Global Convergence Newton

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Abstract

- The abstract paragraph should be indented ½ inch (3 picas) on both the left- and right-hand margins. Use 10 point type, with a vertical spacing (leading) of 11 points.

 The word **Abstract** must be centered, bold, and in point size 12. Two line spaces precede the abstract. The abstract must be limited to one paragraph.
- 5 1 Introduction
- 6 In this paper we consider problems of the

$$\min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) \tag{1}$$

where $f: \mathbb{R}^d \to \mathbb{R}$ is a twice-differentiable function. First-order optimization methods are widely used for such problems due to their low per-iteration computational cost and their suitability for parallelization they often suffer from slow convergence for ill-conditioned objective functions [1]. Newton's method is a popular optimization algorithm that is commonly used to solve optimization 10 problems. It is a second-order optimization algorithm since it uses second-order information of 11 the objective function. Newton's method is known to have fast local convergence guarantees for 12 convex functions. However, the global convergence properties of Newton's method are still an active 13 area of research [2] [3]. In contrast to first-order methods such as gradient descent, second-order 14 methods such as Newton's method can achieve much faster convergence when presented with ill 15 conditioned Hessians by transferring the problem into a more isotropic optimization problem at the cost of an increase to cubic run time. Newton's method yields local quadratic convergence if 17 f is twice differentiable (or we have suitable regularity conditions), which degrades to sublinear 18 convergence outside of the local regions. 19

In this paper, we explore the theoretical foundations of several Newton-type methods that achieve different global convergence guarantees, compare their performance in a classification-type problem for two loss functions on four different datasets. Finally we will propose two modifications of the algorithms to achieve an increase in runtime, by either coupling the Newton-type method with a conjugate gradient method for Hessian vector multiplication or Strassen's algorithm for fast matrix inversion.

Background

2.1 Loss function and Datasets

28 Let
$$X = \begin{bmatrix} \dots x_1^\top \dots \\ \vdots \\ \dots x_i^\top \dots \end{bmatrix} \in \mathbb{R}^{n \times d}$$
 be the set of data for n datapoints with d features, i.e. $x_i \in \mathbb{R}^d$

29 and labels $y^\top = [y_1, \dots, y_n]$

29 For $\sigma(x) := \frac{\exp(x)}{1 + 1}$ the loss functions were available $x \in \mathbb{R}^d$

For $\sigma(x) := \frac{\exp(x)}{1 + \exp(x)}$ the loss functions w.r.t. weights ω are given by

$$L_1(\omega) = -\frac{1}{n} \sum_{i=1}^n \left(y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i) \right), \quad \hat{y}_i = \sigma(x_i^\top \omega)$$
 (2)

$$L_2(\omega) = \frac{1}{n} \sum_{i=1}^n \log \left(1 + \exp(-y_i x_i^{\top} \omega) \right) + r(\omega), \quad r(\omega) = \lambda \sum_{j=1}^d \frac{\alpha \omega_j^2}{1 + \alpha \omega_j^2}$$
 (3)

(4)

which yields the two optimization problems

$$\min L_1(\omega) \tag{5}$$

$$\min_{\omega} L_2(\omega) \tag{6}$$

The corresponding gradients of L_i are

$$\nabla L_1(x) = \frac{1}{n} X^{\top} (\hat{y} - y) \tag{7}$$

$$\nabla L_2(x) = -\frac{1}{n} X^{\top} \left(y \odot \sigma(-y \odot (X\omega)) \right) + \nabla r(x)$$
(8)

$$\text{with} \quad \nabla r(\omega)^\top = \lambda \cdot \left[\frac{2\alpha\omega_1}{(1+\alpha\omega_1^2)^2}, ..., \frac{2\alpha\omega_d}{(1+\alpha\omega_d^2)^2} \right] \quad \text{and } \sigma(\;\cdot\;) \text{ applied elementwise}$$

and \odot denotes the entrywise multiplication of vectors

Differentiating again yields the Hessians

$$\nabla^2 L_1(\omega) = \frac{1}{n} X^\top D X \tag{9}$$

$$\nabla^2 L_2(\omega) = \frac{1}{n} X^{\top} D X + \nabla^2 r(\omega), \nabla^2, \quad r(\omega) = \operatorname{diag}\left(\lambda \frac{2\alpha (1 - 3\alpha \omega_j^2)}{(1 + \alpha \omega_j^2)^3}\right)$$
(10)

where the diagonal matrix D has entries

$$D_{ii} = \hat{y}_i (1 - \hat{y}_i) = \sigma(-y_i z_i^{\mathsf{T}} \omega) \left(1 - \sigma(-y_i z_i^{\mathsf{T}} \omega)\right),\tag{11}$$

Observation: 35

Since $\log(\hat{y}_i)$, $\log(1-\hat{y}_i)$ are concave on $(0,\infty)$ it follows that $-\log(\hat{y}_i)$, $-\log(1-\hat{y}_i)$ are convex

and thus L_1 is a linear combination of convex functions (which is agian convex). Meanwhile L_2 is 37

not guaranteed to be convex due to the non-convex regularization term $r(\omega)$. 38

2.2 Classic Newton's Method 39

The classical origin of Newton's method is as an algorithm for finding the roots of functions. In

this paper it is used to find the roots x^* of $\nabla(f(x))$ s.t. $\nabla(f(x^*)) = 0$ and x^* a local minimum of f.

Newton's method combined with a stepsize η uses the update rule [1]:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \eta(\nabla^2 f(\mathbf{x}_k))^{-1} \nabla f(\mathbf{x}_k)$$
(12)

The inverse Hessian can be interpreted as transforming the gradient landscape to be more isotropic,

thereby improving the conditioning of the problem.

2.3 Cubic Newton

- The cubic Newton method was one of the first to achieve a good complexity guarantee globally
- [REFERENCE TO DO: What convergence rate exactly?]. It is based on cubic regularization and uses 47
- the update rule:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - (\nabla^2 f(\mathbf{x}_k) + H||\mathbf{x}_{k+1} - \mathbf{x}_k||\mathbf{I})^{-1} \nabla f(\mathbf{x}_k)$$
(13)

2.4 Levenberg and Marquardt method

- The Levenberg-Marquardt's algorithm [REFERENCE] is an early form of regularized Newton's
- method that modifies the Hessian. For ill conditioned (or singular) H this can increase conergence (or 51
- make the problem solvable as $H + \lambda I$ is always invertible for sufficiently large $eiq(H) > -\lambda, \lambda >$ 52
- 0).he update rule is:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - (\nabla^2 f(\mathbf{x}_k) + \lambda_k \mathbf{I})^{-1} \nabla f(\mathbf{x}_k)$$
(14)

Regularized Newton

In their 2023 article Michenko presents a variation of Newton's method that uses the update rule [2]:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - (\nabla^2 f(\mathbf{x}_k) + \sqrt{H||\nabla f(\mathbf{x}_k)||\mathbf{I}|})^{-1} \nabla f(\mathbf{x}_k)$$
(15)

- where H>0 is a constant. The convergence rate of this algorithm is $\mathcal{O}(\frac{1}{k^2})$. This method uses an adaptive variant of the Levenberg-Marquardt regularization.
- 2.6 TODO 58
- Jorge Nocedal & Stephen J. Wright, Numerical Optimization (2nd ed), Springer (2006). Chapter 7 59 (Newton-CG methods for large-scale optimization) Section 7.2: "Newton-CG Algorithm" 60

2.7 Inexact Newton Method

Given that Newton has cubic complexity we now outline how we aim to reduce the runtime by extending CG and MINRES methods to the Newton-type methods described in our paper. In order for the modified algorithms to inherit the convergence guarantees of the algorithms we want to approximate p s.t.

$$||Hp + \nabla f|| \le \epsilon$$
 (absolute tolerance) $< \epsilon = 10^{-8}$

Since $H_{1,2} = \nabla^2 L_{1,2}$ are clearly symmetric (as both $X^{\top}DX$ and $\nabla^2 r(x)$ are) we can apply the conjugate gradient method if the H is positive definite or have to fall back on MINRES if it is not pd. Positive definiteness depends on the data matrix and the regularizer curvature. [TODO: runtime for MINRES and CG]

Every iteration of Vanilla Newton takes $O(n^3)$ per iteration because inversion of the Hessian costs $O(n^3)$.

for symmetric applying CG to newton drops the effort for conversion down to

$$O(k \cdot n^2) = O(\sqrt{\kappa} \log{(1/\epsilon)} \cdot n^2)$$

- where $\kappa(H)=\frac{\lambda_{max}(H)}{\lambda_{max}(H)}$ Precondition with SSOR to reduce condition number.

References

- [1] Jorge Nocedal and Stephen J. Wright. Numerical Optimization. Springer, 2nd edition, 2006.
- [2] Konstantin Mishchenko. Regularized newton method with global convergence. SIAM Journal on 67 Optimization, 33(3):1440-1462, 2023. 68

[3] Slavomír Hanzely, Dmitry Kamzolov, Dmitry Pasechnyuk, Alexander Gasnikov, Peter Richtárik, and Martin Takác. A damped newton method achieves global $(o)(\frac{1}{k^2})$ and local quadratic convergence rate. *Advances in Neural Information Processing Systems*, 35:25320–25334, 2022.

2 Checklist

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- The checklist follows the references. Please read the checklist guidelines carefully for information on how to answer these questions. For each question, change the default **[TODO]** to **[Yes]**, **[No]**, or **[N/A]**. You are strongly encouraged to include a **justification to your answer**, either by referencing the appropriate section of your paper or providing a brief inline description. For example:
 - Did you include the license to the code and datasets? [Yes] See Section
 - Did you include the license to the code and datasets? [No] The code and the data are proprietary.
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Please do not modify the questions and only use the provided macros for your answers. Note that the Checklist section does not count towards the page limit. In your paper, please delete this instructions block and only keep the Checklist section heading above along with the questions/answers below.

- 1. For all authors...
 - (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? **[TODO]**
 - (b) Did you describe the limitations of your work? [TODO]
 - (c) Did you discuss any potential negative societal impacts of your work? [TODO]
 - (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [TODO]
- 2. If you are including theoretical results...
 - (a) Did you state the full set of assumptions of all theoretical results? [TODO]
 - (b) Did you include complete proofs of all theoretical results? [TODO]
- 3. If you ran experiments...
 - (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [TODO]
 - (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [TODO]
 - (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [TODO]
 - (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [TODO]
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 - (b) Did you mention the license of the assets? [TODO]
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 - (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [TODO]
 - (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [TODO]
 - (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [TODO]

A Appendix

Optionally include extra information (complete proofs, additional experiments and plots) in the appendix. This section will often be part of the supplemental material.