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**MASTER Data Science et BIG Data**

**Projet de Fin De Module**

**Comparaison Systématique des Algorithmes d’Optimisation pour l’Apprentissage**

**Automatique et Profond : Étude Empirique et Analyse Critique**

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**Abstract**

Optimization algorithms play a critical role in training machine learning (ML) and deep learning (DL) models, impacting both convergence speed and predictive accuracy. This report evaluates four widely used optimization algorithms—Stochastic Gradient Descent (SGD) with momentum, Adam, Limited-memory Broyden–Fletcher–Goldfarb–Shanno (L-BFGS), and Newton-CG—on two datasets (Boston Housing and California Housing). The evaluation is performed on two models: linear regression (ML) and a neural network with one hidden layer (DL). Metrics include convergence speed, generalization (test Mean Squared Error), and sensitivity to hyperparameters. Results highlight trade-offs between speed and accuracy, providing insights for practitioners to select appropriate optimizers based on dataset and model complexity.

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# 1 Introduction

## Problem Statement

Optimization is at the core of training ML and DL models, influencing model performance and training efficiency. Despite advances in optimization techniques, selecting the best algorithm for specific datasets and models remains challenging due to the variability in performance.

## 1.2 Objectives

**This study aims to:**

* Perform an empirical comparison of four optimization algorithms (SGD with momentum, Adam, L-BFGS, Newton-CG).
* Evaluate their performance on a linear regression model and a neural network with one hidden layer.
* Analyze metrics such as convergence speed, generalization ability, and sensitivity to hyperparameters.

## 1.3 Contributions

* A systematic benchmark of four optimization algorithms.
* Quantitative metrics for comparing speed, accuracy, and robustness.
* Practical recommendations for optimization algorithm selection.

# 2 Literature Review

## 2.1 Optimization Algorithms

**SGD with Momentum:** Accelerates convergence by incorporating momentum, reducing oscillations in the gradient.

**Adam**: Combines momentum and adaptive learning rates, offering robustness across various applications.

**L-BFGS**: A quasi-Newton method that approximates second-order gradients, suitable for smaller models.

**Newton-CG**: A second-order optimizer leveraging exact or approximate Hessians, often used inconstrained problems.

## 2.2 Existing Comparative Studies

**P**revious studies, such as Kingma & Ba (2014) for Adam, emphasize algorithm advantages in various contexts. For instance, Kingma & Ba highlighted Adam's efficiency in handling sparse gradients and adapting learning rates dynamically, making it suitable for deep learning tasks.

**H**owever, comparative studies focusing on both ML and DL across datasets of varying complexity remain limited. Research gaps include a lack of systematic evaluations of second-order optimizers like Newton-CG and L-BFGS in ML contexts and the performance variability of optimizers across different architectures and dataset sizes. This project aims to address these gaps by providing a unified analysis framework, quantifying trade-offs between convergence speed, generalization, and sensitivity to hyperparameters.

# 3 Methodology

## 3.1 Datasets

* **Boston Housing**: Predicts median housing prices based on 13 features.
* **California Housing**: Predicts median house values using 8 features.

## 3.2 Models

* **Linear Regression (ML):** A simple linear model predicting continuous outcomes.
* **Neural Network (DL):** One hidden layer with 32 units and ReLU activation.

## 3.3 Experimental Protocol

**Train/test split :**

* **80%** training, **20%** testing.

**Hyperparameters:**

* **Learning rates:** {0.01, 0.001} for SGD and Adam.
* Default parameters for L-BFGS and Newton-CG.

**Metrics:**

* Training time (seconds).
* Test MSE.
* Convergence epochs (**loss threshold**).

### 3.4 Tools

* **Python libraries:** PyTorch, Scikit-learn, SciPy.
* **Hardware:** Intel **i7** processor, **16GB** RAM.

# Results

## Boston Housing Dataset

## Linear Regression

|  |  |  |  |
| --- | --- | --- | --- |
| **Optimizer** | **Test MSE** | **Training Time (s)** | **Epochs to Threshold** |
| **SGD (lr=0.01)** | **0.2950** | **2.18** | **Not reached** |
| **Adam (lr=0.01)** | **0.2870** | **2.40** | **Not reached** |
| **L-BFGS** | **0.3985** | **0.15** | **2** |
| **Newton-CG** | **0.2877** | **0.02** | **-** |

#### **Neural Network**

|  |  |  |  |
| --- | --- | --- | --- |
| **Optimizer** | **Test MSE** | **Training Time (s)** | **Epochs to Threshold** |
| **SGD (lr=0.01)** | **0.2667** | **0.12** | **5** |
| **Adam (lr=0.01)** | **0.2347** | **0.08** | **3** |
| **L-BFGS** | **0.3707** | **0.18** | **2** |

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**Figure 1:Convergence Curves for Boston Housing (Linear Regression vs. Neural Network)**

## Description:

## Training Loss (MSE) vs. Epochs for:

## Linear Regression: SGD (lr=0.01, 0.001), Adam (lr=0.01, 0.001), L-BFGS (lr=0.1).

## Neural Network (1 hidden layer): Same optimizers.

## Key Observations:

## Linear Regression: L-BFGS converges fastest (2 epochs) but generalizes poorly (high test MSE). Newton-CG (not plotted) matches Adam’s MSE but is faster.

## Neural Network: Adam (lr=0.01) achieves the lowest loss and fastest convergence (3 epochs). SGD is slower and unstable.

## California Housing Dataset

## Linear Regression

|  |  |  |  |
| --- | --- | --- | --- |
| **Optimizer** | **Test MSE** | **Training Time (s)** | **Epochs to Threshold** |
| **SGD (lr=0.01)** | **0.4057** | **75.88** | **Not reached** |
| **Adam (lr=0.01)** | **0.4204** | **85.05** | **Not reached** |
| **L-BFGS** | **0.4751** | **0.15** | **2** |
| **Newton-CG** | **0.4175** | **0.05** | **-** |

#### **Neural Network**

|  |  |  |  |
| --- | --- | --- | --- |
| **Optimizer** | **Test MSE** | **Training Time (s)** | **Epochs to Threshold** |
| **SGD (lr=0.01)** | **0.2995** | **3.70** | **4** |
| **Adam (lr=0.01)** | **0.2779** | **2.37** | **2** |
| **L-BFGS** | **0.5927** | **0.15** | **2** |

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**Figure 2:Convergence Curves for California Housing (Linear Regression vs. Neural Network)**

## Description:

## Training Loss (MSE) vs. Epochs for the same optimizers as Figure 1.

## Key Observations :

## Linear Regression: SGD (lr=0.001) is stable but slow. Newton-CG (not plotted) has the best test MSE (0.4175).

## Neural Network: Adam (lr=0.01) outperforms others (MSE: 0.2779). L-BFGS fails to converge properly (flat curve).

# Discussion

## 5.1 Interpretation of Results

## ****Figures 1 & 2 demonstrate that:****

## **For linear regression, second-order methods (Newton-CG, L-BFGS) are fastest but sensitive to hyperparameters. Adam balances speed and accuracy.**

## **For neural networks, Adam consistently outperforms due to adaptive learning rates. SGD requires careful tuning (e.g., lr=0.001).**

## 5.2 Hyperparameter Sensitivity

## ****SGD:** Highly sensitive to learning rate (diverges at lr=0.01, stabilizes at lr=0.001).**

## ****Adam:** Robust across learning rates (lr=0.01 optimal).**

## ****L-BFGS:** Fails in DL due to non-convexity (Figure 2)**

## 5.3 Sensitivity to Hyperparameters

* Learning rate tuning significantly impacts SGD and Adam. L-BFGS is less sensitive but slower for complex models.

## 5.4 Limitations

* Single DL architecture.
* Results may not generalize to larger datasets or more complex models.

# Conclusion

## 6.1 Summary

* **Newton-CG** is optimal for small **ML** models.
* **Adam** demonstrates superior performance for **DL** tasks.
* **Trade-offs** between speed, accuracy, and stability depend on the optimizer and problem.

## 6.2 Recommendations

* **For small datasets:** Use **Newton-CG** or **SGD** with tuning.
* **For DL:** Use **Adam** for faster convergence and robust generalization.

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# 8. Annexe

# https://github.com/safaaafhamni/projet-optimisation-.git