Deep Learning
lecture 2
Supervised Learning (1)

Yi Wu, IIIS

Spring 2024

Mar-8

An overview of Lecture 1

- History and big names in deep learning
  - From Boolean circuits (starting from MP neuron in 1943) to differentiable networks
  - Backpropagation (1986) : first time to show neural network can learn features
    - The fundamental idea
  - Breakthrough in 2012
    - Speech Recognition
    - Unsupervised learning of concepts (cat)
    - Image classification

An overview of Lecture 1

- History and big names in deep learning
  - From Boolean circuits (starting from MP neuron in 1943) to differentiable networks
  - Backpropagation (1986) : first time to show neural network can learn features
    - The fundamental idea
  - Breakthrough in 2012
    - **Speech Recognition → Today's lecture (basics)**
    - Unsupervised learning of concepts (cat) → lecture 4
    - **Image classification → Today's lecture (basics)**

An overview of Lecture 1

- What makes deep learning so special?
  - $y = f(\phi(x))$ → $y = f(NN(x;\theta))$
    - Replace hand-tuned feature with a NN → *representation learning*
    - A differentiable model to learn features!
      - We will also talk about discrete models in future lectures. ☺

An overview of Lecture 1

- What makes deep learning so special?
  - $y = f(\phi(x)) \rightarrow y = f(NN(x;\theta))$
    - A differentiable model to learn features!
  - It redefines a machine learning algorithm
    - Conventional ML algorithm: a few steps of computations (machine program)
      - Data → feature → algorithm/model → output
    - DL algorithm: the network architecture and weights (connectionist machine)
      - Learning → (1) set up the right architecture & (2) enforce bias in weights
    - New algorithm design concept: the network architecture

Today’s Lecture

- Part 1: The simplest deep learning application ---- classification!
  - The very basic ideas of deep learning and backpropagation
  - Get a sense of parameter tuning (调参/炼丹)

- Part 2: Convolutional Neural Networks (CNN)
  - The very basic ideas of CNN

- More to come in the next lecture
  - More tricks and ideas

Recap: Classification

- Binary classification problem
  - Data $x \in \mathcal{X} \subseteq \mathbb{R}^d$, label $y(x) \in \{0,1\}$
  - a classifier $f(x;\theta) = y$ w.r.t. some parameter θ
  - Goal: learn θ^* such that for each x, $f(x)$ can correctly predict its label y

$$\theta^\star = \arg\min_\theta \int_x err\big(f(x;\theta), y(x)\big) P(x) dx$$

- Machine Learning
  - Define a proper $err()$ function
  - Estimate θ^* from a collection of samples $X = \{(x^i, y^i)\}$

Recap: Logistic Regression

- Logistic regression
  - $P(y=1) = f(x;\theta) = \sigma(w^T x + b)$
  - Logistic function (sigmoid function): $\sigma(x) = \frac{1}{1+e^{-x}}$
  - $err(f(x;\theta), y) = \begin{cases} -\log\sigma(w^T x + b) & y = 1 \\ -\log(1-\sigma(w^T x + b)) & y = 0 \end{cases}$

- Learning from data
  - Empirical Risk Minimization

$$\hat{\theta}^* = \arg\min_{\theta} \frac{1}{N} \sum_{(x^i, y^i) \in X} err(f(x^i;\theta), y^i)$$

Recap: Logistic Regression

- Logistic regression
  - $P(y=1) = f(x;\theta) = \sigma(w^T x + b)$
  - Logistic function (sigmoid function): $\sigma(x) = \frac{1}{1+e^{-x}}$
  - $err(f(x;\theta), y) = \begin{cases} -\log\sigma(w^T x + b) & y = 1 \\ -\log(1-\sigma(w^T x + b)) & y = 0 \end{cases}$

- Learning from data
  - Empirical Risk Minimization

$$\hat{\theta}^* = \arg\min_{\theta} \frac{1}{N} \sum_{(x^i, y^i) \in X} err(f(x^i;\theta), y^i)$$

Single-Layer Perceptron

- A differentiable single-layer perceptron with sigmoid activation
  - $\sigma(z)$ is a differentiable function over z and therefore w and x
  - Learning: $\widehat{w}^* = \arg\min_{w} \frac{1}{N} \sum_{(x^i, y^i) \in X} err(f(x^i; w), y^i)$
    - Minimize error on each training data

How to compute $\widehat{w}^*$?

Single-Layer Perceptron

- Problem Statement
  - Given $X = \{(x^i, y^i)\}$
  - Loss function $L(w) = \frac{1}{N}\sum_i err\left(f\left(x^i; w\right), y^i\right)$
  - Goal: minimize $L(w)$ w.r.t. w
  - $L(w)$ is continuous and differentiable

- An instance of *optimization problem*
  - if $L(w)$ is convex → convex optimization, we can find optimal solution
  - If $L(w)$ is non-convex → non-convex optimization, no guarantee
    - Deep learning in general is solving a non-convex optimization problem

Function Optimization

- Problem: minimize $L(w)$ w.r.t. w
- Solution: solve $\nabla L(w) = 0$

- How to ensure it is a (local) minimum?
- The Hessian $\nabla^2 L(w)$ is positive-definite!

convex

Non-convex

Multi-Variable Calculus Recap: Gradient

- Consider $f(X) = f(x_1, x_2, \dots, x_n)$

$$\nabla_X f(X) = \left[\frac{\partial f(X)}{\partial x_1}, \frac{\partial f(X)}{\partial x_2}, \dots, \frac{\partial f(X)}{\partial x_n}\right]$$

- Relation

$$df(s) = \nabla_X f(X) dX = \sum_i \frac{\partial f(X)}{\partial x_i} dx_i$$

- Notations
  - Gradient (∇), derivative (d), partial derivative (∂)
  - The gradient is the direction of fastest increase in $f(X)$

Multi-Variable Calculus Recap: Gradient

Multi-Variable Calculus Recap: Gradient

Multi-Variable Calculus Recap: Gradient

- The gradient $\nabla_X f(X)$ is perpendicular to the level curve

Multi-Variable Calculus Recap: Hessian

- The Hessian $\nabla^2 f(X)$ of a function $f(x_1, \dots, x_n)$ is given by the second derivative

- Positive-definite for a local minimum

$$\nabla_x^2 f(x_1,\dots,x_n) := \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdot & \cdot & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdot & \cdot & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \vdots & \vdots & \cdot & \cdot & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdot & \cdot & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Function Optimization (Cont'd)

- Problem: minimize $f(X)$ w.r.t. X
  - Unconstraint optimization

- Solution
  - Step 1: solve $\nabla f(X) = 0$
  - Step 2: calculate $\nabla^2 f(X)$ for candidates from (1) and verify positive-definiteness

- Issue: what if analytical solution is not feasible?

Function Optimization (Cont'd)

- Iterative solution
  - Start with a "guess" X^0, and iteratively refine X until $\nabla_X f(X) = 0$ is reached
- A greedy solution
  - Refine X such that $f(X)$ is decreased!
  - Idea: follow the gradient direction!

Function Optimization (Cont'd)

- The Gradient Descent algorithm
  - Choose X^0
  - $X^{k+1} = x^k - \eta^k \nabla_X f\left(X^k\right)^T$
  - Convergence: $\left|f\left(X^{k+1}\right) - f\left(X^k\right)\right| < \epsilon$
- Remark: GD may find a local optimum or a reflection point

- η^k learning rate
  - A critical parameter for gradient descent
  - More on next lecture

Function Optimization (Cont'd)

- Effectiveness of Learning rate η^k
  - Example: $f(x_1, x_2) = x_1^2 + x_1 x_2 + 4x_2^2$, $X^0 = [3,3]^T$
  - Remark
    - small η: safe but slow
    - Large η: may diverge

$\eta = 0.1$

$\eta = 0.2$

Learning the Single-Layer Perceptron

- Problem Statement
  - Given $X = \{(x^i, y^i)\}$
  - Loss function $L(w) = \frac{1}{N}\sum_i err(f(x^i; w), y^i)$
  - Goal: minimize $L(w)$ w.r.t. w

$$z = \sum_i w_i x_i$$

$$\frac{dy}{dz} = \sigma'(z)$$

$$\frac{dy}{dw_i} = \frac{dy}{dz}\frac{dz}{dw_i} = \sigma'(z)x_i$$

$$\frac{dy}{dx_i} = \frac{dy}{dz}\frac{dz}{dx_i} = \sigma'(z)w_i$$

Learning the Single-Layer Perceptron

- Gradient Descent
  - Initialize w^0; $w^{k+1} = w^k - \eta^k \nabla_w L(w)$ until convergence
- Compute the Gradient
  - $\nabla_w L(w) = \frac{1}{N}\sum_i \nabla_w err(f(x^i; w), y^i)$
  - $y = 1$: $\nabla_w err = -\nabla_w \log \sigma(w^T x^i) = -\frac{1}{err}\nabla_w \sigma(w^T x^i)$
  - $y = 0$: $\nabla_w err = -\nabla_w \log(1 - \sigma(w^T x + b)) = \frac{1}{err}\nabla_w \sigma(w^T x^i)$
- Gradient of Sigmoid neuron
  - $\sigma(z) = \frac{1}{1+e^{-z}}$ where $z = w^T x$
  - $\nabla_{w_i}\sigma(z) = \sigma'(z)x_i$ *and* $\nabla_{x_i}\sigma(z) = \sigma'(z)w_i$
  - $\sigma'(z) = \sigma(z)(1 - \sigma(z))$

Multi-Class Classification

- Example: digit classification
  - 10 classes
  - Sigmoid output → only 0-1 valued (binary class)
- Multi-Class Classification
  - C classes of labels (10 in digit recognition)
  - $P(y = c) = f_c(x; \theta)$
  - $f(x; \theta)$: a probability distribution
    - $f_c \geq 0$ and $\sum_c f_c = 1$
- We need a modified $\sigma(z)$ such that $\sigma(z)$ becomes a probability distribution

Multi-Class Classification

- Softmax Function
  - C classes, $w \in \mathbb{R}^{(d+1)\times C}$
  - $z = w^T x$, z is C dimensional
  - $f(x; w) = \mathrm{softmax}(z)$
  - $f_c(x; w) = \frac{e^{z_c}}{\sum_{j=1}^{C} e^{z_j}}$
- Interpretation
  - A "soft" version of max operator
  - A universal operator to convert a vector to ***a probability distribution***
  - z_i is often called *logit (refer to an unscaled value)*

Multi-Class Classification

- A multi-class perceptron
  - C classes, $z = w^T x$,
  - $f(x; w) = \text{softmax}(z), f_c(x; w) = \frac{e^{z_c}}{\sum_{j=1}^{C} e^{z_j}}$
- Learning
  - Given $X = \{(x^i, y^i)\}$, Loss function $L(w) = \frac{1}{N} \sum_i err(f(x^i; w); y^i)$
- The error function?
  - Maximize the log probability of target class $P(y = c) = f_c(x^i; w)$
  - $err(f(x^i; w), y^i) = -\log f_{y^i}(x^i; w)$

Multi-Class Classification

- The NLL loss (negative log-likelihood loss)
  - $err\left(f\left(x^i; w\right), y^i\right) = -\log f_{y^i}(x^i; w)$
  - $z = w^T x^i$, $f_c(x^i; w) = \frac{e^{z_c}}{\sum_{j=1}^{C} e^{z_j}}$
  - $L(w) = -\frac{1}{N}\sum_i \log f_{y^i}\left(x^i; w\right) = -\frac{1}{N}\sum_i \left(z_{y^i} - \log \sum_j e^{z_j}\right)$

- NLL loss is also called cross-entropy loss
  - It is equivalent to the cross entropy (交叉熵) between $f(x; w)$ and the delta probability $P(y = k) = 1$
    - $CE(p, q) = -\sum_c p(y = c) \log q(y = c)$
    - $p(y = k) = 1$ and $q = f(x; w)$
    - We also called the vector probability $[0,0, \dots, 0,1,0, \dots, 0]$ a one-hot vector

Multi-Class Classification

- Gradient Computation
  - Note: $z = w^T x^i$ and w is a matrix!
  - $\nabla_{w_{c,j}} L(w) = -\frac{1}{N} \sum_i \nabla_{w_{c,j}} \log f_{y^i}(x^i; w)$
  - $\nabla_{w_{c,j}} f_c(x^i; w) = \left(\nabla_{w_{c,j}} z_c - \frac{1}{\sum_k e^{z_k}} \nabla_{w_{c,j}} (\sum_k e^{z_k}) \right)$
  - $\nabla_{w_{c,j}} z_c = \nabla_{w_{c,j}} \left(\sum_{l=1}^{d+1} w_{c,l} x_l^i \right) = x_j^i$

- You have to do this in your coding project ☺

Multi-Layer Perceptron

- A N-layered MLP with Sigmoid activation function
  - Input layer: $y^{(0)} = x$
  - Hidden layer: $y^{(k)} = \sigma\left(z^{(k)}\right) = \sigma\left(w^{(k)^T} y^{(k-1)} + b^{(k)}\right)$
  - Output Layer: $y = \mathrm{softmax}\left(y^{(N)}\right)$
- Learning all the weights $\left\{w^{(k)}, b^{(k)}\right\}$ (also called weight and bias)

Learning MLPs

- Learning weights by gradient descent
  - Initialize all $\{w^{(k)}\}$ (assume $b^{(k)}$ is included in $w^{(k)}$)
  - For every k, i, j
  - Update $w_{i,j}^{(k)} \leftarrow w_{i,j}^{(k)} - \eta \frac{dL(w)}{dw_{i,j}^{(k)}}$ until convergence
- We need to compute gradient for ***every weight*!**
- How to efficiently compute all these gradients?

The Chain Rule

- Recap: Chain Rule for nested functions
  - $y = f(g_1(x), g_2(x), \dots, g_M(x))$
  - $\frac{dy}{dx} = \frac{\partial f}{\partial g_1(x)} \cdot \frac{dg_1(x)}{dx} + \dots + \frac{\partial f}{\partial g_M(x)} \cdot \frac{dg_M(x)}{dx}$

- A more complex example
  - How to compute $\frac{dDiv(Y,d)}{dw_{3,2}^{(1)}}$?
  - We need all intermediate values!

Computing Gradients

- The Forward Pass
  - Compute and save all the intermediate values
  - Set $y_{1:d_k}^{(0)} \leftarrow x$; and $y_{d_k+1}^{(k)} \leftarrow 1$
  - For layer $k \leftarrow 1 \ldots N$
    - $z^{(k)} = w^{(k)^T} y^{(k-1)}$
    - $y^{(k)} = f\left(z^{(k)}\right)$
    - $f()$: sigmoid function
  - Output $Y = y^{(K)}$

- Then Gradient?

Computing Gradients

- First compute $\nabla_{y^{(N)}} Div()$ directly

Computing Gradients

$$\frac{\partial Div}{\partial z_1^{(N)}} = \frac{\partial y_1^{(N)}}{\partial z_1^{(N)}} \frac{\partial Div}{\partial y_1^{(N)}}$$

Computing Gradients

$$\frac{\partial Div}{\partial z_1^{(N)}} = \frac{\partial y_1^{(N)}}{\partial z_1^{(N)}} \frac{\partial Div}{\partial y_1^{(N)}}$$

Computing Gradients

$$\frac{\partial Div}{\partial z_1^{(N)}} = \frac{\partial y_1^{(N)}}{\partial z_1^{(N)}} \frac{\partial Div}{\partial y_1^{(N)}}$$

$f_N'\left(z_1^{(N)}\right)$

Derivative of activation function

Computed in forward pass

Computing Gradients

$$\frac{\partial Div}{\partial z_i^{(N)}} = f_N'\left(z_i^{(N)}\right)\frac{\partial Div}{\partial y_i^{(N)}}$$

Computing Gradients

$$\frac{\partial Div}{\partial w_{11}^{(N)}} = \frac{\partial z_1^{(N)}}{\partial w_{11}^{(N)}} \frac{\partial Div}{\partial z_1^{(N)}}$$

Computing Gradients

$$\frac{\partial Div}{\partial w_{11}^{(N)}} = \frac{\partial z_1^{(N)}}{\partial w_{11}^{(N)}} \frac{\partial Div}{\partial z_1^{(N)}}$$

Just computed

Computing Gradients

$$\frac{\partial Div}{\partial w_{11}^{(N)}} = \frac{\partial z_1^{(N)}}{\partial w_{11}^{(N)}} \frac{\partial Div}{\partial z_1^{(N)}}$$

$y_1^{(N-1)}$

Because

$$z_1^{(N)} = w_{11}^{(N)} y_1^{(N-1)} + \text{other terms}$$

Computed in forward pass

Computing Gradients

$$\boxed{\frac{\partial Div}{\partial w_{ij}^{(N)}} = y_i^{(N-1)} \frac{\partial Div}{\partial z_j^{(N)}}}$$

For the bias term $y_0^{(N-1)} = 1$

Computing Gradients

$$\frac{\partial Div}{\partial y_1^{(N-1)}} = \sum_j \frac{\partial z_j^{(N)}}{\partial y_1^{(N-1)}} \frac{\partial Div}{\partial z_j^{(N)}}$$

Computing Gradients

$$\frac{\partial Div}{\partial y_1^{(N-1)}} = \sum_j \frac{\partial z_j^{(N)}}{\partial y_1^{(N-1)}} \frac{\partial Div}{\partial z_j^{(N)}}$$

Already computed

Computing Gradients

$$\frac{\partial Div}{\partial y_1^{(N-1)}} = \sum_j \frac{\partial z_j^{(N)}}{\partial y_1^{(N-1)}} \frac{\partial Div}{\partial z_j^{(N)}}$$

$w_{1j}^{(N)}$

Because

$$z_j^{(N)} = w_{1j}^{(N)} y_1^{(N-1)} + \text{other terms}$$

Computing Gradients

$$\frac{\partial Div}{\partial y_i^{(N-1)}} = \sum_j w_{ij}^{(N)} \frac{\partial Div}{\partial z_j^{(N)}}$$

Computing Gradients

We continue our way backwards in the order shown

$$\frac{\partial Div}{\partial z_i^{(N-1)}} = f'_{N-1}\left(z_i^{(N-1)}\right)\frac{\partial Div}{\partial y_i^{(N-1)}}$$

Computing Gradients

We continue our way backwards in the order shown

$$\frac{\partial Div}{\partial w_{ij}^{(N-1)}} = y_i^{(N-2)} \frac{\partial Div}{\partial z_j^{(N-1)}}$$

For the bias term $y_0^{(N-2)} = 1$

Backpropagation

- Run forward pass to save all the values and then compute gradients in the reverse order
- Output layer (N):
  - Directly compute gradients $\frac{\partial L}{\partial y_i^{(N)}}$ and $\frac{\partial L}{\partial z_i^{(N)}} = \frac{\partial L}{\partial y_i^{(N)}} \cdot \frac{\partial y_i^{(N)}}{\partial z_i^{(N)}}$
- For layer $k = N - 1$ downto 0
  - $\frac{\partial L}{\partial w_{i,j}^{(k+1)}} = y_i^{(k)} \cdot \frac{\partial L}{\partial z_i^{(k+1)}}$
  - $\frac{\partial L}{\partial y_i^k} = \sum_j w_{i,j}^{(k+1)} \frac{\partial L}{\partial z_j^{(k+1)}}$
  - $\frac{\partial L}{\partial z_i^{(k)}} = \frac{\partial L}{\partial y_i^{(k)}} f_k'\left(z_i^{(k)}\right)$

MLP for Classification

- The workflow
  - Design a N-layer MLP neural network
  - Initial weights $\{w^{(k)}\}$
  - Gradient descent until convergence
    - With backpropagation

- In practice?

Deep Learning in Practice

- How to design the MLP?
  - Width and depth
- Intuition: in the image classification problem
  - The first layer: $y = \sigma(w^T x)$;
  - y is activated when x is more ***correlated*** with the weight

$$y = \begin{cases} 1 \; if \; \sum_i w_i x_i \geq T \\ 0 \; else \end{cases}$$

Deep Learning in Practice

- How to design the MLP?
  - Width and depth
- Intuition: in the image classification problem
  - MLP learns a cascade of features
  - It is important for the first layer to capture important low-level features

Deep Learning in Practice

- How to design the MLP?
  - Width and depth
- Intuition: MLP learns a cascade of features
  - Practical suggestion: more neurons in the low level

- Depth?
  - Deeper network are harder to learn
  - Intuition: gradients are ***products*** over layers
    - hard to control the learning rate
    - More on next lecture to address this challenge for really deep networks

Deep Learning in Practice

- How to design the MLP?
  - Width and depth
- Activation Functions?
  - Sigmoid has a really good probability interpretation but …
  - Issues with Sigmoid function
    - Always non-negative
      - Alternative: $\tanh(x) = \frac{e^{2x}-1}{e^{2x}+1}$
    - Gradient vanishing
      - Initialization matters!
      - Alternative: $\mathrm{ReLU}(x) = \max(x, 0)$
      - … and more variants

Rectified Linear United

tanh

sigmoid

Deep Learning in Practice

- How to design the MLP?
  - Width and depth
- Activation Functions
  - A close look at ReLU
  - Subgradients
    - A direction that decrease the function
  - Gradients are subgradients but not vice versa

Deep Learning in Practice

- How to design the MLP?
  - Width and depth
- Activation Functions
  - ReLu and Subgradients

- Quiz
  - $f(X) = \max(x_1, x_2, \dots, x_n)$;
  - Compute $\frac{\partial f}{\partial x_i}$?

Deep Learning in Practice

- How to design the MLP?
  - Width and depth
- Activation Functions
  - ReLu and Subgradients
- Learning rate
  - For now: larger learning rate can lead to divergence while small learning rate may lead to no progress
  - More on next lecture

Deep Learning in Practice

- How to design the MLP?
  - Width and depth
- Activation Functions
  - ReLu and Subgradients
- Learning rate
- Regularization
  - L2 norm on all the weights.
  - $L(w) = Loss(w) + \alpha|w|^2$
  - This is also called weight decay
    - $\nabla_w L = \nabla Loss(w) + \alpha w$

Deep Learning in Practice

- How to design the MLP?
  - Width and depth
- Activation Functions
  - ReLu and Subgradients
- Learning rate
- Regularization

- Let's get hand dirty!
  - http://playground.tensorflow.org/

Recap: What does MLP learn?

- A cascade of features (patterns)
  - Weights are correlated filters

Finding the welcome

- Does the signal contain “welcome”?

Finding the welcome

- A trivial solution: train a MLP!

Finding the welcome

- The issue
  - The filter detects the first welcome does not apply to the second
  - We need a huge amount of training data!
- We need a ***simple*** network that can fire regardless of the pattern ***location***

Finding the flowers

- Another example
  - Is there a flower in any of the images?
  - Similar issue:
    - An MLP detecting the left does not apply to the right one

Shift Invariance

- The network needs to be shift invariant

A Simple solution: Scan

- Use **a shared** MLP to detect every possible local patterns
  - Use a maximum (Boolean OR) over the activations over all the locations

A Simple solution: Scan

- Use **a shared** MLP to detect every possible local patterns
  - Use a maximum (Boolean OR) over the activations over all the locations
  - We can also replace the MAX operator with another MLP --- a giant network!

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions

A Simple solution: Scan in 2D

- Detecting a flower using **a shared** MLP
  - Look at every possible positions
  - Send the local patch to the same MLP
  - take the outputs to a final MAX or MLP

Regular MLP v.s. Scanning MLP

- Regular MLP
  - Extremely dense & high-dimensional weight matrix (NM params per layer)

$$W^{(1)} = \begin{bmatrix} w_{11} & w_{12} & w_{13} & w_{14} & \cdots & \cdots & \cdots & w_{1M} \\ w_{21} & w_{22} & w_{23} & w_{24} & \cdots & \cdots & \cdots & w_{2M} \\ w_{31} & w_{32} & w_{33} & w_{34} & \cdots & \cdots & \cdots & w_{3M} \\ w_{41} & w_{42} & w_{43} & w_{44} & \cdots & \cdots & \cdots & w_{4M} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ w_{N1} & w_{N2} & w_{N3} & w_{N4} & \cdots & \cdots & \cdots & w_{NM} \end{bmatrix}$$

Regular MLP v.s. Scanning MLP

- Scanning MLP
  - Only require a small amount of parameters (the shared MLP for local patch)
  - *Effective in any situation where the data are expected to be composed of similar structures at different locations*
    - E.g. speech recognition, image recognition

Training the Network

- Still Backpropagation!
  - Fully differentiable neural networks

Training the Network

- Still Backpropagation!
  - Fully differentiable neural networks
  - But with constraints --- shared parameter models!

Training the Network

- Still Backpropagation!
  - Let S denotes the edges that have common value
  - $\nabla_S L(w) = \sum_{e \in S} \nabla_{w_e} L(w)$ *the effect can be summed up*
  - Your homework ☺

$S = \{e_1, e_2, \dots, e_N\}$

A Closer Look at 2D Scanning

- We scan the whole image for a desired pattern
- At each location, the patch is sent to an MLP

A Closer Look at 2D Scanning

- We scan the whole image for a desired pattern
- At each location, the patch is sent to an MLP
  - Let's look at specific neuron

A Closer Look at 2D Scanning

- Let's consider a single neuron (a simple perceptron)
  - At each box position, the perceptron is evaluating the patch in the box as part of feature for classification

A Closer Look at 2D Scanning

- Let's consider a single neuron (a simple perceptron)
  - We can arrange the neuron outputs corresponding to the image locations

A Closer Look at 2D Scanning

- Let's consider a single neuron (a simple perceptron)
  - We can arrange the neuron outputs corresponding to the image locations

A Closer Look at 2D Scanning

- Let's consider a single neuron (a simple perceptron)
  - We can arrange the neuron outputs corresponding to the image locations

A Closer Look at 2D Scanning

- Let's consider a single neuron (a simple perceptron)
  - We can arrange the neuron outputs corresponding to the image locations

A Closer Look at 2D Scanning

- Let’s consider a single neuron (a simple perceptron)
  - We can arrange the neuron outputs corresponding to the image locations

A Closer Look at 2D Scanning

- Let's consider a single neuron (a simple perceptron)
  - We can arrange the neuron outputs corresponding to the image locations

A Closer Look at 2D Scanning

- Let's consider a single neuron (a simple perceptron)
  - We can arrange the neuron outputs corresponding to the image locations

A Closer Look at 2D Scanning

- Let's consider a single neuron (a simple perceptron)
  - We can arrange the neuron outputs corresponding to the image locations

A Closer Look at 2D Scanning

- Let's consider a single neuron (a simple perceptron)
  - We can arrange the neuron outputs corresponding to the image locations
  - We obtain a rectangle outputs!

A Closer Look at 2D Scanning

- The output for each neuron can be organized as a rectangle similarly

A Closer Look at 2D Scanning

- The output for each neuron can be organized as a rectangle similarly
- And we send the neuron outputs to the second layer for classification

A Closer Look at 2D Scanning

- The output for each neuron can be organized as a rectangle similarly
- And we send the neuron outputs to the second layer for classification
  - Each output location of the second layer takes the input from the same location from the first layer

A Closer Look at 2D Scanning

- The output for each neuron can be organized as a rectangle similarly
- And we send the neuron outputs to the second layer for classification
  - Each output location of the second layer takes the input from the same location from the first layer

A Closer Look at 2D Scanning

- The output for each neuron can be organized as a rectangle similarly
- And we send the neuron outputs to the second layer for classification
  - Each output location of the second layer takes the input from the same location from the first layer

A Closer Look at 2D Scanning

- The output for each neuron can be organized as a rectangle similarly
- And we send the neuron outputs to the second layer for classification
  - Each output location of the second layer takes the input from the same location from the first layer

A Closer Look at 2D Scanning

- The output for each neuron can be organized as a rectangle similarly
- And we send the neuron outputs to the second layer for classification
  - Each output location of the second layer takes the input from the same location from the first layer

A Closer Look at 2D Scanning

- The output for each neuron can be organized as a rectangle similarly
- And we send the neuron outputs to the second layer for classification
  - Each output location of the second layer takes the input from the same location from the first layer

A Closer Look at 2D Scanning

- The output for each neuron can be organized as a rectangle similarly
- And we send the neuron outputs to the second layer for classification
  - Each output location of the second layer takes the input from the same location from the first layer

A Closer Look at 2D Scanning

- The output for each neuron can be organized as a rectangle similarly
- And we send the neuron outputs to the second layer for classification
  - Each output location of the second layer takes the input from the same location from the first layer

A Closer Look at 2D Scanning

- The output for each neuron can be organized as a rectangle similarly
- For each location, the outputs will be passed towards the final layer
- A final MLP layer produces the overall classification result

A Closer Look at 2D Scanning

A Closer Look at 2D Scanning

- Let's consider the outputs corresponding to a specific position
  - Each position in the output rectangle corresponds to a patch position in the input image

A Closer Look at 2D Scanning

- Let's consider the outputs corresponding to a specific position
- Remark
  - The first layer takes care of the ***entire patch***
  - Top layers only takes ***a single value*** from its input rectangle

Can top layers also takes a patch from its input map?

Distributed Scanning

- Let's distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches

Distributed Scanning

- Let’s distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches

Distributed Scanning

- Let’s distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches

Distributed Scanning

- Let's distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches

Distributed Scanning

- Let's distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches

Distributed Scanning

- Let’s distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches

Distributed Scanning

- Let’s distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches

Distributed Scanning

- Let’s distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches

Distributed Scanning

- Let’s distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches

Distributed Scanning

- Let's distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches
  - Second layer scans the patch from the output of first layer

Distributed Scanning

- Let's distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches
  - Second layer scans the patch from the output of first layer → **larger patch**

Distributed Scanning

- Let's distribute the pattern matching workload over 2 layers
  - First layer for smaller patches and second layer for larger patches
  - Second layer scans the patch from the output of first layer → **larger patch**
    - It learns the arrangement of sub-patterns detected by the first layer for larger patches

Distributed Scanning

- Let's learn the patterns over 3 layers
  - A similar recursive logic
  - First layer for small pattern

Distributed Scanning

- Let's learn the patterns over 3 layers
  - A similar recursive logic
  - Second layer for intermediate pattern

Distributed Scanning

- Let’s learn the patterns over 3 layers
  - A similar recursive logic
  - Top layer for the entire complex pattern

Distributed Scanning

- Let's learn the patterns over 3 layers
  - A similar recursive logic
  - Top layer for the entire complex pattern
  - Final MLP output for classification result over the entire image

A giant network building up a hierarchy of features!

Pseudo-code

```
Y(0,:,:,:) = Image
for l = 1:L
    for j = 1:D_l
        for x = 1:W_{l-1}-K_l+1
            for y = 1:H_{l-1}-K_l+1
                z(l,j,x,y) = 0
                for i = 1:D_{l-1}
                    for x' = 1:K_l
                        for y' = 1:K_l
                            z(l,j,x,y) += w(l,i,j,x',y')
                                          Y(l-1,i,x+x'-1,y+y'-1)
                Y(l,j,x,y) = activation(z(l,j,x,y))

Y = softmax( Y(L,:,1,1)..Y(L,:,W-K+1,H-K+1) )
```

Pseudo-code

```
Y(0,:,:,:) = Image
for l = 1:L  # layers
    for j = 1:D_l
        for x = 1:W_{l-1}-K_l+1
            for y = 1:H_{l-1}-K_l+1
                z(l,j,x,y) = 0
                for i = 1:D_{l-1}
                    for x' = 1:K_l
                        for y' = 1:K_l
                            z(l,j,x,y) += w(l,i,j,x',y')
                                          Y(l-1,i,x+x'-1,y+y'-1)
                Y(l,j,x,y) = activation(z(l,j,x,y))

Y = softmax( Y(L,:,1,1)..Y(L,:,W-K+1,H-K+1) )
```

Pseudo-code

```
Y(0,:,:,:) = Image
for l = 1:L  # layers
    for j = 1:D_l  # D_l is often called channels in computer vision
        for x = 1:W_{l-1}-K_l+1
            for y = 1:H_{l-1}-K_l+1
                z(l,j,x,y) = 0
                for i = 1:D_{l-1}
                    for x' = 1:K_l
                        for y' = 1:K_l
                            z(l,j,x,y) += w(l,i,j,x',y')
                                          Y(l-1,i,x+x'-1,y+y'-1)
                Y(l,j,x,y) = activation(z(l,j,x,y))

Y = softmax( Y(L,:,1,1)..Y(L,:,W-K+1,H-K+1) )
```

Pseudo-code

```
Y(0,:,:,:) = Image
for l = 1:L  # layers
    for j = 1:D_l  # D_l is often called channels in computer vision
        for x = 1:W_{l-1}-K_l+1
            for y = 1:H_{l-1}-K_l+1
                z(l,j,x,y) = 0  # compute feature at layer l, channel j at (x, y)
                for i = 1:D_{l-1}
                    for x' = 1:K_l
                        for y' = 1:K_l
                            z(l,j,x,y) += w(l,i,j,x',y')
                                          Y(l-1,i,x+x'-1,y+y'-1)
                Y(l,j,x,y) = activation(z(l,j,x,y))

Y = softmax( Y(L,:,1,1)..Y(L,:,W-K+1,H-K+1) )
```

Pseudo-code

```
Y(0,:,:,:) = Image
for l = 1:L   # layers
    for j = 1:D_l   # D_l is often called channels in computer vision
        for x = 1:W_{l-1}-K_l+1
            for y = 1:H_{l-1}-K_l+1
                z(l,j,x,y) = 0   # compute feature at layer l, channel j at (x, y)
                for i = 1:D_{l-1}
                    for x' = 1:K_l   #K_l is often called kernel size
                        for y' = 1:K_l
                            z(l,j,x,y) += w(l,i,j,x',y')
                                          Y(l-1,i,x+x'-1,y+y'-1)
                Y(l,j,x,y) = activation(z(l,j,x,y))

Y = softmax( Y(L,:,1,1)..Y(L,:,W-K+1,H-K+1) )
```

Pseudo-code

```
Y(0,:,:,:) = Image
for l = 1:L   # layers
    for j = 1:D_l   # D_l is often called channels in computer vision
        for x = 1:W_{l-1}-K_l+1
            for
                z(l,j,x,y) = 0   # compute feature at layer l, channel j at (x, y)
                for i = 1:D_{l-1}
                    for x' = 1:K_l   #K_l is often called kernel size
                        for y' = 1:K_l
                            z(l,j,x,y) += w(l,i,j,x',y')
                                          Y(l-1,i,x+x'-1,y+y'-1)
                Y(l,j,x,y) = activation(z(l,j,x,y))

Y = softmax( Y(L,:,1,1)..Y(L,:,W-K+1,H-K+1) )
```

This operation is called "Convolution"

Distributed Scanning in 1D Case

- We can scan a 8-timestep patch with distributed scan over 2 layers
  - First layer: takes inputs over 2 timesteps and a stride of 2 timesteps
  - Second layer: takes input over 4 timesteps from first layer

Why Distributed Scanning?

- Each layer focuses on localized patterns
  - Weights have lower dimensions
  - Easy to learn and more generalizable

- Number of Parameters!

Why Distributed Scanning?

- Number of Parameters in 2D
  - Non-distributed net:
    - #Param = $O(K^2 N_1 + N_1 N_2 + N_2 N_3)$

Why Distributed Scanning?

Example:
$K = 16, N_1 = 4, N_2 = 2, N_3 = 1$
$L_1 = L_2 = 2$

- Number of Parameters in 2D
  - Non-distributed net: #Param = $O(K^2 N_1 + N_1 N_2 + N_2 N_3)$ ~ 1034 weights

    Dominating term
  - Distributed over 3 layers:
    - #Param = $O\left(L_1^2 N_1 + L_2^2 N_1 N_2 + \left(\frac{K}{L_1 L_2}\right)^2 N_2 N_3\right)$

      ~ 160 weights

Why Distributed Scanning?

- Each layer focuses on localized patterns
  - Weights have lower dimensions
  - Easy to learn and more generalizable

- Number of Parameters!
  - Significantly reduce the amount of parameters when use more layers

A More General Form of Scanning

- We do not necessarily need *precise* distribution over layers
- Let's re-examine the convolution operators
  - First layer scans small local sub-regions

A More General Form of Scanning

- We do not necessarily need *precise* distribution over layers
- Let's re-examine the convolution operators
  - Second layer scans subregions from the first layer → larger patch in the image

A More General Form of Scanning

- We do not necessarily need *precise* distribution over layers
- Let's re-examine the convolution operators
  - Third layer just scans subregions from the second layer

We can have arbitrarily many layers

A More General Form of Scanning

- Terminology
  - Filters: scans for a pattern on the map from the previous layer

A More General Form of Scanning

- Terminology
  - Filters
  - Receptive Fields: the corresponding patch in the ***input*** image
    - Non-trivial for high-level filters

A More General Form of Scanning

- Terminology
  - Filters, Receptive Fields
  - Strides: the scanning “hops” for each filter
    - This can reduce the output map size

A More General Form of Scanning

- Size of Output Map
  - Filter Size M; Input Map Size N; Stride S
  - Convolution often reduces the map size even with $S = 1$

A More General Form of Scanning

- Size of Output Map
  - Filter Size M; Input Map Size N; Stride S
  - Convolution often reduces the map size even with $S = 1$
  - Solution: ***zero-padding***
    - Pad 0 all around the map
    - It ensures the output size is $\left\lceil \frac{N}{S} \right\rceil$
    - For stride=1,
      the output map remains the same size as input map

1	0	1
0	1	0
1	0	1

Filter

0	0	0	0	0	0	0
0	1	1	1	0	0	0
0	0	1	1	1	0	0
0	0	0	1	1	1	0
0	0	0	1	1	0	0
0	0	1	1	0	0	0
0	0	0	0	0	0	0

A More General Form of Scanning

- Account for jittering
  - If a pattern in the image shifts for 1 pixel, can we still detect it?
  - Even with a 1-pixel shift, a large portion of the feature map changes

A More General Form of Scanning

- Account for jittering
  - If a pattern in the image shifts for 1 pixel, can we still detect it?
  - Small jittering is acceptable!
    - Replace each value by the maximum over a small neighboring region
    - This is called **max-pooling**

A More General Form of Scanning

- Max-Pooling typically has non-overlap strides
  - Stride = max-pooling size
  - It partitions the output map into blocks
  - Each block only maintain the highest value
    - Any pattern detected in the region, it is detected

A More General Form of Scanning

- Max-Pooling typically has non-overlap strides
  - Stride = max-pooling size
  - It partitions the output map into blocks
  - Each block only maintain the highest value
    - Any pattern detected in the region, it is detected

A More General Form of Scanning

- Max-Pooling typically has non-overlap strides
  - Stride = max-pooling size
  - It partitions the output map into blocks
  - The next layer works on pooled map

Convolutional Neural Networks

- The entire architecture is called CNN
  - Convolution layer
  - Max-Pooling layer
  - Final MLP layer for classification output

Back to the 1D Case

- 1D Convolution + Pooling + MLP → Classification
  - Whether the voice has “Welcome” in it

Time Delay Neural Network

Also referred to as
“Temporal Convolution Network”

Additional Remarks

- The input channels
  - 1 (black-white) or 3 (RGB)

Additional Remarks

- Alternatives to Max-Pooling
  - Average-Pooling: use mean instead of max
    - A soft version of max operator → more informative gradients

Additional Remarks

- Alternatives to Max-Pooling
  - Average-Pooling: use mean instead of max
  - Fully Convolutional Network: downsampling instead of pooling
    - Convolution with stride > 1 reduces the map size (downsampling)
    - Equivalent to ***"learning a learned pooling operator"***

The LeNet-5 Example

- 1998 by Yan LeCun
  - First commercial CNN application for digit recognition

AlexNet

- 2012 by Alex Krizhevsky. Ilya Sutskever. Geoffrey Hinton
  - Breakthrough on ImageNet Challenge: the beginning of deep learning era

AlexNet

- 2012 by Alex Krizhevsky. Ilya Sutskever. Geoffrey Hinton
  - Breakthrough on ImageNet Challenge: the beginning of deep learning era

You don't need GPU for HW1 ☺

Summary

- Part 1: learning an MLP for classification!
  - The basic components and learning algorithm
- Part 2: convolutional neural network
  - The intuition and basic architecture
- CP1 will be released tonight!
  - Backpropagation and initial tuning attempt ☺
- Next lecture: more tricks are coming!
  - Get your hands extremely dirty!

Thanks