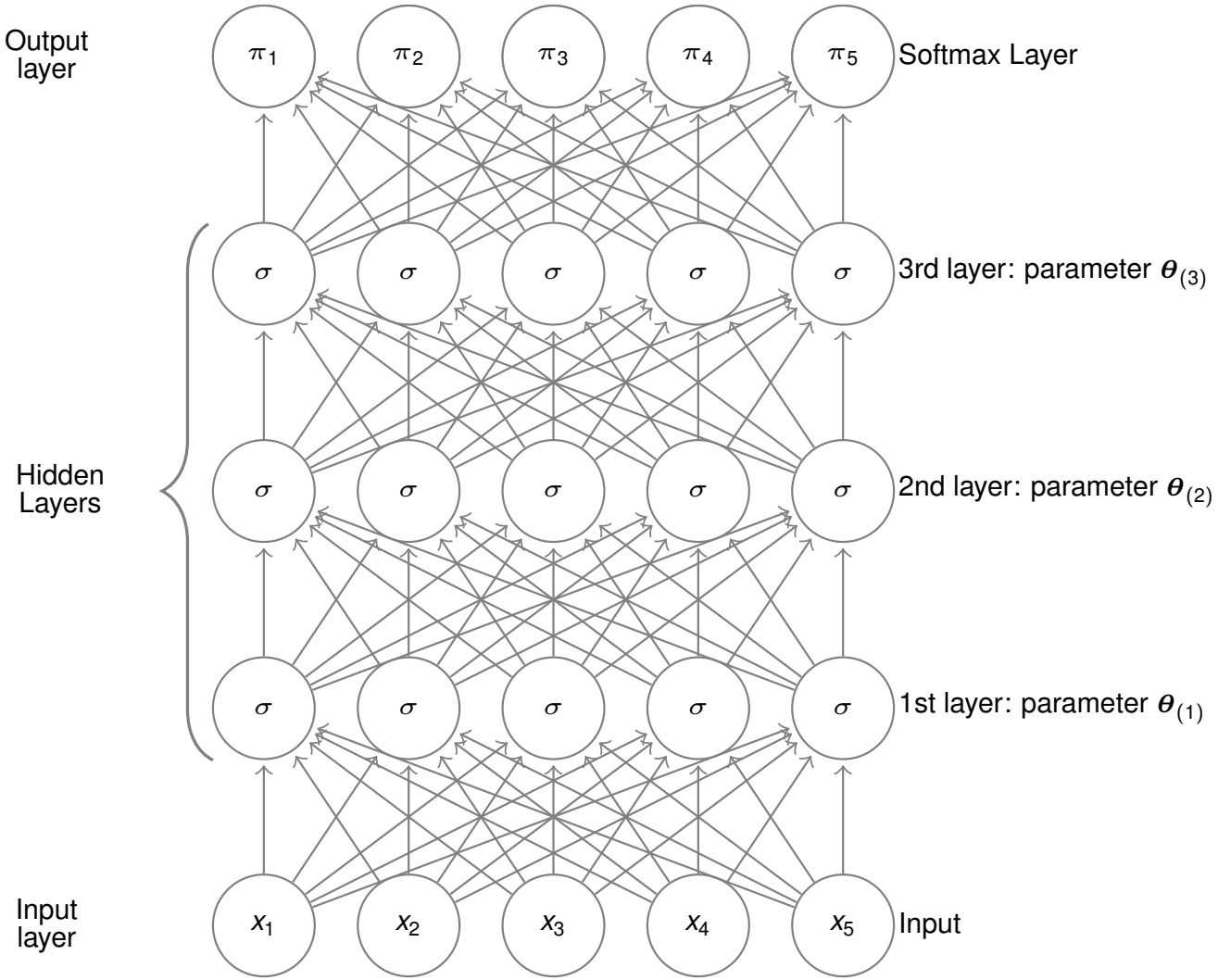
Convolution Neural Net: Basics to Recent Reseach

A/Prof Richard Yi Da Xu
Yida.Xu@uts.edu.au
Wechat: aubedata
https://github.com/roboticcam/machine-learning-notes

University of Technology Sydney (UTS)

January 28, 2020

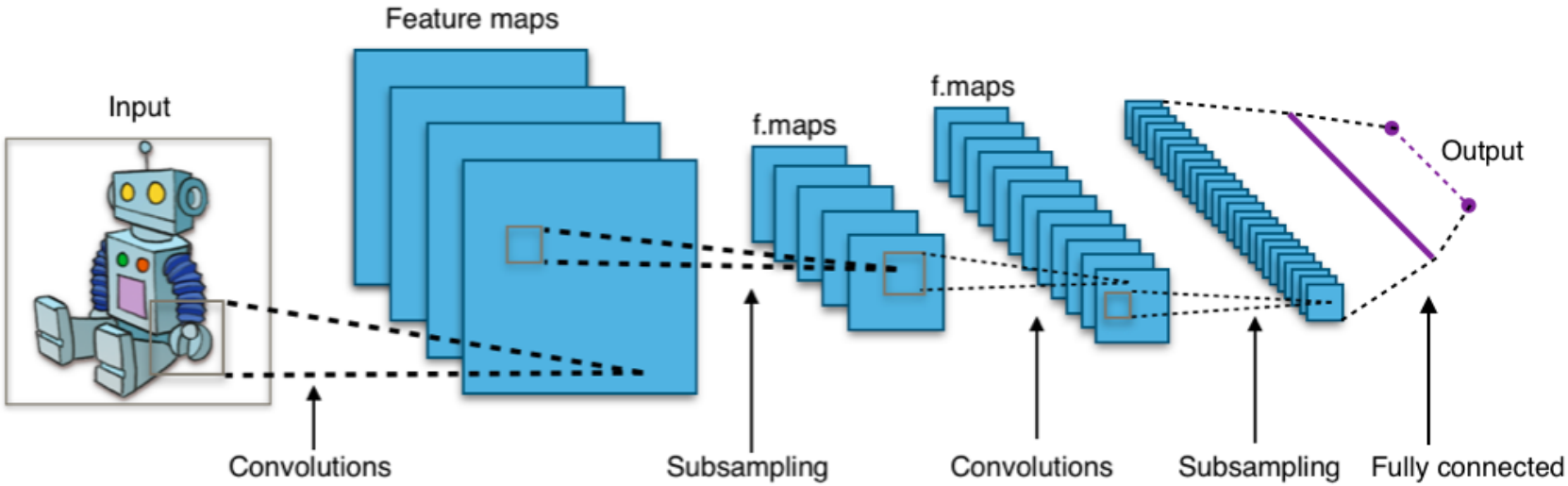
Good old Feedforward Neural Network with Many layers



Feedforward Neural Network with Many layers

- For complicated problem, one hidden layer may NOT be enough.
- σ Layers can be flexibly designed: linear, Softmax, ReLU or any other
- Each layers may have their own parameters $\theta_{(l)}$
- There are many such layers, hence many parameters
- Think about the case of **one meg pixel image**.
- How may we reduce the number of parameters from the fully connected network?
- keyword of the day: **parameter sharing**

A high level view of Convolution Neural Network (CNN)



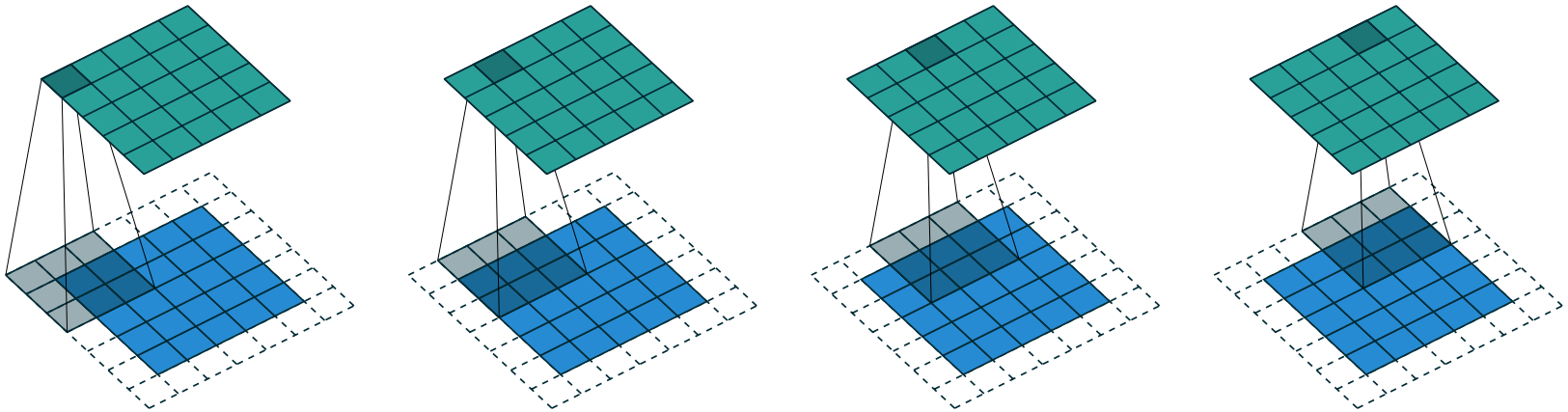
Convolution Neural Networks: What is a convolution?

- from a signal processing perspective:

$$(f * g)(t) \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} f(\tau)\, g(t-\tau)\, d\tau = \int_{-\infty}^{\infty} f(t-\tau)\, g(\tau)\, d\tau.$$

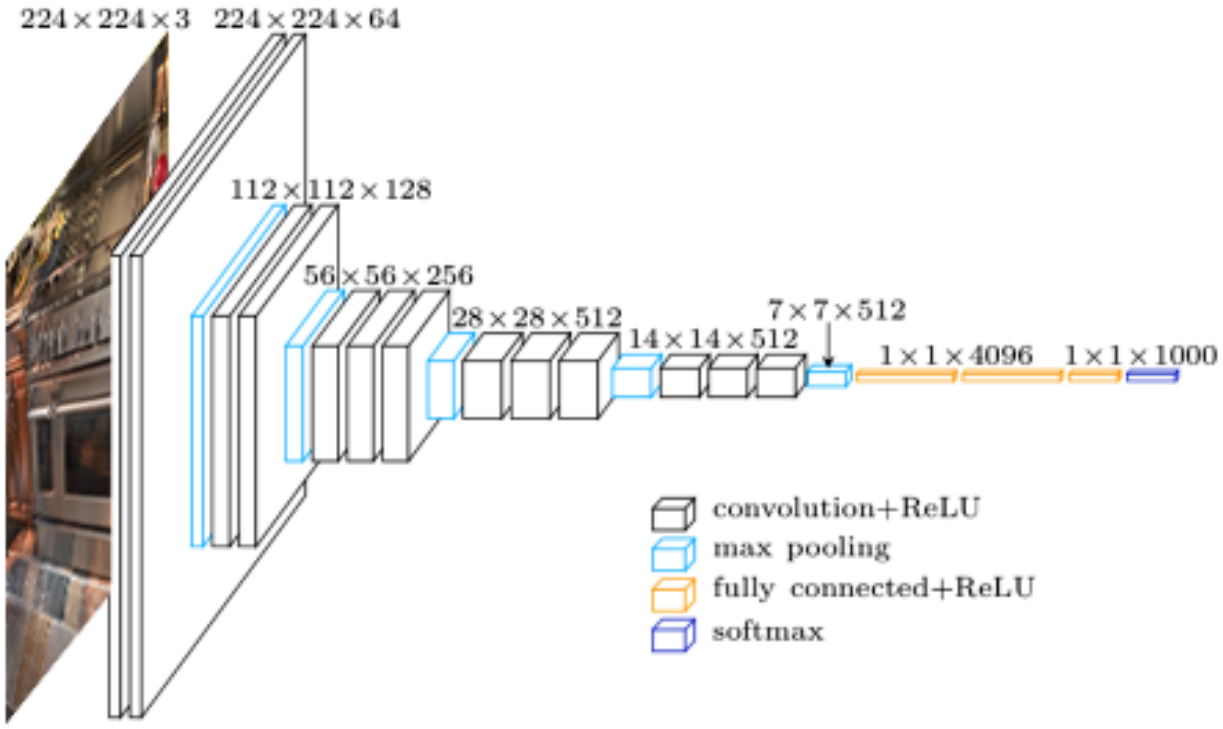
What is a 2D Convolution in Discrete Imaging?

An example of Convolving a 3×3 kernel over a 5×5 input with padding1.

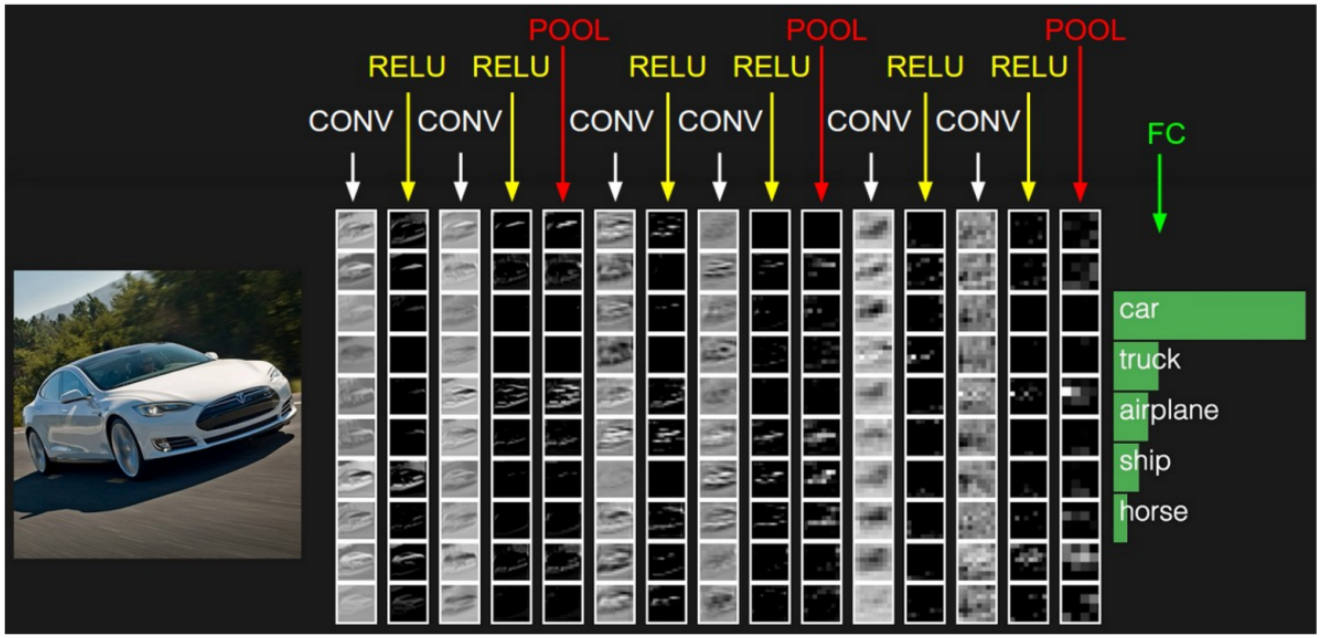


- Exploiting the strong spatially local correlation present in natural images.
- In term of number of parameters, assume in a layer, you have 128 convolution Kernels (the grey square), you create 64 “copies” of the image.
- Assume in a layer, if each kernel is 5×5 in size, we have something like $128x5x5 = 3200$ parameters.
- A lot less than fully connected neural networks

CNN for image classification: look at it again



What does the “learnt” image feature represent?



CNN Feed-forward: convolution as a linear operator

- let's forget about only considers:

$$x_{ij}^{(l)} = W * (y^{(l-1)}) \qquad y_{ij}^{(l)} = \sigma\left(x_{ij}^{(l)}\right)$$

- as matter of fact, in $1-D$ convolution, one may replace convolution by matrix multiplication:

$$x^l = W * y^{l-1} = \begin{bmatrix} w_1 & 0 & \dots & 0 & 0 \\ w_2 & w_1 & \dots & \vdots & \vdots \\ w_3 & w_2 & \dots & 0 & 0 \\ \vdots & w_3 & \dots & w_1 & 0 \\ & \vdots & & & \\ w_{m-1} & & \dots & w_2 & w_1 \\ & & \vdots & \vdots & \\ w_m & w_{m-1} & & & w_2 \\ & & & & \vdots \\ 0 & w_m & \dots & w_{m-2} & \\ 0 & 0 & \dots & w_{m-1} & w_{m-2} \\ \vdots & \vdots & \vdots & & \\ \vdots & \vdots & \vdots & w_m & w_{m-1} \\ 0 & 0 & 0 & \dots & w_m \end{bmatrix} \begin{bmatrix} y_1^{l-1} \\ y_2^{l-1} \\ y_3^{l-1} \\ \vdots \\ y_n^{l-1} \end{bmatrix}$$

CNN Feed-forward: looking at one layer only

- say at layer $(l-1)$: $y^{(l-1)}$ has $N \times N$ square neurons
- use $m \times m$ filter ω
- when stride 0 used, $x^{(l)}$ will be of size $(N-m+1) \times (N-m+1)$
- for simplicity - shift the centre by $(\frac{m}{2}, \frac{m}{2})$

$$x_{ij}^{(l)} = \sum_{a=0}^{m-1} \sum_{b=0}^{m-1} \omega_{ab} y_{(i+a)(j+b)}^{(l-1)}$$

$$y_{ij}^{(l)} = \sigma(x_{ij}^{(l)})$$

CNN back-propagation

- we need four derivative quantities:
  - $\frac{\partial y_{ij}^{(l)}}{\partial x_{ij}^{(l)}} = \sigma'(x_{ij}^{(l)})$
  - $\frac{\partial x_{ij}^{(l)}}{\partial \omega_{a,b}} = y_{(i+a)(j+b)}^{(l-1)}$
  - $\frac{\partial x_{(i-a)(j-b)}^{(l)}}{\partial y_{ij}^{(l-1)}} = \omega_{a,b}$
- say we already knew $\frac{\partial E}{\partial y_{ij}^{(l)}}$,

find $\frac{\partial E}{\partial y_{ij}^{(l-1)}}$: it involves a "filter-window" of $x_{ij}^{(l)}$

$$\frac{\partial E}{\partial y_{ij}^{(l-1)}} = \sum_{a=0}^{m-1}\sum_{b=0}^{m-1} \frac{\partial E}{\partial x_{(i-a)(j-b)}^{(l)}} \frac{\partial x_{(i-a)(j-b)}^{(l)}}{\partial y_{ij}^{(l-1)}}$$

$$= \sum_{a=0}^{m-1}\sum_{b=0}^{m-1} \frac{\partial E}{\partial y_{ij}^{(l)}} \sigma'\left(x_{(i-a)(j-b)}^{(l)}\right) \omega_{a,b}$$

sum over a filter window

find $\frac{\partial E}{\partial \omega_{a,b}}$: it involves entire $x_{ij}^{(l)}$

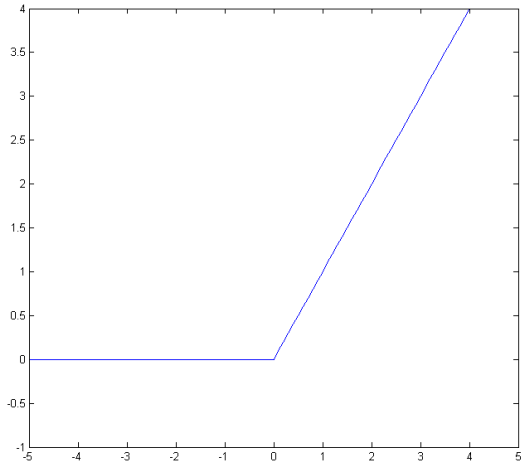
$$\frac{\partial E}{\partial \omega_{a,b}} = \sum_{i=0}^{N-m+1}\sum_{j=0}^{N-m+1} \frac{\partial E}{\partial x_{i,j}^{(l)}} \frac{\partial x_{i,j}^{(l)}}{\partial \omega_{a,b}}$$

$$= \sum_{i=0}^{N-m+1}\sum_{j=0}^{N-m+1} \frac{\partial E}{\partial y_{ij}^{(l)}} \sigma'\left(x_{i,j}^{(l)}\right) y_{(i+a)(j+b)}^{(l-1)}$$

sum over an entire image

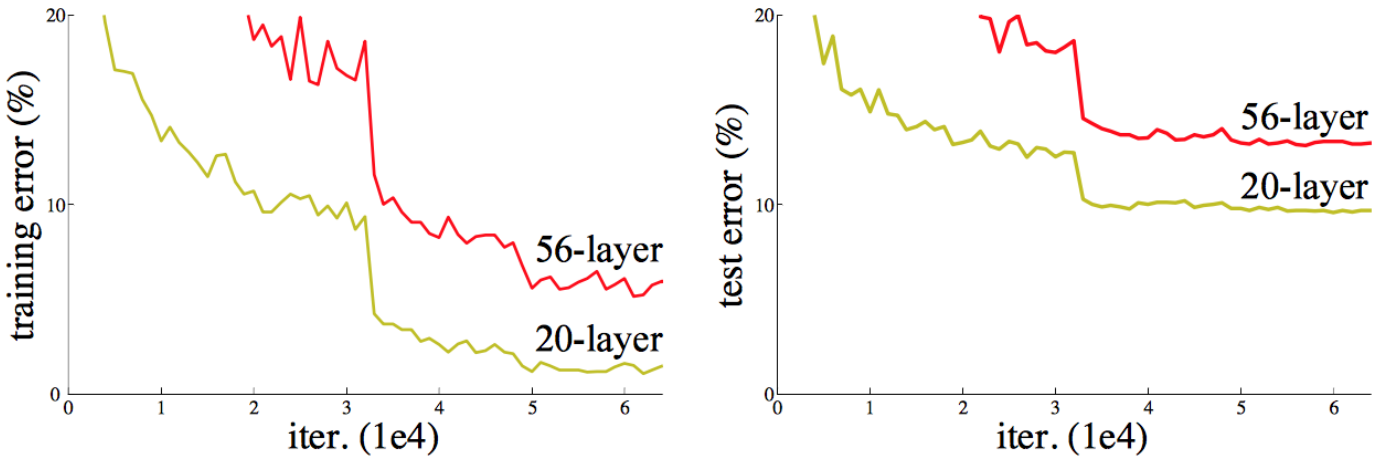
The winning ingredient: **Re**ctified **L**inear **U**nit

- How to combine the different “convolved” images together?
- A Linear + **Activation function** $f(x) = \mathbf{max}(0, x)$



- High school mathematics is useful
- **its derivative can only be** $\{0, 1\}$. This is useful to prevent gradient vanishing and exploding
- They do not require any exponential computation (such as those required in sigmoid)
- reported around 6X speed over existing activation functions

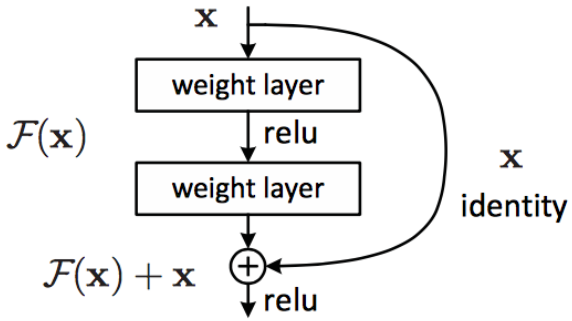
New network designs: Deep Residual Learning



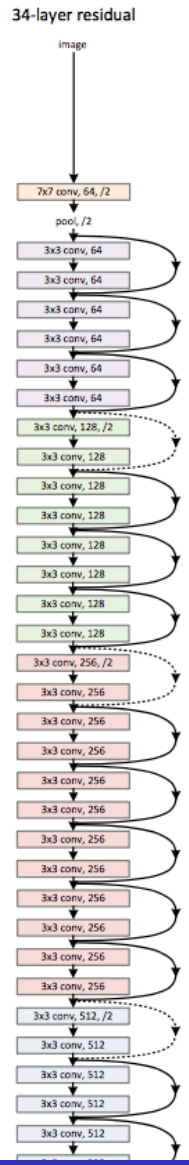
- when network depth increasing, accuracy gets saturated and then degrades rapidly.
- authors claim such degradation is **not** caused by overfitting

New network designs: Deep Residual Learning:

He., et al, (2016), Deep Residual Learning for Image Recognition, CVPR, pp. 770-778



- instead of few stacked layers directly fit a desired underlying mapping $H(x)$
- explicitly let these layers fit a residual mapping $F(x)$: $H(x) = F(x) + x$
- **hypothesize**: easier to optimize residual mapping than optimize original unreferenced mapping.
- if an identity mapping were optimal, it would be easier to push the residual to zero than to fit an identity mapping by a stack of nonlinear layers.



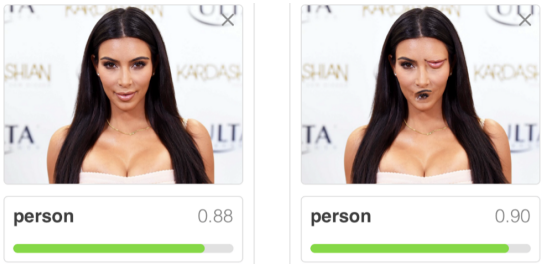
One way we may able to argue its advantage

$$x_2 = F(x_1) + x_1 \qquad \dots \qquad x_t = F(x_{t-1}) + x_{t-1}$$

$$\begin{aligned}
\frac{\partial x_t}{\partial x_1} &= \frac{\partial x_t}{\partial x_{t-1}} \frac{\partial x_{t-1}}{\partial x_{t-2}} \cdots \frac{\partial x_2}{\partial x_1} \\
&= \left(F'(x_{t-1}) + 1\right)\left(F'(x_{t-2}) + 1\right) \dots \left(F'(x_1) + 1\right) \\
&= (\text{some polynomial terms of } x_1, \dots x_t) + 1
\end{aligned}$$

Therefore, change x_1 propagates some of it to x_t even though t may be large

Capsule Networks



neural network

$$z_j = W_{j,:}^{\top} x_i \qquad a_j = \sigma(z_j)$$

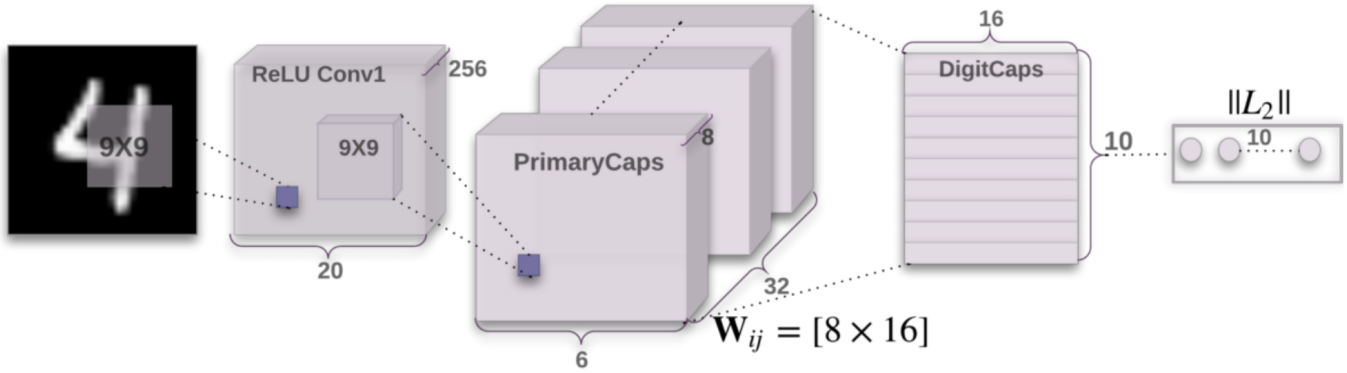
capsule layer

$\hat{\mathbf{u}}_{j|i} = \mathbf{W}_{ij}\mathbf{u}_i$ a unique matrix link between capsules of adjacent layers

$\mathbf{s}_j = \sum_i c_{ij}\hat{\mathbf{u}}_{j|i}$ dynamic routing

$\mathbf{v}_j = \frac{\|\mathbf{s}_j\|^2}{1+\|\mathbf{s}_j\|^2}\frac{\mathbf{s}_j}{\|\mathbf{s}_j\|}$ normalise a vector to ensure $\|\mathbf{v}_j\| \leq 1$

Capsule Networks - diagram



- Each PrimaryCaps contains 8 convolutional units with a 9×9 kernel and stride 2:
- in its **loss function**:
  - it doesn't use **softmax** loss
  - its loss function is:

$$L_c = T_c \max(0, m^+ - \|\mathbf{v}_c\|)^2 + \lambda(1 - T_c) \max(0, \|\mathbf{v}_c\| - m^-)^2$$

  - $m^+ = 0.9$ and $m^- = 0.1$:
  - it penalise correctly classified data if it's below 0.9
  - it penalise incorrectly classified data if it's above 0.1

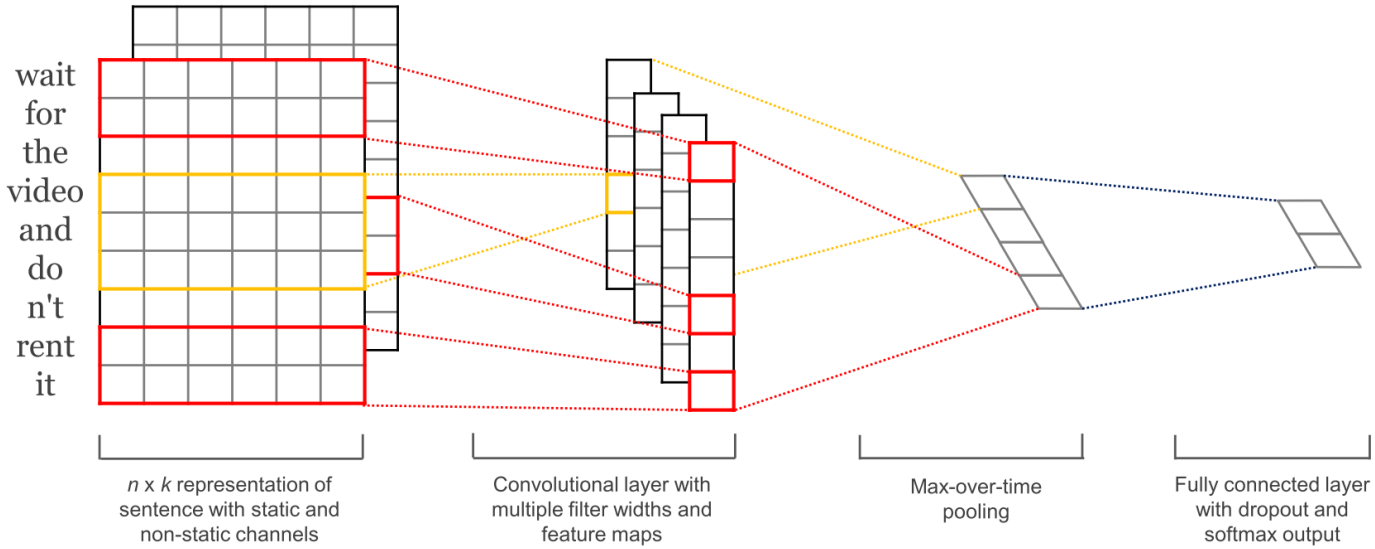
Capsule Networks - Dynamic Routing

Procedure 1 Routing algorithm.

1: **procedure** ROUTING($\hat{\boldsymbol{u}}_{j|i}$, r, l)
2: for all capsule i in layer l and capsule j in layer $(l+1)$: $b_{ij} \leftarrow 0$.
3: **for** r iterations **do**
4: for all capsule i in layer l: $\mathbf{c}_i \leftarrow \texttt{softmax}(\mathbf{b}_i)$ ▷ `softmax` computes Eq. 3
5: for all capsule j in layer $(l+1)$: $\mathbf{s}_j \leftarrow \sum_i c_{ij}\hat{\mathbf{u}}_{j|i}$
6: for all capsule j in layer $(l+1)$: $\mathbf{v}_j \leftarrow \texttt{squash}(\mathbf{s}_j)$ ▷ `squash` computes Eq. 1
7: for all capsule i in layer l and capsule j in layer $(l+1)$: $b_{ij} \leftarrow b_{ij} + \hat{\mathbf{u}}_{j|i}.\mathbf{v}_j$
return $\mathbf{v}_j$

- lower layer is sent to higher level capsule that agrees with it
- the agreement is iterative updated through its value c_{ij}

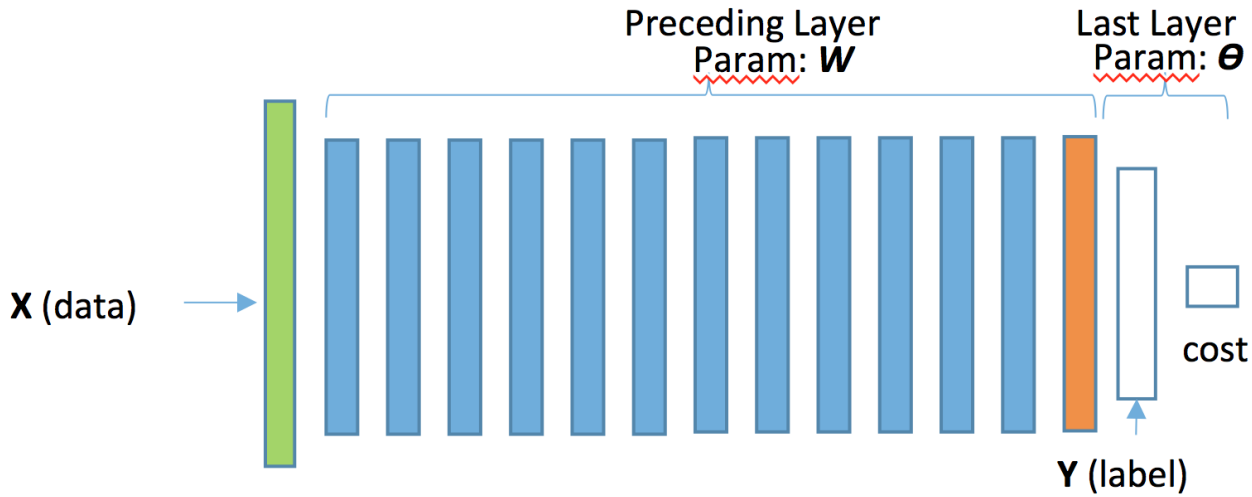
CNN for text classification



excercise why can't we perform 2-D in text classification?
excercise how does it solve the problem of variable text length?

Generic Deep Neural Network Structure

- The generic framework for deep learning:



The Last layer of Convolution Neural Network

The structure can be thought of as:

- The **last layer**: dictating the **objective** of the neural network.
  - It has parameter set θ. Usually, its dimension has been just a few.
- The **preceding layers**: **data transformation/preparation** to serve the objective (specified in the **last layer**) better
  - It has parameter set W. Usually, Its dimension is HUGE!
- A more "scholarly" way of saying this: **preceding** layers brings **feature embeddings** to serve the function of the last layer.
- When data is less complex, one may apply the **last layer** directly without the preceding layers, i.e., **no embeddings** is required.

We will look at some of the **Last layer** of CNN

- Softmax
- Linear
- Centre
- Contrastive
- Triplet
- and some of the unique last layers for **object detection**

First of them all: Softmax Layer

$$\mathcal{C}(\boldsymbol{\theta}) = -\sum_{i=1}^{N}\sum_{k=1}^{K} \underbrace{y_{i,k}}_{\text{label}} \underbrace{\log\left[\frac{\exp(\mathbf{x}_i^T\boldsymbol{\theta}_k)}{\sum_{l=1}^{K}\exp(\mathbf{x}_i^T\boldsymbol{\theta}_l)}\right]}_{\text{prob of belong to a class } k}$$

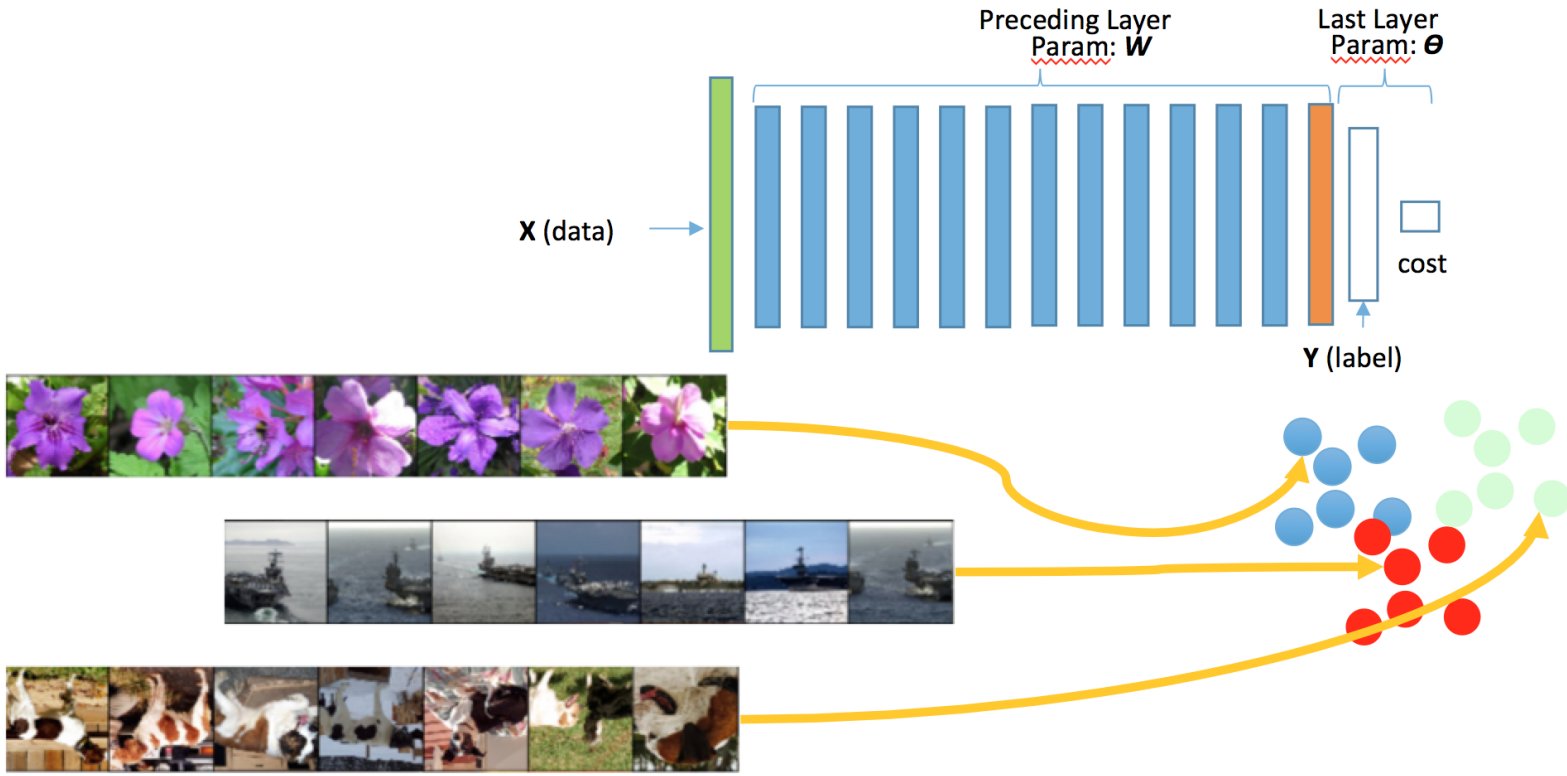
- Used for classification (Most commonly used)
- See `soft_max.m` where Softmax is applied **without** the preceding networks.
- Just for fun: $\arg\min\left(\mathcal{C}(\boldsymbol{\theta})\right) \implies \arg\max\left(\exp(-\mathcal{C}(\boldsymbol{\theta}))\right)$:

$$\begin{aligned}
\exp(-\mathcal{C}(\boldsymbol{\theta})) &= \exp\left(\sum_{i=1}^{N}\sum_{k=1}^{K} y_{i,k}\log\left[\frac{\exp(\mathbf{x}_i^T\boldsymbol{\theta}_k)}{\sum_{l=1}^{K}\exp(\mathbf{x}_i^T\boldsymbol{\theta}_l)}\right]\right)\\
&= \prod_{i=1}^{N}\prod_{k=1}^{K}\exp\left(y_{i,k}\log\left[\frac{\exp(\mathbf{x}_i^T\boldsymbol{\theta}_k)}{\sum_{l=1}^{K}\exp(\mathbf{x}_i^T\boldsymbol{\theta}_l)}\right]\right)\\
&= \prod_{i=1}^{N}\prod_{k=1}^{K}\left[\frac{\exp(\mathbf{x}_i^T\boldsymbol{\theta}_k)}{\sum_{l=1}^{K}\exp(\mathbf{x}_i^T\boldsymbol{\theta}_l)}\right]^{y_{i,k}}
\end{aligned}$$

- It is not hard to tell $\exp(-\mathcal{C}(\boldsymbol{\theta}))$ is maximised, when red and blue parts are **identical**.

Softmax Layer

- **Without** using preceding networks, Softmax does NOT work well for complicated input, e.g., faces:



- the **preceding networks** plays the role of the **feature embedding**.
- Sometimes, pre-trained networks are used to generate **feature embedding** for unseen data (in the same context), i.e., last layer do NOT involved.

Centre loss

- Wen, et. al, (2016) A Discriminative Feature Learning Approach for Deep Face Recognition, ECCV
- introduce so-called center loss to minimize the intra- class distances of the deep features
- c_j are also variables

$$\mathcal{L} = \mathcal{L}_s + \lambda \mathcal{L}_c = \underbrace{-\sum_{i=1}^{N} \log \frac{\exp^{W_{y_i} x_i}}{\sum_{j=1}^{M} \exp^{W_j x_i}}}_{\text{softmax}} + \underbrace{\frac{\lambda}{2} \sum_{i=1}^{N} \| x_i - c_{y_i} \|^2}_{\text{centre}}$$

while not converge **do**
  $t \leftarrow t + 1$
  Compute the joint loss $\mathcal{L}^t = \mathcal{L}_s^t + \lambda \mathcal{L}_c^t$
  Compute the backpropagation error:
  $\frac{\partial \mathcal{L}^t}{\partial x_i^t} = \frac{\partial \mathcal{L}_s^t}{\partial x_i^t} + \lambda \frac{\partial \mathcal{L}_c^t}{\partial x_i^t}$ $\quad W^{t+1} = W^t - \mu^t \frac{\partial \mathcal{L}^t}{\partial W^t} = W^t - \mu^t \frac{\partial \mathcal{L}_s^t}{\partial W^t}$
  Update each centre: $c_j^{t+1} = c_j^t - \alpha \nabla c_j^t$
  Update convolution parameters: $\theta_C^{t+1} = \theta_j^t - \mu^t \sum_{i=1}^{N} \frac{\partial \mathcal{L}^t}{\partial x_i^t} \frac{\partial x_i^t}{\partial \theta_C^t}$
end while

Centre Loss

- Wen, et. al, (2016) A Discriminative Feature Learning Approach for Deep Face Recognition, ECCV

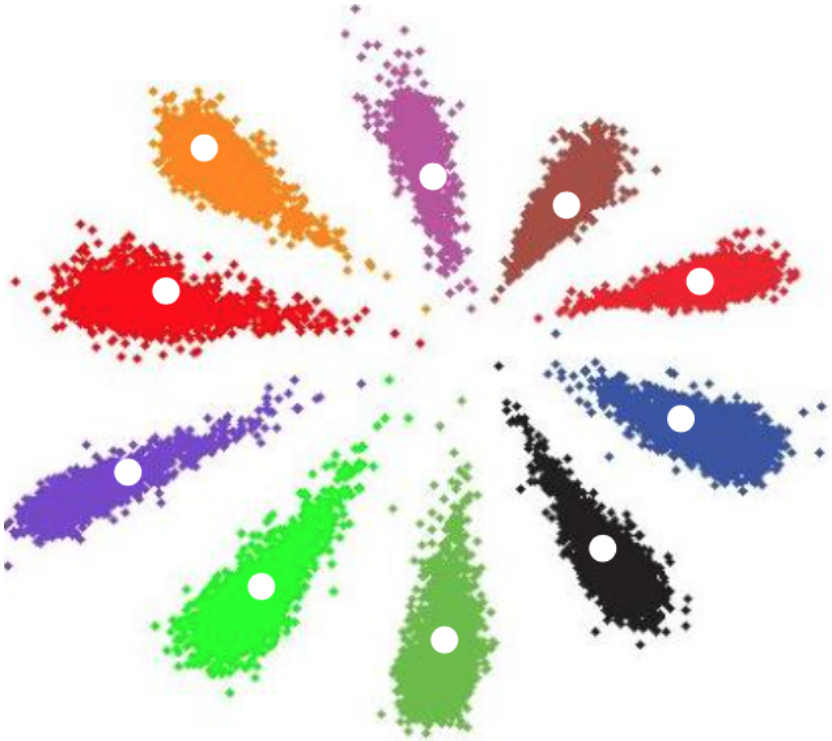


Figure: Softmax only

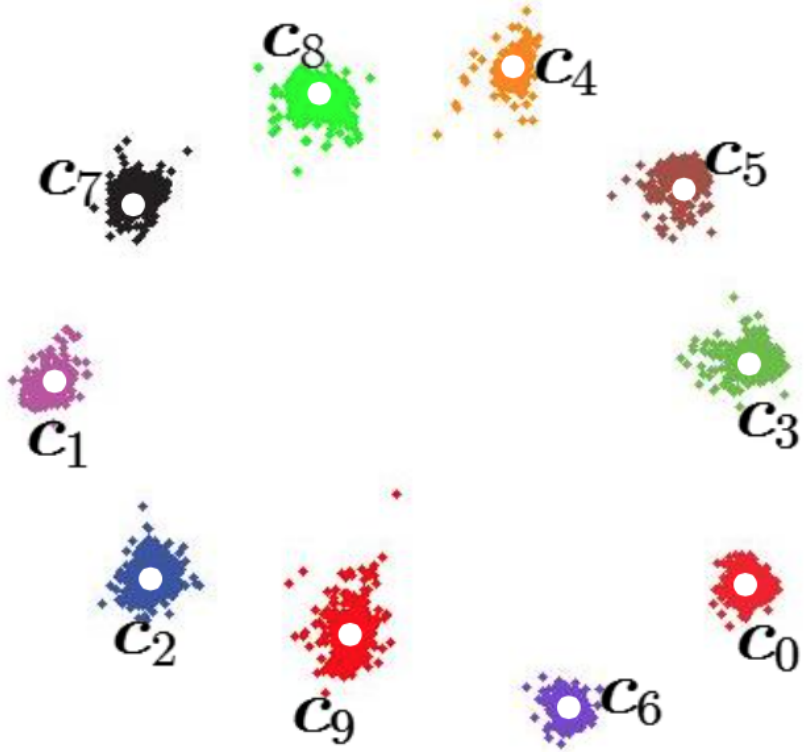


Figure: Softmax + Centre Loss

Center Loss

Our own experiments using Centre Loss training for job descriptions + VET courses

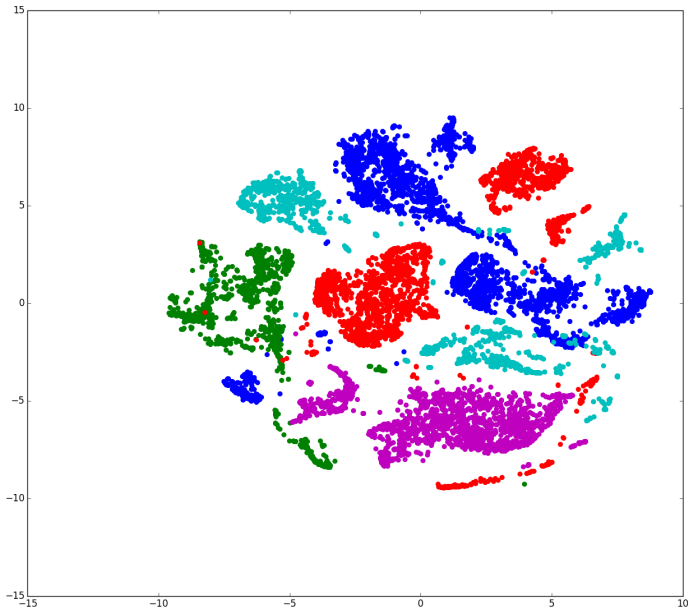


Figure: Softmax only

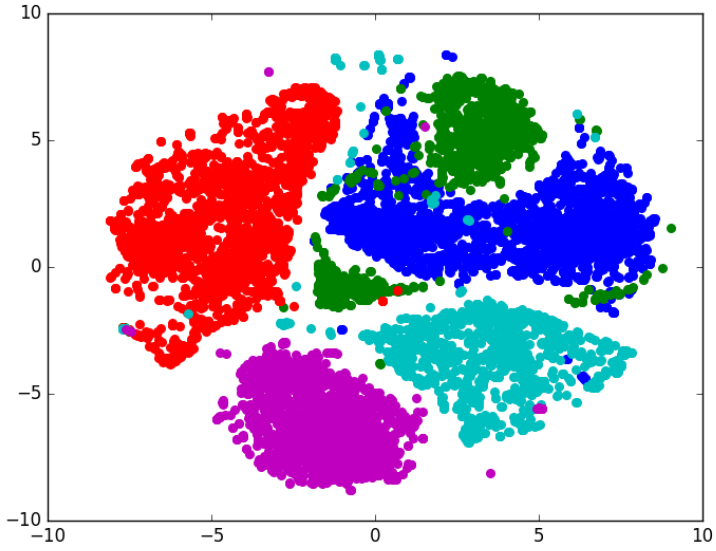


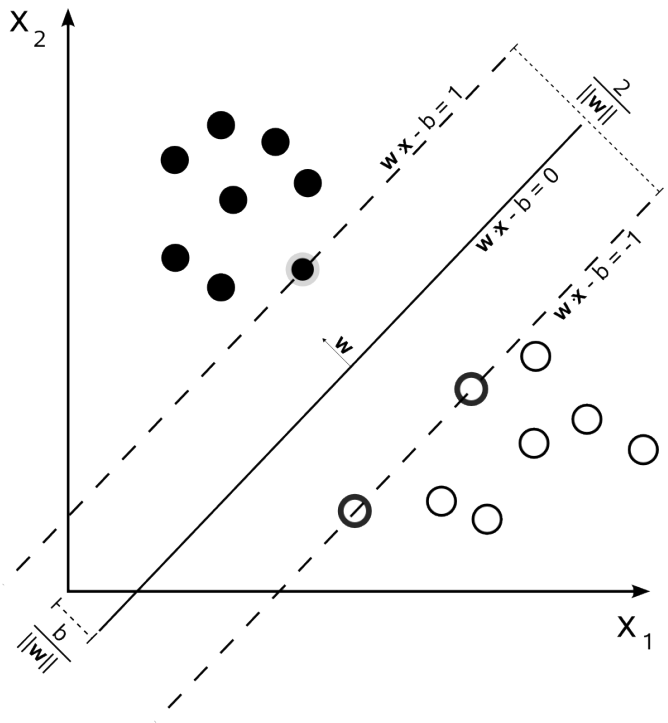
Figure: Softmax + Centre Loss

Support Vector Machine Layer

- Instead of Softmax layer, one may try SVM layer
- Tang, Yichuan. ”Deep learning using linear support vector machines (2013): author claimed it works better on certain dataset

- Soft Margin: allow “some ” wrong sides:

$$\min \left(\frac{1}{2}\|\mathbf{w}\|^2 + C \underbrace{\sum_{i=1}^{n} \mathbf{1}\left[y_i(\mathbf{w}^T x_i + b) < 0\right]}_{\text{sum of number of mis-classified}} \right)$$



- Add a convex upper bound to the indicator function:

$$\min \left(\frac{1}{2}\|\mathbf{w}\|^2 + C \sum_{i=1}^{n} h\left[y_i(\mathbf{w}^T x_i + b)\right] \right)$$

- Hinge loss function $h(x)$:

$$h(x) = \begin{cases} 1 - x & 1 - x > 0 \\ 0 & \text{otherwise} \end{cases}$$

Linear Layer

- Deep Learning can be used for Regression: The last layer can be:

$$U^\top x^{(f)}$$

- In words, the preceding layers are "embedding the data", such that the output from the final linear layer, $x_i^{(f)}$ and response variable y_i forms a linear relationship.

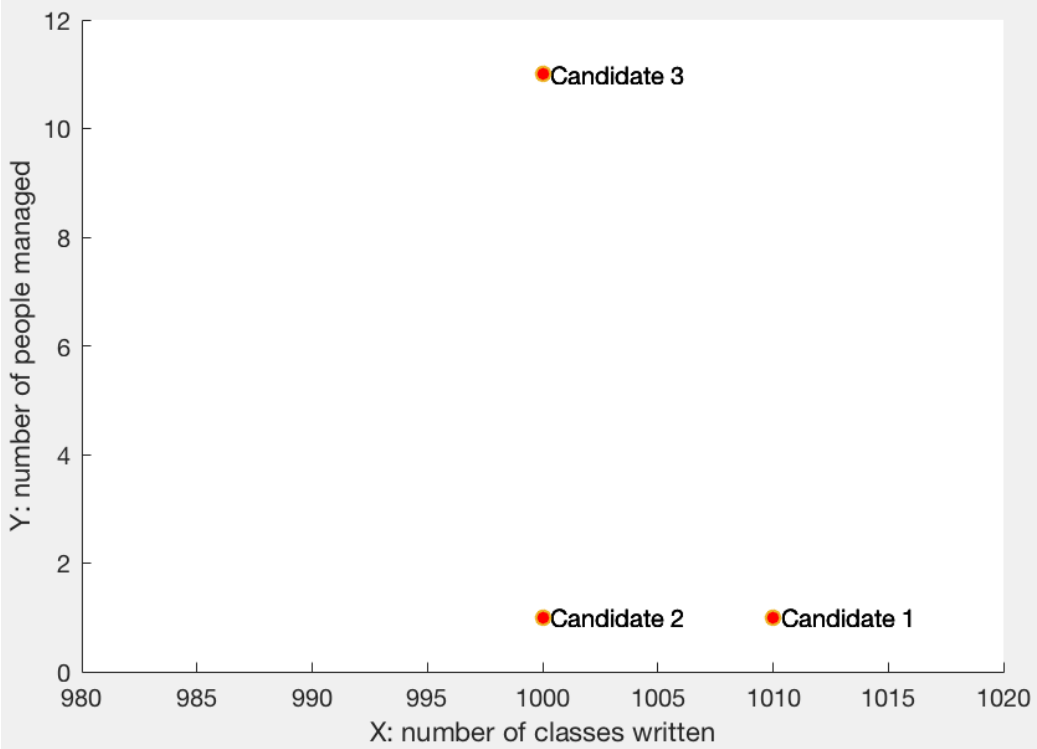
Is there any other task can be carried by Deep Learning dictated by using a different last layer?

- Let's look at **Learning a Similarity Metric**

Distance Metric Learning

To understand **Contrastive** or **Triplet** loss, we need to know **metric learning**:

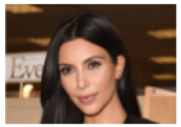
- Suppose 3 candidates competing for technical lead role: (both manager and software skills are essential)
- You want to decide between candidate 1 and candidate 3, whom is more closely matched with candidate 2:
- candidate 1 and candidate 2, **differs 10 in (OO) classes of code**.
- candidate 3 and candidate 2, **differs 10 in number of people managed**.
- It is obvious that number of people managed should attract higher weight



$$d(\text{candidate}_i, \text{candidate}_j) = \left(\begin{bmatrix} X_i \\ Y_i \end{bmatrix} - \begin{bmatrix} X_i \\ Y_i \end{bmatrix} \right)^\top \begin{bmatrix} w_1^{-1} & 0 \\ 0 & w_2^{-1} \end{bmatrix} \left(\begin{bmatrix} X_i \\ Y_i \end{bmatrix} - \begin{bmatrix} X_i \\ Y_i \end{bmatrix} \right)$$

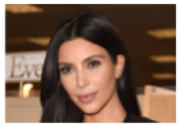
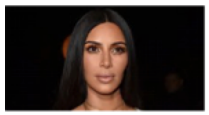
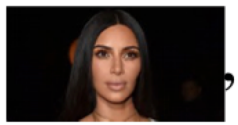
Distance Metric Learning (2)

- In some situations, setting the weight matrix isn't intuitive, but under many scenarios, external labelling can be used:
- **triplet**

$$d_\theta(\ \text{  }\ ,\ \text{  }\ ) \leq d_\theta(\ \text{  }\ ,\ \text{  }\ )$$

- **constrastive**

$$(\ \text{  }\ ,\ \text{  }\ ) \in S \quad (\ \text{  }\ ,\ \text{  }\ ) \in D$$

$$(\ \text{  }\ ,\ \text{  }\ ) \in S \quad (\ \text{  }\ ,\ \text{  }\ ) \in D$$

Traditional Metric Learning

A distance between two vectors x and y can be defined as:

$$d(x,y) = d_W(x,y) = \|x-y\|_W = \sqrt{(x-y)^T W (x-y)}$$

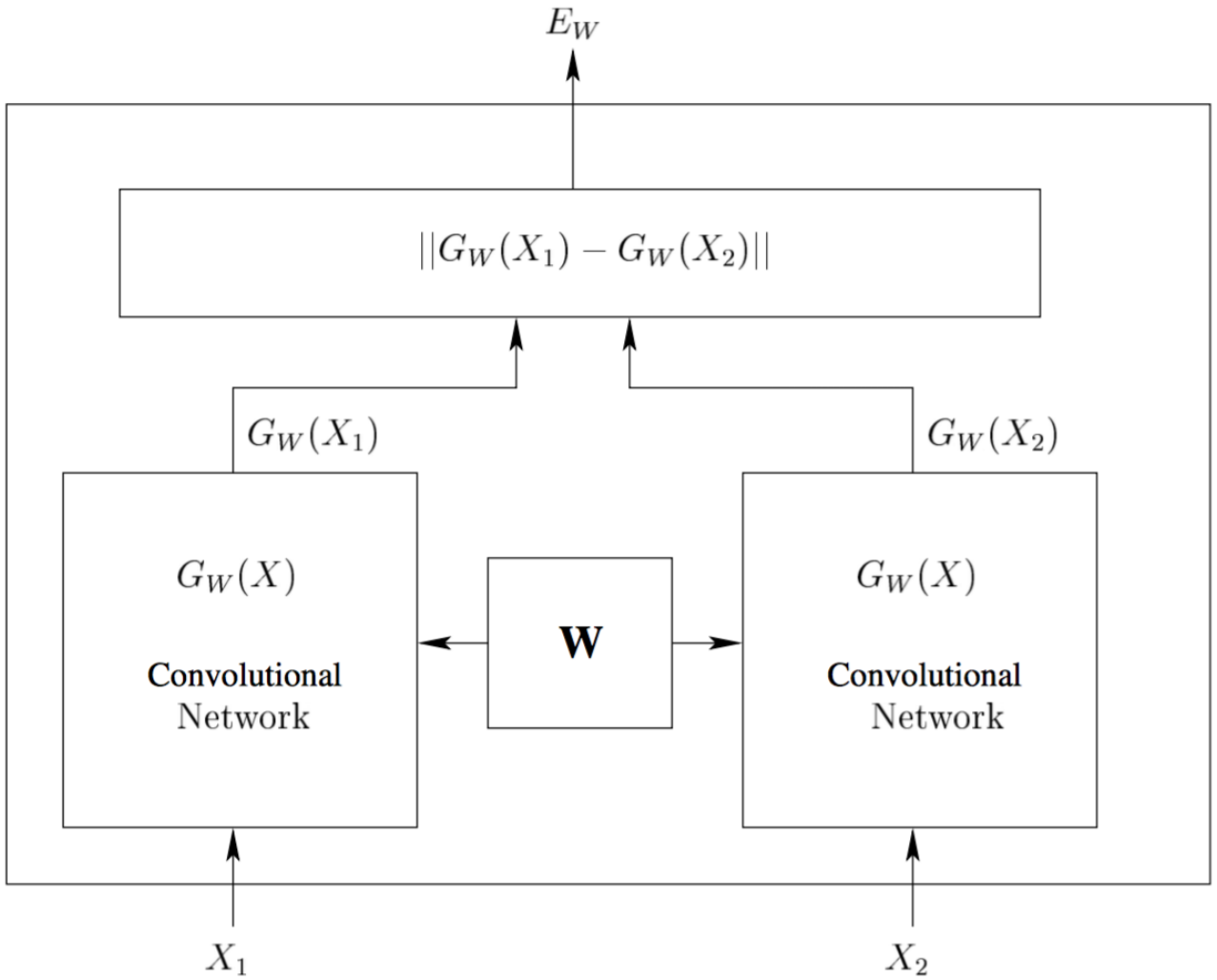
where M is a positive semi-definite (PSD) matrix, or a metric:

$$\min_W \sum_{(x_i,x_j)\in\mathcal{S}} \|x_i - x_j\|_W^2$$

$$\text{s.t.} \sum_{(x_i,x_j)\in\mathcal{D}} \|x_i - x_j\|_W \geq c$$

for some arbitary scalar c.

Bring on the Deep Learning! The Siamese Network



Contrastive Loss

$$\mathcal{C}(X_i, X_j) = \frac{2}{m} \sum_{(i,j)}^{m} y_{i,j} \|G_W(X_i) - G_W(X_j)\| + (1 - y_{i,j}) \max\left(0, \alpha - \|G_W(X_i) - G_W(X_j)\|\right)^2$$

Training process encourages the network to find an embedding where:

- $y_{i,j} \in \{0, 1\}$ indicates whether a pair (x_i, x_j) is from the same class or not
- Minimises the distance between a pair of examples with the same class label
- penalises the negative pair distances for being smaller than the margin α
- $\max(0, .)$ is called the **hinge-loss**

Triplet Loss

$$\mathcal{C}(X_i, X_j) = \frac{2}{m} \sum_{i}^{m} \max\left(0, \|G_W(X_i^a) - G_W(X_i^p)\| - \|G_W(X_i^a) - G_W(X_i^n)\| + \alpha\right)$$

Training process encourages the network to find an embedding where:

- the distance between x_a and x_n cost function is larger than the distance between x_a and x_p plus some margin α

What other examples of Loss function are available?

- Energy Loss

$$\mathcal{L}\left(Y_i, \mathcal{E}(W, Y, X_i)\right) = \mathcal{E}(W, Y_i, X_i)$$

- Generalized Perceptron Loss

$$\mathcal{L}\left(Y_i, \mathcal{E}(W, Y, X_i)\right) = \mathcal{E}(W, Y_i, X_i) - \min_{y \in \mathcal{Y}} \mathcal{E}(W, Y, X_i)$$

- Let $\bar{Y} = \arg\min_{Y \in Y, Y = Y_i} \mathcal{E}(W, Y, X_i)$, the label that has the lowest energy among all answers that are incorrect
- Generalized Margin Losses - Hinge loss:

$$\mathcal{L}\left(Y_i, \mathcal{E}(W, Y, X_i)\right) = \max\left(0, m + \mathcal{E}(W, Y_i, X_i) - \mathcal{E}(W, \bar{Y}_i, X_i)\right)$$

Penalized linearly when $E(W, \bar{Y}_i, X_i) - \mathcal{E}(W, Y_i, X_i) < m$. Loss only depends on energy differences, hence individual energies are not constrained to take any particular value.

- Generalized Margin Losses - Log loss:

$$\log\left(1 + \exp^{\mathcal{E}(W, Y_i, X_i) - \mathcal{E}(W, \bar{Y}_i, X_i)}\right)$$

This is a softer version of hinge loss.

All about that loss: Negative Log-Likelihood Loss

- A Gibbs distribution is defined as:

$$p(Y|X) = \frac{p(X,Y)}{p(X)} = \frac{\exp -\beta \mathcal{E}(Y,X)}{\int_{y\in\mathcal{Y}} exp -\beta \mathcal{E}(Y,X)}$$

- Energy can measure in arbitrary units, but the fraction can cancel the effect.

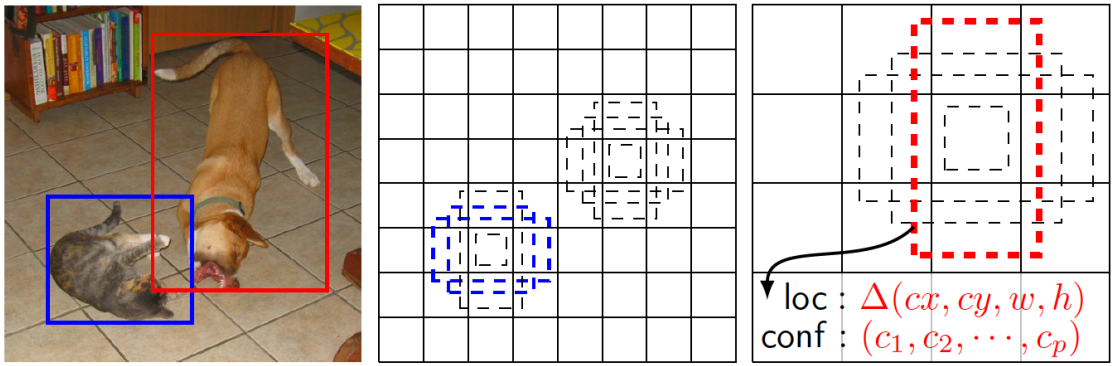
$$\begin{aligned}
-\log \prod_{i=1}^{N} p(Y_i|X_i,W) &= -\sum_{i=1}^{N} \log\left(p(Y_i|X_i,W)\right) \\
&= -\sum_{i=1}^{N} \log\left(\frac{\exp -\beta \mathcal{E}(Y_i,X_i|W)}{\int_{y\in\mathcal{Y}} exp -\beta \mathcal{E}(Y,X_i|W)}\right) \\
&= -\sum_{i=1}^{N} \log\left(\exp -\beta \mathcal{E}(Y_i,X_i|W)\right) + \sum_{i=1}^{N} \int_{y\in\mathcal{Y}} exp -\beta \mathcal{E}(Y,X_i|W) \\
&= \sum_{i=1}^{N} \beta \mathcal{E}(Y_i,X_i|W) + \sum_{i=1}^{N} \int_{y\in\mathcal{Y}} exp -\beta \mathcal{E}(Y,X_i|W)
\end{aligned}$$

In the previous example, $\beta = -1$
When $\beta > 0$:

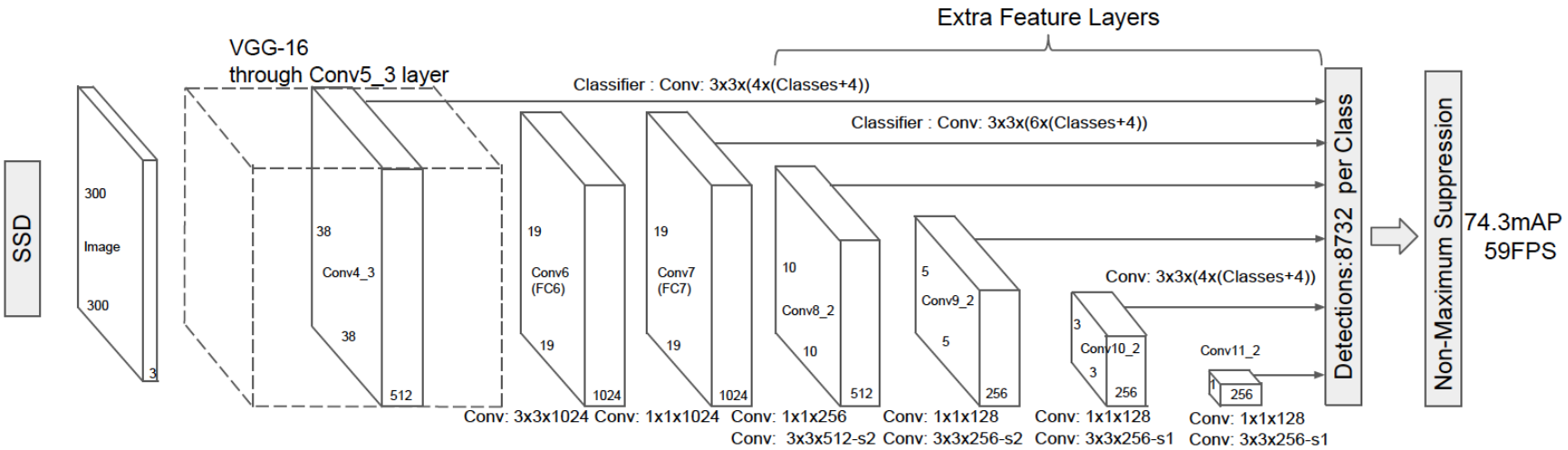
$$\mathcal{C}(W) = \frac{1}{N}\left(\sum_{i=1}^{N} \mathcal{E}(Y_i,X_i|W) + \frac{1}{\beta}\int_{y\in\mathcal{Y}} exp -\beta \mathcal{E}(Y,X_i|W)\right)$$

CNN for detection: Single Shot MultiBox Detector (SSD)

Liu., et. al., (2016) SSD: Single Shot MultiBox Detector, ECCV2016



(a) Image with GT boxes (b) 8×8 feature map (c) 4×4 feature map



CNN for detection: Single Shot MultiBox Detector (SSD)

- $x_{i,j}^p = \{1, 0\}$ indicator for matching ***i*-th default box** to ***j*-th ground truth box** of category p
- $l \equiv (l^{cx}, l^{cy}, l^w, l^h)$: predicted box (transformed represenation)
- $d \equiv (d^{cx}, d^{cy}, d^w, d^h)$: default box (original representation)
- $g \equiv (g^{cx}, g^{cy}, g^w, g^h)$: ground-truth box (original representation)
- $\hat{g} \equiv (\hat{g}^{cx}, \hat{g}^{cy}, \hat{g}^w, \hat{g}^h)$: ground-truth box (transformed representation)

Training objective:

$$\mathcal{C}(x, c, l, g) = \frac{1}{N}\left(\mathcal{C}_{\text{conf}}(x, c) + \alpha \mathcal{C}_{\text{loc}}(x, l, g)\right)$$

- $\mathcal{C}_{\text{conf}}(x, c)$:

$$\mathcal{C}_{\text{conf}}(x, c) = -\sum_{i \in \text{pos}}^{N} x_{i,j}^p \log(\hat{c}_i^p) - \sum_{i \in \text{neg}} \log(\hat{c}_i^0) \qquad \text{where } \hat{c}_i^p = \frac{\exp(c_i^p)}{\sum_p \exp(c_i^p)}$$

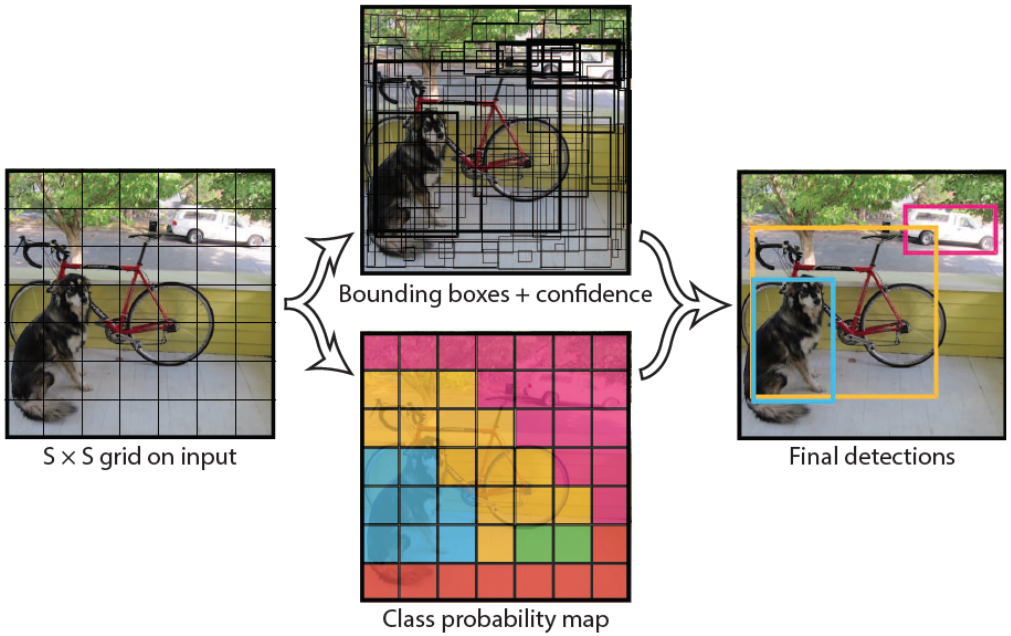
- $\mathcal{C}_{\text{loc}}(x, l, g)$:

$$\mathcal{C}_{\text{loc}}(x, l, \hat{g}) = \sum_{i \in \text{pos}}^{N} \sum_{m \in \{cx, cy, w, h\}} x_{ij}^k \text{smooth}_{L1}(l_i^m - \hat{g}_j^m)$$

- all the parameters making them happen are **convolution filters**

CNN for detection: You Only Look Once (YOLO)

- divides input image into an $S \times S$ grid
- if center of object falls into a grid cell, that grid cell is responsible for detecting that object
- each bounding box consists of 5 predictions: (x, y, w, h, C)
- (x, y) centre of box relative to bounds of grid cell
- (w, h) weight and height of bound relative to the whole image
- C confidence prediction: Intersection Over Union (IOU) between predicted box and any ground truth box



CNN for detection: You Only Look Once (YOLO)

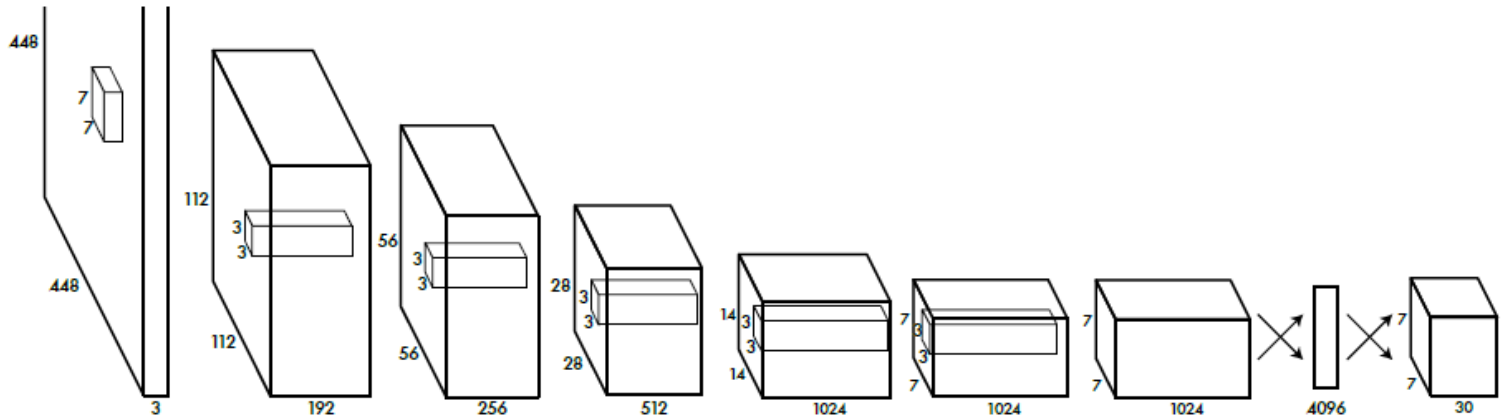
Redmon, et. al., (2016) You Only Look Once: Unified, Real-Time Object Detection, ICCV

- objective function:

$$
\begin{aligned}
\mathcal{C} = & \lambda_{\text{coord}} \sum_{i=1}^{S^2} \sum_{j=1}^{B} \mathbf{1}_{i,j}^{\text{obj}} \left[(x_i - \hat{x}_i)^2 + (y_i - \hat{y}_i)^2 \right] \\
& + \lambda_{\text{coord}} \sum_{i=1}^{S^2} \sum_{j=1}^{B} \mathbf{1}_{i,j}^{\text{obj}} \left[(\sqrt{(w_i)} - \sqrt{\hat{w}_i})^2 + (\sqrt{h_i} - \sqrt{\hat{h}_i})^2 \right] \\
& + \sum_{i=1}^{S^2} \sum_{j=1}^{B} \mathbf{1}_{i,j}^{\text{obj}} \left[(C_i - \hat{C}_i)^2 \right] \\
& + \lambda_{\text{noobj}} \sum_{i=1}^{S^2} \sum_{j=1}^{B} \mathbf{1}_{i,j}^{\text{noobj}} \left[(C_i - \hat{C}_i)^2 \right] \\
& + \sum_{i=1}^{S^2} \mathbf{1}_{i}^{\text{obj}} \sum_{c \in \text{classes}} (p_i(c) - \hat{p}_i(c))^2
\end{aligned}
$$

- $\mathbf{1}_{i,j}^{\text{obj}}$: j-th bounding box predictor in cell i is responsible for that prediction
- $\mathbf{1}_{i}^{\text{obj}}$: if object appears in cell i

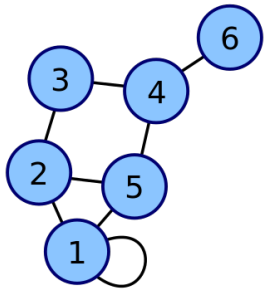
CNN for detection: You Only Look Once (YOLO)



degree matrix

Given a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, the associated degree matrix D is a $n \times n$ diagonal matrix:

$$d_{i,j} := \deg(v_i) \quad \text{if } i = j, \qquad d_{i,j} := 0 \text{ otherwise}$$



$$\begin{pmatrix} 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

- $\deg(v_i)$ counts the number of times an edge terminates at that vertex
- in undirected graph, each new loop increases degree of vertex by **two**, see node 1 above

matrix representation of a graph

- Given a simple graph $\mathcal{G}$ with n vertices, its Laplacian matrix $L^{n\times n}$:

$$L^{\mathcal{G}} = D - A$$

- D is the degree matrix and A is the adjacency matrix of the graph.

$$L^{\mathcal{G}}_{i,j} := \begin{cases} \deg(v_i) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } v_i \text{ is adjacent to } v_j \\ 0 & \text{otherwise} \end{cases}$$

- Since $\mathcal{G}$ is a simple graph, A only contains 1s or 0s and its diagonal elements are all 0s.
- Symmetric normalized Laplacian:

$$L^{\text{sym}} := D^{-1/2} L D^{-1/2} = I - D^{-1/2} A D^{-1/2}$$

About Graph Laplacian

- For a twice differentiable function f on the euclidean space, the Laplacian of f, Δf is **div(grad(f))** (divergence of the gradient of f)
- consider Laplacian in two dimensions:

$$\Delta f(x,y) = \nabla \cdot \nabla f(x,y) = \frac{d^2 f(x,y)}{dx^2} + \frac{d^2 f(x,y)}{dy^2}$$

- knowing that in 1-d, second derivative is approximated by:

$$f''(x) = \lim_{h \to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

- then we can see the approximation of

$$\begin{aligned} \Delta f(x,y) &= \lim_{t \to 0} \frac{f(x+h,y) + f(x-h,y) + f(x,y+h) + f(x,y-h) - 4f(x,y)}{h^2} \\ &\approx \frac{f(x+h,y) + f(x-h,y) + f(x,y+h) + f(x,y-h) - 4f(x,y)}{h^2} \end{aligned}$$

- this means that $\Delta f(x,y)$ is a **local gradient averaging operator**, is zero at a smooth image

f and ∇f

- Consider a function (or vector) **f** over vertices $\mathcal{V}$, $\mathbf{f} : \mathcal{V} \to \mathbb{R}$. This function is indexed by vertices, say v_i is the node value for i^{th} node, i.e., **f** is a vector, for example:

$$\mathbf{f} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$$

- then the product $\nabla\mathbf{f}$ is indexed by edges $\mathcal{E}$:
- each element of $\nabla\mathbf{f}$ is the difference between two end points of an edge e i.e. $v_i - v_j$:

$$\nabla\mathbf{f} = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} = \begin{bmatrix} v_1 - v_2 \\ v_2 - v_3 \end{bmatrix}$$

- Matrix ∇ acts like a difference or gradient operator on $\mathcal{G}$

g and $\nabla^T \mathbf{g}^T$

- Consider a real function $\mathbf{g}$ over edges $\mathcal{E}$, $\mathbf{g} : \mathcal{E} \to \mathbb{R}$ indexed by edges.
- then, the product $\nabla^\top g^\top$ is a vector indexed by $\mathcal{V}$.
- Value at i^{th} vertex:

$$(\mathbf{g}\nabla)_i = \sum_{e \text{ exit node } i} g_e - \sum_{e \text{ enters node } i} g_e$$

- $(\mathbf{g}\nabla)_i$ is the net outbound flow on the vertex v which is **divergence**

combine together

- Consider the quantity $\nabla^T \nabla \mathbf{f}$
- this is divergence of the gradient.
- the matrix $L^{\mathcal{G}} = \nabla^T \nabla$ is the **Graph Laplacian**:

$$\nabla^\top \nabla = \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & 1 & -1 \end{bmatrix}$$

$$\implies \nabla^\top \nabla \mathbf{f} = \begin{bmatrix} 1 & -1 & 0 \\ 1 & 2 & -1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} = \begin{bmatrix} v_1 - v_2 \\ 2v_2 + v_1 - v_3 \\ v_2 - v_3 \end{bmatrix}$$

- for each i, j element of $L^{\mathcal{G}}$:

$$L^{\mathcal{G}}_{i,j} := \begin{cases} \deg(v_i) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } v_i \text{ is adjacent to } v_j \\ 0 & \text{otherwise} \end{cases}$$

- easy to see that $L^{\mathcal{G}} = D - A$:
- Laplacian is positive semidefinite:

$$\mathbf{f}^\top \nabla^\top \nabla \mathbf{f} = \|\nabla \mathbf{f}\|^2 = \sum_{(i,j) \in \mathcal{E}} (\mathbf{f}_i - \mathbf{f}_j)^2$$

Spectral Decomposition

- A Laplacian is written as:

$$L^{\mathcal{G}}\phi_k = \lambda_k \phi_k$$

- eigenvectors:

$$\langle \phi_k, \phi_{k'} \rangle = \delta_{k,k'}$$

- eigenvalues are non-negative:

$$0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$$

- eigendecomposition of graph Laplacian:

$$L^{\mathcal{G}} = \Phi^\top \Lambda \Phi$$

where:

$$\Phi = [\phi_1, \ldots, \phi_n] \qquad \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$$

Fourier Transform

- **traditional** Fourier series of a function:

$$f(x) = \sum_{k \geq 0} \underbrace{\frac{1}{2\pi} \int_{-\pi}^{\pi} f(t) \exp^{-ikt} \, \mathrm{d}t}_{\hat{f}_k = \langle \mathbf{f}, \exp^{-ikx} \rangle \text{ coefficient}} \underbrace{\exp^{-ikx}}_{\text{Fourier basis}}$$

- **graph** Fourier series: for the i^{th} element:

$$f_i = \sum_{k=1}^{n} \underbrace{\langle f, \phi_k \rangle}_{\hat{f}_k \text{ coefficient}} \qquad \underbrace{\phi_{k,i}}_{\text{graph Fourier basis}}$$

in matrix notation:

$$\hat{\mathbf{f}} = \Phi^\top \mathbf{f} \qquad \text{and } \mathbf{f} = \Phi^\top \hat{\mathbf{f}}$$

Convolution in Euclidean space

- convolution theorem:

$$\widehat{\mathbf{f} \circledast \mathbf{g}} = \hat{\mathbf{f}} \odot \hat{\mathbf{g}}$$

- $\mathbf{f} = (f_1, \ldots, f_n)^\top$ and $\mathbf{g} = (g_1, \ldots, g_n)^\top$

$$(\mathbf{f} \circledast \mathbf{g})_i = \sum_k g(i-k) \bmod n \cdot f_m$$

$$\implies \mathbf{f} \circledast \mathbf{g} = \underbrace{\begin{bmatrix} g_1 & g_2 & \cdots & \cdots & g_n \\ g_n & g_1 & g_2 & \cdots & g_{n-1} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ g_3 & g_4 & \cdots & g_1 & g_2 \\ g_2 & g_3 & \cdots & \cdots & g_1 \end{bmatrix}}_{\text{Circulant matrix}} \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}$$

$$= \Phi \underbrace{\begin{bmatrix} \hat{g}_1 & & \\ & \ddots & \\ & & \hat{g}_n \end{bmatrix}}_{\Phi^\top \mathbf{g}} \Phi^\top \mathbf{f}$$

$$= \Phi(\Phi^\top \mathbf{g} \odot \Phi^\top \mathbf{f})$$

Convolution on graphs

- spectral convolution:

$$\begin{aligned}\mathbf{f} \circledast \mathbf{g} &= \Phi(\Phi^\top \mathbf{g} \odot \Phi^\top \mathbf{f}) \\ &= \underbrace{\Phi \mathrm{diag}(\hat{g}_1, \ldots, \hat{g}_n)\Phi^\top}_{G} \mathbf{f}\end{aligned}$$

What is missing?

- CNN has a pooling step
- GraphCNN has Graph downsampling(**coarsening**) step