I Robot
Isaac Asimov
1950
Future Vision

Eye Robot
CSCI 1430
2017 MWF 1pm
Computer Vision
**Convolutional Layer**

Perceptron: \[ \text{output} = \begin{cases} 0 & \text{if } w \cdot x + b \leq 0 \\ 1 & \text{if } w \cdot x + b > 0 \end{cases} \]

\[ w \cdot x \equiv \sum_j w_j x_j. \]

*This is convolution!*

Share the same parameters across different locations (assuming input is stationary):

Convolutions with learned kernels
Convolutional Layer

\[
\begin{bmatrix}
-1 & 0 & 1 \\
-1 & 0 & 1 \\
-1 & 0 & 1
\end{bmatrix}
\]

Shared weights
Convolutional Layer

Learn multiple filters.
Filter = ‘local’ perceptron.
Also called kernel.

E.g.: 200x200 image
100 Filters
Filter size: 10x10
10K parameters
By *pooling* responses at different locations, we gain robustness to the exact spatial location of image features.
AlexNet diagram (simplified) [Krizhevsky et al. 2012]

Input size
227 x 227 x 3

Conv 1
11 x 11 x 3
Stride 4
96 filters

Conv 2
5 x 5 x 96
Stride 1
256 filters

Conv 3
3 x 3 x 256
Stride 1
384 filters

Conv 4
3 x 3 x 192
Stride 1
384 filters

Conv 4
3 x 3 x 192
Stride 1
256 filters
Architecture for Classification

Total nr. params: 60M

4M

LINEAR

16M

FULLY CONNECTED

37M

FULLY CONNECTED

MAX POOLING

442K

CONV

74M

1.3M

CONV

224M

884K

CONV

149M

MAX POOLING

LOCAL CONTRAST NORM

307K

CONV

223M

MAX POOLING

LOCAL CONTRAST NORM

35K

CONV

105M

Total nr. flops: 832M

4M

16M

37M
Training Neural Networks

Learning the weight matrices $W$
Gradient descent
General approach

Pick random starting point.
General approach

Compute gradient at point (analytically or by finite differences)
General approach

Move along parameter space in direction of negative gradient

\[ a_2 = a_1 - \gamma \nabla f(a_1) \]

\( \gamma = \text{amount to move} \)

= learning rate
General approach

Move along parameter space in direction of negative gradient.

\[ a_3 = a_2 - \gamma \nabla f(a_2) \]

\( \gamma = \) amount to move
\( = \) learning rate
General approach

Stop when we don’t move any more.

\[ a_{n-1} - \gamma \nabla f(a_{n-1}) = 0 \]
Gradient descent

• Optimizer for functions.
• Guaranteed to find optimum for convex functions.
  • Non-convex = find *local* optimum.
  • Most vision problems aren’t convex.

• Works for multi-variate functions.
  • Need to compute matrix of *partial derivatives* (“*Jacobian*”)
Train NN with Gradient Descent

- $x^i, y^i = n$ training examples
- $f(x) =$ feed forward neural network
- $L(x, y; \theta) =$ some loss function

- *Loss function* measures how ‘good’ our network is at classifying the training examples wrt. the parameters of the model (the perceptron weights).
Train NN with Gradient Descent

Loss function
(Evaluate NN on training data)

Model parameters (perceptron weights)
How Good is a Network?

\[ y = [0 \ldots 0 \ 1 \ldots 0] \]
What is an appropriate loss?

- Define some output threshold on detection
- Classification: compare training class to output class
- Zero-one loss $L$ (per class)

$$
y = \text{true label} \quad \hat{y} = \text{predicted label} \quad L(\hat{y}, y) = I(\hat{y} \neq y),$$

- Is it good?
  - Nope – it’s a step function.
  - I need to compute the gradient of the loss.
  - This loss is not differentiable, and ‘flips’ easily.
Classification has binary outputs

Special function on last layer - ‘Softmax’:

• "squashes" a $C$-dimensional vector $\mathbf{O}$ of arbitrary real values to a $C$-dimensional vector $\sigma(\mathbf{O})$ of real values in the range $(0, 1)$ that add up to 1.

• Turns the output into a probability distribution on classes.

\[
p(c_k = 1 | \mathbf{x}) = \frac{e^{o_k}}{\sum_{j=1}^{C} e^{o_j}}
\]
How Good is a Network?

Probability of class $k$ given input (softmax):

$$p(c_k = 1 | x) = \frac{e^{o_k}}{\sum_{j=1}^{c} e^{o_j}}$$
**Cross-entropy loss function**

- Negative log-likelihood

\[ L(x, y; \theta) = - \sum_j y_j \log p(c_j | x) \]

- Is it a good loss?
  - Differentiable
  - Cost decreases as probability increases
How Good is a Network?

\[ y = \begin{bmatrix} 0 & 0 & \cdots & 1 & 0 & \cdots & 0 \end{bmatrix} \]

Probability of class \( k \) given input (softmax):

\[
p(c_k = 1|x) = \frac{e^{o_k}}{\sum_{c} e^{o_j}}
\]

(Per-sample) Loss; e.g., negative log-likelihood (good for classification of small number of classes):

\[
L(x, y; \theta) = -\sum_{j} y_j \log p(c_j|x)
\]
Learning consists of minimizing the loss (plus some regularization term) w.r.t. parameters over the whole training set.

$$\theta^* = \arg \min_\theta \sum_{n=1}^{P} L(x^n, y^n ; \theta)$$
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\[ \theta^* = \arg \min_{\theta} \sum_{n=1}^{P} L(x^n, y^n; \theta) \]

**Question:** How to minimize a complicated function of the parameters?

**Answer:** Chain rule, a.k.a. **Backpropagation**! That is the procedure to compute gradients of the loss w.r.t. parameters in a multi-layer neural network.

Rumelhart et al. “Learning internal representations by back-propagating..” Nature 1986
Key Idea: Wiggle To Decrease Loss

Let's say we want to decrease the loss by adjusting $W_{i,j}^1$. We could consider a very small $\epsilon = 1e-6$ and compute:

$$L(x, y; \theta)$$

$$L(x, y; \theta \setminus W_{i,j}^1, W_{i,j}^1 + \epsilon)$$
Key Idea: Wiggle To Decrease Loss

Let's say we want to decrease the loss by adjusting $W_{i,j}^1$. We could consider a very small $\epsilon = 1 \times 10^{-6}$ and compute:

$$L(x, y; \theta)$$

$$L(x, y; \theta \setminus W_{i,j}^1, W_{i,j}^1 + \epsilon)$$

Then, update:

$$W_{i,j}^1 \leftarrow W_{i,j}^1 + \epsilon \text{sgn}(L(x, y; \theta) - L(x, y; \theta \setminus W_{i,j}^1, W_{i,j}^1 + \epsilon))$$
Derivative w.r.t. Input of Softmax

\[
p(c_k = 1|x) = \frac{e^{o_k}}{\sum_j e^{o_j}}
\]

\[
L(x, y; \theta) = -\sum_j y_j \log p(c_j|x) \quad y = [0 \ldots 0 \ 1 \ 0 \ldots 0]
\]

By substituting the first formula in the second, and taking the derivative w.r.t. \( o \) we get:

\[
\frac{\partial L}{\partial o} = p(c|x) - y
\]
Given $\frac{\partial L}{\partial o}$ and assuming we can easily compute the Jacobian of each module, we have:

$$\frac{\partial L}{\partial W^3} = \frac{\partial L}{\partial o} \frac{\partial o}{\partial W^3}$$
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$$\frac{\partial L}{\partial W^3} = \frac{\partial L}{\partial \mathbf{o}} \frac{\partial \mathbf{o}}{\partial W^3}$$

$$\frac{\partial L}{\partial h^2} = \frac{\partial L}{\partial \mathbf{o}} \frac{\partial \mathbf{o}}{\partial h^2}$$

$$\frac{\partial L}{\partial W^3} = (p(c|x) - y) h^{2T}$$

$$\frac{\partial L}{\partial h^2} = W^{3T} (p(c|x) - y)$$
Given $\frac{\partial L}{\partial h^2}$, we can compute now:

$$\frac{\partial L}{\partial W^2} = \frac{\partial L}{\partial h^2} \frac{\partial h^2}{\partial W^2}$$

$$\frac{\partial L}{\partial h^1} = \frac{\partial L}{\partial h^2} \frac{\partial h^2}{\partial h^1}$$
Backward Propagation

\[ \frac{\partial L}{\partial h^1} \]

\[ \frac{\partial L}{\partial h^2} \]

\[ \frac{\partial L}{\partial o} \]

Given \( \frac{\partial L}{\partial h^1} \), we can compute now:

\[ \frac{\partial L}{\partial W^1} = \frac{\partial L}{\partial h^1} \frac{\partial h^1}{\partial W^1} \]
Backward Propagation

**Question:** Does BPROP work with ReLU layers only?

**Answer:** Nope, any a.e. differentiable transformation works.
But the ReLU is not differentiable at 0!

Right. Fudge!

- ‘0’ is the best place for this to occur, because we don’t care about the result (it is no activation).
- ‘Dead’ perceptrons
- ReLU has unbounded positive response:
  - Faster convergence
  - But can cause your gradient response to ‘explode’.
Backward Propagation

**Question:** Does BPROP work with ReLU layers only?

**Answer:** Nope, any a.e. differentiable transformation works.

**Question:** What's the computational cost of BPROP?

**Answer:** About twice FPROP (need to compute gradients w.r.t. input and parameters at every layer).

**Note:** FPROP and BPROP are dual of each other. E.g.,:
Optimization demo


- Thank you Matt Mazur
Toy Code (Matlab): Neural Net Trainer

% F-PROP
for i = 1 : nr_layers - 1
    [h{i}  jac{i}] = nonlinearity(W{i} * h{i-1} + b{i});
end
h{nr_layers-1} = W{nr_layers-1} * h{nr_layers-2} + b{nr_layers-1};
prediction = softmax(h{l-1});

% CROSS ENTROPY LOSS
loss = - sum(sum(log(prediction) .* target)) / batch_size;

% B-PROP
dh{l-1} = prediction - target;
for i = nr_layers - 1 : -1 : 1
    Wgrad{i} = dh{i} * h{i-1}';
    bgrad{i} = sum(dh{i}, 2);
    dh{i-1} = (W{i}' * dh{i}) .* jac{i-1};
end

% UPDATE
for i = 1 : nr_layers - 1
    W{i} = W{i} - (lr / batch_size) * Wgrad{i};
    b{i} = b{i} - (lr / batch_size) * bgrad{i};
end
Stochastic Gradient Descent

• Dataset can be too large to strictly apply gradient descent.

• Instead, randomly sample a data point, perform gradient descent per point, and iterate.
  • True gradient is approximated only
  • Picking a subset of points: “mini-batch”

Pick starting $W$ and learning rate $\gamma$

While not at minimum:
  • Shuffle training set
  • For each data point $i=1...n$ (maybe as mini-batch)
    • Gradient descent

“Epoch”
Stochastic Gradient Descent

Loss will not always decrease (locally) as training data point is random.

Still converges over time.
Gradient descent oscillations
Gradient descent oscillations

Slow to converge to the (local) optimum
Momentum

• Adjust the gradient by a weighted sum of the previous amount plus the current amount.

• Without momentum: \[ \theta_{t+1} = \theta_t - \gamma \frac{\partial L}{\partial \theta} \]

• With momentum (new \( \alpha \) parameter):

\[
\theta_{t+1} = \theta_t - \gamma \left( \alpha \left[ \frac{\partial L}{\partial \theta} \right]_{t-1} + \left[ \frac{\partial L}{\partial \theta} \right]_t \right)
\]
But James...

...I thought we were going to treat machine learning like a black box? I like black boxes.

Deep learning is:
- a black box
But James...

...I thought we were going to treat machine learning like a black box? I like black boxes.

Deep learning is:
- a black box
- also a black art.
But James...

...I thought we were going to treat machine learning like a black box? I like black boxes.

Many approaches and hyperparameters:

   Activation functions, learning rate, mini-batch size, momentum...

Often these need tweaking, and you need to know what they do to change them intelligently.
Nailing hyperparameters + trade-offs

agokasla 6:56 PM
uploaded and commented on this image: image.png

"WOOT! Nailed the hyperparameters. 4 generator updates per discriminator update. Wait extra long before you initiate the switch.

jamestompkin 6:57 PM
Well done - I wonder if we can turn hyperparameter nailing into the next e-Sport?

agokasla 4:30 AM
I am starting to think that the numeric instability of the model is starting to become a real issue. Lowering the learning rate could make it more stable, but it would require lowering it by two orders of magnitude which would make it take 100x longer to train right? 😞
Lowering the learning rate = smaller steps in SGD

- Less ‘ping pong’
- Takes longer to get to the optimum
Flat regions in energy landscape
Problem of fitting

• Too many parameters = overfitting
• Not enough parameters = underfitting

• More data = less chance to overfit

• How do we know what is required?
Regularization

- Attempt to guide solution to *not overfit*
- But still give freedom with many parameters
Data fitting problem
Which is better?
Which is better *a priori*?

9th order polynomial

1st order polynomial
Regularization

• Attempt to guide solution to *not overfit*
• But still give freedom with many parameters

• Idea:
  *Penalize the use of parameters to prefer small weights.*
Regularization:

- Idea: add a cost to having high weights
- $\lambda =$ regularization parameter

$$C = C_0 + \lambda \sum_w w^2,$$
Both can describe the data...

• ...but one is simpler.

• Occam’s razor:
  "Among competing hypotheses, the one with the fewest assumptions should be selected"

For us:

Large weights cause large changes in behaviour in response to small changes in the input.
Simpler models (or smaller changes) are more robust to noise.
Regularization

- Idea: add a cost to having high weights
- \( \lambda = \text{regularization parameter} \)

\[
C = C_0 + \lambda \sum_w w^2,
\]

\[
C = -\frac{1}{n} \sum_{x_j} \left[ y_j \ln a_j^L + (1 - y_j) \ln (1 - a_j^L) \right] + \lambda \sum_w w^2.
\]

- Normal cross-entropy loss (binary classes)
- Regularization term
Regularization: Dropout

• Our networks typically start with random weights.
• Every time we train = slightly different outcome.

• Why random weights?
• If weights are all equal, response across filters will be equivalent.
  • Network doesn’t train.
Regularization

• Our networks typically start with random weights.
• Every time we train = slightly different outcome.

• Why not train 5 different networks with random starts and vote on their outcome?
  • Works fine!
  • Helps generalization because error is averaged.
Regularization: Dropout
Regularization: Dropout

At each mini-batch:
- Randomly select a subset of neurons.
- Ignore them.

On test: half weights outgoing to compensate for training on half neurons.

Effect:
- Neurons become less dependent on output of connected neurons.
- Forces network to learn more robust features that are useful to more subsets of neurons.
- Like averaging over many different trained networks with different random initializations.
- Except cheaper to train.

[Nielson]
More regularization

• Adding more data is a kind of regularization
• Pooling is a kind of regularization
• Data augmentation is a kind of regularization