An Introduction to Multi-label Learning
(ML-KNN & BP-MLL)

Bobby Lumpkin

Overview

1. Introduction to Multi-label Learning
   - Overview and Advantages
2. ML-KNN Approach
   - Model Outline
   - Computing Model Probabilities
   - Implementation (in scikit-multilearn)
3. BP-MLL Approach
   - Feed-forward Neural Networks
   - Neural Network Loss Functions & Training for MLL
   - Implementation (in TensorFlow/Keras)

Introduction to Multi-label Learning

Multi-label Learning

What is it?

→ Multi-label learning (mll) is a form of classification where each instance may be associated with more than one label.

→ Plenty of tasks, such as text categorization, functional genomics, and supervised product recommendation fit naturally into the mll paradigm.

  * **EX:** A news article discussing White House Covid press briefings might belong to each of the categories: "News", "Health" and "Government".

Why use novel approaches?

→ Naive Approach: Train a sequence of independent binary classifiers (one per category)

→ Doesn't capitalize on the information in the correlations between the different labels of each instance.

Multi-label Paradigm: Definitions & Notation

- Let χ denote the domain of instances and $\mathcal{Y} = \{1, ..., Q\}$ be the finite set of labels.
- Given $x \in \chi$ and its associated $Y \subseteq \mathcal{Y}$, let $\vec{y}_x$ be the category vector for x such that (for all $\ell \in \mathcal{Y}$) $\vec{y}_x(\ell) = 1$ if $\ell \in Y$. Otherwise, $\vec{y}_x(\ell) = 0$.

ML-KNN Approach

ML-KNN Algorithm: More Notation

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- Let H_0^ℓ denote the event that test instance t does not have a label ℓ and let H_1^ℓ denote the event that it does have label ℓ.
- Let E_j^ℓ $(j \in \{1, ..., K\})$ denote the event that, among the K nearest neighbors of t, there are exactly j instances which have label ℓ.

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\vec{y}_t(\ell) &= \underset{b \in \{0,1\}}{\operatorname{argmax}} \, \mathbb{P}\left(\mathrm{H}_b^\ell | E^\ell_{\vec{C}_t(\ell)}\right), \quad \ell \in \mathcal{Y} \\
&= \underset{b \in \{0,1\}}{\operatorname{argmax}} \, \frac{\mathbb{P}\left(\mathrm{H}_b^\ell\right) \cdot \mathbb{P}\left(E^\ell_{\vec{C}_{t(\ell)}} | \mathrm{H}_b^\ell\right)}{\mathbb{P}\left(E^\ell_{\vec{C}_t(\ell)}\right)} \\
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\end{aligned}$$

- Where we take a Bayesian approach towards estimating the prior probabilities, $\mathbb{P}\left(\mathrm{H}_b^\ell\right)$, and conditional probabilities, $\mathbb{P}\left(E^\ell_{\vec{C}_{t(\ell)}} | \mathrm{H}_b^\ell\right)$.

ML-KNN Algorithm: Overall Approach continued...

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$\Rightarrow$ Thus, given training data, $\mathcal{X}$, and a test instance, t, we wish to compute $[\vec{y}_t(\ell), \vec{r}_t(\ell)]$.

ML-KNN Algorithm: Computing the Prior Probabilities, $\widehat{\mathbb{P}(\mathrm{H}_b^\ell)}$

We model $\mathbb{P}(\mathrm{H}_1^\ell)$ with a $\mathrm{Beta}(s, s)$ prior and $\mathrm{Binomial}(m,\ \mathbb{P}(\mathrm{H}_1^\ell))$ likelihood. (When $s = 1$, $\mathrm{Beta}(s, s)$ reduces to the uniform distribution on $[0, 1]$.)

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$\Rightarrow$ The posterior distribution for $\mathbb{P}(\mathrm{H}_1^\ell)$ is:

$$\mathrm{Beta}\left(s + \sum_{i=1}^{m} \vec{y}_{x_i}(\ell),\ s + m - \sum_{i=1}^{m} \vec{y}_{x_i}(\ell)\right).$$

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$\Rightarrow$ We will estimate $\mathbb{P}(\mathrm{H}_1^\ell)$ with the expectation of it's posterior Beta distribution:

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where m is the number of training instances.

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(i) Let c be a vector of length $K+1$, where $c(j) =$ the number of training instances where $\vec{C}_{x_i}(\ell) = j$ when $\vec{y}_{x_i}(\ell) = 1$.

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* We use a $\mathrm{Multinomial}(K+1, (\frac{c(0)}{m_1}, ..., \frac{c(K)}{m_1}))$ likelihood, where $m_1 = \sum_{i=1}^m \vec{y}_{x_i}(\ell)$ (analogously for $\overrightarrow{\mathbb{P}(E_j^\ell|\mathrm{H}_0^\ell)}$).

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Using our previous derivation:

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NOTE: The larger the value for s, the less importance assigned to the training data: As $s \to \infty$, $\vec{r}_t(\ell) \to \frac{1}{2}$.

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→ MLkNN() from the scikit-multilearn module can be used to instantiate a ML-KNN object.

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classifier = MLkNN(k=3)

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→ “MLkNN” class methods like “fit()” and “predict()” mirror those for standard scikit-learn objects.

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BP-MLL Approach

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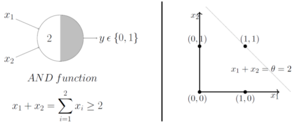

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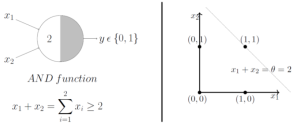

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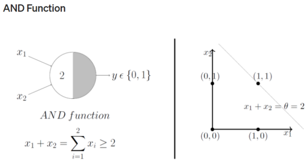

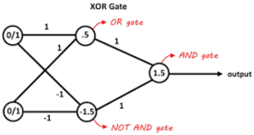

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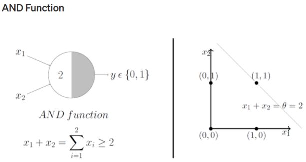
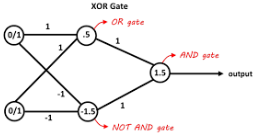
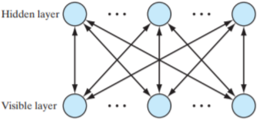
- In the early 1980s, research on neural networks resurged largely due to successful learning algorithms for multi-layer neural networks and are used today for various tasks such as computer vision, associative memory, representation learning, NLP, etc..

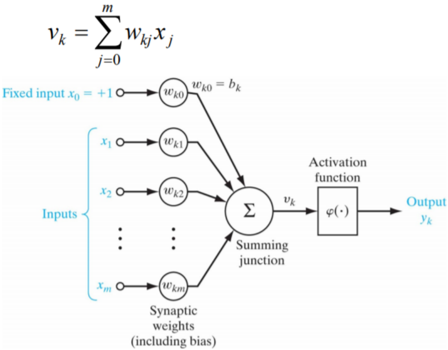






Introduction to Feed-forward Networks: Perceptron Model

The perceptron model (the building block for feed-forward networks) can be viewed as a connected, directed, loop-free graph like the one below.



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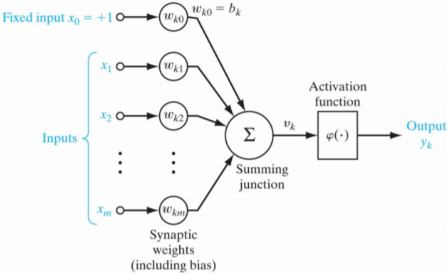

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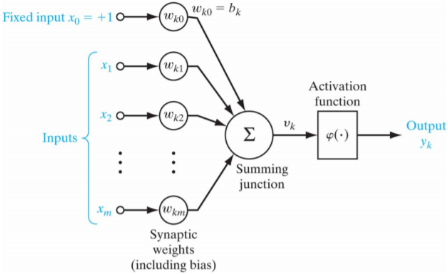

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- Rosenblatt's Perceptron model uses a step function non-linearity, but other common activation functions include the sigmoid function ($\sigma()$), tanh(), ReLU, Leaky ReLU, softmax, etc..

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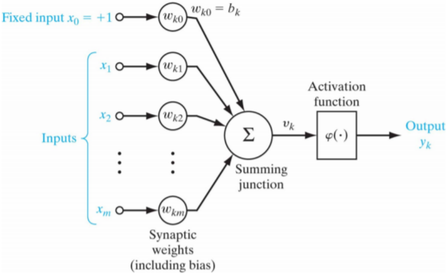
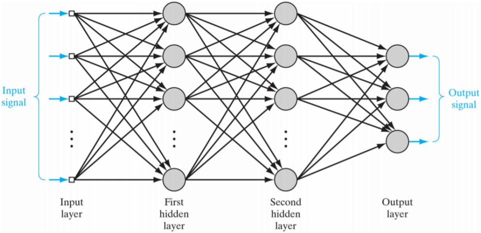


Multilayer Networks & Training

- Adding additional layers and units (like in the network pictured below) significantly expands the class of discrimination problems a network can learn.



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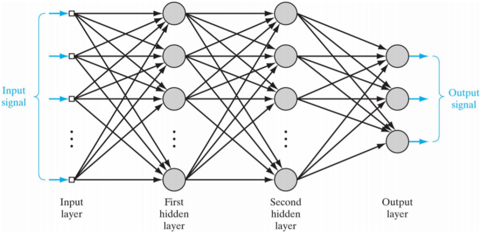

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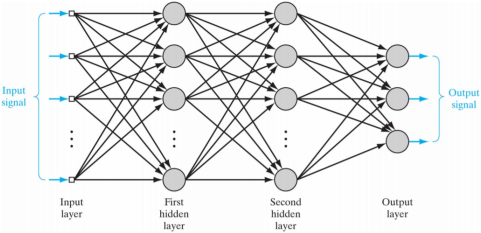
- "Online" training involves evaluating an instance, and updating weights using gradient descent.
- For multi-label learning with Q instances, networks will have Q output layers, each with a tanh() activation.



Designing a Cost Function

As for standard networks, BP-MLL uses gradient descent & back propagation for learning. The novelty of the approach is in the design of the cost function.

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Naive Approach ("BasicBP"):

- Standard MSE:

$$E = \sum_{i=1}^{m} E_i = \sum_{i=1}^{m} \sum_{j=1}^{q} (c_j^i - d_j^i)^2$$

where $c_j^i = c_j(x_i)$ is the output of the network on x_i on the j^{th} class.

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Novel Approach ("BP-MLL"):

- BP-MLL Cost function:

$$E = \sum_{i=1}^{m} E_i = \sum_{i=1}^{m} \frac{1}{|Y_i||\overline{Y}_i|} \sum_{(k,l) \in Y_i \times \overline{Y}_i} \exp(-(c_k^i - c_l^i))$$

so that the i^{th} error term is severely penalized if c_k^i is much smaller than c_l^i.

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- Back-propagation for training is derived just as in the standard (MSE) case (details omitted here, but can be found in Zhang and Zhou's paper).

Deep Learning APIs in Python: TensorFlow/Keras

TensorFlow: an open source python library for numerical computation and large-scale machine learning, created by the Google Brain team.

→ One of the most widely used APIs for deep learning, along with PyTorch and Keras.

→ Later versions of TensorFlow began incorporating the Keras API, since users found its high-level design to be simpler.

```
import tensorflow as tf
mnist = tf.keras.datasets.mnist

(x_train, y_train),(x_test, y_test) = mnist.load_data()
x_train, x_test = x_train / 255.0, x_test / 255.0

model = tf.keras.models.Sequential([
  tf.keras.layers.Flatten(),
  tf.keras.layers.Dense(512, activation=tf.nn.relu),
  tf.keras.layers.Dropout(0.2),
  tf.keras.layers.Dense(10, activation=tf.nn.softmax)
])
model.compile(optimizer='adam',
              loss='sparse_categorical_crossentropy',
              metrics=['accuracy'])

model.fit(x_train, y_train, epochs=5)
model.evaluate(x_test, y_test)
```

BP-MLL in TensorFlow:

→ Data Scientist, Lukas Huwald, published an implementation of the bp-mll cost function for the TensorFlow API as part of the module "bpmll".

→ After installation, the bp-mll loss function can be utilized just as any other TensorFlow loss function.

```
# create simple mlp
model = Sequential()
model.add(Dense(128, input_dim=dim_no, activation='relu', kernel_initializer='glorot_uniform'))
model.add(Dense(64, activation='relu', kernel_initializer='glorot_uniform'))
model.add(Dense(class_no, activation='sigmoid', kernel_initializer='glorot_uniform'))
model.compile(loss=bp_mll_loss, optimizer='adagrad', metrics=[])

# train a few epochs
model.fit(X_train, Y_train, epochs=100)
```

References (Original Method Papers)

Min-Ling Zhang and Zhi-Hua Zhou. Ml-knn: A lazy learning approach to multi-label learning. *Pattern Recognition*, 40(7):2038–2048, 2007. doi: 10.1016/j.patcog.2006.12.019.

Min-Ling Zhang and Zhi-Hua Zhou. Multilabel neural networks with applications to functional genomics and text categorization. *IEEE Transactions on Knowledge and Data Engineering*, 18(10):1338–1351, 2006. doi: doi:10.1109/TKDE.2006.162.