Etivity_1_CA

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1 Artificial Intelligence - MSc

ET5003 - MACHINE LEARNING APPLICATIONS

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1.0.2 ET5003_Etivity-1

1.1 MNIST dataset

The MNIST database is a dataset of handwritten digits that has been and is extensively used in machine learning. There are 10 classes, each image is 28×28 pixels and, therefore, each input is $x_i \in \mathbb{R}^{784}$.

1.2 Task

You have to extend the code to manage any arbitrary number of classes, in other words you have to implement a general-recipe multinomial logistic classifier and Bayesian multinomial logistic classifier.

You must then select 3 digits at random and perform the following task.

1. Your goal is to use Bayesian multinomial logistic regression (as in the road-sign notebook) to solve this classification problem.

- 2. You can downsize the training dataset (e.g., 40% training and 60% testing) if the computation of the posterior takes too much time in your computer.
- 3. Use the posterior uncertainty to detect the instances (digits) in the test set that are hard to classify and remove them from the test-set.
- 4. Then you need to compute again the accuracy of the general-recipe logistic regression on the remaining (non-difficult) instances and comment on the result.
- 5. In practice, the task is to use uncertainty estimation to detect the difficult instances in the test-set. This is equivalent to refuse to classify all high-uncertainty instances or, in other words, when we are uncertain we say "I don't know" and we do not return any class. In this way, you will learn how uncertainty can be used to make safer decisions, by detecting the instances that are difficult to classify.

1.3 Libraries

```
[5]: # Import libraries
   import pandas as pd
   import numpy as np
   from tqdm import tqdm
   import random
   import pickle
   import pymc3 as pm
   import theano as tt
   import arviz as az
   from sklearn.linear_model import LogisticRegression
   from sklearn.metrics import accuracy_score, precision_score, recall_score
   from sklearn.model_selection import train_test_split
   from sklearn.utils import shuffle
   from scipy.special import softmax
   import matplotlib.image as mpimg
   import matplotlib.pyplot as plt
   import matplotlib
   %matplotlib inline
[6]: # Setting a seed:
   np.random.seed(123)
```

2 Data preparation

2.0.1 Loading the MNIST dataset

```
[7]: from google.colab import drive drive.mount('/content/drive')
```

Mounted at /content/drive

```
[8]: # Path, copy the path from your Drive
Path = "/content/drive/MyDrive/UL Masters/ET5003/Week-1/"

# MNIST Data
train_data = Path + 'mnist_train.csv'
test_data = Path + 'mnist_test.csv'

# train data
df_train = pd.read_csv(train_data)
X_train = df_train.drop("label",axis=1).values
y_train = df_train.label.values
print(X_train.shape)

# test data
df_test = pd.read_csv(test_data)
X_test = df_test.drop("label",axis=1).values
y_test = df_test.label.values
print(X_test.shape)
```

```
(60000, 784)
(10000, 784)
```

```
[9]: # Normalizing the Inputs:
X_train = X_train/255
X_test = X_test/255

# Printing the new input range of values:
minv = np.min(X_train)
maxv = np.max(X_train)
print(minv, maxv)
```

0.0 1.0

2.0.2 Description of Data:

```
[10]: # Number of examples
    n_train = len(X_train)
    n_test = len(X_test)

# Shape of an traffic sign image
    image_shape = X_train.shape[1]

# unique classes/labels in the training dataset.
    alltotal = set(y_train)
    n_classes = len(alltotal)

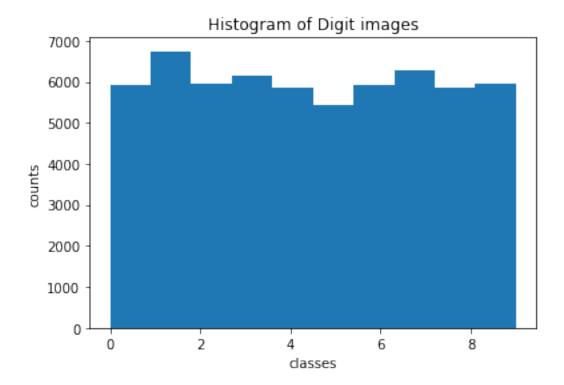
print("Number of Training examples =", n_train)
    print("Number of Test examples =", n_test)
    print("Image input shape =", image_shape)
    print("Number of classes =", n_classes)
```

```
Number of Training examples = 60000
Number of Test examples = 10000
Image input shape = 784
Number of classes = 10
```

2.0.3 Class Distribution:

```
[11]: fig, ax = plt.subplots()
  ind = np.arange(n_classes)

  ax.hist(y_train, bins=n_classes)
  ax.set_xlabel('classes')
  ax.set_ylabel('counts')
  ax.set_title(r'Histogram of Digit images')
  plt.show()
```



The classes are mostly uniformly distributed with a few digits having more or less labels than the average

2.1 Downsampling

2.1.1 Randomly selecting 3 of the 10 Digit Classes

```
[12]: # We select the number of Classes we want:
n_classes = 3

classes = np.random.choice(range(10), size=n_classes, replace=False)
classes.sort()
print("Classes selected:", classes)
```

Classes selected: [0 4 7]

```
[13]: # The number of instances we'll keep for each of our 3 digits:
n_instances = 500

inputs, labels = [], []

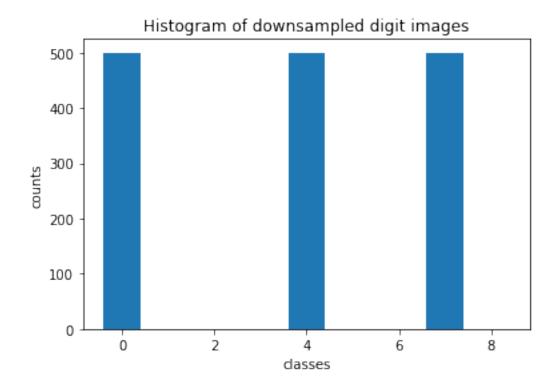
# Loop to randomly sample the instances for each digit:
for r in classes:
   imgs = X_train[np.where(y_train==r)[0],:]
```

```
inputs.append(
    imgs
    [np.random.permutation(imgs.shape[0]), :] # shuffle the data
    [:n_instances, :] # Reduce dataset size to n_instances
)
    labels.append(np.ones(n_instances)*r)

# Shaping inputs and labels in the right format
X_train = np.vstack(inputs).astype(np.float64)
y_train = np.hstack(labels)
```

New Classes Distribution

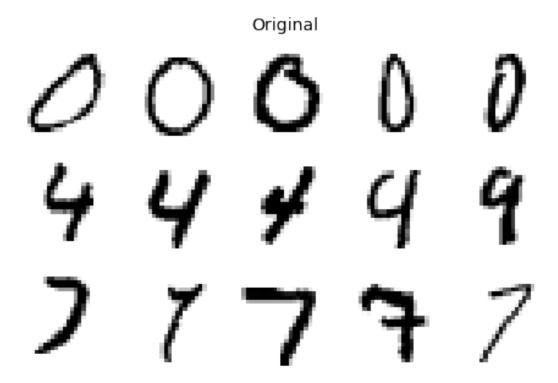
```
[14]: # new histogram
plt.hist(y_train, bins=range(10), align="left", rwidth=0.8)
plt.xlabel('classes')
plt.ylabel('counts')
plt.title('Histogram of downsampled digit images')
plt.show()
```



As expected, we have 500 instances form each class.

```
[15]: # plot digits
def plot_digits(instances, images_per_row=5, **options):
    size = 28
    images_per_row = min(len(instances), images_per_row)
```

```
images = [instance.reshape(size,size) for instance in instances]
         n_rows = (len(instances) - 1) // images_per_row + 1
         n_empty = n_rows * images_per_row - len(instances)
         images.append(np.zeros((size, size * n_empty)))
         row_images = []
         for row in range(n_rows):
             rimages = images[row * images_per_row : (row + 1) * images_per_row]
             row_images.append(np.concatenate(rimages, axis=1))
         image = np.concatenate(row_images, axis=0)
         plt.imshow(image, cmap='gist_yarg', **options)
         plt.axis("off")
[16]: # Show a few instances from each Digit:
     plt.figure(figsize=(8,8))
     # Selecting a few label indices from each of the 3 classes to show:
     label_indices = np.hstack([
         np.random.choice(
             np.where(y_train==label)[0], size=5
         for label in classes
     ])
     # Plotting 'original' image
     plot_digits(X_train[label_indices, :], images_per_row=5)
     plt.title("Original", fontsize=14)
     plt.show()
```



2.1.2 Splitting the Training data into both Training and Validation Sets:

- Although this is the Training set, we can still set aside some samples (for instance 20%) of the 1,500 instances we have for Model Validation purposes.
- With that Validation Set, we can then select the amount of Uncertainty we are happy with from our Model to use out of sample on other unseen data.
- We can then test out how well our decision performs on the Test Set that we put aside earlier.

```
[18]: # print shape of your validation and training set print("Training set shape", X_train.shape) print("Validation set shape", X_val.shape)
```

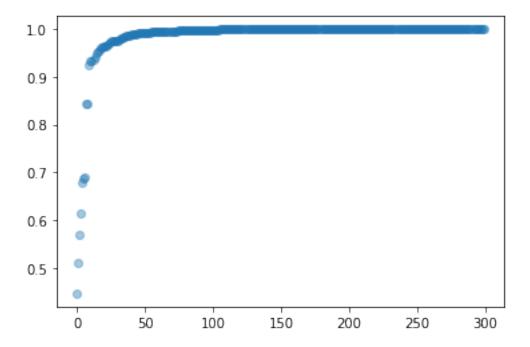
Training set shape (1200, 784) Validation set shape (300, 784)

3 General-Recipe ML

```
[19]: def print_metrics(y_true, y_hat):
         print(f"\tPrecision: {precision_score(y_hat, y_true, average='macro'):.2%}")
         print(f"\tRecall: {recall_score(y_hat, y_true, average='macro'):.2%}")
         print(f"\tAccuracy: {accuracy_score(y_hat, y_true):.2%}")
[20]: # model
     log_clf = LogisticRegression(
         random_state=123,
         max_iter=1000,
         multi_class="multinomial"
     log_clf.fit(X_train, y_train)
     # Classification:
     y_pred_log = log_clf.predict(X_val)
     y_pred_logi_prob = log_clf.predict_proba(X_val)
[21]: print("General Logistic Regression scores:")
     print_metrics(y_val, y_pred_log)
    General Logistic Regression scores:
            Precision: 98.31%
            Recall: 98.29%
            Accuracy: 98.33%
```

Below we plot the sorted probabilities of the model predictions for the validation set.

```
[22]: plt.scatter(
    range(len(X_val)),
    sorted(np.max(y_pred_logi_prob, axis=1)),
    alpha=0.4
)
plt.show()
```



From the plot above we see that the general Logistic Regression model only has a few instances where it is not confident of the result (those near the bottom left of the plot)

4 Probabilistic Multinomial Logistic Regression:

4.0.1 Encoding the Class labels for the Probabilistic ML Model:

This is an example:

- [1,0,0] for first digit
- [0,1,0] for second digit
- [0,0,1] for third digit

The Multinomial Logistic Regression has some parameters:

- α , which is the intercept term:
- β , which is a vector of coefficients which give a weighting to the importance of each input feature:

```
[23]: from sklearn.preprocessing import LabelBinarizer

binarizer = LabelBinarizer()
y_train_bin = binarizer.fit_transform(y_train.reshape(-1, 1))

n_classes = len(classes)
n_features = X_train.shape[-1]
```

```
init_a = np.random.randn(n_classes-1).astype(tt.config.floatX)
init_b = np.random.randn(n_features, n_classes-1).astype(tt.config.floatX)
with pm.Model() as model:
    # setting up the priors
    = pm.Normal(
        "beta",
        mu=0.
        sigma=100,
        shape=(n_features, n_classes-1),
        testval=init_b,
    = pm.Normal(
        "alpha",
        mu=0,
        sigma=100,
        shape=(n_classes-1, ),
        testval=init_a
    )
    # 33
    _1 = tt.tensor.concatenate(
        [np.zeros((n_features, 1)), ],
        axis=1
    _1 = tt.tensor.concatenate([[0], ])
    # Likelihood, our assumption of what the data looks like.
    # We use logistic regression by applying softmax to a simple
    # Linear relationship between the parameters
    p = tt.tensor.nnet.nnet.softmax(
        pm.math.matrix_dot(X_train, _1) + _1
    )
    likelihood = pm.Multinomial("likelihood", p=p, observed=y_train_bin, n=1)
    # Fit the model
    approx = pm.fit(3000, method="advi")
approx.model
```

WARNING (theano.tensor.blas): We did not find a dynamic library in the library_dir of the library we use for blas. If you use ATLAS, make sure to compile it with dynamics library.

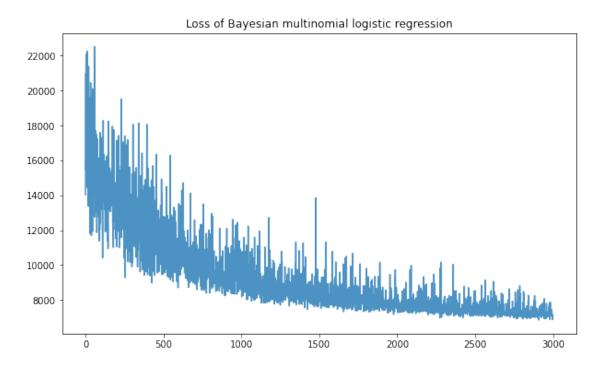
<IPython.core.display.HTML object>

```
Finished [100%]: Average Loss = 7,506.1
```

[23]:

 $\begin{array}{ccc} \text{beta} & \sim & \text{Normal} \\ \text{alpha} & \sim & \text{Normal} \\ \text{likelihood} & \sim & \text{Multinomial} \end{array}$

```
[24]: fig, ax = plt.subplots(figsize=(10, 6))
    ax.plot(approx.hist, alpha=0.8)
    ax.set_title("Loss of Bayesian multinomial logistic regression")
    plt.show()
```



Let's use Arviz plot_trace functionality to examine the posterior distribution.

```
[25]: n_samples = 400
posterior = approx.sample(n_samples)

az.plot_trace(posterior)
plt.show()
```

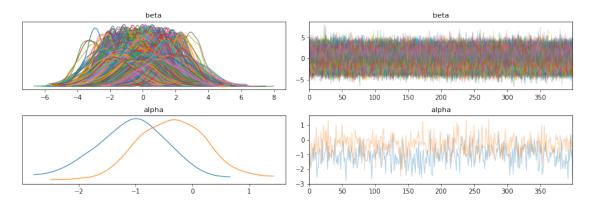
/usr/local/lib/python3.7/dist-packages/arviz/data/io_pymc3.py:100: FutureWarning: Using `from_pymc3` without the model will be deprecated in a future release. Not using the model will return less accurate and less useful results. Make sure you use the model argument or call from_pymc3 within a model context.

FutureWarning,

/usr/local/lib/python3.7/dist-packages/arviz/data/io_pymc3.py:100:

FutureWarning: Using `from_pymc3` without the model will be deprecated in a future release. Not using the model will return less accurate and less useful results. Make sure you use the model argument or call from_pymc3 within a model context.

FutureWarning,



The kernel density estimate for β is unreadable as we have 784 features per class for our data. The plot for α however is more interesting and shows that the model was able to identify that each class has a different mean intercept and standard deviation

Now let's examine the predictions

```
[26]: def zero_pad(arr):
         """Pads the last axis of arr with zeros.
         Args
             arr : np.ndarray
                 Array to be padded
         Returns
             np.ndarray
         return np.concatenate(
             np.zeros(arr.shape[:-1] + (1, )),
             ],
             axis=-1
         )
     def predict(posterior, X):
         """Generates Bayesian Logistic regression predictions based on a learned
         posterior.
```

```
Parameters
         _____
         posterior : pymc3.backends.base.MultiTrace
             The learned posterior parameters
         X : np.ndarray
             Dataset features
         Returns
         _____
         y_probas : np.ndarray
             Class probabilities obtained with softmax
         y_preds : np.ndarray
             Predicted classes
         alpha = zero_pad(posterior["alpha"])
         beta = zero_pad(posterior["beta"])
         # Take softmax along the last axis which represents each class
         logits = softmax(X.dot(beta) + alpha, axis=-1)
         y_probas = (
             np.sum(logits, axis=1) # Sum logits across all samples
             / len(posterior) # Then normalize them
         )
         y_preds = np.argmax(y_probas, axis=1)
         return y_probas, y_preds
[27]: y_probas, y_preds = predict(posterior, X_val)
     y_preds[:10]
[27]: array([0, 0, 2, 0, 2, 2, 1, 0, 0, 2])
[28]: print("Probabilistic Bayesian Logistic Regression scores:")
     print_metrics(y_val, (np.array(classes)[y_preds]))
    Probabilistic Bayesian Logistic Regression scores:
            Precision: 97.28%
```

Recall: 97.30% Accuracy: 97.33%

Calculating posterior uncertainty

To identify which instances the model found easy and hard to classify, we will look at the standard deviation of the prediction across all samples for each instance.

This means that for each instance we will have a 2-D array of shape (n_samples, n_classes) where entries will be 1 if the model assigned the highest probability to that class. For example

```
[[1, 0, 0],
[0, 1, 0],
```

```
[1, 0, 0], ..., [0, 0, 1], [1, 0, 0], [0, 1, 0]],
```

We call this the rank matrix. Next we calculate the standard deviation across each class (i.e. axis 0 - columns) and sort the instances across this dimension in descending order. This will give us the instanced that had highest deviation in the prediction, i.e. the hardest ones to classify!

Note that there are three levels of dimensionality here: instance, sample and class. By instance we mean each data point in the dataset being evaluated (in this case X_val). By sample, we mean each value drawn from the posterior. Finally by class, we mean which label we're predicting.

```
[29]: def assign_ranks(logits):
         """Helper function to create a rank matrix.
         The rank matrix is of shape (len(X), n\_samples, n\_classes) and its entries
         are marked 1 for the class that has the highest logits for each sample.
         Adapted from: https://stackoverflow.com/questions/42519475/
      \neg python-numpy-argmax-to-max-in-multidimensional-array
         Parameters
         _____
         logits : np.ndarray
             A matrix of shape (len(X), n\_samples, n\_classes)
         Returns
         _____
         np.ndarray
             A matrix of shape (len(X), n\_samples, n\_classes) where each entries
             with 1 indicate the class with highest probability
         pred_idx = np.argmax(logits, axis=-1)
         m, n = logits.shape[:2]
         I, J = np.ogrid[:m, :n]
         ranks = np.zeros(shape=logits.shape, dtype=int)
         ranks[I, J, pred_idx] = 1
         return ranks
     def posterior_uncertainty(posterior, X):
         """Generates statistics for Bayesian prediction.
         Parameters
         posterior : pymc3.backends.base.MultiTrace
```

```
The learned posterior parameters
X : np.ndarray
   Dataset features
Returns
stats : np.ndarray
    An array of shape (len(X), 3) with prediction statistics
Notes
The columns of the returned array are as follows
    0: The predicted class
    1: Predicted class probability
    2: Standard deviation of predicted classes across all samples
To calculate the last metric we create an (n samples, n classes) matrix
where each entry is assigned 1 if that is the class with highest
probability.
alpha = zero_pad(posterior["alpha"])
beta = zero_pad(posterior["beta"])
logits = softmax(X.dot(beta) + alpha, axis=-1)
mean_logits = np.mean(logits, axis=1) # mean logits across all samples
y_pred = np.argmax(mean_logits, axis=1) # idx of highest mean logit
y_pred_proba = mean_logits[range(len(X)), y_pred].reshape(-1, 1)
ranks = assign_ranks(logits)
rank_std = np.std(ranks, axis=1)[range(len(X)), y_pred].reshape(-1, 1)
return np.hstack((y_pred.reshape(-1, 1), y_pred_proba, rank_std))
```

Now the array below has columns predicted class, mean predicted probability, standard deviation. (mean and standard deviation calculated across samples)

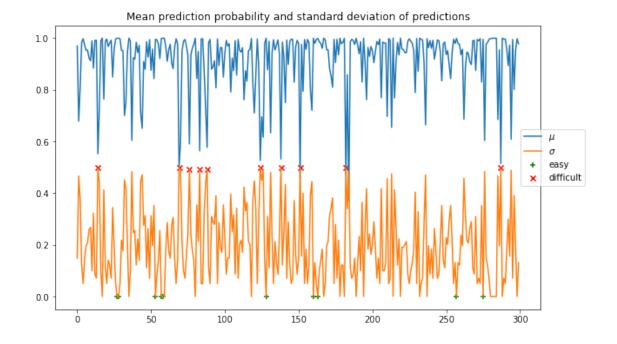
5.1 Easy and difficult instances

By sorting the standard deviations we identify difficult/easy instances

The plot below shows the mean probabilty prediction across all samples (μ) and the standard deviation of the predictions (σ). Note that the instances that are hard to classify have high σ and low μ .

We also mark a few easy/difficult instances with markers to understand their behaviour

```
[33]: n_instances = 10
     plt.figure(figsize=(10, 6))
     plt.plot(range(len(X_val)), uncertainty[:, 1], label="$\mu$")
     plt.plot(range(len(X_val)), uncertainty[:, 2], label="$\sigma$")
     plt.scatter(
         np.arange(len(X_val))[difficult[-n_instances:]],
         uncertainty[difficult[-n_instances:], 2],
         label="easy",
         marker="+",
         c="g"
     plt.scatter(
         np.arange(len(X_val))[difficult[:n_instances]],
         uncertainty[difficult[:n_instances], 2],
         label="difficult",
         marker="x",
         c="r"
     plt.title("Mean prediction probability and standard deviation of predictions")
     plt.legend(bbox_to_anchor=(.95, .65))
     plt.show()
```

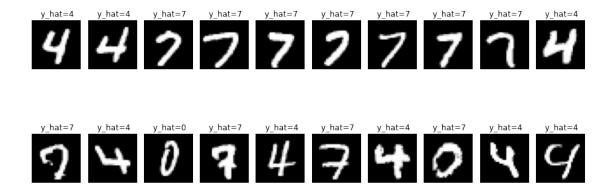


```
[34]: fig, axes = plt.subplots(2, 10, figsize=(12, 6))
# fig.subplots_adjust(hspace = .2, wspace=.001)

for ax, mult in zip(axes, [-1, 1]):
    for idx, axis in enumerate(ax):
        arr = easy if mult==-1 else difficult
        img = X_val[arr[idx]].reshape(28, 28)

        axis.imshow(img, cmap="Greys_r")
        # title_type = "Easy" if mult==-1 else "Difficult"
        title_pred = f" y_hat={y_pred_log[arr[idx]]:.0f}"
        axis.set_title("" + title_pred)
        axis.axis("off")

fig.suptitle("Easy (top) and hard (bottom) to label instances")
fig.tight_layout()
plt.show()
```



As the classifier is very strong, even the difficult instances are mostly well labeled, with only a few having being incorrectly labelled.

5.2 Classifier accuracy on easy/hard instances

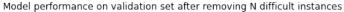
Now that we identified the easy and hard instances, let'see how the general logistic regression classifier performs on these

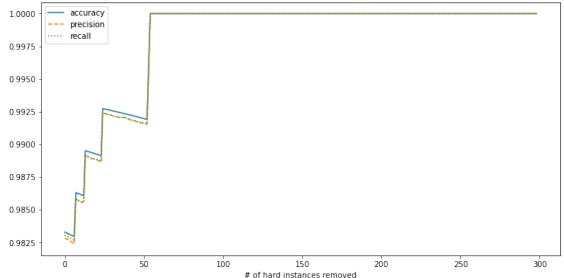
[36]: uncertainty[uncertainty[:, 2] > 0.49]

Recall: 92.59% Accuracy: 90.00%

```
[0.
                       , 0.56364692, 0.49314678],
            [1.
                       , 0.57718666, 0.49183331],
            [0.
                       , 0.52616442, 0.49959984],
            [1.
                       , 0.5321281 , 0.49937461],
            Γ2.
                       , 0.45687319, 0.4987735 ],
                       , 0.46895868, 0.49909919],
            [1.
            Γ2.
                       , 0.51476434, 0.49989999]])
[46]: def calc_metrics(y_true, y_hat):
         """Helper function to calculate model metrics"""
         return np.array([
             accuracy_score(y_true, y_hat),
             precision_score(y_true, y_hat, average="macro"),
             recall_score(y_true, y_hat, average="macro")
         ])
     def log_performance(y_true, y_hat, difficult=difficult):
         scores = np.array([
             calc_metrics(
                 y_true[difficult[-idx:]],
                 y_hat[difficult[-idx:]]
             for idx in range(1, len(easy))
         ])
         return scores
     def plot_performance(*args):
         scores = log_performance(*args)[::-1]
         x = range(len(scores))
         plt.figure(figsize=(12, 6))
         plt.plot(x, scores[:, 0], "-", label="accuracy")
         plt.plot(x, scores[:, 1], "--", label="precision")
         plt.plot(x, scores[:, 2], ":", label="recall")
         plt.legend()
         plt.title("Model performance on validation set after removing N difficult⊔

→instances")
         plt.xlabel("# of hard instances removed")
         plt.show()
[47]: plot_performance(y_val, y_pred_log)
```





As expected, the performance improves as we remove the difficult instances. The shape of the curve is somewhat peculiar, with spikes where the performance increases and then decreases for a while. I suspect this is due to the way np.argsort works in this case: there are ties in the data where some instances have the same standard deviation but different prediction probabilities (which is not taken into account when sorting).

5.3 Summary

We explored the Bayesian approach to Multinomial Logistic regression using Pymc3 and comparing the results to a general Logistic Regression classifier. Overall the performance of the general classifier was marginally higher, however the Bayesian approach offers us a way to identify hard to classify instances and re-evaluate the model after removing these.

6 References

Koehrsen, W. (2018) *Introduction to Bayesian Linear Regression* Available at: https://towardsdatascience.com/introduction-to-bayesian-linear-regression-e66e60791ea7 (Accessed: 18 September 2021)

Salvatier J., Wiecki T., Fonnesbeck C., (2018) "Getting started with PyMC3" https://docs.pymc.io/notebooks/getting_started.html (Accessed: 9 September 2021)

The PyMC Development Team (no date) *Probability Distributions* https://docs.pymc.io/Probability_Distributions.html (Accessed: 9 September 2021)

PDF Using the library below to convert this colab notebook to pdf

```
[56]: %%capture # !wget -nc https://raw.githubusercontent.com/brpy/colab-pdf/master/colab_pdf. \rightarrow py
```

```
from colab_pdf import colab_pdf
     colab_pdf('Etivity_1_CA.ipynb')
 []:
[58]: colab_pdf('Etivity_1_CA.ipynb')
    WARNING: apt does not have a stable CLI interface. Use with caution in scripts.
    WARNING: apt does not have a stable CLI interface. Use with caution in scripts.
    [NbConvertApp] Converting notebook /content/drive/MyDrive/Colab
    Notebooks/Etivity_1_CA.ipynb to pdf
    [NbConvertApp] Support files will be in Etivity_1_CA_files/
    [NbConvertApp] Making directory ./Etivity_1_CA_files
    [NbConvertApp] Making directory ./Etivity 1 CA files
    [NbConvertApp] Making directory ./Etivity_1_CA_files
    [NbConvertApp] Writing 85479 bytes to ./notebook.tex
    [NbConvertApp] Building PDF
    [NbConvertApp] Running xelatex 3 times: [u'xelatex', u'./notebook.tex',
    '-quiet']
    [NbConvertApp] Running bibtex 1 time: [u'bibtex', u'./notebook']
    [NbConvertApp] WARNING | bibtex had problems, most likely because there were no
    citations
    [NbConvertApp] PDF successfully created
    [NbConvertApp] Writing 451745 bytes to /content/drive/My Drive/Etivity_1_CA.pdf
    <IPython.core.display.Javascript object>
    <IPython.core.display.Javascript object>
[58]: 'File ready to be Downloaded and Saved to Drive'
```

[]: