Building AI Models to Improve Medical Diagnosis

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Motivation

Main Problem

"About 12 million people in the U.S. are misdiagnosed in outpatient care every year." - Harvard School of Public Health

AI as a promising solution to misdiagnoses

Convolutional Neural Network performed better at detecting melanomas in comparison to 58 dermatologists from 17 countries (The International Oncology Network, 2018)

Today's talk

- Heart Disease Diagnosis AI and Medical Imaging Interpreter
  - Mathematical Algorithms
  - Results
- Contribution
  - First model outperformed some other algorithms at detecting absence of heart disease
  - Second model achieved 94.55% accuracy in detecting meningioma tumors. The second best method got an accuracy of 85.64%.

First Model: Heart Disease Diagnosis

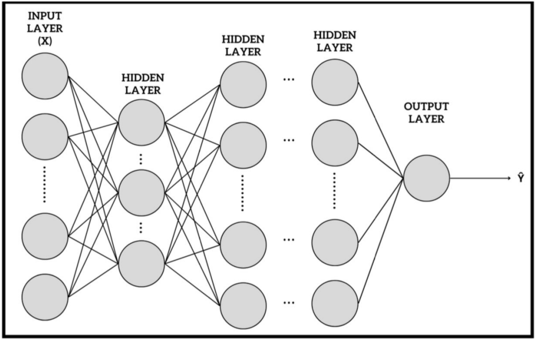


Figure 1: *Simplification of the Neural Network Architecture*

Initial Layers

Input Layer: Cardiovascular Risk Factors and Indicators

Columns: # of samples; Rows: # of features (symptoms)

$$X^{[0]} = \begin{pmatrix} x_{1,1} & \cdots & x_{1,237} \\ x_{2,1} & \cdots & x_{2,237} \\ \cdots & \ddots & \cdots \\ x_{13,1} & \cdots & x_{13,237} \end{pmatrix}$$

First Hidden Layer Calculation:

$$Z^{[1]} = W^{[1]}X^{[0]} + B^{[1]}$$

- $Z^{[n]}$: Matrix representation of the n layer
- $W^{[n]}$: Randomly initialized weights matrix
- $B^{[n]}$: Randomly initialized bias matrix

Sample Information to Matrix | Matrices Dimensionalities

Forward Propagation

1) $Z^{[1]} = W^{[1]}X^{[0]} + B^{[1]} :=$ Layer 1

2) $ReLU(x) = \begin{cases} x & \text{if } x > 0 \\ 0 & \text{if } x \leq 0 \end{cases}$

3) $A^{[1]} = ReLU(Z^{[1]})$

4) $Z^{[2]} = W^{[2]}A^{[1]} + B^{[2]} :=$ Layer 2

5) Process is repeated until reaching the output layer composed of one neuron

6) $Sigmoid(z) = \frac{1}{1+e^{-z}}, D : (-\infty, \infty), R : (0, 1)$

7) Binary Classifications: $\hat{Y} = \begin{cases} 1 & \text{if } Sigmoid(z) \geq 0.5 \\ 0 & \text{if } Sigmoid(z) < 0.5 \end{cases}$

Backpropagation

Loss Function: Binary Cross Entropy Loss

$$BCE = -\frac{1}{N}\sum_{i=0}^{N}[y_i log(\hat{y}_i) + (1 - y_i) log(1 - \hat{y}_i)]$$

- y_i: Actual target (0 or 1)
- $\hat{y}_i$: Predicted probability of the target (not yet rounded, that is just the $Sigmoid(z)$ of the last layer)
- N: # Samples fed to the model at a time

- We have to sufficiently minimize the loss function. Let's use partial derivates and the chain rule to do it.

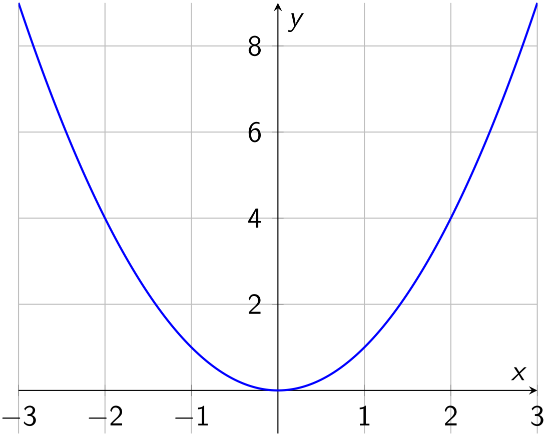
$$\frac{\partial BCE}{\partial W} = \frac{\partial BCE}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial Z} \cdot \frac{\partial Z}{\partial W}$$
$$\frac{\partial BCE}{\partial B} = \frac{\partial BCE}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial Z} \cdot \frac{\partial Z}{\partial B}$$

- We can update the weights' and bias' parameters to make the loss get closer to zero. (This happens in every layer from the end to the beginning)

$$\text{New } W^{[5]}_{numbers} = W^{[5]}_{numbers} - \alpha \frac{\partial BCE}{\partial W^{[5]}_{variables}}(W^{[5]}_{numbers})$$
$$\text{New } B^{[5]}_{numbers} = B^{[5]}_{numbers} - \alpha \frac{\partial BCE}{\partial B^{[5]}_{variables}}(B^{[5]}_{numbers})$$

Note: One random sample is loaded at a time (SGD).
Definition: An epoch is when all the samples in the training dataset have gone through the model.

Gradient Descent Intuition



Determination of Number of Epochs

Accuracy Analysis

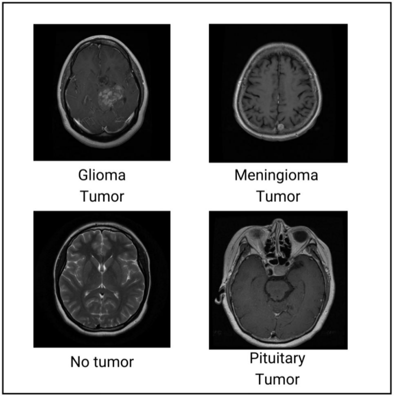
$$VD_{acc,n} = \frac{PTE_n}{TT_{VD}} \cdot 100$$
$$95\%\ \text{CI Margin}_n = \left(196\sqrt{\frac{VD_{acc,n}(1-VD_{acc,n})}{N}}\right)$$

- PTE_n = Correct Predicted Targets after the Epoch n
- $VD_{acc,n}$ = Validation Data Accuracy
- TT_{VD} = Total Targets in the Validation Dataset (same as # samples in VD)

Note: The data was standarized but regarding their corresponding feature and the dataset was split in three: X_{test}, X_{train}, and X_{val}

Second Model: Medical Imaging Interpreter

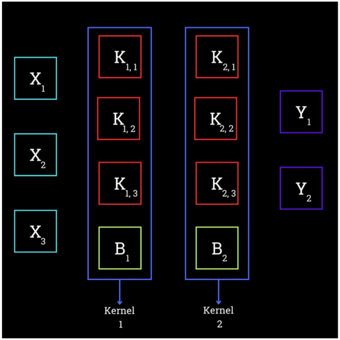
Four classes:



Convolutional Neural Network (CNN)

Convolutional Layer

Example:



Valid Cross-Correlation

$$Y_1 = B_1 + X_1 \star K_{1,2} + X_2 \star K_{1,2} + X_3 \star K_{1,3}$$

$$Y_2 = B_2 + X_1 \star K_{2,1} + X_2 \star K_{2,2} + X_3 \star K_{2,3}$$

In general,

$$Y_1 = B_1 + X_1 \star K_{1,2} + X_2 \star K_{1,2} + \cdots + X_n \star K_{1,n}$$

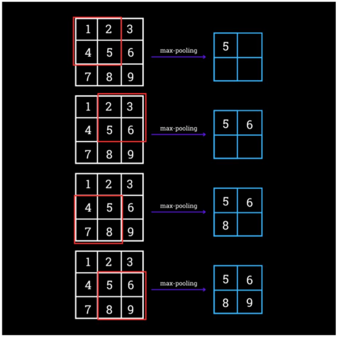
$$Y_2 = B_2 + X_1 \star K_{2,1} + X_2 \star K_{2,2} + \cdots + X_n \star K_{1,n}$$

$$\cdots$$

$$Y_d = B_d + X_1 \star K_{d,1} + X_2 \star K_{d,2} + \cdots + X_n \star K_{d,n}$$

Other types of layers used

Max-pooling:



Average-pooling: Same process as max-pooling but computing the average

Backpropagation

One Hot Encoding:

- glioma_tumor: [1,0,0,0]
- meningioma_tumor: [0,1,0,0]
- no_tumor: [0,0,1,0]
- pituitary_tumor: [0,0,0,1]

Cross Entropy Loss:

$$CEL = -\left(\frac{1}{n}\right) \sum_{i=1}^{n} \sum_{j=1}^{c} (y\_true_{i,j}) log(y\_pred_{i,j})$$

- n = Number of samples in the batch
- i = index of the sample (ranges from 1 to 16)
- j = index of possible labels (ranges from 1 to 4)
- $y\_true_{i,j}$ = true label for sample i and label j
- $y\_pred_{i,j}$ = predicted probability for sample i and label j

The parameters' updates of the outer layer would look like this (slightly modified because of momentum):

$$K_{i,j}{}^{(3)}_{numbers} \leftarrow K_{i,j}{}^{(3)}_{numbers} - \alpha \frac{\partial L}{\partial K_{i,j}{}^{(3)}_{variables}} (K_{i,j}{}^{(3)}_{numbers})$$
$$B_{i,j}{}^{(3)}_{numbers} \leftarrow B_{i,j}{}^{(3)}_{numbers} - \alpha \frac{\partial L}{\partial B_{i,j}{}^{(3)}_{variables}} (B_{i,j}{}^{(3)}_{numbers})$$

In order to change the parameters for hidden layers, keep in mind that $Y^{(2)} = X^{(3)}$.

$$\frac{\partial L}{\partial K_{i,j}^{(2)}} = X_j^{(2)} \star \frac{\partial L}{\partial Y_i^{(2)}} = X_j^{(2)} \star \frac{\partial L}{\partial X_i^{(3)}}$$
$$\frac{\partial L}{\partial B_i^{(2)}} = \frac{\partial L}{\partial Y_i^{(2)}} = \frac{\partial L}{\partial X_j^{(3)}}$$

The same algorithm can be used to find the partials of the other hidden layers and update those parameters.

What's momentum?

$$V_t = \beta V_{t-1} + \alpha \nabla_{w_t} L(W_t, X, y)\ ,\ \ W_{t+1} = W_t - V_t$$

- $\nabla_{w_t} L(W_t, X, y)$:Gradient of the Loss Function w.r.t a learnable parameter (will be applied to all contained in the model)
- α: Learning rate
- V_t: Velocity at time step t
- W_t: A model parameter at time step t
- β: Momentum coefficient

Note: V_{t-1} is initialized as $V_0 = 0$. Accelerates convergence.

Both models' specific details

Note:

$$ReLU(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases}, \quad ReLU'(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ 1 & \text{if } x > 0 \end{cases}$$

<u>Workflows</u>:

First Model:

- Layers' output neurons:
  - First (after the input layer): 360
  - Second: 180
  - Third: 90
  - Fourth: 45
  - Fifth (last): 1
- Activation functions: ReLU, Sigmoid (end)
- Learning Rate: 0.01
- Loss: BCE
- Optimization Algorithm: SGD
- # Epochs: 482

Second Model:

1. Conv. Layer: 16 kernels with K matrices of shape 3x3; ReLU; Batch Normalization, Max-pooling
2. The same process is repeated but now the inputs are the results obtained.
3. After that, the same happens with the additional step of average pooling.
4. Then, all the information is converted into a matrix where each row is a sample, and each column the information extracted per sample.
5. Standard Feedforward Neural Network: first layer with 120 neurons, ReLU, Second Layer with 84 neurons, ReLu, output layer with 4 neurons. Output Layer: 16x4 matrix where each row is a sample and each column the predicted probability for the classes.

Second model details

- Learning rate: 0.01
- Momentum coefficient: 0.9
- Batch Normalization: Each batch of size 16 is fed to the network

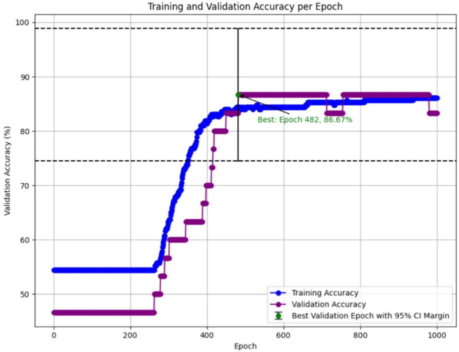
$$\hat{x} = \frac{x - \bar{x}}{\sqrt{V(x) + 10^{-5}}}, \quad y = \gamma \hat{x} + \beta$$

where γ and β are learnable parameters

Results

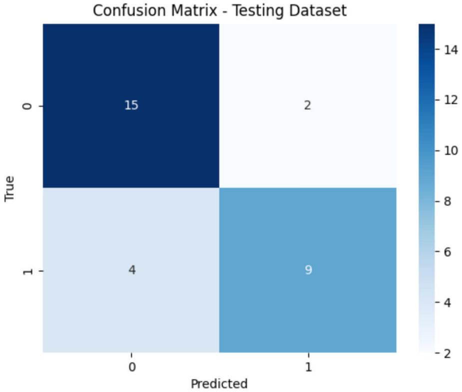
First Model: Heart Disease Diagnosis AI

Epoch selection



Data Sizes:
Training: 237 (79.8%)
Validation: 30 (10.1%)
Testing: 30 (10.1%)
Validation Accuracy: 86.67%

Confusion Matrix for First Model (Testing Dataset)



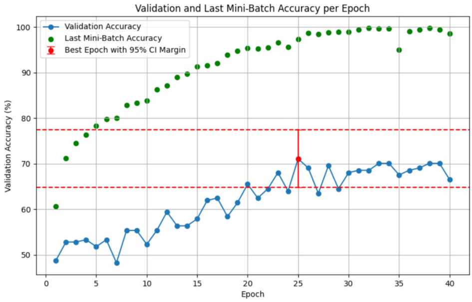
Note: 0 indicates absence and 1 presence.

- Overall Accuracy: 80%
- Absence: 88.2%
- Presence: 69.2%

Results

Second Model: Medical Imaging Interpreter AI

Epoch selection



Data Sizes:
Training: 2870 (87.92%)
Validation: 197 (6.03%)
Testing: 197 (6.03%)
Validation Accuracy: 70.56%

Confusion Matrix for Second Model (Testing Dataset)

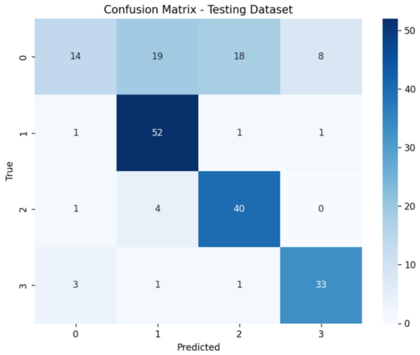


Figure: 0 represents Glioma Tumor, 1 Meningioma Tumor, 2 No Tumor, and 3 Pituitary Tumor

- Overall Accuracy: 71.07%
- Meningioma: 94.55%
- No Tumor: 88.89%
- Pituitary: 86.8%
- Glioma: 23.7%

Discussion and Conclusion

- **First Model:** The meaningful contribution of the model is that it outperforms other proposed machine learning algorithms published from the scientific community at detecting absence (Nashif, Raihan, Islam, & Imam, 2018) such as an artificial neural network by 24.78% and a Naive Bayes algorithm by 5.32%.
- **Second Model:** For the four-class classification task, the model achieves 94.55% accuracy in detecting meningioma tumors. As a reference, the second-best method (Google Vision Transformer) from recent machine learning research projects in the community acquired a 85.64% accuracy for the same task.

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Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.
Research Mentors: Peter Mucha and Rebecca Hardenbrook

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Appendix Slides - Matrix presentation of sample information

Consider 237 samples as vectors (there are 13 features per each):

$$\begin{aligned}
s_1 &= < v_{1,1}, v_{1,2}, \ldots, v_{1,13} > \\
s_2 &= < v_{2,1}, v_{2,2}, \ldots, v_{2,13} > \\
&\ldots \\
s_{237} &= < v_{237,1}, v_{237,2}, \ldots, v_{237,13} >
\end{aligned}$$

Each node in the input layer represents the data per feature:

$$\begin{aligned}
x_1 &= < v_{1,1}, v_{2,1}, \ldots, v_{237,1} > \\
x_2 &= < v_{1,2}, v_{2,2}, \ldots, v_{237,2} > \\
&\ldots \\
x_{13} &= < v_{1,13}, v_{2,13}, \ldots, v_{237,13} >
\end{aligned}$$

Appendix Slides - Matrix dimensionalities

Note:

- # Rows in weights', bias matrix, and z matrix: # Neurons in the layer
- # Cols in weights' matrix: # Neurons in the previous layer.
- # Cols in the z matrix and 1's matrix: # Samples in the previous layer

$$\begin{bmatrix} z_{1,1} & \cdots & z_{1,237} \\ z_{2,1} & \cdots & z_{2,237} \\ \vdots & \ddots & \vdots \\ z_{360,1} & \cdots & z_{360,237} \end{bmatrix} = \begin{bmatrix} w_{1,1} & \cdots & w_{1,13} \\ w_{2,1} & \cdots & w_{2,13} \\ \vdots & \ddots & \vdots \\ w_{360,1} & \cdots & w_{360,13} \end{bmatrix} \begin{bmatrix} x_{1,1} & \cdots & x_{1,237} \\ x_{2,1} & \cdots & x_{2,237} \\ \vdots & \ddots & \vdots \\ x_{13,1} & \cdots & x_{13,237} \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_{360} \end{bmatrix} \begin{bmatrix} 1_1 & 1_2 & \dots & 1_{237} \end{bmatrix}$$

Further Reading

- **Complete Research Paper:** Daza Vigo, E. S. (2023). *Machine Learning Approaches for Precision Medicine*. Retrieved from `https://www.researchgate.net/publication/383692584_Machine_Learning_Approaches_for_Precision_Medicine`

You can also scan the QR code to access the paper.