Bachelor Thesis

Investigating Probabilistic Preconditioning on Deep Learning using DeepOBS

Ludwig Bald

Tübingen

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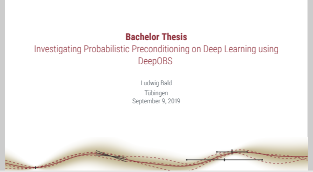
2019-09-09



- Introduce myself, I study Cognitive Science
- I chose this topic because I wanted to get to know deep learning from the inside. I had never done Deep Learning before and wanted to learn it hands-on.
- In this talk I will talk about the science, but also about the process I used.
- If you have questions during the talk, ask them right away!

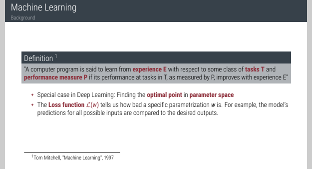
Machine Learning

Definition [1]

"A computer program is said to learn from **experience E** with respect to some class of **tasks T** and **performance measure P** if its performance at tasks in T, as measured by P, improves with experience E"

- Special case in Deep Learning: Finding the **optimal point** in **parameter space**
- The **Loss function** $\mathcal{L}(w)$ tells us how bad a specific parametrization $\boldsymbol{w}$ is. For example, the model's predictions for all possible inputs are compared to the desired outputs.

[1] Tom Mitchell, "Machine Learning", 1997



- Most of you will have seen this definition before.
- As an example, have a look at this 2-parametrical problem

Gradient Descent

Optimization

Gradient Descent uses knowledge of the **gradient** at a point in parameter space to take an update step:

$$w_{i+1} = w_i - \alpha \cdot \nabla \mathcal{L}(w_i)$$

where α is the learning rate.

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└─Background

└─Gradient Descent

Gradient Descent
Optimization
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where α is the learning rate.

- In real life, we have Big Data. The true $\nabla \mathcal{L}(w)$ is expensive to compute.
- To speed things up, we compute the noisy estimate $\hat{\mathcal{L}}(w_i)$ on a minibatch of for example 128 data points.

The update rule still looks the same:

$$w_{i+1} = w_i - \alpha \cdot \nabla \hat{\mathcal{L}}(w_i)$$

where α is the learning rate.

Preconditioning

The condition number of the Hessian

- The performance of (S)GD depends heavily on the shape of the loss landscape
- The **condition number** is defined as

$$\kappa = \frac{\lambda_n}{\lambda_1} > 1$$

  where λ_n, λ_1 are the largest/smallest eigenvalues of the Hessian $\nabla\nabla\mathcal{L}(w)$
- For larger κ, (S)GD can converge slower.
- The condition number can be changed by carefully rescaling the gradient before taking the optimization step

Probabilistic Preconditioning

by Filip & Philipp, 2019

In the stochastic (minibatched) setting and while only having access to **Hessian-vector products**, it isn't obvious how to construct the preconditioner. This is the method I'm testing:

1. Empirically construct a prior for the multivariate Gaussian distribution and set the learning rate for SGD
2. Gather observations and update the posterior estimate for the Hessian, using Bayes
3. Create a rank-2 approximation of the Preconditioner
4. apply the preconditioner at every step and do SGD

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If I'm grossly misrepresenting the algorithm, please correct me now! For an exact description check out the paper

Deep learning

Neural nets

For the purposes of this talk, a neural net is a model

- with many ($>$ hundreds of thousands) parameters, weights $\boldsymbol{w}$
- with an available noisy gradient $\nabla\hat{\mathcal{L}}(\boldsymbol{w}_0)$, which was obtained by backpropagation

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Evaluating an Optimizer

Empirically

This is a hard problem in itself! How do you chose:

- Data Set
- Batch Size
- Model architecture
- Hyperparameter tuning method
- Measure of success

Comparing results between papers is very hard.

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Measure of success
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Now that we have roughly defined the algorithm, how do we test it?

DeepOBS

by Frank & Aaron

- A library for Tensorflow and Pytorch
- In order to test an optimizer, you have to specify only
  - The optimizer class
  - The hyperparameters of my optimizer
  - One of the provided testproblems
- DeepOBS then returns a json file
- And automatically generates figures

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Implementation Details

The class Preconditioner

```
Preconditioner(params, est_rank=2, num_observations=5, prior_iterations=10,
               weight_decay=0, lr=None,
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start_estimate()
step()
get_log()
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How to use the TCML Cluster

Cloud Computing

1. Request an account by sending an email
2. If you have any special code requirements, build a Singularity container (kind of like a virtual machine). Alternatively use a provided one.
3. Create & Submit a Slurm Batch job file
4. Get an e-mail when your jobs start of finish
5. Download the output files to your local machine. You can mount the cluster as a virtual drive.

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Experiments

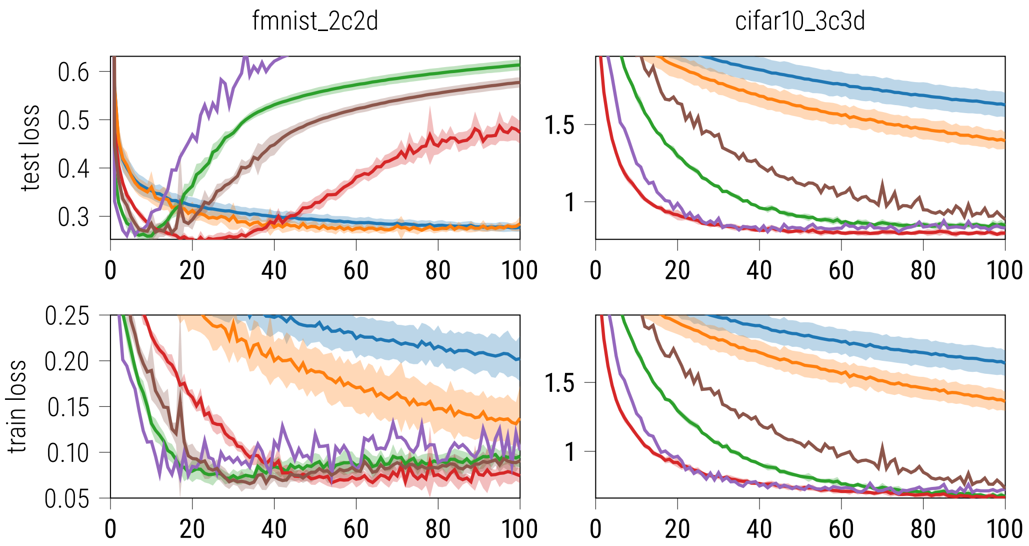
Overview

- Effectiveness of Preconditioning
- Computational Complexity
- Stability
- Learning Rate sensitivity

Experiments
Overview
Effectiveness of Preconditioning
Computational Complexity
Stability
Learning Rate sensitivity

Effectiveness of Preconditioning

AdaptiveSGD PreconditionedSGD



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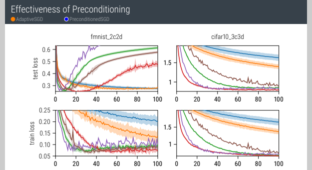
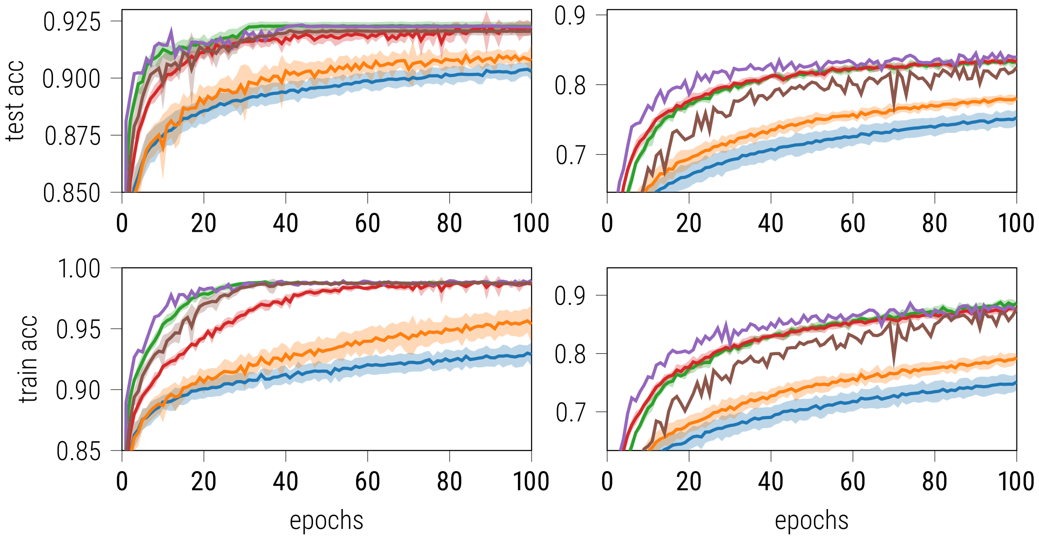


Effectiveness of Preconditioning

AdaptiveSGD   PreconditionedSGD



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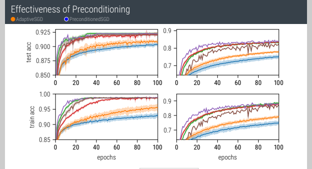

Discussion: Effectiveness

Why might it be worse than plain SGD?

- It’s very noisy: Noise from the Hessian is amplified through the whole epoch.
- The constructed learning rate is not optimal
- PreconditionedSGD is worse than AdaptiveSGD, so the Preconditioning makes things worse
- The preconditioner has only rank 2, while there might be thousands large eigenvalues (usually 10%)
- The other optimizers are exhaustively tuned
- The other optimizers use more data for actual parameter updates: 1920/50.000 images per epoch are only used for the Hessian

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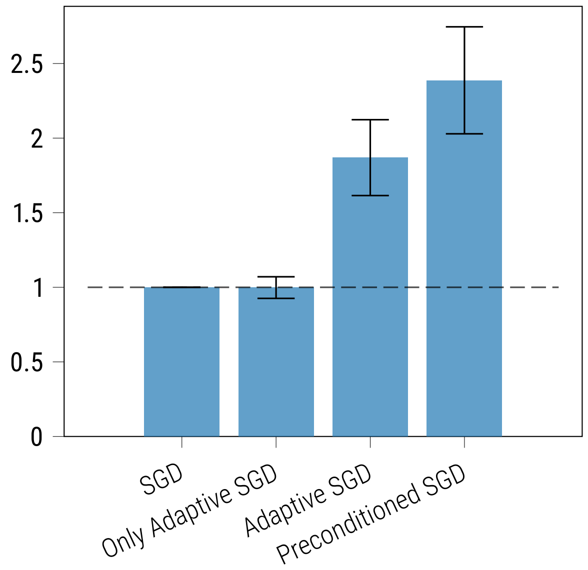
Performance penalty

Computational overhead



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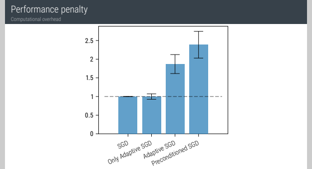
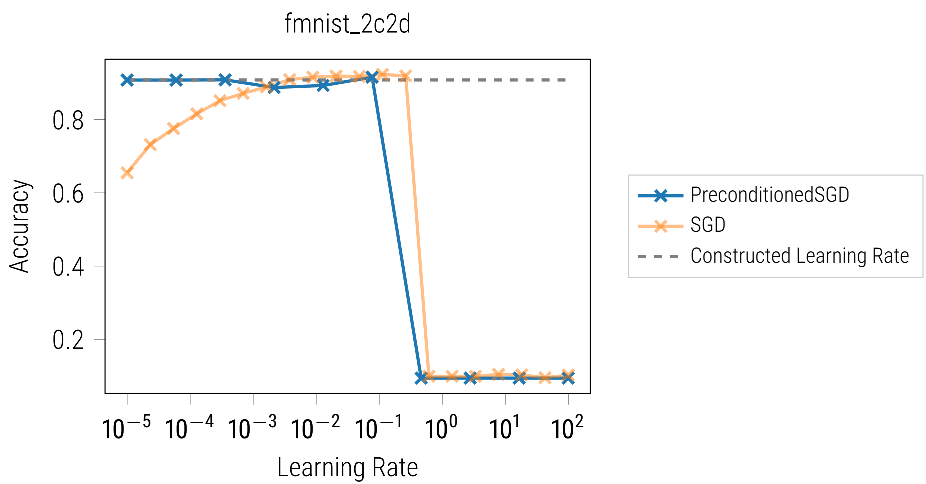
└Experiments + Results + Discussion

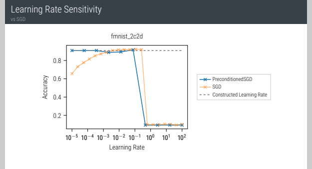
└Performance penalty



Learning Rate Sensitivity

vs SGD





Conclusion/Final Remarks

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