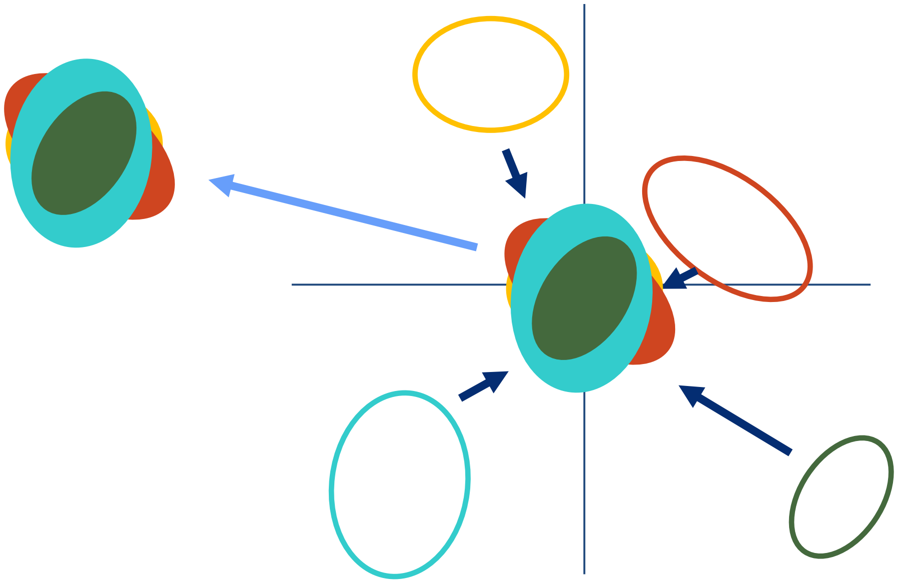

→ Then, move entire collection to desirable location: **Batch normalization**

Ioffe, S., & Szegedy, C. (2015). Batch normalization: Accelerating deep network training by reducing internal covariate shift. arXiv:1502.03167.

Batch Normalization

- If we want unit Gaussian activations, let's make them that!

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

This function is differentiable (backprop!)

- Rather then pre-conditioning data and hoping that nice properties are preserved, at each layer we re-condition during every forward pass

Batch Normalization

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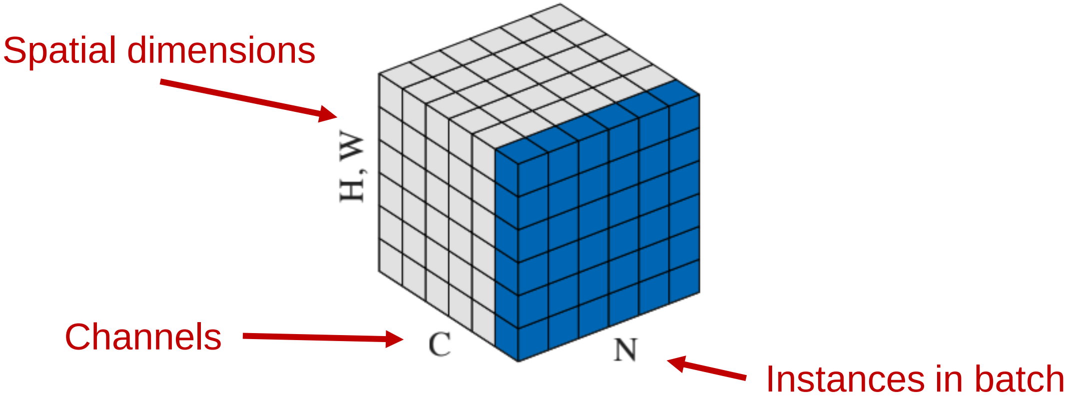
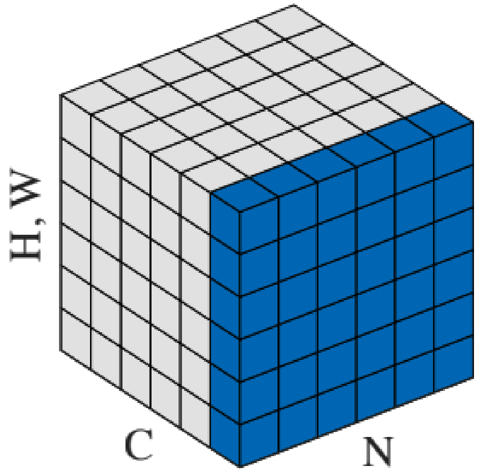


Wu, Y. and He, K., 2018. Group normalization. arXiv preprint arXiv: 1803.08494.

Batch Normalization



1. Compute empirical mean and variance for each channel
$$E[x^{(k)}], \mathrm{Var}[x^{(k)}]$$

2. Normalize to unit Gaussian
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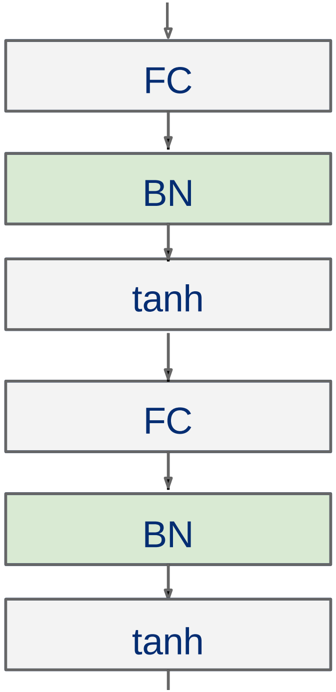

Usually inserted right after fully connected
or convolutional layers, right before activation.

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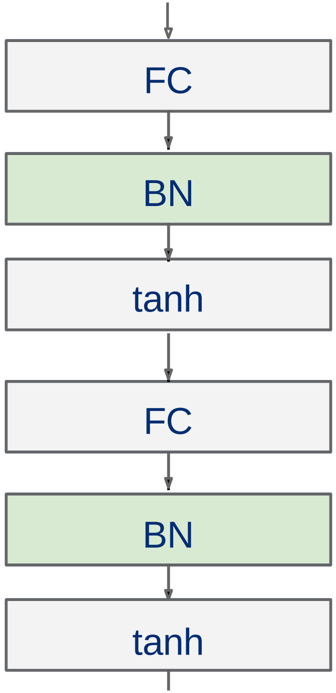

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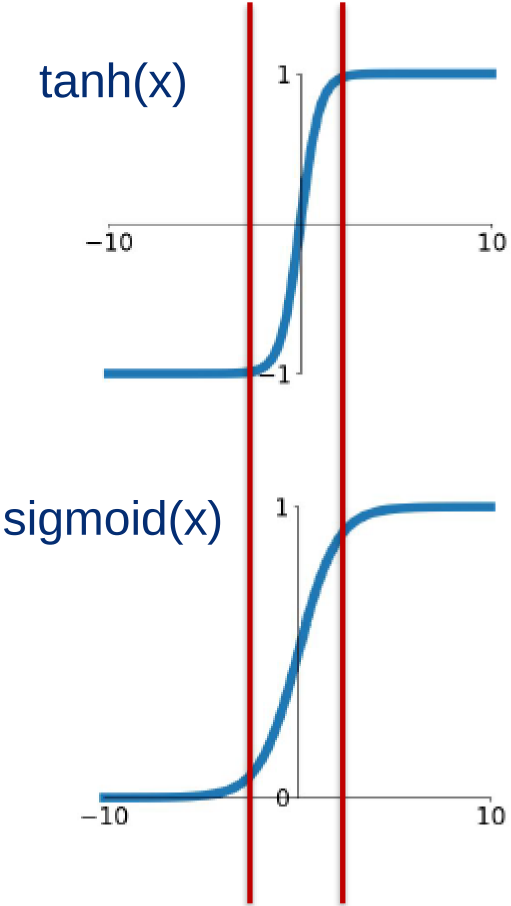
Q: Is unit Gaussian activation necessarily what we want?

Batch Normalization



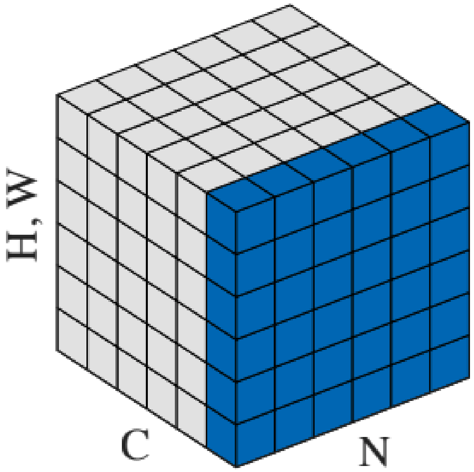
Consider tanh or sigmoid activation

→ Batch normalization will limit the activation to the linear regime of these activation functions!

→ In such case, negatively affects performance

There are other cases where you also would not want BN, e.g. when magnitude matters.

Batch Normalization



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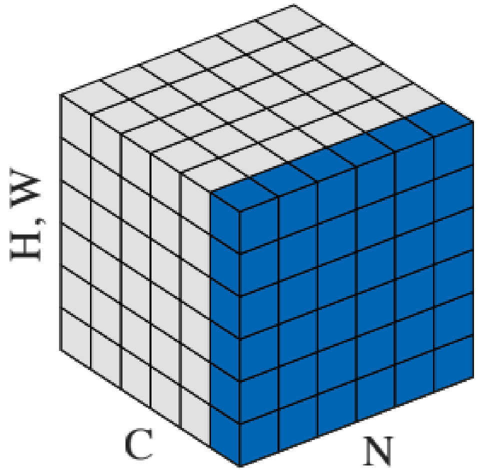
3. Squash output to beneficial range
$$y^{(k)} = \gamma^{(k)} \hat{x}^{(k)} + \beta^{(k)}$$

These are parameters and are learned during training.

Ioffe, S., & Szegedy, C. (2015). Batch normalization: Accelerating deep network training by reducing internal covariate shift. arXiv:1502.03167.

Batch Normalization



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These are parameters and are learned during training.

Network can learn identity!

$$\gamma^{(k)} = \mathrm{Var}[x^{(k)}]$$
$$\beta^{(k)} = E[x^{(k)}]$$

Ioffe, S., & Szegedy, C. (2015). Batch normalization: Accelerating deep network training by reducing internal covariate shift. arXiv:1502.03167.

Batch Normalization

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

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

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

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

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

Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.

- Improves gradient flow through network and allows for higher learning rates
  - Avoids saturating activations
  - Avoids exploding/vanishing gradients
  - Higher learning rates usually produce larger weights leading to explosion
    → Can be avoided here since re-normalized
- Reduces strong dependence on initialization
- Acts as regularization
  - Single instance is now seen in conjuncture with other samples of the batch
  - Network outputs per sample no longer deterministic

Ioffe, S., & Szegedy, C. (2015). Batch normalization: Accelerating deep network training by reducing internal covariate shift. arXiv:1502.03167.

Batch Normalization During Testing

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

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

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

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

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

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Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.

Q: What to do at testing time?

Batch Normalization During Testing

Train N_{BN}^{tr} to optimize the parameters $\Theta \cup \{\gamma^{(k)}, \beta^{(k)}\}_{k=1}^{K}$

$N_{BN}^{inf} \leftarrow N_{BN}^{tr}$ // Inference BN network with frozen // parameters

for $k = 1 \dots K$ **do**

// For clarity, $x \equiv x^{(k)}, \gamma \equiv \gamma^{(k)}, \mu_{\mathcal{B}} \equiv \mu_{\mathcal{B}}^{(k)}$, etc.

Process multiple training mini-batches $\mathcal{B}$, each of size m, and average over them:

$$\mathrm{E}[x] \leftarrow \mathrm{E}_{\mathcal{B}}[\mu_{\mathcal{B}}]$$
$$\mathrm{Var}[x] \leftarrow \frac{m}{m-1}\mathrm{E}_{\mathcal{B}}[\sigma_{\mathcal{B}}^2]$$

In N_{BN}^{inf}, replace the transform $y = \mathrm{BN}_{\gamma,\beta}(x)$ with $y = \frac{\gamma}{\sqrt{\mathrm{Var}[x]+\epsilon}} \cdot x + \left(\beta - \frac{\gamma\,\mathrm{E}[x]}{\sqrt{\mathrm{Var}[x]+\epsilon}}\right)$

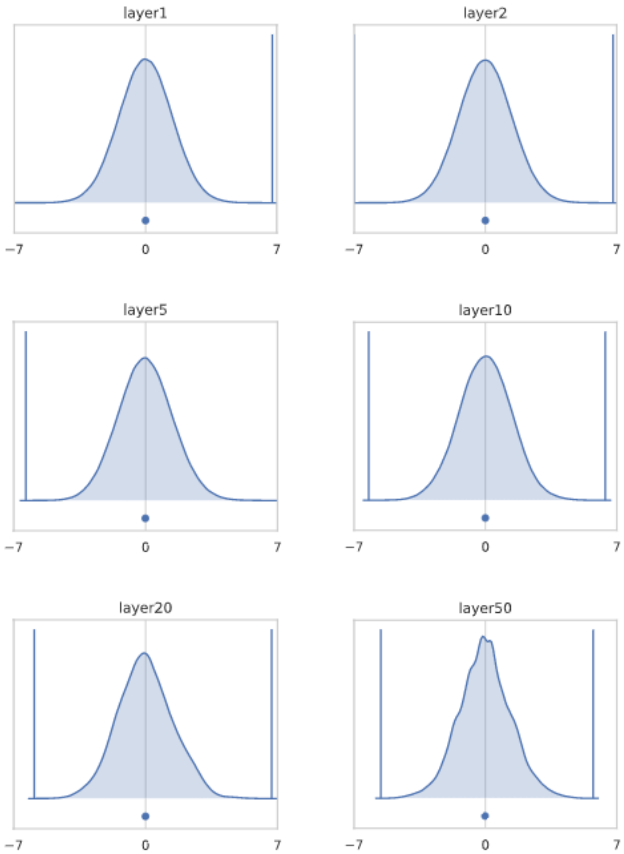
end for

Q: What to do at testing time?

Compute average mean and standard deviation across multiple batches, then save these values for inference.

Batch Norm: New Insights

- Is it really about covariate shift?
- Let's reconsider He initialization
  - Goal: Preserve mean and variance of outputs if marginalized over the weight distribution

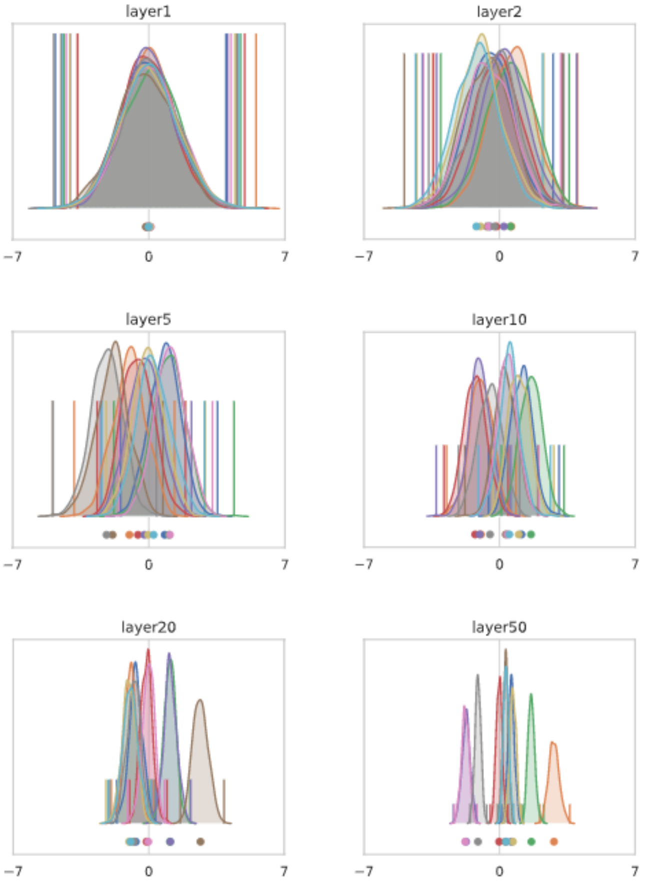


Channel activation at different depths with independent N(0,1) inputs

Santurkar, S., Tsipras, D., Ilyas, A., & Madry, A. (2018). How does batch normalization help optimization?. NeurIPS (pp. 2483-2493).
https://myrtle.ai/how-to-train-your-resnet-7-batch-norm/

Batch Norm: New Insights

- Is it really about covariate shift?
- Let's reconsider He initialization
  - Goal: Preserve mean and variance of outputs if marginalized over the weight distribution
- Every channel has chosen a constant value!
  - Peaked, narrow distribution
  - Most inputs would be classified as the orange class

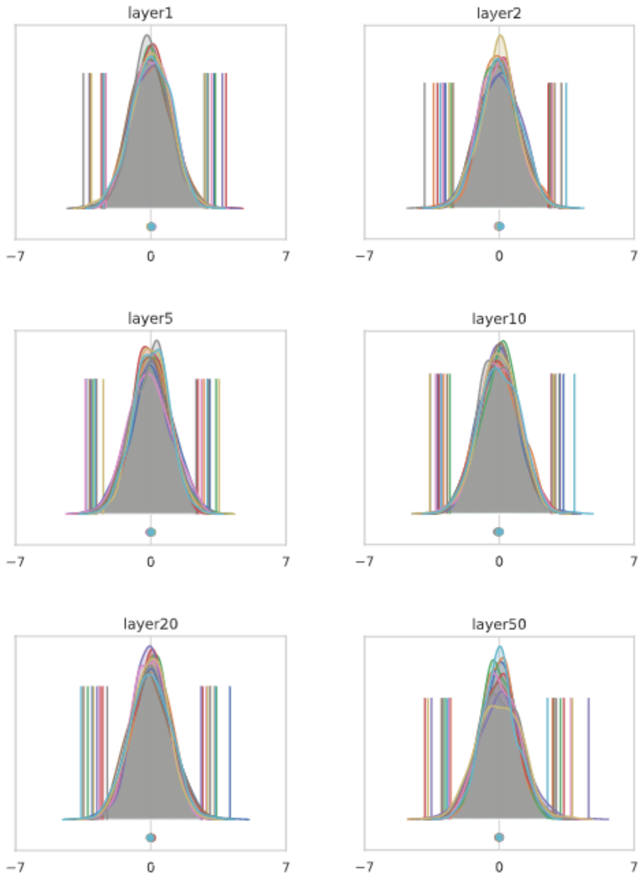


Channel activation at different depths with independent N(0,1) inputs **split by channel**

Santurkar, S., Tsipras, D., Ilyas, A., & Madry, A. (2018). How does batch normalization help optimization?. NeurIPS (pp. 2483-2493).
https://myrtle.ai/how-to-train-your-resnet-7-batch-norm/

Batch Norm: New Insights

- Is it really about covariate shift?
- Let's reconsider He initialization
  - Goal: Preserve mean and variance of outputs if marginalized over the weight distribution
- Every channel has chosen a constant value!
  - Peaked, narrow distribution
  - Most inputs would be classified as the orange class
- Removing ReLU: Problem disappears
  - Non-zero channel means
  - Decreasing variance due to increasing mean (see blog)



Channel activation at different depths with independent N(0,1) inputs

split by channel, no ReLU

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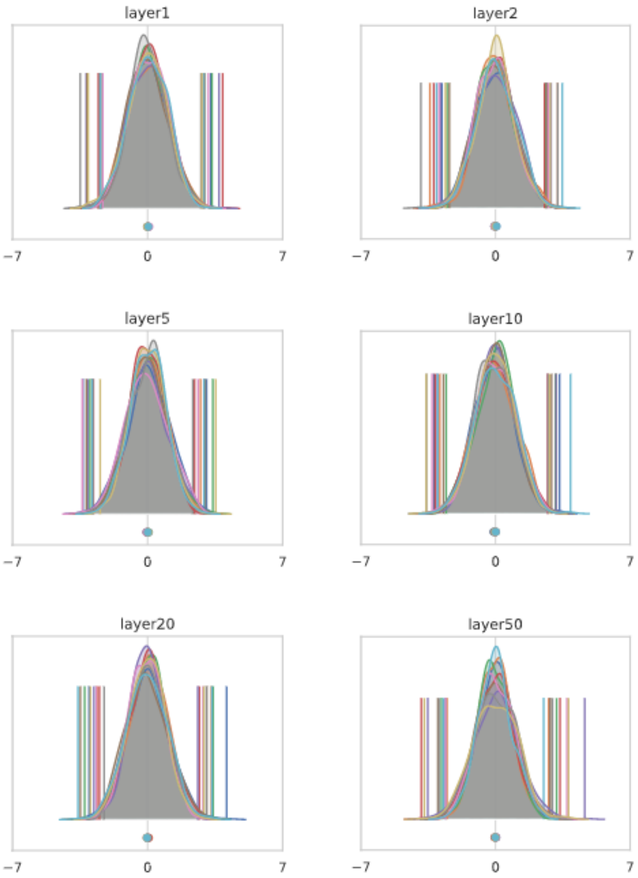
https://myrtle.ai/how-to-train-your-resnet-7-batch-norm/

Batch Norm: New Insights

- → Without batch norm
  - → Standard initialization leads to bad configurations
  - → Network will predict near constant outputs
- → Batch norm fixes this by design

What happens during training?



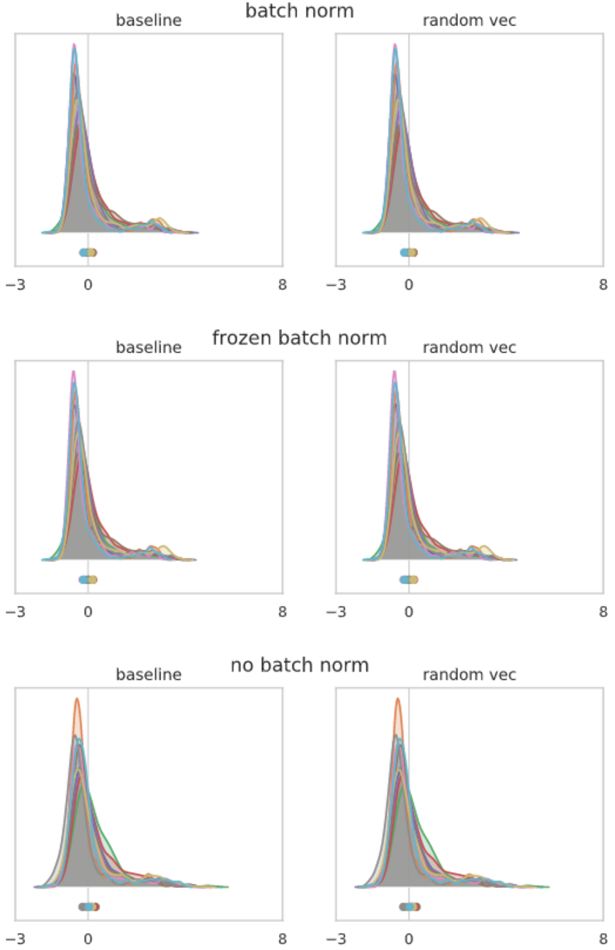
Channel activation at different depths with independent N(0,1) inputs

split by channel, no ReLU

[Santurkar, S., Tsipras, D., Ilyas, A., & Madry, A. (2018). How does batch normalization help optimization?. NeurIPS (pp. 2483-2493).](#)
https://myrtle.ai/how-to-train-your-resnet-7-batch-norm/

Batch Norm: New Insights

- Random perturbation of the weight
  Strength of 1% of parameter vector length
  - Similar output distributions
  - Main mode and second smaller mode: Network starting to make confident predictions



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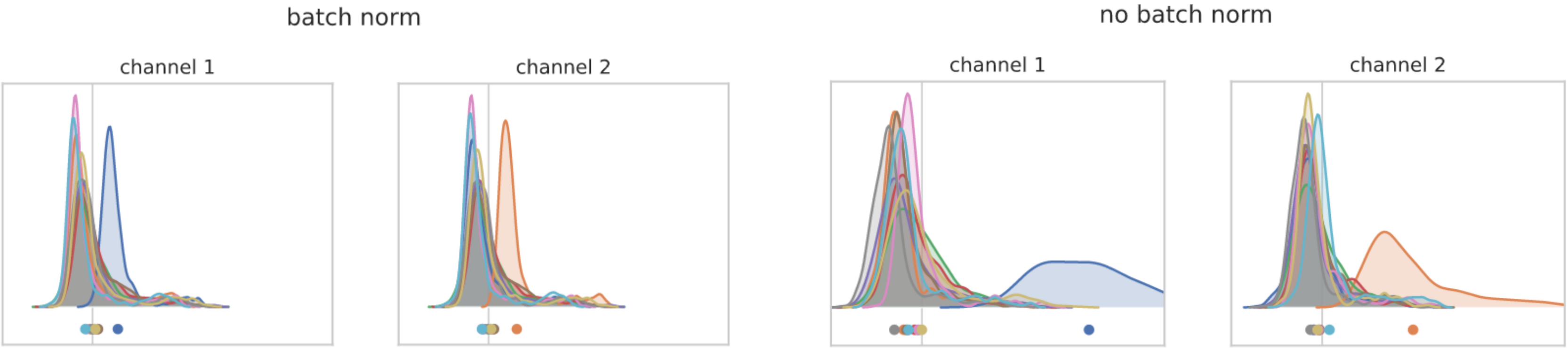
https://myrtle.ai/how-to-train-your-resnet-7-batch-norm/

Batch Norm: New Insights

- **Targeted** perturbation of the weight
  Strength of 1% of parameter vector length
  Gradient of channel mean
  - Network will predict perturbed class in majority of inputs!
  - Internal covariate shift can propagate to external covariate shift in non-batch norm networks!



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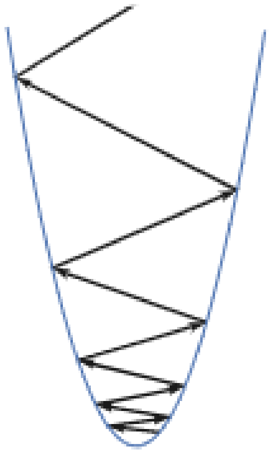
Batch Norm: New Insights



- **Targeted** perturbation of the weight
  Strength of 1% of parameter vector length
  Gradient of channel mean
  - Network will predict perturbed class in majority of inputs!
  - Internal covariate shift can propagate to external covariate shift in non-batch norm networks!

- What does this mean for optimization?
  - Without batch norm, small perturbations lead to immense increases in loss!
  - This means that we are in a narrow valley-type loss landscape (see also next lecture)

[Santurkar, S., Tsipras, D., Ilyas, A., & Madry, A. (2018). How does batch normalization help optimization?. NeurIPS (pp. 2483-2493).](https://myrtle.ai/how-to-train-your-resnet-7-batch-norm/)
https://myrtle.ai/how-to-train-your-resnet-7-batch-norm/

Batch Norm: New Insights

- Investigate the Hessian of parameters
  - **Leading eigenvector** (direction of largest curvature)
    → This direction makes SGD spiral out of control
  - Computed via a power method (not important)
- Also, compute gradients w.r.t.
  mean channel activation (as in perturbation)

→ **Compute overlap between eigenvectors and output-mean gradients**

Santurkar, S., Tsipras, D., Ilyas, A., & Madry, A. (2018). How does batch normalization help optimization?. NeurIPS (pp. 2483-2493).
https://myrtle.ai/how-to-train-your-resnet-7-batch-norm/

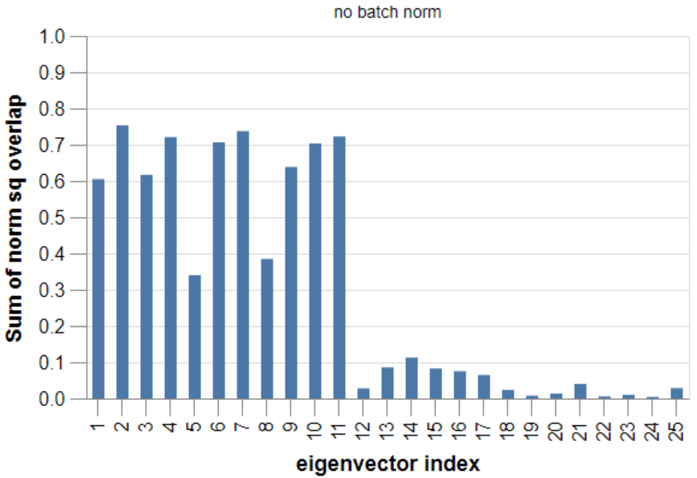
Batch Norm: New Insights

→ **Compute overlap between eigenvectors and output-mean gradients**

- Largest eigenvectors lie almost entirely in the 9-dim subspace spanned by the mean-output gradients!

- **This de-stabilizes SGD optimization!**

- **Batch norm: Smoothens the optimization landscape.**



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Activation, Initialization, Preprocessing, Dropout, Batch Norm

Regularization with Dropout

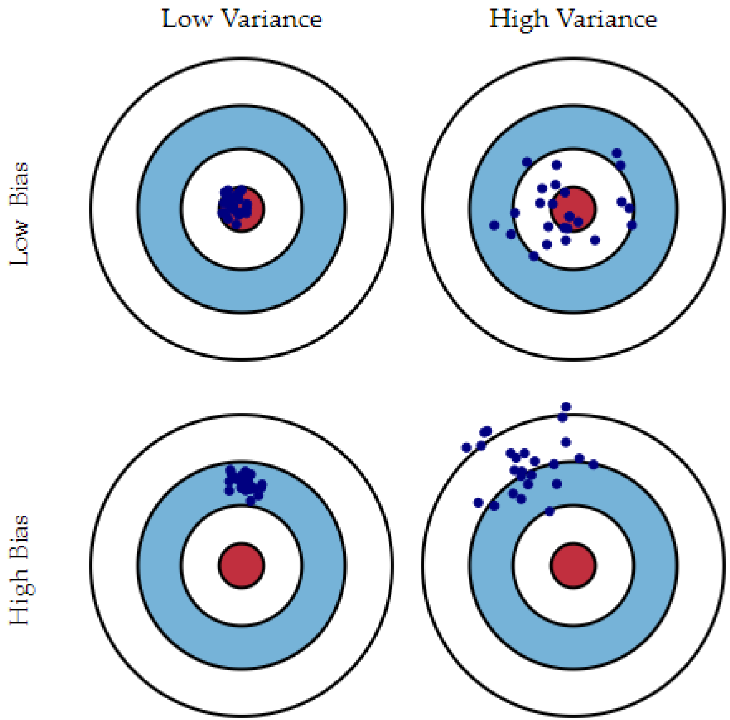
The Bias-Variance Tradeoff and Regularization

Decomposition into bias and variance

$$L(W) = \underbrace{(E[\hat{y}] - y)^2}_{\text{Bias}^2} + \underbrace{E[(\hat{y} - E[\hat{y}])^2]}_{\text{Variance}} + \sigma$$

Adding regularization

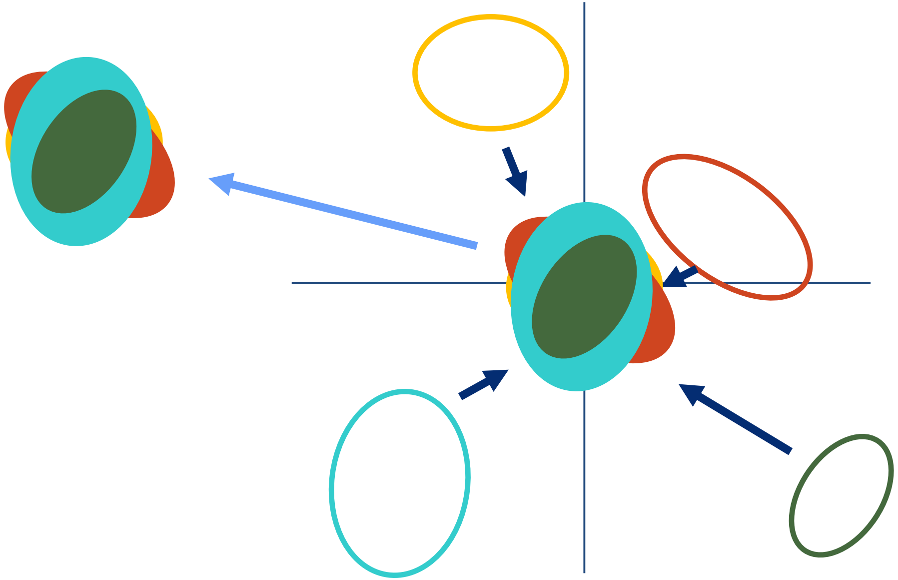
$$L(W) = \underbrace{\frac{1}{N}\sum_i L_i\left(f(x_i, W), y_i\right)}_{\textbf{Data fidelity}} + \underbrace{\lambda R(W)}_{\textbf{Regularization}}$$



[Hastie, T., Tibshirani, R, and Friedman, J. (2017) The Elements of Statistical Learning]

Batch Normalization

Regularization “in a funny way” by seeing samples in conjuncture with others



Other approaches

- L2 on weights
- L1 on activations
- Adding noise to inputs

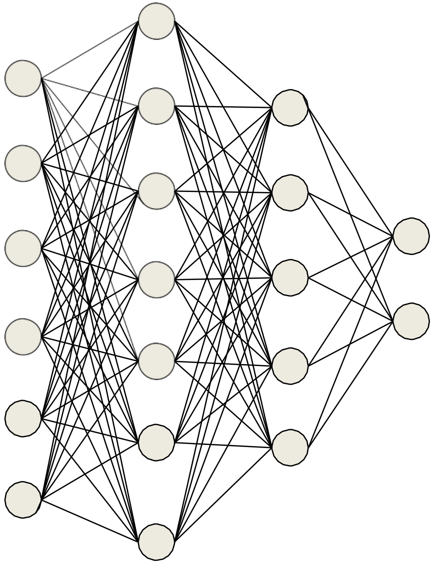
Q: Can we regularize “in a less funny” way?

[Ioffe, S., & Szegedy, C. (2015). Batch normalization: Accelerating deep network training by reducing internal covariate shift. arXiv:1502.03167.]

Dropout

No, not like this!

Dropout

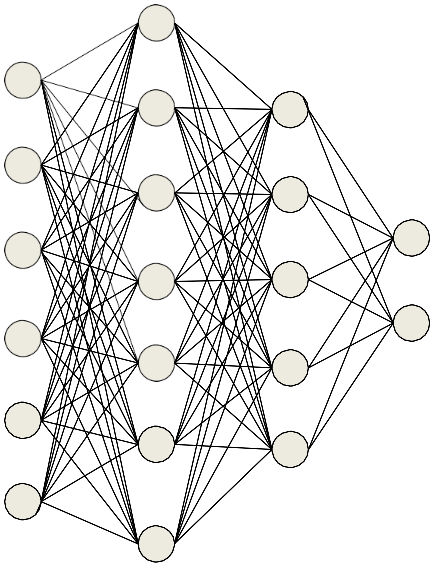


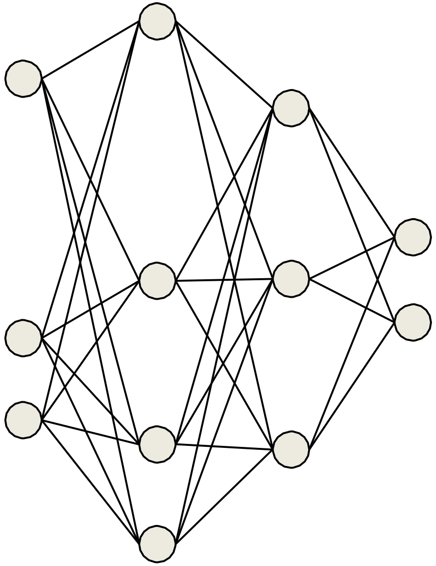
During training

- At each iteration, in each layer, “knock out” each neuron with probability 1-α

[Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., & Salakhutdinov, R. (2014). Dropout: a simple way to prevent neural networks from overfitting. JMLR, 15(1), 1929-1958.]

Dropout





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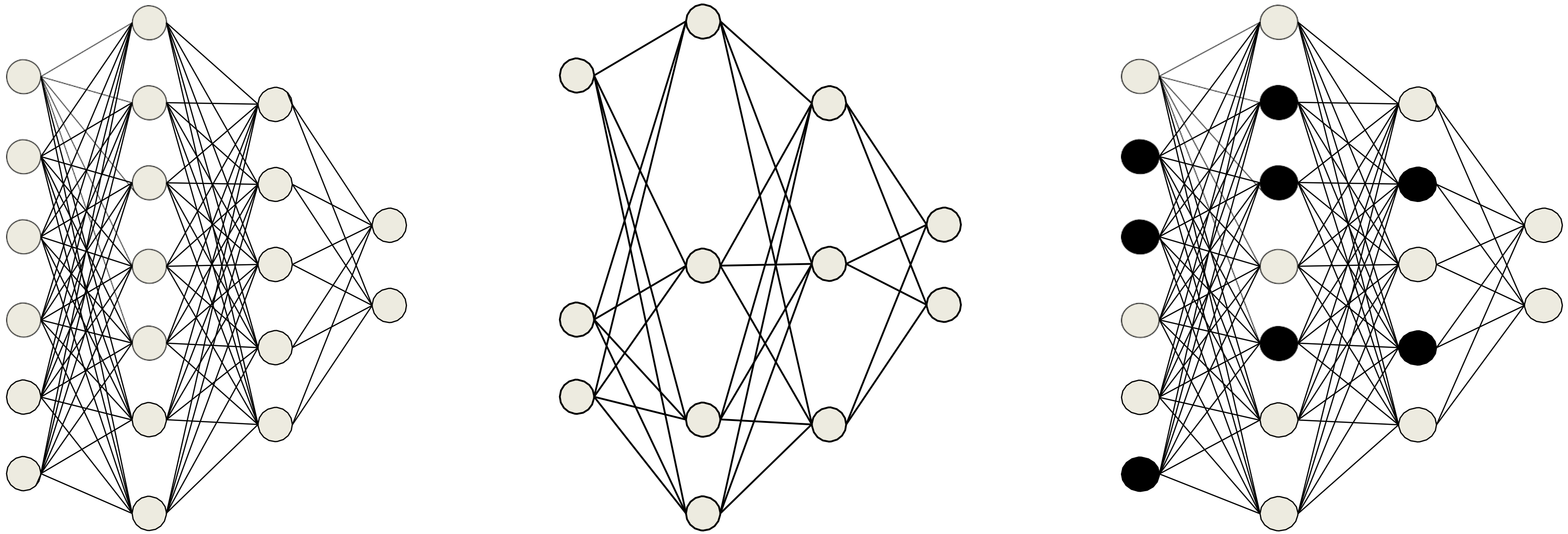
Dropout



During training

- At each iteration, in each layer, “knock out” each neuron with probability 1-α
- In practice, we do not drop connections but set inputs/outputs to zero

Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., & Salakhutdinov, R. (2014). Dropout: a simple way to prevent neural networks from overfitting. JMLR, 15(1), 1929-1958.

Dropout in Forward Pass

Without dropout:

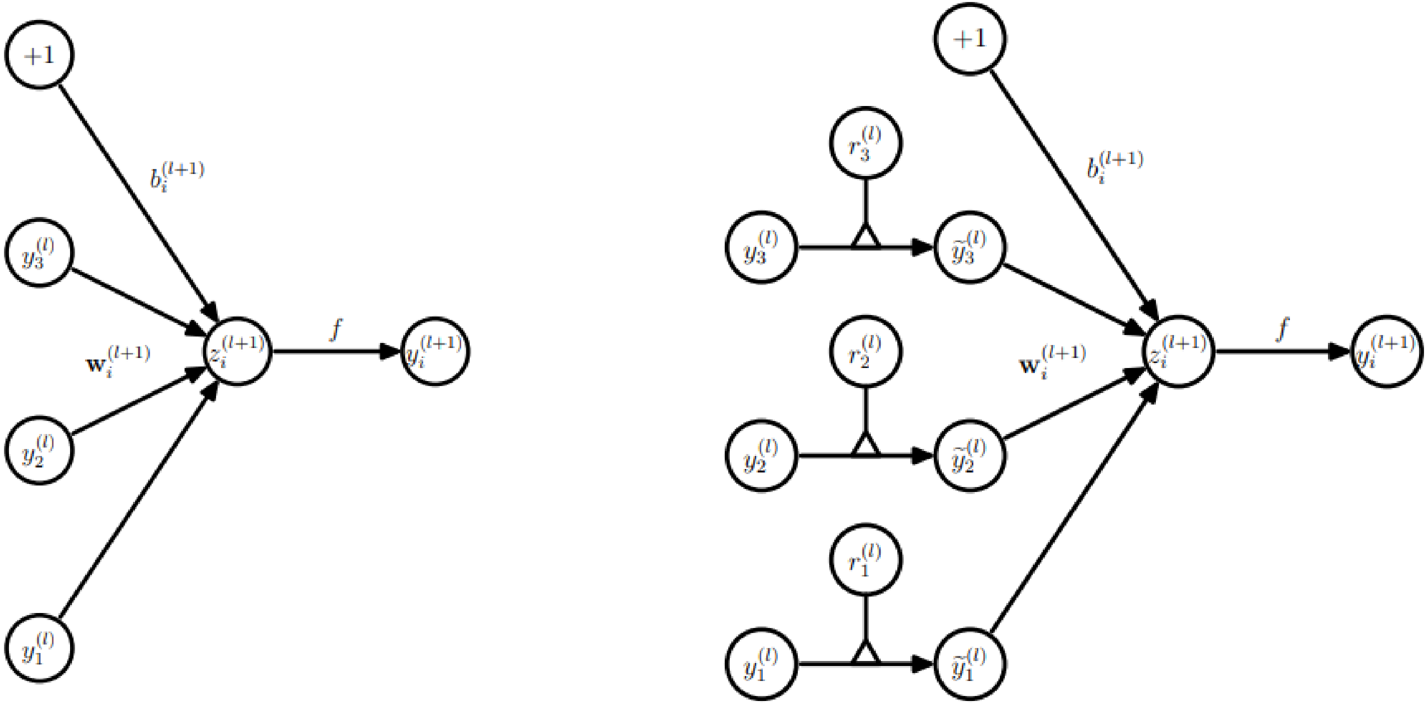
$$
\begin{aligned}
z_i^{(l+1)} &= \mathbf{w}_i^{(l+1)} \mathbf{y}^l + b_i^{(l+1)}, \\
y_i^{(l+1)} &= f(z_i^{(l+1)}),
\end{aligned}
$$

With dropout:

$$
\begin{aligned}
r_j^{(l)} &\sim \mathrm{Bernoulli}(p), \\
\widetilde{\mathbf{y}}^{(l)} &= \mathbf{r}^{(l)} * \mathbf{y}^{(l)}, \\
z_i^{(l+1)} &= \mathbf{w}_i^{(l+1)} \widetilde{\mathbf{y}}^l + b_i^{(l+1)}, \\
y_i^{(l+1)} &= f(z_i^{(l+1)}).
\end{aligned}
$$

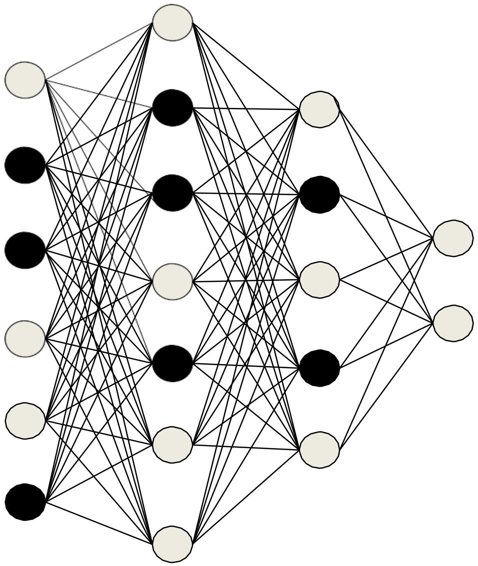
1. For every node j and layer l, determine Bernoulli number {0,1}
2. Drop outputs
3. ???
4. Profit.

Dropout in Forward Pass



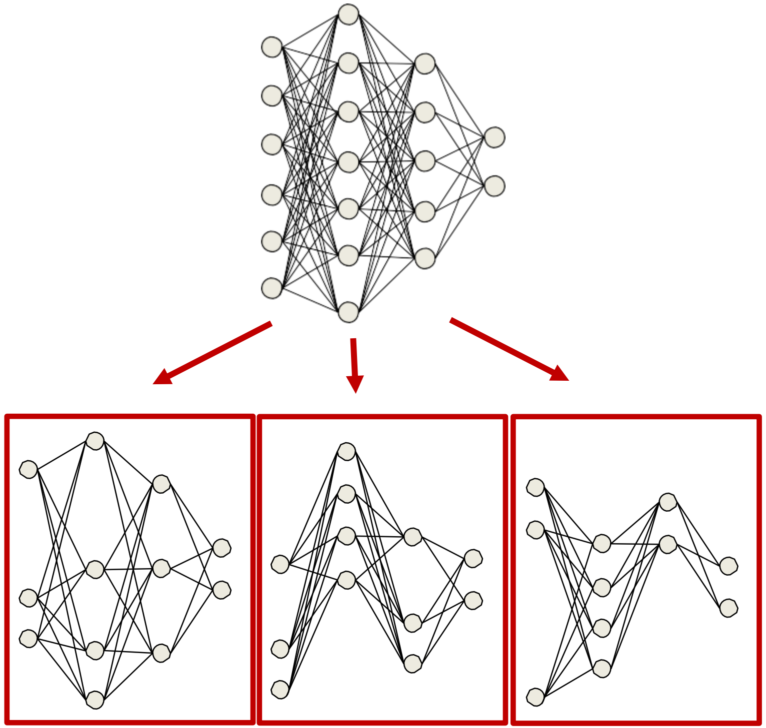
(a) Standard network (b) Dropout network

Dropout in Backward Pass



- Backpropagation as usual, but
  Set updates to zero for dropped out weights
- Tricks of the trade still work

Dropout at Inference Time

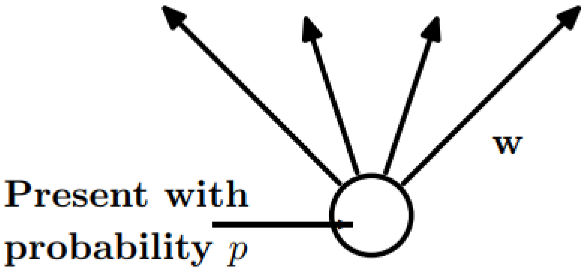


A slightly different view onto dropout

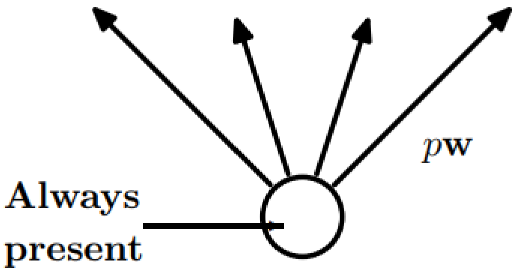
- 2^N sub-networks for N-neuron network
- Dropout samples over these sub-networks

→ Learns a network that averages over all possible networks

Dropout at Inference Time



(a) At training time



(b) At test time

During training

- Fewer activations present

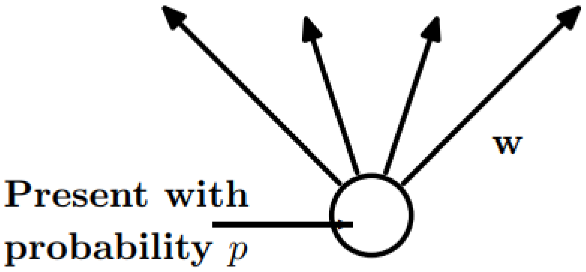
→ Overall activation smaller

During testing

- All activations present

→ Weights or activations scaled by *p*

Dropout at Inference Time



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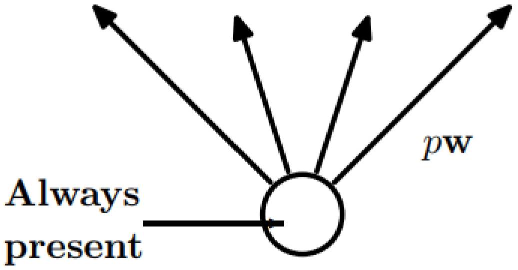

(b) At test time

During training

- Fewer activations present

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During testing

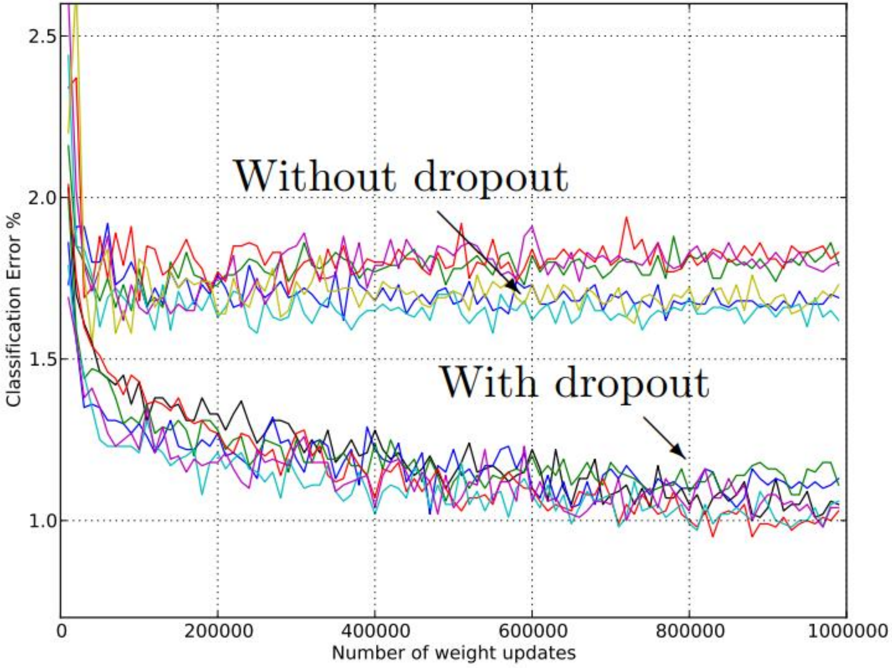
- All activations present

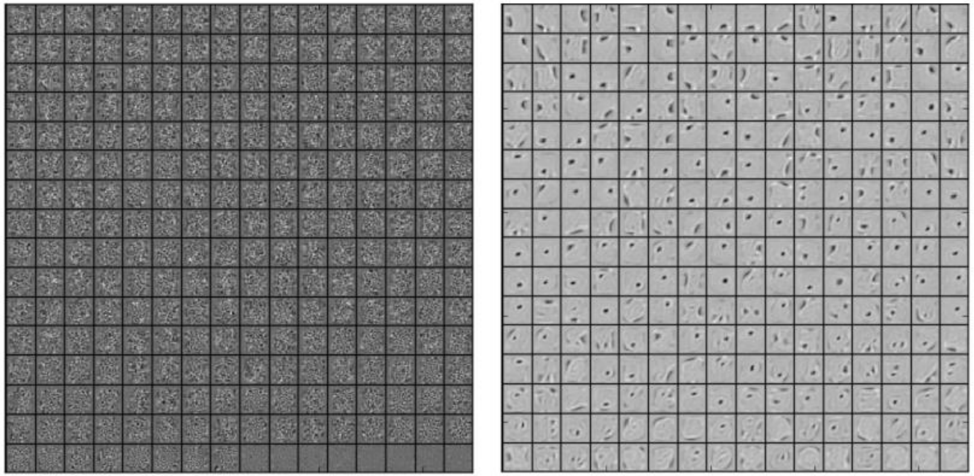
→ Weights or activations scaled by *p*

Some research on test time dropout.

Q: Why would you want to do this?

Dropout: Typical Values and Results





(a) Without dropout (b) Dropout with $p = 0.5$.

This experiment considers an autoencoder. We will see this behavior again later.

Typical values

- Input unit dropout: 0.2
- Hidden unit dropout: 0.5

Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., & Salakhutdinov, R. (2014). Dropout: a simple way to prevent neural networks from overfitting. JMLR, 15(1), 1929-1958.

Activation, Initialization, Preprocessing, Dropout, Batch Norm

Questions?