CS 540 Introduction to Artificial Intelligence
Deep Learning III

University of Wisconsin-Madison

Fall 2022

Outline

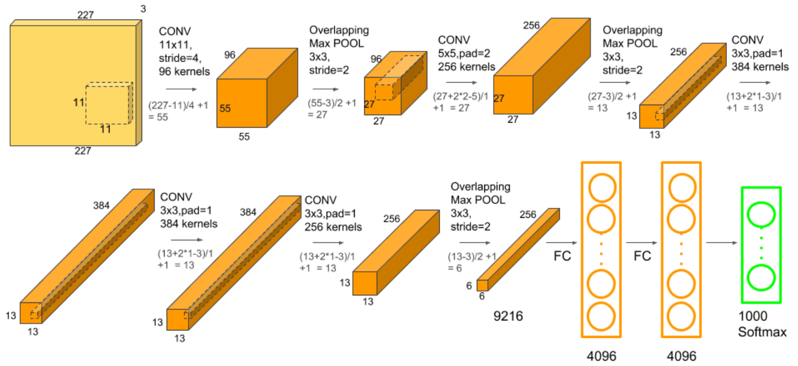
- CNNs with more layers: ResNets
  - Layer problems, residual connections, identity maps
- Data Augmentation & Regularization
  - Expanding the dataset, avoiding overfitting
- More Signal From our Data
  - Graph-structured data, graph neural networks

Last Time: CNNs

We talked about CNN components & architectures

- **Components**: convolutional layers, pooling layers (recall kernels, channels, strides, padding)
- **Architectures**: LeNet, AlexNet, VGG

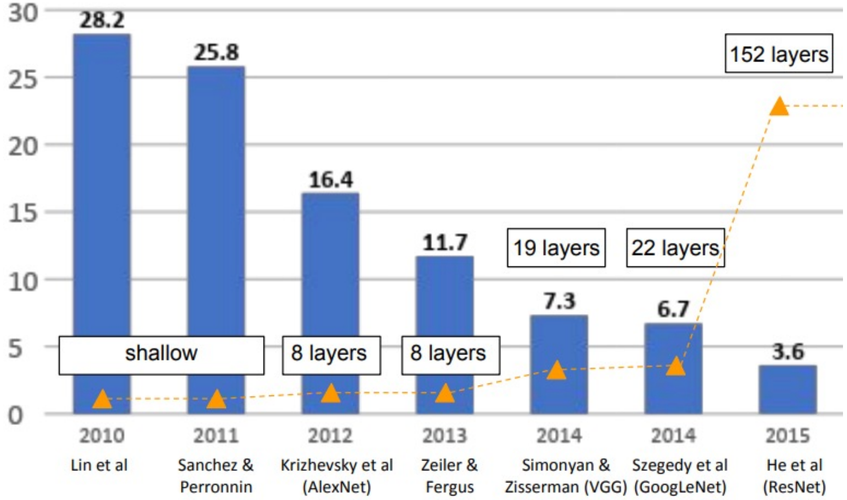
- Trend: bigger, deeper.



Credit: Mathworks

Evolution of CNNs

ImageNet competition (error rate)



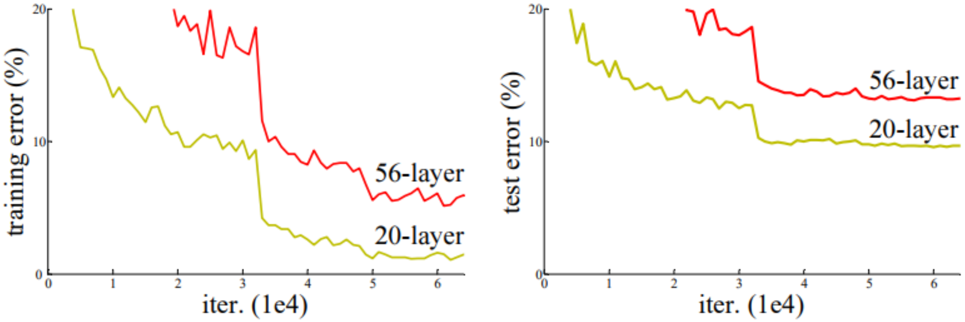
Credit: Stanford CS 231n

Simple Idea: Add More Layers

VGG: 19 layers. ResNet: 152 layers. **Add more layers**… sufficient?

- No! Some problems:
  - i) Vanishing gradients: more layers ➔ more likely
  - ii) Instability: deeper models are harder to optimize

Reflected in training error:

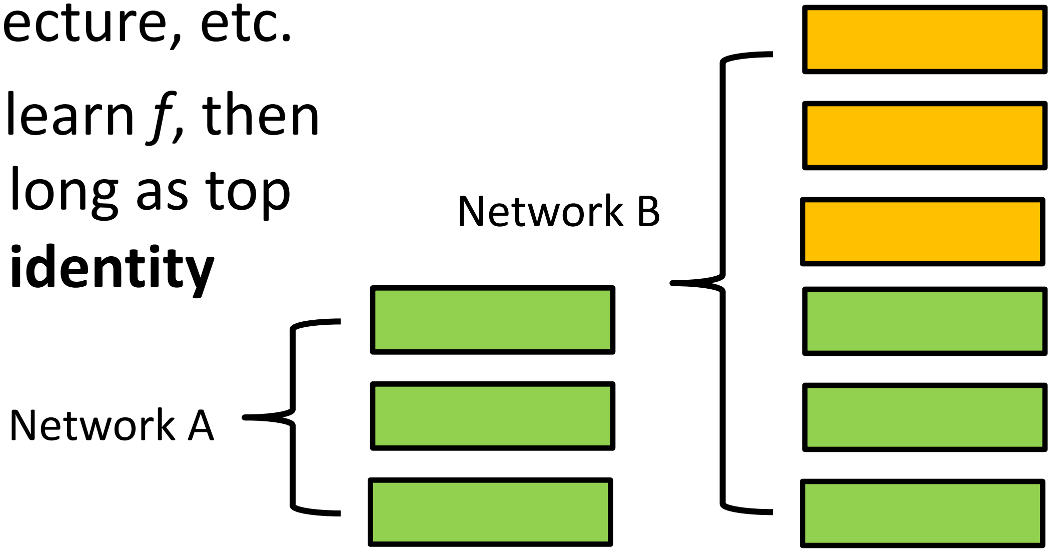


He et al: "Deep Residual Learning for Image Recognition"

Depth Issues & Learning Identity

Why would more layers result in **worse** performance?

- Same architecture, etc.
- If the A can learn *f*, then so can B, as long as top layers learn **identity**



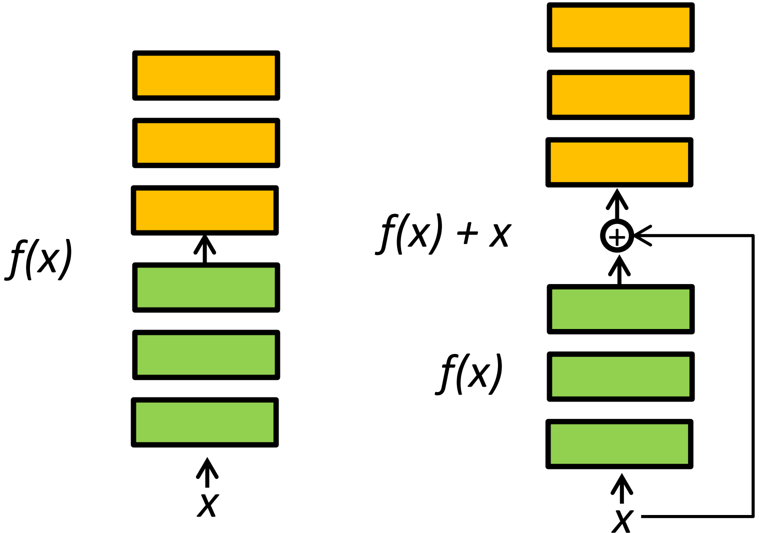
Q: can we learn identity here?

Idea: if layers can learn identity, **can't get** worse.

Residual Connections

Idea: Identity might be hard to learn, but zero is easy!

- Make all the weights tiny, produces zero for output
- Can easily transform learning identity to learning zero:



Left: Conventional layers block

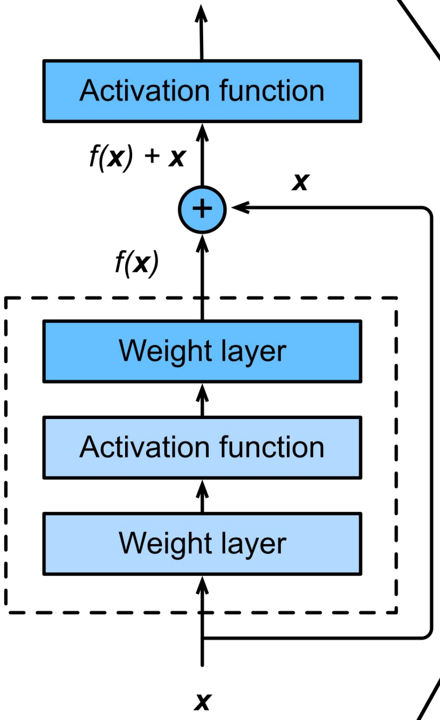
Right: **Residual** layer block

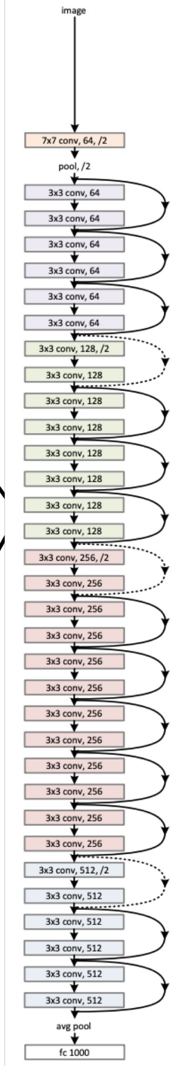
To learn identity $f(x) = x$, layers now need to learn $f(x) = 0$ ➔ easier

Full ResNet Architecture

[He et al. 2015]

- Stack residual blocks
- Every residual block has two 3x3 conv layers
- Periodically, double # of filters and downsample spatially using stride of 2 (/2 in each dimension)



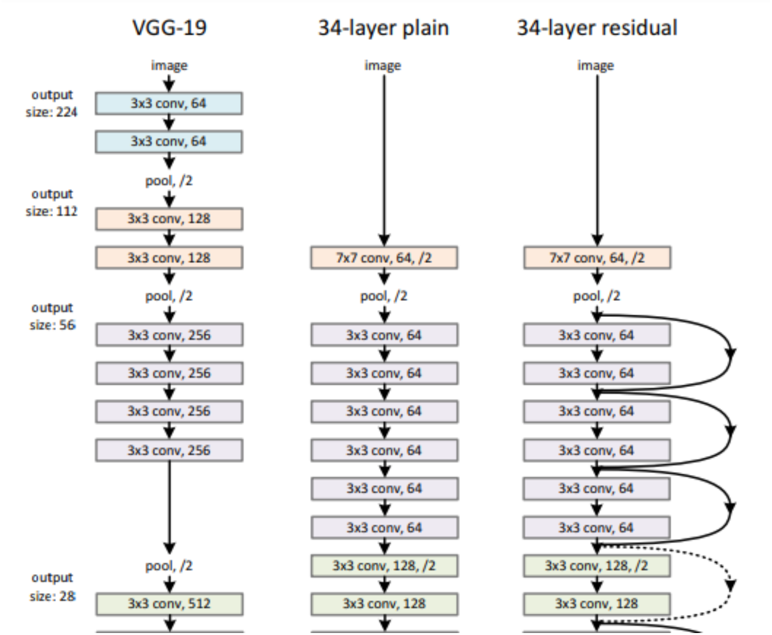


(Figure from Stanford CS231n)

ResNet Architecture

Idea: Residual (skip) connections help make learning easier

- Example architecture:
- Note: residual connections
  - Every two layers for ResNet34
- **Vastly better** performance
  - No additional parameters!
  - Records on many benchmarks



He et al: “Deep Residual Learning for Image Recognition”

ResNet Architecture

Various depth

layer name	output size	18-layer	34-layer	50-layer	101-layer	152-layer
conv1	112×112	7×7, 64, stride 2				
conv2_x	56×56	3×3 max pool, stride 2				
		$\begin{bmatrix} 3\times3, 64 \\ 3\times3, 64 \end{bmatrix}\times2$	$\begin{bmatrix} 3\times3, 64 \\ 3\times3, 64 \end{bmatrix}\times3$	$\begin{bmatrix} 1\times1, 64 \\ 3\times3, 64 \\ 1\times1, 256 \end{bmatrix}\times3$	$\begin{bmatrix} 1\times1, 64 \\ 3\times3, 64 \\ 1\times1, 256 \end{bmatrix}\times3$	$\begin{bmatrix} 1\times1, 64 \\ 3\times3, 64 \\ 1\times1, 256 \end{bmatrix}\times3$
conv3_x	28×28	$\begin{bmatrix} 3\times3, 128 \\ 3\times3, 128 \end{bmatrix}\times2$	$\begin{bmatrix} 3\times3, 128 \\ 3\times3, 128 \end{bmatrix}\times4$	$\begin{bmatrix} 1\times1, 128 \\ 3\times3, 128 \\ 1\times1, 512 \end{bmatrix}\times4$	$\begin{bmatrix} 1\times1, 128 \\ 3\times3, 128 \\ 1\times1, 512 \end{bmatrix}\times4$	$\begin{bmatrix} 1\times1, 128 \\ 3\times3, 128 \\ 1\times1, 512 \end{bmatrix}\times8$
conv4_x	14×14	$\begin{bmatrix} 3\times3, 256 \\ 3\times3, 256 \end{bmatrix}\times2$	$\begin{bmatrix} 3\times3, 256 \\ 3\times3, 256 \end{bmatrix}\times6$	$\begin{bmatrix} 1\times1, 256 \\ 3\times3, 256 \\ 1\times1, 1024 \end{bmatrix}\times6$	$\begin{bmatrix} 1\times1, 256 \\ 3\times3, 256 \\ 1\times1, 1024 \end{bmatrix}\times23$	$\begin{bmatrix} 1\times1, 256 \\ 3\times3, 256 \\ 1\times1, 1024 \end{bmatrix}\times36$
conv5_x	7×7	$\begin{bmatrix} 3\times3, 512 \\ 3\times3, 512 \end{bmatrix}\times2$	$\begin{bmatrix} 3\times3, 512 \\ 3\times3, 512 \end{bmatrix}\times3$	$\begin{bmatrix} 1\times1, 512 \\ 3\times3, 512 \\ 1\times1, 2048 \end{bmatrix}\times3$	$\begin{bmatrix} 1\times1, 512 \\ 3\times3, 512 \\ 1\times1, 2048 \end{bmatrix}\times3$	$\begin{bmatrix} 1\times1, 512 \\ 3\times3, 512 \\ 1\times1, 2048 \end{bmatrix}\times3$
	1×1	average pool, 1000-d fc, softmax				
FLOPs		1.8×10^9	3.6×10^9	3.8×10^9	7.6×10^9	11.3×10^9

Table 1. Architectures for ImageNet. Building blocks are shown in brackets (see also Fig. 5), with the numbers of blocks stacked. Down-sampling is performed by conv3_1, conv4_1, and conv5_1 with a stride of 2.

ResNet Architecture

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ResNet Architecture

Various depth

Repeat x3 times

# of filters

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ResNet Architecture

Various depth

1+ 2x3 + 2x4 + 2x6 + 2x3 +1 = 34

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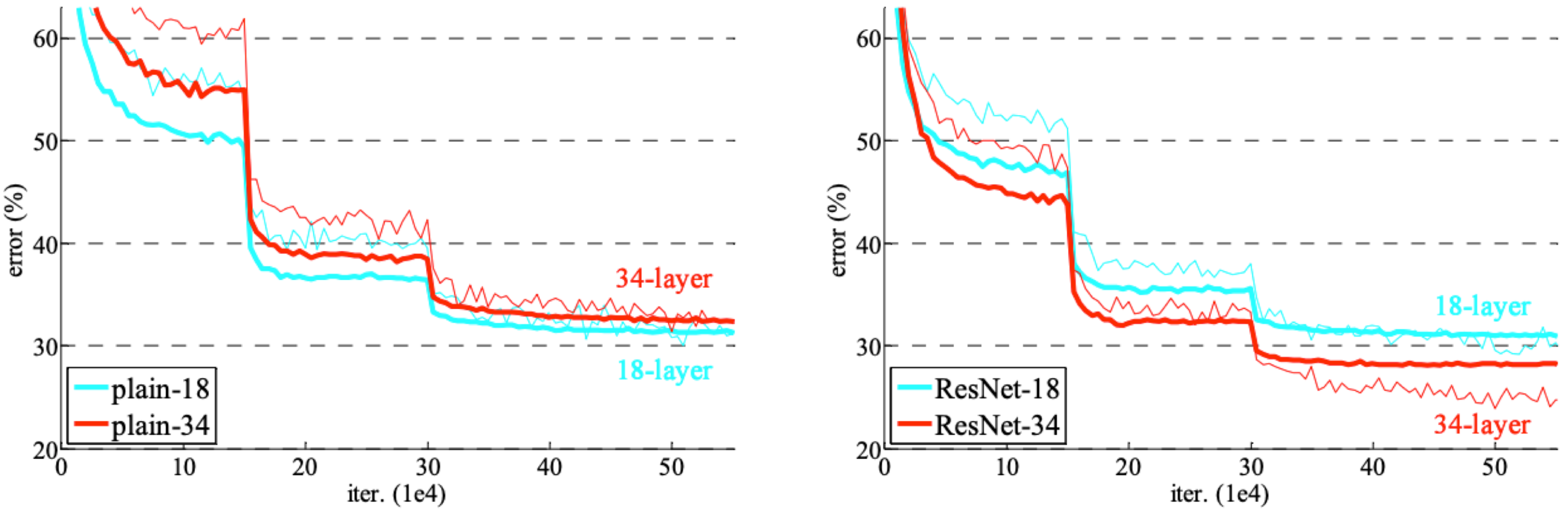
ResNet Training Curves on ImageNet

[He et al., 2015]



A Bit More on ResNets

Idea: Residual (skip) connections help make learning easier

- Note: Can also analyze from **backpropagation** p.o.v
  - Residual connections add paths to computation graph
- Also uses **batch normalization**
  - Normalize the features at each layer to have same mean/variance
  - Common deep learning trick
- Highway networks: learn weights for residual connections

Ioffe and Szegedy: "Batch Normalization: Accelerating Deep Network Training b y Reducing Internal Covariate Shift"

Break & Quiz

Q 1.1: Which of the following is **not** true?

- A. Adding more layers can improve the performance of a neural network.
- B. Residual connections help deal with vanishing gradients.
- C. CNN architectures use no more than ~20 layers to avoid problems such as vanishing gradients.
- D. It is usually easier to learn a zero mapping than the identity mapping.

Break & Quiz

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- B. Residual connections help deal with vanishing gradients.
- **C. CNN architectures use no more than ~20 layers to avoid problems such as vanishing gradients.**
- D. It is usually easier to learn a zero mapping than the identity mapping.

Break & Quiz

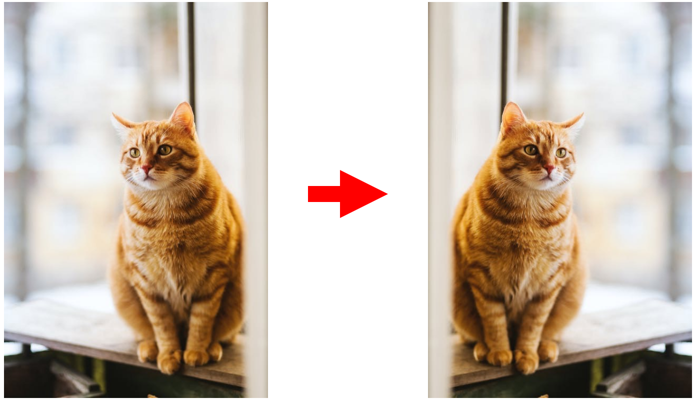
Q 1.1: Which of the following is **not** true?

- A. Adding more layers can improve the performance of a neural network. (Yes, as long as we're careful, e.g., ResNets.)
- B. Residual connections help deal with vanishing gradients. (Yes, this is an explicit consideration for residual connections.)
- **C. CNN architectures use no more than ~20 layers to avoid problems such as vanishing gradients.** (No, much deeper networks.)
- D. It is usually easier to learn a zero mapping than the identity mapping. (Yes: simple way to learn zero is to make weights zero)

Data Concerns

What if we don't have a lot of data?

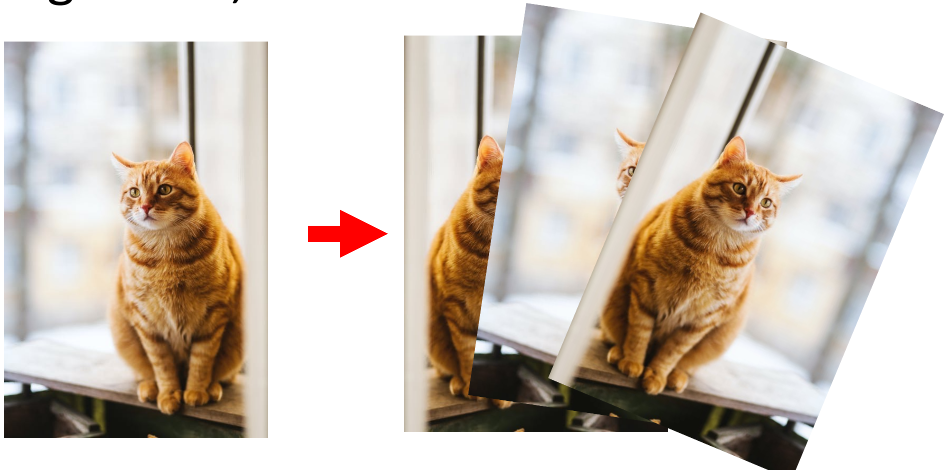
- We risk overfitting
- Avoiding overfitting: **regularization** methods
- Data augmentation: a classic way to regularize



Data Augmentation

Augmentation: transform + add new samples to dataset

- Transformations: based on domain
- Idea: build **invariances** into the model
  - **Ex**: if all images have same alignment, model learns to use it
- Keep the label the same!



Transformations

Examples of transformations for images

- **Crop** (and zoom)
- **Color** (change contrast/brightness)
- **Rotations+** (translate, stretch, shear, etc)

Many more possibilities. Combine as well!

Q: how to deal with this at **test time**?

- A: transform, test, average

Combining & Automating Transformations

One way to automate the process:

- Apply every transformation and combinations
- **Downside:** most don’t help…

Want a good policy, ie, → → → → →

- Active area of research: search for good policies

1. **Ratner et al**: “Learning to Compose Domain-Specific Transformations for Data Augmentation”
2. **Cubuk et al**: “AutoAugment: Learning Augmentation Strategies from Data”

Other Domains

Not just for image data. For example, on text:

- Substitution
  - E.g., “It is a **great** day” → “It is a **wonderful** day”
  - Use a thesaurus for particular words
  - Or, use a model. Pre-trained word embeddings, language models
- Back-translation
  - “Given the low budget and production limitations, this movie is very good.” → “There are few budget items and production limitations to make this film a really good one”

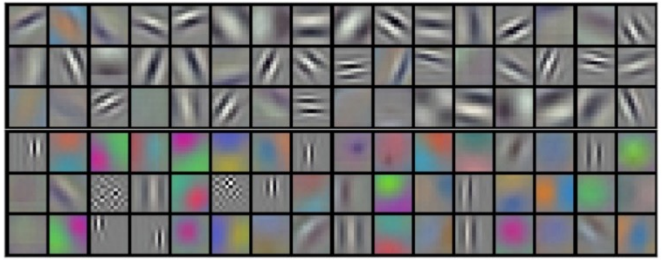
Xie **et al**: “Unsupervised Data Augmentation for Consistency Training”

Importance of Augmentation

Data augmentation is critical for top performance!

- You should use it!
- **AlexNet**: used (many papers re-used as well)
  - Random crops, rotations, flips.

Krizhevsky et al: “ImageNet Classification with Deep Convolutional Neural Networks”



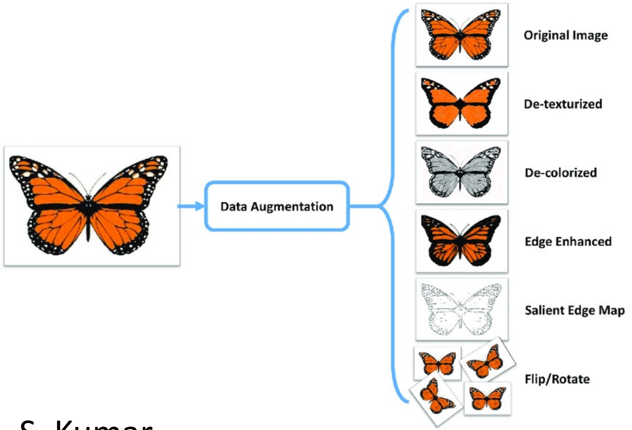
Other Forms of Regularization

Regularization has many interpretations

- **Goodfellow**: “any modification… to a learning algorithm that is intended to reduce its generalization error but not its training error.”

- A way of adding knowledge / side informatio

- Enforcing parsimony/simplicity



S. Kumar

Other Forms of Regularization

Classic regularizations

1. Modify loss functions

   Ex: regularized least squares LR

$$\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} (\theta_0 + x_i^T \theta - y_i)^2 + \lambda \|\theta\|_2^2$$

Regularizer

$$\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \ell(f_\theta(x_i), y_i) + \lambda R(f_\theta)$$

Standard loss

Regularization parameter

2. Modify architecture/training/data

   a) Dropout, batch normalization, augmentation

Break & Quiz

Q 2.1: If we apply data augmentation blindly, we might

(i) Change the label of the data point

(ii) Produce a useless training point

- A. (i) but not (ii)
- B. (ii) but not (i)
- C. Neither
- D. Both

Break & Quiz

Q 2.1: If we apply data augmentation blindly, we might

(i) Change the label of the data point

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Break & Quiz

Q 2.1: If we apply data augmentation blindly, we might

(i) Change the label of the data point

(ii) Produce a useless training point

- A. (i) but not (ii) (Can do (ii): imagine turning up the contrast till the image is completely black and is unusable).
- B. (ii) but not (i) (Can change label: rotate a 6 into a 9).
- C. Neither (Can do either).
- **D. Both**

Break & Quiz

Q 2.2: What are some consequences of data augmentation?

(i) We have to store a much bigger dataset in memory

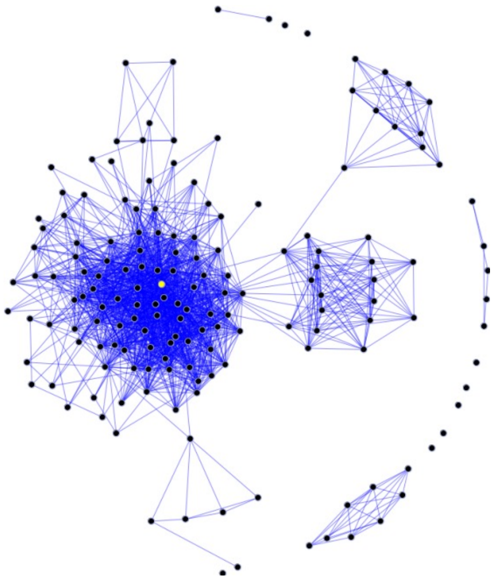
(ii) For a fixed batch size, there will be more batches per epoch

- A. (i) but not (ii)
- B. (ii) but not (i)
- C. Neither
- D. Both

Relationships in Data

So far, all of our data consists of points

- Assume all are independent, "unrelated" in a sense $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$
- Pretty common to have relationships between points
  - **Social networks**: individuals related by friendship
  - **Biology/chemistry**: bonds between compounds, molecules
  - **Citation networks**: Scientific papers cite each other

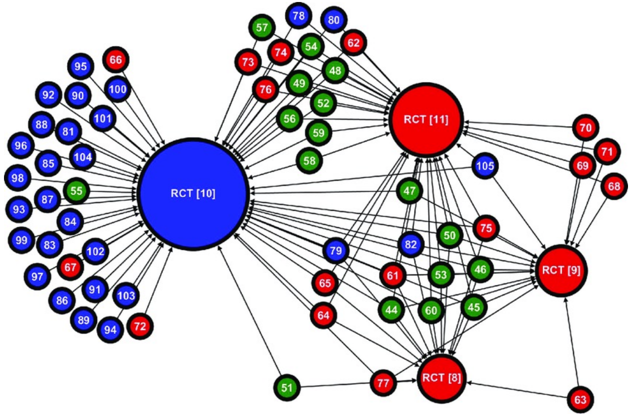


Wiki

Signal from Relationships

Suppose we are classifying scientific papers

- **Features**: title, abstract, authors. **Labels**: math/science/eng.
- Could build a reasonable classifier with the above data
- **More signal** from relationships
  - Cite each other, more likely from the same field
  - Note: citations are not features; they're **links**
  - Need a new type of network to handle



Leng

Graph Neural Networks

Have: $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n), G = (V, E)$

How should our new architecture look?

- Still want layers
  - linear transformation + non-linearity

Parameters

Non-Linearity

Hidden Layer Representation

$$H^{(\ell+1)} = \sigma(H^{(\ell)} W^{(\ell)})$$

- Now want to integrate neighbors
- Bottom: graph convolutional network

$$H^{(\ell+1)} = \sigma(A_G H^{(\ell)} W^{(\ell)})$$

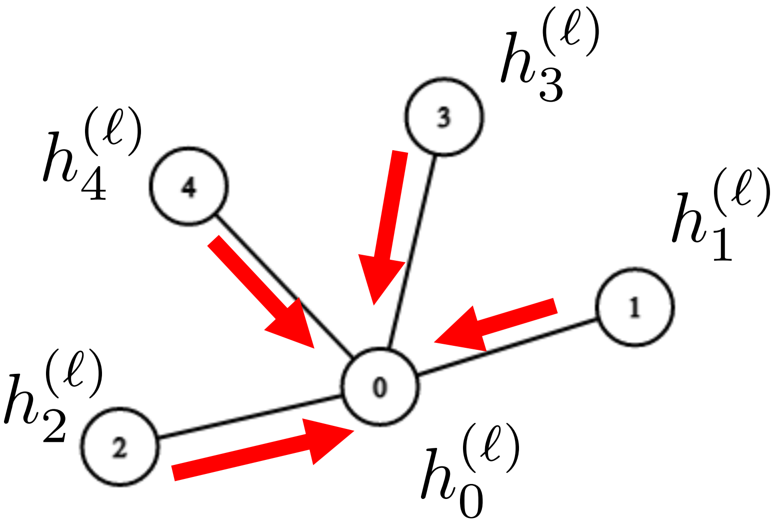
Kipf and Welling: "Semi-Supervised Classification with Graph Convolutional Networks"

Graph Mixing

Graph Convolutional Networks

Let's examine the GCN architecture in more detail

- Difference: "graph mixing" component
- At each layer, get representation at each node
- Combine node's representation with neighboring nodes
- "**Aggregate**" and "**Update**" rules

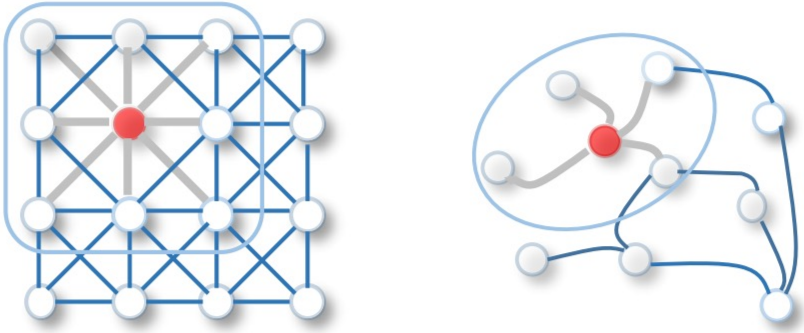


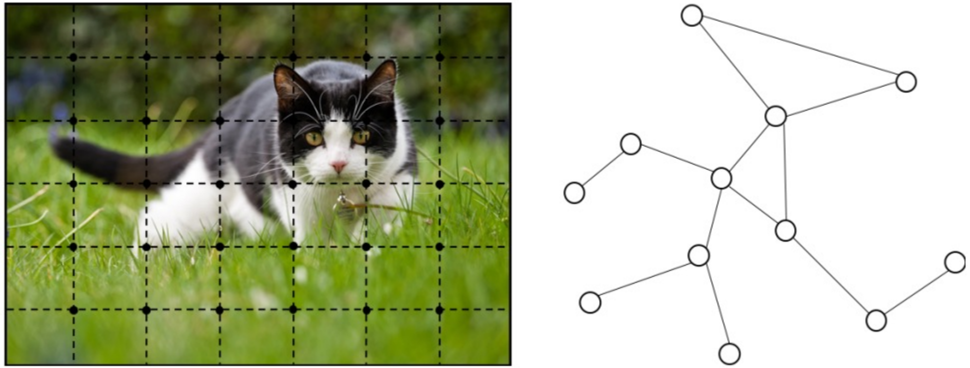
Graph Convolutional Networks

Note the resemblance to CNNs:

- Pixels: arranged as a very regular graph
- Want: more general configurations (less regular)

Wu et al, A Comprehensive Survey on Graph Neural Networks





Zhou et al, Graph Neural Networks: A Review of Methods and Applications

Summary

- Intro to deeper networks (resnets)
  - Dealing with problems by adding skip connections
- Intro to regularization
  - Data augmentation + other regularizers
- Basic graph neural networks

Acknowledgements: Inspired by materials by Fei-Fei Li, Ranjay Krishna, Danfei Xu (Stanford CS231n)