Simulating the ground truth

Practical Course: Hands-on Deep Learning for Computer Vision and Biomedicine

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Motivation

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- In many applications the ground truth cannot be directly obtained
- One field where data and labels are expensive to obtain is in diffusion MRI
- Is it good enough to build and train models from computer simulations of the ground truth?

Diffusion MRI

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- Molecules such as water floats freely through our bodies
- In some medical conditions, such as stroke, these molecules can become restricted.
- With diffusion MRI we measure the ability of these molecules to move freely within each voxel.

Diffusion MRI

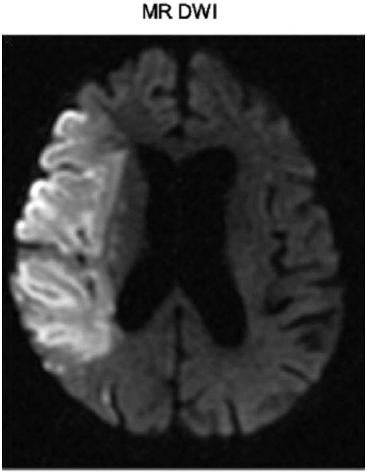

Figure: White area shows restricted diffusion

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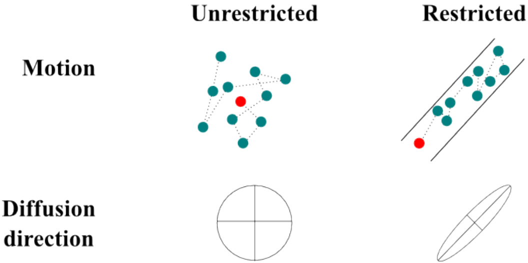

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- Want similar to HPC (Human Connectome Project) - Diffusion MRI dataset from scanned persons
- Idea: Try wide spread of settings with Camino, use kNN to compare with HPC data.
- Run many simulations with these settings.

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- Simulated data divided into training 60%, validation 20% and test 20%.

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- L1 or L2 loss function
- Which optimizer and what learning rate
- Dropout and regularization
- Standardization, scaling and batch normalization

Evaluation

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For n samples:

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- Mean squared error between prediction y and target t as $\frac{1}{n}\sum_{i=1}^{n}(y_i - t_i)^2$
- R^2-score, $1 - \frac{SS_{res}}{SS_{tot}}$ where $SS_{res} = \sum_{i=1}^{n}(y_i - t_i)^2$ and $SS_{tot} = \sum_{i=1}^{n}(t_i - \overline{t})^2$.
  Best possible score 1.0.

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- L2 loss works better, expected since we simulate data and should not have many outliers
- Batch normalization does not improve, expected since data is already normalized and network not too deep
- Scaling outputs to $[0, 1]$ was essential to get any presentable score, since targets very small, around 10^{-7}

Model comparison

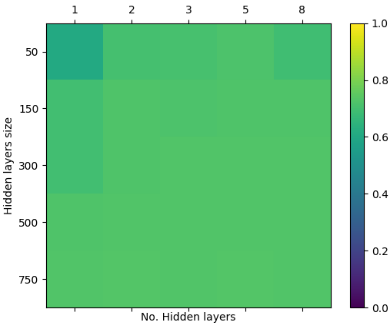

Figure: Heat plot showing R^2-score for hidden layer size vs depth

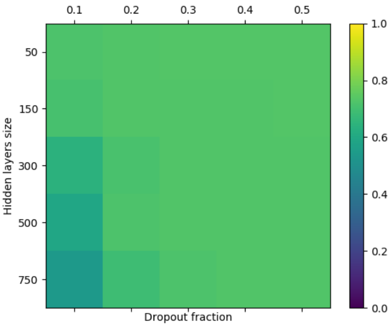

Figure: Heat plot showing R^2-score for hidden layer size vs dropout fraction

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Test set performance:

- $R^2 = 0.80701$
- $MSE = 1.77545 \times 10^{-14}$

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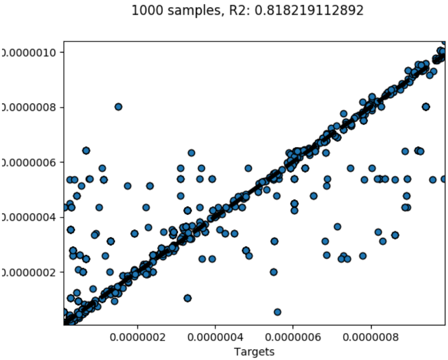

Figure: Predictions vs Targets on 1000 unseen random samples on best performing model

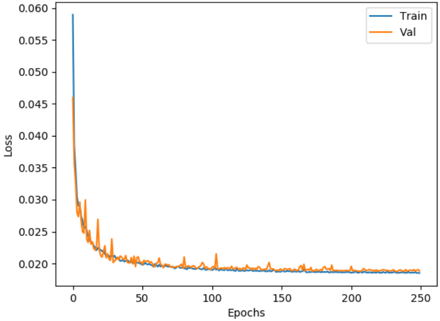

Figure: Loss vs Epochs on best performing model

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- Using more complex simulations, i.e not cylinders, would probably be closer to actual diffusion MRI data
- Training and test error very similar even without regularization, may indicate very similar inputs.
- Very easy to learn an "OK" network, very hard to improve on those results.
- Difficulty to get high train accuracy may indicate that the problem is ill-posed, i.e inputs are not uniquely mappable to targets.

Thank you for your attention

Questions?