Neural Networks II: Deep Learning

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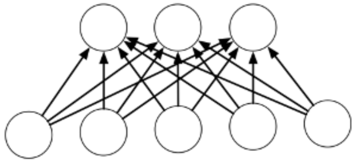
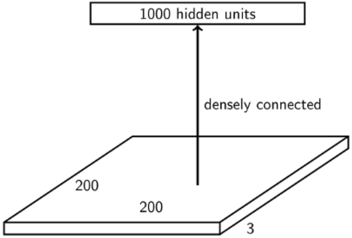
Nov 28, 2023

Fully connected vs. locally connected

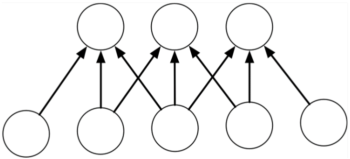
- So far we apply a layer where all output neurons are connected to all input neurons.
- In matrix form, $z = Wx$.
- This is also called a fully connected layer or a dense layer or a linear layer.
- For 200×200 image and 1000 hidden units, the matrix of a single layer will have 40M parameters!

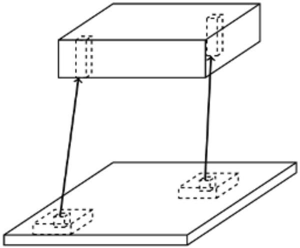




Fully connected vs. locally connected

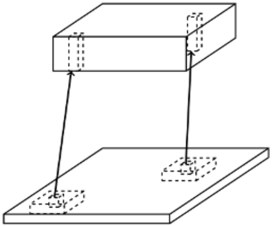
- An alternative strategy is to use local connection.
- For neuron i, only connects to its neighborhood (e.g. [i+k, i-k])
- For images, we index neurons with three dimensions i, j, and c.
- i = vertical index, j = horizontal index, c = channel index.





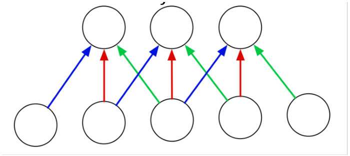
Local connection patterns

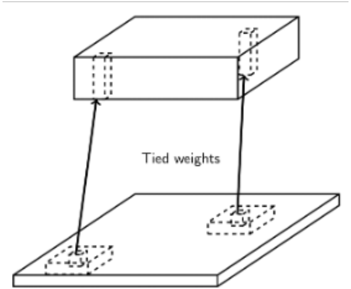
- The typical image input layer has 3 channels R G B for color or 1 channel for grayscale.
- The hidden layers may have C channels, at each spatial location (i, j).
- Now each hidden neuron $z_{i,j,c}$ receives inputs from $x_{i \pm k, j \pm k, \cdot}$
- k is the "kernel" size - do not confuse with the other kernel we learned.
- $z_{i,j,c} = \sum_{i' \in [i \pm k], j' \in [j \pm k], c'} x_{i'j'c'} w_{i,j,i'-i,j'-j,c',c}$
- The spatial awareness (receptive field) of the neighborhood grows bigger as we go deeper.



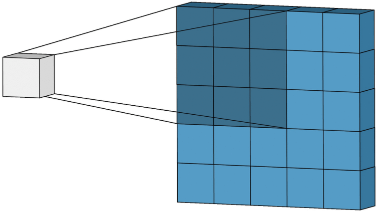
Weight sharing

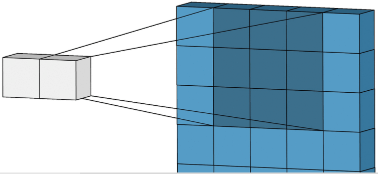
- Still a lot of weights: If we have 100 channels in the second layer, then $200 \times 200 \times 3 \times 100 = 12M$
- Local information is the same regardless of the position of an element.
- Solution: We can tie the weights at different locations.



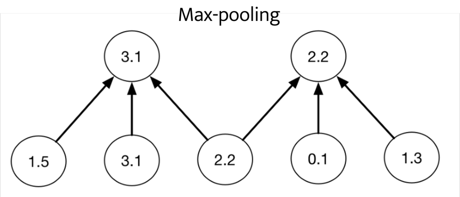


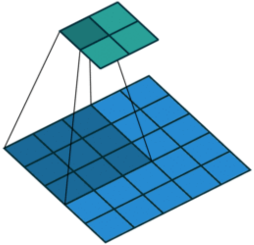
2D convolution





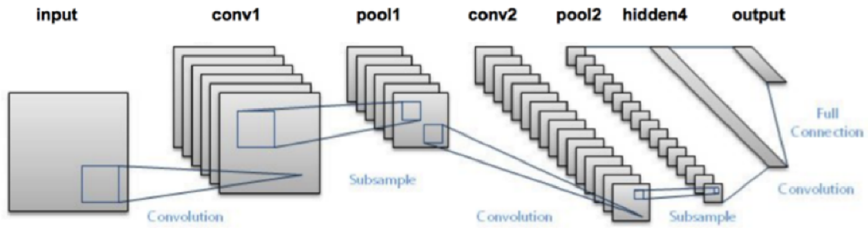
Pooling





- Need to summarize global information more efficiently

Assembling together: LeNet



- Used by USPS to read post code in the 90s.

Historical development

- LeNet has worked and being put to practice in the 1990s.
- Neural networks for images start to dominate in the last 10 years (starting 2012) for understanding general high resolution natural images.
- During the years:
  - Neural networks were difficult to work
  - People focused on feature engineering
  - Then apply SVM or random forest (e.g. AdaBoost face detector)
  - What has changed?

Gradient learning conditioning

Optimization challenges

- Larger images require deeper networks (more stages of processing at different resolutions)
- Optimizing deeper layers of networks is not trivial.
- Loss often stalls or blows up.
- Why?
  - Backpropagation: multiplying the Jacobian $\frac{\partial y}{\partial x}$ by each layer.
  - If the maximum singular value of each layer of Jacobian is less than 1: then the gradient will converge to 0 with more layers.
  - If the greater than 1: then the gradient will explode with more layers.
  - The bottom (input) layer may get 0 or infinite gradients.

Weight initialization

- Even with a few layers (>3), optimization is still hard.
- If weight initialization is bad (too small or too big), then optimization is hard to kick off.
- Consider the distribution of whole dataset in the activation space.
    - Intuition: upon initialization, the variance of the activations should stay the same across every layer.

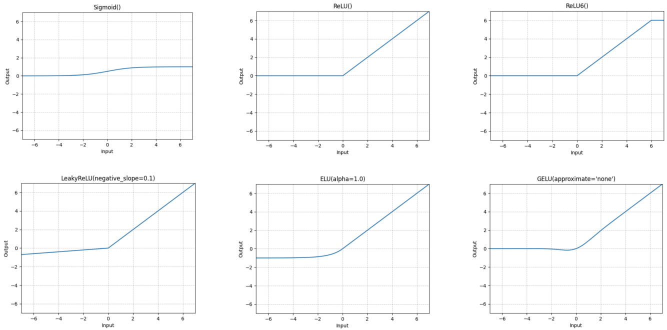
Kaiming Initialization

- Suppose each neuron and weight connection are sampling from a random distribution.
- At l-th layer, $Var[z_l] = n_l Var[w_l x_l]$ ($n_l =$ num. input neurons to l-th layer)
- If we suppose that ReLU is used as the activation, and w_l is symmetric and zero-mean, $x_{l+1} = \frac{1}{2} Var[z_l]$.
- Putting altogether, $x_{l+1} = \frac{1}{2} n_l Var[w_l] Var[x_l]$.
- To make the variance constant, we need $\frac{1}{2} n_l Var[w_l] = 1$, $Std[w_l] = \sqrt{2/n_l}$[1].

[1] He et al. Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet. ICCV, 2015.

Activation functions

- ReLU was proposed in 2009-2010[2,3], and was successfully used in AlexNet in 2012[4].
- Address the vanishing gradient issue in activations, comparing to sigmoid or tanh.



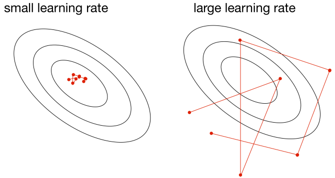
[2] Jarrett et al. What is the Best Multi-Stage Architecture for Object Recognition? ICCV, 2009.
[3] Nair & Hinton/ Rectified Linear Units Improve Restricted Boltzmann Machines. ICML, 2010.
[4] Krizhevsky et al. ImageNet Classification with Deep Convolutional Neural Networks. NIPS, 2012.

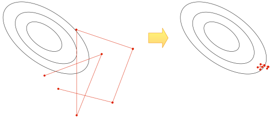
SGD Learning Rate

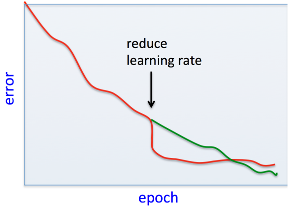
- In stochastic training, the learning rate also influences the fluctuations due to the stochasticity of the gradients.
- Typical strategy:
  - Use a large learning rate early in training so you can get close to the optimum.
  - Gradually decay the learning rate to reduce the fluctuations.

Learning Rate Decay

- We also need to be aware about the impact of learning rate due to the stochasticity.







RMSprop and Adam

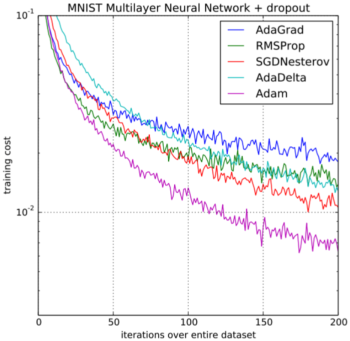
- Recall: SGD takes large steps in directions of high curvature and small steps in directions of low curvature.
- RMSprop is a variant of SGD which rescales each coordinate of the gradient to have norm 1 on average. It does this by keeping an exponential moving average s_j of the squared gradients.
- The following update is applied to each coordinate j independently:

$$s_j \leftarrow (1-\gamma)s_j + \gamma[\tfrac{\partial L}{\partial \theta_j}]^2$$

$$\theta_j \leftarrow \theta_j - \frac{\alpha}{\sqrt{s_j + \epsilon}} \frac{\partial L}{\partial \theta_j}$$

Adam optimizer

- Adam = RMSprop + momentum = Adaptive Momentum estimation
- Smoother estimate of the average gradient and gradient norm.
- m_t: exponential moving average of gradient.
- v_t: exponential moving average of gradient squared.
- $\hat{m}_t$, $\hat{v}_t$: Bias correction.
- $\theta_t \leftarrow \theta_{t-1} - \alpha \hat{m}_t / (\sqrt{\hat{v}_t} + \epsilon)$
- The "default" optimizer for modern networks.

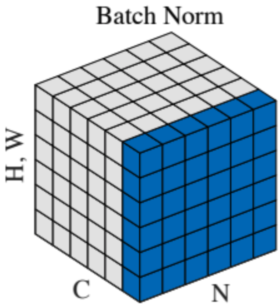


Normalization

- Weight initialization is tricky, and there is no guarantee that the distribution of activations will stay the same over the learning process.
- What if the weights keep grow bigger and activation may explode?
- We can "normalize" the activations.
- The idea is to control the activation within a normal range: zero-mean, uni-variance.

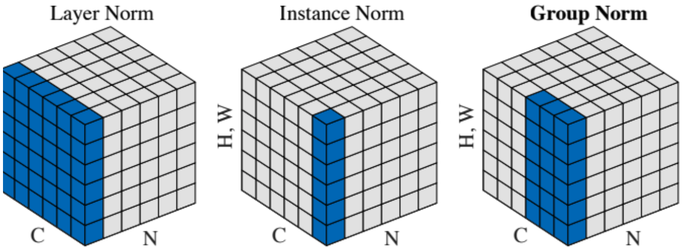
Batch Normalization (BN)

- In CNNs, neurons across different spatial locations are also samples of the same feature channel.
- Batch norm: Normalize across N H W dimensions, leaving C channels.
- $\tilde{x} = \gamma \frac{x-\mu}{\sigma} + \beta$
- γ, β: learnable parameters. μ, σ: statistics from the training batch.
- Test time: using the mean and variance from the entire training set.



BN Alternatives

- Need a considerable batch size to estimate mean and variance correctly.
- Training is different from testing.
- Alternatives consider the C channel dimension instead of N batch dimension.



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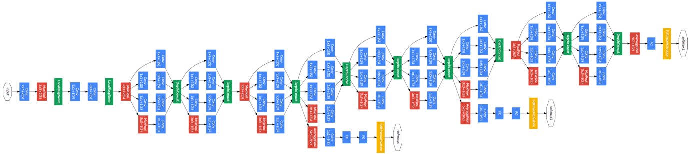
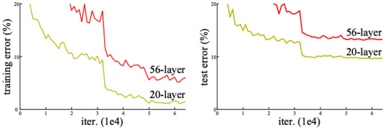
[5] Wu and He. Group normalization. ECCV 2018.

Going Deeper

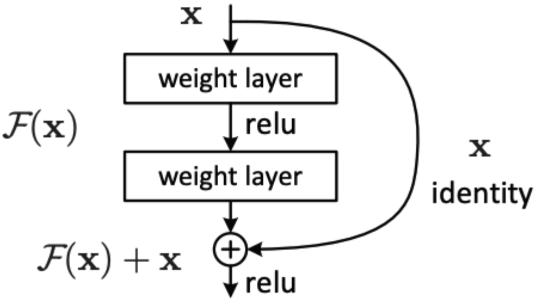
- The progress of normalization allowed us to train even deeper networks.
- The networks are no longer too sensitive with initialization.
- But the best networks were still around 20 layers and deeper results in worse performance.





Residual Networks (ResNet)

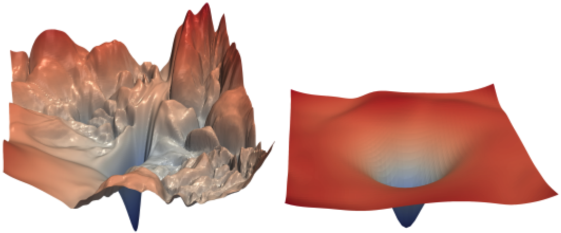
- Recall in gradient boosting, we are iteratively adding a function to the model to expand the capacity.
- Residual connection: Skip connection to prevent gradient vanishing.[6]



[6] He et al. Deep Residual Learning for Image Recognition. CVPR 2016.

ResNet Success

- Now able to train over 100 layers.
- One of the most important network design choices in the past decade.
- Prevalent in almost all network architectures, including Transformers.
- Loss landscape view: Skip connections makes loss smoother -> easier to optimize [7].

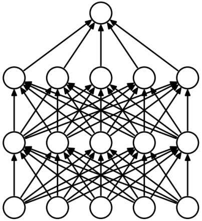


(a) without skip connections (b) with skip connections

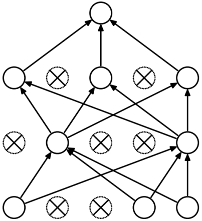
[7] Li et al. Visualizing the Loss Landscape of Neural Nets. NIPS 2018.

Dropout[8]

- Want to reduce overfitting in neural networks.
- Stochastically turning off neurons in propagation.
- Training to preserve redundancy.
- Test time: multiplying activations with probability. Model ensembling effect.



(a) Standard Neural Net

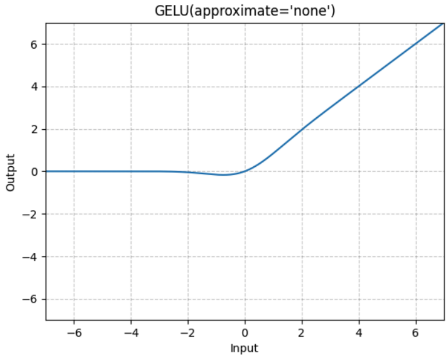


(b) After applying dropout.

[8]Srivastava et al. A Simple Way to Prevent Neural Networks from Overfitting. JMLR, 2014.

GELU[9]

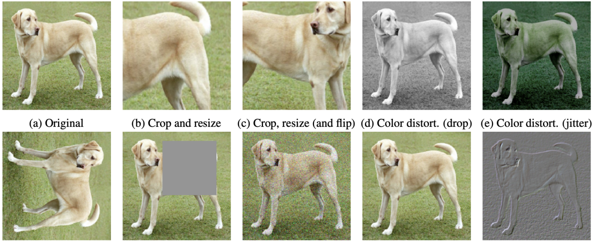
- Gaussian Error Linear Unit - A smoother activation function.
- Motivated by Dropout.
- $f(x) = \mathbb{E}[x \cdot m]$.
- $m \sim Bernoulli(\Phi(x))$.
- $\Phi(x) = P(X \leqslant x)$.
- $X \sim \mathcal{N}(0, 1)$.



[9] Hendrycks & Gimpel. Gaussian Error Linear Unit (GELU). CoRR abs/1606.08415, 2016.

Data augmentation

- Leverage the invariances of images
- Create more data points for free
    - Random cropping
    - Left+right flipping
    - Random color jittering
    - Random blurring
    - Affine warping
    - Etc.



(a) Original (b) Crop and resize (c) Crop, resize (and flip) (d) Color distort. (drop) (e) Color distort. (jitter)
(f) Rotate {90°, 180°, 270°} (g) Cutout (h) Gaussian noise (i) Gaussian blur (j) Sobel filtering

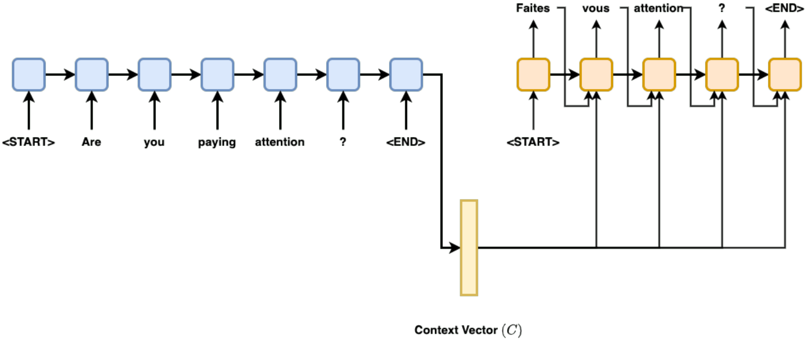
Image credit[10]

[10] Chen et al. A Simple Framework for Contrastive Learning of Visual Representations. ICML 2020.

Language and sequential signals

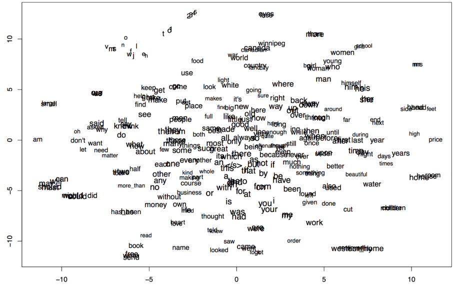
What about natural language

- Neural networks are great for dealing with naturalistic and unstructured signals.
- Past lectures: Feature functions in structured models, but still primitive.
- Design neural networks to accomodate sequential signals such as language.



Word embeddings

- Neural networks are best dealing with real valued vectors.
- Need to convert words (discrete) into vectors (continuous).
- A large matrix of $V \times D$. V = vocab size, D = network embedding size.

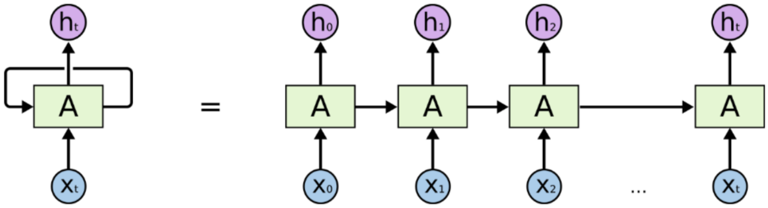


[11]

[11]https://aelang.github.io/word-embeddings.html

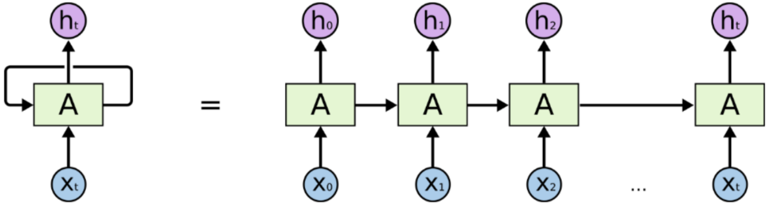
Convolutional vs. recurrent networks

- Recall in images we used the convolution operation.
- We can also use the idea of convolution for temporal signals.
- Another alternative is to use a type of network called recurrent networks.
- Two inputs: x_t is the current input, and h_t is the historical hidden state.
- We can unroll the computation graph into a direct acyclic graph (DAG).



Recurrent neural networks (RNNs)

- A simple RNN can be made similar to a standard NN with one hidden layer.
- $h_t = \tanh(Wh_{t-1} + Ux_t)$.
- $y_t = \text{Softmax}(Vh_t)$.



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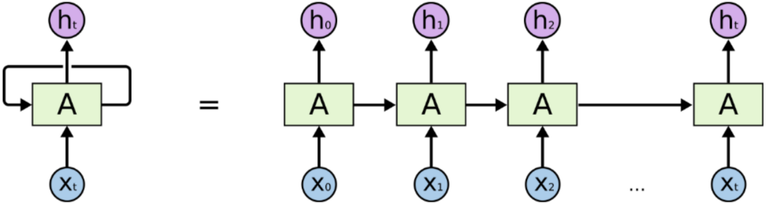
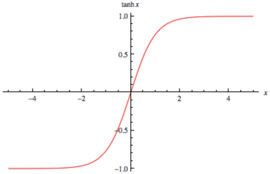
[12] Image credit: Chris Olah https://colah.github.io/posts/2015-08-Understanding-LSTMs/

Gradient vanishing

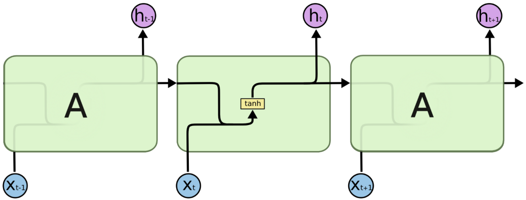
- Every iteration, we multiply the hidden state h_{t-1} from the previous iteration with the same W. Recall the definition of Jacobian.
- If the largest singular value of W is less than one then back-propagation will be attenuated.
- Similarly, we apply tanh activation every iteration – further reducing gradient flow.

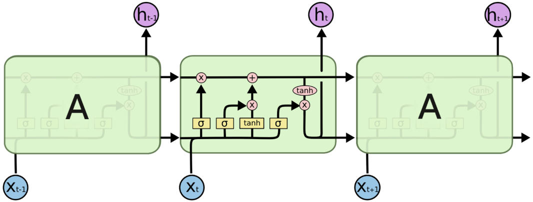




Gating functions in LSTM

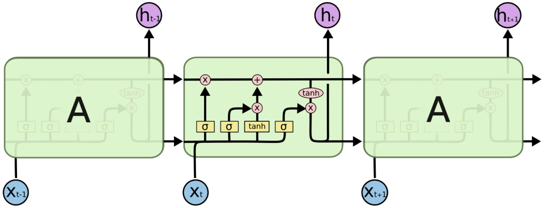
- Long short-term memory is a network that addresses the gradient vanishing problem by introducing gating functions.
- Gating functions provide "shortcuts", like ResNet.
- Originally proposed by Hochreiter and Schmidhuber in 1997.





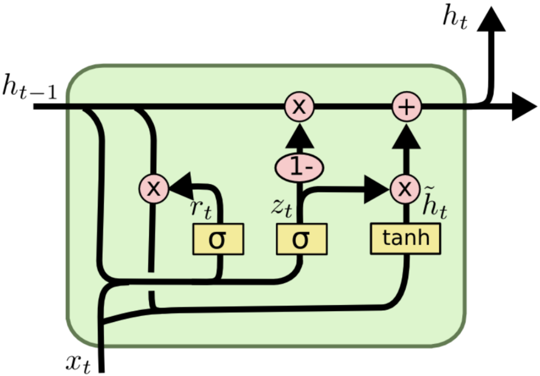
Gating functions in LSTM

- Input gate: $i_t = \sigma(W_i[h_{t-1}, x_t] + b_i)$.
- Forget gate: $f_t = \sigma(W_f[h_{t-1}, x_t] + b_f)$.
- $z_t = \tanh(w_z[h_{t-1} x_t] + b_z)$.
- $c_t = f_t \odot c_{t-1} + i_t \odot z_t$.
- Output gate: $o_t = \sigma(W_o[h_{t-1}, x_t] + b_o)$.
- $h_t = o_t \odot \tanh(c_t)$.



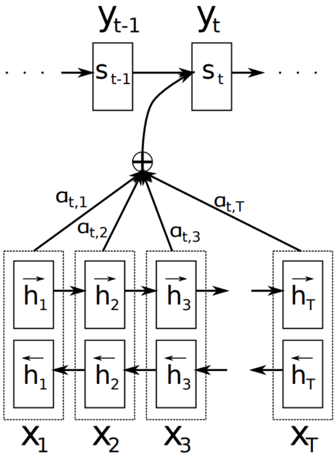
Gated Recurrent Unit

- Proposed by Chung et al. in 2015, a simplified variant compared to LSTM.
- Input gate $i_t = \sigma(W_i[h_{t-1}, x_t] + b_i)$.
- Reset gate $r_t = \sigma(W_r[h_{t-1}, x_t] + b_r)$.
- $\tilde{h}_t = \tanh(W_h[r_t \odot h_t, x_t] + b_h)$.
- $h_t = (1 - i_t) \odot h_{t-1} + i_t \odot \tilde{h}_t$.



Attention Mechanisms

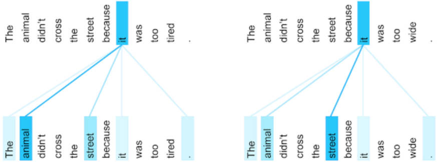
- Earlier content will decay more.
- Hard to refer back to the raw content.
- Reverse order better than forward order [abcde -> a'b'c'd'e' vs. abcde -> e'd'c'b'a'].
- Attending to arbitrary sequence tokens.
- $s_t = f(s_{t-1}, y_{t-1}, c_t)$
- $c_t = \sum_\tau \alpha_{t,\tau} h_\tau$, $\alpha_{t,\tau} = \frac{\exp(a(s_{t-1}, h_k))}{\sum_k \exp(a(s_{t-1}, h_k))}$
- $a(s_{t-1}, h_k) = v_a^\top \tanh(W_a[s_{i-1}, h_k])$



Bahdanau et al., 2014

Transformers ("Attention is All You Need")

- The previous architecture is very complicated.
  - 1 RNN for encoding the tokens.
  - Attention mechanisms for accessing content
  - 1 RNN for combining attended tokens.
- RNNs have the ability to incorporate past information, so does attention.



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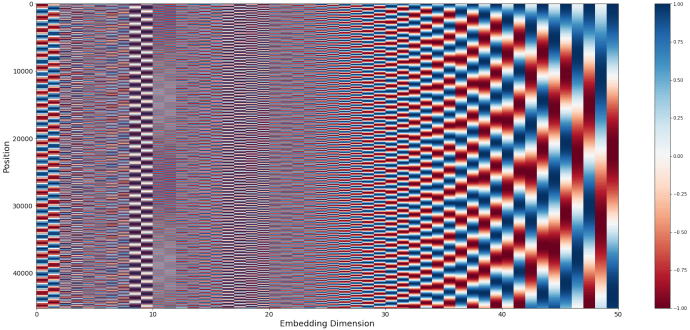
[13] Image credit: Google Research Blog

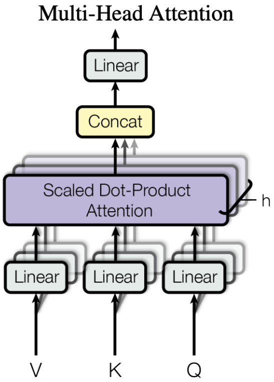
Positional encoding

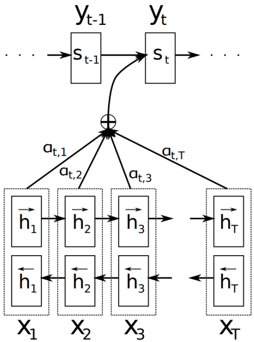
- Attention operation is permuation equivariant.
- Solution: Encode the position of each token.
- $PE(pos, 2i) = \sin(p/k^{2i/d}), PE(pos, 2i+1) = \cos(p/k^{2i/d})$.



Multi-headed attention

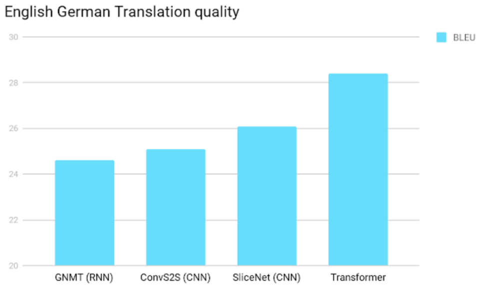
- Map tokens into query, key, and value.
- $Attention(Q, K, V) = \text{Softmax}(\frac{QK^\top}{\sqrt{d_k}})V$.
- $H_i = Attention(QW_i^Q, KW_i^K, VW_i^V)$.
- $MultiHead(Q, K, V) = [H_1, ..., H_n]W^O$
- More advantageous to have multiple set of attentions for each token, so it can more efficiently incorporate information from multiple sources.

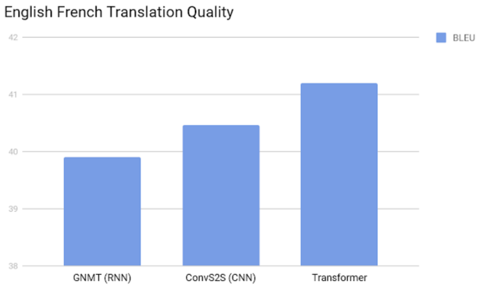




Machine Translation

- Achieved superior performance on machine translation.
- Animation link





Autoregressive modeling

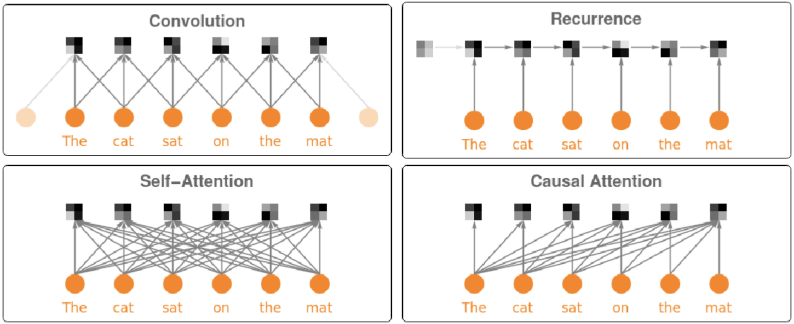
- Recall the chain rule on joint distribution:

$$p(x_{1:t}) = p(x_1, \ldots, x_t) = p(x_1)p(x_2|x_1)\ldots p(x_t|x_{t-1}) = p(x_1)\prod_i p(x_i|x_{1:i-1}).$$

- In Naive Bayes, we treat each variable as independent, but this cannot perform sequence generation.
- How do we model a conditional distribution $p(x_i|x_{1:i-1})$ using an RNN or a Transformer?
- RNN is naturally autoregressive: h_t contains all information up to time t.
- For Transformers, h_t contains information about the future.

Causal Attention

- For Transformers, we need to "mask" the attention so that each token can only attend to tokens prior to itself.
- This is called "causal attention".

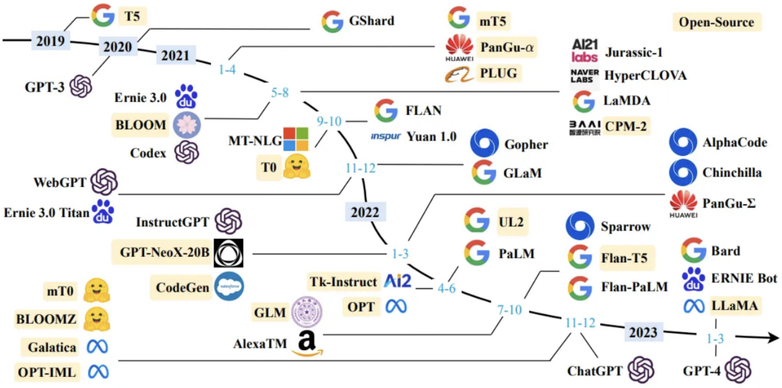


14

[14] Image credit: Wolfram.com

Large Language Models

- Most LLMs today are large-scale decoder-only autoregressive (causal) Transformers (>1B parameters).



[15]

15 Image credit: Medium.com

Interim Summary

- Optimization: Learning rate, initialization, activation functions, normalization, shortcut skip connection, attention, etc.
- Overfitting: Dropout, Data augmentation, etc.
- Architecture Motifs: MLP, CNN, RNN, Transformers, etc.
- Why deep learning works? Data, optimization, compute.
- Still many open questions: Interpretability, fairness, uncertainty, data efficiency, energy efficiency, theory, etc.

Interpretability in Deep Neural Networks

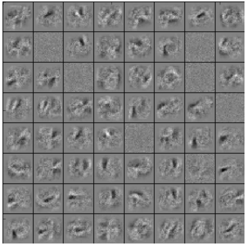
ML Interpretability

- Linear regression: Weights represent feature selection strength.
- SVMs: Dual weights represent sample selection.
- Bayesian methods: Model the generative process as a probabilistic model, fully transparent.
- Decision trees: If-else decision making process.
- Neural networks: ?

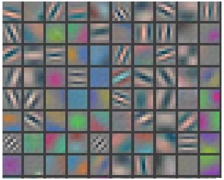
Feature Visualization

- Recall: we can understand what first-layer features are doing by visualizing the weight matrices.

Fully connected



Convolutional



Zeiler and Fergus, Visualizing and understanding convolutional networks, ECCV 2014.

- The better the input matches these weights, the more the feature activates.
- Higher-level weight matrices are hard to interpret.
  - Obvious generalization: visualize higher-level features by seeing what inputs activate them.

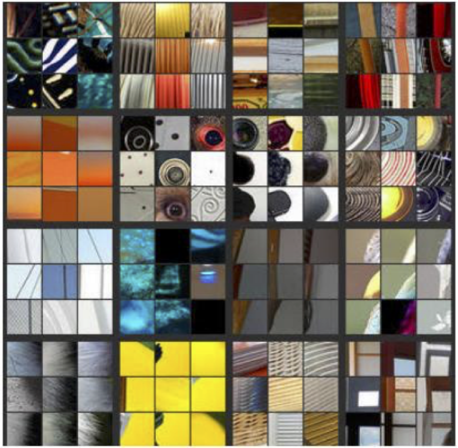
Feature Visualization

- One way to formalize: pick the images in the training set which activate a unit most strongly.
- Here's the visualization for layer 1:

Zeiler and Fergus, Visualizing and understanding convolutional networks, ECCV 2014.

Feature Visualization

- Layer 3:



Zeiler and Fergus, Visualizing and understanding convolutional networks, ECCV 2014.

Feature Visualization

- Layer 4:

Feature Visualization

- Layer 5:

Feature Visualization

- Higher layers seem to pick up more abstract, high-level information.
- Problems?
  - Can't tell what the unit is actually responding to in the image.
  - We may read too much into the results, e.g. a unit may detect red, and the images that maximize its activation will all be stop signs.
- Can use input gradients to diagnose what the unit is responding to.

- Input gradients can be hard to interpret.
- Take a good object recognition conv net (Alex Net) and compute the gradient of $\log p(y = \text{“cat”}|\mathrm{x})$:

Original image

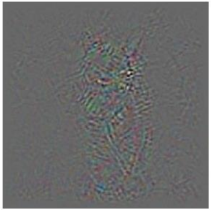
Gradient for “cat”

Feature Visualization

- Guided backprop is a total hack to prevent this cancellation.
- Do the backward pass as normal, but apply the ReLU nonlinearity to all the activation error signals.

$$y = \mathrm{ReLU}(z) \qquad \bar{z} = \begin{cases} \bar{y} & \text{if } z > 0 \text{ and } \bar{y} > 0 \\ 0 & \text{otherwise} \end{cases}$$

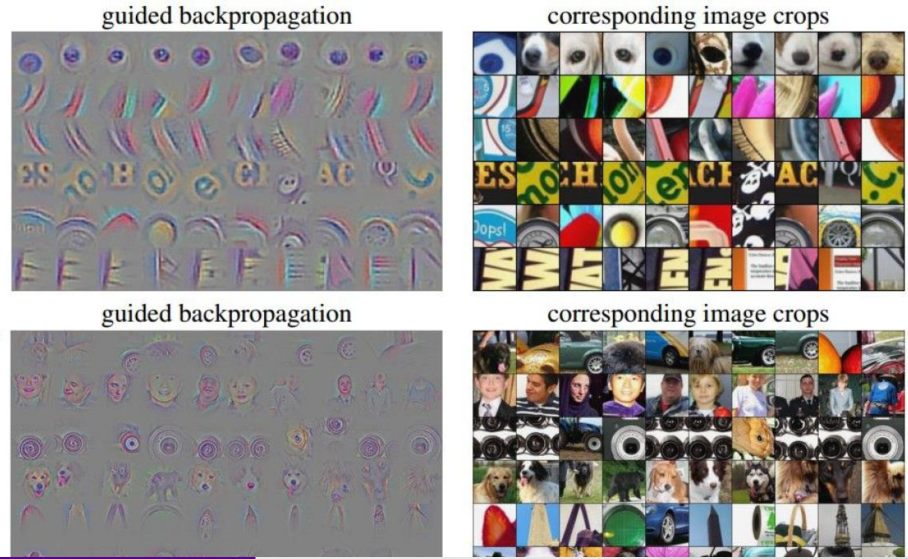
- We want to visualize what excites given unit, not what suppresses it.



Backprop

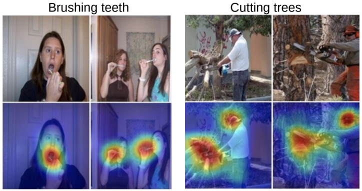
Guided Backprop

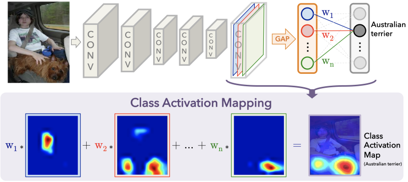
Guided Backprop



Class activation map (CAM)

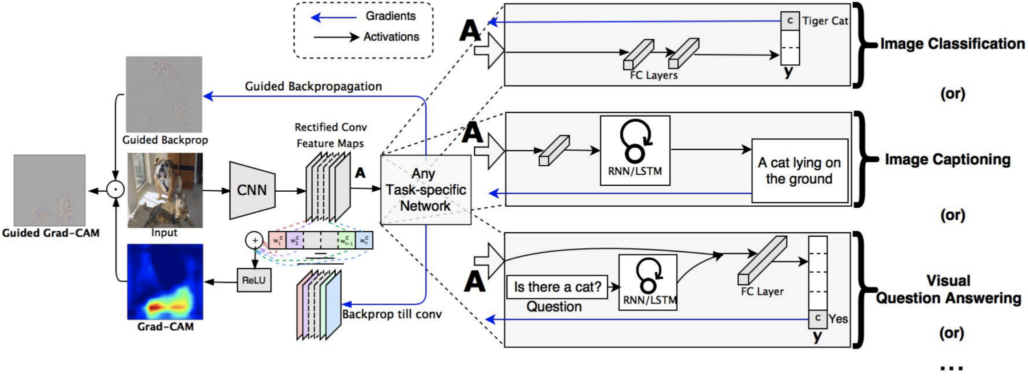
- Classification networks typically use global avg pooling before the final layer.
- This pooling layer can already contain semantic information.
- We can visualize a heat map





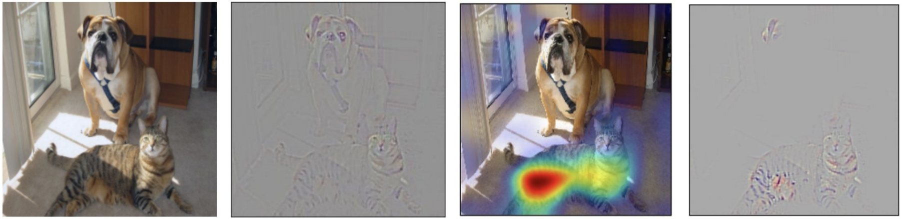
Zhou et al. Learning deep features for discriminative localization. CVPR 2016.

GradCAM

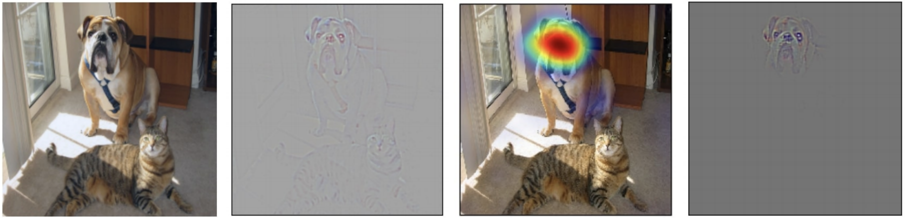


Selvaraju et al. Grad-CAM: Visual explanations from deep networks via gradient-based localization. ICCV 2017.

GradCAM



(a) Original Image (b) Guided Backprop 'Cat' (c) Grad-CAM 'Cat' (d)Guided Grad-CAM 'Cat'



(g) Original Image (h) Guided Backprop 'Dog' (i) Grad-CAM 'Dog' (j)Guided Grad-CAM 'Dog'

DeepDream[16]

- Start with an image, and run a conv net on it.
- Change the image such that units which were already highly activated get activated even more strongly. "Rich get richer."

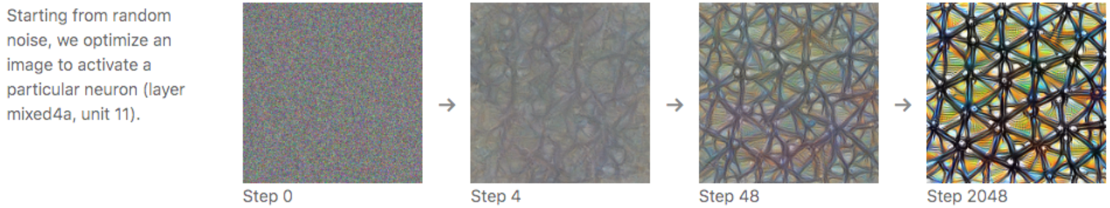
[16] Google Research Blog

"Admiral Dog!" "The Pig-Snail" "The Camel-Bird" "The Dog-Fish"

DeepDream

Gradient Ascent on Images

- Doing gradient ascent on an image to maximize the activation of a given neuron.



https://distill.pub/2017/feature-visualization/

Gradient Ascent on Images

Dataset Examples show us what neurons respond to in practice

Optimization isolates the causes of behavior from mere correlations. A neuron may not be detecting what you initially thought.

Baseball—or stripes? *mixed4a, Unit 6*

Animal faces—or snouts? *mixed4a, Unit 240*

Clouds—or fluffiness? *mixed4a, Unit 453*

Buildings—or sky? *mixed4a, Unit 492*

https://distill.pub/2017/feature-visualization/

Gradient Ascent on Images

- Higher layers in the network often learn higher-level, more interpretable representations

Edges (layer conv2d0) **Textures** (layer mixed3a) **Patterns** (layer mixed4a)

https://distill.pub/2017/feature-visualization/

Gradient Ascent on Images

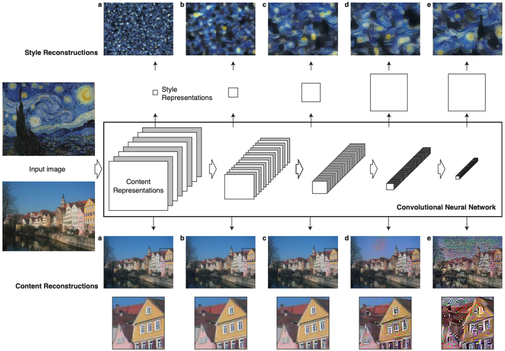
- Higher layers in the network often learn higher-level, more interpretable representations

Parts (layers mixed4b & mixed4c) **Objects** (layers mixed4d & mixed4e)

https://distill.pub/2017/feature-visualization/

Artistic style transfer

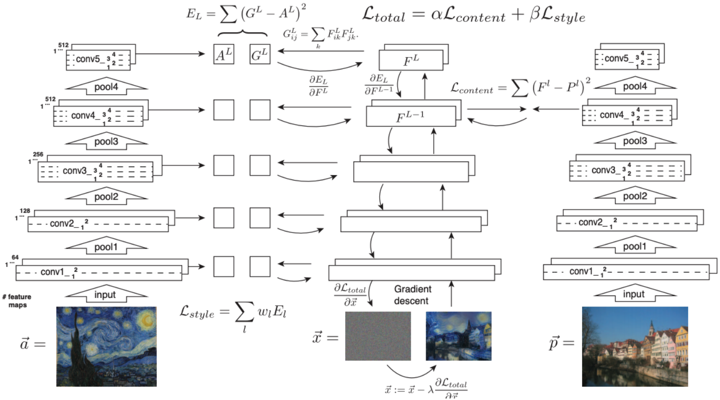
- Activations store content information
- Activation correlation stores style/texture information: $G^l_{ij} = \sum_k F^l_{ik} F^l_{jk}$



Gatys et al., Image style transfer using convolutional neural networks, CVPR 2016.

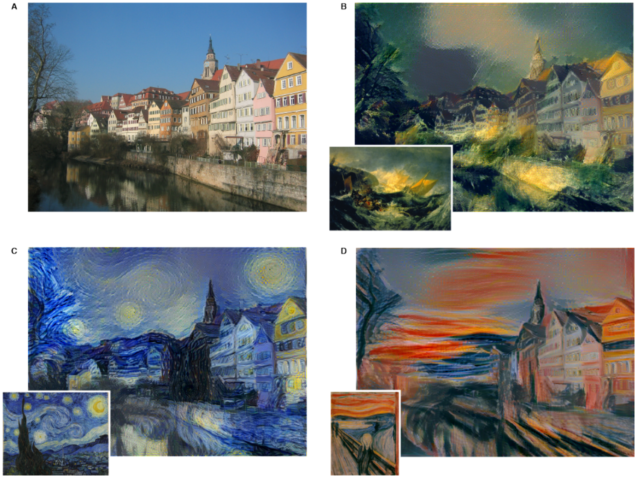
Artistic style transfer

- Optimizing both content & style from random noise



Gatys et al., Image style transfer using convolutional neural networks, CVPR 2016.

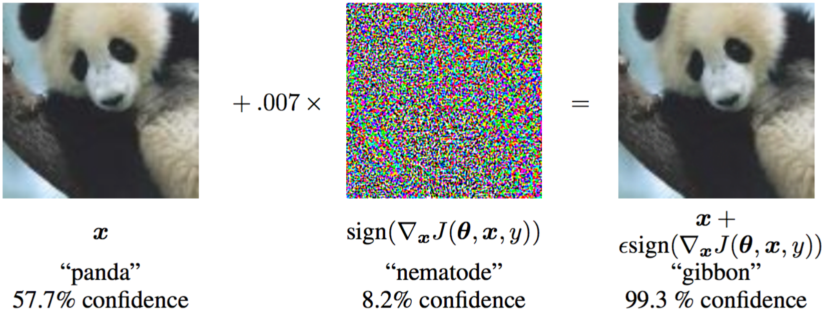
Artistic style transfer



Gatys et al., Image style transfer using convolutional neural networks, CVPR 2016.

Adversarial Examples

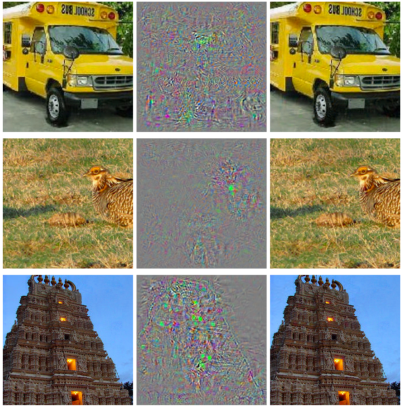
- One of the most surprising findings about neural nets has been the existence of adversarial inputs, i.e. inputs optimized to fool an algorithm.

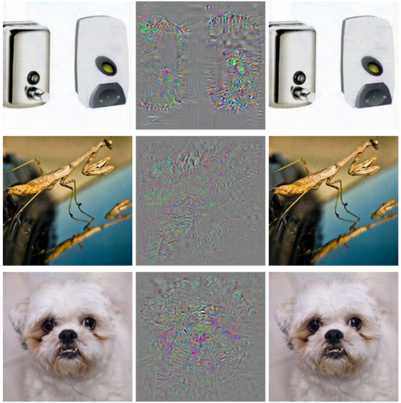


Goodfellow et al., Explaining and harnessing adversarial examples, ICLR 2015.

Adversarial Examples

- The following adversarial examples are misclassified as ostriches. ($10\times$ perturbation visualized in middle.)





Szegedy et al., Intriguing properties of neural networks, ICLR 2014.

Adversarial Examples

- You can print out an adversarial image and take a picture of it, and it still works!

(a) Printout (b) Photo of printout (c) Cropped image

Kurakin et al., Adversarial examples in the physical world, ICLR workshop 2017.

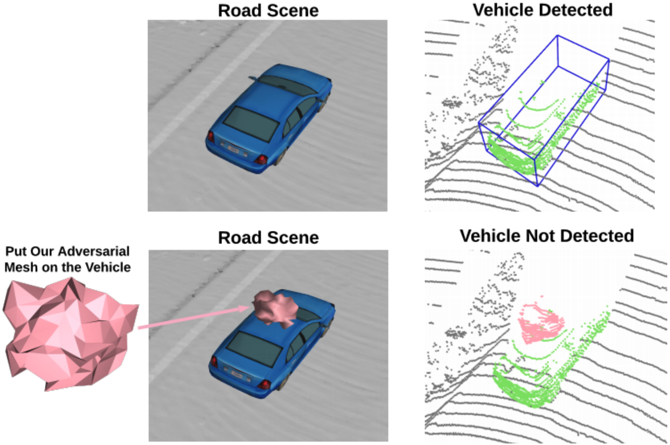
Adversarial Examples

- An adversarial example in the physical world (network thinks it's a gun, from a variety of viewing angles!)

Athalye et al., Synthesizing robust adversarial examples, ICML 2018.

Adversarial Examples

- An adversarial mesh object that can hide cars from LiDAR detector



Tu et al., Physically realizable adversarial examples for LiDAR object detection, CVPR 2020.

Adversarial Defense

- How to defend from adversarial perturbation is still an active research area.
- Blackbox vs. whitebox attacks.
- One common approach is to train with millions of adversarial examples.
- Needs to train much longer, and also suffers a drop in accuracy.
- Data augmentation and label smoothing also help.

Summary

- Interpretability - ways to open up the black box of neural networks
- Knowing what each neuron does is like studying a “brain” with perfect observation and measurement.
- Still very open research area.
- Adversarial examples are safety vulnerabilities of deep neural networks.
- Need more data and innovations in more robust learning objectives.