Comparison of different techniques for image augmentation.

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1. Introduction

Convolutional Neural Networks (CNNs) have become a major aproach for the task of Semantic Segmentation and are nowadays used widely over many different fields of applications. Although for some use cases large datasets with thousands of (manually) labeled images have been published (such as CamVid or CityScape in the context of city traffic), in many situations appropriate training data still remains sparse. As a consequence Deep Neural Networks with lots of trainable parameters tend to overfit small and monotonous datasets while generating poor predictions for new (unseen) observations. In order to improve generalization of such CNNs existing training data can be extended by employing different techniques of image augmentation.

2. Architecture

In our case study we use a hierarchical encoderdecoder network with skip connections (CNN of exercise 3) to compare different settings:

- (1) No Augmentation
- (2) Shape Augmentation by applying different geometric transformation and dropouts (Horizontal Flip, Scaling, Crop and Padding, rectangular Cutouts)
- (3) Color Augmentation by varying the intensity values (Adjustment of Brightness and Contrast, Color shifts)
- (4) Shape and Color Augmentation

3. Training

The network is trained on CamVid dataset, which contains ???? different labeled images. To allow for a fair comparison between the 4 different configurations, we use the same hyperparameters (namely the total amount of iterations and batch size) for all types of augmentation. Batches are created by sampling images from the original dataset with pseudo-random numbers and then applying augmentations for setting (2) - (4) on 90% of the images. To facilitate multiple independent modifications A_k (e.g. cropping and flipping an image) we implemented our own probabilistic framework based on the principle of inclusion and exclusion, where:

$$P\left(\bigcup_{k=1}^{n} A_k\right) = \sum_{k=1}^{n} (-1)^{(k+1)} \binom{n}{k} P(A_k)^k,$$

which randomly selects different types of augmentations in varying order. We use the same probability for shape or color modification when investigating setting (4). Because of storage limitations all augmentations are calculated "on the fly" using Python 3.? together with the Numpy, Scipy, OpenCV and Scikit-Image packages, before feeding them into the CNN.

7. References

4. Examples

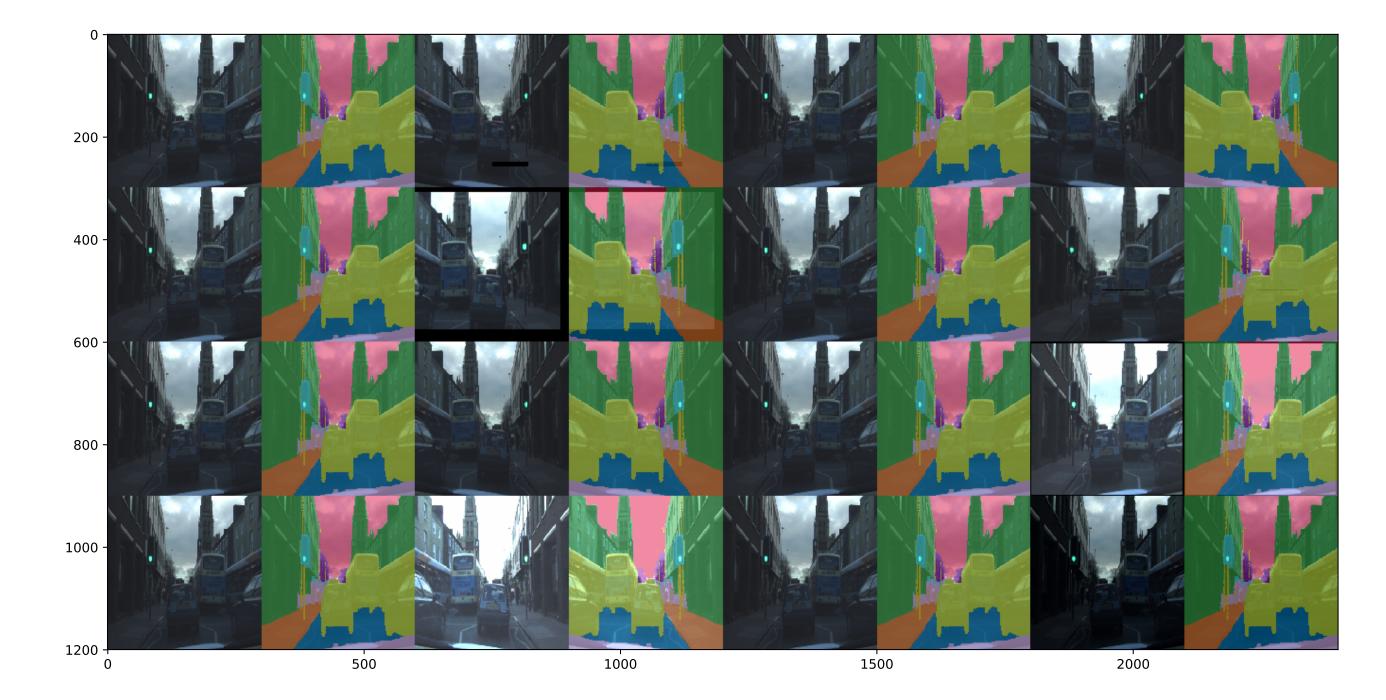


Figure 1: Different types of augmentation applied to a single image. From left to right: original image, original segmentation map, augmented image, augmented segmentation map.

order parametrize shape and color modifications we draw samples different from of distritypes bution (uniform distribution, truncated normal distribution and truncated exponential distribution) depending on the type of augmentation. Hyperparameters (scale and marginal values of the distributions) are adjusted by manually applying random augmen-

tations on some arbitrary images of the CamVid dataset. The range of possible modifications is thereby limited to realistic variations that correspond to natural changes of lightning conditions and scale transformations. Cutout and cropping operations are chosen to cover at most 1/4 of all pixels.

5. Results

We tested DeCAF in 35 case studies taken from the DUD-E database, to evaluate its power to discriminate between active and inactive molecules. We used DeCAF as a classifier and compared it to the SEA (Similarity Ensemble Approach) algorithm [?]. To compare sets of ligands, we adapted the approach used in SEA, replacing Tc by DCAF. We prepared datasets as shown in the left diagram. Then, we tested both classifiers calculating ROC AUC values for every target (below).

6. Conclusions