TBMI26 Neural Networks and Learning Systems Lecture 6 Deep Networks

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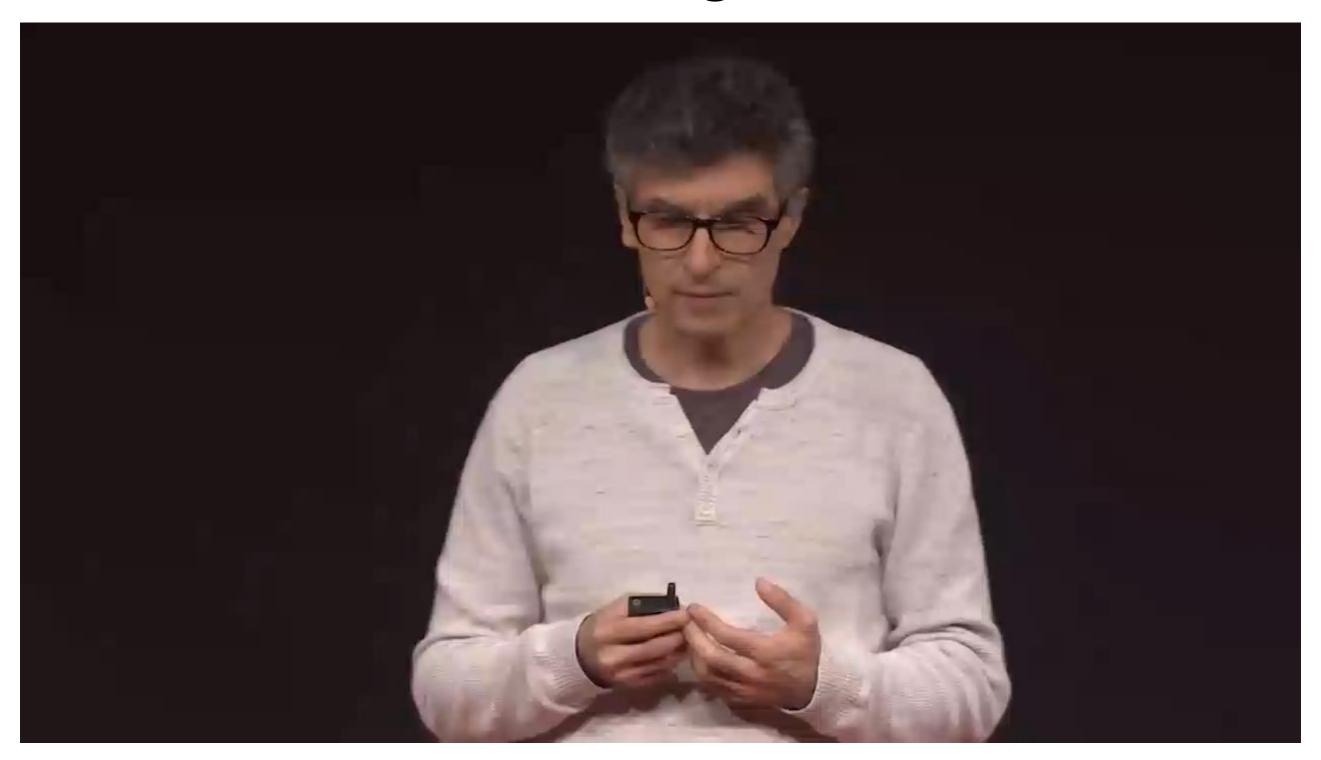
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Introduction



TEDx-talk Yoshua Bengio

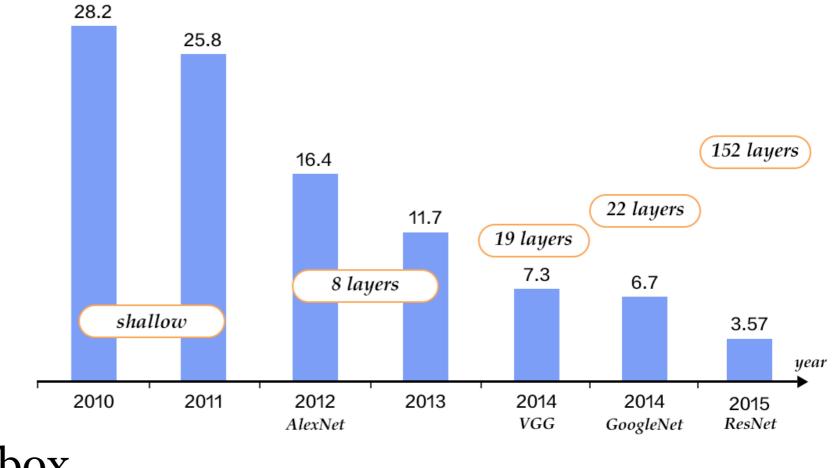




ILSVRC-2010

 ImageNet Large Scale Visual Recognition Challenge [Deng et al. 2009]

- more than 14million images
- More than 10
 million images
 annotated
- More than 1
 million images
 with bounding box





Loss functions (cont.)



Motivation: maximum likelihood estimation

- Probability distribution $P(X=x; \theta) = C \exp(-(x-\theta)^2/(2\sigma^2))$
- The maximum likelihood estimate for θ is (assuming independence and i.i.d.)

$$\theta_{\text{ML}} = \arg \max_{\theta} \sum_{i=1}^{N} \log P(X = x^{(i)}; \theta)$$

$$= \arg\min_{\theta} \sum_{i=1}^{N} (x^{(i)} - \theta)^2$$

 Note: this example is parametric

$$= \frac{1}{N} \sum_{i=1}^{N} x^{(i)}$$



Conditional log-likelihood

- Supervised learning: learn a conditional probability distribution over target values y, given features x.
- The assumption that the samples are i.i.d. yields

$$\theta_{\text{ML}} = \arg \max_{\theta} \sum_{i=1}^{N} \log P(y^{(i)} | x^{(i)}; \theta)$$

- Same as minimizing *cross-entropy* $E_X[-\log P(Y|X)]$
- Principled way to derive the cost function (incl. L2)

$$cost(\{(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})\}) = -\frac{1}{N} \sum_{i=1}^{N} \log P(\mathbf{y}^{(i)} | \mathbf{x}^{(i)}; \boldsymbol{\theta})$$



Cross-entropy cost function

• Back to logistic activation: $h(\mathbf{x}_i) = f(\theta \cdot \mathbf{x}_i) = \frac{1}{1 + e^{-\theta \cdot \mathbf{x}_i}}$

interpretation: conditional probability $P(y_i = 1 \mid x)$ for binary random variable y_i . $P(y_i = 0 \mid x) = 1 - P(y_i = 1 \mid x)$

The cross-entropy is the "natural" error function:

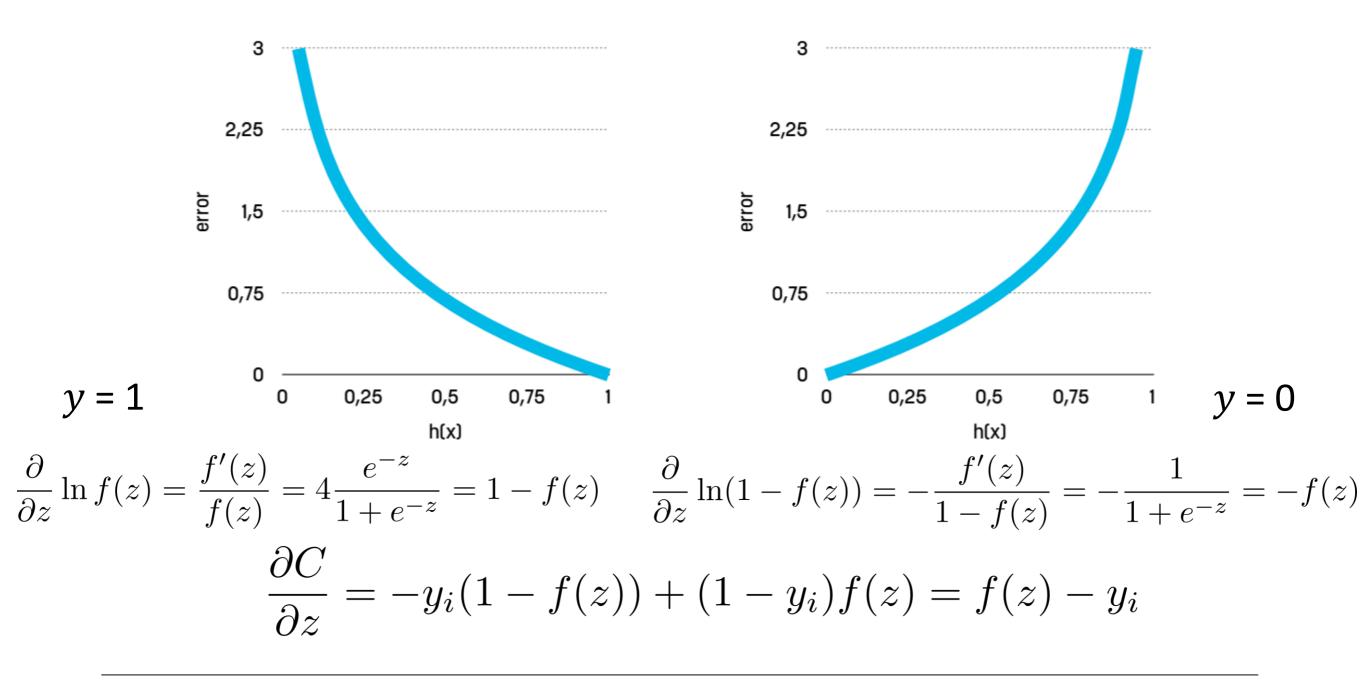
$$C = \begin{cases} -\ln h(\mathbf{x}_i) & \text{if } y_i = 1\\ -\ln(1 - h(\mathbf{x}_i)) & \text{if } y_i = 0 \end{cases}$$

This is usually written as

$$C = -(y_i \ln h(\mathbf{x}_i) + (1 - y_i) \ln(1 - h(\mathbf{x}_i)))$$



Sigmoid and cross-entropy balance each other





Cross-entropy cost function

• Back to soft-max activation: $h_k(\mathbf{x}_i) = f_k(\boldsymbol{\theta}\mathbf{x}_i) = \frac{e^{\theta_k \cdot \mathbf{x}_i}}{\sum_l e^{\theta_l \cdot \mathbf{x}_i}}$

interpretation: conditional probability $P(y_i = (0, 1, 0, ...) \mid x)$ for one-hot random vector y_i .

$$P(\mathbf{y}|\mathbf{x}) = \Pi_k h_k(\mathbf{x})^{y_k} = h_{k:y_k=1}(\mathbf{x})$$

• The cross-entropy is the "natural" error function:

$$-\ln P(\mathbf{y}_n|\mathbf{x}_n; n=1\dots N) = -\sum_{n} \sum_{k} y_{kn} \ln h_k(\mathbf{x}_n)$$

• Often the soft-max is (wrongly) called to be the cost



Surrogate loss function

- Example: 0-1 loss for class membership (one-hot coding) surrogated / replaced with log-likelihood (cross-entropy)
 - Motivation 1: Gradient descent does not allow for 0-1 loss (discontinuous loss) – cross-entropy is continuously differentiable
 - Motivation 2: Test error with 0-1 loss might be lower for training with cross-entropy than 0-1 loss cross-entropy pushes classes apart even if 0-1 loss on training set is zero



Example: Handwritten digit recognition



Handwritten digit recognition

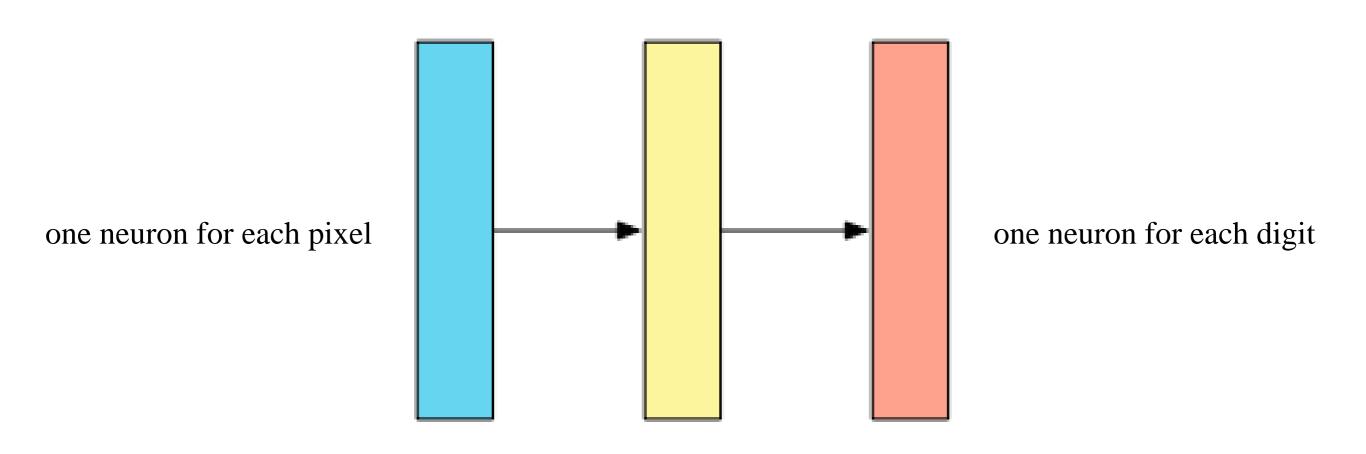
You are to build a feedforward net that takes in a greyscale image of a handwritten digit and outputs the digit (an integer).

supervised learning

```
5 0 5 9 7 7
6 8 6 6 3 6
7 1 5 8 3
```



Basic network architecture



 $1 + 28 \times 28$

7

10



How to use the network

• Translate each image to a vector \mathbf{x} with $1 + 28 \times 28$ components, where component x_i is the greyscale value for pixel i in the image.

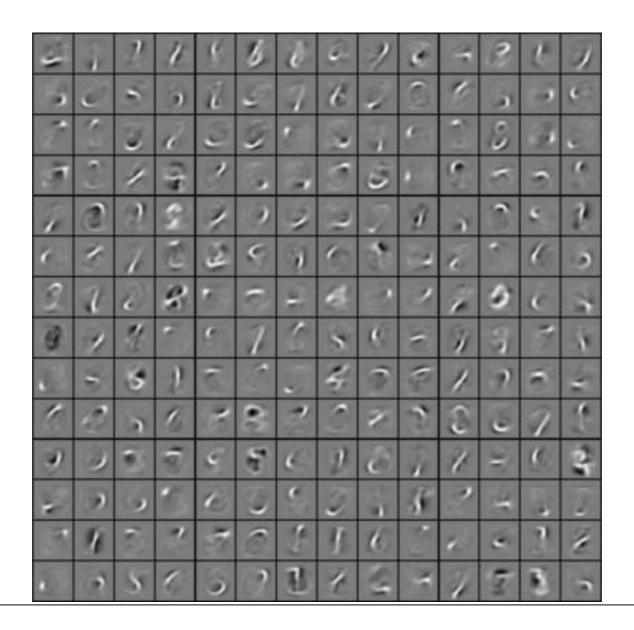
The greyscale value is a fraction k/255 between 0 (black) and 1 (white).

- Feed the image to the network.
- Find the neuron y_i in the output layer that has the highest activation and predict the digit i.

Softmax layer



What does the net learn?







How to train the network

- To train the network we use the MNIST database, which consists of 70,000 handwritten labelled digits.
- Each target is translated into a vector y with 10 components, where y_i is 1 if the target equals i and 0 otherwise (one-hot).

Example: If the target is 3 then $y_3 = 1$, and all other components zero.



Regularization



Norm-based regularisation

- We can regularise the training of a neural network by adding an additional term to the error function.
- L2-regularisation: Give preference to parameter vectors with smaller Euclidean norms ('lengths'):

$$\|\boldsymbol{\theta}\|_2^2 = \boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\theta}$$

• L1-regularisation: Give preference to parameter vectors with smaller absolute-value norms:

$$\|\boldsymbol{\theta}\|_1 = \sum_i |\theta_i|$$



Selected regularization techniques

• Dataset augmentation. Generate new training data by systematically transforming the existing data.

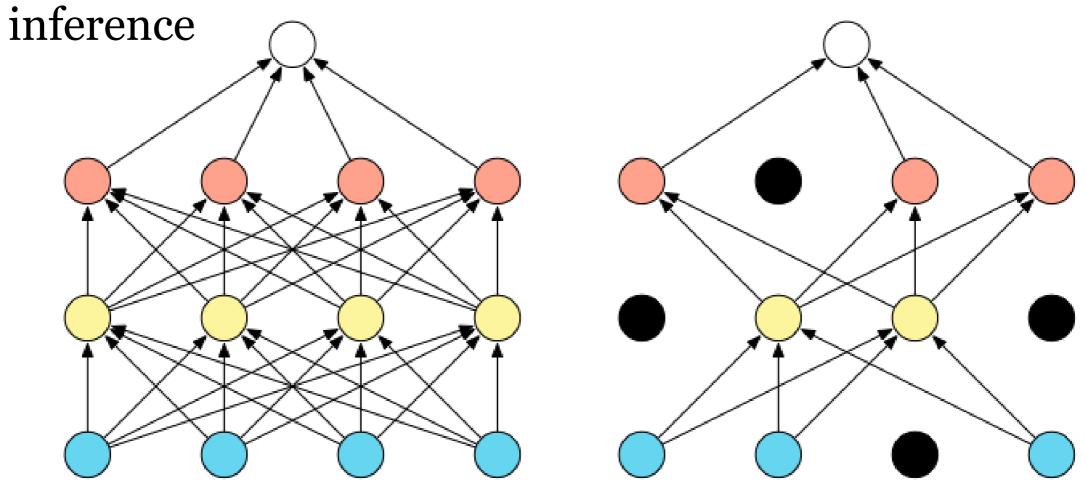
example: rotating and scaling images

- *Early stopping*. Stop the training when the validation set error goes up and backtrack to the previous set of parameters.
- Bagging / ensemble methods. Train several different models separately, then have all of the models vote on the output.



Dropout

Randomly set a fraction of units to zero during training /



unmodified neural net

net after applying dropout



Discussion: Local minima

- Deep networks always lead to local minima (model identifiability problem)
- Not necessarily a problem: mostly similarly low cost
- True global minimum not relevant
- Test: plot norm of gradient over time
 - if local minima are the problem, the norm needs to shrink close to zero
- In high dimensions, saddle points are much more likely than local minima; local minima have low costs



Initialization and Normalization



Initialization

- Gradient-based learning might lead to wrong directions or long trajectories
- Initialization in an area connected to a solution results in faster learning
- Initial weights *may not* be symmetric or identical, as this will just lead to redundancy
- Initial values should be large to break symmetry
- Initial values should not be too large to avoid numerical issues



Initialization

- Determining intial values is costly
- Good heuristic: draw weights from Gaussian or uniform distribution
- Normalized (Xavier) intialization for *m* inputs, *n* outputs (tanh; add factor 4 for sigmoid):

$$\theta_{ij} \sim U\left(-\sqrt{\frac{6}{m+n}}, \sqrt{\frac{6}{m+n}}\right)$$

• Other approaches: random orthogonal matrices, sparse initialization, ...



Batch normalization

- In deep networks, the simultaneous update of layers will have second, third, ... order effects
- To reduce this effect, z is replaced during learning

$$z_i' = \frac{z_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \varepsilon}} \qquad \mu_{\mathcal{B}} = \frac{1}{m} \sum_{i=1}^m z_i \qquad \sigma_{\mathcal{B}}^2 = \frac{1}{m} \sum_{i=1}^m (z_i - \mu_{\mathcal{B}})^2$$

where the empirical mean and variance are computed over the (mini)batch of size *m*

• This normalized activation is transformed $z_i'' = \gamma z_i' + \beta$ with moving-average parameters



Optimization Algorithm



Minibatch methods

- *Batch* deterministic: whole training set
- Stochastic gradient descent: single training samples
- *Minibatch*: subsets from training set
 - Large enough to exploit multicore architecture
 - Size coincides with accuracy of e.g. gradients
 - Small enough to fit into memory
 - Often power of 2: 32 .. 256
 - Number of minibatches coincides with regularization
 - Repeated drawing: *epochs*



Learning rate

- Stochastic methods (SGD, MB) require decaying learning rate
- Conditions for convergence:
 - Sum of learning rates goes to infinity
 - Sum of squared learning rates is bounded
- Often applied: linear combination of initial and final learning rate

$$\alpha_k = (1 - \lambda)\alpha_0 + \lambda\alpha_{\tau} \qquad \lambda = \frac{k}{\tau}$$

- Rule of thumb:
 - Initial rate larger than what initial results suggests
 - Final rate at about 1%

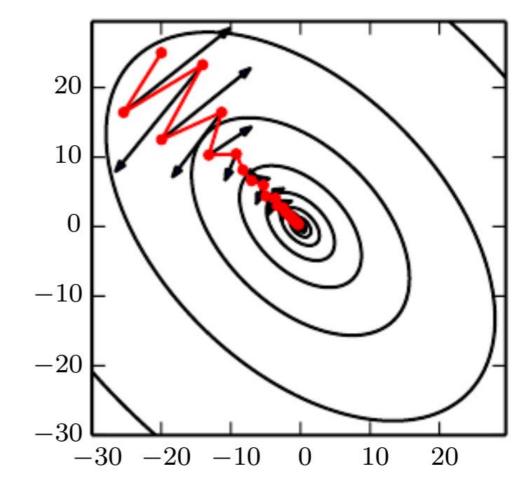


Momentum

- Gradient is problematic due to curvature, small scale, or noise
- Introduce velocity as exponentially decaying moving average of gradients

$$\begin{array}{cccc} \Delta \boldsymbol{\theta} & \leftarrow & \lambda \Delta \boldsymbol{\theta} - (1 - \lambda) \nabla_{\boldsymbol{\theta}} J \\ \boldsymbol{\theta} & \leftarrow & \boldsymbol{\theta} + \alpha \Delta \boldsymbol{\theta} \end{array}$$

 Hyperparameter of 0.9 gives about factor 10 speed-up





Adam [Kingma & Ba, 2015]

Based on RMSProp (adaptive gradient weight)

$$\mathbf{n} \leftarrow \nu \mathbf{n} + (1 - \nu) \nabla_{\boldsymbol{\theta}} J \odot \nabla_{\boldsymbol{\theta}} J$$
 element-wise operations

Combined with momentum and bias correction

$$\Delta \boldsymbol{\theta} \leftarrow \lambda \Delta \boldsymbol{\theta} - (1 - \lambda) \nabla_{\boldsymbol{\theta}} J$$

$$\hat{\Delta} \boldsymbol{\theta} \leftarrow \Delta \boldsymbol{\theta} / (1 - \lambda^{t})$$

$$\mathbf{n} \leftarrow \nu \mathbf{n} + (1 - \nu) \nabla_{\boldsymbol{\theta}} J \odot \nabla_{\boldsymbol{\theta}} J$$

$$\hat{\mathbf{n}} \leftarrow \mathbf{n} / (1 - \nu^{t})$$

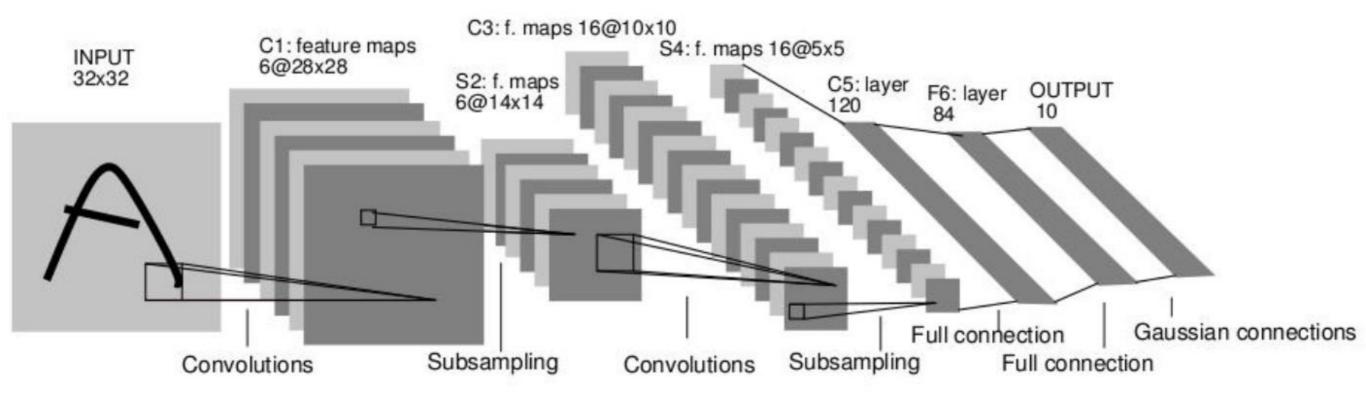
$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha \hat{\Delta} \hat{\boldsymbol{\theta}} / (\sqrt{\hat{\mathbf{n}}} + \varepsilon)$$



Network Architectures



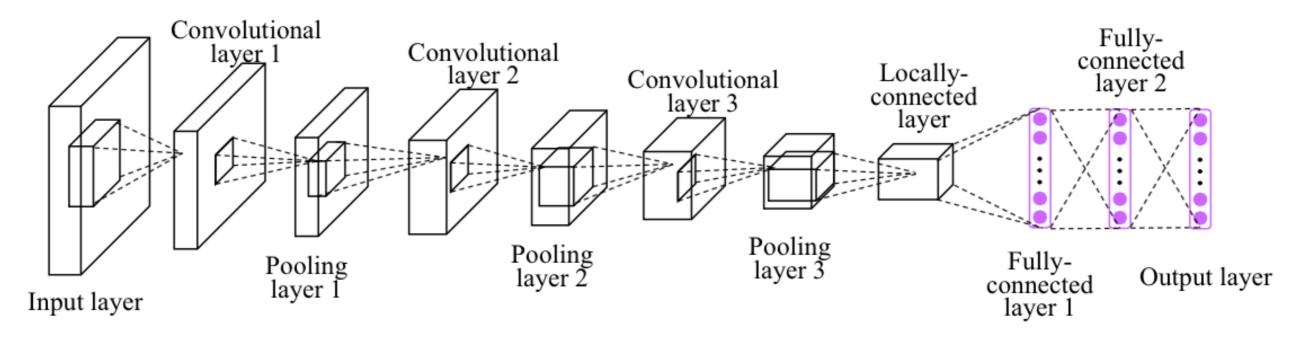
LeNet 5 [LeCun et al. 1998]

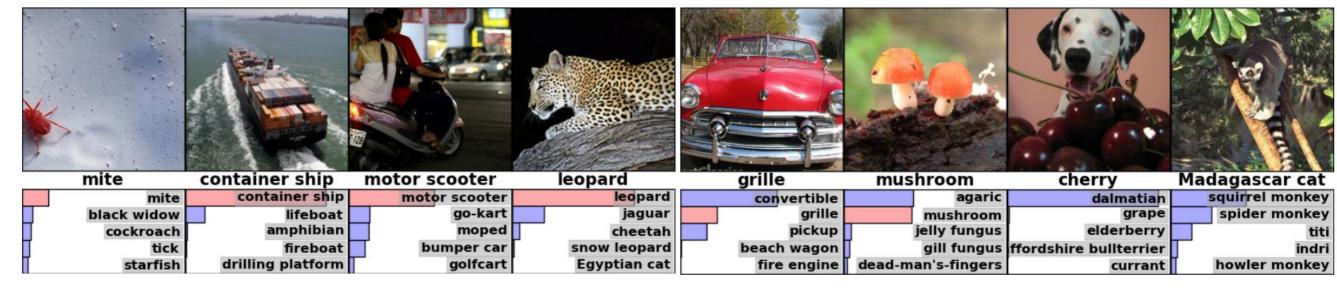


- Average pooling
- Sigmoid/tanh activation
- 60K training samples, 10 classes (MNIST)



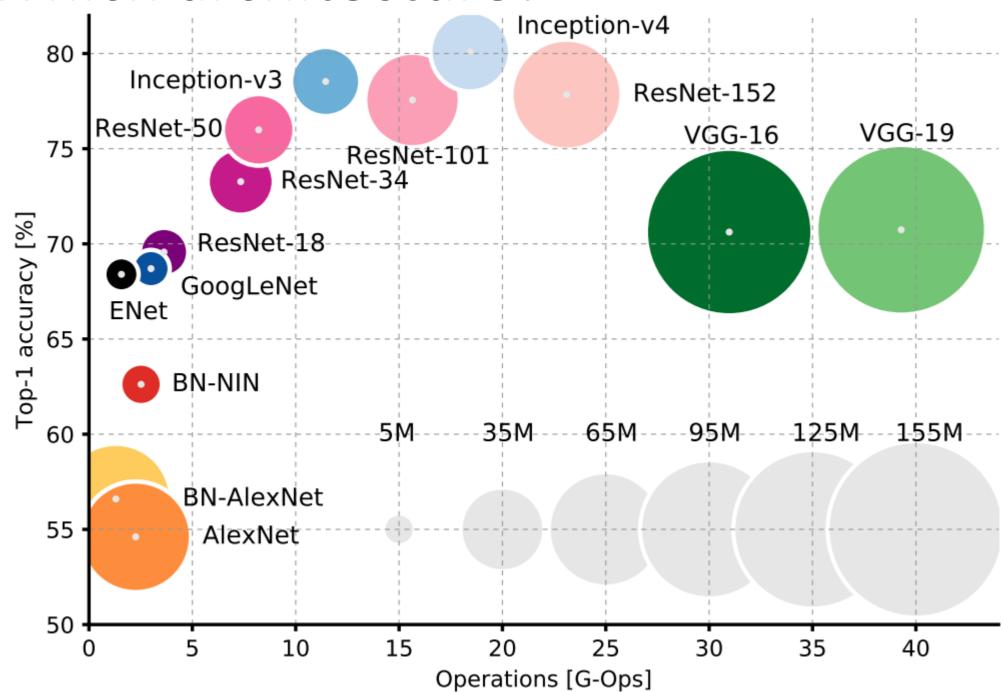
Deep Neural Networks (simple)



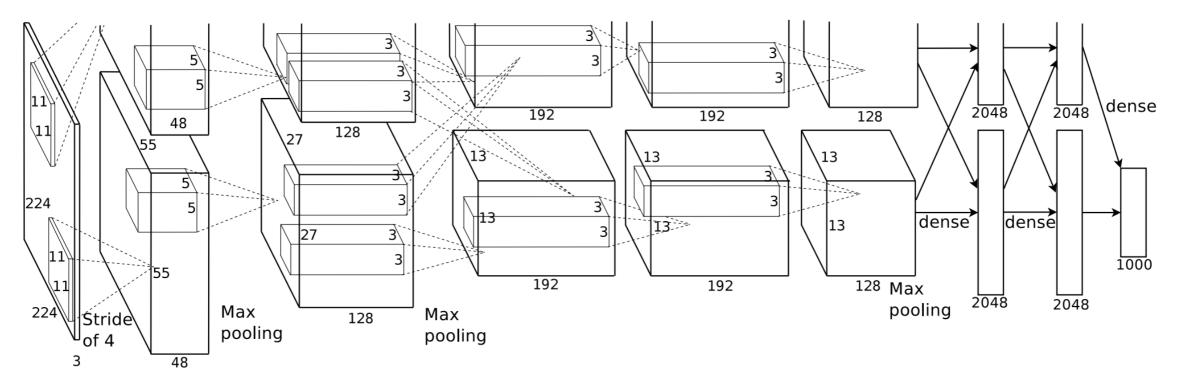




Which architecture?



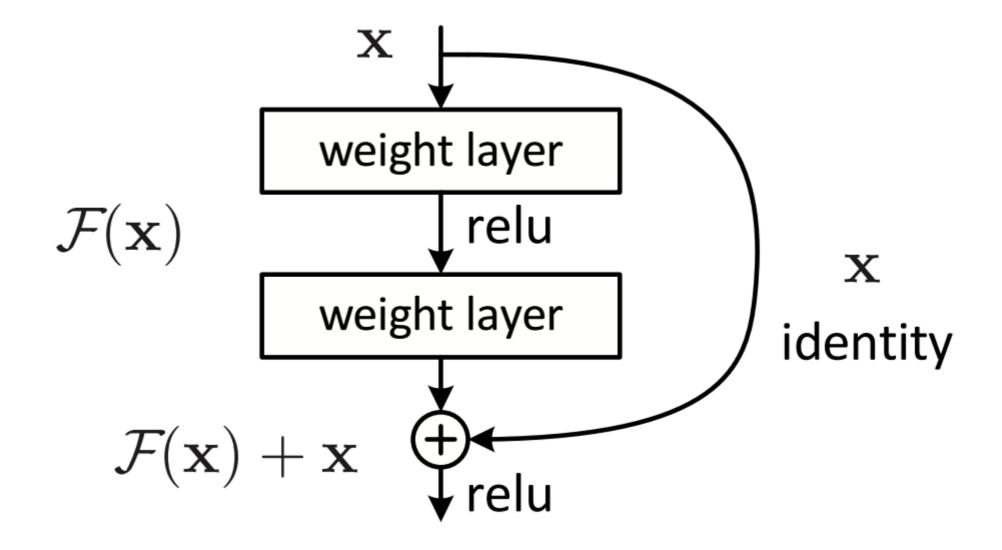
AlexNet [Krizhevsky et al. 2012]



- Max pooling
- ReLU activation
- Dropout regularization
- 1.2M training samples, 1000 classes (ILSVRC)



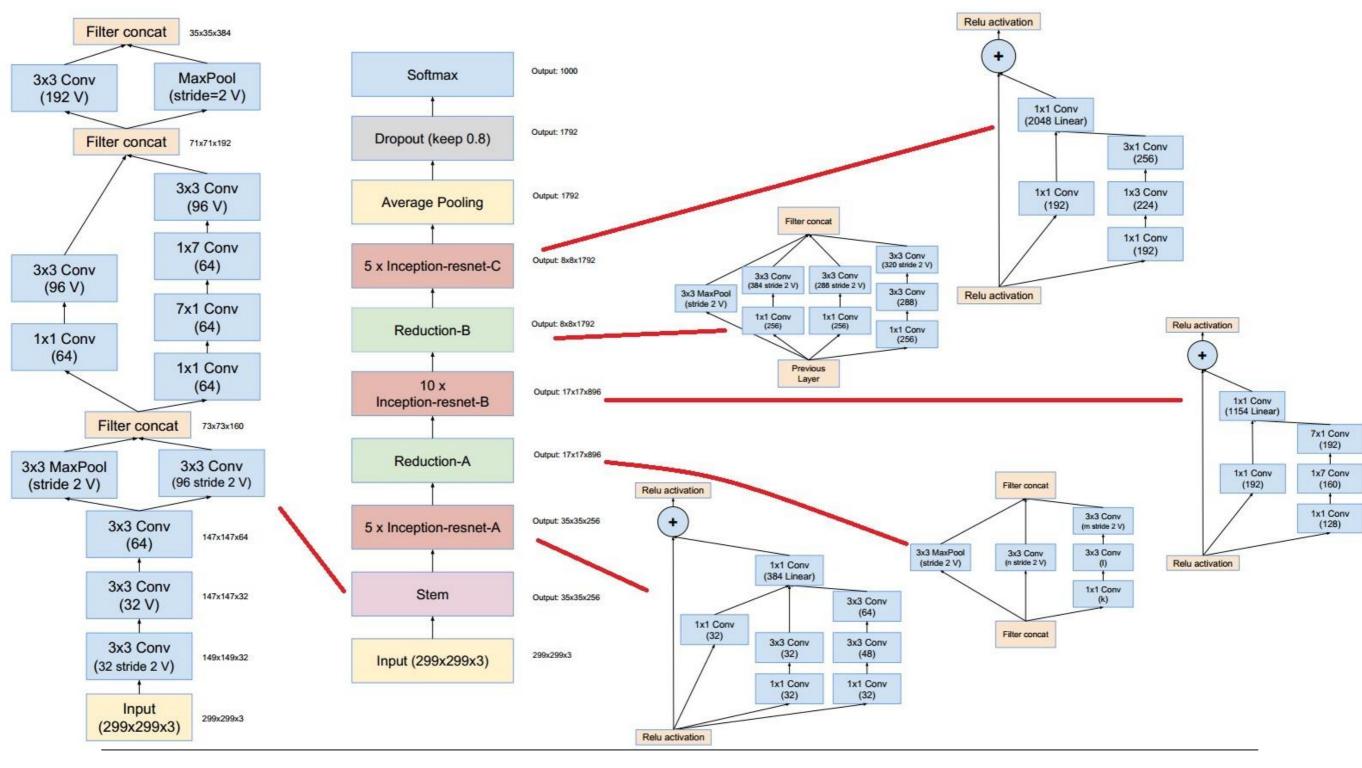
Shortcuts / ResNet (152 layers!)



He et al. Deep Residual Learning for Image Recognition. CVPR, IEEE Press, 2016



Inception v4





C. Szegedy et al., Inception-v4, Inception-ResNet and the Impact of Residual Connections on Learning, arXiv 2016

Definition of Visual Tasks



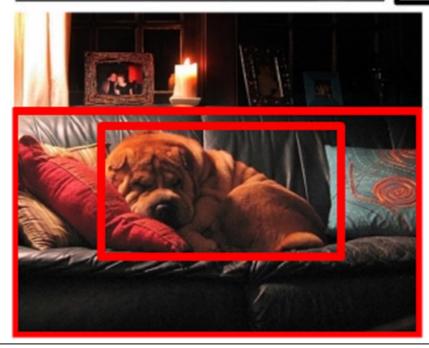


Classification Task:

Is there a dog in the image? Is there a sofa in the image?

Categorization Task:

Is this an indoor scene?



Localization Task:

Where is the dog in the image?

Detection Task:

Where are known objects (dog, sofa) in the image?

Tracking Task (generic/specific):

Where is the object/dog from the first frame in all subsequent frames of the image sequence?



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