unmixing

June 15, 2021

If you plan on using this implementation, please cite our work:

@INPROCEEDINGS{Tulczyjew2021IGARSS, author={Tulczyjew, Lukasz and Nalepa, Jakub}, booktitle={IGARSS 2021 - 2021 IEEE International Geoscience and Remote Sensing Symposium}, title={Investigating the impact of the training set size on deep learning-powered hyperspectral unmixing}, year={2021}, note={in press}}

1 Parameters description for the unmixing experiments

Train and evaluate the convolutional neural network (CNN) as well as the deep convolutional autoencoder (DCAE) for the unmixing problem. The CNN architecture utilizes several convolutional operations, concluded with fully-connected layers. The first part could be treated as a feature extractor, whereas the final segment of the model, basing on the selected representation, estimates the abundance for each endmember in the hyperspectral image. The dropout technique is utilized to prevent from overfitting in the spectral-spatial variant. Consequently, in the pixel-based approach, max pooling operations are employed. The DCAE architecture constitutes an autoencoder-powered approach. The encoding part incorporates several convolutional layers, whereas the decoder constitutes a single fully-connected layer. Furthermore, the weights of the decoder are set to the endmembers matrix of a particular HSI, hence the condensed representation in the latent space, expresses the abundance of a particular pixel. Exemplary hyperparameters to set:

- –data-file-path - path to the hyperspectral image (HSI).
- –ground-truth-path - path to the ground truth map containing the fractions of abundances for entire HSI.
- –train-size - magnitude of the learning set that is utilized to fine-tune the weights of the model.
- –sub-test-size - size of the test set to evaluate the generalization of the model. It is sampled from the remaining HSI excluding the training subset. If not specified, all non-training samples constitute the test set.Can be employed in the case of experiments when changing the magnitudes of training sets while keeping the size of testing sets constant.
- –val-size - fraction or size of the validation subset, it is designed to monitor the overfitting.
- –channels-idx - index of the spectral dimension in input HSI.
- batch-size - number of samples per update step in the training phase.
- –shuffle - indicates whether to shuffle the dataset in experiment.
- –patience - stopping condition for a specific number of epochs without improvement.
- –model-name - name of the utilized model, possible values: unmixing_pixel_based_cnn, unmixing_cube_based_cnn, unmixing_pixel_based_dcae, unmixing_cube_based_dcae. The

cnn suffix specifies the CNN architecture, whereas the *dcae* represents the autoencoder approach. Cube-based variant incorporates additional features in a form of a spatial extent of the neighboring pixels of a particular sample, whereas the pixel-based approach utilizes only the spectral information of a given sample.
- –sample-size - number of spectral bands in a given HSI.
- –neighborhood-size - size of the spatial extent which is employed for each sample in the form of local neighboring pixels. Most cases allows to leverage the quality of the segmentation as well as the unmixing.
- –n-classes - number of endmembers in the HSI for which the abundances will be estimated by the model.
- –lr - learning rate regulates the step size during weights updates in the training phase.
- –epochs - second stopping condition, i.e., the maximum number of epochs.
- –verbose - verbosity mode.
- –save-data - indicates whether to save the training and test data.

2 Cube-based DCAE

We specify the necessary parameters for the experiment.

[1]:
```
# Execute cube-based DCAE:
from os.path import join

base_path = r'../datasets/urban'
data_file_path = join(base_path, 'urban.npy')
ground_truth_path = join(base_path, 'urban_gt.npy')
endmembers_path = join(base_path, 'urban_m.npy')
train_size = 15500
sub_test_size = 47249
val_size = 0.1
channels_idx = -1
batch_size = 256
shuffle = True
patience = 3
model_name = 'unmixing_cube_based_dcae'
sample_size = 162
neighborhood_size = 5
n_classes = 6
dest_path = join('../examples', 'unmixing_results')
lr = 0.0005
epochs = 10
verbose = 0
save_data = False
use_mlflow = False
seed = 1
```

[2]:
```
import os
import warnings
warnings.filterwarnings('ignore')

import tensorflow as tf

from ml_intuition import enums
from ml_intuition.data.utils import parse_train_size, subsample_test_set, \
    plot_training_curve, show_statistics
from scripts import prepare_data
from scripts.unmixing import train_unmixing, evaluate_unmixing

os.makedirs(dest_path, exist_ok=True)

dcae_dest_path = join(dest_path, 'cube-based-dcae')
os.makedirs(dcae_dest_path, exist_ok=True)
```

3 Prepare data

We prepare data for the unmixing by utilizing the *prepare_data.main* method. It accepts various parameters such as path to the data file or ground-truth for a specific HSI. Furthermore, magnitude of the learning set can be also specified. Moreover, the method accepts the neighborhood size parameter, which specifies the spatial extent of each sample. For each run in the experiment, for the sake of reproducibility, it is possible to set a specific seed. The returned object is a dictionary with three keys: *train*, *test* and *val*. Each of them contains an additional dictionary with *data* and *labels* keys, holding corresponding *numpy.ndarray* objects with the data. For more details about the parameters, refer to the documentation of *prepare_data.main* function (located in *scripts/prepare_data*).

[3]:
```
# Prepare data for unmixing:
data = prepare_data.main(data_file_path=data_file_path,
                         ground_truth_path=ground_truth_path,
                         train_size=parse_train_size(train_size),
                         val_size=val_size,
                         stratified=False,
                         background_label=-1,
                         channels_idx=channels_idx,
                         neighborhood_size=neighborhood_size,
                         save_data=save_data,
                         seed=seed,
                         use_unmixing=True)
# Subsample the test set to constitute a constant size:
if sub_test_size is not None:
    subsample_test_set(data[enums.Dataset.TEST], sub_test_size)
```

4 Train and evaluate the model

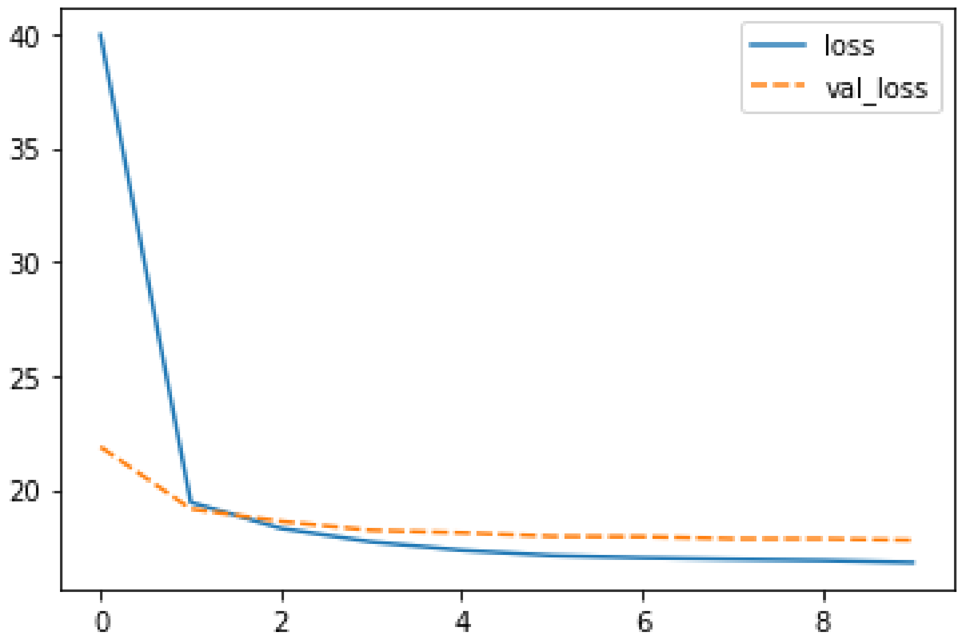
Few parameters previously initialized are employed in this step e.g., the name of the model, size of the spectral extent, learning rate and batch size. The results including the metrics are stored in *dcae_dest_path* directory.

[4]:
```
# Train the model:
train_unmixing.train(model_name=model_name,
                     dest_path=dcae_dest_path,
                     data=data,
                     sample_size=sample_size,
                     neighborhood_size=neighborhood_size,
                     n_classes=n_classes,
                     lr=lr,
                     batch_size=batch_size,
                     epochs=epochs,
                     verbose=verbose,
                     shuffle=shuffle,
                     patience=patience,
                     endmembers_path=endmembers_path,
                     seed=seed)
# Evaluate the model:
evaluate_unmixing.evaluate(
    model_path=os.path.join(dcae_dest_path, model_name),
    data=data,
    dest_path=dcae_dest_path,
    neighborhood_size=neighborhood_size,
    batch_size=batch_size,
    endmembers_path=endmembers_path)
tf.keras.backend.clear_session()
```

```
c:\users\łukasz\desktop\machine-learning\venv\lib\site-
packages\tensorflow\python\framework\tensor_util.py:125: DeprecationWarning:
np.asscalar(a) is deprecated since NumPy v1.16, use a.item() instead
  tensor_proto.float_val.extend([np.asscalar(x) for x in proto_values])

_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv3d (Conv3D)              (None, 3, 3, 160, 16)     448
_________________________________________________________________
conv3d_1 (Conv3D)            (None, 1, 1, 158, 32)     13856
_________________________________________________________________
conv3d_2 (Conv3D)            (None, 1, 1, 156, 64)     6208
_________________________________________________________________
conv3d_3 (Conv3D)            (None, 1, 1, 154, 128)    24704
_________________________________________________________________
flatten (Flatten)            (None, 19712)             0
```

```
_________________________________________________________________
dense (Dense)                (None, 256)               5046528
_________________________________________________________________
dropout (Dropout)            (None, 256)               0
_________________________________________________________________
dense_1 (Dense)              (None, 6)                 1542
_________________________________________________________________
softmax (Softmax)            (None, 6)                 0
_________________________________________________________________
dense_2 (Dense)              (None, 162)               1134
=================================================================
Total params: 5,094,420
Trainable params: 5,093,286
Non-trainable params: 1,134
_________________________________________________________________
```

[5]:
```
plot_training_curve(os.path.join(dcae_dest_path, 'training_metrics.csv'),
                    curve_names=['loss', 'val_loss'],
                    y_limit=False)
show_statistics(os.path.join(dcae_dest_path, 'inference_metrics.csv'))
```



[5]:
```
      aRMSE      aSAM  overallRMSE    rmsAAD  perClassSumRMSE  class0RMSE  \
0  0.052665  0.167482     0.080721  0.285665         0.474069    0.085252

   class1RMSE  class2RMSE  class3RMSE  class4RMSE  class5RMSE     rRMSE  \
0    0.102679    0.083158    0.052504    0.087284    0.063191  0.060676
```

```
        rSID  inference_time
0  3085.67749       28.327313
```

5 Pixel-based CNN

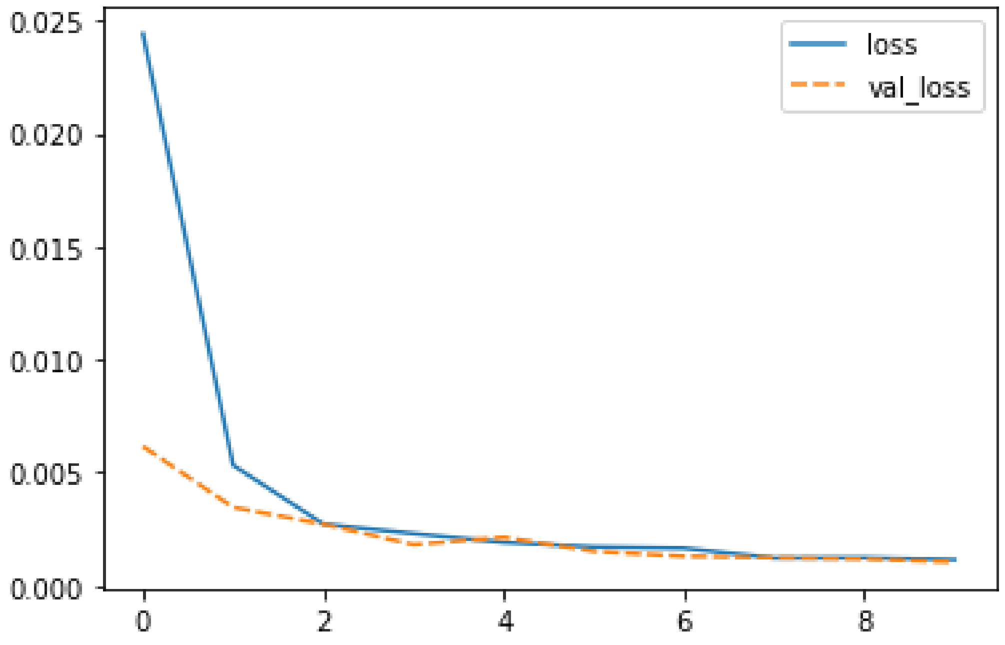
We perform the same steps for the pixel-based CNN model, however a few parameters must be altered. Since we utilize only the spectral dimension, the *neighborhood_size* is set to *None*, the learning rate is also adjusted. The *endmembers_path* is also not needed anymore, since we train the model on the fractions of abundances of each endmember. The pipeline looks similar to the DCAE model.

[6]:
```
# Execute the pixel-based CNN:
endmembers_path = None
model_name = 'unmixing_pixel_based_cnn'
lr = 0.01
neighborhood_size = None
cnn_dest_path = join(dest_path, 'pixel-based-cnn')
os.makedirs(cnn_dest_path, exist_ok=True)

# Prepare data for unmixing:
data = prepare_data.main(data_file_path=data_file_path,
                         ground_truth_path=ground_truth_path,
                         train_size=parse_train_size(train_size),
                         val_size=val_size,
                         stratified=False,
                         background_label=-1,
                         channels_idx=channels_idx,
                         neighborhood_size=neighborhood_size,
                         save_data=save_data,
                         seed=seed,
                         use_unmixing=True)
# Subsample the test set to constitute a constant size:
if sub_test_size is not None:
    subsample_test_set(data[enums.Dataset.TEST], sub_test_size)
# Train the model:
train_unmixing.train(model_name=model_name,
                     dest_path=cnn_dest_path,
                     data=data,
                     sample_size=sample_size,
                     neighborhood_size=neighborhood_size,
                     n_classes=n_classes,
                     lr=lr,
                     batch_size=batch_size,
                     epochs=epochs,
                     verbose=verbose,
                     shuffle=shuffle,
                     patience=patience,
                     endmembers_path=endmembers_path,
                     seed=seed)
# Evaluate the model:
evaluate_unmixing.evaluate(
    model_path=os.path.join(cnn_dest_path, model_name),
    data=data,
    dest_path=cnn_dest_path,
    neighborhood_size=neighborhood_size,
    batch_size=batch_size,
    endmembers_path=endmembers_path)
tf.keras.backend.clear_session()
```

```
c:\users\łukasz\desktop\machine-learning\venv\lib\site-
packages\tensorflow\python\framework\tensor_util.py:125: DeprecationWarning:
np.asscalar(a) is deprecated since NumPy v1.16, use a.item() instead
  tensor_proto.float_val.extend([np.asscalar(x) for x in proto_values])

_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv3d (Conv3D)              (None, 1, 1, 158, 3)      18
_________________________________________________________________
max_pooling3d (MaxPooling3D) (None, 1, 1, 79, 3)       0
_________________________________________________________________
conv3d_1 (Conv3D)            (None, 1, 1, 76, 6)       78
_________________________________________________________________
max_pooling3d_1 (MaxPooling3 (None, 1, 1, 38, 6)       0
_________________________________________________________________
conv3d_2 (Conv3D)            (None, 1, 1, 34, 12)      372
_________________________________________________________________
max_pooling3d_2 (MaxPooling3 (None, 1, 1, 17, 12)      0
_________________________________________________________________
conv3d_3 (Conv3D)            (None, 1, 1, 14, 24)      1176
_________________________________________________________________
max_pooling3d_3 (MaxPooling3 (None, 1, 1, 7, 24)       0
_________________________________________________________________
flatten (Flatten)            (None, 168)               0
_________________________________________________________________
dense (Dense)                (None, 192)               32448
_________________________________________________________________
dense_1 (Dense)              (None, 150)               28950
_________________________________________________________________
dense_2 (Dense)              (None, 6)                 906
=================================================================
Total params: 63,948
Trainable params: 63,948
```

```
Non-trainable params: 0
_________________________________________________________________
```

[7]:
```
plot_training_curve(os.path.join(cnn_dest_path, 'training_metrics.csv'),
                    curve_names=['loss', 'val_loss'],
                    y_limit=False)
show_statistics(os.path.join(cnn_dest_path, 'inference_metrics.csv'))
```



[7]:
```
      aRMSE      aSAM  overallRMSE    rmsAAD  perClassSumRMSE  class0RMSE  \
0  0.023885  0.073451     0.032043  0.109212         0.189771    0.037084

   class1RMSE  class2RMSE  class3RMSE  class4RMSE  class5RMSE  inference_time
0    0.036499    0.033178    0.024482    0.024789    0.033738        1.865043
```