Binary Classification of Graphene Flakes

Samuel Rager and Alvin Wang

Main References

- Krizhevsky, Alex, Ilya Sutskever, and Geoffrey E. Hinton. "ImageNet Classification with Deep Convolutional Neural Networks."
- Ioffe, Sergey. "Batch normalization: Accelerating deep network training by reducing internal covariate shift." *arXiv preprint arXiv:1502.03167* (2015).
- Kingma, Diederik P. "Adam: A method for stochastic optimization." *arXiv preprint arXiv:1412.6980* (2014).
- Gabbard & Miller. “Machine Learning from Scratch: Stochastic Gradient Descent and Adam Optimizer.”

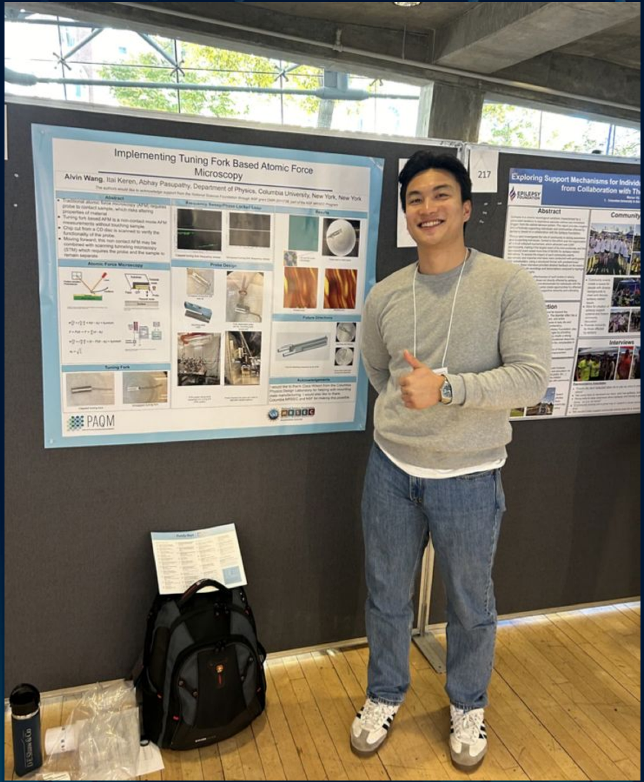
Reproducibility

- GitHub Repository: https://github.com/56sarager/Graphene-Classification
- Medium Article: https://medium.com/@56sarager/alexnet-and-the-binary-classification-of-graphene-ad07dc595867

Outline

- Speakers' Backgrounds
- The Problem
- State of the Field
- Alternative Solution
- AlexNet Architecture
- Batch Normalization Pseudocode
- Adam Optimizer Pseudocode
- Backpropagation Pseudocode
- Code Demonstration
- Project Results
- Additional Model Architectures and Results
- Future Work

About Us


Implementing Tuning Fork Based Atomic Force Microscopy
Alvin Wang, Itai Keren, Abhay Pasupathy, Department of Physics, Columbia University, New York, New York
Abstract
Atomic Force Microscopy
Probe Design
Tuning Fork
PAQM
217
Abstract
Community
Interviews

Why Do We Care?/Why Should You Care?

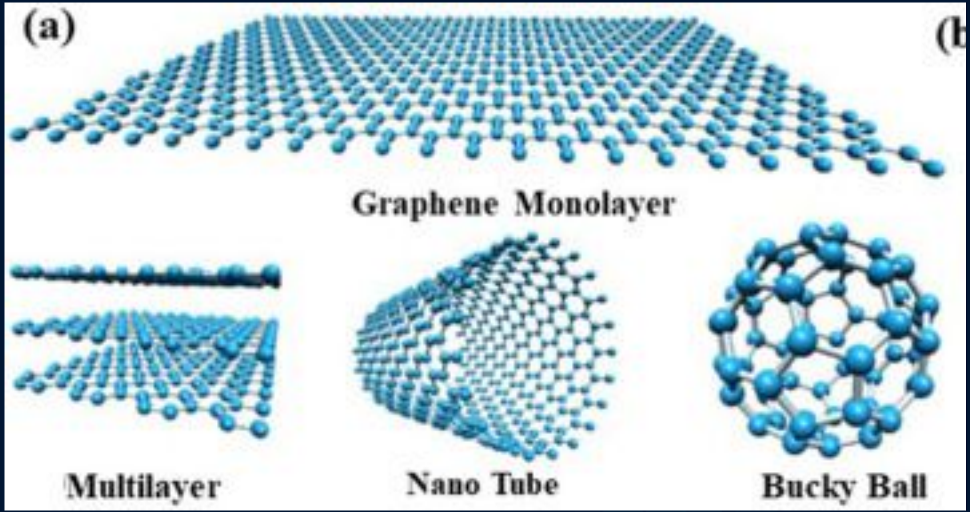
Condensed Matter Experiment: Studying the electronic properties of 2D materials

COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK

DEPARTMENT OF PHYSICS

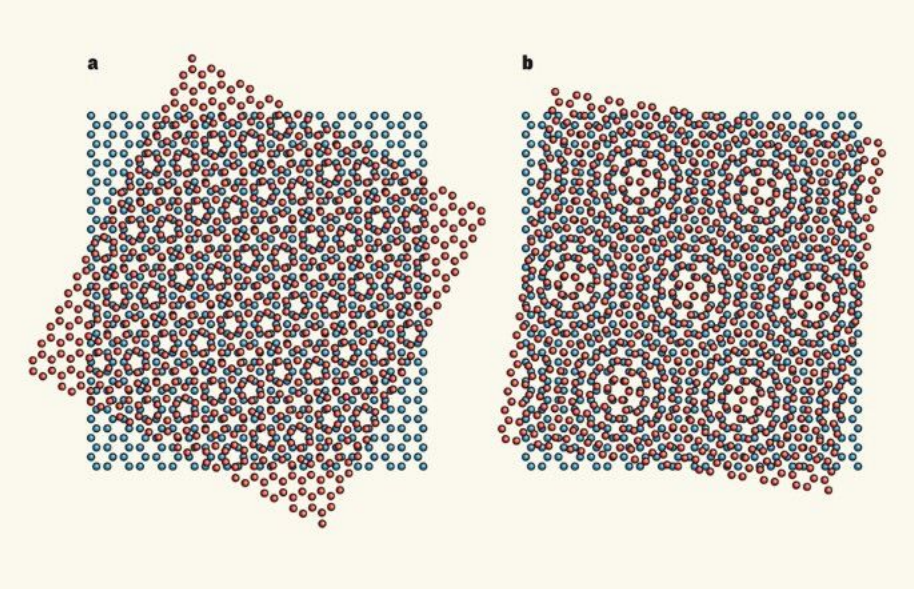
Condensed Matter Physics | Department of Physics, www.physics.columbia.edu/content/condensed-matter-physics. Accessed 7 Dec. 2024.

Discovery of Graphene: Professor Andre Geim and Professor Kostya Novoselov



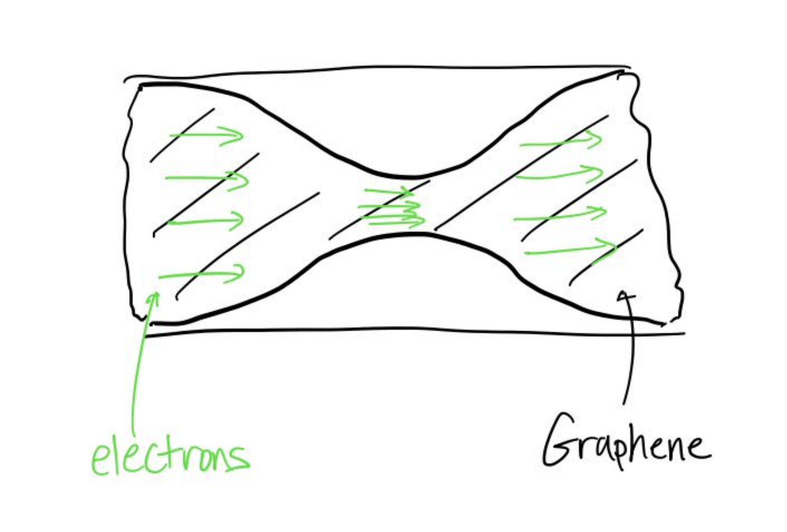
Lloyd-Hughes, James & Jeon, Tae-In. (2012). A Review of the Terahertz Conductivity of Bulk and Nano-Materials. J Infrared Milli Terahz Waves. 33. 871. 10.1007/s10762-012-9905-y.

Superconductivity in Moire Superlattices



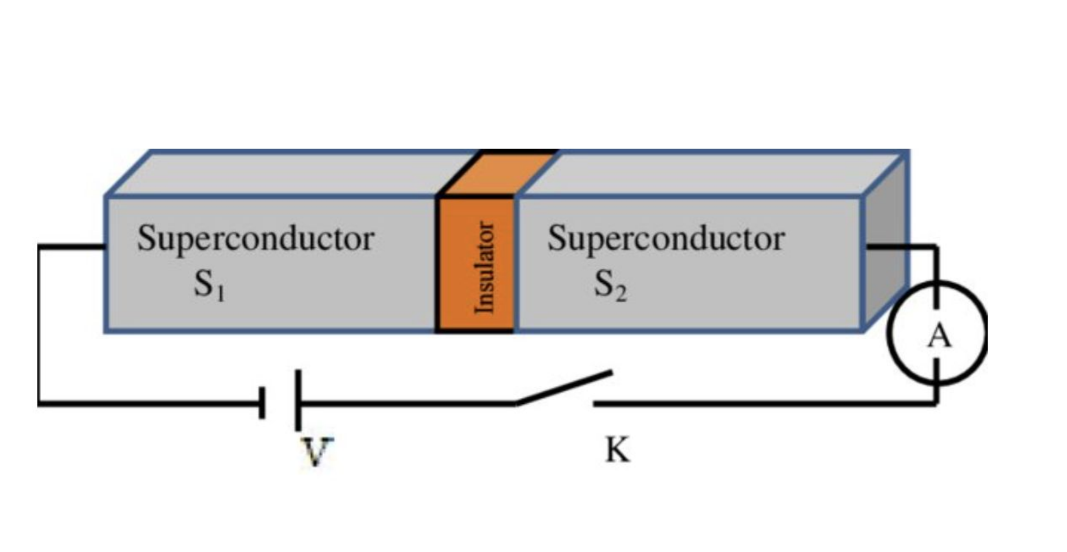
MacDonald, A., Bistritzer, R. Graphene moiré mystery solved?. *Nature* 474, 453–454 (2011).
https://doi.org/10.1038/474453a

Work in Pasupathy Lab: Electron Hydrodynamics



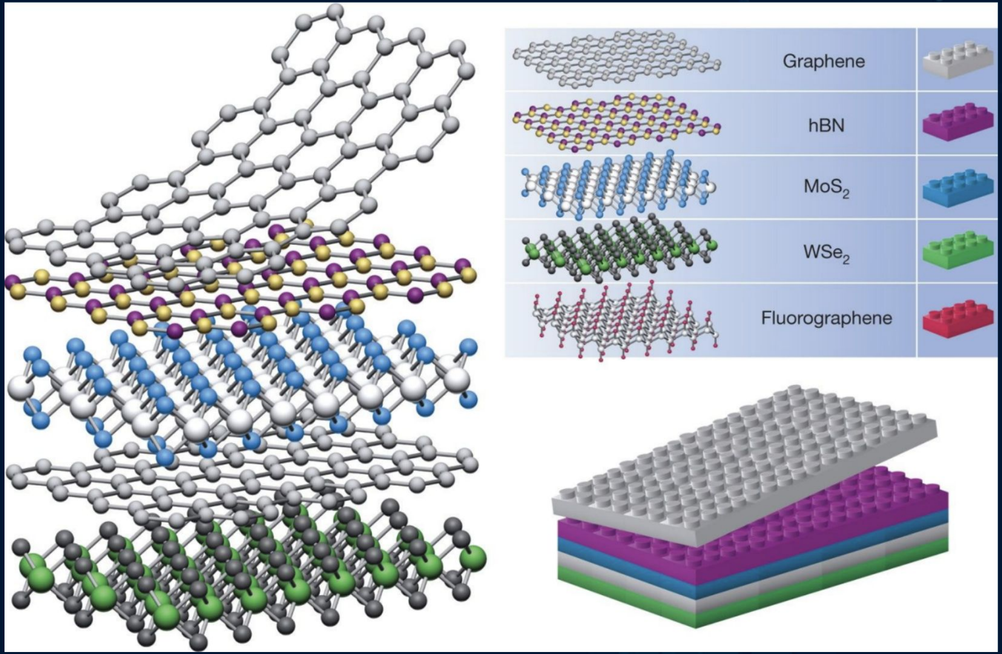
BEIJING IWHR CORPORATION. "Spillway Crest Gates: Controlling Water Flow in Dam Structures." BEIJING IWHR CORPORATION, 2024, www.bic-iwhr.com/news/spillway-crest-gates-controlling-water-flow-in-dam-structures.html. Accessed 8 Dec. 2024.

Work in Pasupathy Lab: Josephson Junction



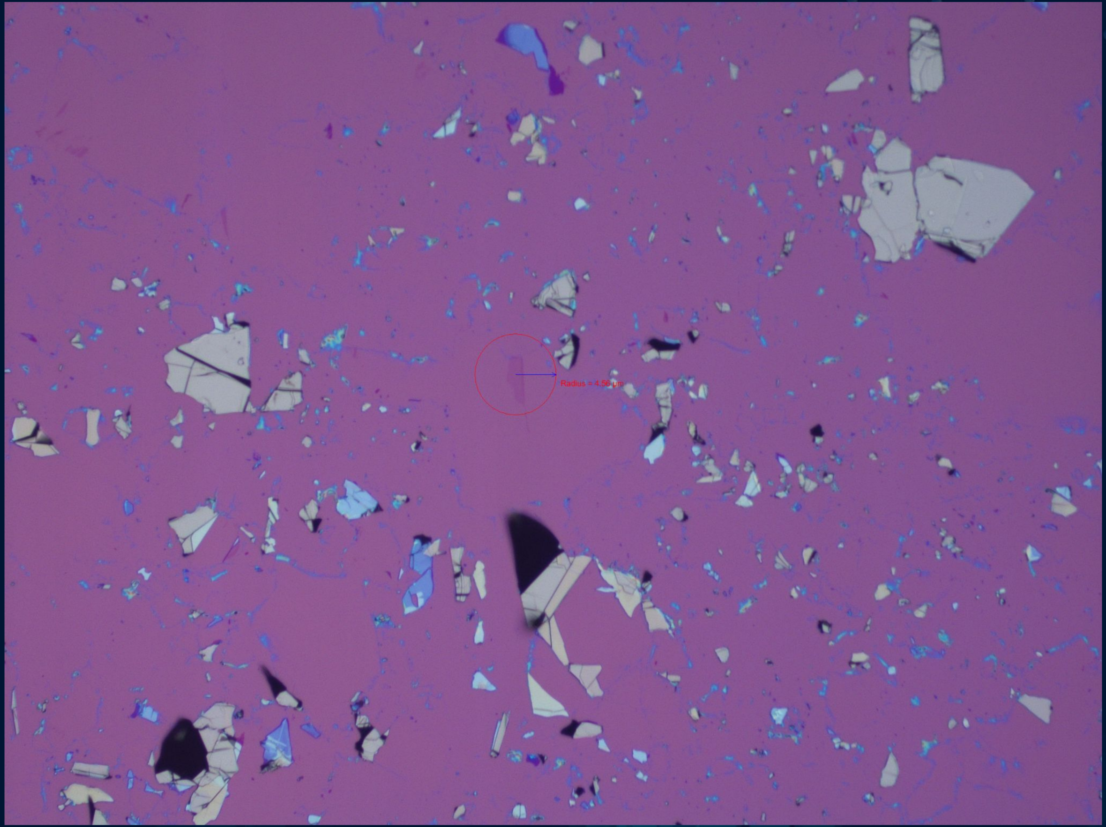
Maruf, H M & Islam, Md. Rafiqul & Chowdhury, F.-U.-Z. (2018). ANALOGY BETWEEN AC JOSEPHSON JUNCTION EFFECTS AND OPTICAL PHENOMENA IN SUPERCONDUCTORS. 105-113.

Everything done in-house

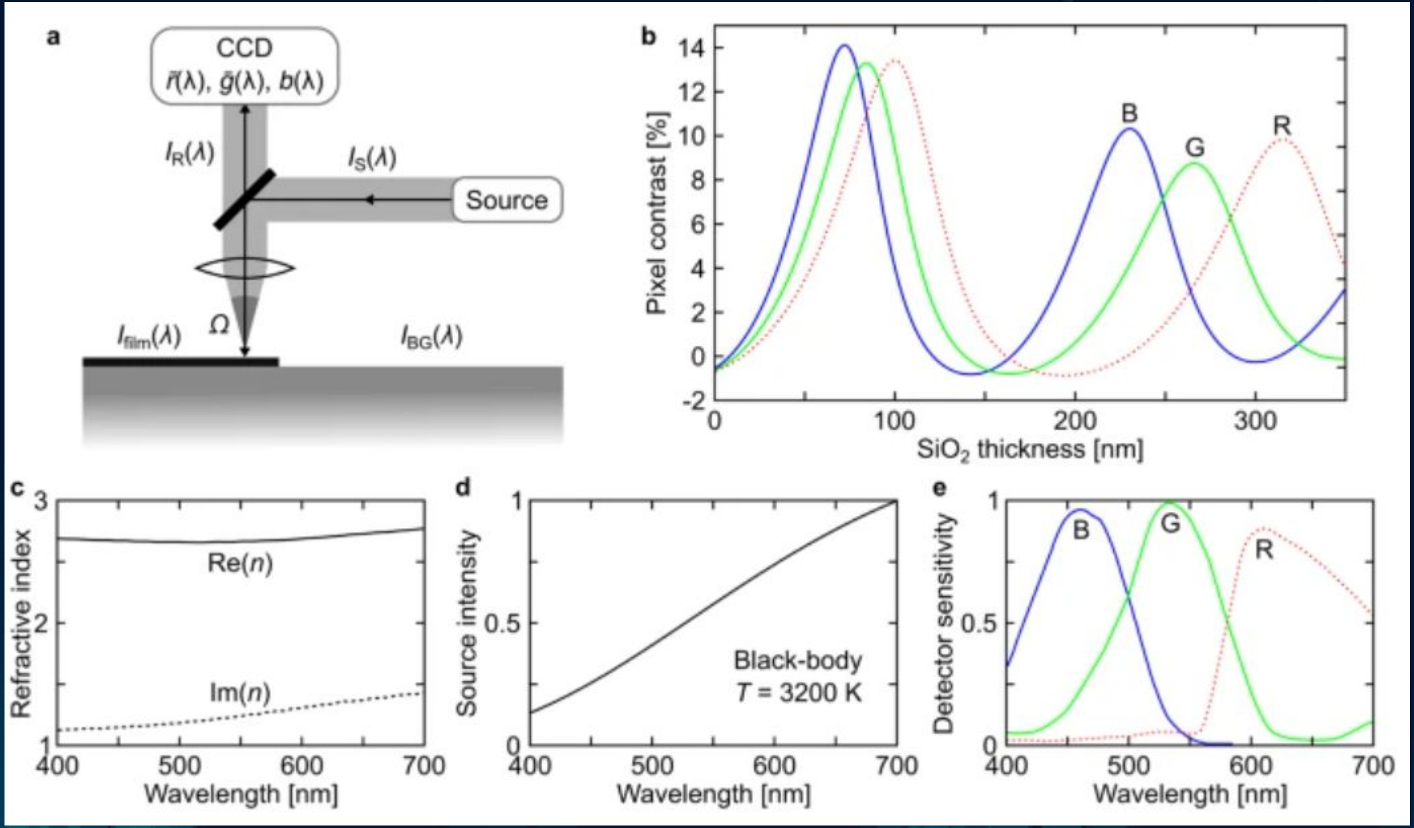


Geim, A. K., and I. V. Grigorieva. “Van Der Waals Heterostructures.” Nature, vol. 499, no. 7459, 1 July 2013, pp. 419–425, www.nature.com/articles/nature12385, https://doi.org/10.1038/nature12385.

Everything done in-house…Problem



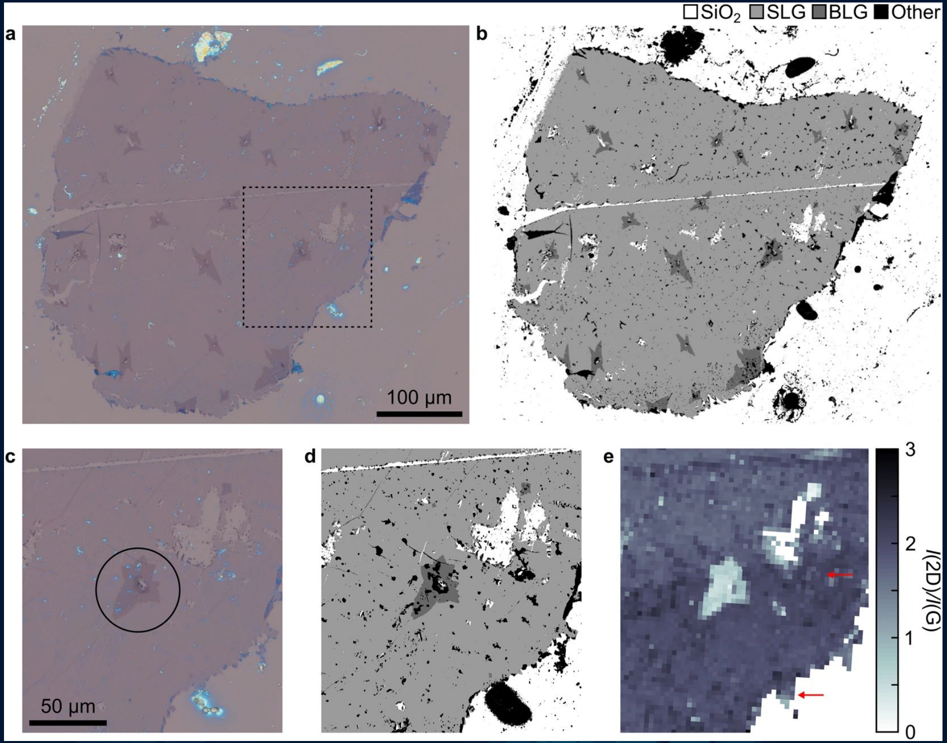
State of the Field- Fresnel Approach



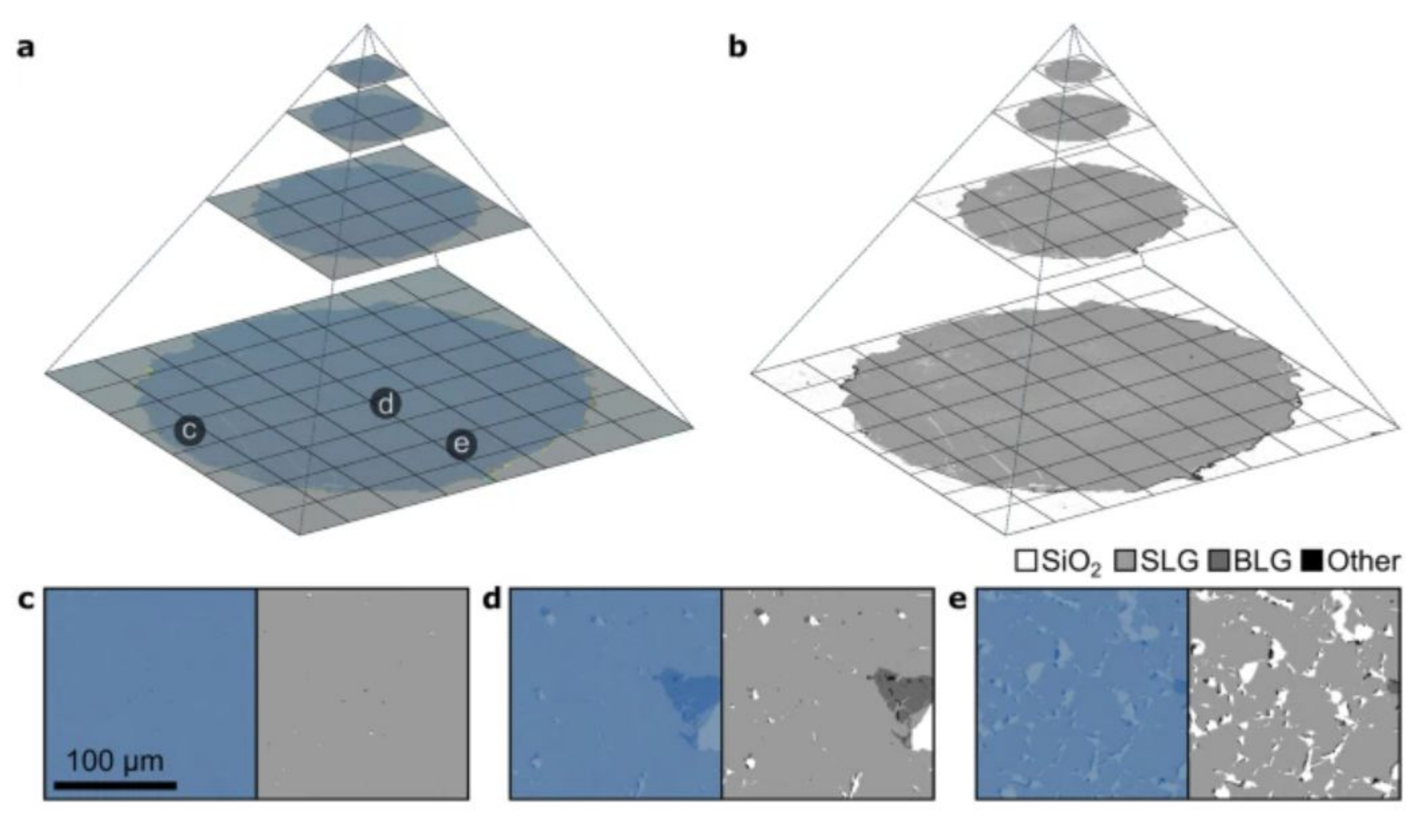
Jessen, B.S., Whelan, P.R., Mackenzie, D.M.A. *et al*. Quantitative optical mapping of two-dimensional materials. *Sci Rep* 8, 6381 (2018). https://doi.org/10.1038/s41598-018-23922-1

State of the Field- Quality

Jessen, B.S., Whelan, P.R., Mackenzie, D.M.A. *et al.* Quantitative optical mapping of two-dimensional materials. *Sci Rep* 8, 6381 (2018). https://doi.org/10.1038/s41598-018-23922-1

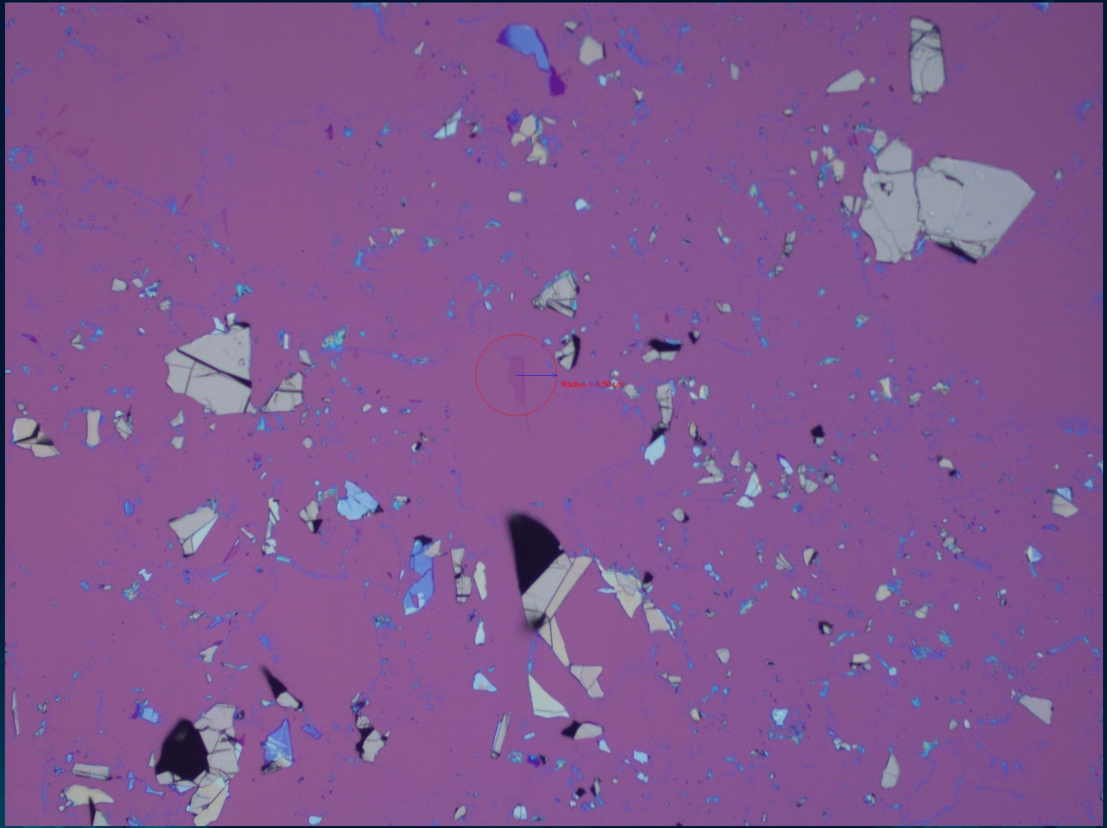


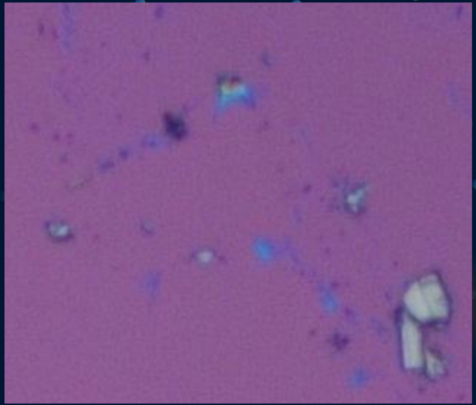
State of the Field- Data Parsing



Jessen, B.S., Whelan, P.R., Mackenzie, D.M.A. *et al.* Quantitative optical mapping of two-dimensional materials. *Sci Rep* 8, 6381 (2018). https://doi.org/10.1038/s41598-018-23922-1

Data Cleaning Methodology

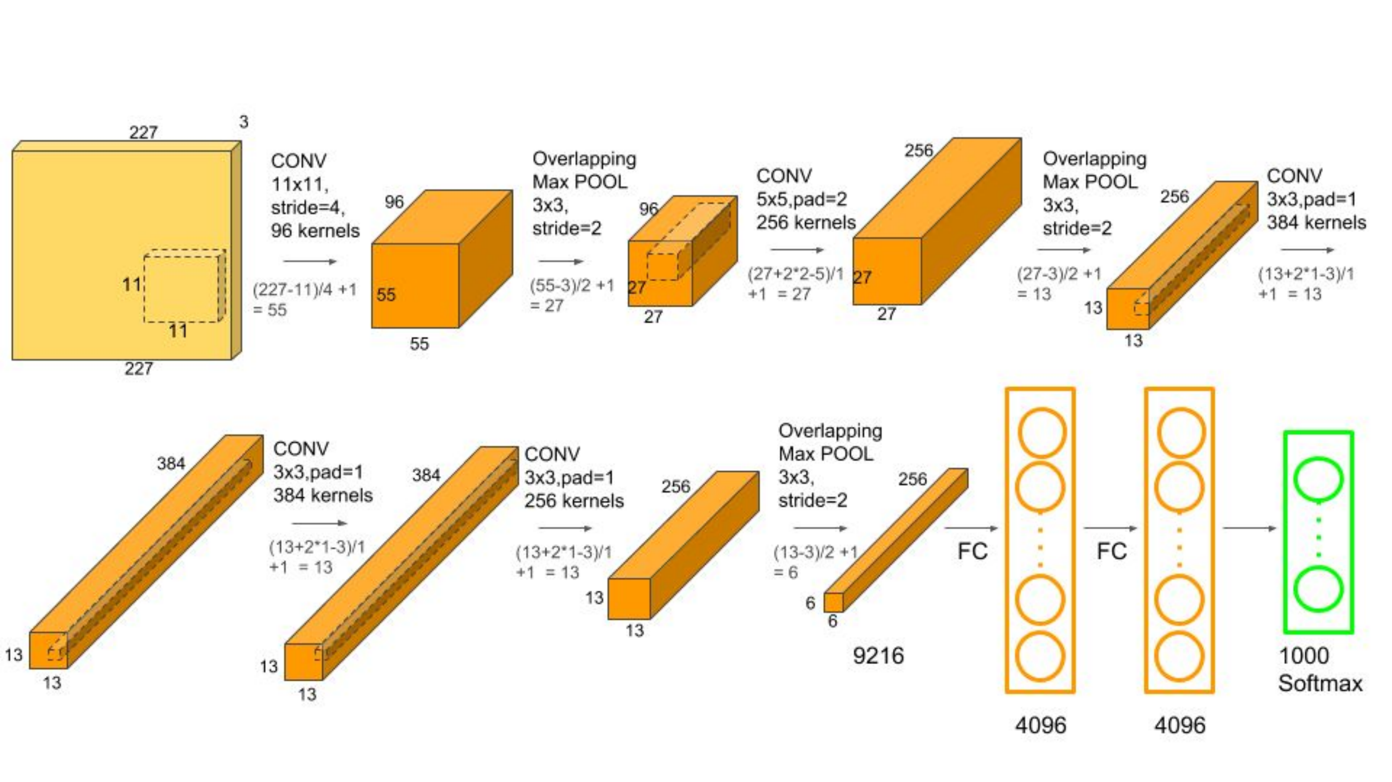




Timeline

2010	2012	2014	2015	2016	2017	2018	2019	2023
• First ImageNet challenge	• AlexNet	• Adam • VGG • GoogleNet	• ResNet • Batch Norm. • GoogleNet renamed Inception • Yolo V1	• Inception v3	• AdamW • Transformer • Last Imagenet Challenge	• Mobile Net v2 (Inverted Residual)	• Efficient Net	• Yolo V8

AlexNet



Askari, Syed Sajjad. "Alex-Net Explanation and Implementation in Tensorflow and Keras." *Medium*, Medium, 14 Jan. 2023, medium.com/@syedsajjad62/alex-net-explanation-and-implementation-in-tensorflow-and-keras-8047efeb7a0f.

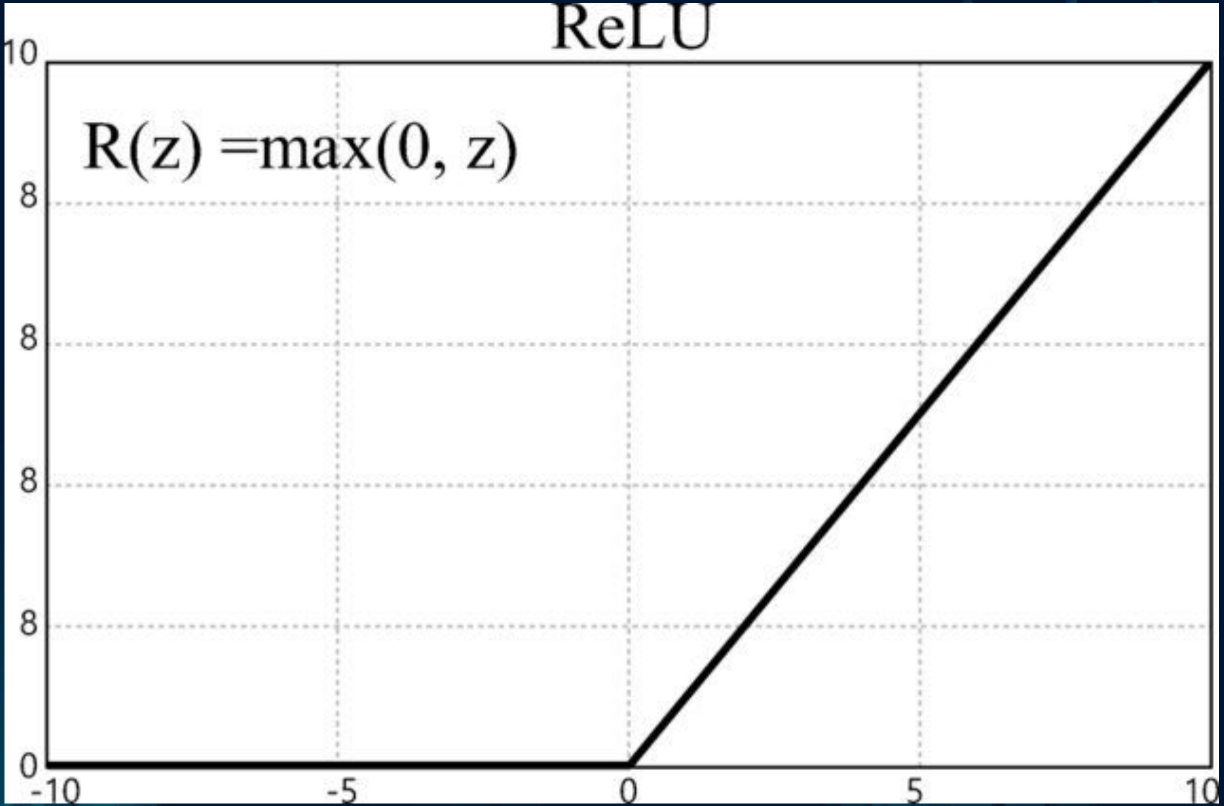
Convolution

Sanderson, Grant. “But What is a Convolution?” *Youtube*, 3blue1brown, 29 Dec. 2023, https://www.youtube.com/shorts/kpG7I2MOcnI.

Max Pooling

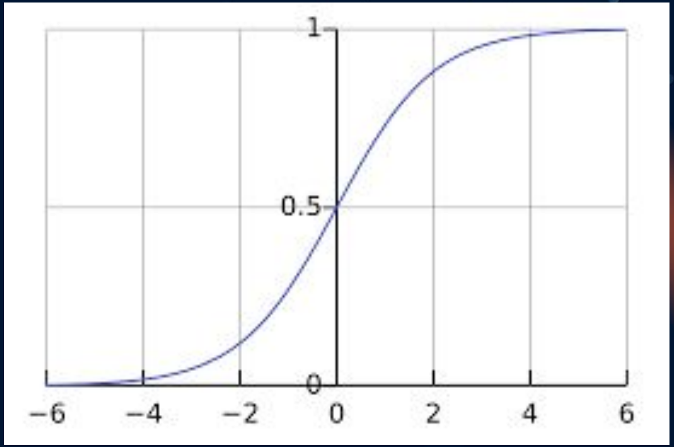
Ave Coders. “101 Concepts of Data Science and Machine Learning” *Youtube*, AveCoders, 28 May. 2024, https://www.youtube.com/shorts/ykt5PUxs3z8.

Rectified Linear Function



Chima, Precious. "Activation Functions: ReLU & Softmax." *Medium*, Medium, 5 Apr. 2020, https://medium.com/@preshchima/activation-functions-relu-softmax-87145bf39288.

Softmax- Reduces to Sigmoid in Binary Case



$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

Alexander, Giffah. “Softmax Activation function explained” Youtube, Giffah_Alexander, 22 Oct. 2024, https://www.youtube.com/shorts/SrJN_hpiuAs.

Sigmoid function. “Sigmoid function.” *Wikipedia*, Wikipedia, 14 Nov. 2024, https://en.wikipedia.org/wiki/Sigmoid_function.

Local Response Normalization

$$b^i_{x,y} = a^i_{x,y} / \left(k + \alpha \sum_{j=\max(0,i-n/2)}^{\min(N-1,i+n/2)} (a^j_{x,y})^2 \right)^{\beta}$$

For AlexNet, k=2, n=5, alpha=10^-4, beta=0.75

Alex Krizhevsky, Ilya Sutskever, and Geoffrey E. Hinton. 2017. ImageNet classification with deep convolutional neural networks. Commun. ACM 60, 6 (June 2017), 84–90. https://doi.org/10.1145/3065386

Batch Normalization

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_\mathcal{B} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_\mathcal{B}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (x_i - \mu_\mathcal{B})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_\mathcal{B}}{\sqrt{\sigma_\mathcal{B}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.

Input: Network N with trainable parameters Θ;
subset of activations $\{x^{(k)}\}_{k=1}^{K}$

Output: Batch-normalized network for inference, $N_{\mathrm{BN}}^{\mathrm{inf}}$

$N_{\mathrm{BN}}^{\mathrm{tr}} \leftarrow N$ // Training BN network
for $k = 1 \dots K$ **do**
  Add transformation $y^{(k)} = \mathrm{BN}_{\gamma^{(k)},\beta^{(k)}}(x^{(k)})$ to $N_{\mathrm{BN}}^{\mathrm{tr}}$ (Alg. 1)
  Modify each layer in $N_{\mathrm{BN}}^{\mathrm{tr}}$ with input $x^{(k)}$ to take $y^{(k)}$ instead
end for
Train $N_{\mathrm{BN}}^{\mathrm{tr}}$ to optimize the parameters $\Theta \cup \{\gamma^{(k)}, \beta^{(k)}\}_{k=1}^{K}$
$N_{\mathrm{BN}}^{\mathrm{inf}} \leftarrow N_{\mathrm{BN}}^{\mathrm{tr}}$ // Inference BN network with frozen
  // parameters
for $k = 1 \dots K$ **do**
  // For clarity, $x \equiv x^{(k)}, \gamma \equiv \gamma^{(k)}, \mu_\mathcal{B} \equiv \mu_\mathcal{B}^{(k)}$, etc.
  Process multiple training mini-batches $\mathcal{B}$, each of size m, and average over them:

$$\mathrm{E}[x] \leftarrow \mathrm{E}_\mathcal{B}[\mu_\mathcal{B}]$$
$$\mathrm{Var}[x] \leftarrow \frac{m}{m-1}\mathrm{E}_\mathcal{B}[\sigma_\mathcal{B}^2]$$

  In $N_{\mathrm{BN}}^{\mathrm{inf}}$, replace the transform $y = \mathrm{BN}_{\gamma,\beta}(x)$ with $y = \frac{\gamma}{\sqrt{\mathrm{Var}[x]+\epsilon}} \cdot x + \left(\beta - \frac{\gamma\,\mathrm{E}[x]}{\sqrt{\mathrm{Var}[x]+\epsilon}}\right)$
end for

Algorithm 2: Training a Batch-Normalized Network

Ioffe, Sergey. "Batch normalization: Accelerating deep network training by reducing internal covariate shift." *arXiv preprint arXiv:1502.03167* (2015).

Logits and Sigmoid Function

Logits: Raw outputs of neural networks.

- Numerical values, hard to interpret

Sigmoid function: $\hat{y} = \sigma(z) = \frac{1}{1 + e^{-z}}$

- Turns logits into probabilities, easier to interpret

Binary Cross Entropy Loss

$$L = -\frac{1}{N}\sum_{i=1}^{N}[y_i \log(p_i) + (1-y_i)\log(1-p_i)]$$

$> N$ *is the number of samples*

$> y_i\ i$ *is the true label for the* i^{th} *sample (0 or 1)*

$> p_i$ *is the predicted probability that the* i^{th} *sample belongs to Positive class*

Sahilcarterr. "Mathematics Behind Simple Linear Regression using Gradient Descent." *Medium*, Medium, 5 Apr. 2020, https://medium.com/@sahilcarterr/mathematics-behind-simple-linear-regression-using-gradient-descent-a09595bf701d.

Binary Cross Entropy with Logits Loss

$$\ell_n := \begin{cases} w_n \cdot [(1 - y_n) \cdot x_n + \ln(1 + e^{-x_n})] & \text{if } x_n > 0 \\ w_n \cdot [-x_n \cdot y_n + \ln(e^{x_n} + 1)] & \text{otherwise} \end{cases}$$

jodag. “How Is Pytorch’s Class BCEWITHLOGITSLOSS Exactly Implemented?” *Stack Overflow*, 11 July 2022, stackoverflow.com/questions/66906884/how-is-pytorchs-class-bcewithlogitsloss-exactly-implemented.

Backpropagation

Algorithm 1 Backpropagation

procedure BACKPROPAGATION(X, θ)
    $a^0 \leftarrow x$ ▷ Set Input
    for $l \leftarrow [1, L]$ **do** ▷ Forward Pass: Compute weighted inputs and activations
        $z^l \leftarrow W^l a^{l-1} + b^l$
        $a^l \leftarrow \sigma(z^l)$
    end for

    $\delta_L \leftarrow (a^L - y) \odot \sigma'(z^L)$ ▷ Compute Error in Final Layer
    for $l \leftarrow [L-1, 1]$ **do** ▷ Backpropagate Error
        $\delta^l \leftarrow (W^{l+1})^T \delta^{l+1} \odot \sigma'(z^l)$
    end for

    for $l \leftarrow [1, L]$ **do** ▷ Compute gradients w.r.t. network parameters
        $\nabla_{b^l} = \delta^l$
        $\nabla_{W^l} = \delta^l (a^{l-1})^T$
    end for
    return $\nabla_\theta = (\nabla_{W^l}, \nabla_{b^l})$
end procedure

Gabbard & Miller. “Machine Learning from Scratch: Stochastic Gradient Descent and Adam Optimizer.” *18.0851 Project*, accessed 17 November 2024, https://www.mit.edu/~jgabbard/assets/18085_Project_final.pdf .

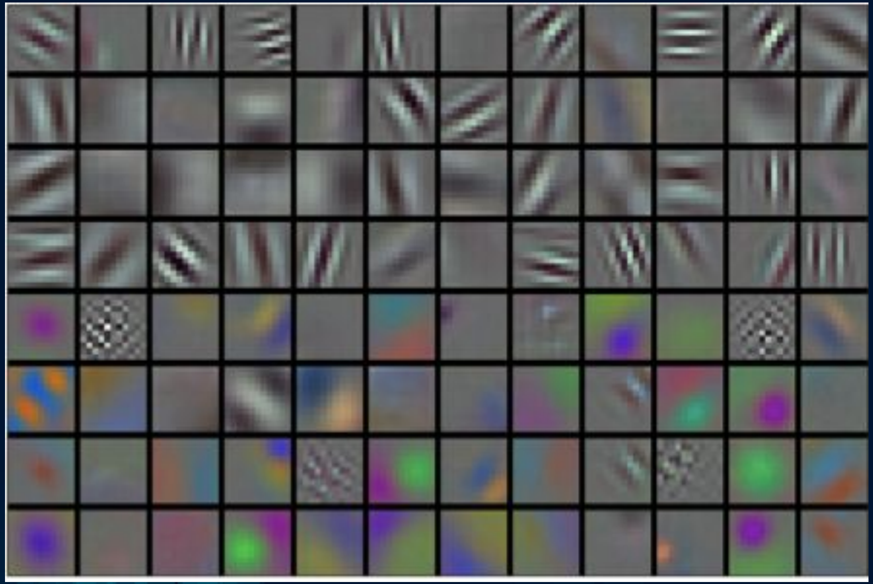
ADAM (Adaptive Moment Estimation/ Gradient Descent with Momentum)

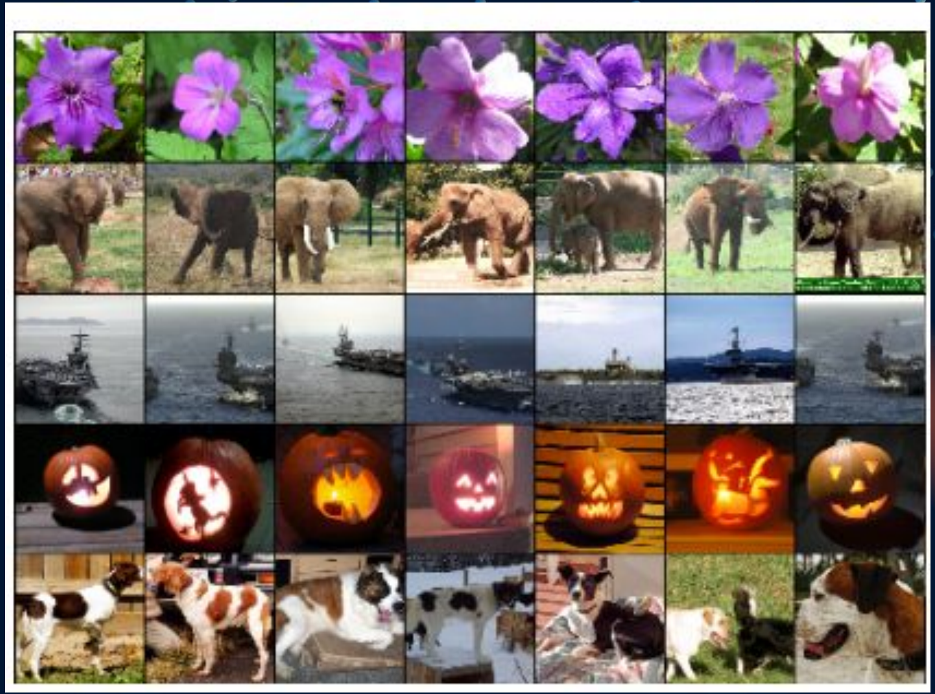
Algorithm 1: *Adam*, our proposed algorithm for stochastic optimization. See section 2 for details, and for a slightly more efficient (but less clear) order of computation. g_t^2 indicates the elementwise square $g_t \odot g_t$. Good default settings for the tested machine learning problems are $\alpha = 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 10^{-8}$. All operations on vectors are element-wise. With β_1^t and β_2^t we denote β_1 and β_2 to the power t.

Require: α: Stepsize
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector
  $m_0 \leftarrow 0$ (Initialize 1st moment vector)
  $v_0 \leftarrow 0$ (Initialize 2nd moment vector)
  $t \leftarrow 0$ (Initialize timestep)
  while θ_t not converged **do**
    $t \leftarrow t + 1$
    $g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$ (Get gradients w.r.t. stochastic objective at timestep t)
    $m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (Update biased first moment estimate)
    $v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2$ (Update biased second raw moment estimate)
    $\widehat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ (Compute bias-corrected first moment estimate)
    $\widehat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (Compute bias-corrected second raw moment estimate)
    $\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \widehat{m}_t / (\sqrt{\widehat{v}_t} + \epsilon)$ (Update parameters)
  end while
  return θ_t (Resulting parameters)

Kingma, Diederik P. "Adam: A method for stochastic optimization." *arXiv preprint arXiv:1412.6980* (2014).

AlexNet





Alex Krizhevsky, Ilya Sutskever, and Geoffrey E. Hinton. 2017. ImageNet classification with deep convolutional neural networks. Commun. ACM 60, 6 (June 2017), 84–90. https://doi.org/10.1145/3065386

Data Structure for Colab Models

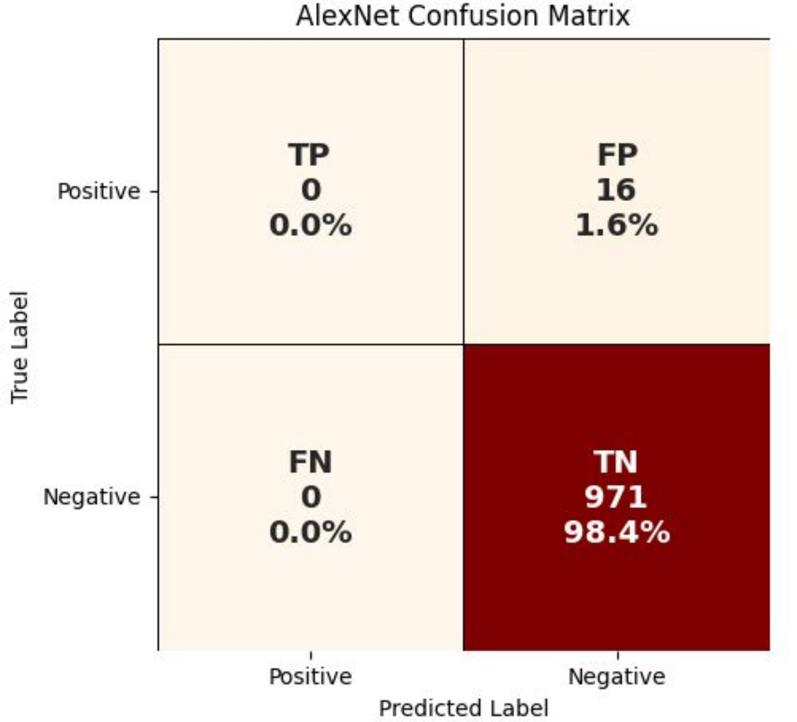
```
Data Structure

Dataset-|
            | _>train---| _> graphene
                        |_> non_graphene

            | _>test---| _> graphene
                       |_> non_graphene
```

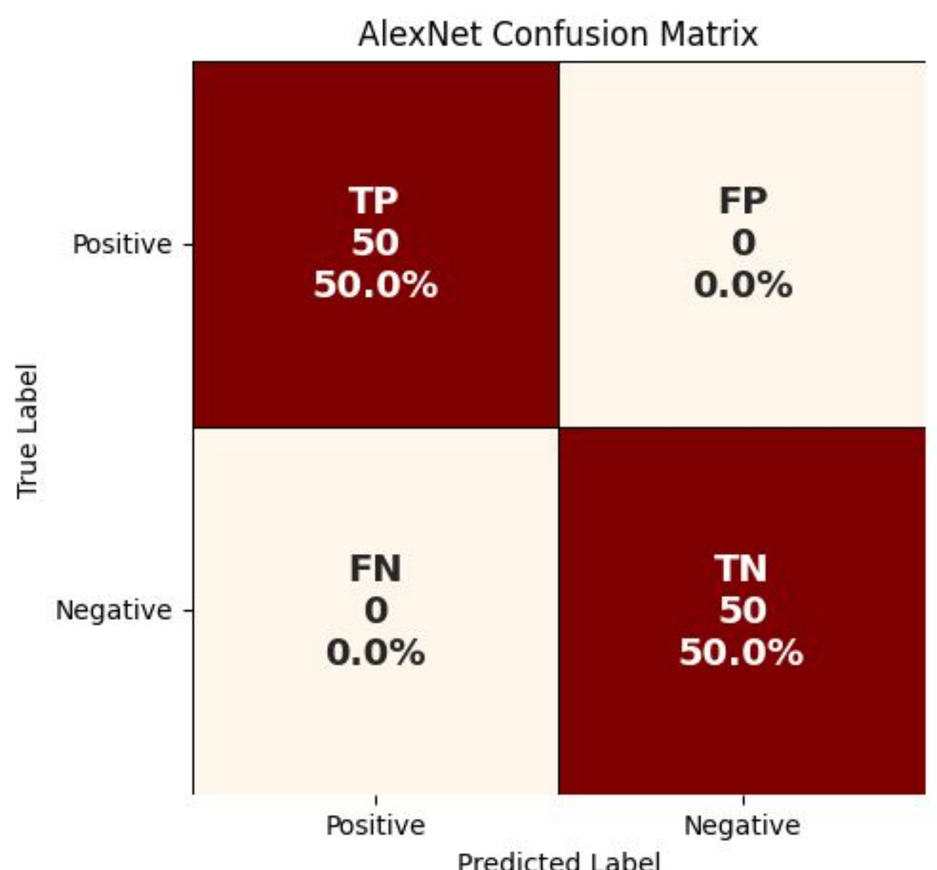
Pre-Trained Models Used & Metrics

	Metric	AlexNet	VGG16	ResNet50	EfficientNet b0	Inception v3
0	Accuracy	0.98	0.98	0.98	0.99	0.99
1	Precision	0.98	0.98	1.00	0.99	0.99
2	F1	0.99	0.99	0.99	1.00	1.00
3	ROC AUC	0.50	0.40	0.96	1.00	0.97
4	Runtime (sec)	173.46	676.63	484.59	301.84	662.06

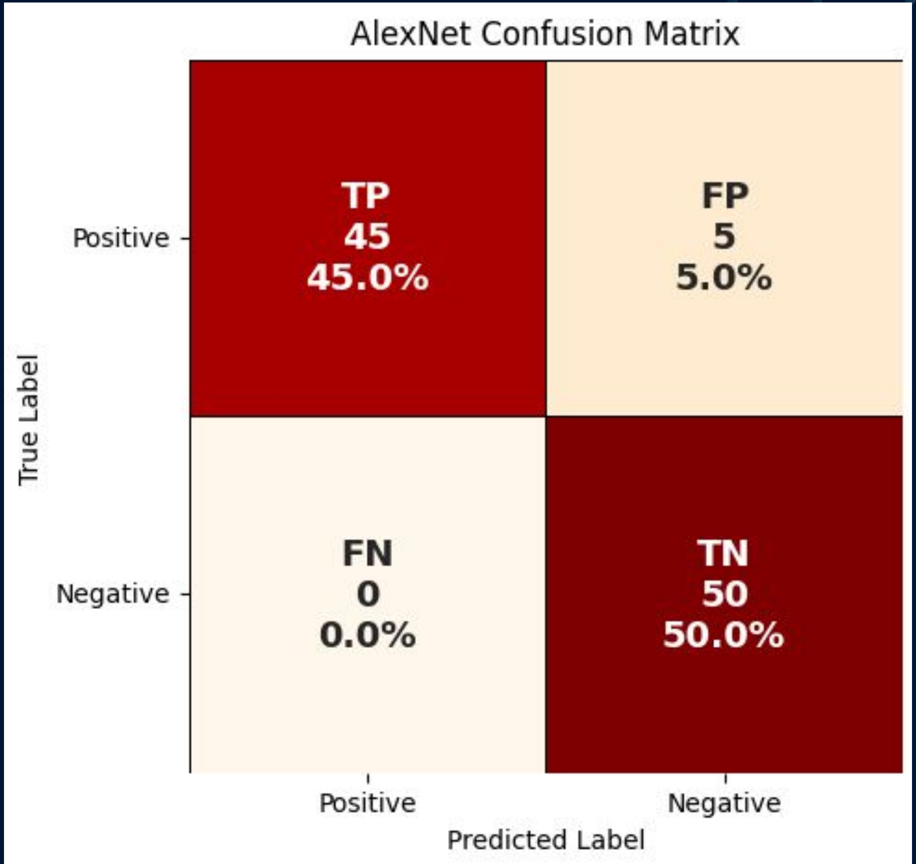
Metric	AlexNet	VGG16	ResNet50	EfficeintNet b0	Inception v3
Accuracy	0.95	0.91	0.84	0.89	0.96
Precision	0.91	0.85	0.77	0.82	0.93
F1	0.95	0.92	0.86	0.90	0.96
AUC of ROC	0.97	0.91	0.99	0.97	1
Runtime(sec)	189.64	418.92	583.52	355.70	816.22
Parameter #	61,100,840	138,357,544	25,557,032	5.3M	27,161,264

AlexNet Confusion Matrix





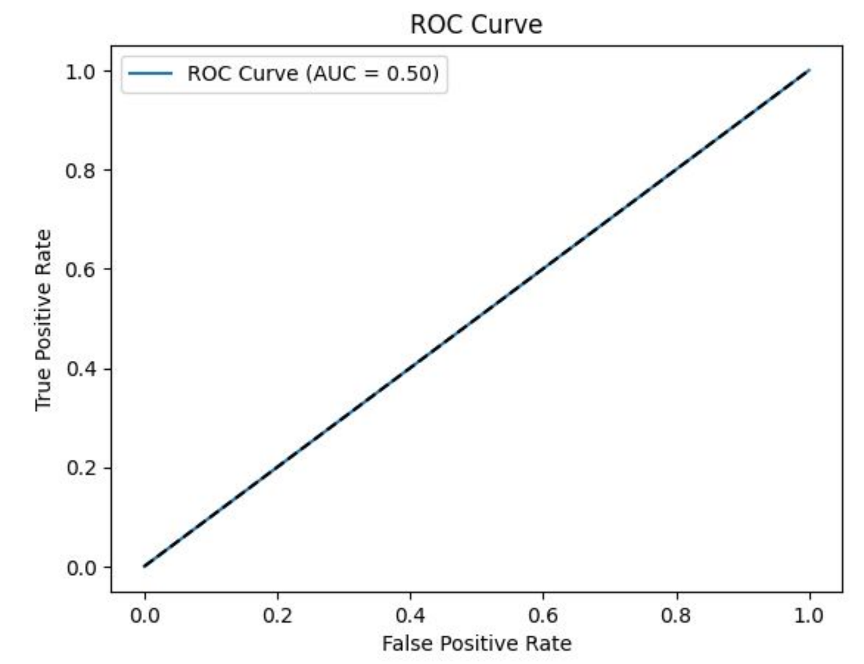
AlexNet Confusion Matrix

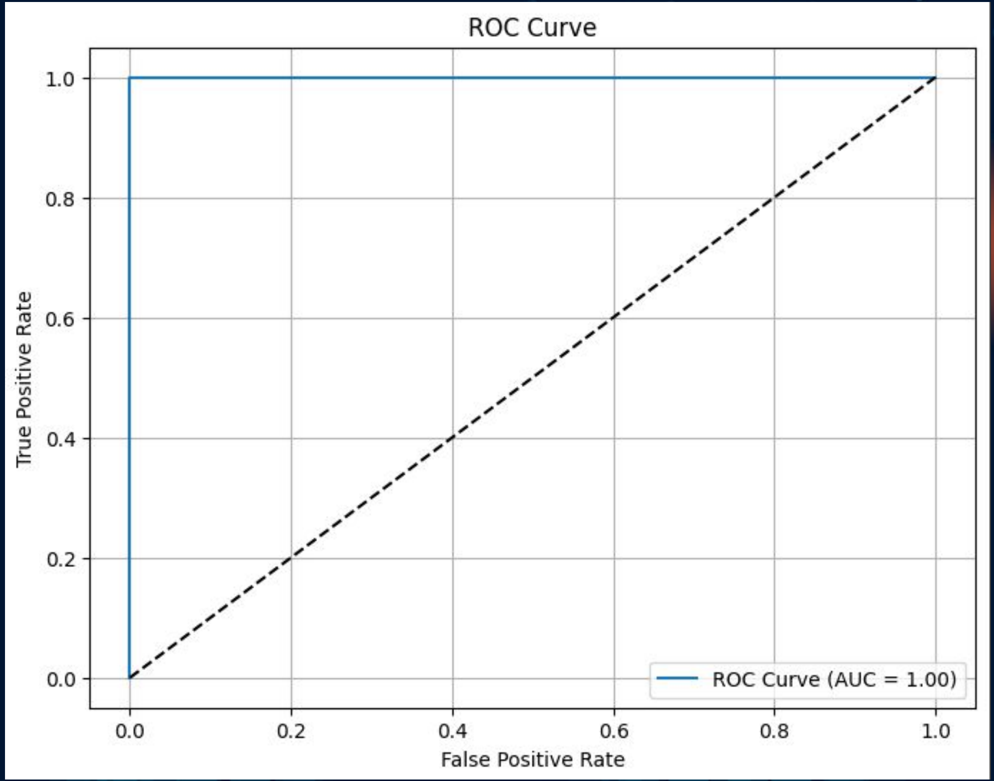


AlexNet ROC/ AUC Plot

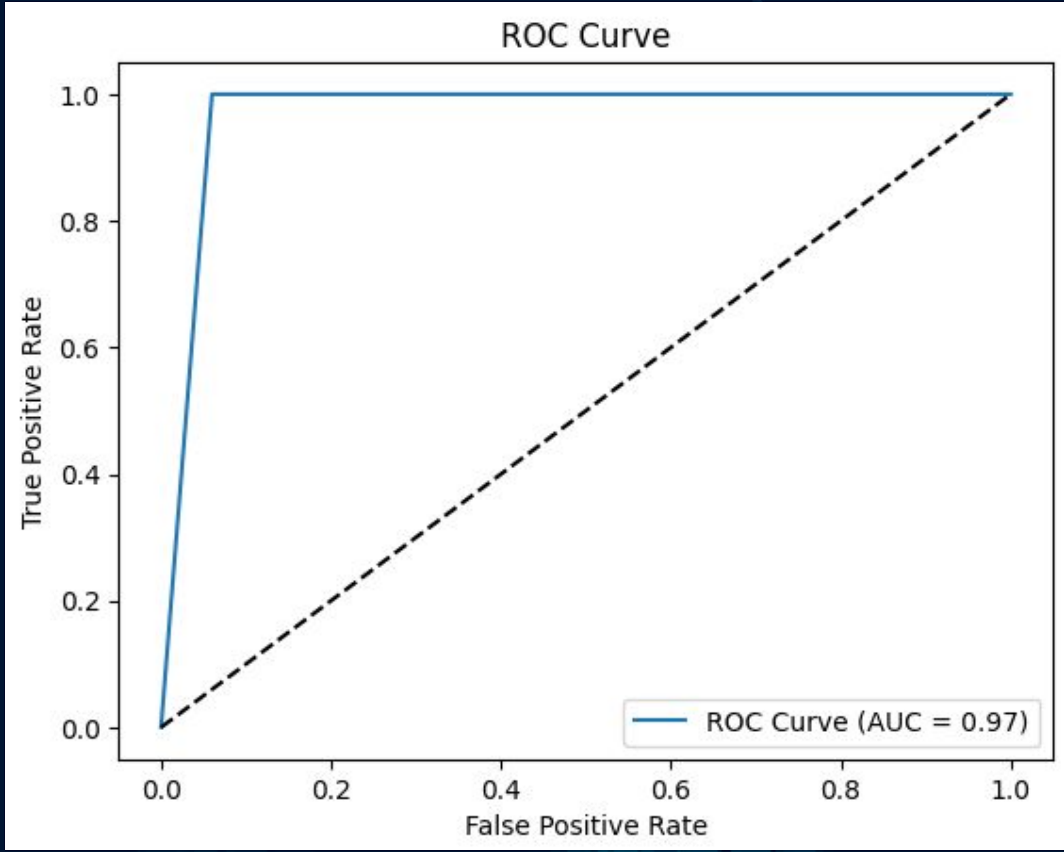
$$TPR = \frac{TP}{TP + FN}$$

$$FPR = \frac{FP}{FP + TN}$$

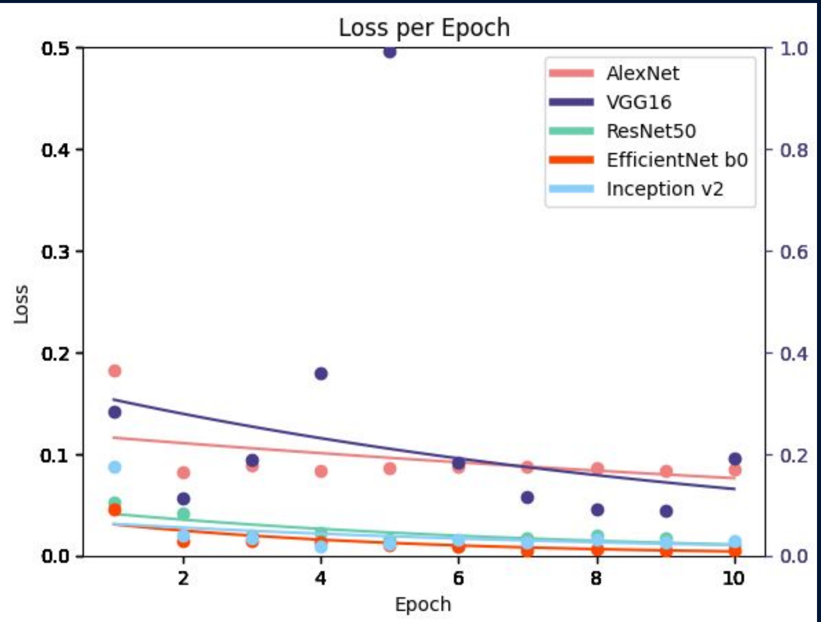


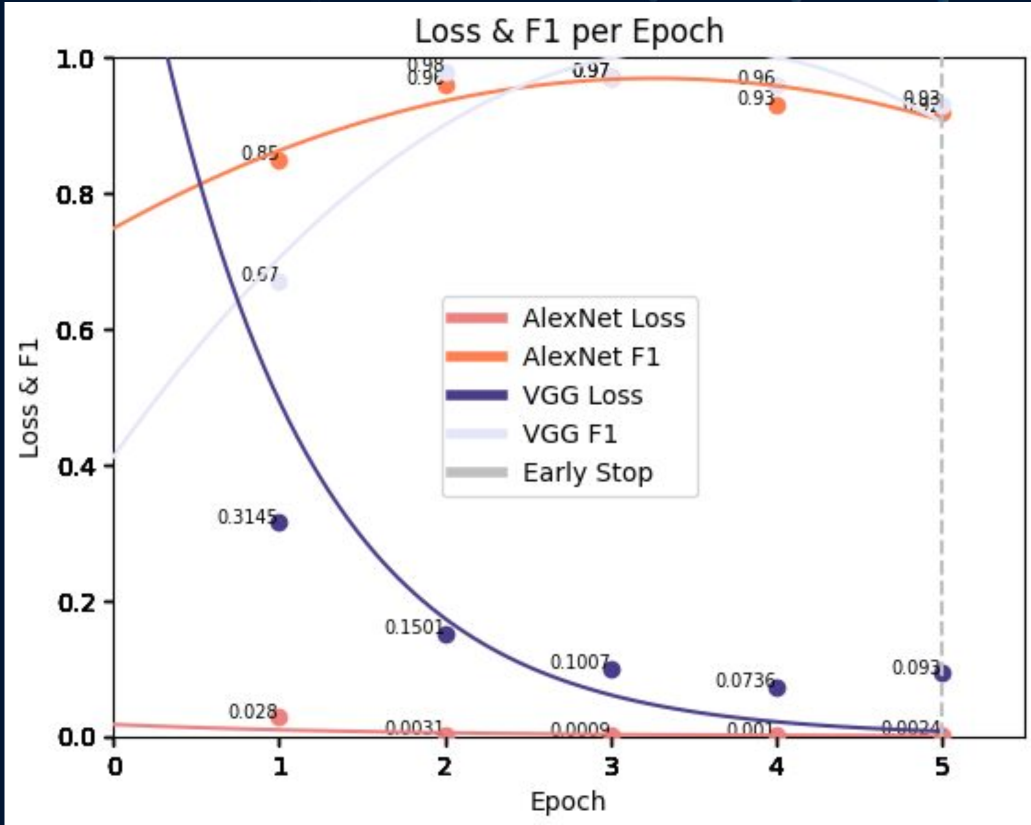


AlexNet ROC/ AUC Plot

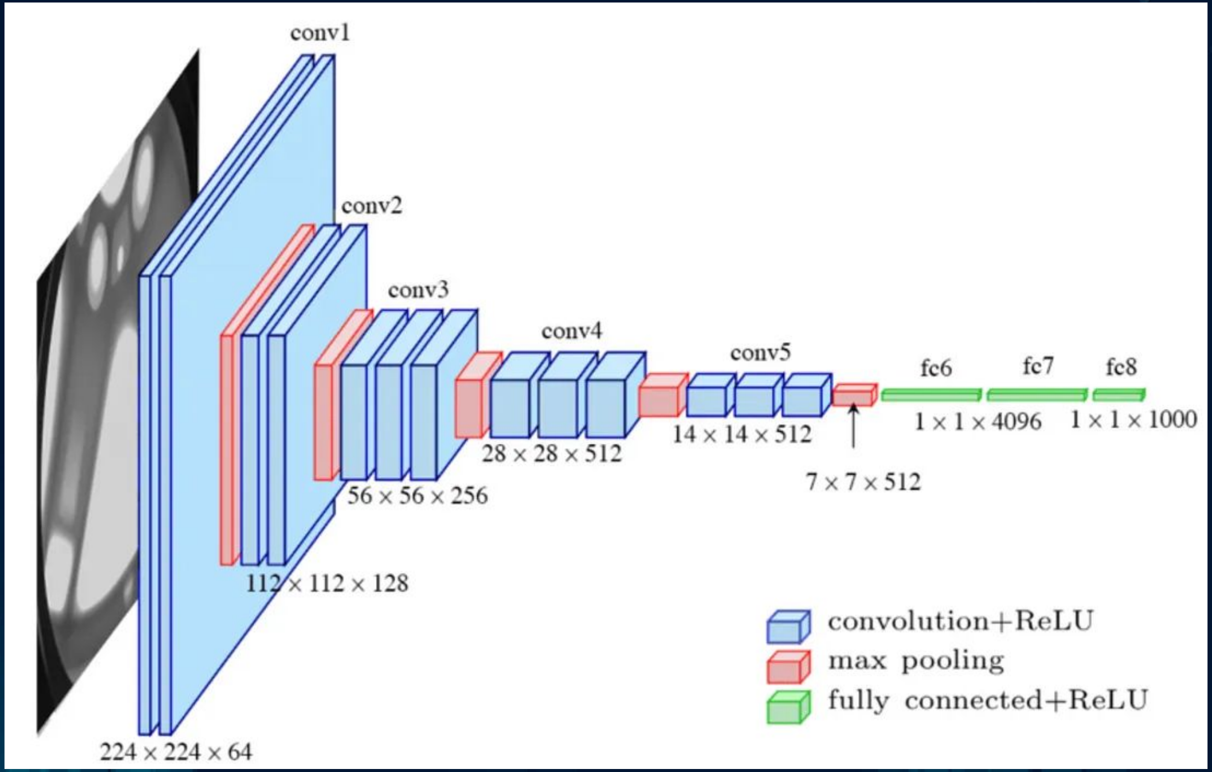


Loss Per Epoch w/ Curve Fit



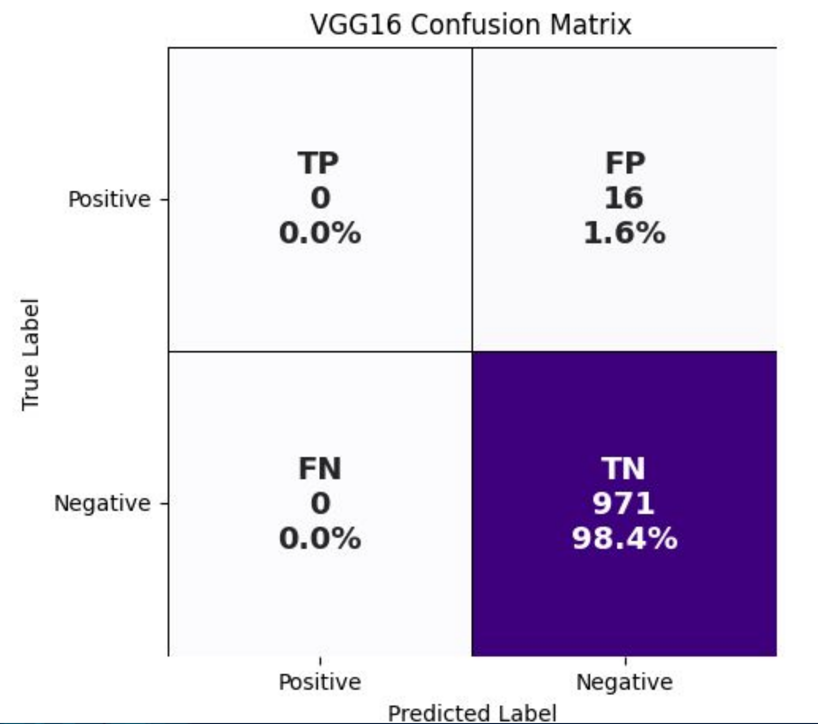


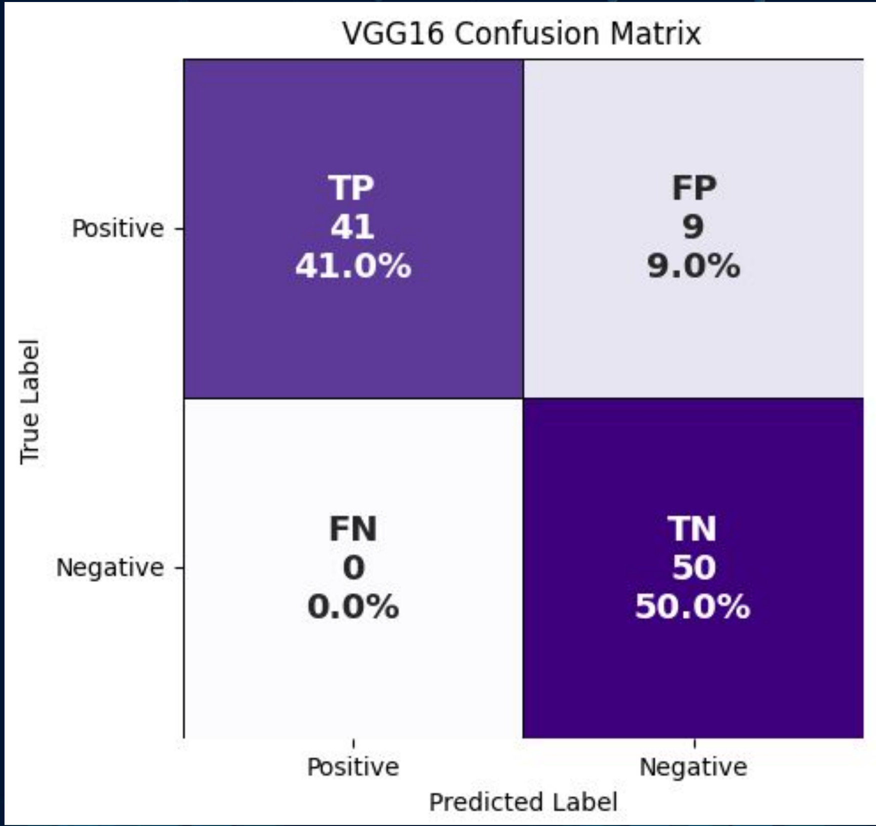
Visual Geometry Group (VGG) 16



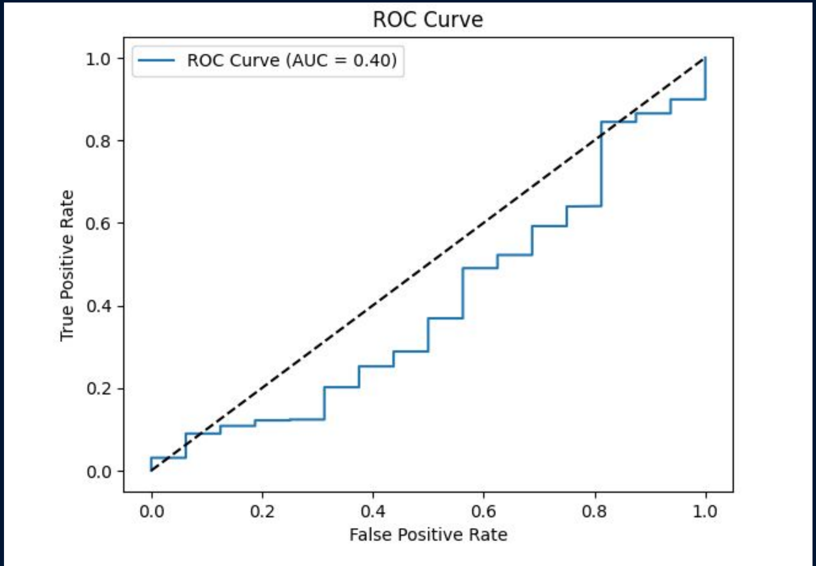
Bangar, Siddhesh. "VGG-Net Architecture Explained." *Medium*, Medium, 28 Jun. 2022, https://medium.com/@siddheshb008/vgg-net-architecture-explained-71179310050f.

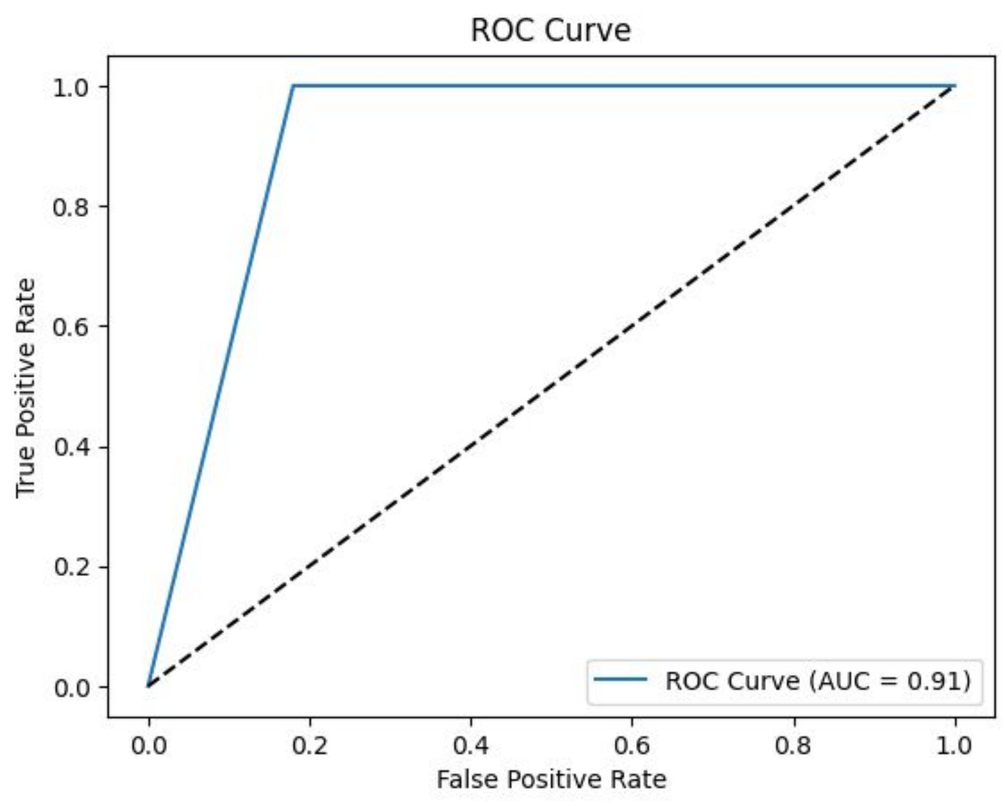
VGG16 Confusion Matrix





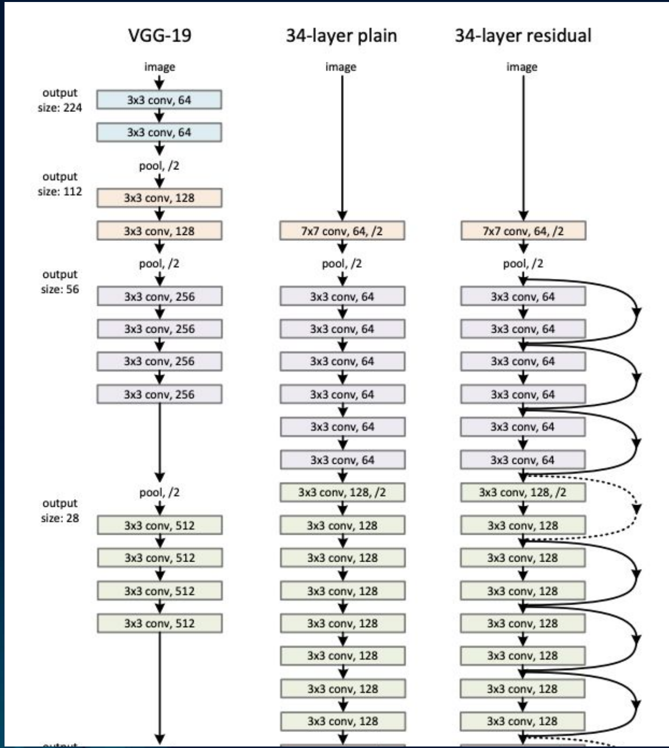
VGG16 ROC/ AUC Plot

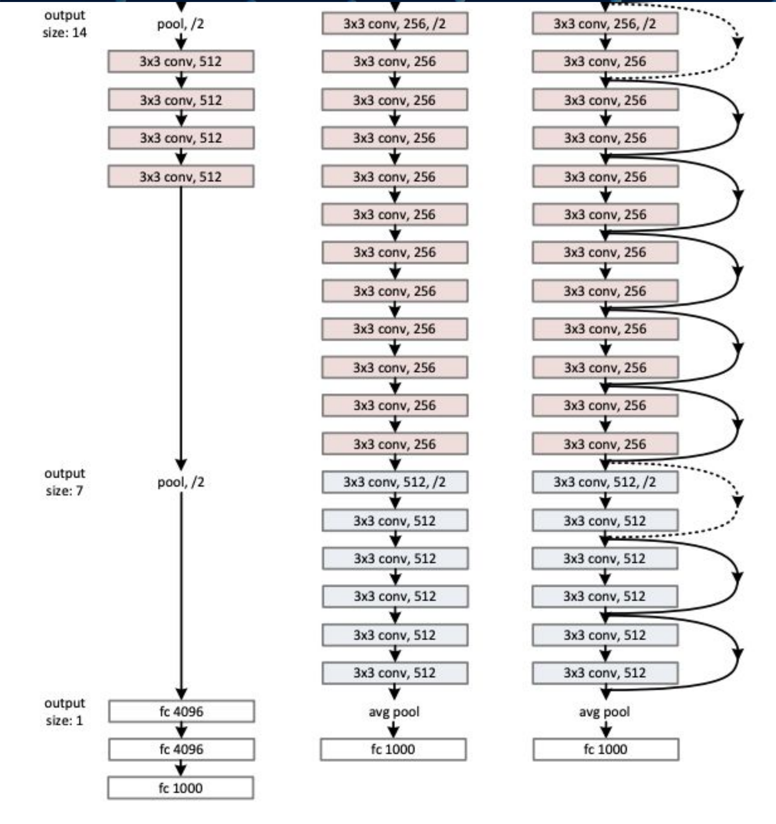




Note sign flip^

ResNet Architecture





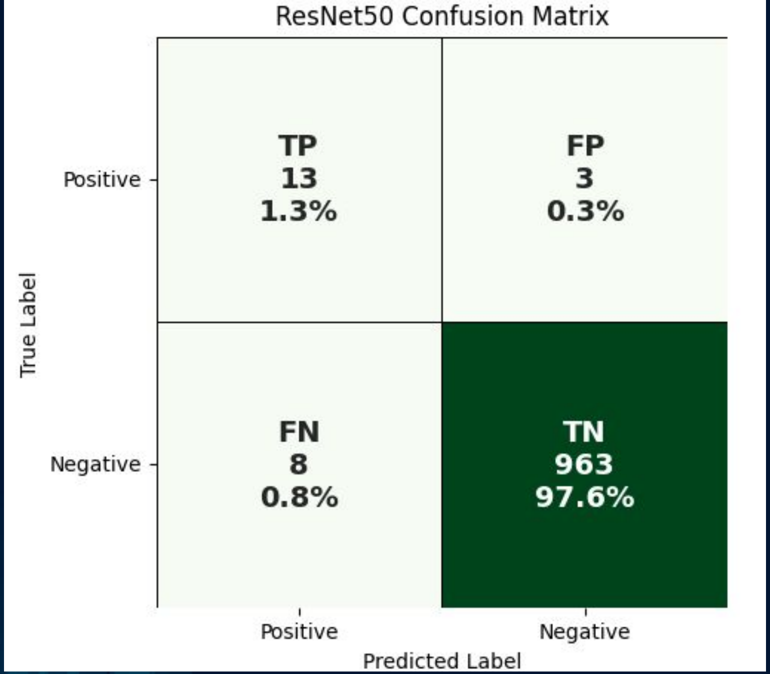
He, Kaiming, et al. "Deep residual learning for image recognition." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

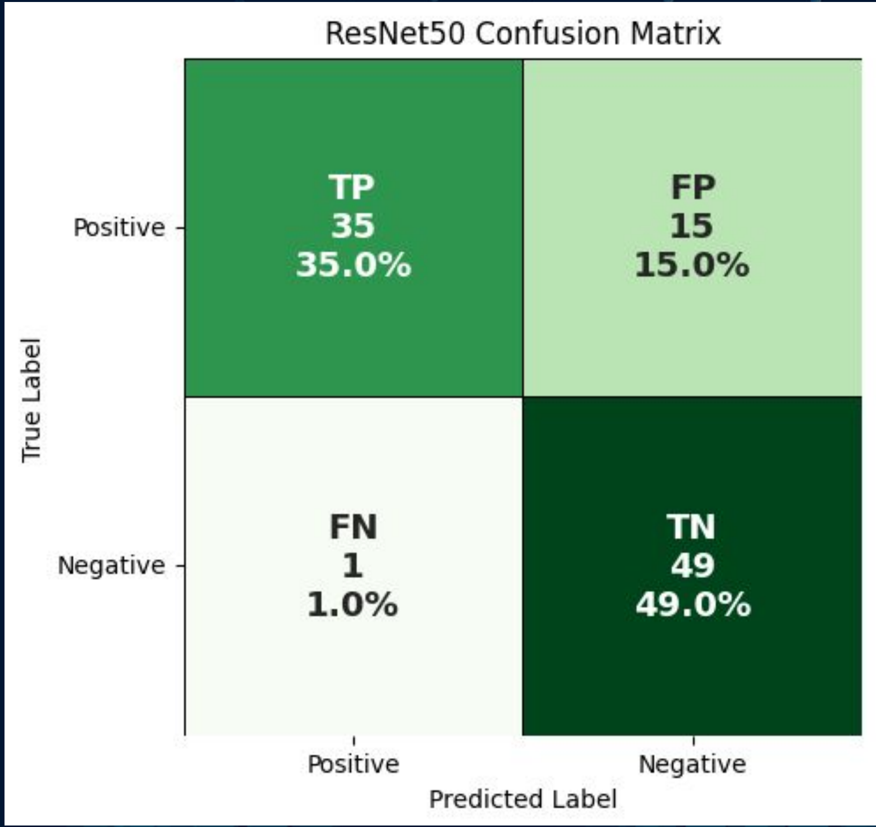
ResNet 50 Architecture

layer name	output size	18-layer	34-layer	50-layer	101-layer	152-layer
conv1	112×112	7×7, 64, stride 2				
conv2_x	56×56	3×3 max pool, stride 2				
		[3×3, 64 3×3, 64] ×2	[3×3, 64 3×3, 64] ×3	[1×1, 64 3×3, 64 1×1, 256] ×3	[1×1, 64 3×3, 64 1×1, 256] ×3	[1×1, 64 3×3, 64 1×1, 256] ×3
conv3_x	28×28	[3×3, 128 3×3, 128] ×2	[3×3, 128 3×3, 128] ×4	[1×1, 128 3×3, 128 1×1, 512] ×4	[1×1, 128 3×3, 128 1×1, 512] ×4	[1×1, 128 3×3, 128 1×1, 512] ×8
conv4_x	14×14	[3×3, 256 3×3, 256] ×2	[3×3, 256 3×3, 256] ×6	[1×1, 256 3×3, 256 1×1, 1024] ×6	[1×1, 256 3×3, 256 1×1, 1024] ×23	[1×1, 256 3×3, 256 1×1, 1024] ×36
conv5_x	7×7	[3×3, 512 3×3, 512] ×2	[3×3, 512 3×3, 512] ×3	[1×1, 512 3×3, 512 1×1, 2048] ×3	[1×1, 512 3×3, 512 1×1, 2048] ×3	[1×1, 512 3×3, 512 1×1, 2048] ×3
	1×1	average pool, 1000-d fc, softmax				
FLOPs		1.8×10^9	3.6×10^9	3.8×10^9	7.6×10^9	11.3×10^9

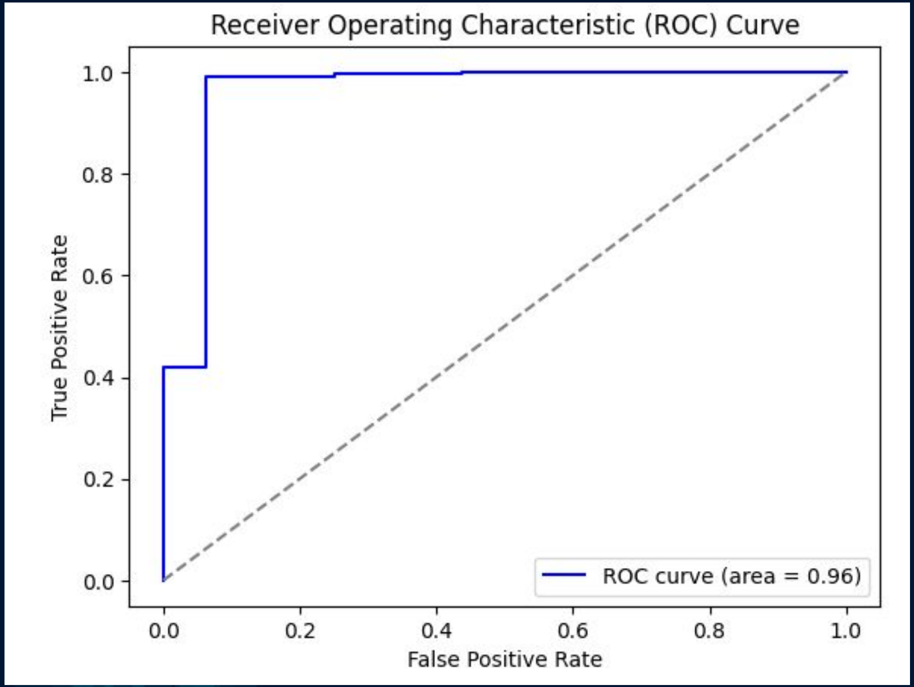
He, Kaiming, et al. "Deep residual learning for image recognition." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

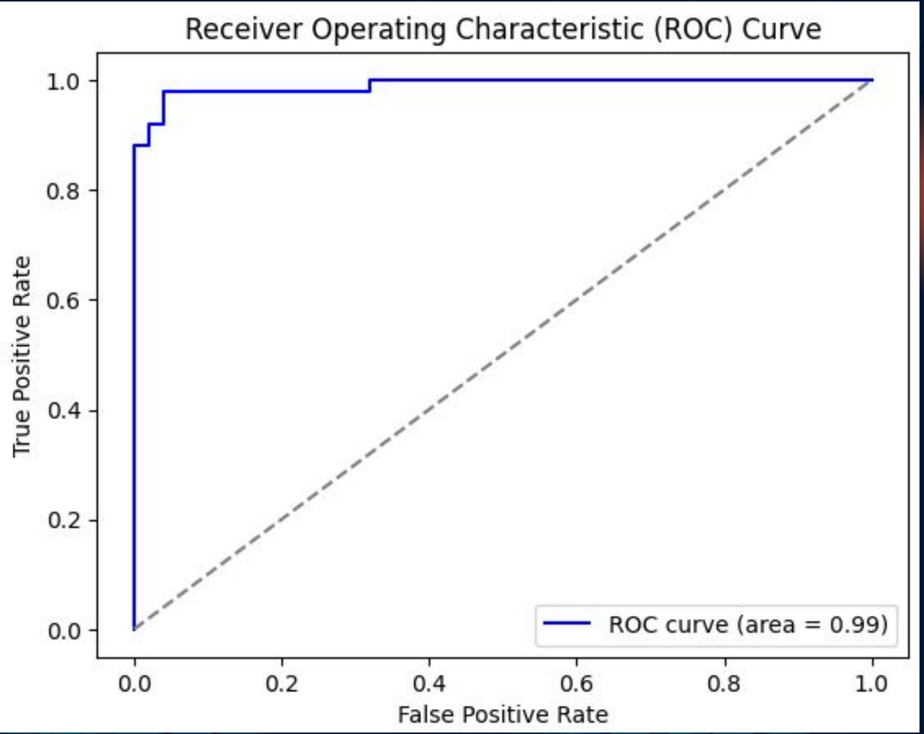
ResNet50 Confusion Matrix



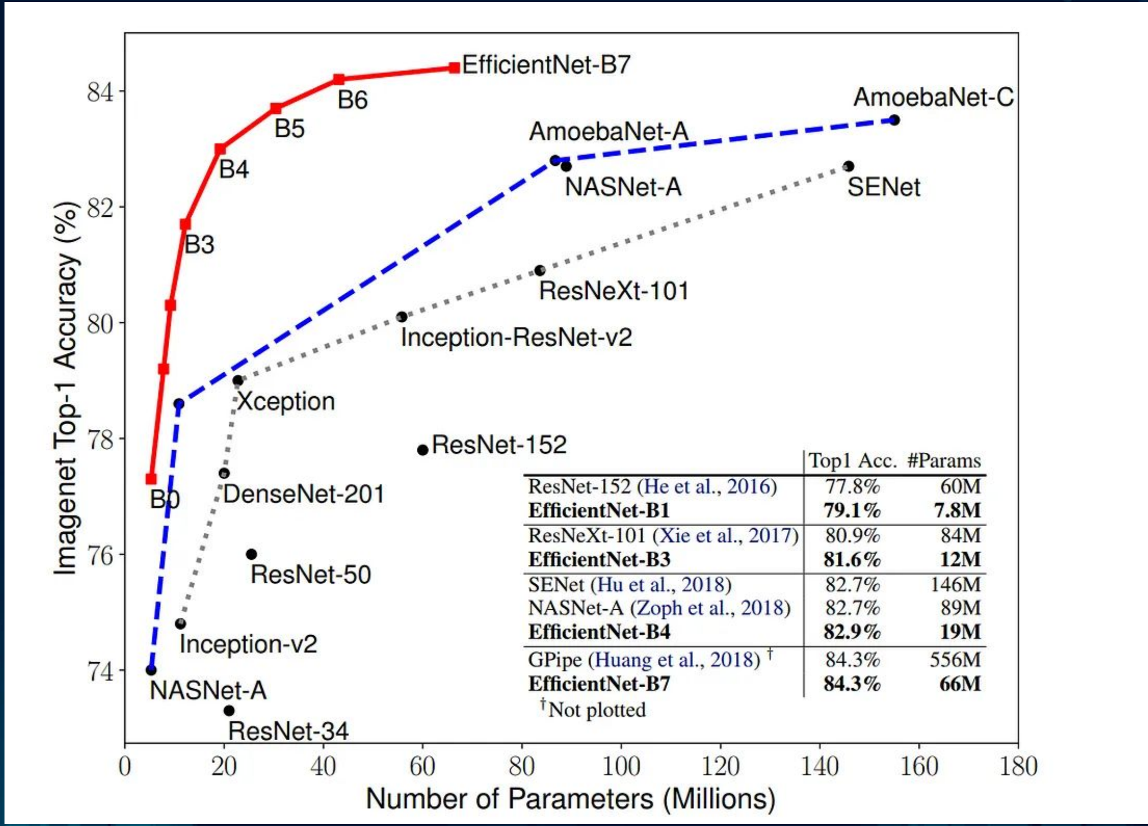


ResNet50 ROC/ AUC Plot





EfficientNet B0



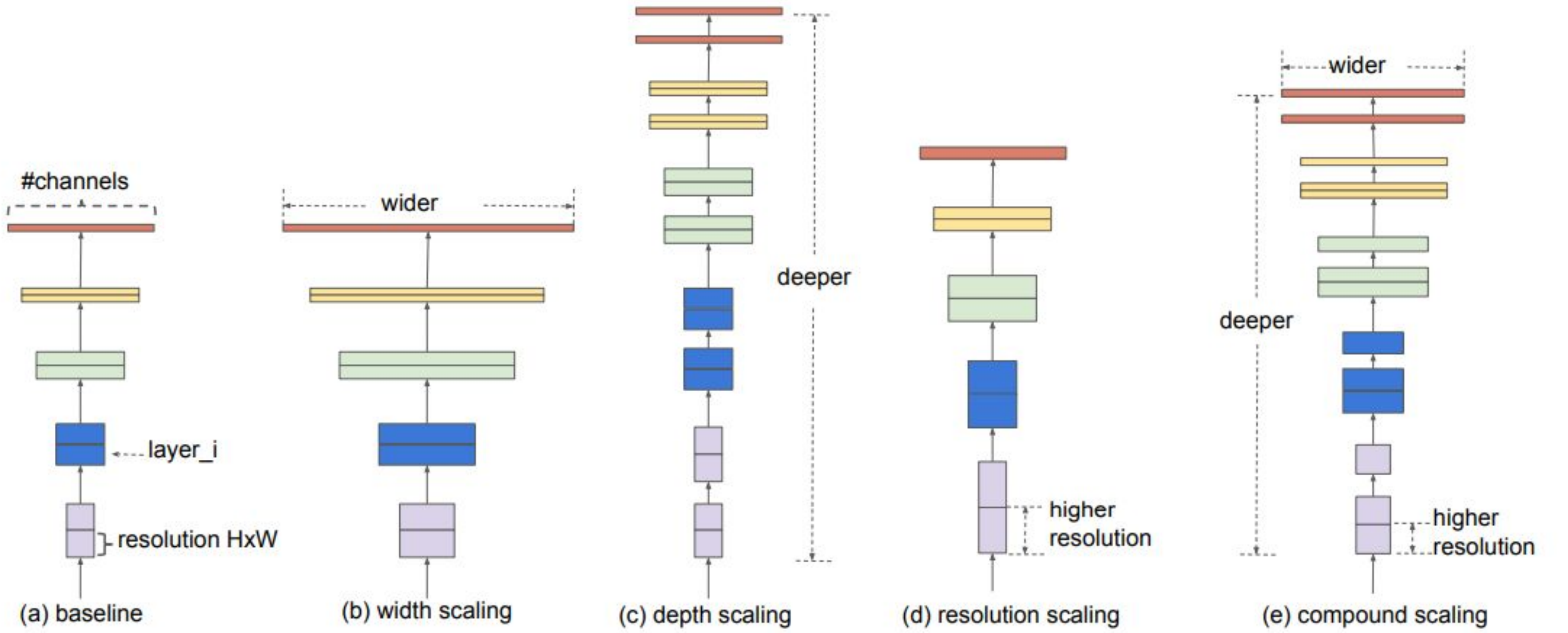
	Top1 Acc.	#Params
ResNet-152 (He et al., 2016)	77.8%	60M
EfficientNet-B1	**79.1%**	**7.8M**
ResNeXt-101 (Xie et al., 2017)	80.9%	84M
EfficientNet-B3	**81.6%**	**12M**
SENet (Hu et al., 2018)	82.7%	146M
NASNet-A (Zoph et al., 2018)	82.7%	89M
EfficientNet-B4	**82.9%**	**19M**
GPipe (Huang et al., 2018) [†]	84.3%	556M
EfficientNet-B7	**84.3%**	**66M**

[†]Not plotted

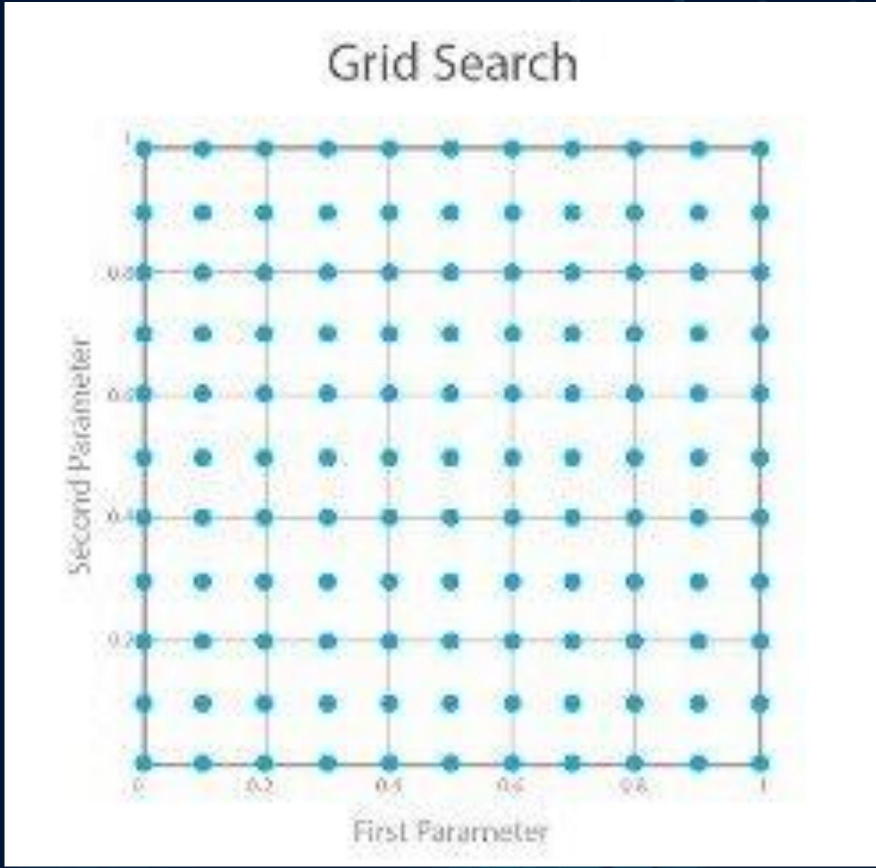
Tan, Mingxing, and Quoc Le. "Efficientnet: Rethinking model scaling for convolutional neural networks." *International conference on machine learning*. PMLR, 2019.

EfficientNet B0

Tan, Mingxing, and Quoc Le. "Efficientnet: Rethinking model scaling for convolutional neural networks." *International conference on machine learning*. PMLR, 2019.



Grid Search



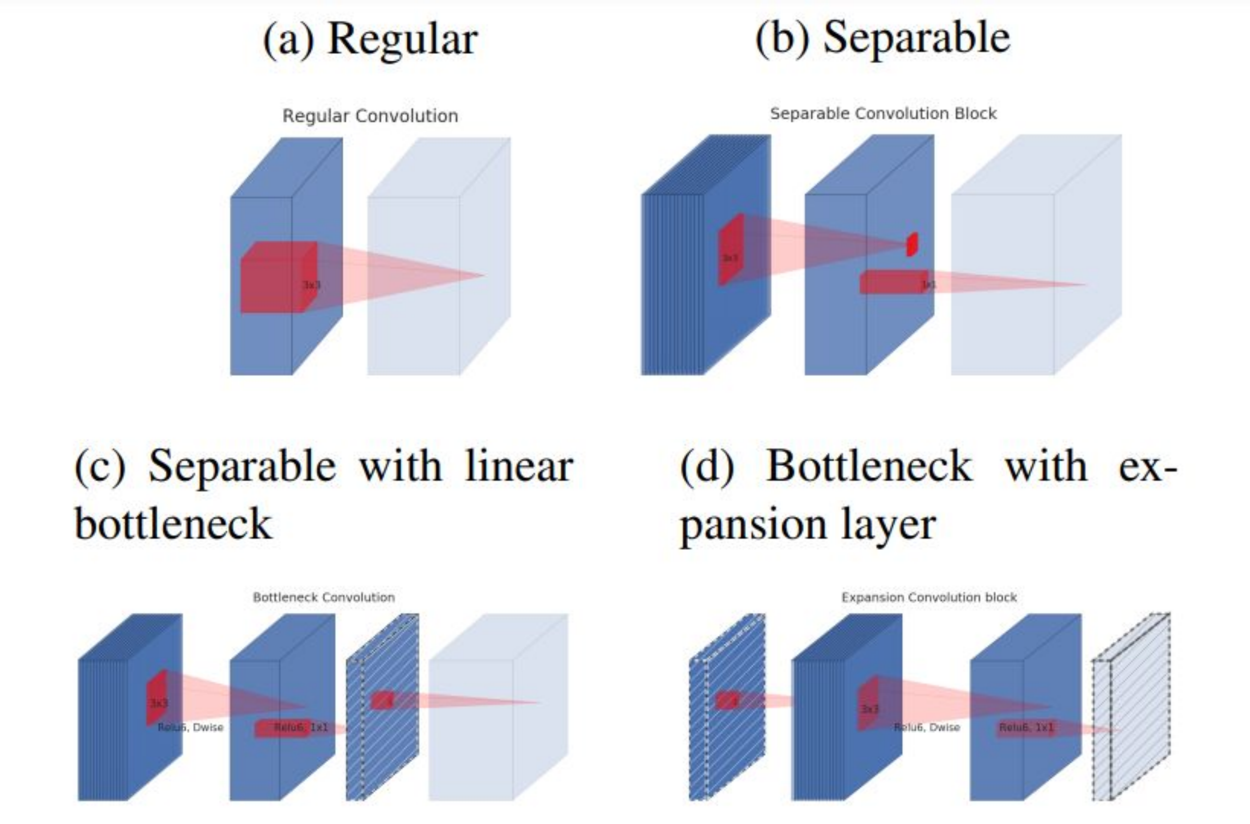
Hien, Ngo Le Huy. "Grid Search space Illustration" *ResearchGate*, ResearchGate, https://www.researchgate.net/figure/Grid-Search-space-illustration_fig9_346571789.

EfficientNet B0 Architecture

Tan, Mingxing, and Quoc Le. "Efficientnet: Rethinking model scaling for convolutional neural networks." *International conference on machine learning*. PMLR, 2019.

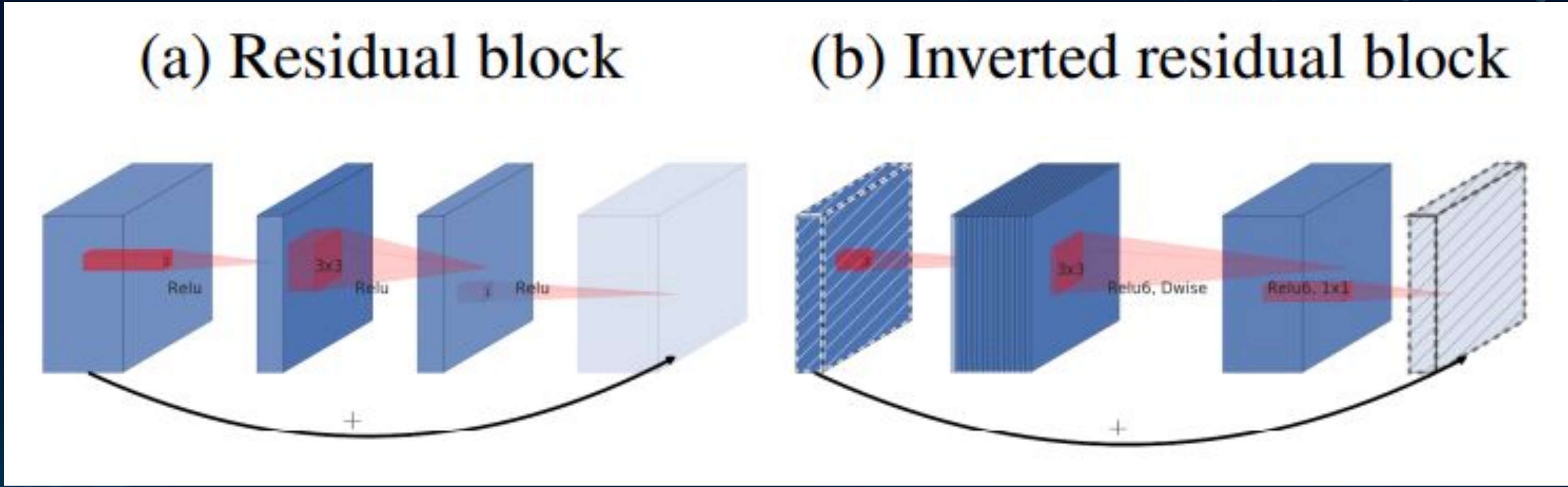
Stage i	Operator $\hat{\mathcal{F}}_i$	Resolution $\hat{H}_i \times \hat{W}_i$	#Channels $\hat{C}_i$	#Layers $\hat{L}_i$
1	Conv3x3	224×224	32	1
2	MBConv1, k3x3	112×112	16	1
3	MBConv6, k3x3	112×112	24	2
4	MBConv6, k5x5	56×56	40	2
5	MBConv6, k3x3	28×28	80	3
6	MBConv6, k5x5	14×14	112	3
7	MBConv6, k5x5	14×14	192	4
8	MBConv6, k3x3	7×7	320	1
9	Conv1x1 & Pooling & FC	7×7	1280	1

Inverted Residual Block



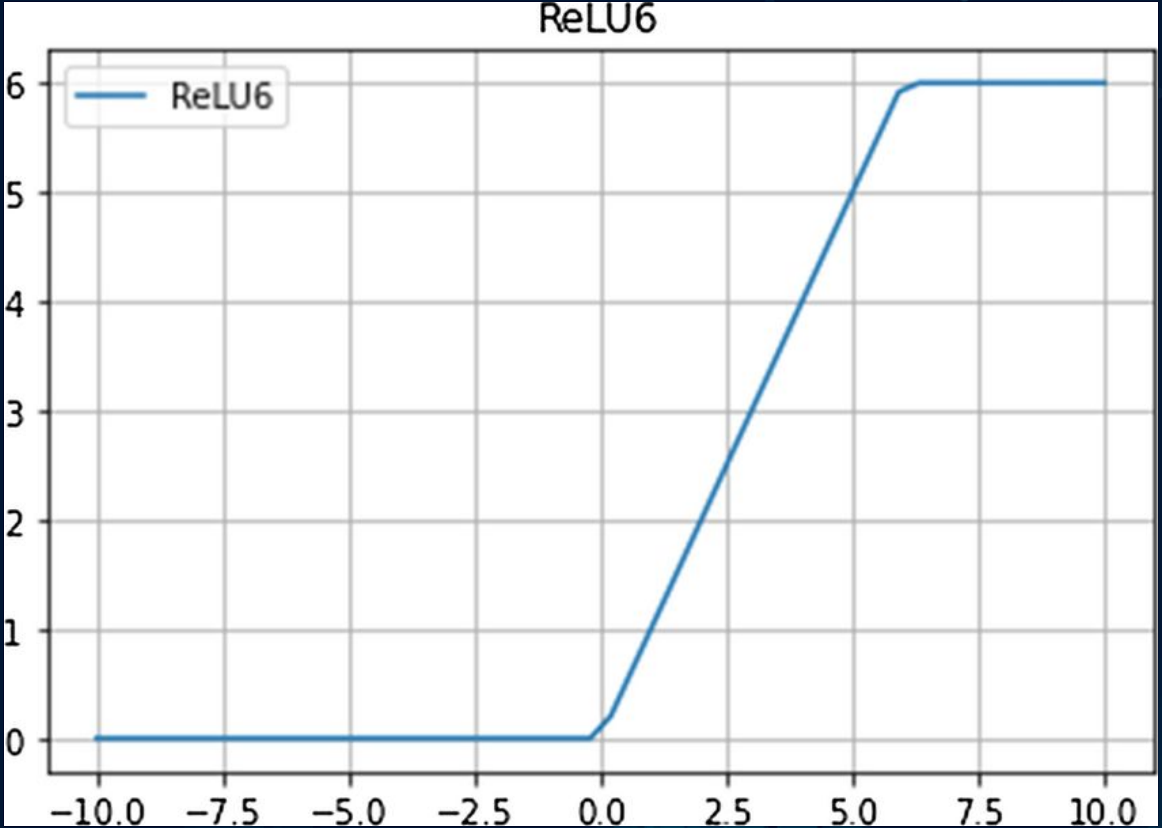
Sandler, Mark, et al. "Mobilenetv2: Inverted residuals and linear bottlenecks." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2018.

Inverted Residual Block



Sandler, Mark, et al. "Mobilenetv2: Inverted residuals and linear bottlenecks." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2018.

ReLU6



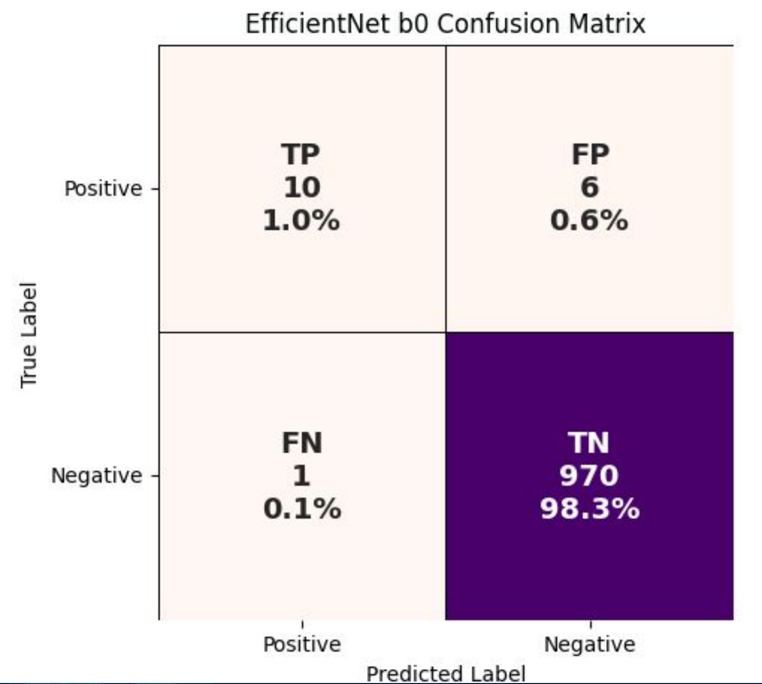
Neural Computing and Applications. “Graph for ReLU6 activation function” *ResearchGate*, ResearchGate, https://www.researchgate.net/figure/Graph-for-ReLU6-activation-function_fig5_371374851.

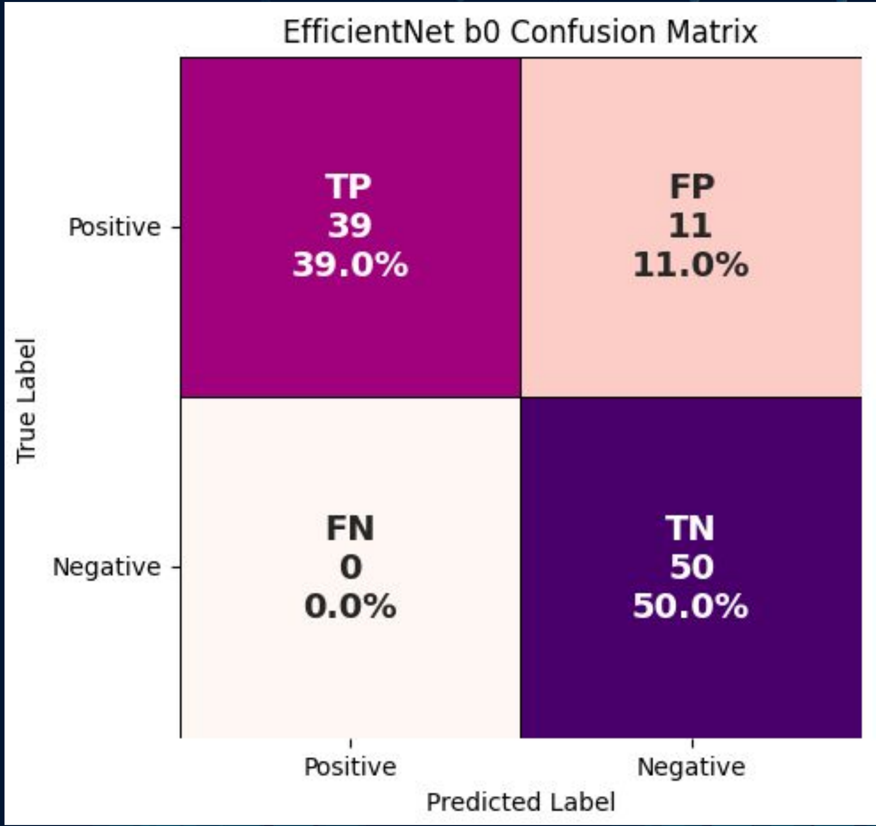
Compound Scaling

Baseline ResNet-50 (He et al., 2016)	4.1B	76.0%
Scale ResNet-50 by depth (d=4)	16.2B	78.1%
Scale ResNet-50 by width (w=2)	14.7B	77.7%
Scale ResNet-50 by resolution (r=2)	16.4B	77.5%
ResNet-50 compound scale	**16.7B**	**78.8%**

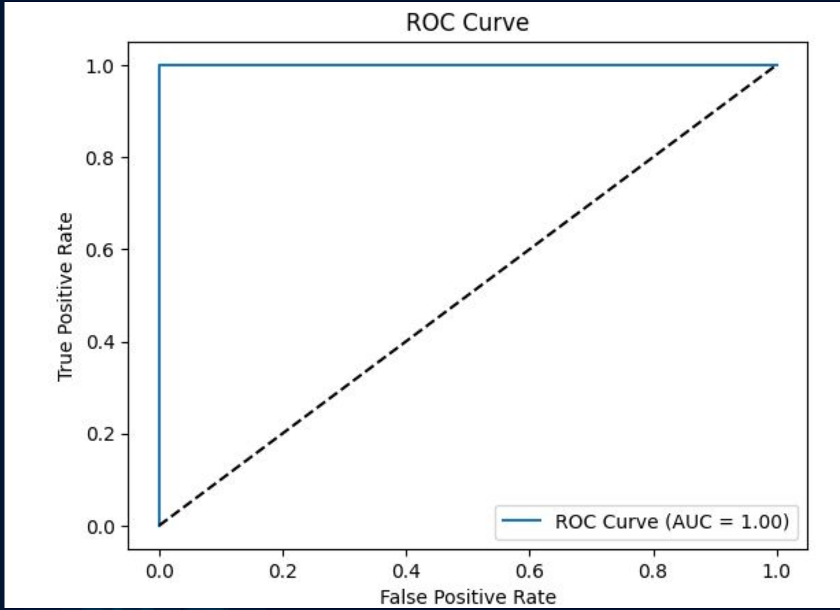
Tan, Mingxing, and Quoc Le. "Efficientnet: Rethinking model scaling for convolutional neural networks." *International conference on machine learning*. PMLR, 2019.

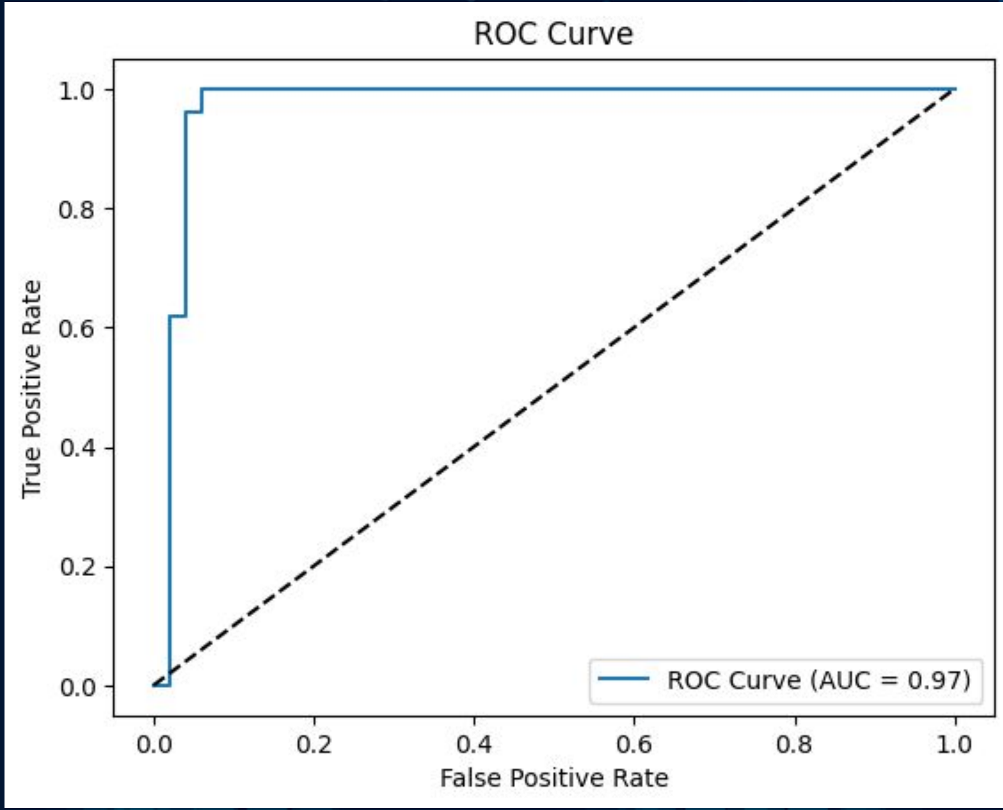
EfficientNet b0 Confusion Matrix





EfficientNet b0 ROC/ AUC Plot





Inception (GoogleNet)

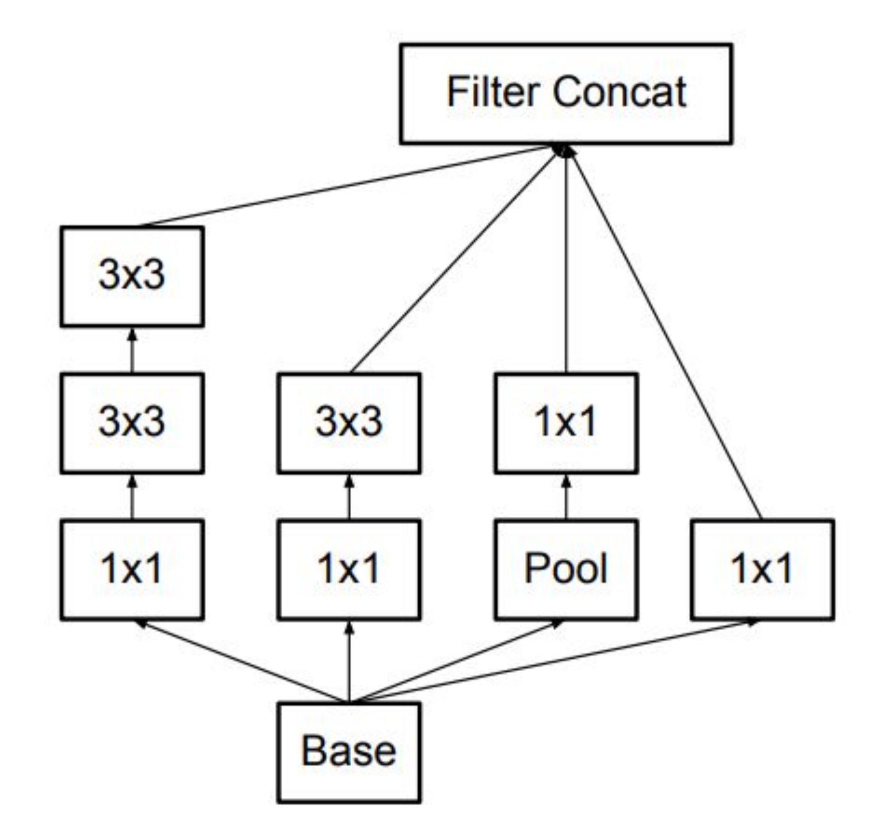
Derevianko, Ivan. “BLAZOR - IT’S TIME TO FORGET JAVASCRIPT” *Ivan Derevianko*, Ivan Derevianko, 16 July 2019, https://ivanderevianko.com/2019/07/blazor-its-time-to-forget-javascript.

Inception v3 Architecture

type	patch size/stride or remarks	input size
conv	$3\times3/2$	$299\times299\times3$
conv	$3\times3/1$	$149\times149\times32$
conv padded	$3\times3/1$	$147\times147\times32$
pool	$3\times3/2$	$147\times147\times64$
conv	$3\times3/1$	$73\times73\times64$
conv	$3\times3/2$	$71\times71\times80$
conv	$3\times3/1$	$35\times35\times192$
$3\times$Inception	As in figure 5	$35\times35\times288$
$5\times$Inception	As in figure 6	$17\times17\times768$
$2\times$Inception	As in figure 7	$8\times8\times1280$
pool	8×8	$8\times8\times2048$
linear	logits	$1\times1\times2048$
softmax	classifier	$1\times1\times1000$

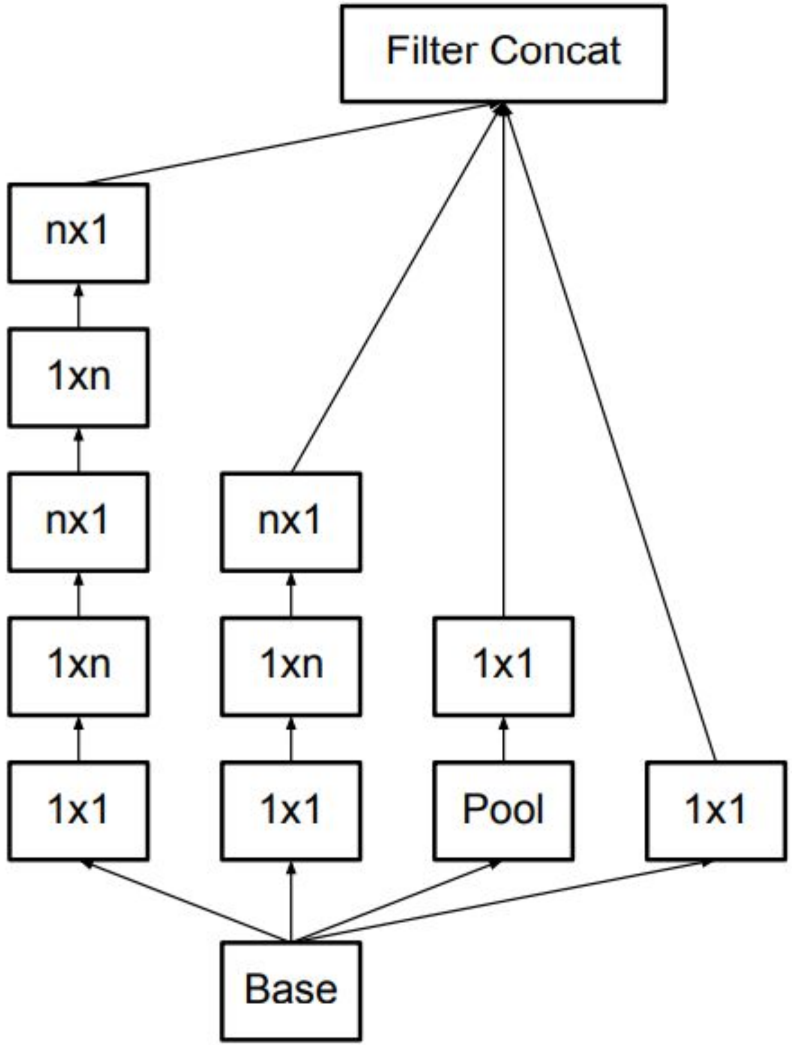
Szegedy, Christian, et al. "Rethinking the inception architecture for computer vision." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

Figure 5



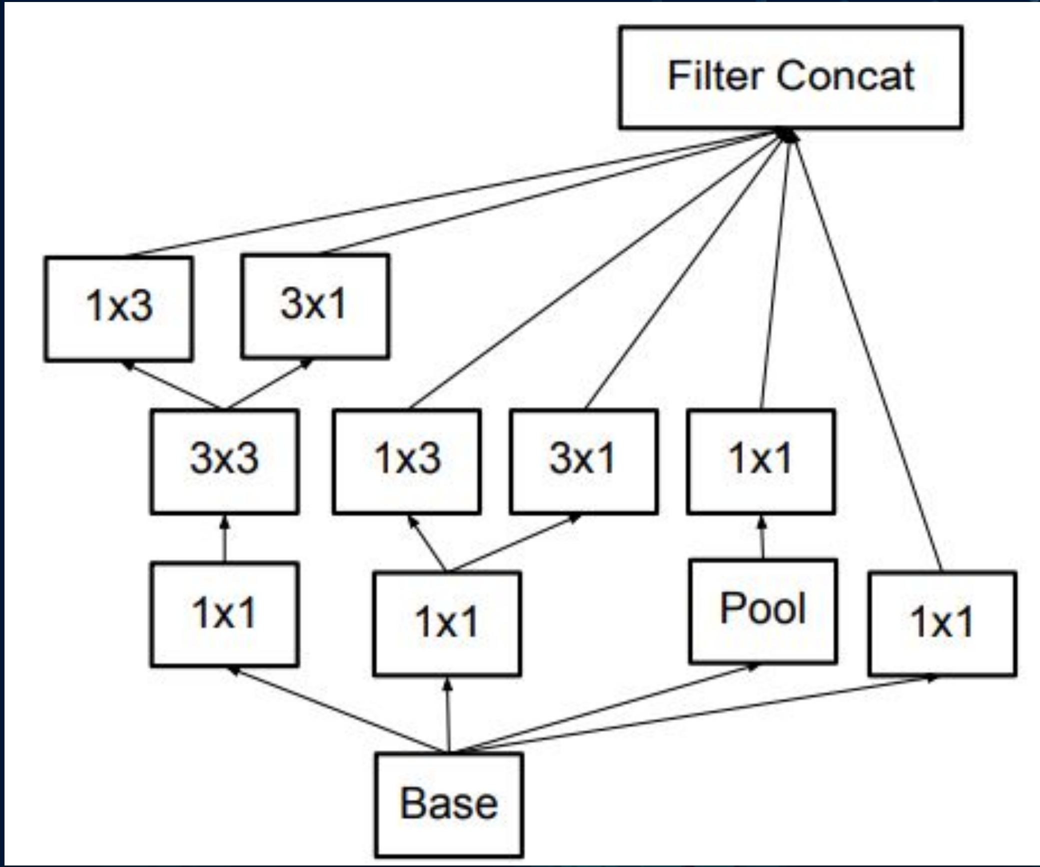
Szegedy, Christian, et al. "Rethinking the inception architecture for computer vision." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

Figure 6



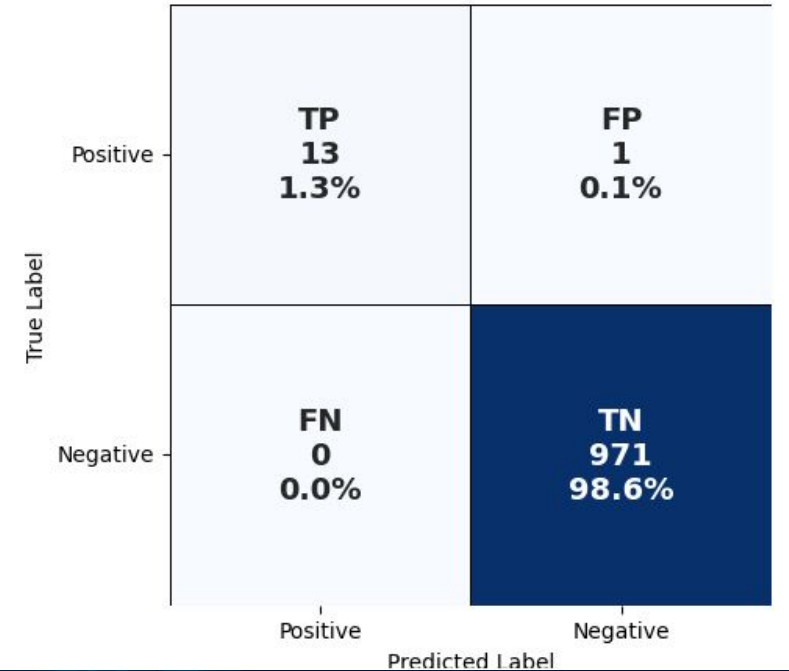
Szegedy, Christian, et al. "Rethinking the inception architecture for computer vision." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

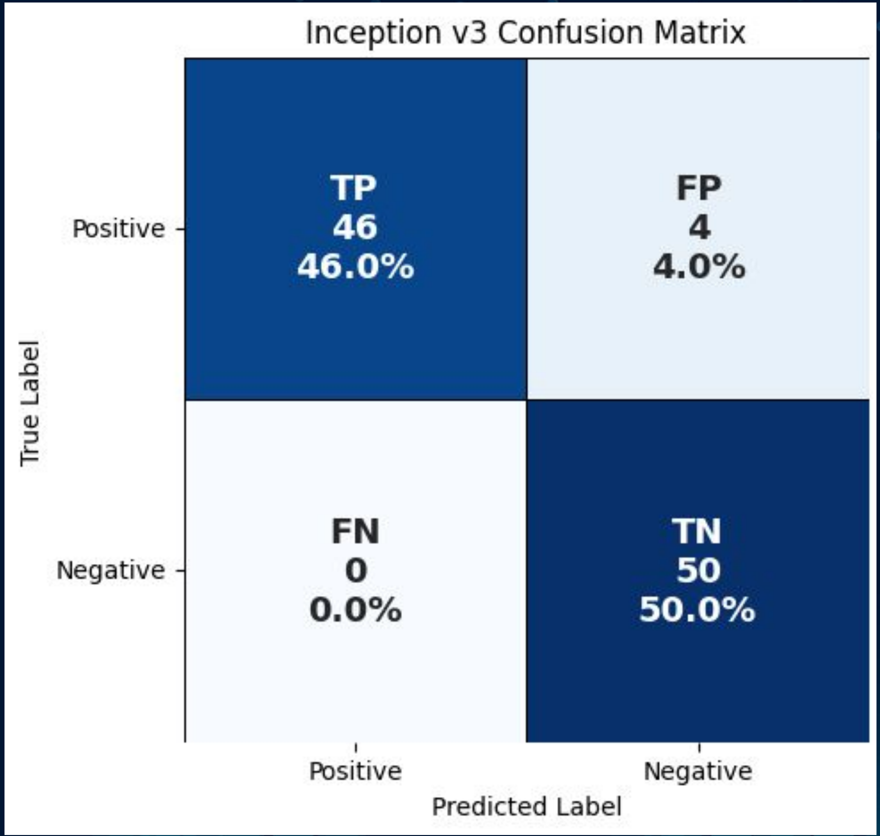
Figure 7



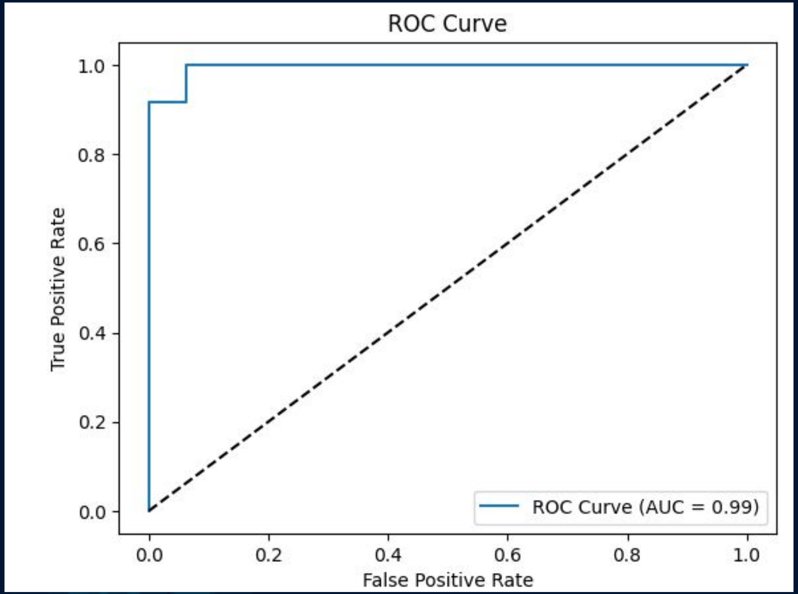
Szegedy, Christian, et al. "Rethinking the inception architecture for computer vision." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.

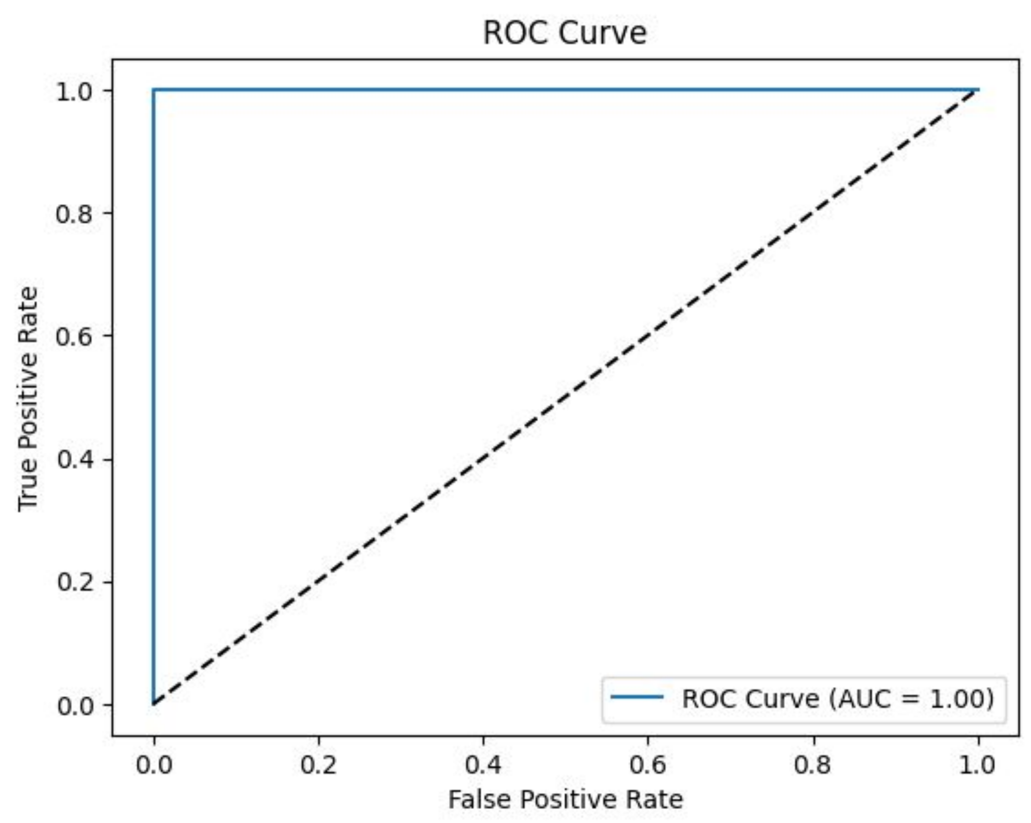
Inception v3 Confusion Matrix





Inception v3 ROC/ AUC Plot





AdamW Optimizer Psuedocode (Algo. 1 is

Algorithm 2 Adam with L_2 regularization and Adam with decoupled weight decay (AdamW)

given $\alpha = 0.001, \beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}, \lambda \in \mathbb{R}$
initialize time step $t \leftarrow 0$, parameter vector $\boldsymbol{\theta}_{t=0} \in \mathbb{R}^n$, first moment vector $\boldsymbol{m}_{t=0} \leftarrow \boldsymbol{0}$, second moment vector $\boldsymbol{v}_{t=0} \leftarrow \boldsymbol{0}$, schedule multiplier $\eta_{t=0} \in \mathbb{R}$
repeat
  $t \leftarrow t + 1$
  $\nabla f_t(\boldsymbol{\theta}_{t-1}) \leftarrow \text{SelectBatch}(\boldsymbol{\theta}_{t-1})$ ▷ select batch and return the corresponding gradient
  $\boldsymbol{g}_t \leftarrow \nabla f_t(\boldsymbol{\theta}_{t-1}) \; +\lambda\boldsymbol{\theta}_{t-1}$
  $\boldsymbol{m}_t \leftarrow \beta_1 \boldsymbol{m}_{t-1} + (1 - \beta_1)\boldsymbol{g}_t$ ▷ here and below all operations are element-wise
  $\boldsymbol{v}_t \leftarrow \beta_2 \boldsymbol{v}_{t-1} + (1 - \beta_2)\boldsymbol{g}_t^2$
  $\hat{\boldsymbol{m}}_t \leftarrow \boldsymbol{m}_t / (1 - \beta_1^t)$ ▷ β_1 is taken to the power of t
  $\hat{\boldsymbol{v}}_t \leftarrow \boldsymbol{v}_t / (1 - \beta_2^t)$ ▷ β_2 is taken to the power of t
  $\eta_t \leftarrow \text{SetScheduleMultiplier}(t)$ ▷ can be fixed, decay, or also be used for warm restarts
  $\boldsymbol{\theta}_t \leftarrow \boldsymbol{\theta}_{t-1} - \eta_t \left(\alpha \hat{\boldsymbol{m}}_t / (\sqrt{\hat{\boldsymbol{v}}_t} + \epsilon) \; +\lambda\boldsymbol{\theta}_{t-1} \right)$
until *stopping criterion is met*
return optimized parameters $\boldsymbol{\theta}_t$

Loshchilov, I. "Decoupled weight decay regularization." *arXiv preprint arXiv:1711.05101* (2017).

Future Work

“BNL | QPress Cluster Tool.” Bnl.gov, 2024, www.bnl.gov/qpress/modules/cluster-tool.php. Accessed 8 Dec. 2024.

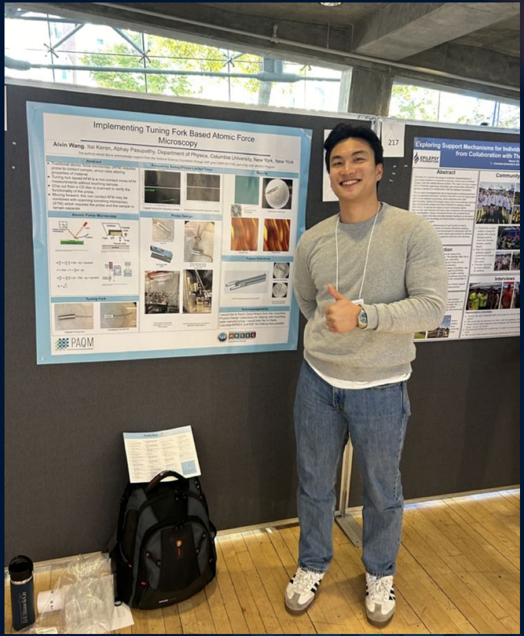
Our Futures

R&D

Boster, Seth. “Smokejumping, Other Outdoor Extremes Shape Life of Colorado Woman.” *Colorado Springs Gazette*, 25 Apr. 2022, gazette.com/premium/smokejumping-other-outdoor-extremes-shape-life-of-colorado-woman/article_55b68c42-bc07-11ec-8b01-c3ddee3115f4.html.

COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK

DEPARTMENT OF PHYSICS



References

1. *Condensed Matter Physics | Department of Physics*, www.physics.columbia.edu/content/condensed-matter-physics. Accessed 7 Dec. 2024.
2. Lloyd-Hughes, James & Jeon, Tae-In. (2012). A Review of the Terahertz Conductivity of Bulk and Nano-Materials. J Infrared Milli Terahz Waves. 33. 871. 10.1007/s10762-012-9905-y.
3. MacDonald, A., Bistritzer, R. Graphene moiré mystery solved?. *Nature* 474, 453–454 (2011). https://doi.org/10.1038/474453a
4. Maruf, H M & Islam, Md. Rafiqul & Chowdhury, F.-U.-Z. (2018). ANALOGY BETWEEN AC JOSEPHSON JUNCTION EFFECTS AND OPTICAL PHENOMENA IN SUPERCONDUCTORS. 105-113.
5. BEIJING IWHR CORPORATION. “Spillway Crest Gates: Controlling Water Flow in Dam Structures.” BEIJING IWHR CORPORATION, 2024, www.bic-iwhr.com/news/spillway-crest-gates-controlling-water-flow-in-dam-structures.html. Accessed 8 Dec. 2024.
6. Nanoscience Instruments. “Scanning Tunneling Microscopy - Nanoscience Instruments.” Nanoscience Instruments, 2018, www.nanoscience.com/techniques/scanning-tunneling-microscopy/.
7. Yamada, Yuya, et al. “Fundamental and Higher Eigenmodes of QPlus Sensors with a Long Probe for Vertical-Lateral Bimodal Atomic Force Microscopy.” Nanoscale Advances, vol. 5, no. 3, 26 Dec. 2022, pp. 840–850, pubs.rsc.org/en/content/articlehtml/2023/na/d2na00686c, https://doi.org/10.1039/d2na00686c. Accessed 8 Dec. 2024.
8. Geim, A. K., and I. V. Grigorieva. “Van Der Waals Heterostructures.” Nature, vol. 499, no. 7459, 1 July 2013, pp. 419–425, www.nature.com/articles/nature12385, https://doi.org/10.1038/nature12385.

References

9. Askari, Syed Sajjad. “Alex-Net Explanation and Implementation in Tensorflow and Keras.” *Medium*, Medium, 14 Jan. 2023, medium.com/@syedsajjad62/alex-net-explanation-and-implementation-in-tensorflow-and-keras-8047efeb7a0f.
10. Sanderson, Grant. “But What is a Convolution?” *Youtube*, 3blue1brown, 29 Dec. 2023, https://www.youtube.com/shorts/kpG7I2MOcnI.
11. Ave Coders. “101 Concepts of Data Science and Machine Learning” *Youtube*, AveCoders, 28 May. 2024, https://www.youtube.com/shorts/ykt5PUxs3z8.
12. Chima, Precious. “Activation Functions: ReLU & Softmax.” *Medium*, Medium, 5 Apr. 2020, https://medium.com/@preshchima/activation-functions-relu-softmax-87145bf39288.
13. Alexander, Giffah. “Softmax Activation function explained” *Youtube*, Giffah_Alexander, 22 Oct. 2024, https://www.youtube.com/shorts/SrJN_hpiuAs.
14. Sigmoid function. “Sigmoid function.” *Wikipedia*, Wikipedia, 14 Nov. 2024, https://en.wikipedia.org/wiki/Sigmoid_function.
15. Krizhevsky, Alex, Ilya Sutskever, and Geoffrey E. Hinton. "ImageNet Classification with Deep Convolutional Neural Networks."
16. Ioffe, Sergey. "Batch normalization: Accelerating deep network training by reducing internal covariate shift." *arXiv preprint arXiv:1502.03167* (2015).

References

17. Kingma, Diederik P. "Adam: A method for stochastic optimization." *arXiv preprint arXiv:1412.6980* (2014).
18. Gabbard & Miller. “Machine Learning from Scratch: Stochastic Gradient Descent and Adam Optimizer.” *18.0851 Project*, accessed 17 November 2024, https://www.mit.edu/~jgabbard/assets/18085_Project_final.pdf .
19. Sahilcarterr. “Mathematics Behind Simple Linear Regression using Gradient Descent.” *Medium*, Medium, 5 Apr. 2020, https://medium.com/@sahilcarterr/mathematics-behind-simple-linear-regression-using-gradient-descent-a09595bf701d.
20. Bangar, Siddhesh. “VGG-Net Architecture Explained.” *Medium*, Medium, 28 Jun. 2022, https://medium.com/@siddheshb008/vgg-net-architecture-explained-71179310050f.
21. Simonyan, Karen, and Andrew Zisserman. "Very deep convolutional networks for large-scale image recognition." *arXiv preprint arXiv:1409.1556* (2014).
22. He, Kaiming, et al. "Deep residual learning for image recognition." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.
23. Tan, Mingxing, and Quoc Le. "Efficientnet: Rethinking model scaling for convolutional neural networks." *International conference on machine learning*. PMLR, 2019.
24. Hien, Ngo Le Huy. “Grid Search space Illustration” *ResearchGate*, ResearchGate, https://www.researchgate.net/figure/Grid-Search-space-illustration_fig9_346571789.
25. Sandler, Mark, et al. "Mobilenetv2: Inverted residuals and linear bottlenecks." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2018.

References

26. Neural Computing and Applications. “Graph for ReLU6 activation function” *ResearchGate*, ResearchGate, https://www.researchgate.net/figure/Grid-Search-space-illustration_fig9_346571789.
27. Derevianko, Ivan. “BLAZOR - IT’S TIME TO FORGET JAVASCRIPT” *Ivan Derevianko*, Ivan Derevianko, 16 July 2019, https://ivanderevianko.com/2019/07/blazor-its-time-to-forget-javascript.
28. Szegedy, Christian, et al. "Rethinking the inception architecture for computer vision." *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2016.
29. Pytorch. “Vision/Torchvision/Models/Alexnet.Py at Main · Pytorch/Vision.” *GitHub*, github.com/pytorch/vision/blob/main/torchvision/models/alexnet.py. Accessed 20 Nov. 2024.
30. Pytorch. “Vision/Torchvision/Models/ResNet.Py at Main · Pytorch/Vision.” *GitHub*, https://github.com/pytorch/vision/blob/main/torchvision/models/resnet.py. Accessed 20 Nov. 2024.
31. Pytorch. “Vision/Torchvision/Models/VGG.Py at Main · Pytorch/Vision.” *GitHub*, https://github.com/pytorch/vision/blob/main/torchvision/models/vgg.py. Accessed 20 Nov. 2024.
32. Nvidia. “DeepLearningExamples/Pytorch/Classification/Convnets/Efficientnet at Master · Nvidia/Deeplearningexamples.” *GitHub*, github.com/NVIDIA/DeepLearningExamples/tree/master/PyTorch/Classification/ConvNets/efficientnet. Accessed 20 Nov. 2024.
33. Pytorch. “Vision/Torchvision/Models/Inception.Py at Main · Pytorch/Vision.” *GitHub*, https://github.com/pytorch/vision/blob/main/torchvision/models/inception.py. Accessed 20 Nov. 2024.
34. “BNL | QPress Cluster Tool.” Bnl.gov, 2024, www.bnl.gov/qpress/modules/cluster-tool.php. Accessed 8 Dec. 2024.

References

35. Boster, Seth. “Smokejumping, Other Outdoor Extremes Shape Life of Colorado Woman.” *Colorado Springs Gazette*, 25 Apr. 2022, gazette.com/premium/smokejumping-other-outdoor-extremes-shape-life-of-colorado-woman/article_55b68c42-bc07-11ec-8b01-c3ddee3115f4.html.
36. jodag. “How Is Pytorch’s Class BCEWITHLOGITSLOSS Exactly Implemented?” *Stack Overflow*, 11 July 2022, stackoverflow.com/questions/66906884/how-is-pytorchs-class-bcewithlogitsloss-exactly-implemented.
37. Loshchilov, I. "Decoupled weight decay regularization." *arXiv preprint arXiv:1711.05101* (2017).