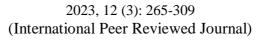
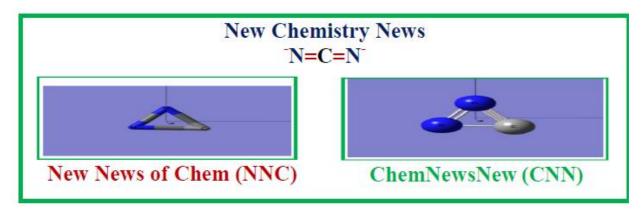
ISSN: 2278-1862



### Journal of Applicable Chemistry







## CNN – 50 Convolution Neural Nets(ConvNN) Part 1.Pretrained Nets

Information Source	ACS.org ; sciencedirect.com
K. Somasekhara Rao,	R. Sambasiva Rao,
Dept. of Chemistry,	Dept. of Chemistry,
Acharya Nagarjuna Univ.,	Andhra University,
Dr. M.R.Appa Rao Campus,	Visakhapatnam 530 003, India
Nuzvid-521 201, India	

**Conspectus:**Neuron is processing unit accepting a scalar input and outputting a scalar. The transformation of input is affected by a transfer function (ranging from identity to tanh, fuzzy and so on). A number of neurons are structured in layers called one input layer, one output layer and single/many hidden layers. The neurons in any layer are not interconnected. The data moves in the forward direction through sequentially connected input-hidden-output layers. These of architectures are popular as feed-forward (FF)-sequential (seq)-single (multiple) (S/M) layer perceptron (SLP/MLP) neural network (NN). When layers are connected in reverse direction also (I $\leftarrow$ [H1 $\leftarrow$ H2] $\leftarrow$  O), the models are called recurrent NNs. In the classical era (1943-1985, 1986 to 1995), the number of hidden layers were restricted to two or a maximum of three. Keeping aside the cognitron (1975) and neo-cognitron (1980) by Fukushima, a new era started with convolution neural nets (CNNs).

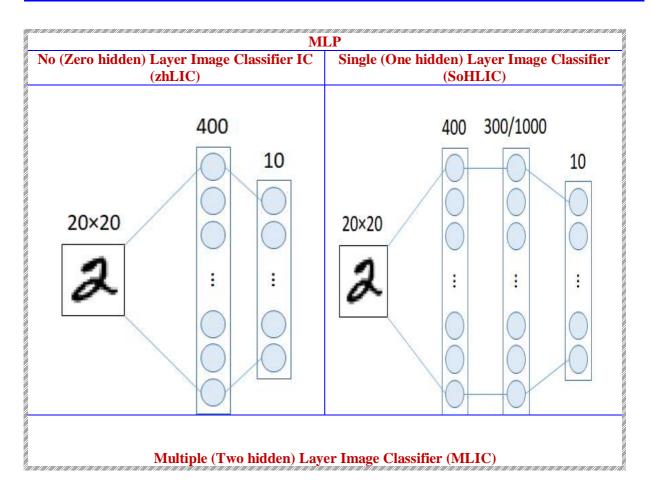
Here, architectural details, performance, depth of net, number of refinable parameters of

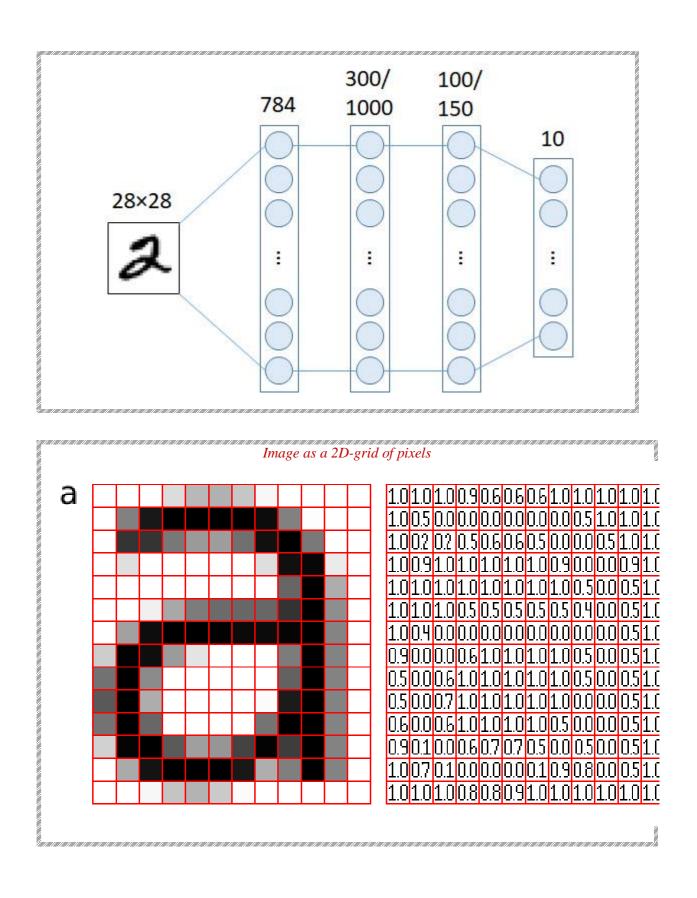
typical large-size CNNs for example LeNet-x, Alex Net, YOLO, VGG, ResNet, Inception, Xception, EfficientNet, MobileNet, DenseNet, ConvNeXt etc. are summarized. The genes i.e. padding, pooling, flattening and normalization express different outcomes.

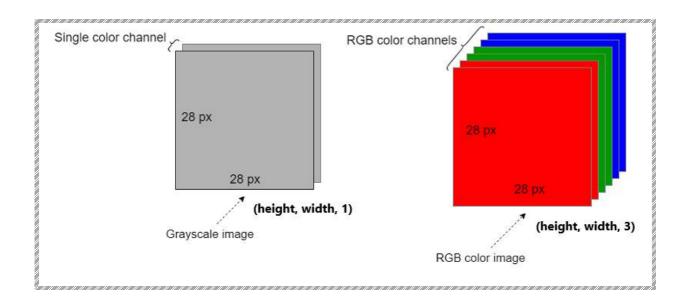
**Keywords:**Single (hidden) layer perceptron (SLP) neural net(NN); M(ulti)LPNN-Convolution neural net(ConvNN)-Images of W\*H-pixels; grey/RBG; AlexNet; VGG;ResNet

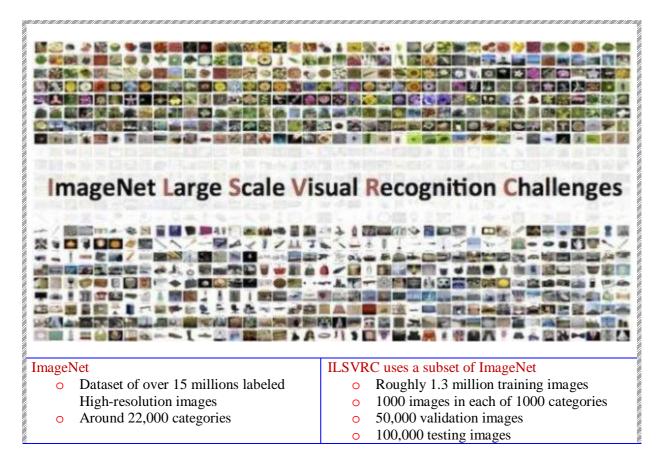
I II	Layout Sequential Layered (seqL) Feed forward (FF) Fully Connected (FulCon) NeuronNets (NNs) Math-DNA- Components of \$\$\$-CNN	V(nowladza)I ab
ш	Architectures and Performance measures Fortypical \$\$\$-ConvNNs	K(nowledge)Lab rsr.chem1979
IV	Anatomy and characteristics of typical \$\$\$-CNN	
V	xAiProbes for ConvNN, CapsNN	

### I. Sequential Layered (seqL) Feed forward (FF) Fully Connected (FulCon) NeuronNets (NNs)

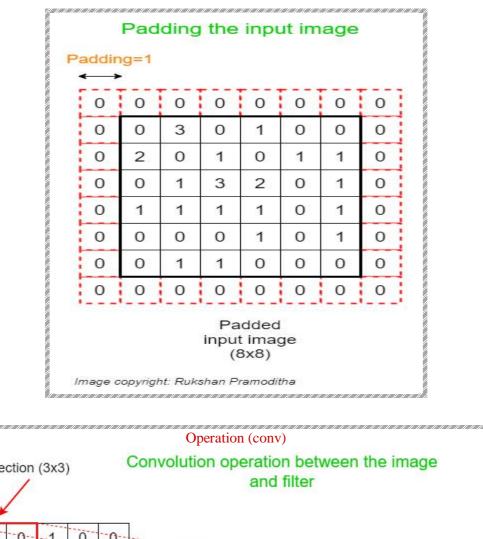


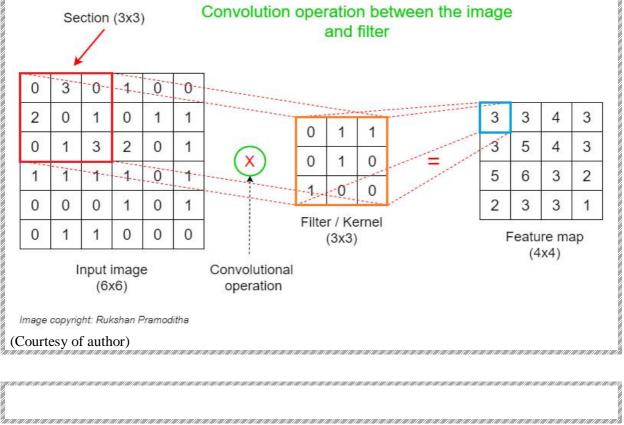


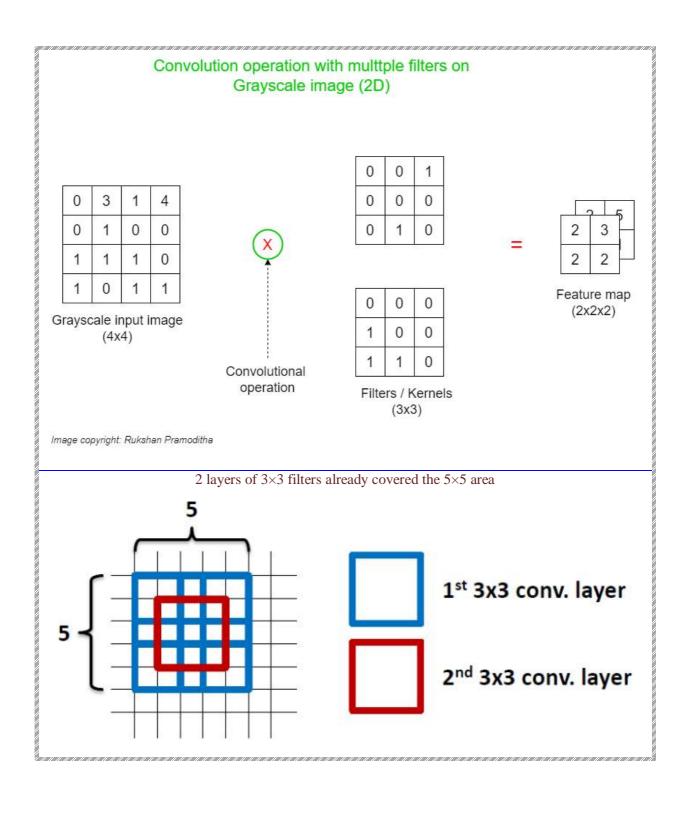


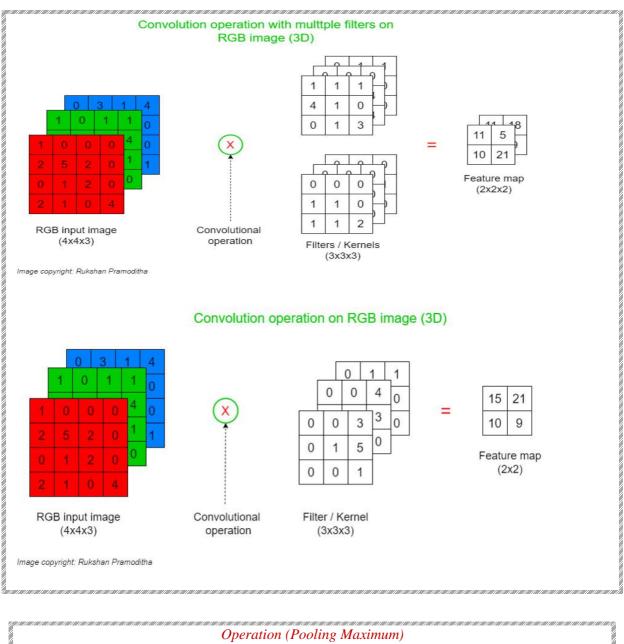


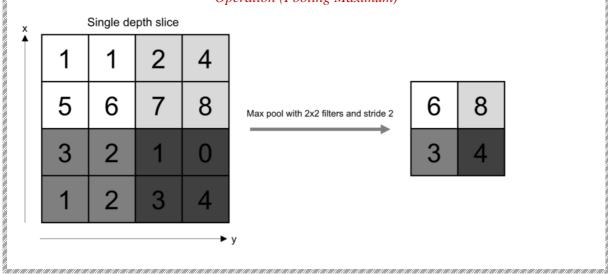
### II. Math-DNA- Components of \$\$\$-CNN

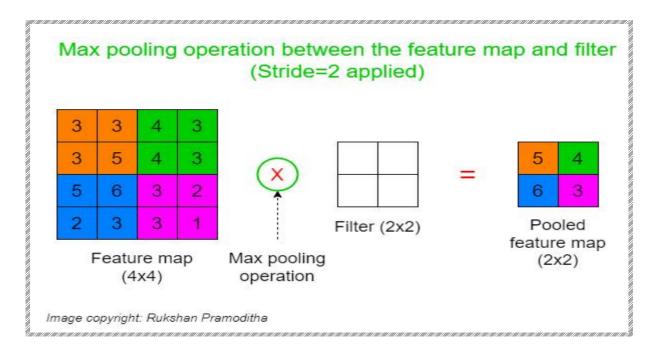


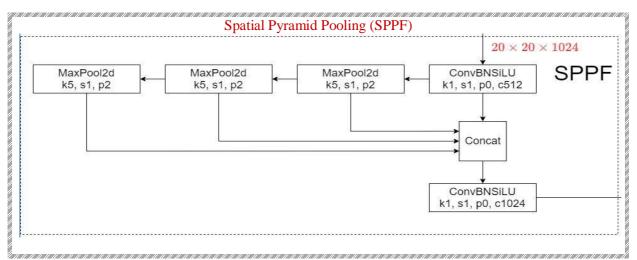


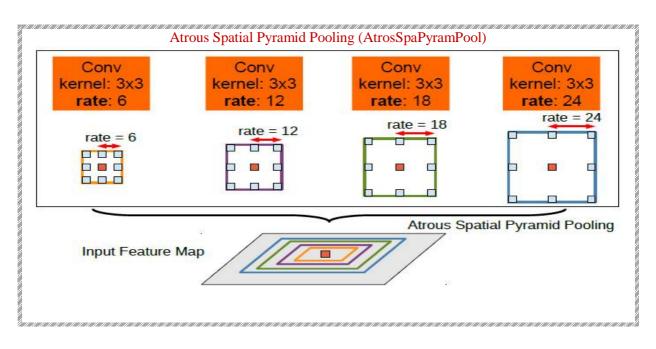


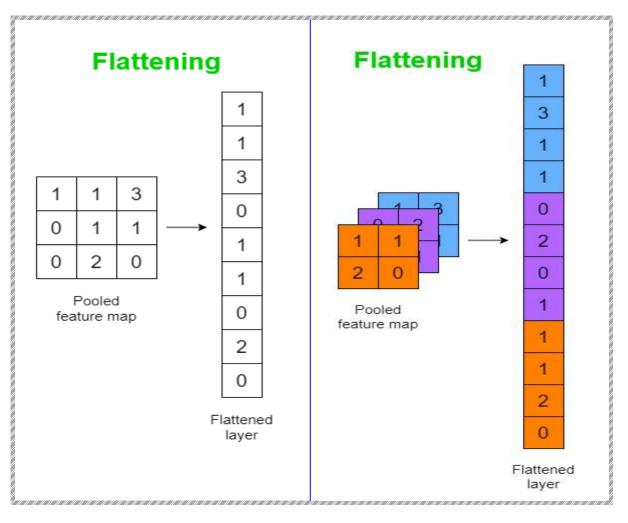


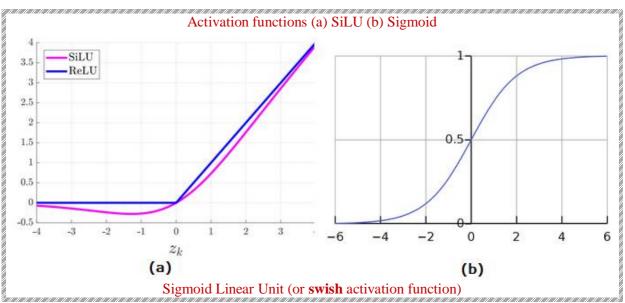


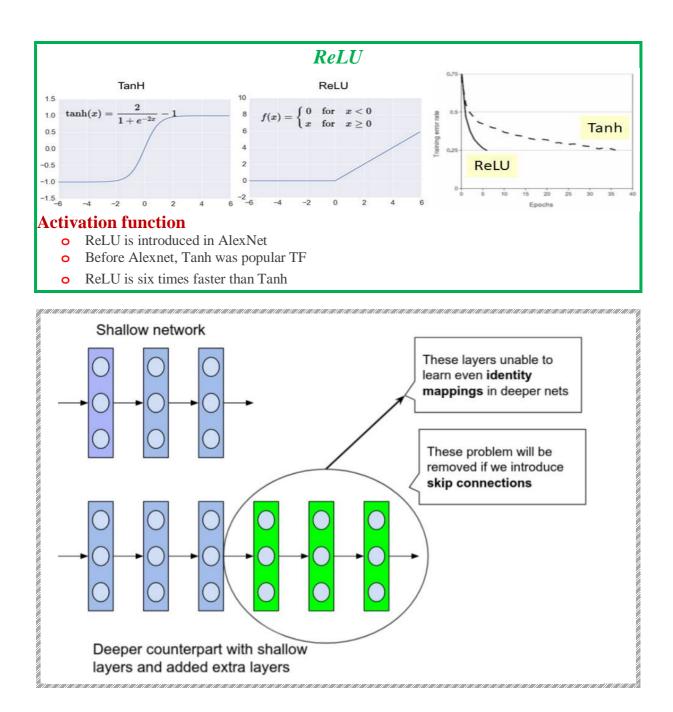


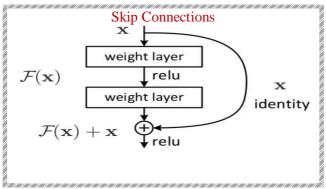


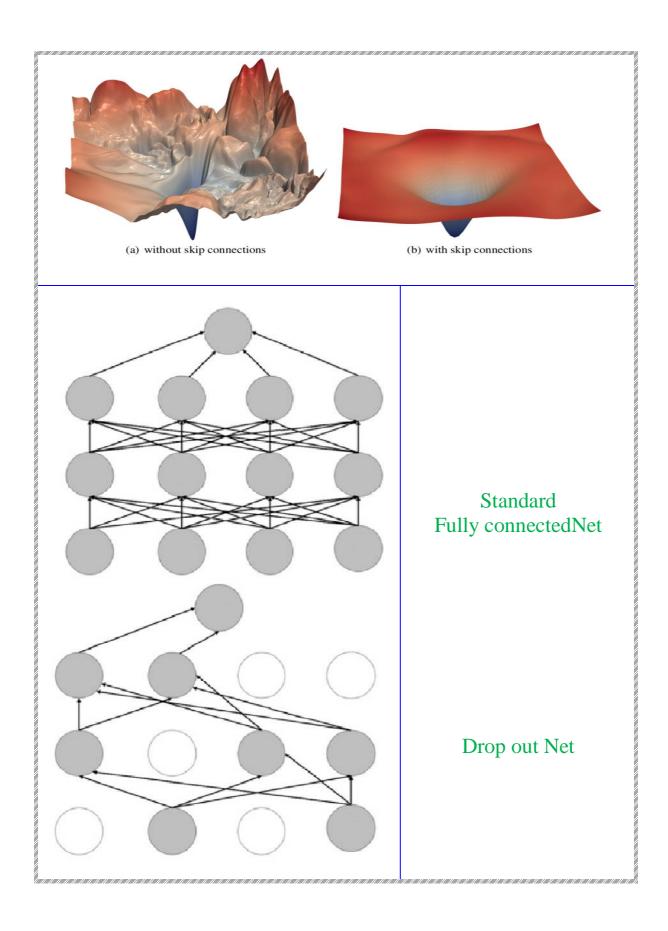


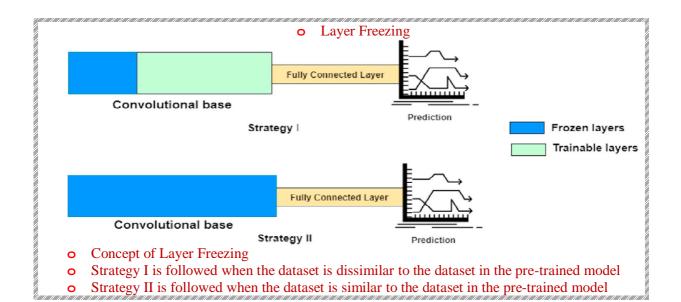


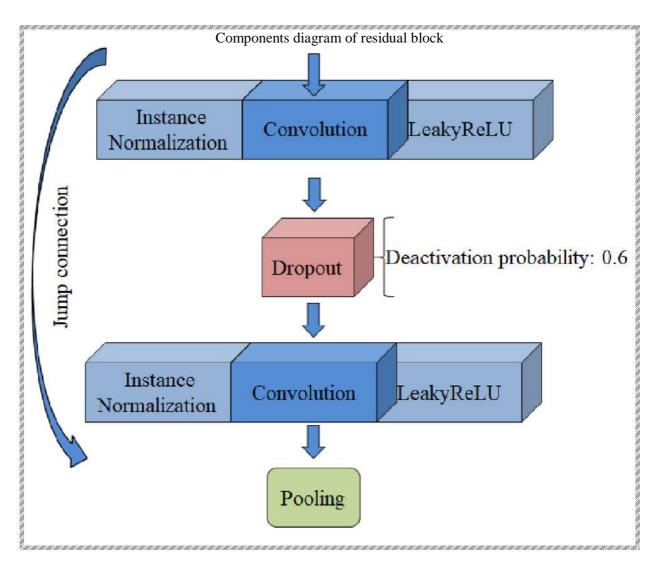










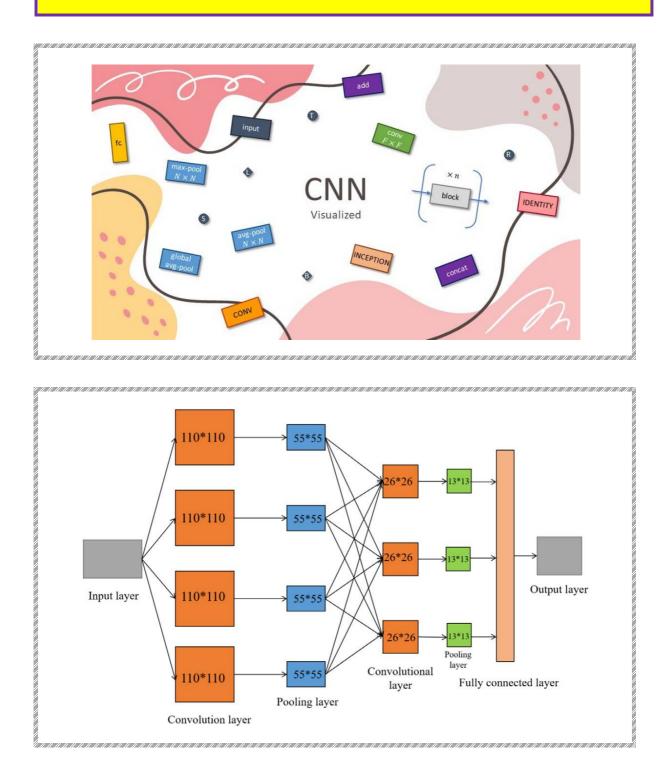


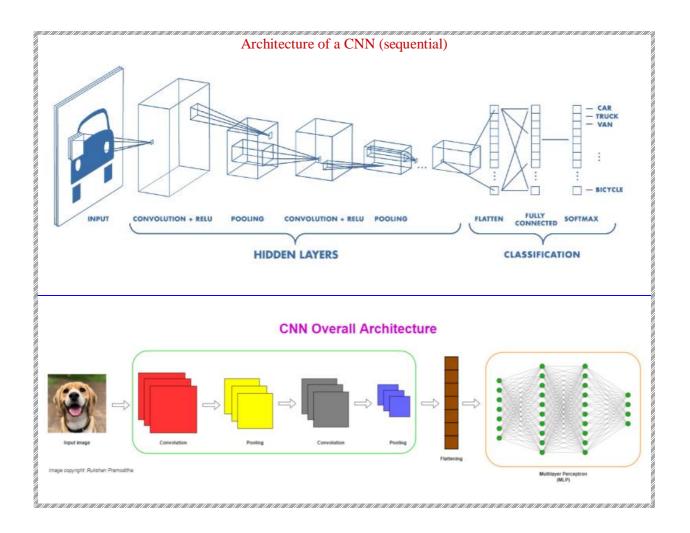
### **III.** Architectures andPerformance measures

## for typical \$\$\$-ConvNNs

Named CNN	version	Depth	Parameters	Size (MB)	Top-1 Accuracy	Top-5 Accuracy
Xception	Xception	81	22.9M	88	79.0%	94.5%
VGG	VGG16	16	138.4M	528	71.3%	90.1%
	VGG19	19	143.7M	549	71.3%	90.0%
ResNet	ResNet50	107	25.6M	98	74.9%	92.1%
	ResNet50V2	103	25.6M	98	76.0%	93.0%
	ResNet101	209	44.7M	171	76.4%	92.8%
	ResNet101V2	205	44.7M	171	77.2%	93.8%
	ResNet152	311	60.4M	232	76.6%	93.1%
	ResNet152V2	307	60.4M	232	78.0%	94.2%
Inception	InceptionV3	189	23.9M	92	77.9%	93.7%
	InceptionResNetV2	449	55.9M	215	80.3%	95.3%
MobileNet	MobileNet	55	4.3M	16	70.4%	89.5%
	MobileNetV2	105	3.5M	14	71.3%	90.1%
DenseNet	DenseNet121	242	8.1M	33	75.0%	92.3%
	DenseNet169	338	14.3M	57	76.2%	93.2%
	DenseNet201	402	20.2M	80	77.3%	93.6%
NASNe	NASNetMobile	389	5.3M	23	74.4%	91.9%
	NASNetLarge	533	88.9M	343	82.5%	96.0%
EfficientNet	EfficientNetB0	132	5.3M	29	77.1%	93.3%
	EfficientNetB1	186	7.9M	31	79.1%	94.4%
	EfficientNetB2	186	9.2M	36	80.1%	94.9%
	EfficientNetB3	210	12.3M	48	81.6%	95.7%
	EfficientNetB4	258	19.5M	75	82.9%	96.4%
	EfficientNetB5	312	30.6M	118	83.6%	96.7%
	EfficientNetB6	360	43.3M	166	84.0%	96.8%
	EfficientNetB7	438	66.7M	256	84.3%	97.0%
	EfficientNetV2B0	-	7.2M	29	78.7%	94.3%
	EfficientNetV2B1	-	8.2M	34	79.8%	95.0%
	EfficientNetV2B2	-	10.2M	42	80.5%	95.1%
	EfficientNetV2B3	-	14.5M	59	82.0%	95.8%
	EfficientNetV2S	-	21.6M	88	83.9%	96.7%
	EfficientNetV2M	-	54.4M	220	85.3%	97.4%
	EfficientNetV2L	-	119.0M	479	85.7%	97.5%
ConvNeXt	ConvNeXtTiny	-	28.6M	109.42	81.3%	-
	ConvNeXtSmall	-	50.2M	192.29	82.3%	-
	ConvNeXtBase	-	88.5M	338.58	85.3%	-
	ConvNeXtLarge	-	197.7M	755.07	86.3%	-
	ConvNeXtXLarge	-	350.1M	1310	86.7%	-

## IV. Anatomy and characteristics of typical \$\$\$-CNN

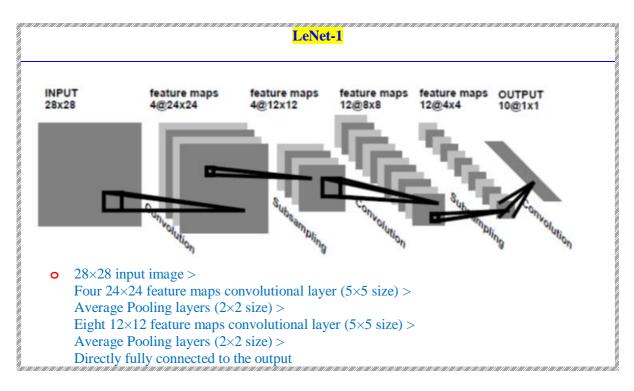


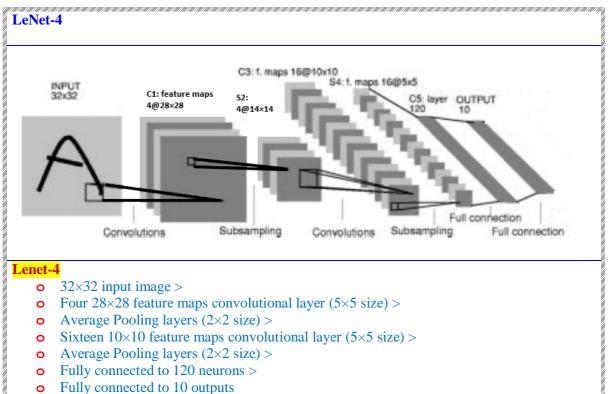


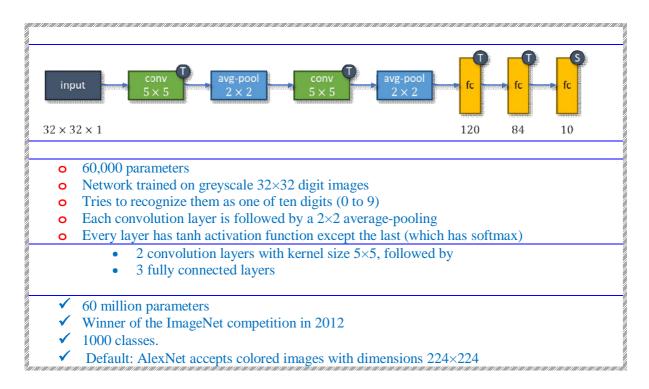
CNN	Default	Default	Number of	Number of	Activation	New Additional Perks
Architecture	Input	Output	Layers	Parameters	Function	
eNet-5	32×32×1	10	5	60K	tanh	Convolution Layer
AlexNet	224×224×3	1000	8	60M	ReLU	Local Response Normalization
VGG-16	224×224×3	1000	16	138M	ReLU	Very deep but still single thread
nception-v1	224×224×3	1000	22	7M	ReLU	Auxiliary Classifiers & Inception Module
ResNet-50	224×224×3	1000	50	26M	ReLU	Batch Normalization & Residual Blocks

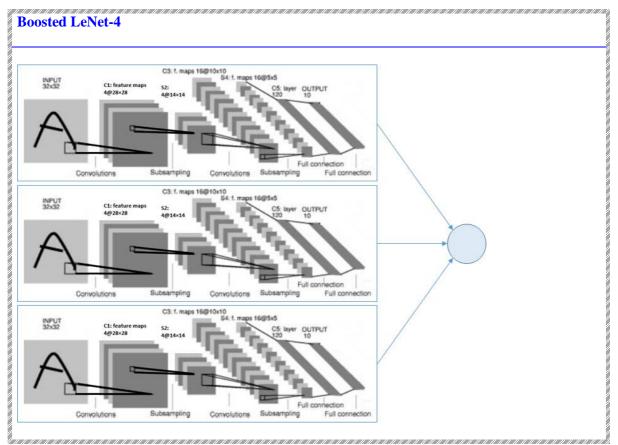
#### **Summary on Error Rate**

- **1.** Baseline Linear Classifier: 8.4%
- 2. One-Hidden-Layer Fully Connected Multilayer NN: 3.6% to 3.8%
- 3. Two-Hidden-Layer Fully Connected Multilayer NN: 2.95% to 3.05%
- **4.** LeNet-1: 1.7%
- **5.** LeNet-4: 1.1%
- **6.** LeNet-5: 0.95%
- 7. Boosted LeNet-4: 0.7%

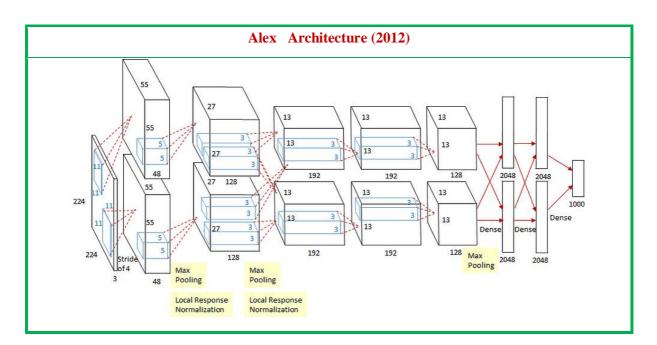






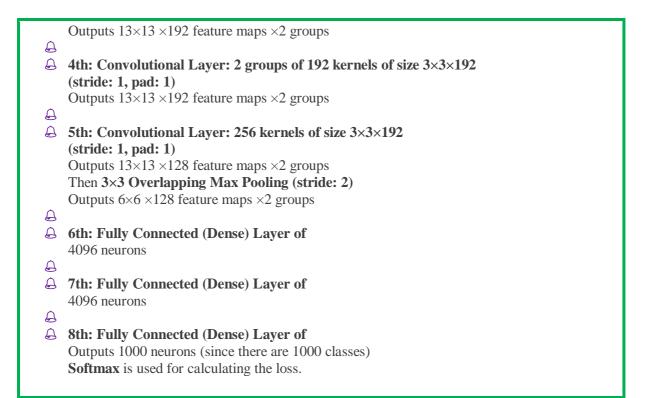


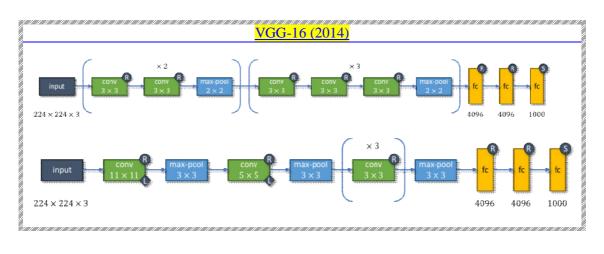
- + Boosting is a technique to combine the results from several/many weak classifiers to obtain more accurate values.
  - ✓ In LeNet-4, the outputs of three LeNet-4 are simply added together
  - ✓ one with maximum value would be the predicted classification class
  - ✓ And there is an enhancement that when the first net has a high confidence answer, the other nets would not be called.
  - + With boosting, the **error rate** on test data is **0.7%** which is even smaller than that of LeNet-5.

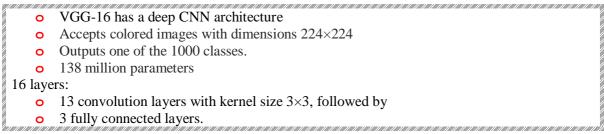


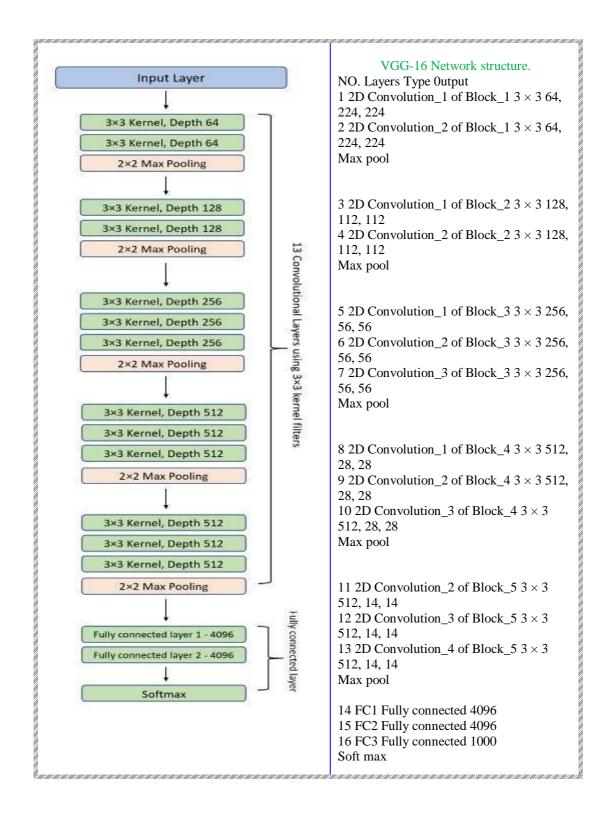
#### Architecture of Alex Net in object mode

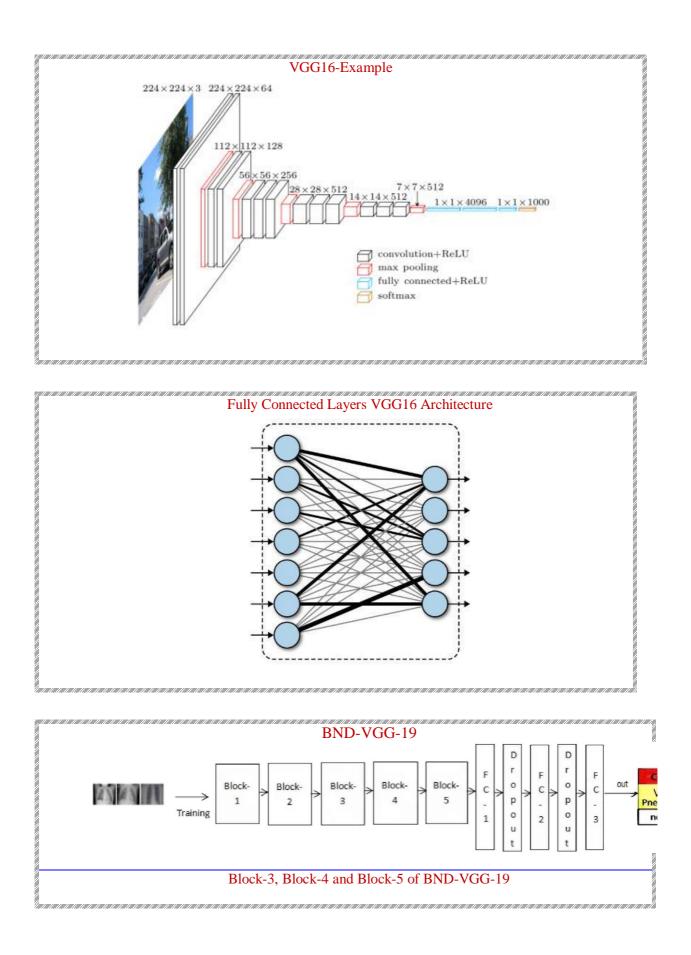
- ✓ Input: 224×224×3 ; original :
- $227 \times 227 \times 3$  if padded during1st convolution
  - ✓ Total parameters trained: 60 million
  - **△** 1st: Convolutional Layer: 2 groups of 48 kernels, size 11×11×3 (stride: 4, pad: 0) Outputs  $55\times55\times48$  feature maps  $\times2$  groups Then 3×3 Overlapping Max Pooling (stride: 2) Outputs  $27 \times 27 \times 48$  feature maps  $\times 2$  groups Then Local Response Normalization Outputs  $27 \times 27 \times 48$  feature maps  $\times 2$  groups A **△** 2nd: Convolutional Layer: 2 groups of 128 kernels of size 5×5×48 (stride: 1, pad: 2) Outputs  $27 \times 27 \times 128$  feature maps  $\times 2$  groups Then 3×3 Overlapping Max Pooling (stride: 2) Outputs  $13 \times 13 \times 128$  feature maps  $\times 2$  groups Then Local Response Normalization Outputs  $13 \times 13 \times 128$  feature maps  $\times 2$  groups A **△** 3rd: Convolutional Layer: 2 groups of 192 kernels of size 3×3×256
    - (stride: 1, pad: 1)

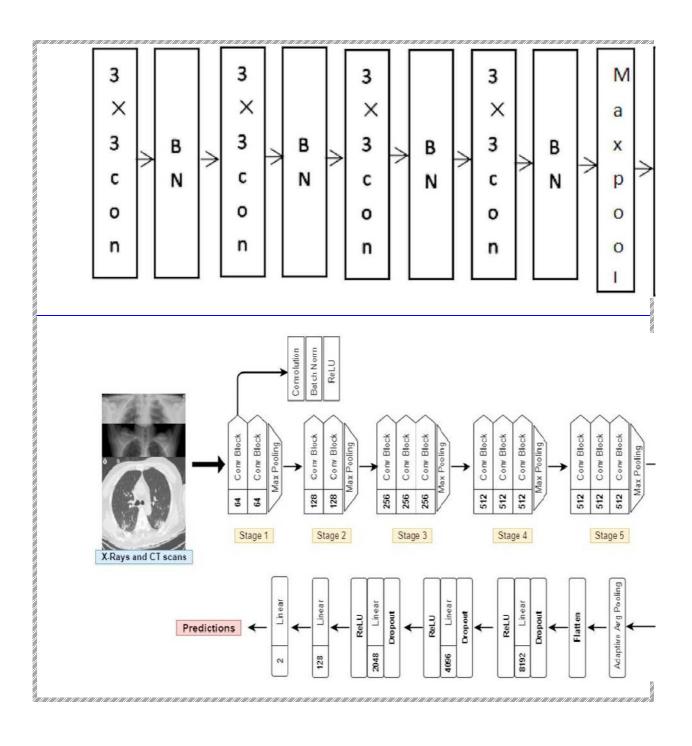


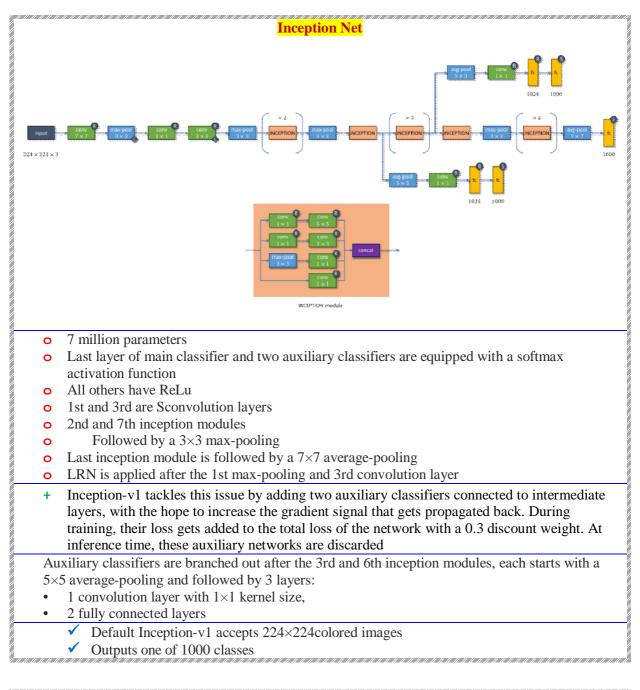


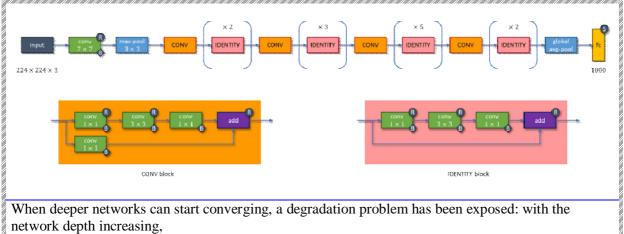




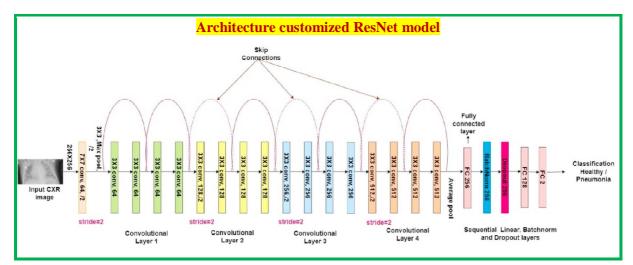


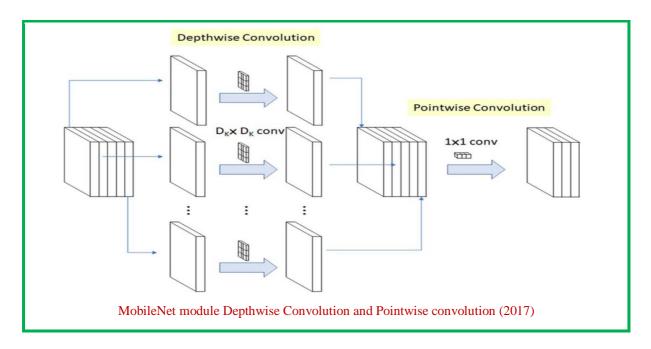






<ul> <li>Accuracy gets saturated and then degrades rapidly</li> <li>Unexpectedly, such degradation is not caused by overfitting (usually indicated by lower training error and higher testing error) since adding more layers to a suitably deep network leads to higher training error</li> </ul>
Notice that both residual blocks have 3 layers.
ResNet-50 has 50 layers and 26 million parameters
<ul> <li>1 convolution layer with BN then ReLU is applied, followed by</li> <li>9 layers that consist of 1 convolution block and 2 identity blocks, followed by</li> <li>12 layers that consist of 1 convolution block and 3 identity blocks, followed by</li> <li>18 layers that consist of 1 convolution block and 5 identity blocks, followed by</li> <li>9 layers that consist of 1 convolution block and 2 identity blocks, followed by</li> </ul>
✓ 1 fully connected layer with softmax
• The first convolution layer is followed by a $3 \times 3$ max-pooling
• Last identity block is followed by a global-average-pooling
• Default ResNet-50 accepts colored images with dimensions 224×224 and outputs one of the 1000 classes.





MobileNet is a lightweight architecture consisting of 30 layers for image classification (71% accuracy)

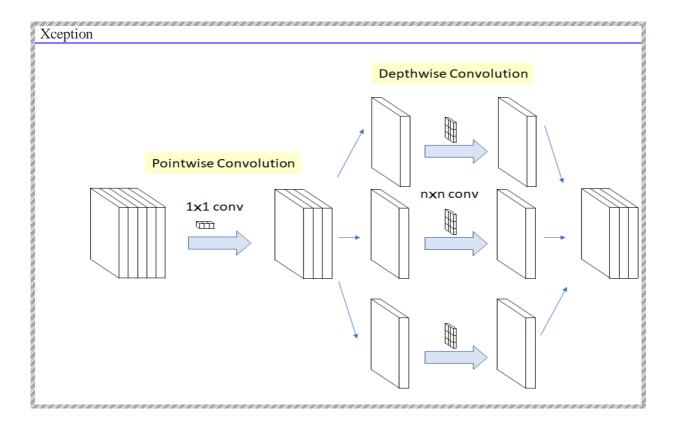
I. Layer of convolution with 2 strides

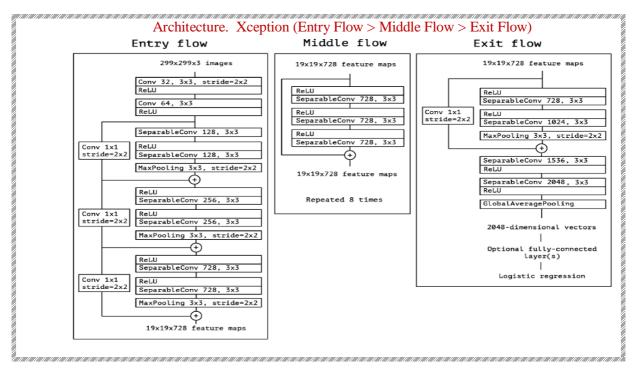
Ii. Depthwise convolution layer

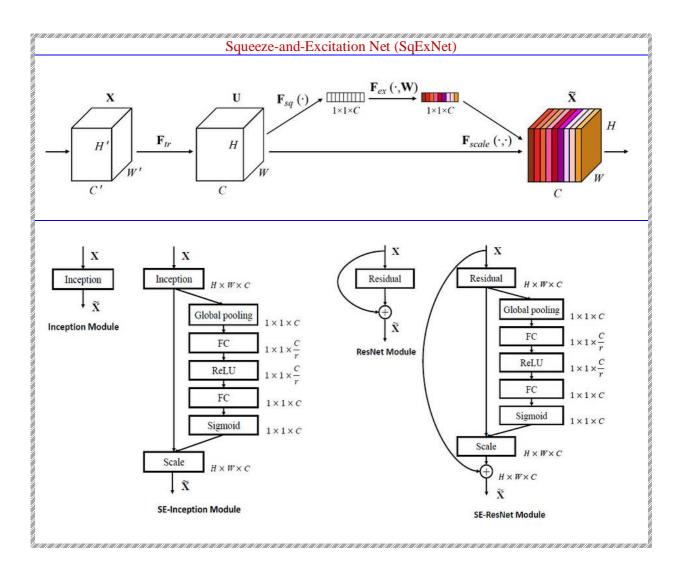
Iii. Pointwise convolution layer which doubles the number of channels

Iv. Depthwise convolution layer with 2 strides

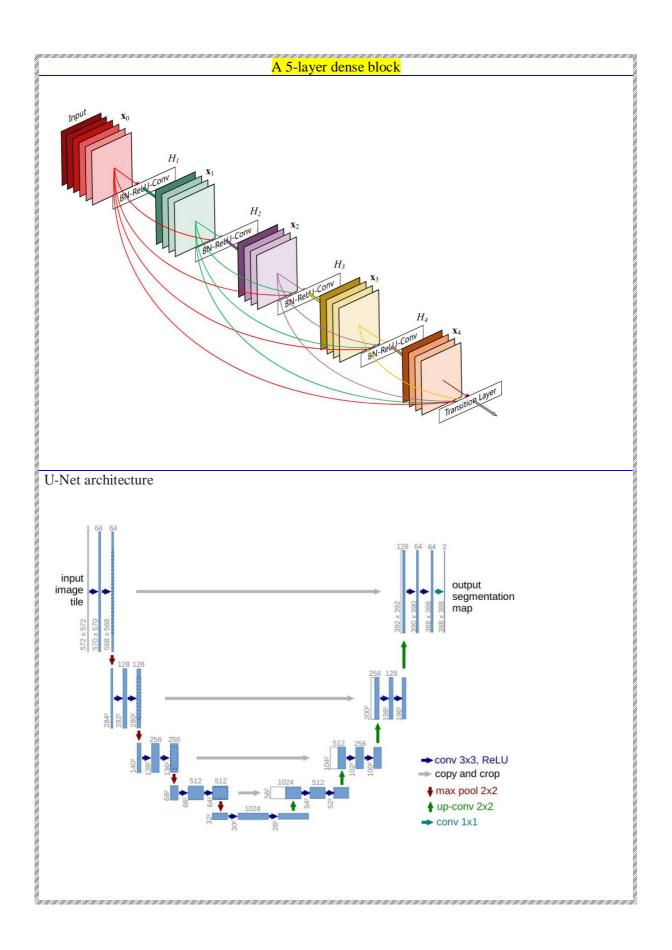
V. Pointwise convolution layer which doubles the number of channels

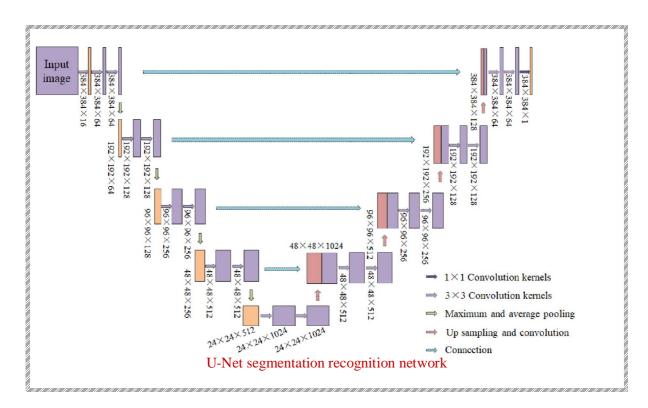


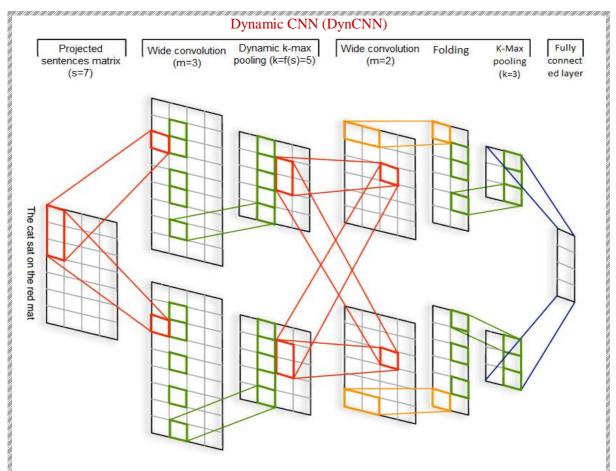


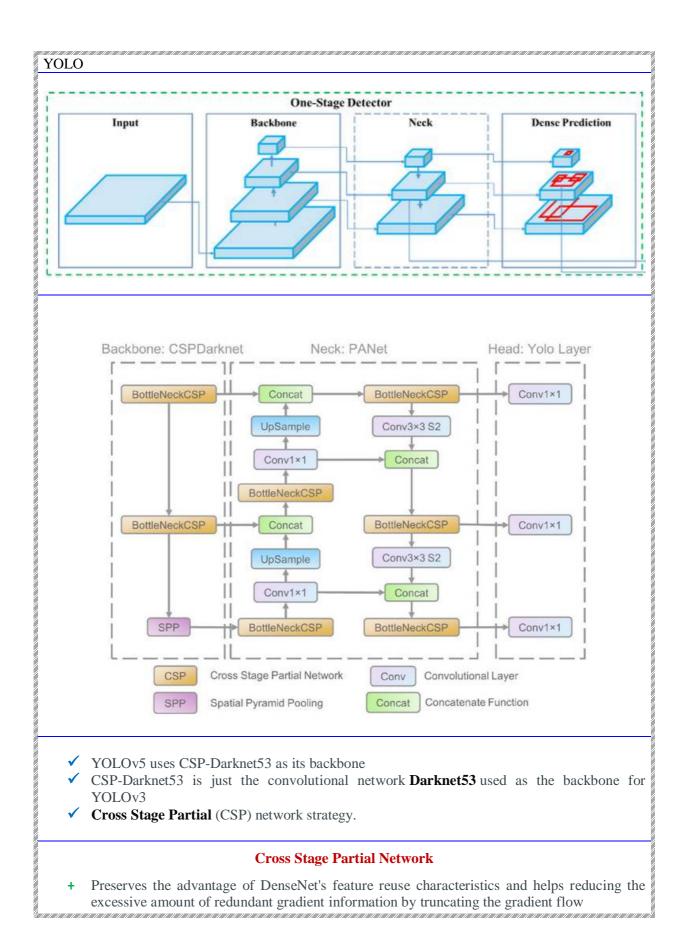


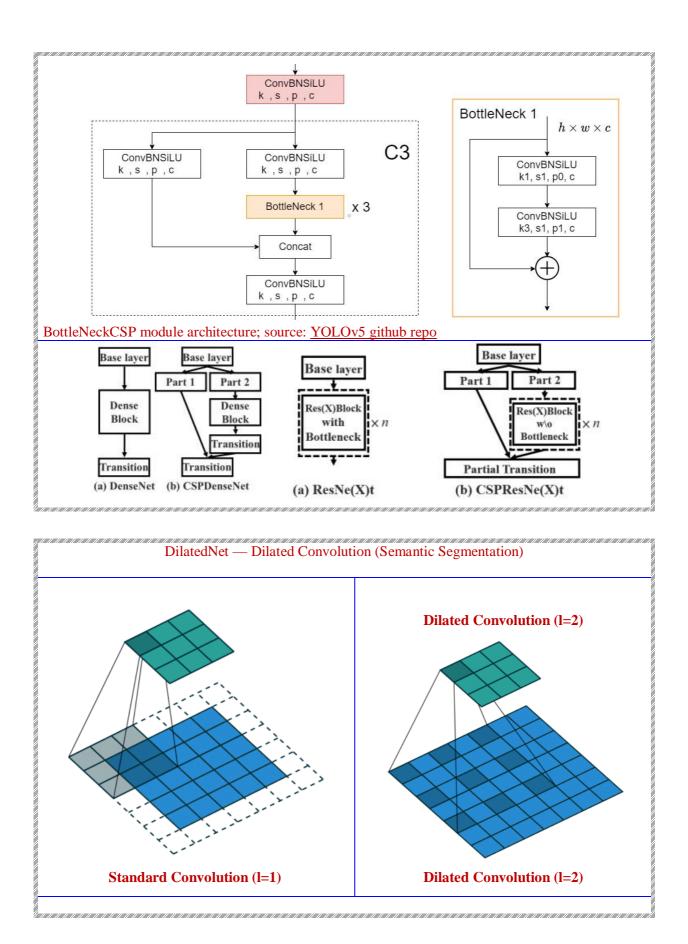
Dutput size	ResNet-50 SE-ResNet-50		SE-ResNeXt-50 $(32 \times 4d)$				
$112 \times 112$		conv, $7 \times 7$ , 64, stride	2				
$56 \times 56$		max pool, $3 \times 3$ , stride 2					
30 X 30	$ \begin{bmatrix} \operatorname{conv}, 1 \times 1, 64 \\ \operatorname{conv}, 3 \times 3, 64 \\ \operatorname{conv}, 1 \times 1, 256 \end{bmatrix} \times 3 $	$\begin{bmatrix} \operatorname{conv}, 1 \times 1, 64 \\ \operatorname{conv}, 3 \times 3, 64 \\ \operatorname{conv}, 1 \times 1, 256 \\ fc, [16, 256] \end{bmatrix} \times 3$	$\begin{bmatrix} \operatorname{conv}, 1 \times 1, 128 \\ \operatorname{conv}, 3 \times 3, 128 \\ \operatorname{conv}, 1 \times 1, 256 \\ fc, [16, 256] \end{bmatrix} \times 3$				
$28 \times 28$	$\begin{bmatrix} \operatorname{conv}, 1 \times 1, 128 \\ \operatorname{conv}, 3 \times 3, 128 \\ \operatorname{conv}, 1 \times 1, 512 \end{bmatrix} \times 4$	$\begin{bmatrix} \operatorname{conv}, 1 \times 1, 128 \\ \operatorname{conv}, 3 \times 3, 128 \\ \operatorname{conv}, 1 \times 1, 512 \\ fc, [32, 512] \end{bmatrix} \times 4$	$\begin{bmatrix} \operatorname{conv}, 1 \times 1, 256 \\ \operatorname{conv}, 3 \times 3, 256 \\ \operatorname{conv}, 1 \times 1, 512 \\ fc, [32, 512] \end{bmatrix} \times 4$				
$14 \times 14$	$\begin{bmatrix} \operatorname{conv}, 1 \times 1, 256 \\ \operatorname{conv}, 3 \times 3, 256 \\ \operatorname{conv}, 1 \times 1, 1024 \end{bmatrix} \times 6$	$\begin{bmatrix} \operatorname{conv}, 1 \times 1, 256\\ \operatorname{conv}, 3 \times 3, 256\\ \operatorname{conv}, 1 \times 1, 1024\\ fc, [64, 1024] \end{bmatrix} \times 6$	$\begin{bmatrix} \operatorname{conv}, 1 \times 1, 512 \\ \operatorname{conv}, 3 \times 3, 512 \\ \operatorname{conv}, 1 \times 1, 1024 \\ fc, [64, 1024] \end{bmatrix} \times 6$				
7×7	$\begin{bmatrix} \operatorname{conv}, 1 \times 1, 512 \\ \operatorname{conv}, 3 \times 3, 512 \\ \operatorname{conv}, 1 \times 1, 2048 \end{bmatrix} \times 3$	$\begin{bmatrix} \operatorname{conv}, 1 \times 1, 512 \\ \operatorname{conv}, 3 \times 3, 512 \\ \operatorname{conv}, 1 \times 1, 2048 \\ fc, [128, 2048] \end{bmatrix} \times 3$	$\begin{bmatrix} \operatorname{conv}, 1 \times 1, 1024 \\ \operatorname{conv}, 3 \times 3, 1024 \\ \operatorname{conv}, 1 \times 1, 2048 \\ fc, [128, 2048] \end{bmatrix} \times 3$				
$1 \times 1$		global average pool, 1000-d fc	c, softmax				

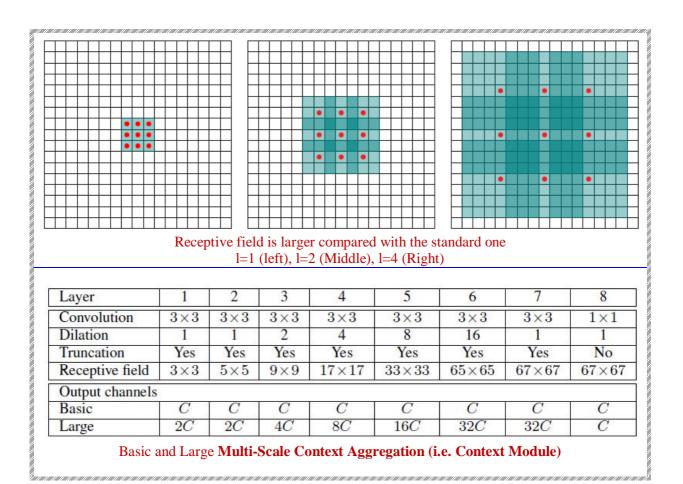


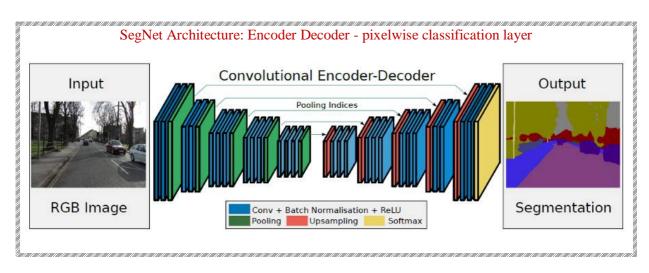


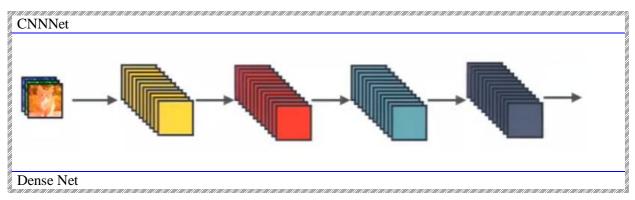


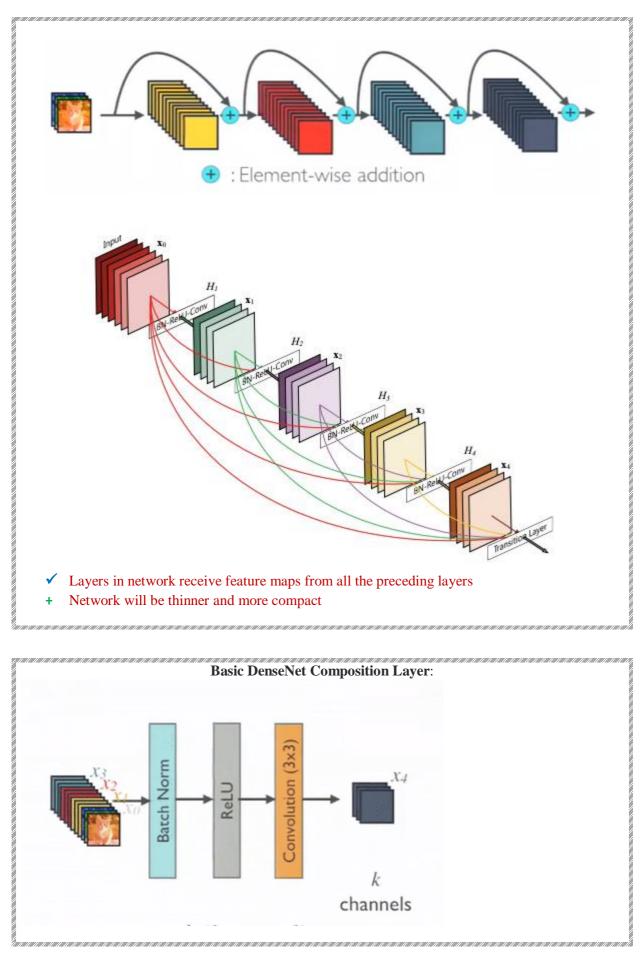




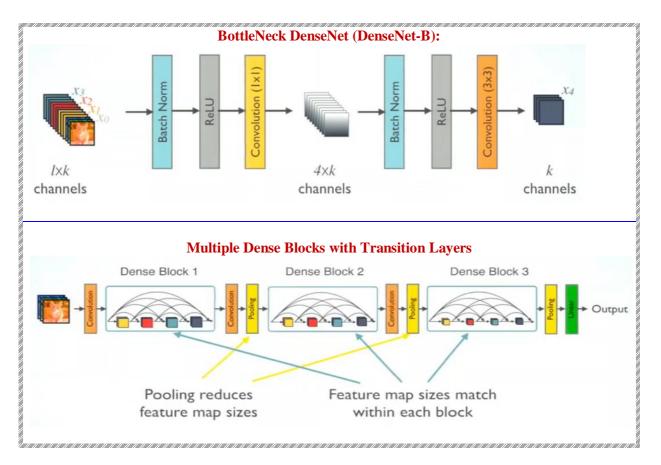


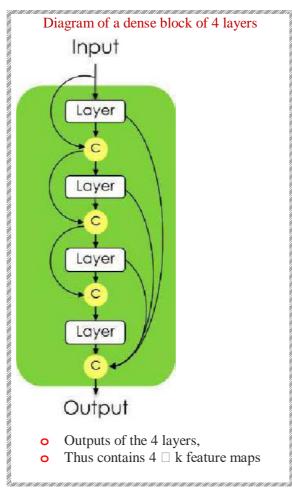




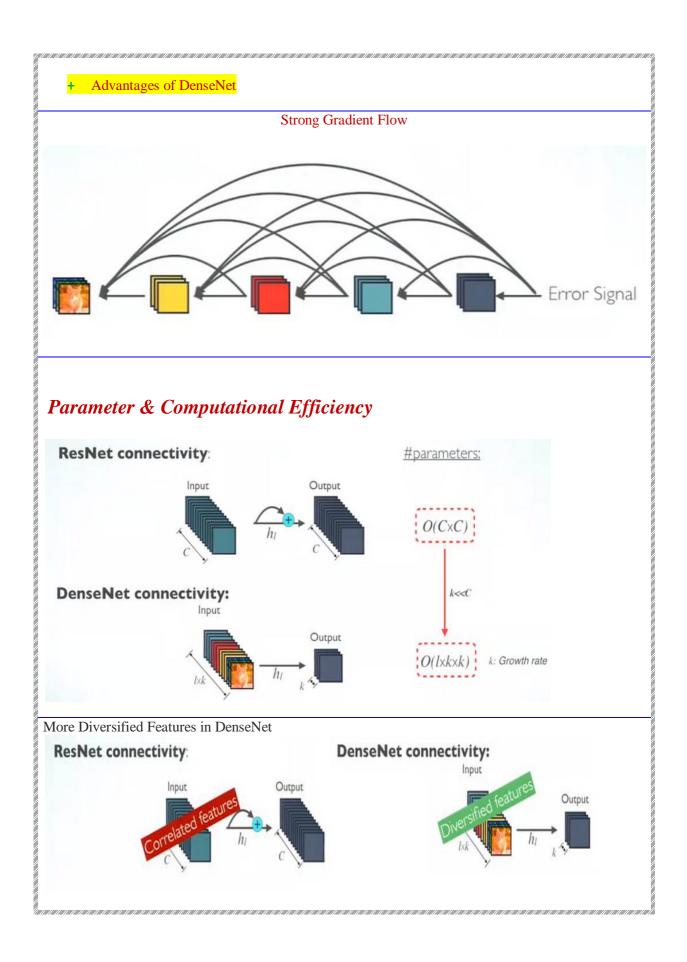


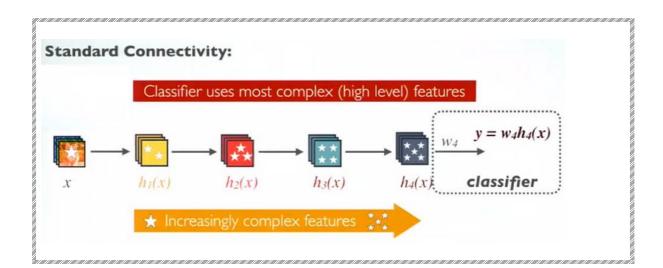
AAA→CNN-50 → ConvNNs—Pretrained Nets

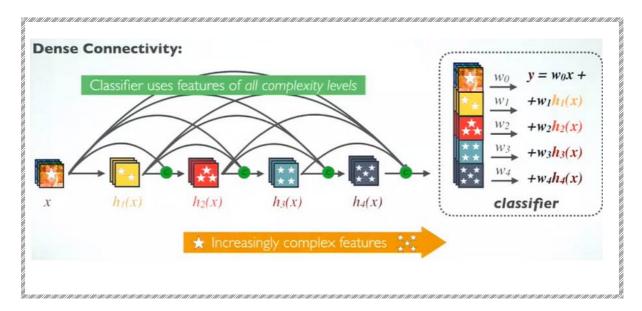


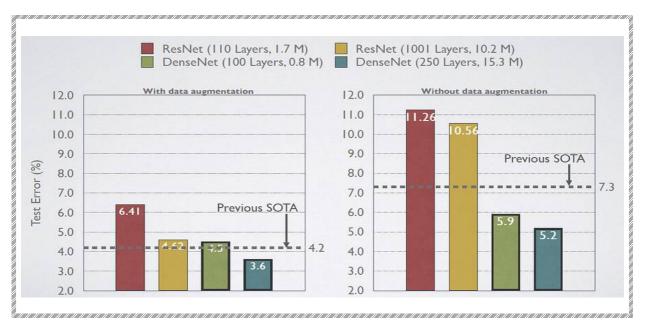


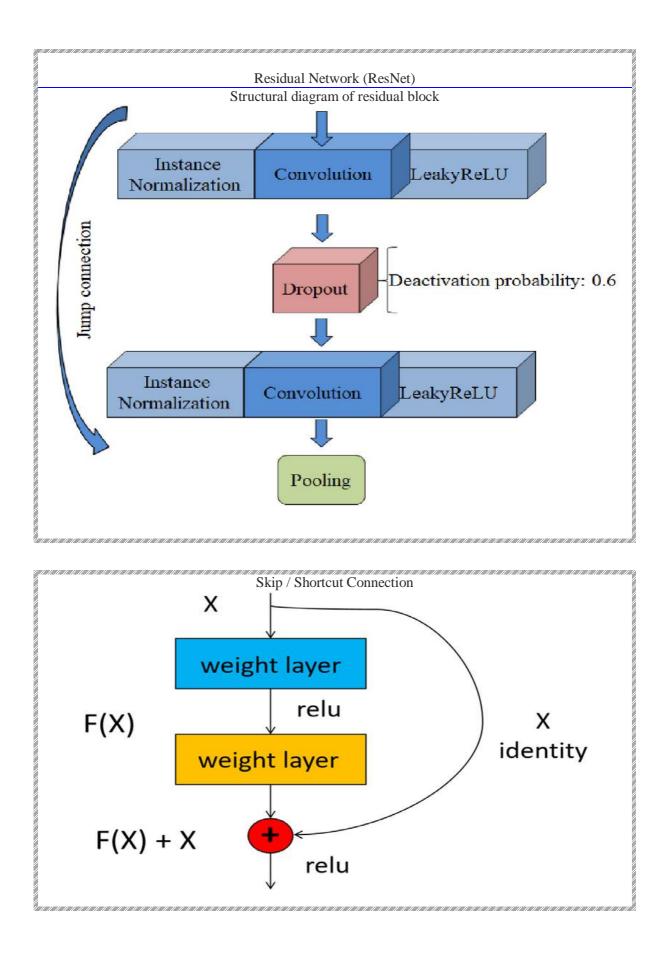
AAA→CNN-50 → ConvNNs—Pretrained Nets

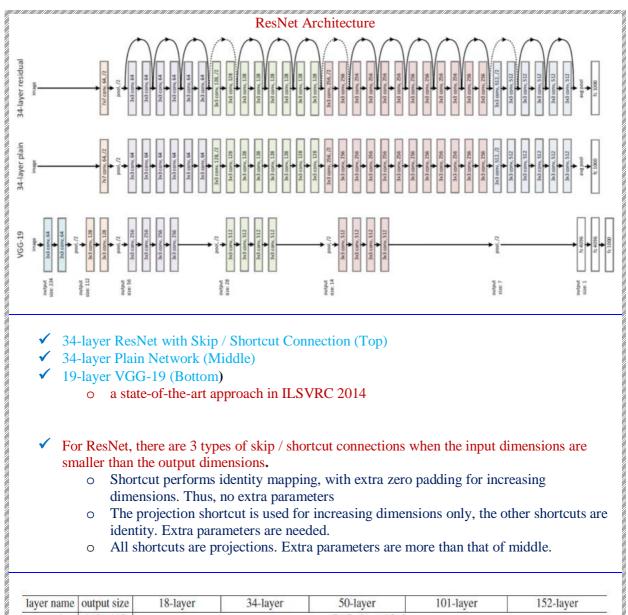




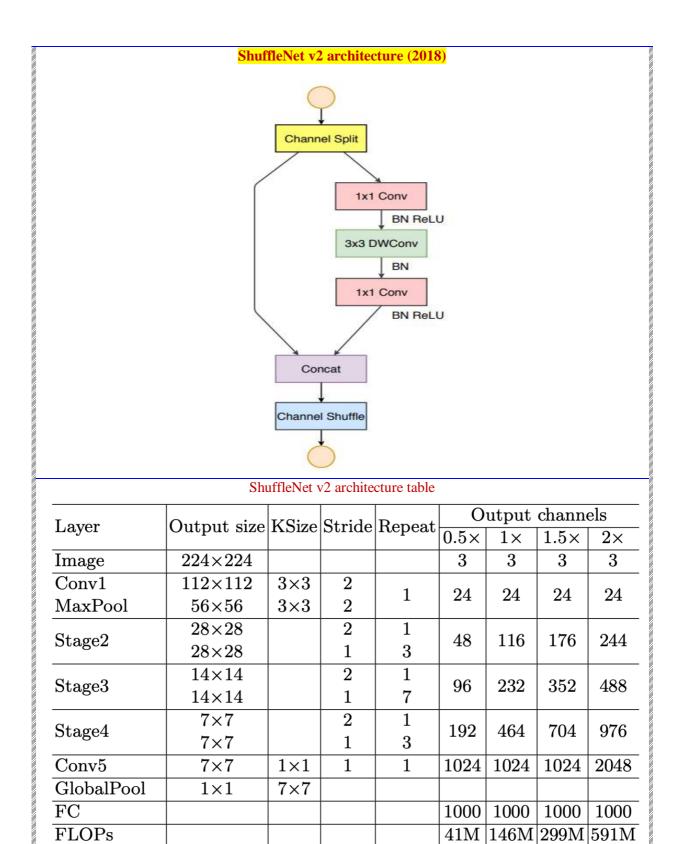






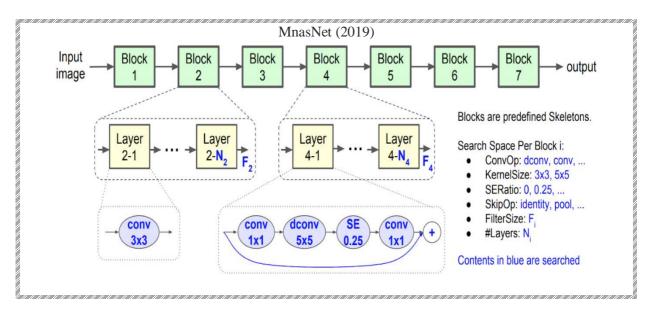


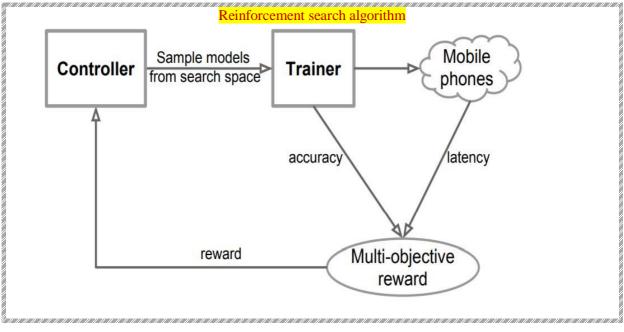
layer name	output size	18-layer	34-layer	50-layer	101-layer	152-layer			
conv1	112×112	*		7×7, 64, stride 2		12 (194			
		$3 \times 3$ max pool, stride 2							
conv2_x	56×56	$\left[\begin{array}{c} 3\times3,64\\ 3\times3,64 \end{array}\right]\times2$	$\left[\begin{array}{c} 3\times3,64\\ 3\times3,64 \end{array}\right]\times3$	$\begin{bmatrix} 1 \times 1, 64 \\ 3 \times 3, 64 \\ 1 \times 1, 256 \end{bmatrix} \times 3$	$\begin{bmatrix} 1 \times 1, 64 \\ 3 \times 3, 64 \\ 1 \times 1, 256 \end{bmatrix} \times 3$	$\begin{bmatrix} 1 \times 1, 64 \\ 3 \times 3, 64 \\ 1 \times 1, 256 \end{bmatrix} \times 3$			
conv3_x	28×28	$\left[\begin{array}{c} 3\times3,128\\ 3\times3,128\end{array}\right]\times2$	$\left[\begin{array}{c} 3\times3,128\\ 3\times3,128\end{array}\right]\times4$	$\begin{bmatrix} 1 \times 1, 128 \\ 3 \times 3, 128 \\ 1 \times 1, 512 \end{bmatrix} \times 4$	$\begin{bmatrix} 1 \times 1, 128 \\ 3 \times 3, 128 \\ 1 \times 1, 512 \end{bmatrix} \times 4$	$\begin{bmatrix} 1 \times 1, 128\\ 3 \times 3, 128\\ 1 \times 1, 512 \end{bmatrix} \times 8$			
conv4_x	14×14	$\left[\begin{array}{c} 3\times3,256\\ 3\times3,256\end{array}\right]\times2$	$\left[\begin{array}{c} 3\times3,256\\ 3\times3,256\end{array}\right]\times6$	$\begin{bmatrix} 1 \times 1, 256 \\ 3 \times 3, 256 \\ 1 \times 1, 1024 \end{bmatrix} \times 6$	$\begin{bmatrix} 1 \times 1, 256 \\ 3 \times 3, 256 \\ 1 \times 1, 1024 \end{bmatrix} \times 23$	$\begin{bmatrix} 1 \times 1, 256 \\ 3 \times 3, 256 \\ 1 \times 1, 1024 \end{bmatrix} \times 36$			
conv5_x	7×7	$\left[\begin{array}{c} 3\times3,512\\ 3\times3,512\end{array}\right]\times2$	$\left[\begin{array}{c} 3\times3,512\\ 3\times3,512\end{array}\right]\times3$	$\begin{bmatrix} 1 \times 1, 512 \\ 3 \times 3, 512 \\ 1 \times 1, 2048 \end{bmatrix} \times 3$	$\begin{bmatrix} 1 \times 1, 512 \\ 3 \times 3, 512 \\ 1 \times 1, 2048 \end{bmatrix} \times 3$	$\begin{bmatrix} 1 \times 1, 512 \\ 3 \times 3, 512 \\ 1 \times 1, 2048 \end{bmatrix} \times 3$			
	1×1		ave	erage pool, 1000-d fc,	softmax				
FLO	OPs	$1.8 \times 10^{9}$	3.6×10 <sup>9</sup>	$3.8 \times 10^{9}$	$7.6 \times 10^{9}$	$11.3 \times 10^{9}$			

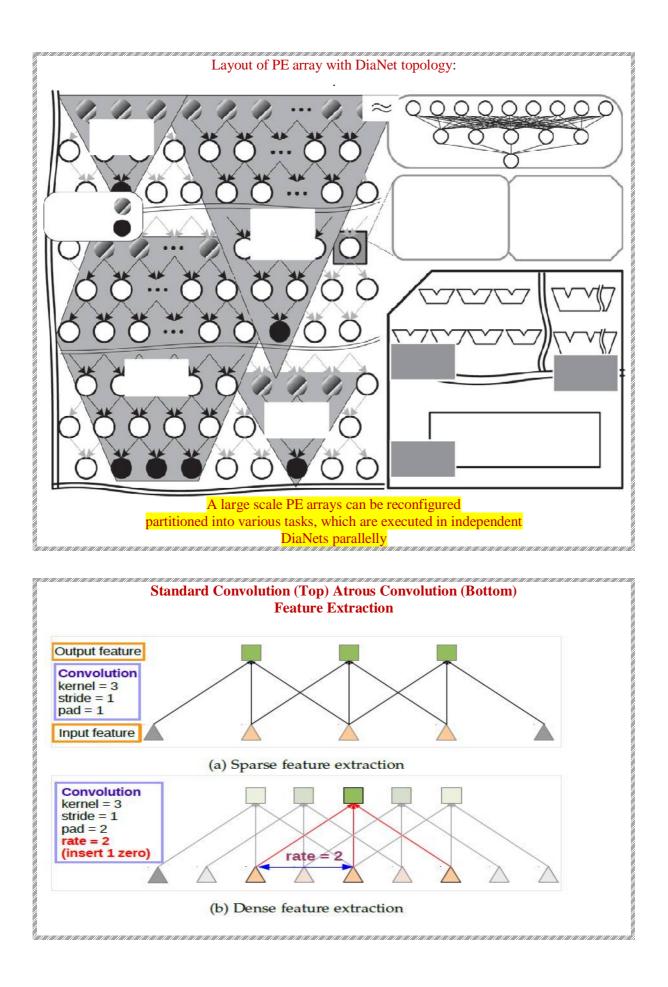


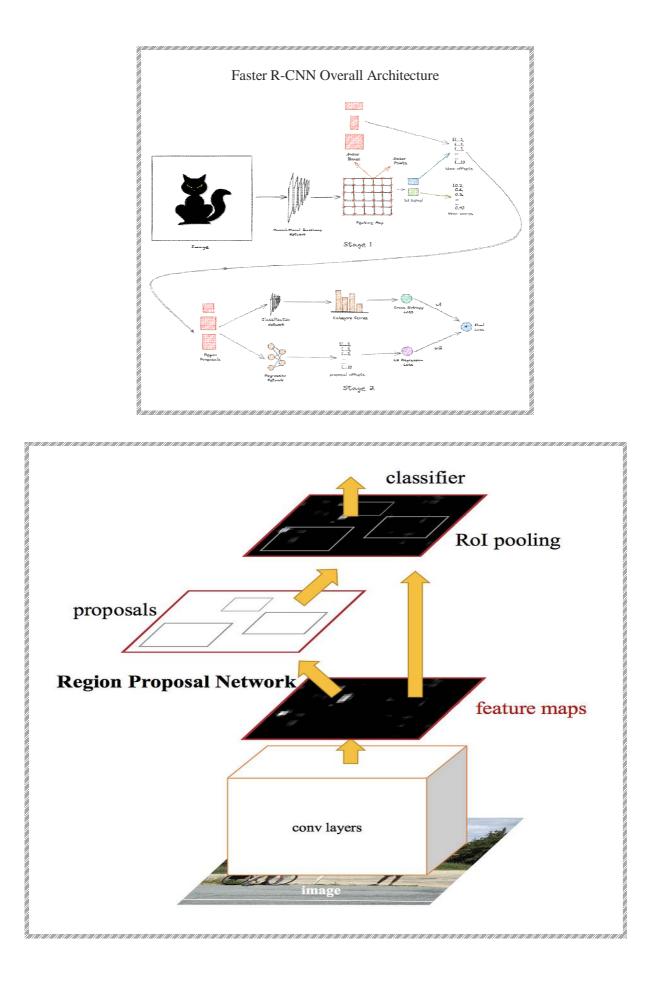
# of Weights

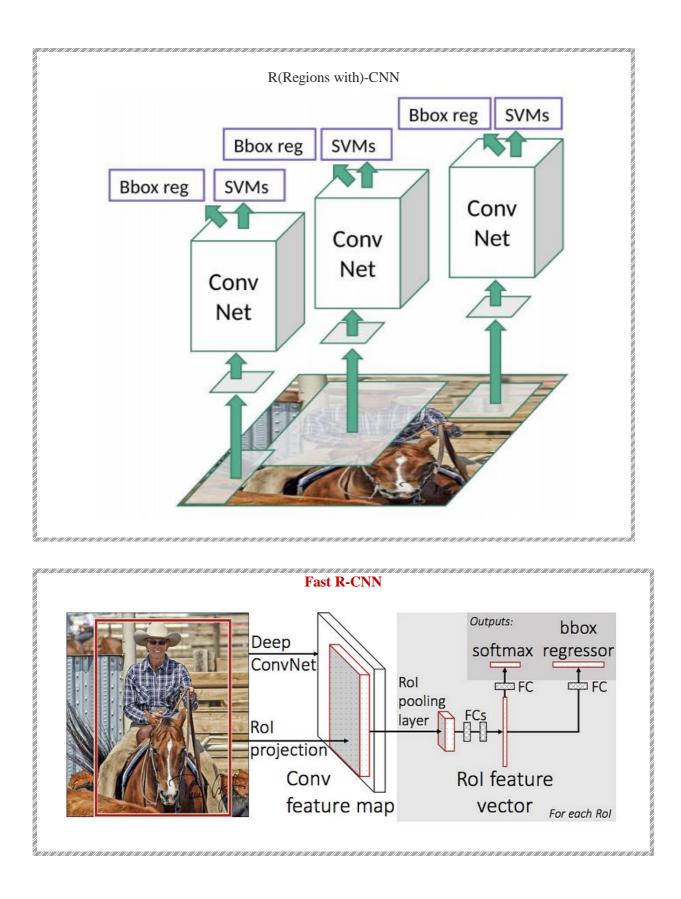
1.4M 2.3M 3.5M 7.4M





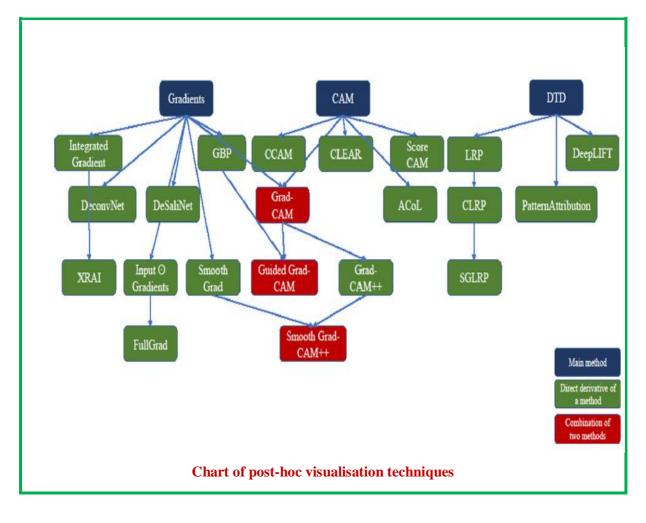






# V. xAiProbes

## for ConvNN, CapsNN



Ref	Displays 73 (2022) 102239;
	/doi.org/10.1016/j.displa.2022.102239
	A review of visualisation-as-explanation techniques for convolutionalneural networks and their evaluation
Au	Elhassan Mohamed, Konstantinos Sirlantzis, Gareth Howells

