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1 new experiments: chemReg with cAdam

1.1 new experiments:chemReg with cAdam sorted by val MAE

| parameter name | best values | | | | |
|--------------------------------|-------------|-----------|-----------|--------------|-----------|
| 'final val loss mae avg' (avg) | 0.1116 | 0.11208 | 0.11416 | 0.11493 | 0.11534 |
| test loss mae avg | 0.11389 | 0.11298 | 0.11493 | 0.11445 | 0.11539 |
| test loss avg | 0.012971 | 0.012764 | 0.0065903 | 0.0065354 | 0.0066426 |
| training time avg | 44.379 | 566.85 | 577.92 | 80.447 | 44.17 |
| neurons per layer | (50, 10) | (50, 10) | (50, 10) | (30, 30, 10) | (40, 20) |
| activation functions | sigmoid | sigmoid | sigmoid | sigmoid | sigmoid |
| last activation function | linear | linear | linear | linear | linear |
| loss function | MSE | MSE | log cosh | log cosh | log cosh |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 500 | 500 | 500 | 500 | 500 |
| batch size | 1000 | 100 | 100 | 1000 | 1000 |
| optimizer | Adam | cAdam | cAdam | cAdam | Adam |
| learning rate | 0.01 | 0.001 | 0.001 | 0.01 | 0.01 |
| ε | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 1.1: best settings regarding *final val loss mae avg* for the chemReg cAdam dataset

| parameter name | parameter values | | | win ratios in % | | | avg. differences | | | best value |
|----------------------|------------------|----------|--------------|-----------------|------|------|------------------|-------|-------|------------|
| neurons per layer | (40, 20) | (50, 10) | (30, 30, 10) | 29.2 | 50.0 | 20.8 | 0.005 | 0.003 | 0.007 | (50, 10) |
| activation functions | ReLU | sigmoid | | 50.0 | 50.0 | | 0.003 | 0.006 | | ReLU |
| loss function | MSE | log cosh | | 31.9 | 68.1 | | 0.004 | 0.002 | | log cosh |
| batch size | 100 | 1000 | 10000 | 52.1 | 45.8 | 2.1 | 0.005 | 0.005 | 0.032 | unclear |
| optimizer | Adam | cAdam | | 41.7 | 58.3 | | 0.005 | 0.002 | | cAdam |
| learning rate | 0.01 | 0.001 | | 63.9 | 36.1 | | 0.004 | 0.015 | | 0.01 |

Table 1.2: parameter influence regarding *final val loss mae avg* for the chemReg cAdam dataset

| parameter name | worst values | | | | |
|--------------------------------|--------------|-----------|-----------|--------------|-----------|
| 'final val loss mae avg' (avg) | 0.19109 | 0.19588 | 0.20277 | 0.21157 | 0.22639 |
| test loss mae avg | 0.18477 | 0.19365 | 0.19938 | 0.20834 | 0.22996 |
| test loss avg | 0.034141 | 0.018634 | 0.019747 | 0.043405 | 0.052883 |
| training time avg | 17.242 | 17.453 | 17.19 | 17.624 | 16.914 |
| neurons per layer | (50, 10) | (50, 10) | (40, 20) | (30, 30, 10) | (40, 20) |
| activation functions | sigmoid | sigmoid | sigmoid | sigmoid | sigmoid |
| last activation function | linear | linear | linear | linear | linear |
| loss function | MSE | log cosh | log cosh | MSE | MSE |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 500 | 500 | 500 | 500 | 500 |
| batch size | 10000 | 10000 | 10000 | 10000 | 10000 |
| optimizer | Adam | Adam | Adam | Adam | Adam |
| learning rate | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| ϵ | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 1.3: worst settings regarding *final val loss mae avg* for the chemReg cAdam dataset

2 MNIST Bachelorthesis new result tables

2.1 accuracy

| parameter name | best values | | | | |
|--------------------------|-------------|-----------|-----------|-----------|-----------|
| final val accuracy avg | 0.97 | 0.9691 | 0.96905 | 0.96885 | 0.9688 |
| test accuracy avg | 0.97006 | 0.96906 | 0.9681 | 0.97048 | 0.97084 |
| training time avg | 46.666 | 43.602 | 86.105 | 86.874 | 23.122 |
| neurons per layer | (50, 10) | (50, 10) | (50, 10) | (50, 10) | (50, 10) |
| activation functions | ReLU | ReLU | ReLU | ReLU | ReLU |
| last activation function | sigmoid | sigmoid | sigmoid | softmax | softmax |
| loss function | cat-cross | cat-cross | cat-cross | cat-cross | cat-cross |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 50 | 25 | 50 | 50 | 25 |
| batch size | 100 | 100 | 100 | 100 | 100 |

| | | | | | |
|---------------|-----------|-------|-------|-------|------|
| optimizer | Adam | cAdam | cAdam | cAdam | Adam |
| learning rate | 0.001 | 0.1 | 0.1 | 0.1 | 0.1 |
| ε | 10^{-7} | 1.0 | 1.0 | 1.0 | 1.0 |

Table 2.1: best settings regarding *final val accuracy avg* for the MNIST BSc dataset

| parameter name | worst values | | | | |
|-------------------------------|--------------|--------------|----------|-----------|----------|
| <i>final val accuracy avg</i> | 0.085333 | 0.0852 | 0.085183 | 0.084467 | 0.0833 |
| test accuracy avg | 0.0845 | 0.0821 | 0.08686 | 0.08748 | 0.08516 |
| training time avg | 1.4319 | 6.3722 | 3.1055 | 3.1968 | 1.3563 |
| neurons per layer | (32,) | (20, 15, 10) | (32,) | (32,) | (50, 10) |
| activation functions | ReLU | ReLU | ReLU | sigmoid | ReLU |
| last activation function | softmax | sigmoid | sigmoid | sigmoid | sigmoid |
| loss function | MSE | MSE | MSE | cat-cross | MSE |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 5 | 5 | 25 | 25 | 5 |
| batch size | 1000 | 100 | 10000 | 10000 | 10000 |
| optimizer | Adam | Adam | Adam | Adam | cAdam |
| learning rate | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| ε | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |

Table 2.2: worst settings regarding *final val accuracy avg* for the MNIST BSc dataset

| parameter name | parameter values | | | win ratios in % | | | avg. differences | | | best value |
|--------------------------|------------------|----------|--------------|-----------------|------|------|------------------|-------|-------|----------------|
| neurons per layer | (32,) | (50, 10) | (20, 15, 10) | 63.8 | 31.4 | 4.9 | 0.003 | 0.117 | 0.17 | (32,) |
| activation functions | ReLU | | sigmoid | 73.1 | | 26.9 | 0.062 | | 0.114 | ReLU |
| last activation function | softmax | | sigmoid | 62.3 | | 37.7 | 0.007 | | 0.069 | softmax |
| loss function | cat-cross | | MSE | 86.7 | | 13.3 | 0.001 | | 0.221 | cat-cross |
| number of epochs | 5 | 25 | 50 | 6.8 | 19.2 | 74.0 | 0.159 | 0.047 | 0.006 | 50 |
| batch size | 100 | 1000 | 10000 | 74.5 | 19.4 | 6.0 | 0.023 | 0.131 | 0.283 | 100 |
| optimizer | Adam | | cAdam | 34.6 | | 65.4 | 0.031 | | 0.01 | cAdam |
| learning rate | 0.1 | 0.01 | 0.001 | 46.9 | 35.1 | 18.1 | 0.175 | 0.096 | 0.202 | <i>unclear</i> |
| ε | 1.0 | | 10^{-7} | 16.2 | | 83.8 | 0.437 | | 0.058 | 10^{-7} |

Table 2.3: parameter influence regarding *final val accuracy avg* for the MNIST BSc dataset

3 MNIST Adam variant comparison

3.1 revised, longer experiments, 1 run

3.2 training time

| parameter name | best values | | | |
|--------------------------|-------------|-----------|-----------|-----------|
| <i>training time avg</i> | 55.489 | 62.251 | 92.568 | 96.35 |
| neurons per layer | (50, 10) | (50, 10) | (50, 10) | (50, 10) |
| activation functions | ReLU | ReLU | ReLU | ReLU |
| last activation function | sigmoid | softmax | sigmoid | softmax |
| loss function | cat-cross | cat-cross | cat-cross | cat-cross |
| training data percentage | 1.0 | 1.0 | 1.0 | 1.0 |
| number of epochs | 250 | 250 | 250 | 250 |
| batch size | 100 | 100 | 100 | 100 |
| optimizer | Adam | Adam | my Adam | my Adam |
| learning rate | 0.001 | 0.001 | 0.001 | 0.001 |
| ε | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 3.1: best settings regarding *training time avg* for the cadam variants dataset

| parameter name | worst values | | | | |
|--------------------------|--------------|-----------|-----------|-----------|-----------|
| <i>training time avg</i> | 96.35 | 104.57 | 110.17 | 113.87 | 115.73 |
| neurons per layer | (50, 10) | (50, 10) | (50, 10) | (50, 10) | (50, 10) |
| activation functions | ReLU | ReLU | ReLU | ReLU | ReLU |
| last activation function | softmax | softmax | sigmoid | softmax | sigmoid |
| loss function | cat-cross | cat-cross | cat-cross | cat-cross | cat-cross |
| training data percentage | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| number of epochs | 250 | 250 | 250 | 250 | 250 |
| batch size | 100 | 100 | 100 | 100 | 100 |

| | | | | | |
|---------------|-----------|------------|------------|-----------|-----------|
| optimizer | my Adam | c adam hat | c adam hat | cAdam | cAdam |
| learning rate | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| ϵ | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 3.2: worst settings regarding *training time avg* for the cadam variants dataset

| parameter name | parameter values | | | | | | | win ratios in % | | | | | avg. differences in % | | best value |
|--------------------------|------------------|---------|-------|----------------------|-------|---|---|-----------------|---|--------|--------|--------|-----------------------|-------|------------|
| last activation function | softmax | | | sigmoid | | | | 50.0 | | 50.0 | | | 4.068 | 1.747 | sigmoid |
| optimizer | Adam | my Adam | cAdam | cAdam _{hat} | 100.0 | 0 | 0 | 0 | 0 | 60.799 | 95.747 | 83.259 | Adam | | |

Table 3.3: parameter influence regarding *training time avg* for the cadam variants dataset

3.3 accuracy

| parameter name | best values | | | | |
|--------------------------|-------------|-----------|-----------|-----------|-----------|
| test accuracy avg | 0.1943 | 0.1941 | 0.19394 | 0.1939 | 0.1938 |
| final val accuracy avg | 0.19403 | 0.19362 | 0.19413 | 0.19363 | 0.1939 |
| final val accuracy std | 0.38807 | 0.38723 | 0.38827 | 0.38727 | 0.3878 |
| final val accuracy min | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| final val accuracy max | 0.97017 | 0.96808 | 0.97067 | 0.96817 | 0.9695 |
| training time avg | 96.35 | 113.87 | 92.568 | 55.489 | 115.73 |
| neurons per layer | (50, 10) | (50, 10) | (50, 10) | (50, 10) | (50, 10) |
| activation functions | ReLU | ReLU | ReLU | ReLU | ReLU |
| last activation function | softmax | softmax | sigmoid | sigmoid | sigmoid |
| loss function | cat-cross | cat-cross | cat-cross | cat-cross | cat-cross |
| training data percentage | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| number of epochs | 250 | 250 | 250 | 250 | 250 |
| batch size | 100 | 100 | 100 | 100 | 100 |
| optimizer | my Adam | cAdam | my Adam | Adam | cAdam |
| learning rate | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| ϵ | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 3.4: best settings regarding *test accuracy avg* for the cadam variants dataset

| parameter name | worst values | | | | |
|--------------------------|--------------|-----------|-----------|------------|------------|
| <i>test accuracy avg</i> | 0.1939 | 0.1938 | 0.19372 | 0.13374 | 0.13306 |
| final val accuracy avg | 0.19363 | 0.1939 | 0.1939 | 0.13457 | 0.13483 |
| final val accuracy std | 0.38727 | 0.3878 | 0.3878 | 0.26913 | 0.26967 |
| final val accuracy min | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| final val accuracy max | 0.96817 | 0.9695 | 0.9695 | 0.67283 | 0.67417 |
| training time avg | 55.489 | 115.73 | 62.251 | 110.17 | 104.57 |
| neurons per layer | (50, 10) | (50, 10) | (50, 10) | (50, 10) | (50, 10) |
| activation functions | ReLU | ReLU | ReLU | ReLU | ReLU |
| last activation function | sigmoid | sigmoid | softmax | sigmoid | softmax |
| loss function | cat-cross | cat-cross | cat-cross | cat-cross | cat-cross |
| training data percentage | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| number of epochs | 250 | 250 | 250 | 250 | 250 |
| batch size | 100 | 100 | 100 | 100 | 100 |
| optimizer | Adam | cAdam | Adam | c adam hat | c adam hat |
| learning rate | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| ϵ | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 3.5: worst settings regarding *test accuracy avg* for the cadam variants dataset

| parameter name | parameter values | | | | | | win ratios in % | | | | avg. differences in % | | best value |
|--------------------------|------------------|---------|-------|----------------------|---|-------|-----------------|---|------|---|-----------------------|--------|------------|
| last activation function | softmax | | | sigmoid | | | 50.0 | | 50.0 | | 0.15 | 0.085 | sigmoid |
| optimizer | Adam | my Adam | cAdam | cAdam _{hat} | 0 | 100.0 | 0 | 0 | 0.16 | 0 | 0.088 | 31.279 | my Adam |

Table 3.6: parameter influence regarding *test accuracy avg* for the cadam variants dataset

4 MNIST with % differences

4.1 training time

| parameter name | best values | | | | |
|--------------------------|-------------|--------|--------|--------|--------|
| <i>training time avg</i> | 1.0347 | 1.0368 | 1.0398 | 1.0412 | 1.0446 |
| neurons per layer | (32,) | (32,) | (32,) | (32,) | (32,) |

| | | | | | |
|--------------------------|-----------|-----------|-----------|---------|---------|
| activation functions | sigmoid | sigmoid | ReLU | ReLU | sigmoid |
| last activation function | sigmoid | sigmoid | sigmoid | sigmoid | sigmoid |
| loss function | MSE | MSE | MSE | MSE | MSE |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 5 | 5 | 5 | 5 | 5 |
| batch size | 10000 | 10000 | 10000 | 10000 | 10000 |
| optimizer | Adam | Adam | Adam | Adam | Adam |
| learning rate | 0.001 | 0.01 | 0.001 | 0.1 | 0.1 |
| ϵ | 10^{-7} | 10^{-7} | 10^{-7} | 1.0 | 1.0 |

Table 4.1: best settings regarding *training time avg* for the MNIST revised dataset

| parameter name | worst values | | | | |
|--------------------------|--------------|--------------|--------------|--------------|--------------|
| <i>training time avg</i> | 106.16 | 106.61 | 106.64 | 106.92 | 106.93 |
| neurons per layer | (20, 15, 10) | (20, 15, 10) | (20, 15, 10) | (20, 15, 10) | (20, 15, 10) |
| activation functions | sigmoid | sigmoid | sigmoid | sigmoid | sigmoid |
| last activation function | softmax | softmax | softmax | softmax | softmax |
| loss function | cat-cross | cat-cross | cat-cross | cat-cross | cat-cross |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 50 | 50 | 50 | 50 | 50 |
| batch size | 100 | 100 | 100 | 100 | 100 |
| optimizer | cAdam | cAdam | cAdam | cAdam | cAdam |
| learning rate | 0.001 | 0.01 | 0.1 | 0.01 | 0.1 |
| ϵ | 1.0 | 1.0 | 1.0 | 10^{-7} | 10^{-7} |

Table 4.2: worst settings regarding *training time avg* for the MNIST revised dataset

| parameter name | parameter values | | | win ratios in % | | | avg. differences in % | | | best value |
|--------------------------|------------------|----------|--------------|-----------------|-----|------|-----------------------|---------|--------|------------|
| neurons per layer | (32,) | (50, 10) | (20, 15, 10) | 98.6 | 1.2 | 0.2 | 0.036 | 12.017 | 22.725 | (32,) |
| activation functions | ReLU | | sigmoid | 49.9 | | 50.1 | 0.716 | | 0.602 | sigmoid |
| last activation function | softmax | | sigmoid | 24.8 | | 75.2 | 1.296 | | 0.506 | sigmoid |
| loss function | cat-cross | | MSE | 52.6 | | 47.4 | 1.241 | | 4.097 | cat-cross |
| number of epochs | 5 | 25 | 50 | 100.0 | 0 | 0 | 0 | 264.684 | 596.88 | 5 |

| | | | | | | | | | | |
|---------------|------|------|-----------|-------|------|-------|---------|--------|-------|-------|
| batch size | 100 | 1000 | 10000 | 0 | 0 | 100.0 | 779.878 | 64.515 | 0 | 10000 |
| optimizer | Adam | | cAdam | 100.0 | | 0 | 0 | 39.945 | | Adam |
| learning rate | 0.1 | 0.01 | 0.001 | 34.7 | 30.9 | 34.4 | 0.914 | 1.126 | 1.094 | 0.1 |
| ε | 1.0 | | 10^{-7} | 54.9 | | 45.1 | 0.666 | 0.686 | | 1.0 |

Table 4.3: parameter influence regarding *training time avg* for the MNIST revised dataset

4.2 accuracy

| parameter name | best values | | | | |
|-------------------------------|-------------|-----------|-----------|-----------|-----------|
| <i>final val accuracy avg</i> | 0.97 | 0.9691 | 0.96905 | 0.96885 | 0.9688 |
| test accuracy avg | 0.97006 | 0.96906 | 0.9681 | 0.97048 | 0.97084 |
| training time avg | 46.666 | 43.602 | 86.105 | 86.874 | 23.122 |
| neurons per layer | (50, 10) | (50, 10) | (50, 10) | (50, 10) | (50, 10) |
| activation functions | ReLU | ReLU | ReLU | ReLU | ReLU |
| last activation function | sigmoid | sigmoid | sigmoid | softmax | softmax |
| loss function | cat-cross | cat-cross | cat-cross | cat-cross | cat-cross |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 50 | 25 | 50 | 50 | 25 |
| batch size | 100 | 100 | 100 | 100 | 100 |
| optimizer | Adam | cAdam | cAdam | cAdam | Adam |
| learning rate | 0.001 | 0.1 | 0.1 | 0.1 | 0.1 |
| ε | 10^{-7} | 1.0 | 1.0 | 1.0 | 1.0 |

Table 4.4: best settings regarding *final val accuracy avg* for the MNIST revised dataset

| parameter name | worst values | | | | |
|-------------------------------|--------------|--------------|----------|----------|----------|
| <i>final val accuracy avg</i> | 0.085333 | 0.0852 | 0.085183 | 0.084467 | 0.0833 |
| test accuracy avg | 0.0845 | 0.0821 | 0.08686 | 0.08748 | 0.08516 |
| training time avg | 1.4319 | 6.3722 | 3.1055 | 3.1968 | 1.3563 |
| neurons per layer | (32,) | (20, 15, 10) | (32,) | (32,) | (50, 10) |
| activation functions | ReLU | ReLU | ReLU | sigmoid | ReLU |
| last activation function | softmax | sigmoid | sigmoid | sigmoid | sigmoid |

| | | | | | |
|--------------------------|-------|-------|-------|-----------|-------|
| loss function | MSE | MSE | MSE | cat-cross | MSE |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 5 | 5 | 25 | 25 | 5 |
| batch size | 1000 | 100 | 10000 | 10000 | 10000 |
| optimizer | Adam | Adam | Adam | Adam | cAdam |
| learning rate | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| ε | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |

Table 4.5: worst settings regarding *final val accuracy avg* for the MNIST revised dataset

| parameter name | parameter values | | | win ratios in % | | | avg. differences in % | | | best value |
|--------------------------|------------------|----------|--------------|-----------------|------|------|-----------------------|--------|--------|------------|
| neurons per layer | (32,) | (50, 10) | (20, 15, 10) | 63.8 | 31.4 | 4.9 | 1.091 | 20.613 | 27.614 | (32,) |
| activation functions | ReLU | | sigmoid | 73.1 | | 26.9 | 8.66 | | 20.247 | ReLU |
| last activation function | softmax | | sigmoid | 62.3 | | 37.7 | 2.423 | | 10.791 | softmax |
| loss function | cat-cross | | MSE | 86.7 | | 13.3 | 0.401 | | 33.215 | cat-cross |
| number of epochs | 5 | 25 | 50 | 6.8 | 19.2 | 74.0 | 25.91 | 9.915 | 1.916 | 50 |
| batch size | 100 | 1000 | 10000 | 74.5 | 19.4 | 6.0 | 4.087 | 21.393 | 38.937 | 100 |
| optimizer | Adam | | cAdam | 34.6 | | 65.4 | 7.61 | | 2.37 | cAdam |
| learning rate | 0.1 | 0.01 | 0.001 | 46.9 | 35.1 | 18.1 | 20.242 | 16.717 | 30.161 | unclear |
| ε | 1.0 | | 10^{-7} | 16.2 | | 83.8 | 52.679 | | 7.421 | 10^{-7} |

Table 4.6: parameter influence regarding *final val accuracy avg* for the MNIST revised dataset

5 ChemRegB with % differences

5.1 training time

| parameter name | best values | | | | |
|--------------------------|-------------|----------|----------|----------|----------|
| training time avg | 16.508 | 16.688 | 16.872 | 16.896 | 16.914 |
| neurons per layer | (40, 20) | (40, 20) | (40, 20) | (40, 20) | (40, 20) |
| activation functions | ReLU | ReLU | ReLU | ReLU | sigmoid |
| last activation function | linear | linear | linear | linear | linear |
| loss function | MSE | MSE | log cosh | log cosh | MSE |

| | | | | | |
|--------------------------|-----------|-----------|-----------|-----------|-----------|
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 500 | 500 | 500 | 500 | 500 |
| batch size | 10000 | 10000 | 10000 | 10000 | 10000 |
| optimizer | Adam | Adam | Adam | Adam | Adam |
| learning rate | 0.001 | 0.01 | 0.01 | 0.001 | 0.001 |
| ϵ | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 5.1: best settings regarding *training time avg* for the chemReg Adam dataset

| parameter name | worst values | | | | |
|--------------------------|--------------|--------------|--------------|--------------|--------------|
| <i>training time avg</i> | 678.56 | 691.95 | 692.12 | 696.0 | 697.49 |
| neurons per layer | (30, 30, 10) | (30, 30, 10) | (30, 30, 10) | (30, 30, 10) | (30, 30, 10) |
| activation functions | sigmoid | ReLU | ReLU | sigmoid | sigmoid |
| last activation function | linear | linear | linear | linear | linear |
| loss function | MSE | log cosh | log cosh | log cosh | log cosh |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 500 | 500 | 500 | 500 | 500 |
| batch size | 100 | 100 | 100 | 100 | 100 |
| optimizer | cAdam | cAdam | cAdam | cAdam | cAdam |
| learning rate | 0.01 | 0.01 | 0.001 | 0.001 | 0.01 |
| ϵ | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 5.2: worst settings regarding *training time avg* for the chemReg Adam dataset

| parameter name | parameter values | | | win ratios in % | | | avg. differences in % | | | best value |
|----------------------|------------------|----------|--------------|-----------------|------|-------|-----------------------|---------|--------|------------|
| neurons per layer | (40, 20) | (50, 10) | (30, 30, 10) | 87.5 | 12.5 | 0 | 0.151 | 1.948 | 11.851 | (40, 20) |
| activation functions | ReLU | sigmoid | | 51.4 | 48.6 | | 0.63 | 0.614 | | unclear |
| loss function | MSE | log cosh | | 87.5 | 12.5 | | 0.126 | 2.565 | | MSE |
| batch size | 100 | 1000 | 10000 | 0 | 0 | 100.0 | 2448.099 | 214.332 | 0 | 10000 |
| optimizer | Adam | cAdam | | 100.0 | 0 | | 0 | 47.609 | | Adam |
| learning rate | 0.01 | 0.001 | | 43.1 | 56.9 | | 0.527 | 0.577 | | unclear |

Table 5.3: parameter influence regarding *training time avg* for the chemReg Adam dataset

5.2 validation loss

| parameter name | best values | | | | |
|--------------------------------|-------------|-----------|-----------|--------------|-----------|
| 'final val loss mae avg' (avg) | 0.1116 | 0.11208 | 0.11416 | 0.11493 | 0.11534 |
| test loss mae avg | 0.11389 | 0.11298 | 0.11493 | 0.11445 | 0.11539 |
| test loss avg | 0.012971 | 0.012764 | 0.0065903 | 0.0065354 | 0.0066426 |
| training time avg | 44.379 | 566.85 | 577.92 | 80.447 | 44.17 |
| neurons per layer | (50, 10) | (50, 10) | (50, 10) | (30, 30, 10) | (40, 20) |
| activation functions | sigmoid | sigmoid | sigmoid | sigmoid | sigmoid |
| last activation function | linear | linear | linear | linear | linear |
| loss function | MSE | MSE | log cosh | log cosh | log cosh |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 500 | 500 | 500 | 500 | 500 |
| batch size | 1000 | 100 | 100 | 1000 | 1000 |
| optimizer | Adam | cAdam | cAdam | cAdam | Adam |
| learning rate | 0.01 | 0.001 | 0.001 | 0.01 | 0.01 |
| ϵ | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 5.4: best settings regarding *final val loss mae avg* for the chemReg Adam dataset

| parameter name | worst values | | | | |
|--------------------------------|--------------|----------|----------|--------------|----------|
| 'final val loss mae avg' (avg) | 0.19109 | 0.19588 | 0.20277 | 0.21157 | 0.22639 |
| test loss mae avg | 0.18477 | 0.19365 | 0.19938 | 0.20834 | 0.22996 |
| test loss avg | 0.034141 | 0.018634 | 0.019747 | 0.043405 | 0.052883 |
| training time avg | 17.242 | 17.453 | 17.19 | 17.624 | 16.914 |
| neurons per layer | (50, 10) | (50, 10) | (40, 20) | (30, 30, 10) | (40, 20) |
| activation functions | sigmoid | sigmoid | sigmoid | sigmoid | sigmoid |
| last activation function | linear | linear | linear | linear | linear |
| loss function | MSE | log cosh | log cosh | MSE | MSE |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 500 | 500 | 500 | 500 | 500 |
| batch size | 10000 | 10000 | 10000 | 10000 | 10000 |
| optimizer | Adam | Adam | Adam | Adam | Adam |

| | | | | | |
|---------------|-----------|-----------|-----------|-----------|-----------|
| learning rate | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| ϵ | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 5.5: worst settings regarding *final val loss mae avg* for the chemReg Adam dataset

| parameter name | parameter values | | | win ratios in % | | | avg. differences in % | | | best value |
|----------------------|------------------|----------|--------------|-----------------|------|------|-----------------------|--------|--------|------------|
| neurons per layer | (40, 20) | (50, 10) | (30, 30, 10) | 29.2 | 50.0 | 20.8 | 3.395 | 2.134 | 5.689 | (50, 10) |
| activation functions | ReLU | sigmoid | | 50.0 | 50.0 | | 2.743 | 4.037 | | ReLU |
| loss function | MSE | log cosh | | 31.9 | 68.1 | | 2.961 | 1.155 | | log cosh |
| batch size | 100 | 1000 | 10000 | 52.1 | 45.8 | 2.1 | 4.485 | 4.275 | 26.929 | unclear |
| optimizer | Adam | cAdam | | 41.7 | 58.3 | | 3.458 | 1.781 | | cAdam |
| learning rate | 0.01 | 0.001 | | 63.9 | 36.1 | | 3.241 | 11.151 | | 0.01 |

Table 5.6: parameter influence regarding *final val loss mae avg* for the chemReg Adam dataset

5.3 test loss

| parameter name | best values | | | | |
|--------------------------|-------------|-----------|-----------|-----------|--------------|
| 'test loss avg' (avg) | 0.11298 | 0.11379 | 0.11389 | 0.11409 | 0.11445 |
| test loss mae avg | 0.11298 | 0.11379 | 0.11389 | 0.11409 | 0.11445 |
| final val loss avg | 0.012562 | 0.013544 | 0.012455 | 0.0066663 | 0.0065895 |
| training time avg | 566.85 | 43.583 | 44.379 | 576.57 | 80.447 |
| neurons per layer | (50, 10) | (40, 20) | (50, 10) | (40, 20) | (30, 30, 10) |
| activation functions | sigmoid | sigmoid | sigmoid | sigmoid | sigmoid |
| last activation function | linear | linear | linear | linear | linear |
| loss function | MSE | MSE | MSE | log cosh | log cosh |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 500 | 500 | 500 | 500 | 500 |
| batch size | 100 | 1000 | 1000 | 100 | 1000 |
| optimizer | cAdam | Adam | Adam | cAdam | cAdam |
| learning rate | 0.001 | 0.01 | 0.01 | 0.001 | 0.01 |
| ϵ | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 5.7: best settings regarding *test loss avg* for the chemReg Adam dataset

| parameter name | worst values | | | | |
|--------------------------|--------------|-----------|-----------|--------------|-----------|
| 'test loss avg' (avg) | 0.18477 | 0.19365 | 0.19938 | 0.20834 | 0.22996 |
| test loss mae avg | 0.18477 | 0.19365 | 0.19938 | 0.20834 | 0.22996 |
| final val loss avg | 0.036515 | 0.019063 | 0.020418 | 0.044762 | 0.051253 |
| training time avg | 17.242 | 17.453 | 17.19 | 17.624 | 16.914 |
| neurons per layer | (50, 10) | (50, 10) | (40, 20) | (30, 30, 10) | (40, 20) |
| activation functions | sigmoid | sigmoid | sigmoid | sigmoid | sigmoid |
| last activation function | linear | linear | linear | linear | linear |
| loss function | MSE | log cosh | log cosh | MSE | MSE |
| training data percentage | 1 | 1 | 1 | 1 | 1 |
| number of epochs | 500 | 500 | 500 | 500 | 500 |
| batch size | 10000 | 10000 | 10000 | 10000 | 10000 |
| optimizer | Adam | Adam | Adam | Adam | Adam |
| learning rate | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 |
| ϵ | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} | 10^{-7} |

Table 5.8: worst settings regarding *test loss avg* for the chemReg Adam dataset

| parameter name | parameter values | | | win ratios in % | | | avg. differences in % | | | best value |
|----------------------|------------------|----------|--------------|-----------------|------|------|-----------------------|--------|--------|------------|
| neurons per layer | (40, 20) | (50, 10) | (30, 30, 10) | 27.1 | 50.0 | 22.9 | 3.242 | 1.677 | 5.055 | (50, 10) |
| activation functions | ReLU | sigmoid | | 55.6 | 44.4 | | 2.313 | 4.219 | | ReLU |
| loss function | MSE | log cosh | | 37.5 | 62.5 | | 2.93 | 1.147 | | log cosh |
| batch size | 100 | 1000 | 10000 | 50.0 | 47.9 | 2.1 | 4.201 | 4.151 | 25.616 | unclear |
| optimizer | Adam | cAdam | | 45.8 | 54.2 | | 3.551 | 1.499 | | cAdam |
| learning rate | 0.01 | 0.001 | | 65.3 | 34.7 | | 3.06 | 10.756 | | 0.01 |

Table 5.9: parameter influence regarding *test loss avg* for the chemReg Adam dataset