Machine Learning

Model Evaluation

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Model Evaluation: Outline

- Need of Model Evaluation
- Loss Function
- Regularization: Controlling the Learning Process
- Apply Regularization to Learning Models
- Model Evaluation
    - Underfitting,
    - Overfitting,
    - Lasso regularization,
    - Ridge regularization,
    - Elastic Net regularization.

Model Evaluation: Why Model Evaluation is Important

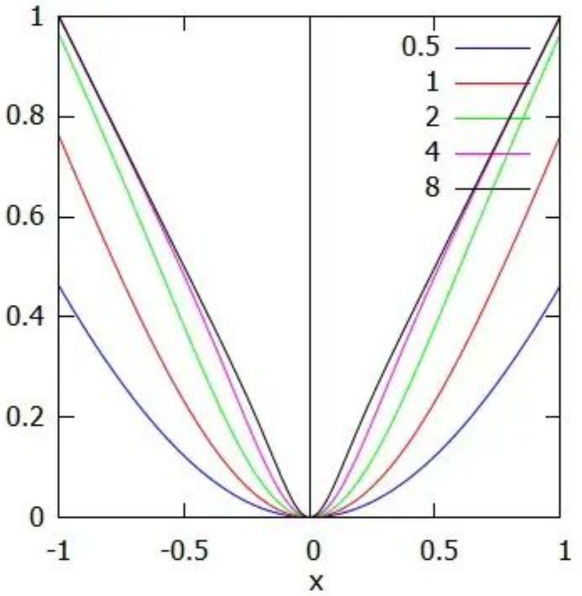
- Need of Model evaluation
    - It is important to assess the efficacy of a model during initial research phases, and
    - It also plays a role in model monitoring.
    - Before deploying your ML model, it is essential to evaluate its performance on real-world data.
    - If your model is trained on a clean dataset,
        - it is important to generate a dataset that simulates real-world data as closely as possible.
- Objectives
    - To understand the concept of overfitting and how regularization helps in reducing overfitting.
    - To understand if your model(s) is working well with new data, you can leverage a # of evaluation metrics.
    - To minimize an error function (loss function) or
    - To maximize the efficiency of production using Optimizers algorithms.

Model Evaluation: Loss function

- **LF** along with **optimization functions** are directly responsible for f**itting the model** to the given training data.
- Learning Objectives:
  - how loss functions are used in neural networks,
  - know different types of loss functions,
  - writing custom loss functions in TensorFlow, and
  - practical implementations of loss functions to process image/video training data
- NN processes the input data at each layer and eventually produces a predicted output value $\hat{y} = AF(X' W + b)$
- To training process makes the model maps the relationship between the training data and the outputs.
- To satisfy the equation $\hat{y} = AF(X' W + b)$, in this training process, the NN updates its **hyperparameters:**
  - W – weights
  - b – biases

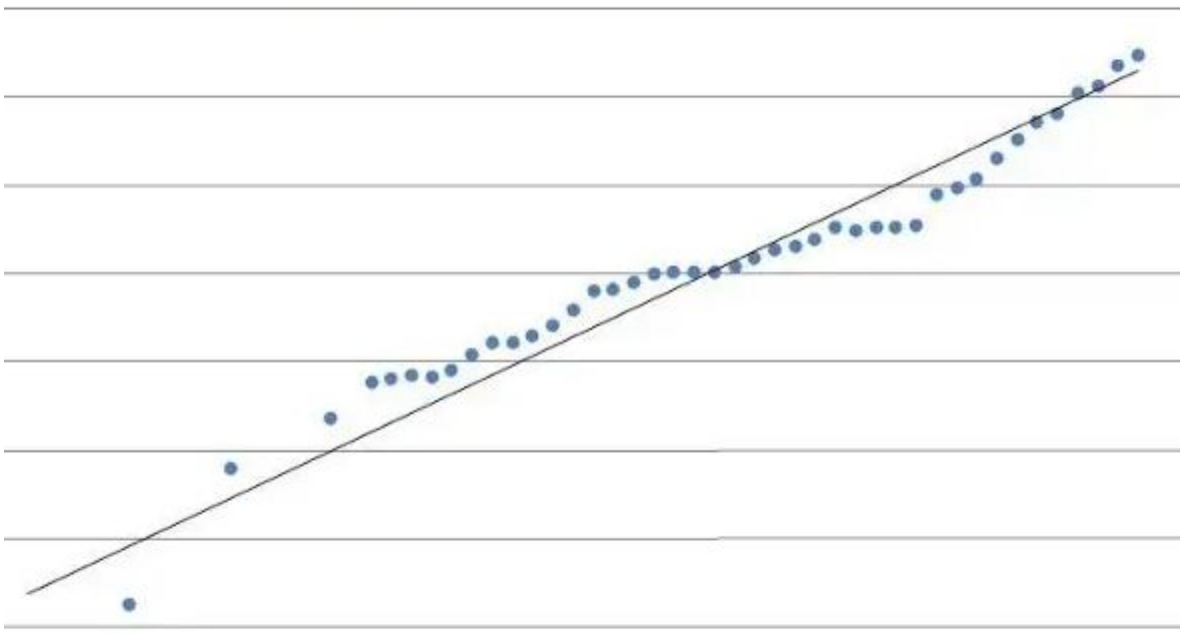
Model Evaluation: Loss function

- Each training input is loaded into the NN in a process called **forward propagation**.
- Once model produces o/p (predicted o/p) is compared against given target o/p in a process called **backpropagation**
- In **backpropagation** process, **hyperparameters** of model are then
  - adjusted to **minimize** (error=predicted-target) output
- This is where loss functions come in.
- A **loss function**
  - compares the target (y) and predicted (ŷ) output values;
  - measures how well the NN models the training data
- When training,
  - we aim to **minimize** this loss bet.ŷ and y
- The hyperparameters are adjusted to minimize the average loss
  - we find w and b, that minimize the value of J (average loss)



Model Evaluation: Loss function

- Loss function is akin to residuals, in statistics.
- Residuals measure the distance of the actual y values from the **regression line** (predicted values)
  - the goal being to minimize the net distance



Model Evaluation: Loss function

- Easy to demonstrate how loss functions are used in models.
  - Using Google's TensorFlow library to implement different loss functions
- In TensorFlow, the LF is specified as a parameter in **model.compile()**
  - This method trains the neural network eg. **model.compile(loss='mse', optimizer='sgd')**
- LF can be inputted either as
  - a String — as shown above — or
  - as a function object — either imported from TensorFlow or written as custom loss functions
  - eg. **from tensorflow.keras.losses import mean_squared_error**
  - **model.compile(loss=mean_squared_error, optimizer='sgd')**
- All loss functions in TensorFlow have a similar structure:
  - def loss_function (y_true, y_pred): return losses
- The **model.compile()** method expects only two input parameters for the loss attribute i.e y_true and y_pred

Model Evaluation: Types of Loss function

- **Regression Loss Functions** — used in regression neural networks;
  - given an input value, the model predicts a corresponding output value (rather than pre-selected labels);
  - Ex. Mean Squared Error, Mean Absolute Error
- **Classification Loss Functions** — used in classification neural networks;
  - given an input, the NN produces a vector of probabilities of the input belonging to various pre-set categories
  - can then select the category with the highest probability of belonging;
  - Ex. Binary Cross-Entropy, Categorical Cross-Entropy
- Loss function in Machine Learning / Deep Learning
- 1. Regression: MSE(Mean Squared Error), MAE(Mean Absolute Error), Huber loss
- 2. Classification: Binary cross-entropy, Categorical cross-entropy
- 3. AutoEncoder: KL Divergence
- 4. GAN: Discriminator loss, Minmax GAN loss

Model Evaluation: Loss function

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y^{(i)} - \hat{y}^{(i)})^2$$

```
def mse (y_true, y_pred):
    return tf.square (y_true - y_pred)
```

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y^{(i)} - \hat{y}^{(i)}|$$

```
def mae (y_true, y_pred):
    return tf.abs(y_true - y_pred)
```

$$CE\ Loss = -\frac{1}{n}\sum_{i=1}^{N}\sum_{j=1}^{M} y_{ij} \cdot log(p_{ij})$$

Binary cross-entropy is a special case of categorical cross-entropy (above), where M = 2 (the number of categories)

$$Huber\ Loss = \begin{cases} \frac{1}{n}\sum_{i=1}^{n}(y^{(i)} - \hat{y}^{(i)})^2 & |y^{(i)} - \hat{y}^{(i)}| \leq \delta \\ \frac{1}{n}\sum_{i=1}^{n}\delta(|y^{(i)} - \hat{y}^{(i)}| - \frac{1}{2}\delta) & |y^{(i)} - \hat{y}^{(i)}| > \delta \end{cases}$$

```
def huber_loss_with_threshold (t = δ):
    def huber_loss (y_true, y_pred):
        error = y_true - y_pred
        within_threshold = tf.abs(error) <= t
        small_error = tf.square(error)
        large_error = t * (tf.abs(error) - (0.5*t))
        if within_threshold:
            return small_error
        else:
            return large_error
    return huber_loss
```

$$CE\ Loss = \frac{1}{n}\sum_{i=1}^{N} -(y_i \cdot log(p_i) + (1 - y_i) \cdot log(1 - p_i))$$

```
def log_loss (y_true, y_pred):
    y_pred = tf.clip_by_value(y_pred, le-7, 1 - le-7)
    error = y_true * tf.log(y_pred + 1e-7) (1-y_true) * tf.log(1-
y_pred + 1e-7)
    return -error
```

Model Evaluation: What is Regularization?

- Model evaluation
  - Process of using different evaluation metrics to understand performance (strengths and weaknesses) of model
  - Assess the efficacy of a model during initial research phases, and it also plays a role in model monitoring.
- Regularization
  - Process of limiting (controlling) the learning process during training of a model
  - by adding another term to the loss (cost) function (trying to minimize).
    - Objective function $(\theta) = L(\theta) + \Omega(\theta)$
    - $L(\theta)$ is loss function
    - $\Omega(\theta)$ is regularization term
  - The main benefit of regularization is to mitigate overfitting.
  - Regularized models are able to generalize well on the unseen data.
  - A complex NN makes training model more prone to overfitting.
  - Regularization makes slight modifications to the learning algorithm such that the model generalizes better.

Model Evaluation: What is Regularization?

- Two ways to apply regularization to learning models:
- By adding another term to the loss function
  - We are trying to minimize
  - The objective function consists of two parts: loss function and regularization term:
    - Objective function $(\theta) = L(\theta) + \Omega(\theta)$
    - $L(\theta)$ is loss function
    - $\Omega(\theta)$ is regularization term
- By early stopping the learning process
  - during the training phase
  - The perfect example of this method is stopping the growth of a decision tree at an early stage.

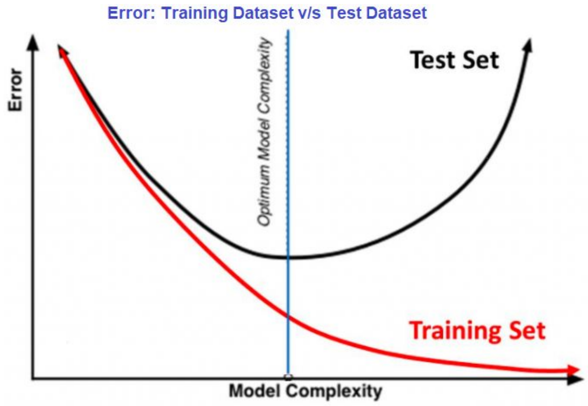
Model Evaluation: What is Regularization?

- Performing L2 regularization encourages the weight values towards zero (but not exactly zero)
- Performing L1 regularization encourages the weight values to be zero
- Intuitively speaking smaller weights reduce the impact of the hidden neurons.
- Less complex models typically avoid modeling noise in the data, and therefore, there is no overfitting.
- When choosing the regularization term α.
- The goal is to strike the right balance between low complexity of the model and accuracy
- If your alpha value is too high, your model will be simple, but you run the risk of underfitting your data.
- Your model won't learn enough about the training data to make useful predictions.
- If α value is too low, your model will be more complex, and you run the risk of overfitting your data.
- Your model will learn **too much** about the particularities of the training data, and
    - won't be able to generalize to new data.

Model Evaluation: What is Regularization?

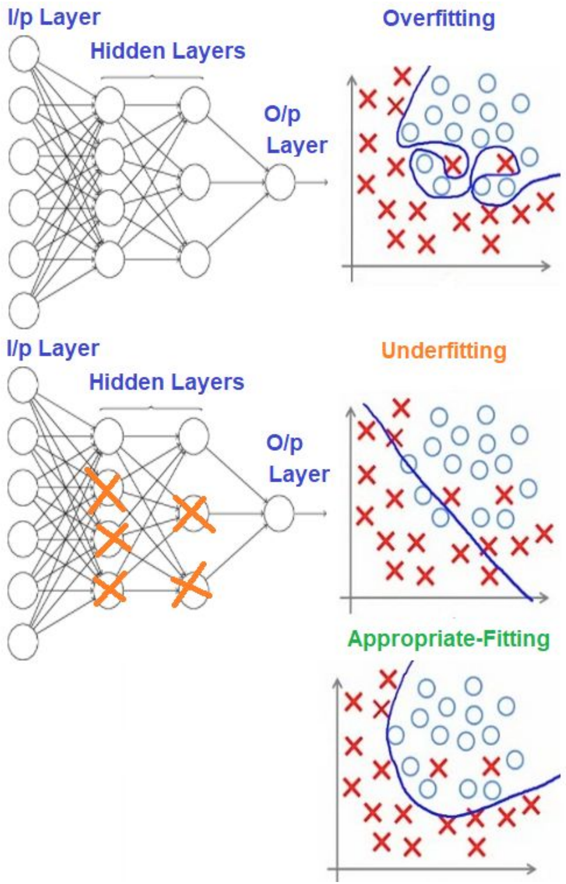
- As we move towards the right in this image our model tries to learn too well the details and
- the noise from the training data, which ultimately results in poor performance on the unseen data.

- While going towards the right
  - Complexity of the model increases such that the training error reduces but the testing error doesn't.



Model Evaluation: Regularization

- How does Regularization help reduce Overfitting?
- NN which is overfitting on the training data (TD) as shown (top)
- In ML, Regularization penalizes the coefficients
- In DL, it actually penalizes the weight matrices of the nodes.
- Assume that our regularization coefficient is so high
    - that some of the weight matrices are nearly equal to zero.
- It result in a much simpler linear NN & slight underfitting of TD (middle)
- Such a large value of the regularization coefficient is not that useful
- We need to **optimize** the value of regularization coefficient in order to obtain a well-fitted model as shown (bottom)



Model Evaluation: Regularization Techniques

- Different techniques in order to apply regularization in learning for reducing overfitting
  - Ridge (apply L2 regularization)
  - Lasso (apply L1 regularization)
  - Elastic Net (Apply both L1 and L2 regularization)
  - Dropout regularization
  - Data augmentation
  - Early stopping
- What does Regularization achieve?
- Performing L2 regularization encourages the weight values towards zero (but not exactly zero)
- Performing L1 regularization encourages the weight values to be zero
  - Intuitively speaking smaller weights reduce the impact of the hidden neurons.
  - These **hidden neurons become neglectable (dropouts)** and
  - Overall complexity of the neural network gets reduced

Model Evaluation: Regularization Techniques

- **L1 and L2 Regularization** update the general **cost function** by adding another term known as regularization term
  - Cost function = Loss (say, binary cross entropy) + Regularization term
- Due to the addition of this regularization term
  - Values of wt. matrices decrease because it assumes NN with smaller wt. matrices leads to simpler models
  - Therefore, it will also reduce overfitting to quite an extent.
- However, this regularization term differs in L1 and L2
- **L2 regularization:**
  - Lambda is the regularization parameter
  - It is the hyperparameter whose value is optimized for better results.
  - It is also known as weight decay as it forces the weights to decay towards zero (but not exactly zero)
- **L1 regularization:**
  - We penalize the absolute value of the weights
  - Unlike L2, the weights may be reduced to zero here.
  - Hence, it is very useful when we are trying to compress our model.
  - Otherwise, we usually prefer L2 over it

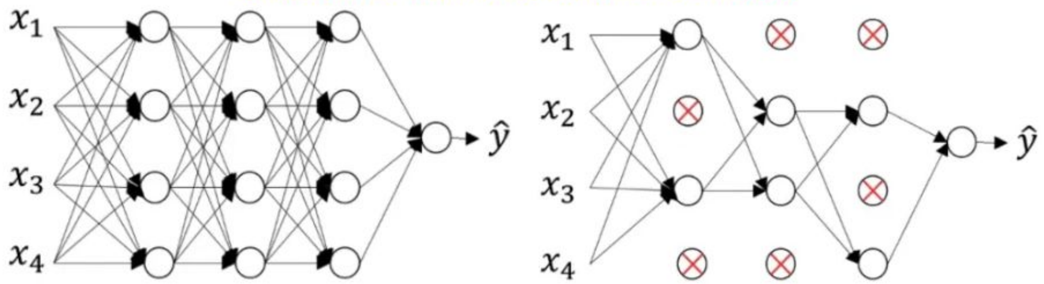
Model Evaluation: Regularization Techniques

- How to apply regularization to any layer in keras
- Sample code to apply L2 regularization to a Dense layer.
  - from keras import regularizers
  - model.add(Dense(64, input_dim=64, kernel_regularizer=regularizers.l2(0.01)
- Note:
  - Here, value of regularization parameter, i.e., lambda = 0.01, which we need to optimize further
  - We can optimize it using the grid-search method.
- Similarly, we can also apply L1 regularization

Model Evaluation: Dropout Regularization

- Dropout Regularization is simple and famous and powerful regularization technique
- Dropout means that with some probability P a neuron of the NN gets turned off **during training** (see figure)
    - Left side of Fig.: Assume we have a feedforward neural network with no dropout
    - Right side of Fig.: Using dropout with say a probability of P=0.5 that a random neuron gets turned off
- Observe that approximately half of the neurons are not active and are not considered as a part of the NN
- Now NN is no more complex rather observe that the NN becomes simpler.
- A simpler version of the NN results in less complexity that can reduce overfitting.
- Deactivation of neurons with a certain probability P is applied at each forward propagation and weight update step.

Neural Network without (left) and with dropout (right)



Model Evaluation: Dropout Regularization

- At every iteration
  - Dropout operation randomly selects few nodes & removes it along with in and outgoing wt. connections
- So each iteration has a different set of nodes and this results in a different set of outputs.
- It can also be thought of as an ensemble technique in machine learning.
- Ensemble models usually perform better than a single model as they capture more randomness.
- Similarly, dropout also performs better than a normal NN model.
- This probability of choosing how many nodes should be dropped is the hyperparameter of the dropout function.
- Dropout can be applied to both the hidden layers as well as the input layers.
- Due to these reasons, dropout is usually preferred when we have a large/complex NN structure
- The probability (say .25) of dropping can decided for tune the model
- We can tune it further for better results using the grid search method.
- In keras, we can implement dropout using the keras core layer.

Model Evaluation: Regularization

- **Data Augmentation**
- The simplest way to reduce overfitting is to increase the size of the training data
- In machine learning, we were not able to increase the size of training data as the labeled data was too costly.
- In case images, there are a few ways of increasing the size (some transformation) of the training data
    - rotating the image, flipping, scaling, shifting, etc.
- This technique of applying transformation is known as data augmentation
- This usually provides a big leap in improving the accuracy of the model
- It can be considered as a mandatory trick in order to improve our predictions.
- In keras, we can perform all of these transformations using ImageDataGenerator.
    - It has a big list of arguments which you you can use to pre-process your training data.

Model Evaluation: Regularization

- **Early stopping**
- If performance on validation set is getting worse, we stop training immediately. This is **known as early stopping**.
- It is a kind of cross-validation strategy where we keep one part of the training set as the validation set
- Stop training at the dotted line since after that our model will start overfitting on the training data.
- In keras, we can apply early stopping using the callbacks function.
  - from keras.callbacks import EarlyStopping
  - EarlyStopping(monitor='val_err', patience=5)
- Here, monitor denotes the quantity that needs to be monitored and ‘val_err’ denotes the validation error.
- Patience denotes the number of epochs with no further improvement after which the training will be stopped
- After the dotted line, each epoch will result in a higher value of validation error.
- So, patience (5 epochs) after the dotted line, our model will stop because no further improvement is seen.
- Note: We need to take extra care while tuning this hyperparameter
  - As after 5 epochs, the model may starts improving again and the validation error starts decreasing as well.

Summary

- Overfitting occurs in more complex neural network models (many layers, many neurons)
- Complexity of the neural network can be reduced by using L1 and L2 regularization as well as dropout
- L1 regularization
  - forces the weight parameters to become zero
- L2 regularization
  - forces the weight parameters towards zero (but never exactly zero)
- Smaller weight parameters make some neurons neglectable → NN becomes less complex → less overfitting
- During dropout
  - Some neurons get deactivated with a random probability P → NN becomes less complex → less overfitting

Model Improvement (Ensemble Learning)

- Refer slide
  - vsat2k_ML_Ch1c Model Improvement (Ensemble Learning) [PDF]

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Thank You.