A Computational Viewpoint for Deep Learning

Liangliang Cao
Jan 28, 2014

http://llcao.net/cu-deeplearning15/

Outline

- An abstract view of deep network
- An abstract view of deep network solver
- Three cases
  - Logistic regression
  - Multiple-layer perceptron (MLP)
  - Convolutional neural network (CNN)
- Q/A; Discussions on course project ideas

Homework and Course Arrangement

- Very easy homework. Deadline passed. Late submissions will be NOT accepted.
- Those who did a good hw#1 will be notified
- Please consider dropping the course if you fail with hw#1
  - Coz you will receive a VERY low score with the course going
- Homework will be explained in class#4
- Why do we assign this homework?

Outline

- **An abstract view of deep network**
- An abstract view of deep network solver
- Three case studies
  - Logistic regression
  - Multiple-layer perceptron (MLP)
  - Convolutional neural network (CNN)
- Q/A; Discussions on course project ideas

An abstract view of deep network

- Estimate the output

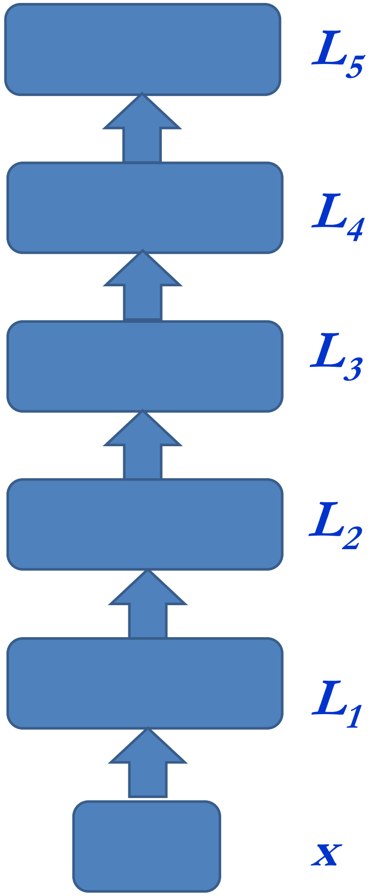
$$o_1 = L_1(x)$$
$$o_2 = L_2(L_1(x))$$
$$\ldots$$
$$o_5 = L_5(L_4(L_3(L_2(L_1(x)))))$$

- Compute the loss function

$$C = Loss(o_5, y)$$

- Compute the gradient $\frac{\partial C}{\partial \mathbf{o}_i} = \frac{\partial C}{\partial \mathbf{o}_{i+1}} \frac{\partial \mathbf{o}_{i+1}}{\partial \mathbf{o}_i}$

$$\frac{\partial C}{\partial \mathbf{o}_1} = \frac{\partial C}{\partial \mathbf{o}_5} \cdot \frac{\partial \mathbf{o}_5}{\partial \mathbf{o}_4} \cdot \frac{\partial \mathbf{o}_4}{\partial \mathbf{o}_3} \cdot \frac{\partial \mathbf{o}_3}{\partial \mathbf{o}_2} \cdot \frac{\partial \mathbf{o}_2}{\partial \mathbf{o}_1}$$



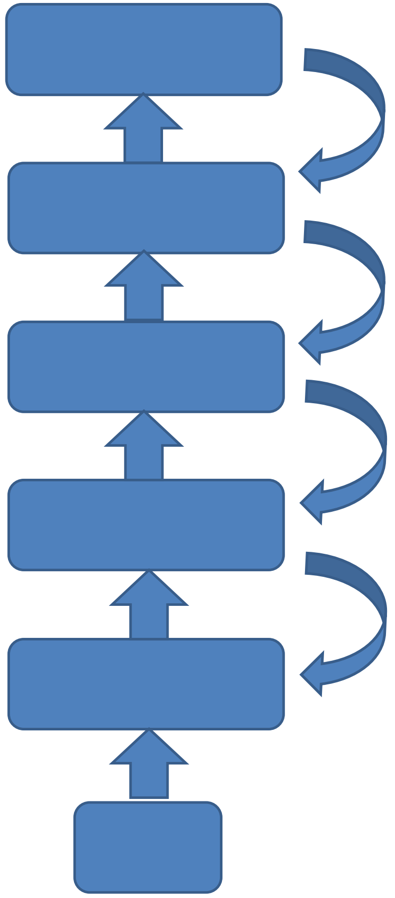
An abstract view of deep network (2)

- Estimate the output (Forward propagation)

$$o_5 = L_5(\,L_4(\,L_3(\,L_2(\,L_1(\mathbf{x})\,)\,)\,)\,)$$

- Compute the gradient (Backward propagation)

$$\frac{\partial C}{\partial \mathbf{o}_1} = \frac{\partial C}{\partial \mathbf{o}_5} \cdot \frac{\partial \mathbf{o}_5}{\partial \mathbf{o}_4} \cdot \frac{\partial \mathbf{o}_4}{\partial \mathbf{o}_3} \cdot \frac{\partial \mathbf{o}_3}{\partial \mathbf{o}_2} \cdot \frac{\partial \mathbf{o}_2}{\partial \mathbf{o}_1}$$



An abstract view of deep network (3)

- Suppose a layer is in the form of

$$o_l = L_l(\mathbf{x}) = f_l(\mathbf{w}^T\mathbf{x} + b)$$

- We can compute the gradients s.t. parameters

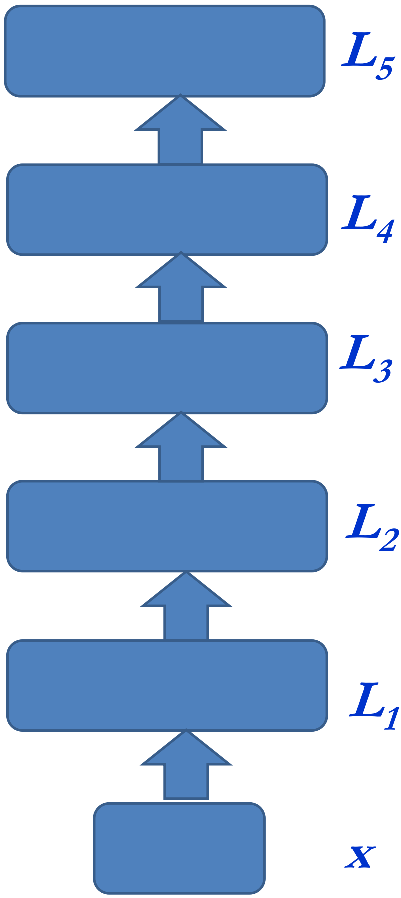
$$\frac{\partial C}{\partial \mathbf{w}} = \sum_i \frac{\partial C}{\partial o_l} \cdot f_l' \cdot \mathbf{x}_i \qquad \frac{\partial C}{\partial b} = \sum_i \frac{\partial C}{\partial o_l} \cdot f_l'$$

- Updating parameters by gradient descent

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial C}{\partial \mathbf{w}} \qquad b \leftarrow b - \alpha \frac{\partial C}{\partial b}$$

An abstract view of deep network (Summary)

- There are many ways to define layers and cost functions
- Layer definitions may differ from field to field
  - Computer vision
  - NLP
  - Speech
  - …
- But there are only **three key steps** in deep network



An abstract view of deep network (Summary)

1. Forward propagation

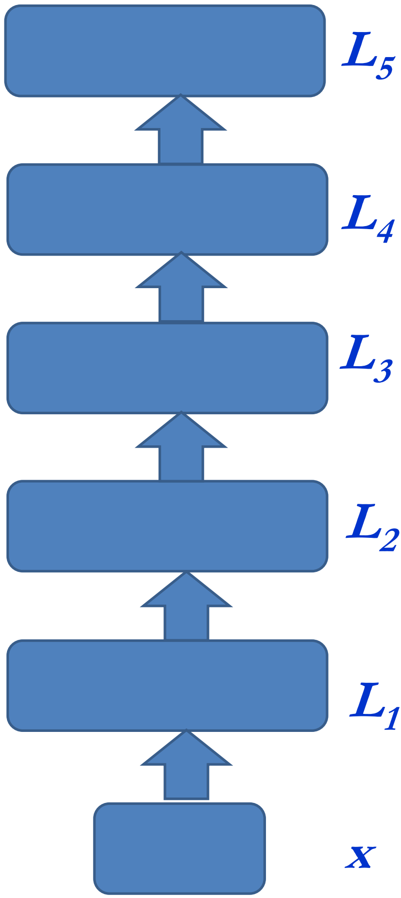
$$o_5 = L_5(\,L_4(\,L_3(\,L_2(\,L_1(\mathbf{x})\,)\,)\,)\,)$$

2. Backward propagation

$$\frac{\partial C}{\partial \mathbf{o}_1} = \frac{\partial C}{\partial \mathbf{o}_5} \cdot \frac{\partial \mathbf{o}_5}{\partial \mathbf{o}_4} \cdot \frac{\partial \mathbf{o}_4}{\partial \mathbf{o}_3} \cdot \frac{\partial \mathbf{o}_3}{\partial \mathbf{o}_2} \cdot \frac{\partial \mathbf{o}_2}{\partial \mathbf{o}_1}$$

3. Updating

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial C}{\partial \mathbf{w}} \qquad b \leftarrow b - \alpha \frac{\partial C}{\partial b}$$



Outline

- An abstract view of deep network
- **An abstract view of deep network solver**
- Three cases
  - Logistic regression
  - Multiple-layer perceptron (MLP)
  - Convolutional neural network (CNN)
- Q/A; Discussions on course project ideas

Brainstorming question:

Deep neural networks have been studied by Hinton, LeCun, Bengio, Schmidhuber, and many others since 1990s.

Why **only recently** it becomes hot (again)?

My understanding

Two reasons

In 1990s we do not have large scale datasets

In 2000s we have not only large scale datasets but also powerful computers (w/o GPUs) to compute them

But what is the algorithm to learn from the large scale datasets?

A typical optimization problem

Very often, a machine learning model with parameter $\mathbf{w}$ aims to minimize

$$\min_{\mathbf{w}} \frac{1}{N}\sum_{i=1}^{N} C(\mathbf{x}_i, y_i|\mathbf{w})$$

with the hope that the cost in the testing set $\boldsymbol{T}$ will be small too.

$$\frac{1}{|T|}\sum_{j\in T} C(\mathbf{x}_j, y_j|\mathbf{w})$$

A typical optimization problem

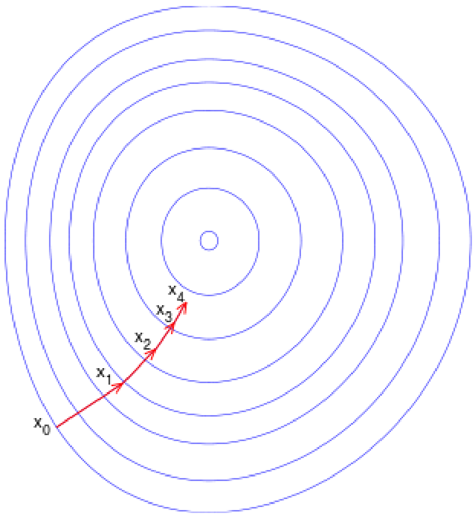
Very often, a machine learning model with parameter $\mathbf{w}$ aims to minimize

$$\min_{\mathbf{w}} \frac{1}{N} \sum_{i=1}^{N} C(\mathbf{x}_i, y_i | \mathbf{w})$$

If C is convex and continuous, we can try

1) gradient descent

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{1}{N} \sum_{i=1}^{N} \frac{\partial C(\mathbf{x}_i, y_i | \mathbf{w})}{\partial \mathbf{w}}$$



A typical optimization problem

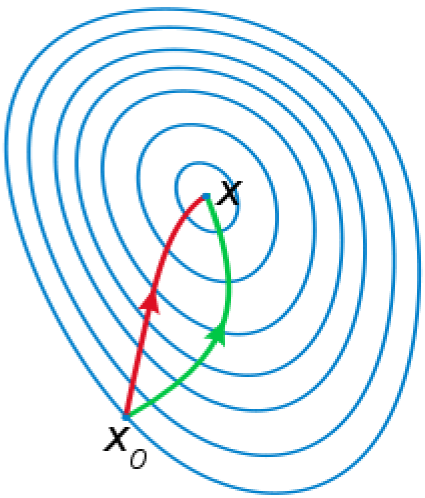
Very often, a machine learning model with parameter **w** aims to minimize

$$\min_{\mathbf{w}} \frac{1}{N}\sum_{i=1}^{N} C(\mathbf{x}_i, y_i|\mathbf{w})$$

If C is convex and continuous, we can try

1) gradient descent

2) Newton's method and its variants



$$w_{t+1} = w_t - \boxed{\Gamma_t}\frac{1}{n}\sum_{i=1}^{n} \nabla_w C(\mathbf{x}_i, y_i|\mathbf{w})$$

inverse of Hessian

A typical optimization problem

Very often, a machine learning model with parameter **w** aims to minimize

$$\min_{\mathbf{w}} \frac{1}{N} \sum_{i=1}^{N} C(\mathbf{x}_i, y_i | \mathbf{w})$$

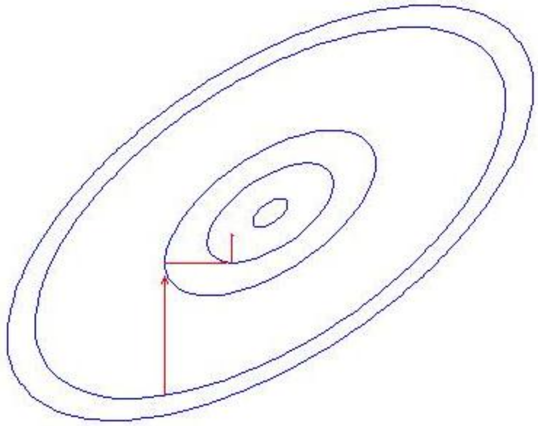
If C is convex and continuous, we can try

1) gradient descent

2) Newton's method and its variants

3) Coordinate descent

4) …



A typical optimization problem

Very often, a machine learning model with parameter $\mathbf{w}$ aims to minimize

$$\min_{\mathbf{w}} \frac{1}{N} \sum_{i=1}^{N} C(\mathbf{x}_i, y_i | \mathbf{w})$$

when N is big, we can see that

- The gradient $\frac{1}{N} \sum_{i=1}^{N} \frac{\partial C(\mathbf{x}_i, y_i|\mathbf{w})}{\partial \mathbf{w}}$ becomes very expensive.
- Even worse, we may not be able to load all ($\mathbf{x}_i$, y_i) in to memory!

Stochastic Gradient Descent (SGD)

Idea: estimate the gradient on a randomly picked sample

- Gradient descent $$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{1}{N} \sum_{i=1}^{N} \frac{\partial C(\mathbf{x}_i, y_i | \mathbf{w})}{\partial \mathbf{w}}$$
- Stochastic gradient descent $$\mathbf{w} \leftarrow \mathbf{w} - \alpha_t \frac{\partial C(\mathbf{x}_t, y_t | \mathbf{w})}{\partial \mathbf{w}}$$

Theoretical requirement for convergence:

$$\sum_t \alpha_t^2 < \infty \qquad \sum_t \alpha_t = \infty$$

in deep learning practice we just choose a small rate and then decrease it

Stochastic gradient descent (SGD) on single machines is much easier to program than many optimization methods!

Example: traditional SVM optimization (SMO)

Classifier $F(\mathbf{x}) = \sum_{i=1}^{N} \alpha_i K(\mathbf{x}, \mathbf{x}_i)$ with the cost function

$$\arg\max_{\alpha} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$0 \le \alpha_i \le \frac{C}{N}, \qquad \sum_{i=1}^{N} \alpha_i y_i = 0$$

SMO algorithm:

1. Heuristically picks 2 variables, say α_i, α_j, and freeze the other variables.
2. Analytically update α_i, α_j
3. Iterate until converges.

You may write hundreds or even thousands of lines of codes to implement SMO

But you can implement a stochastic SVM in 10 lines

```
function w=pegasos_SVM(X,Y,lambda,nepochs)
[m,d] = size(X); w = zeros(d,1); t = 1;
for (i=1:nepochs)          % iterations over the full data
    for (tau=1:m)          % pick a single data point
        if (Y(tau)*X(tau,:)*w < 1)     % data too close or wrongly separa
            w = (1-1/t)*w + 1/(lambda*t)*Y(tau)*X(tau,:)';
        else
            w = (1-1/t)*w;
        end
        t=t+1;             % increment counter
    end
end
```

Can you find the problem of this code?

Pegasos SVM by Shai Shalev-Shwartz

Philosophy of SGD

- One iteration of SGD is way faster than one iteration of GD
- SGD relies on randomness to reduce the cost although it may not find the global minimum
- But SGD fits better data + local minimum than global minimum, esp when
  - Cost function is not convex
  - Training set is not the same distribution as testing set

SGD as a typical deep learning solver

```
for patch = uttL
    self.mlp_.forward(xs(patch,:));
    self.mlp_.backward(ys(patch,:));
    self.mlp_.update();
end
```

For every layer, compute the gradient and update.

```
self.W_ = self.W_ - self.EW_ * self.step_;
self.B_ = self.B_ - self.EB_ * self.step_;
```

SGD and GPUs

```
for patch = uttL
    self.mlp_.forward(xs(patch,:));
    self.mlp_.backward(ys(patch,:));
    self.mlp_.update();
end
```

For every layer, compute the gradient and update.

```
self.W_ = self.W_ - self.EW_ * self.step_;
self.B_ = self.B_ - self.EB_ * self.step_;
```

- Within every batch, SGD is mainly matrix multiplication: perfect task for GPU!
- Beyond every batch, SGD is sequential: so multiple GPUs may help!

Outline

- An abstract view of deep network
- An abstract view of deep network solver
- **Three case studies**
  - **Logistic regression**
  - Multiple-layer perceptron (MLP)
  - Convolutional neural network (CNN)
- Q/A; Discussions on course project ideas

Logistic regression

Logistic regression = one layer neural network + neg-loglikelihood cost

LR can be used separately or as the last layer of MLP.

Consider the binary case:

- Decision function: $p(\mathbf{x}) = Pr(y = 1|\mathbf{x}) = \dfrac{\exp(\beta^T \mathbf{x})}{1 + \exp(\beta^T \mathbf{x})}$
- Cost $\sum_{i=1}^{N} C(\mathbf{x}_i, y_i) = \sum_{i=1}^{N} [y_i \log p(\mathbf{x}) + (1 - y_i) \log(1 - p(\mathbf{x}))]$

Solving logistic regression (traditional methods)

- Compute the gradient

$$L(\beta) = \sum_{i=1}^{N} C(\mathbf{x}_i, y_i)$$

- Solver 1: gradient descent

$$\frac{\partial L(\beta)}{\partial \beta} = \mathbf{X}^T(\mathbf{y} - \mathbf{p}) \qquad \beta = \beta - \alpha \frac{\partial L(\beta)}{\partial \beta}$$

- Solver 2: Newton's method

$$H = \nabla^2 L(\beta) = -\mathbf{X}^T \mathbf{W} \mathbf{X} \qquad \beta = \beta - H^{-1} \frac{\partial L(\beta)}{\partial \beta}$$

W is a diagonal matrix with the element as p(**x**)(1-p(**x**)).

Analyzing the traditional solver

- Solver 1: gradient descent

$$\frac{\partial L(\beta)}{\partial \beta} = \mathbf{X}^T(\mathbf{y} - \mathbf{p}) \qquad \beta = \beta - \alpha \frac{\partial L(\beta)}{\partial \beta}$$

- Solver 2: Newton's method

$$H = \nabla^2 L(\beta) = -\mathbf{X}^T \mathbf{W} \mathbf{X} \qquad \beta = \beta - H^{-1} \frac{\partial L(\beta)}{\partial \beta}$$

Newton's method converges faster than gradient descent, but it requires more time to compute the Hessian matrix

And Newton's method is expensive in large scale.

Comparing optimization methods for Logistic Reg.

	Global minimum	Memory consumption	Convergence speed	More criteria?
GD				
Newton's method				
SGD				

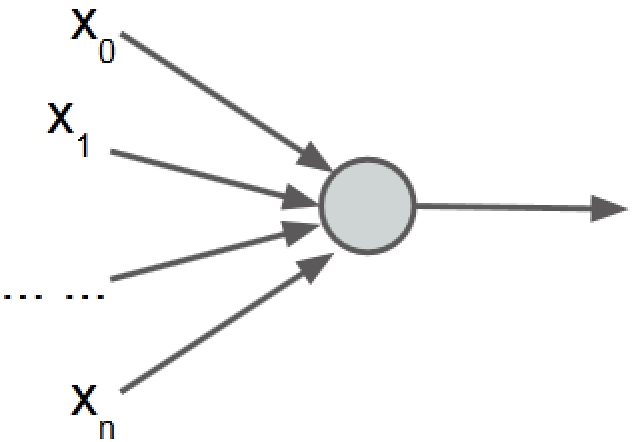
Outline

- An abstract view of deep network
- An abstract view of deep network solver
- **Three case studies**
  - Logistic regression
  - **Multiple-layer perceptron (MLP)**
  - Convolutional neural network (CNN)
- Q/A; Discussions on course project ideas

Multi-layer perceptron

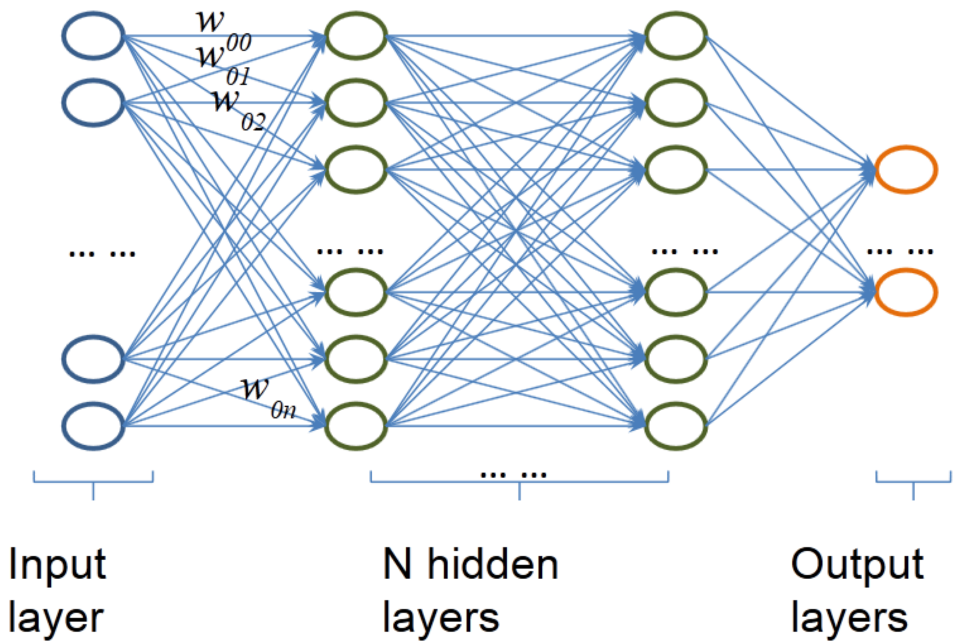
- Generalized from single layer perceptron

$$f(\mathbf{x}) = \begin{cases} 1 & \text{if} \;\; \mathrm{w}^T\mathbf{x} + b > 0 \\ 0 & \text{otherwise} \end{cases}$$



There is an interesting story between single layer perceptron and multi-layer perceptron. See [Minsky and Papert, 1969]

Multi-layer perceptron



The last layer is often logistic regression

The hidden layer is a perceptron with nonlinear function

$$\phi(\mathbf{w}^T\mathbf{x} + b)$$

ϕ can be sigmoid, tanh, or rectifier

Comparing optimization methods for MLP

	Global minimum	Memory consumption	Convergence speed	More criteria?
GD				
Newton's method				
SGD				

Tricks to train MLP with SGD

- Initialize the neurons with random weights
- Randomly shuffle the data
- Use a batch in every SGD iteration
- Choose the learning rate by multiple trials.

More details will be covered by Feb 11 class.

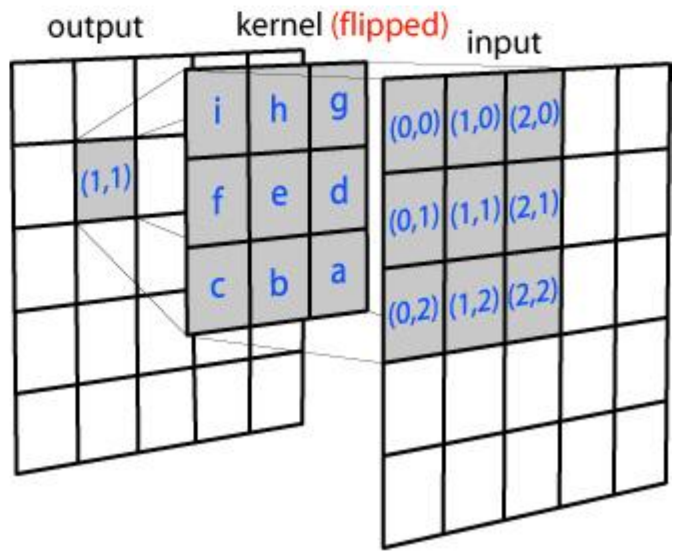
Outline

- An abstract view of deep network
- An abstract view of deep network solver
- **Three case studies**
  - Logistic regression
  - Multiple-layer perceptron (MLP)
  - **Convolutional neural network (CNN)**
- Q/A; Discussions on course project ideas

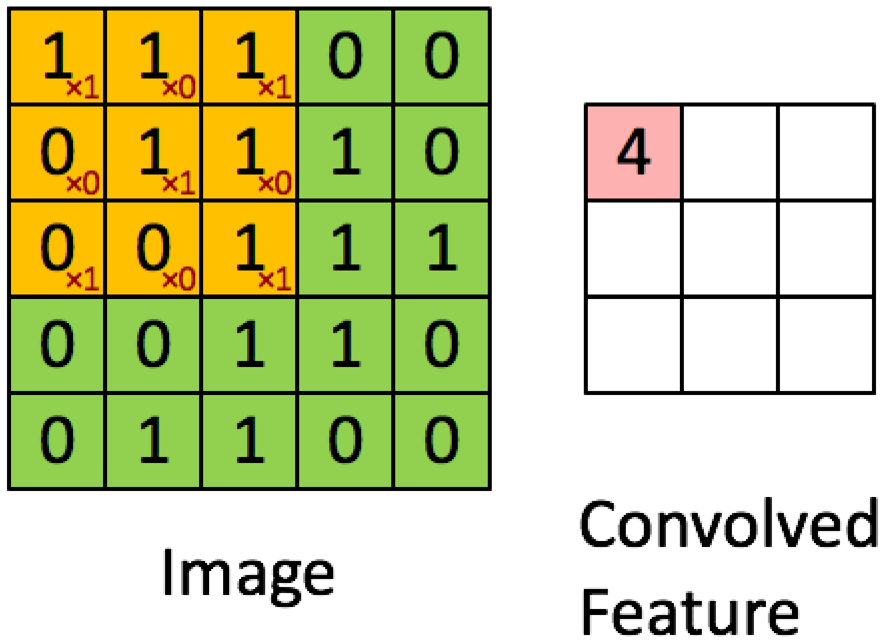
Convolutional Layer

- Almost all image filters can be represented as 2D convolution

$$y[m,n] = x[m,n] * h[m,n] = \sum_{j=-\infty}^{\infty} \sum_{i=-\infty}^{\infty} x[i,j] \cdot h[m-i, n-j]$$



A Nice Illustration of Convolution



Gif picture courtesy to ufldl.Stanford.edu/wiki

Forward and Backward Propagation for Conv Layer

- Forward propagation

$$y_{(s,j)} = \sum_{i \in f} x_{(s,i)} \star w_{(j,i)}$$

- Backward propagation

$$\frac{\partial L}{\partial x_{(s,i)}} = \sum_{j \in f'} \frac{\partial L}{\partial y_{(s,j)}} * w_{(j,i)}$$

$$\frac{\partial L}{\partial w_{(j,i)}} = \sum_{s \in S} \frac{\partial L}{\partial y_{(s,j)}} \star x_{(s,i)}$$

Why Deep CNN Is Powerful?

Conceptually, three reasons:

1. Many many filters

2. A number of layers

3. Conv + Pooling lead to local invariance

An Example of Deep CNN

Krizhevsky, Sutskever and Hinton

1st place, ImageNet LSVRC 2012

Classification output

2 fully connected layers

+

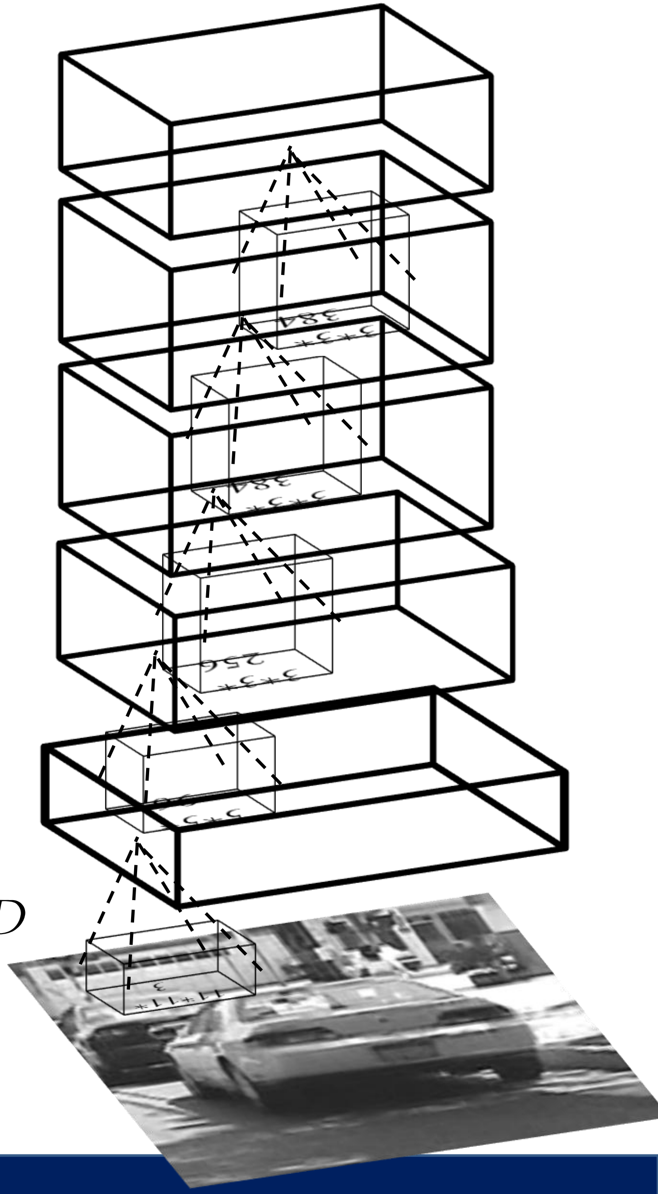
more layers of convolution

1st Conv Output 55*55*96

(11 x 11 x 96) conv3D

(4x4) max pooling

Input: 224*224*3



Local Invariance

Convolution is usually followed by a max-pooling layer

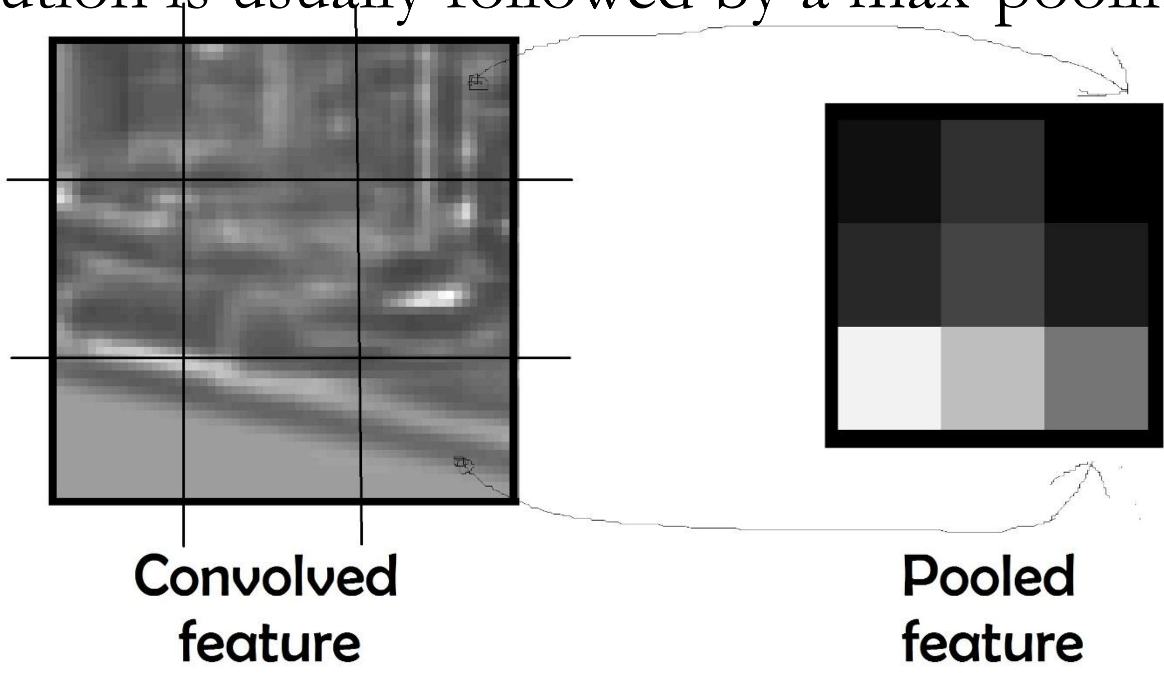


Image courtesy to Amol Mahurkar

- Convolution is translation invariant:
  - any translation invariant operation can be represented as a convolution.
- Convolution + max pooling can find local invariant features

Many Many Filters

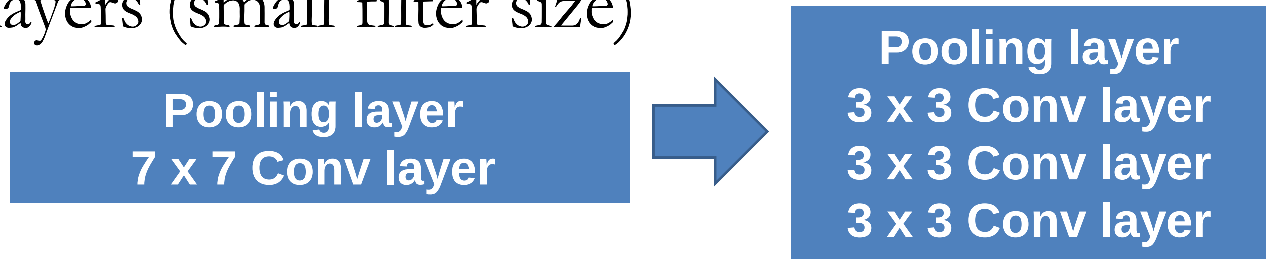
Number of filters in the Alex' CNN

- Filters in 1st conv layer: 3 x 96 (neighborhood 11 x 11)
- Filters in 2^{nd} conv layer: 96 x 128 (neighborhood 5 x 5)
- Filters in 3^{rd} conv layer: 256 x 384 (neighborhood 3 x 3)
- Filters in 4^{th} conv layer: 384 x 192 (neighborhood 3 x 3)
- Filters in 5^{th} conv layer: 384 x 128 (neighborhood 3 x 3)

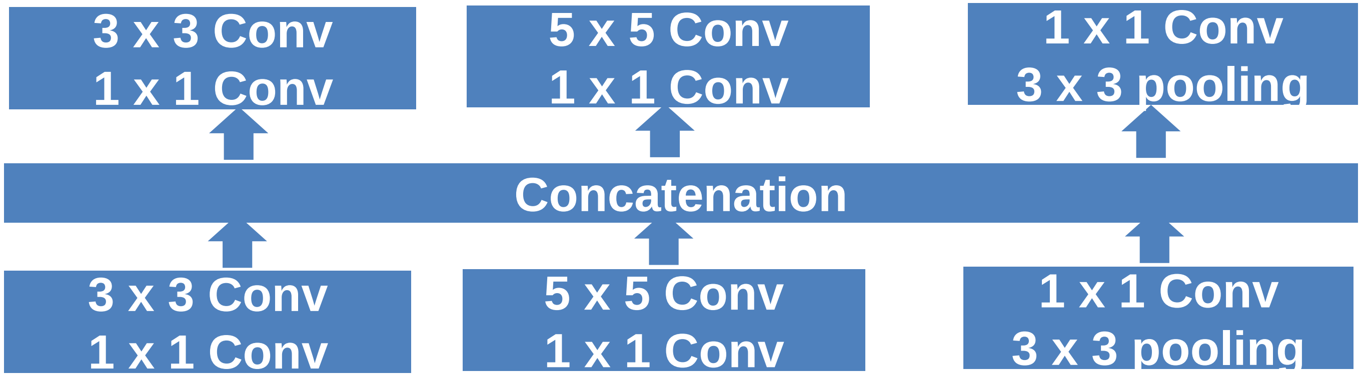
Millions of parameters!

Make the CNN Even Deeper

- [Simonyan and Zisserman 2014] suggests to use replace one conv layer (big filter size) with several concatenated conv layers (small filter size)



- [Szegedy et al 2014] proposes to replace one conv layer with concatenated inceptions



From 1D convolution to 2D convolution

1D convolution is widely used in speech and NLP

- Computational complexity: O(M*m)

2D/3D convolution is mainly used for image/video

- Computational complexity: O(M*N*m*n)

Convolution with 2D Gaussian is efficient by separating 2D into 2*1D

- Computational complexity O(M*N*m * 2)
- But most CNN filters cannot be separated

How Hard to Implement 2D Convolution?

- It is not super hard at the first glance

```
for w in 1..W
  for h in 1..H
    for x in 1..K
      for y in 1..K
        for m in 1..M
          for d in 1..D
            output(w, h, m) += input(w+x, h+y, d) * filter(m, x, y, d)
          end
        end
      end
    end
  end
end
```

- But we overlooked cache, parallelism, or any fancy SSE2 command
- And it becomes 10 times tricky with GPUs!

Three Ways to Implement Fast Convolution in GPU

1. Directly implement convolution algorithm
   - Extremely demanding with memory, data transportation, and model sharing
   - Very challenging for GPU programming skills

2. Change convolution to matrix multiplication
   - Make good use of existing BLAS or cuBLAS library
   - Maybe memory demanding

3. Use FFT instead of directly convolution
   - Convolution in image domain is equivalent to multiplication in frequency domain
   - Performance may depends on the image/filter size.

Projects

What kind of projects would you like to take in this class?

- Theory
- Applications
  1. NLP
  2. Vision
  3. NLP + Vision
  4. Your own data or problem?