CSCE 5218 & 4930
Deep Learning

Neural Network Training

Slides adapted from Adriana Kovashka

Plan for this lecture

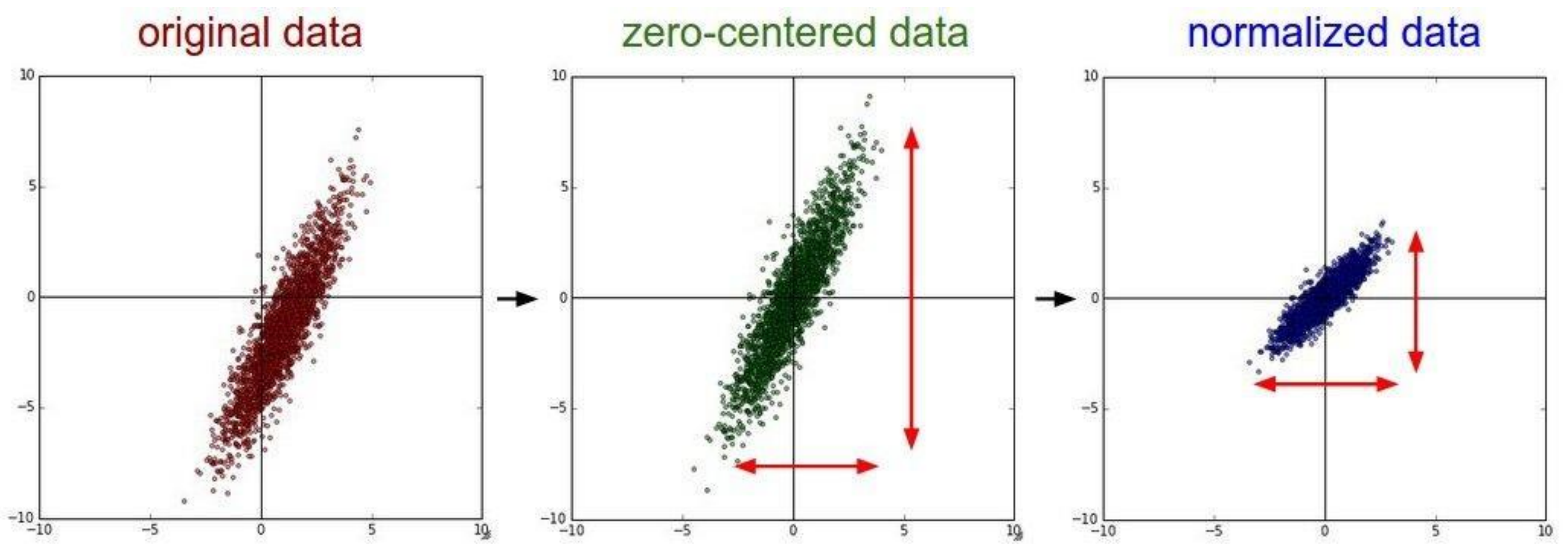
- Tricks of the trade
  - Preprocessing, initialization, normalization
  - Dealing with limited data
- Convergence of gradient descent
  - How long will it take?
  - Will it work at all?
- Different optimization strategies
  - Alternatives to SGD
  - Learning rates
  - Choosing hyperparameters
- How to do the computation
  - Computation graphs
  - Vector notation (Jacobians)

Tricks of the trade

Practical matters

- Getting started: Preprocessing, initialization, normalization, choosing activation functions
- Improving performance and dealing with sparse data: regularization, augmentation, transfer learning
- Hardware and software
- Extra reading/visualization resources
  - https://www.deeplearning.ai/ai-notes/initialization/
  - https://www.deeplearning.ai/ai-notes/optimization/

Preprocessing the Data



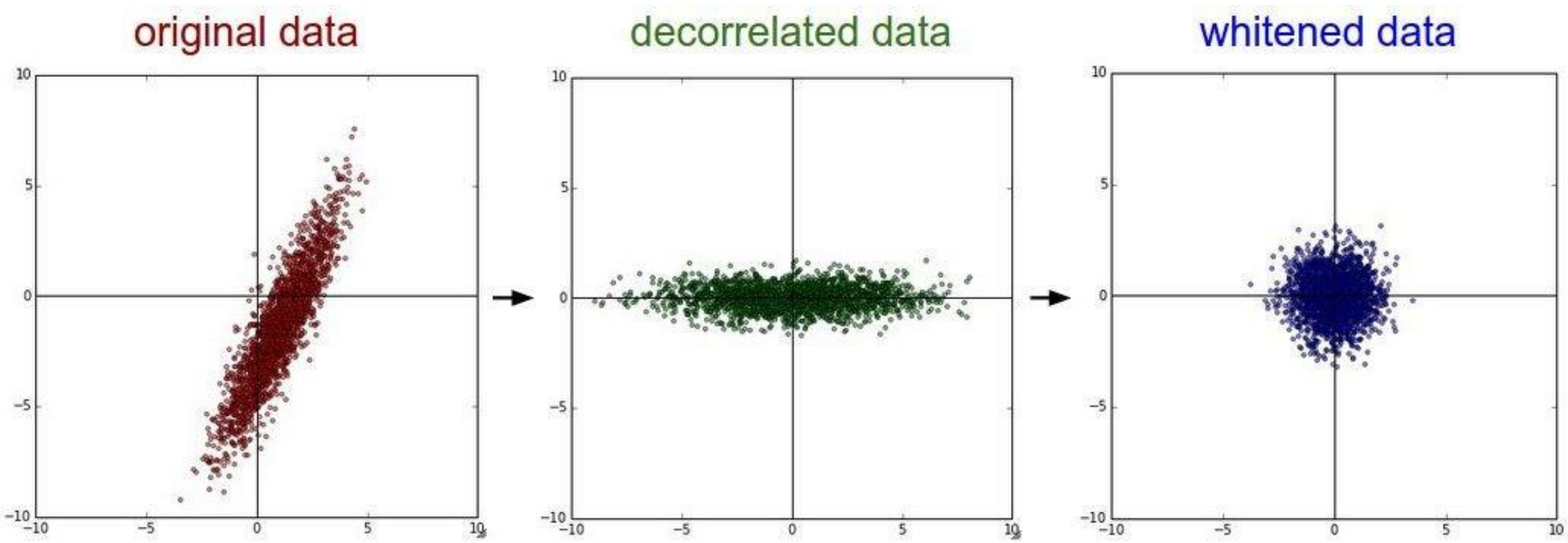

```
X -= np.mean(X, axis = 0)
```

```
X /= np.std(X, axis = 0)
```

(Assume X [NxD] is data matrix, each example in a row)

Preprocessing the Data

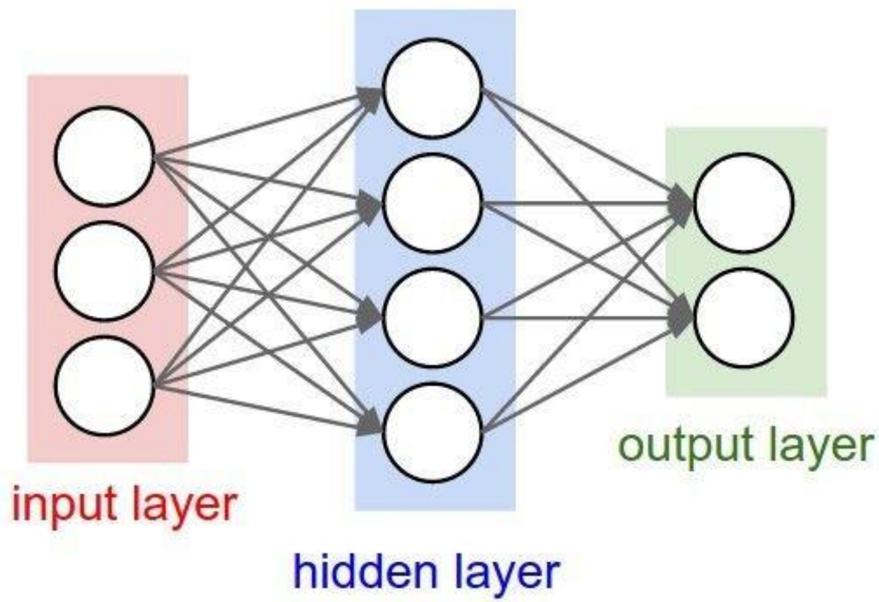
In practice, you may also see **PCA** and **Whitening** of the data



(data has diagonal covariance matrix)

(covariance matrix is the identity matrix)

Weight Initialization



- Q: what happens when W=constant init is used?

Weight Initialization

- Another idea: **Small random numbers**

(gaussian with zero mean and 1e-2 standard deviation)

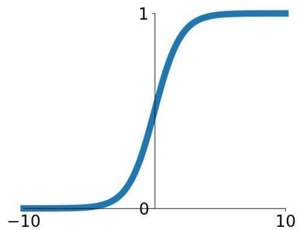
```
W = 0.01* np.random.randn(D,H)
```

Works ~okay for small networks, but problems with deeper networks.

Activation Functions

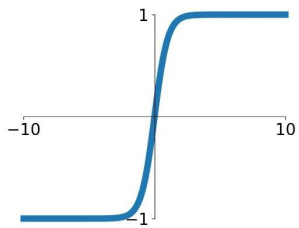
Sigmoid

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



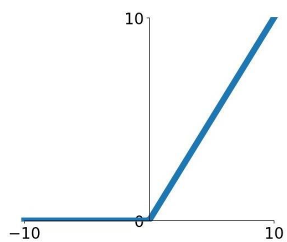
tanh

$\tanh(x)$



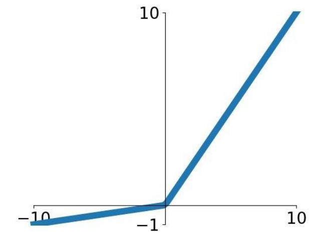
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

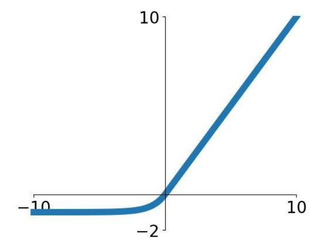


Maxout

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

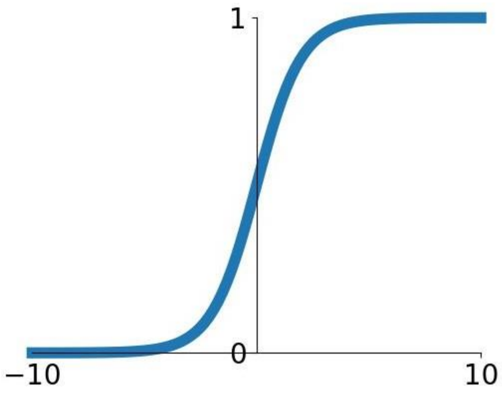
ELU

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



Activation Functions

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



Sigmoid

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

Activation Functions

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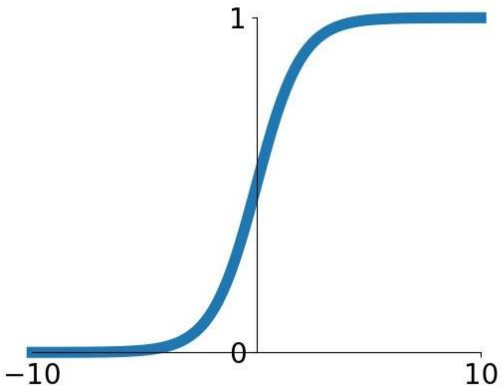

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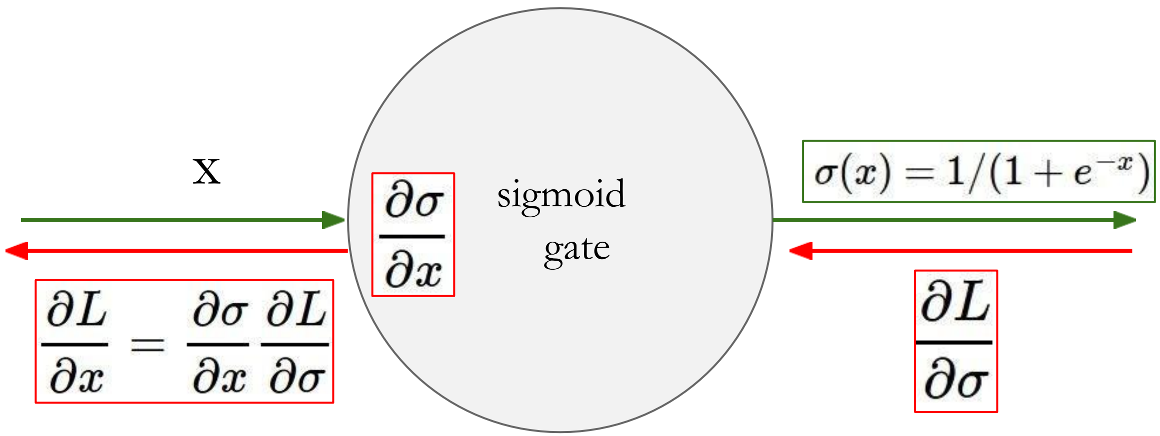
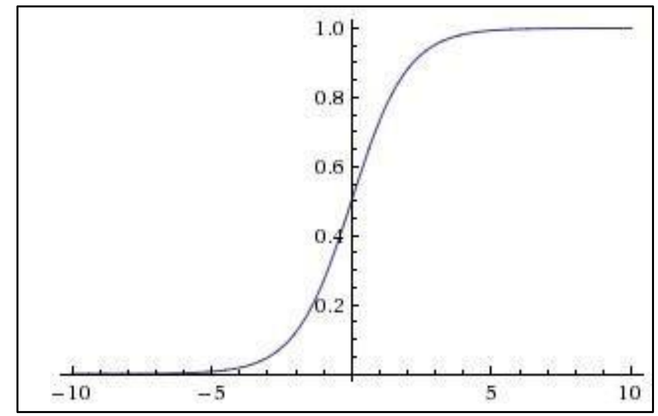
• 3 problems:

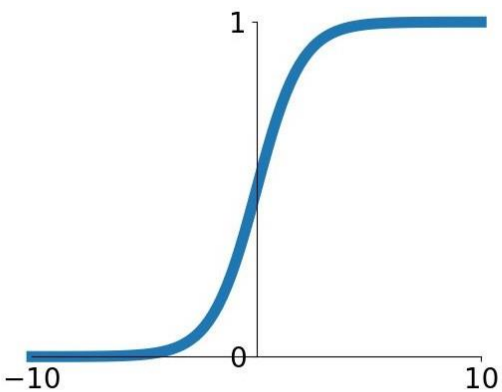
1. Saturated neurons "kill" the gradients





What happens when x = -10?
What happens when x = 0?
What happens when x = 10?

Activation Functions



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- 3 problems:

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2. Sigmoid outputs are not zero-centered

Activation Functions

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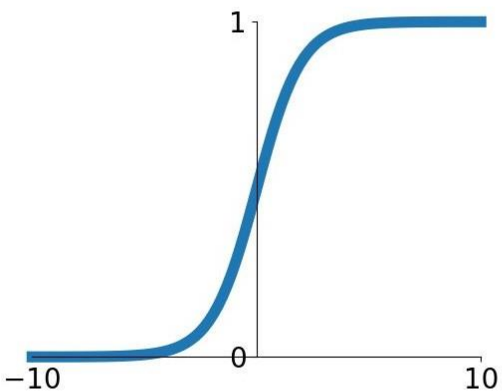


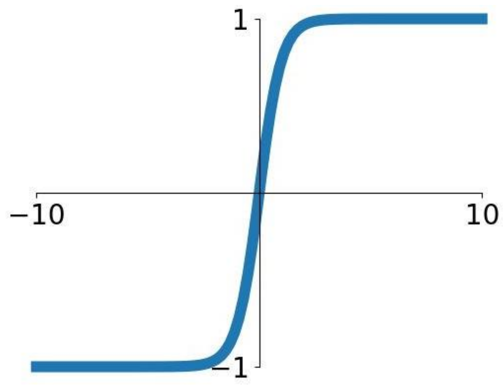
Sigmoid

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

• 3 problems:

1. Saturated neurons "kill" the gradients
2. Sigmoid outputs are not zero-centered
3. exp() is a bit compute expensive

Activation Functions

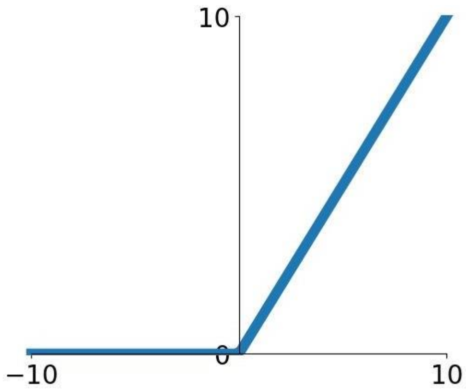


tanh(x)

- Squashes numbers to range [-1,1]
- zero centered (nice)
- still kills gradients when saturated :(

[LeCun et al., 1991]

Activation Functions



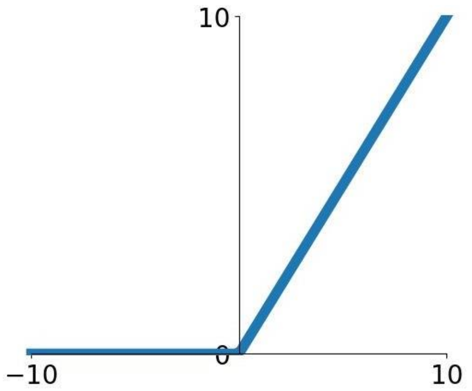
ReLU
(Rectified Linear Unit)

- Computes f(x) = max(0,x)

- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

[Krizhevsky et al., 2012]

Activation Functions



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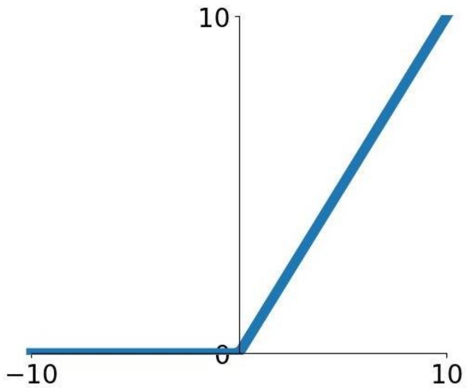
- Not zero-centered output

Activation Functions



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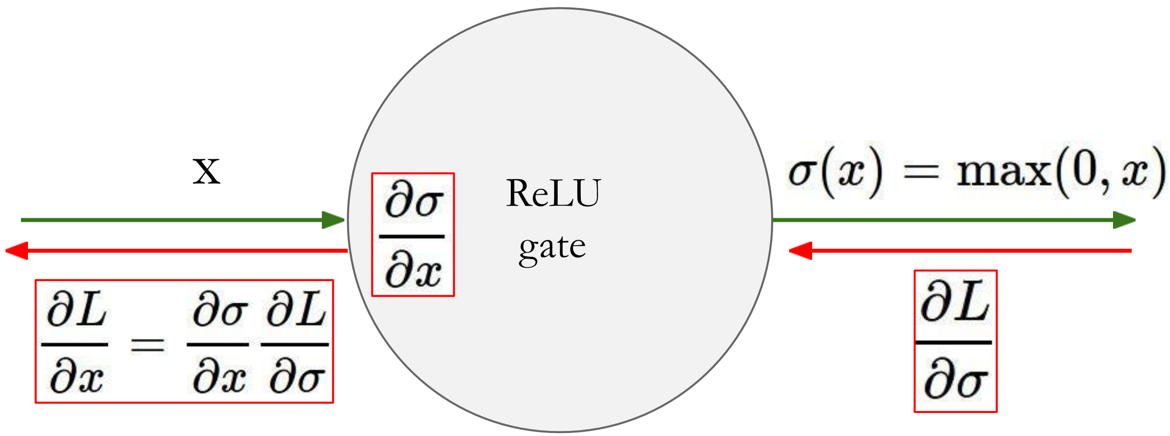
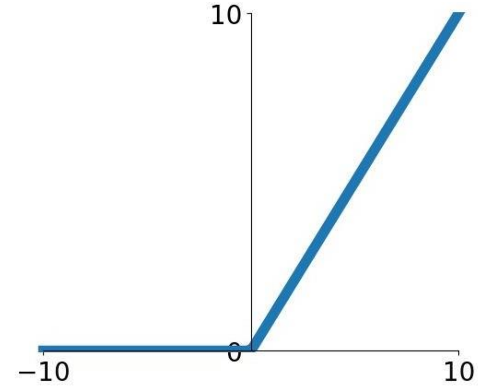
- Not zero-centered output
- An annoyance:

hint: what is the gradient when x < 0?





What happens when x = -10?
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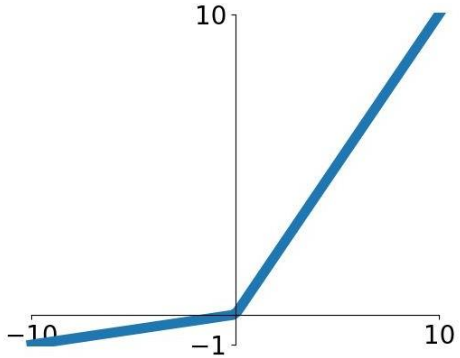
Activation Functions

[Mass et al., 2013]
[He et al., 2015]



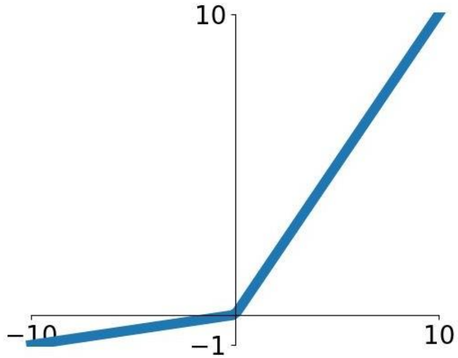
Leaky ReLU

$$f(x) = \max(0.01x, x)$$

- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

Activation Functions

[Mass et al., 2013]
[He et al., 2015]



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Leaky ReLU

$$f(x) = \max(0.01x, x)$$

Parametric Rectifier (PReLU)

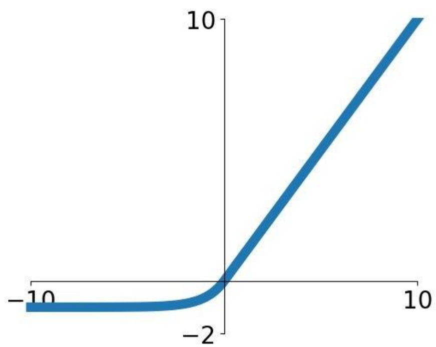
$$f(x) = \max(\alpha x, x)$$

backprop into alpha (parameter)

Activation Functions

[Clevert et al., 2015]

Exponential Linear Units (ELU)



$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\left(\exp(x) - 1\right) & \text{if } x \le 0 \end{cases}$$

- All benefits of ReLU
- Closer to zero mean outputs
- Negative saturation regime compared with Leaky ReLU adds some robustness to noise

- Computation requires exp()

[Goodfellow et al., 2013]

Maxout "Neuron"

- Does not have the basic form of dot product -> nonlinearity
- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

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

Problem: doubles the number of parameters/neuron :(

TLDR: In practice:

- Use ReLU. Be careful with your learning rates
- Try out Leaky ReLU / Maxout / ELU / PReLU
- Try out tanh but don't expect much
- Don't use sigmoid

Adapted from Fei-Fei Li, Andrej Karpathy, Justin Johnson, Serena Yeung

Batch Normalization

[Ioffe and Szegedy, 2015]

"you want zero-mean unit-variance activations? just make them so."

consider a batch of activations at some layer. To make each dimension zero-mean unit-variance, apply:

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

Batch Normalization

[Ioffe and Szegedy, 2015]

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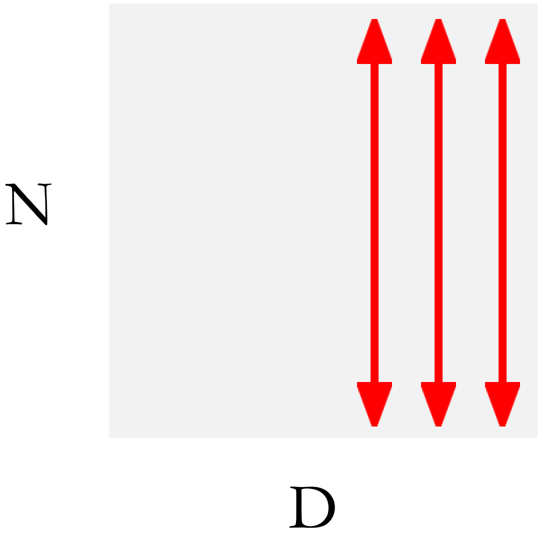

1. compute the empirical mean and variance independently for each dimension.

2. Normalize

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

Batch Normalization

[Ioffe and Szegedy, 2015]

Normalize:

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

And then allow the network to squash the range if it wants to:

$$y^{(k)} = \gamma^{(k)}\widehat{x}^{(k)} + \beta^{(k)}$$

Note, the network can learn:

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

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

to recover the identity mapping.

Batch Normalization

[Ioffe and Szegedy, 2015]

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

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

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

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

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

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

- Improves gradient flow through the network
- Allows higher learning rates
- Reduces the strong dependence on initialization
- Acts as a form of regularization

Batch Normalization

[Ioffe and Szegedy, 2015]

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

Note: at test time BatchNorm layer functions differently:

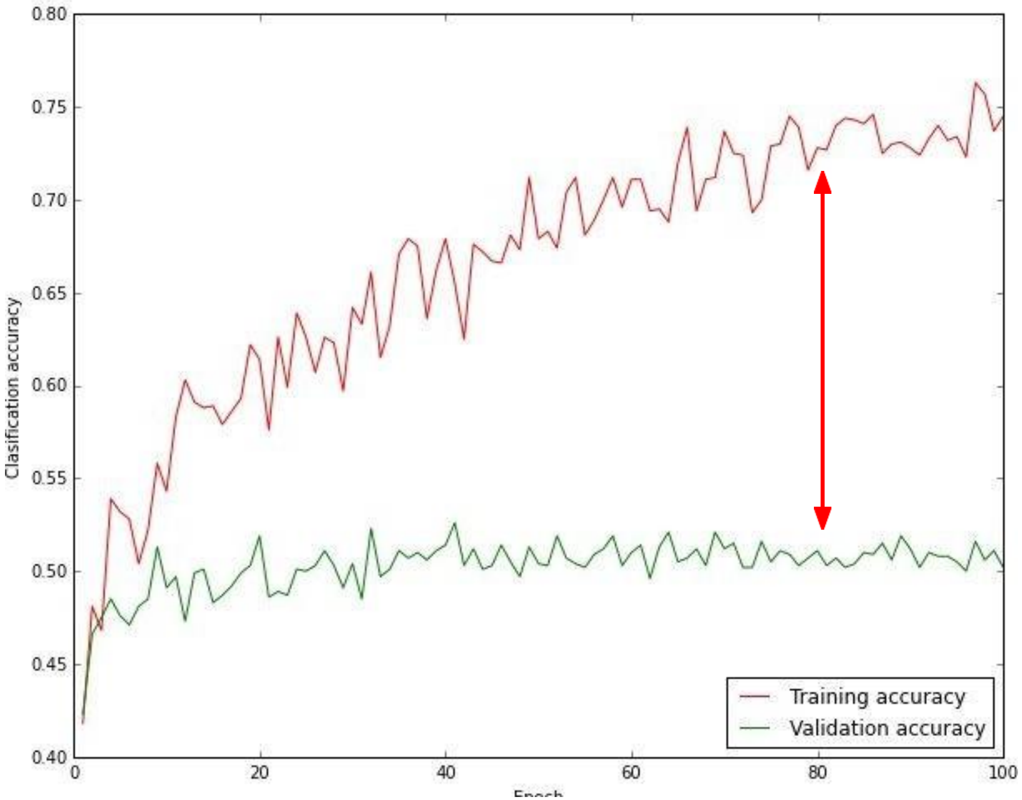
The mean/std are not computed based on the batch. Instead, a single fixed empirical mean of activations during training is used.

(e.g. can be estimated during training with running averages)

Babysitting the Learning Process

- Preprocess data
- Choose architecture
- Initialize and check initial loss with no regularization
- Increase regularization, loss should increase
- Then train – try small portion of data, check you can overfit
- Add regularization, and find learning rate that can make the loss go down
- Check learning rates in range [1e-3 … 1e-5]
- Coarse-to-fine search for hyperparameters (e.g. learning rate, regularization)

Monitor and Visualize Accuracy



big gap = overfitting
=> increase regularization strength?

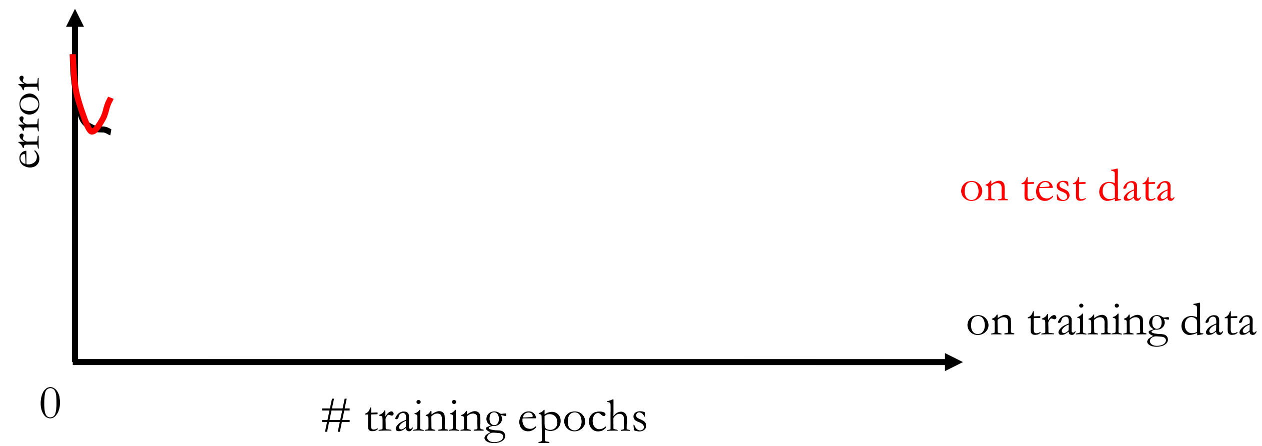
no gap
=> increase model capacity?

Dealing with sparse data

- Deep neural networks require lots of data, and can overfit easily
- The more weights you need to learn, the more data you need
- That's why with a deeper network, you need more data for training than for a shallower network
- Ways to prevent overfitting include:
    - Using a validation set to stop training or pick parameters
    - Regularization
    - Data augmentation
    - Transfer learning

Over-training prevention

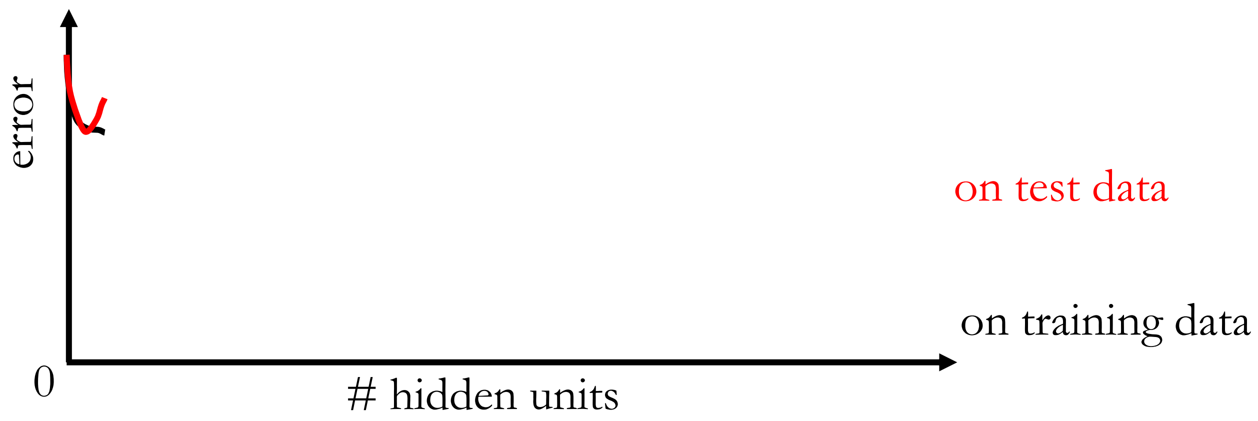
- Running too many epochs can result in over-fitting.



- Keep a hold-out validation set and test accuracy on it after every epoch. Stop training when additional epochs actually increase validation error.

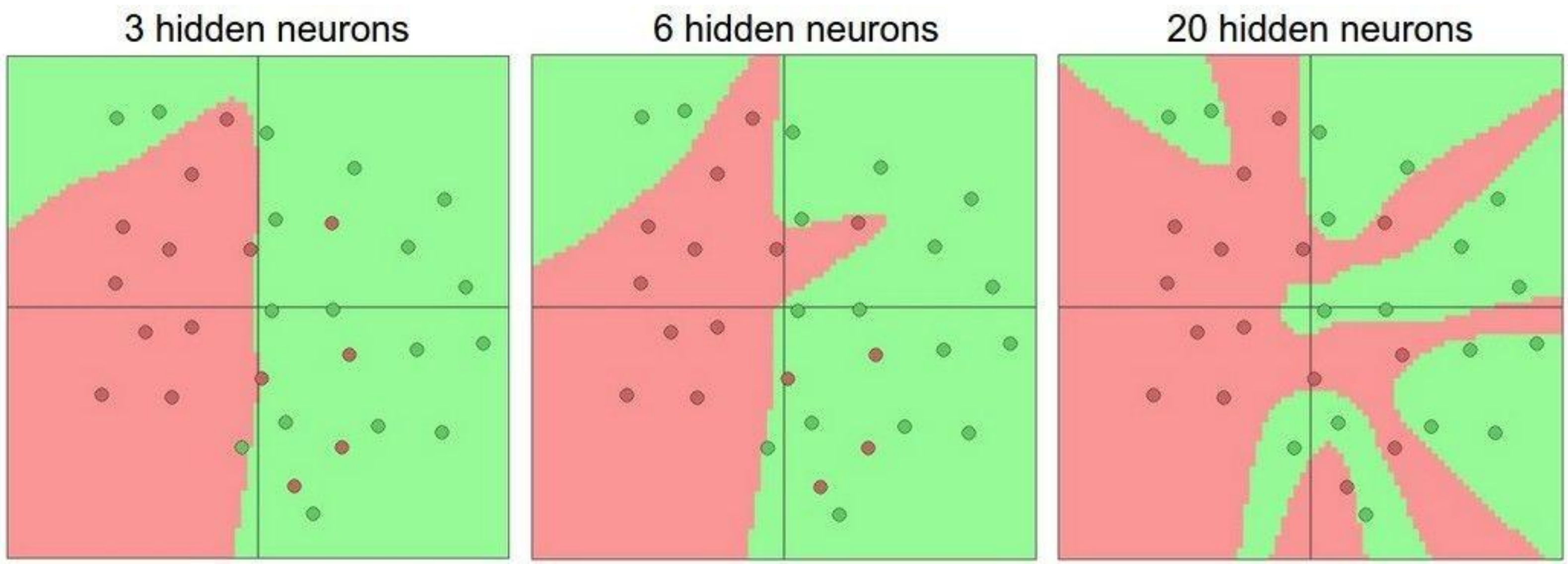
Determining best number of hidden units

- Too few hidden units prevent the network from adequately fitting the data.
- Too many hidden units can result in over-fitting.



- Use internal cross-validation to empirically determine an optimal number of hidden units.

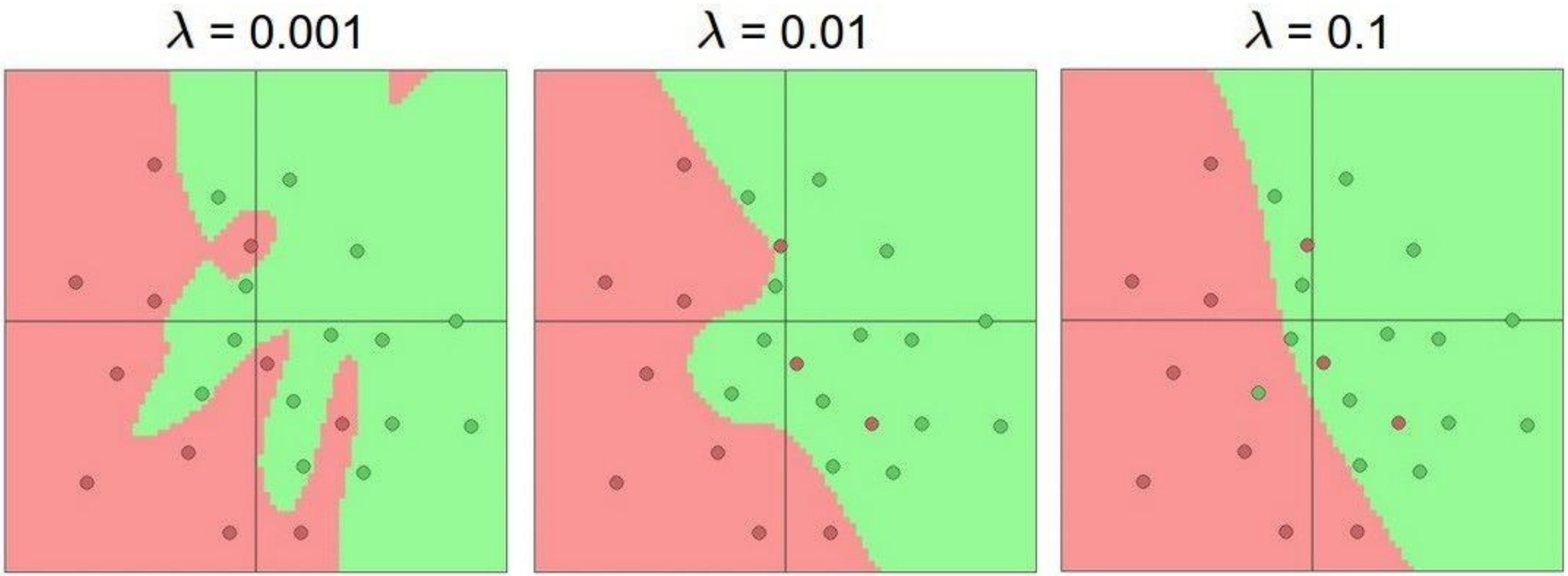
Effect of number of neurons



more neurons = more capacity

Effect of regularization

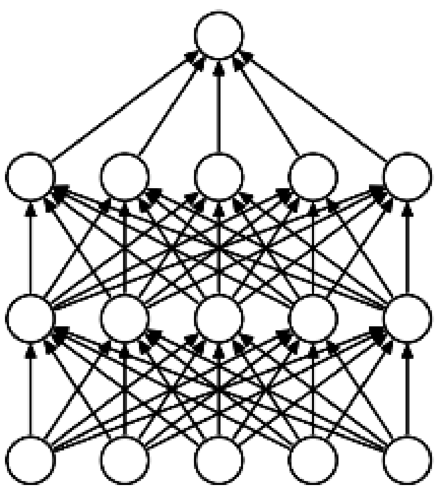
Do not use size of neural network as a regularizer. Use stronger regularization instead:



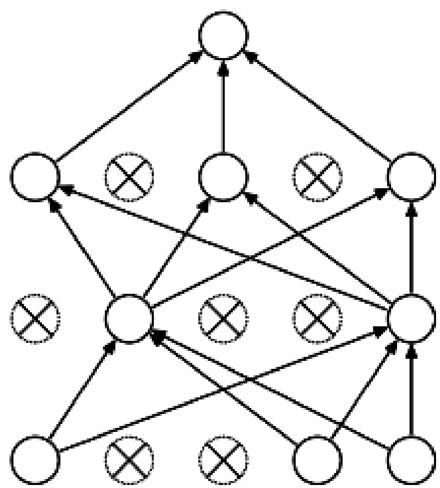
(you can play with this demo over at ConvNetJS: http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html)

Regularization

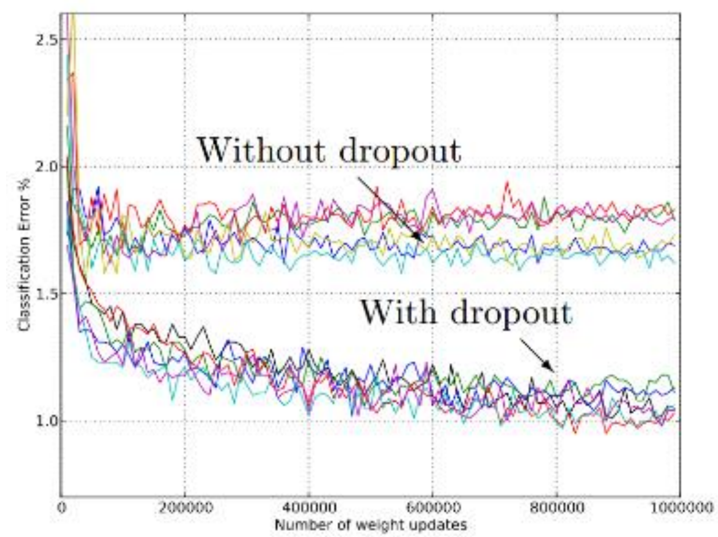
- L1, L2 regularization (*weight decay*)
- Dropout
  - Randomly turn off some neurons
  - Allows individual neurons to independently be responsible for performance



(a) Standard Neural Net



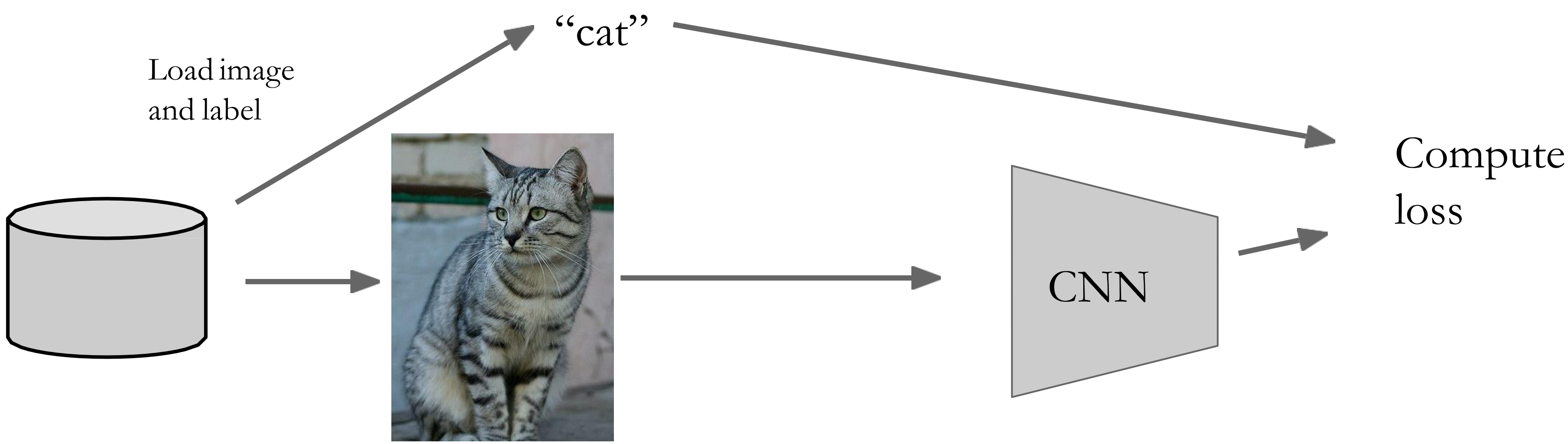
(b) After applying dropout.



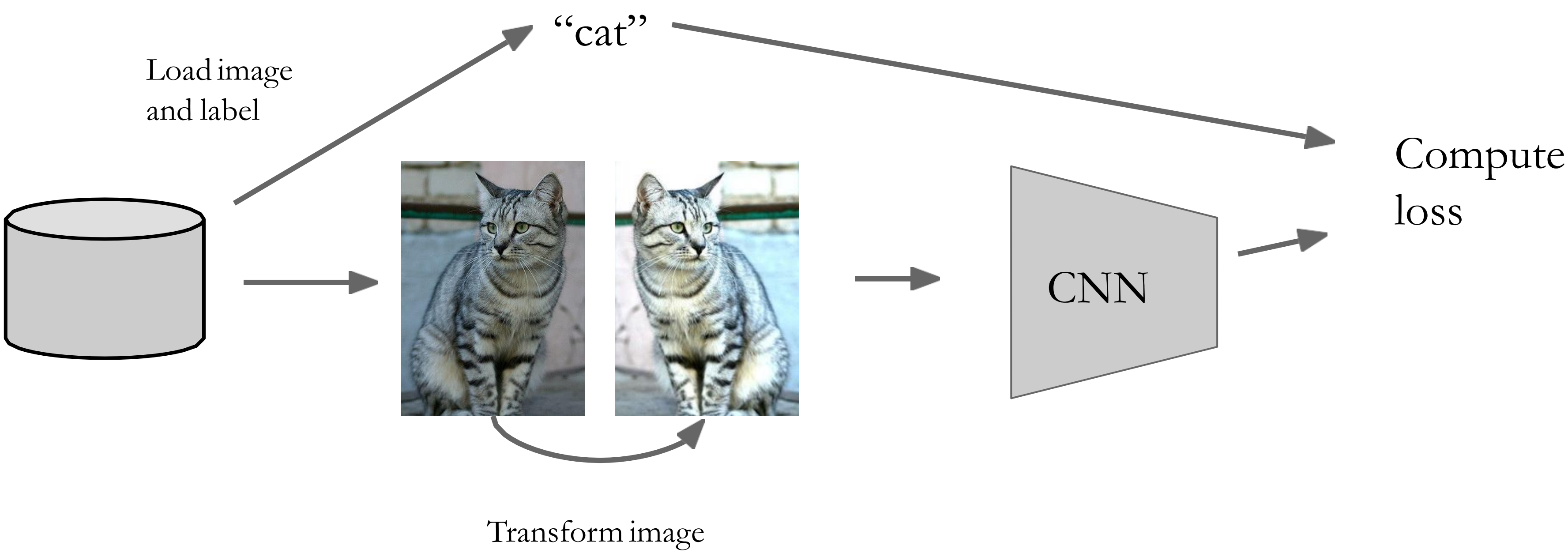
Dropout: A simple way to prevent neural networks from overfitting [Srivastava JMLR 2014]

Adapted from Jia-bin Huang

Data Augmentation

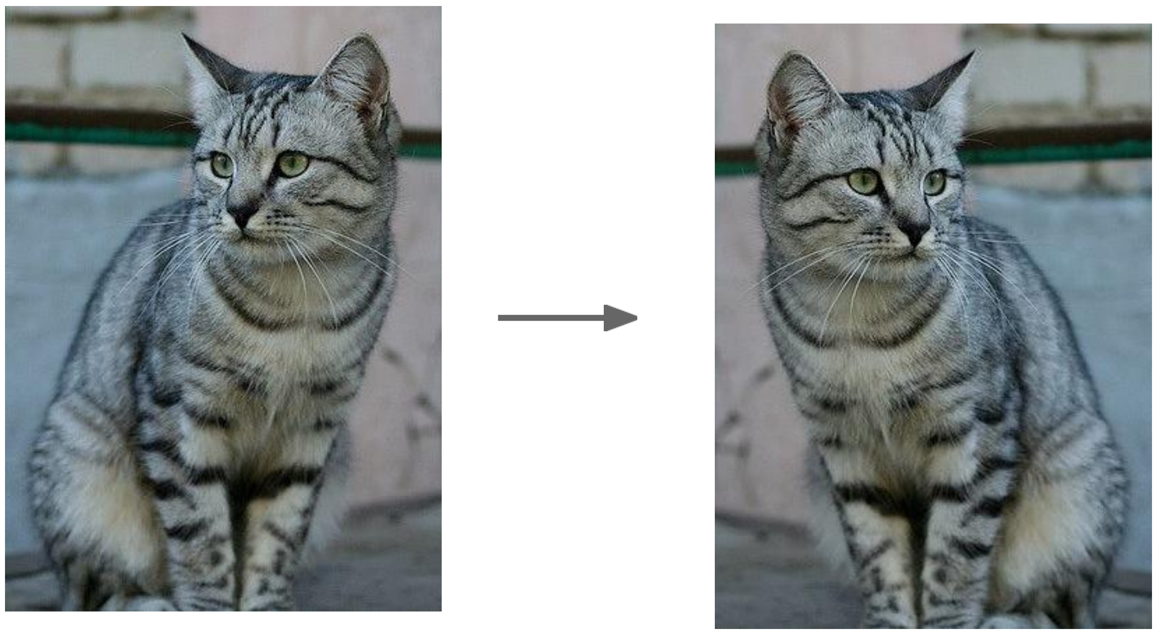


Data Augmentation



Data Augmentation

Horizontal Flips



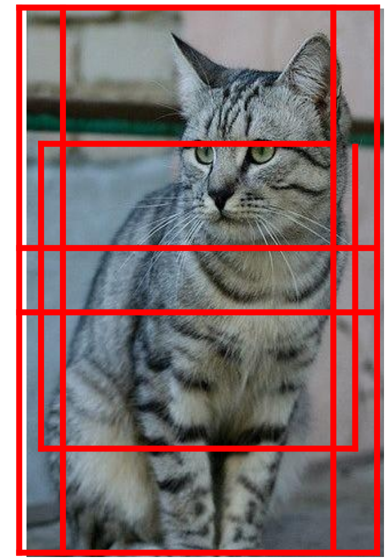
Data Augmentation

Random crops and scales

Training: sample random crops / scales

ResNet:

1. Pick random L in range [256, 480]
2. Resize training image, short side = L
3. Sample random 224 x 224 patch



Testing: average a fixed set of crops

ResNet:

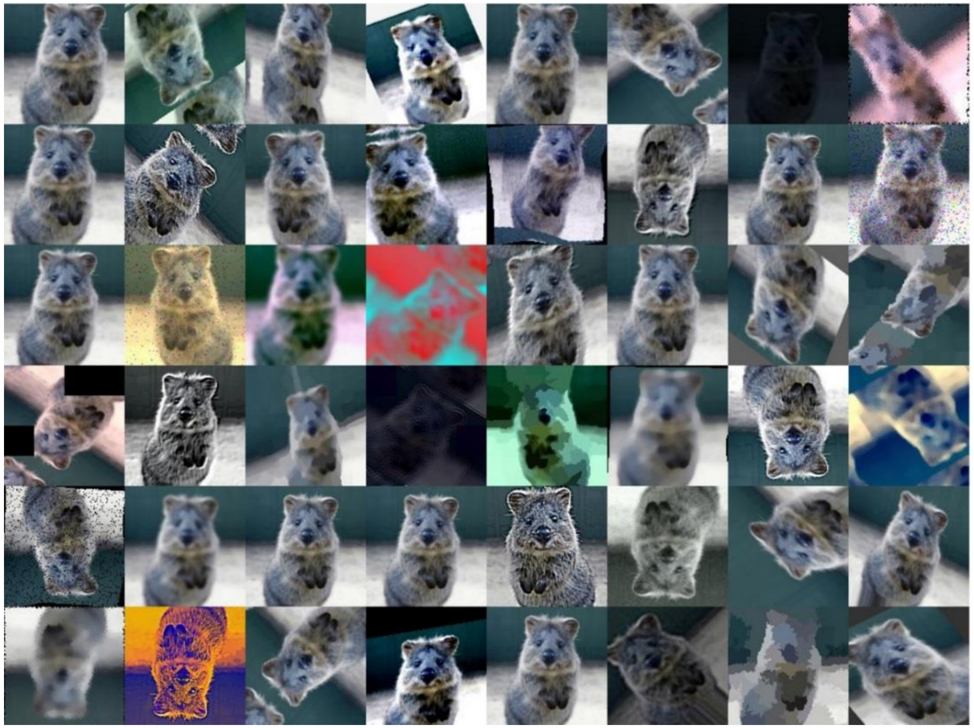
1. Resize image at 5 scales: {224, 256, 384, 480, 640}
2. For each size, use 10 224 x 224 crops: 4 corners + center, + flips

Data Augmentation

Get creative for your problem!

Random mix/combinations of :

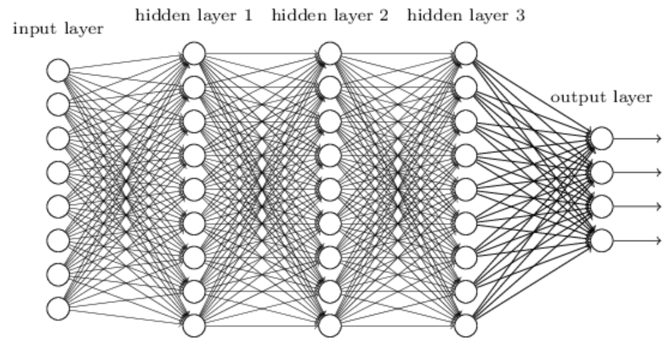
- translation
- rotation
- stretching
- shearing,
- lens distortions
- …



Fei-Fei Li, Andrej Karpathy, Justin Johnson, Serena Yeung; Image: https://github.com/aleju/imgaug

Transfer learning

- If you have sparse data in your domain of interest *(target)*, but have rich data in a disjoint yet related domain *(source)*,
- You can train the early layers on the *source* domain, and only the last few layers on the *target domain:*



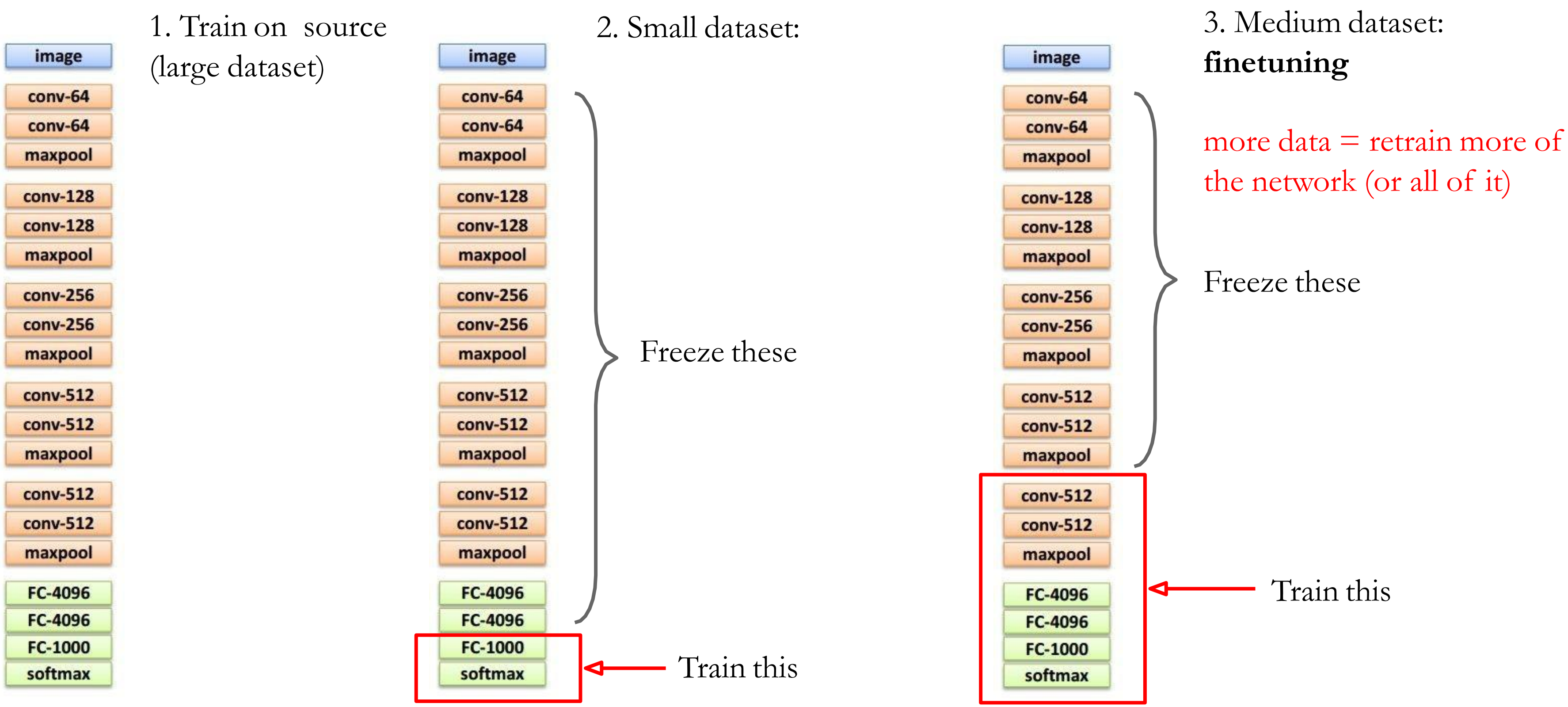
Set these to the already learned weights from another network

Learn these on your own task

Transfer learning

Source: classify 20 animal classes

Target: 10 car classes



Another option: use network as feature extractor, train SVM/LR on extracted features for target task

Adapted from Andrej Karpathy

Mini-batch gradient descent

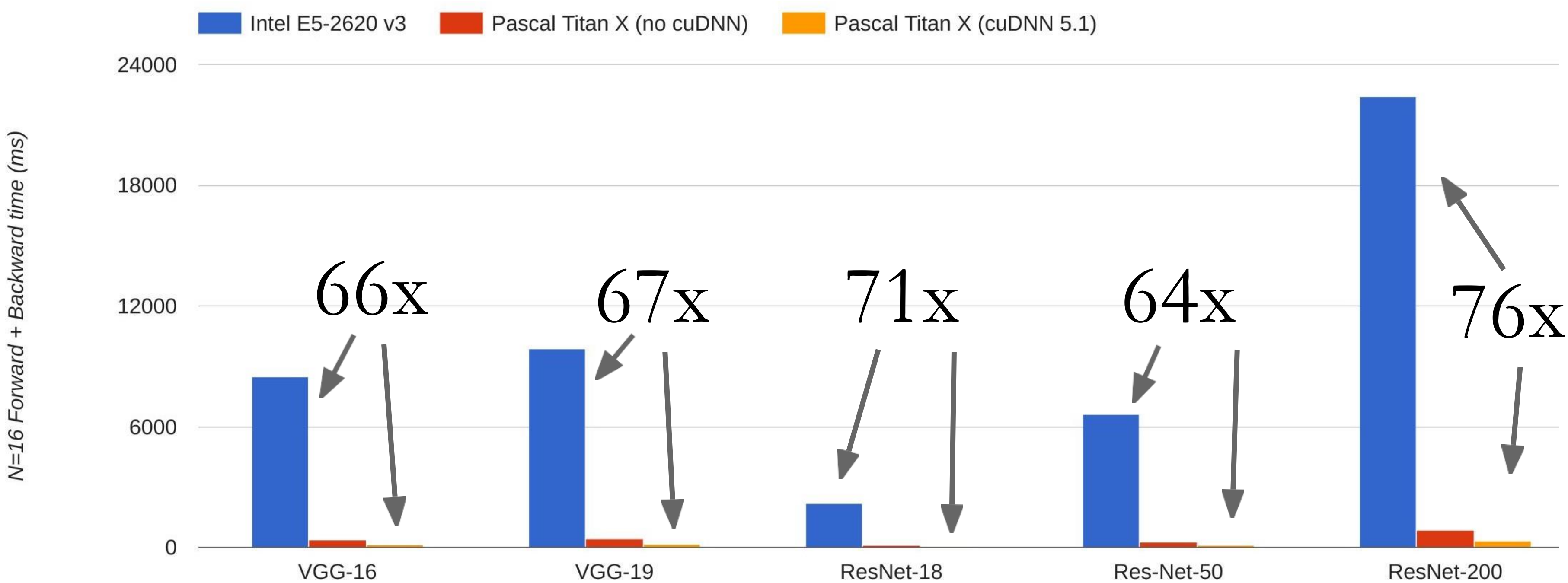
- In classic gradient descent, we compute the gradient from the loss for all training examples
- Could also only use *some* of the data for each gradient update
- We cycle through all the training examples multiple times
- Each time we've cycled through all of them once is called an 'epoch'
- Allows faster training (e.g. on GPUs), parallelization

Training: Best practices

- Center (subtract mean from) your data
- Use careful initialization for weights
- Use RELU or leaky RELU or ELU or PReLU
- Use batch normalization
- Use data augmentation
- Use regularization
- Use mini-batch
- Learning rate: too high? Too low?
- Use cross-validation for hyperparameters

CPU vs GPU in practice

(CPU performance not
well-optimized, a little unfair)



Data from https://github.com/jcjohnson/cnn-benchmarks

Software: A zoo of frameworks!

Caffe
(UC Berkeley) → Caffe2
(Facebook)

Torch
(NYU / Facebook) → PyTorch
(Facebook)

Theano
(U Montreal) → TensorFlow
(Google)

PaddlePaddle
(Baidu)

Chainer

MXNet
(Amazon)

CNTK
(Microsoft)

JAX
(Google)

And others...