
Global Convergence Newton

Raffael Colonnello
University of Basel
Raffael.Colonnello@unibas.ch

Fynn Gohlke
University of Basel
Fynn.Gohlke@stud.unibas.ch

Benedikt Heuser
University of Basel
ben.heuser@unibas.ch

Abstract

1 The abstract paragraph should be indented 1/2 inch (3 picas) on both the left- and
2 right-hand margins. Use 10 point type, with a vertical spacing (leading) of 11 points.
3 The word **Abstract** must be centered, bold, and in point size 12. Two line spaces
4 precede the abstract. The abstract must be limited to one paragraph.

5 1 Introduction

6 In this paper we consider problems of the form

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

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

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

26 2 Background

27 2.1 Loss function and Datasets

28 Let $X = \begin{bmatrix} \dots x_1^\top \dots \\ \vdots \\ \dots x_i^\top \dots \\ \vdots \\ \dots x_n^\top \dots \end{bmatrix} \in \mathbb{R}^{n \times d}$ be the set of data for n datapoints with d features, i.e. $x_i \in \mathbb{R}^d$
 29 and labels $y^\top = [y_1, \dots, y_n]$
 30 For $\sigma(x) := \frac{\exp(x)}{1+\exp(x)}$ the loss functions w.r.t. weights ω are given by

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

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

31 which yields the two optimization problems

$$\min_{\omega} L_1(\omega) \quad (5)$$

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

32 Remark 1: The 0/1 loss function for logistic regression is given by

$$-\sum_{i=1}^N \log \left[\mu_i^{\mathbb{I}(y_i=1)} (1 - \mu_i)^{\mathbb{I}(y_i=0)} \right] = -\sum_{i=1}^N [y_i \log \mu_i + (1 - y_i) \log(1 - \mu_i)]$$

33 for labels $y_i \in \{0, 1\}$ [4, Eq. 8.2–8.3]. If we instead use labels $\tilde{y}_i \in \{-1, +1\}$, the negative
 34 log-likelihood becomes

$$\sum_{i=1}^N \log(1 + \exp(-\tilde{y}_i \mathbf{w}^\top \mathbf{x}_i))$$

35 [4, Eq. 8.4]. To ensure the loss functions correspond to the correct likelihood, the label encoding
 36 must match the loss form [4, Sec. 8.3.1].

37 The corresponding gradients of L_i are

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

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

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

and \odot denotes the entrywise multiplication of vectors.

38 Differentiating again yields the Hessians

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

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

39 where the diagonal matrix D has entries

$$D_{ii} = \hat{y}_i(1 - \hat{y}_i) = \sigma(-y_i x_i^\top \omega)(1 - \sigma(-y_i x_i^\top \omega)), \quad (11)$$

40 Observation:

41 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
 42 and thus L_1 is a linear combination of convex functions (which is again convex). Meanwhile L_2 is
 43 not guaranteed to be convex due to the non-convex regularization term $r(\omega)$.

44 2.2 Classic Newton's Method

45 The classical origin of Newton's method is as an algorithm for finding the roots of functions. In
 46 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 .
 47 Newton's method combined with a stepsize η uses the update rule [1]:

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

48 The inverse Hessian can be interpreted as transforming the gradient landscape to be more isotropic,
 49 thereby improving the conditioning of the problem.

50 2.3 Cubic Newton

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

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

54 2.4 Levenberg and Marquardt method

55 The Levenberg-Marquardt's algorithm [REFERENCE] is an early form of regularized Newton's
 56 method that modifies the Hessian. For ill conditioned (or singular) H regularization can increase
 57 the convergence (or make the problem solvable as $H + \lambda I$ is always invertible for sufficiently large
 58 $\text{eig}(H) > -\lambda, \lambda > 0$). The update rule is:

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

59 2.5 Regularized Newton

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

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

61 where $H > 0$ is a constant. The convergence rate of this algorithm is $\mathcal{O}(\frac{1}{k^2})$. This method uses an
 62 adaptive variant of the Levenberg-Marquardt regularization.

63 2.6 Appendix

$$L_1(\omega) = -\frac{1}{n} \sum_{i=1}^n \left[y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i) \right]$$

$$\hat{y}_i = \sigma(x_i^\top \omega) = \frac{1}{1 + e^{-x_i^\top \omega}}$$

$$\frac{\partial}{\partial \omega} (-y_i \log \hat{y}_i) = -y_i \frac{1}{\hat{y}_i} \hat{y}_i (1 - \hat{y}_i) x_i = -y_i (1 - \hat{y}_i) x_i$$

$$\frac{\partial}{\partial \omega} (-(1 - y_i) \log(1 - \hat{y}_i)) = (1 - y_i) \frac{1}{1 - \hat{y}_i} \hat{y}_i (1 - \hat{y}_i) x_i = (1 - y_i) \hat{y}_i x_i$$

$$\nabla L_1(\omega) = \frac{1}{n} \sum_{i=1}^n [\hat{y}_i - y_i] x_i = \frac{1}{n} X^\top (\hat{y} - y)$$

64 TODO: Hessian von L1 ausrechnen. (Ist aber gesichert korrekt wegen IBM)

$$L_2(\omega) = \frac{1}{n} \sum_{i=1}^n \underbrace{\log(1 + \exp(-y_i x_i^\top \omega))}_{f_i(\omega)} + \lambda \underbrace{\sum_{j=1}^d \frac{\alpha \omega_j^2}{1 + \alpha \omega_j^2}}_{r(\omega)}$$

65 For the gradient we then get

$$\begin{aligned}
\frac{\partial}{\partial \omega_j} r(\omega) &= 2\lambda\alpha \frac{\omega_j}{(1 + \alpha\omega_j^2)^2} \implies \nabla r(\omega) = 2\lambda\alpha \frac{\omega}{(1 + \alpha\omega^2)^2} \\
\nabla f_i(\omega) &= \frac{\partial}{\partial \omega} \log(1 + e^{-y_i x_i^\top \omega}) \\
&= \frac{1}{\underbrace{1 + e^{y_i x_i^\top \omega}}_{\sigma(-y_i x_i^\top \omega)}} \cdot (-y_i x_i) = \sigma(-y_i x_i^\top \omega) \cdot (-y_i x_i) = -y_i x_i \sigma(-y_i x_i^\top \omega) \\
\nabla f(\omega) &= -\frac{1}{n} \sum_{i=1}^n y_i x_i \sigma(-y_i x_i^\top \omega) = -\frac{1}{n} X^\top (y \odot \sigma(-y \odot (X\omega))) \\
\nabla L_2(\omega) &= \nabla f(\omega) + \nabla r(\omega) \\
&= -\frac{1}{n} X^\top (y \odot \sigma(-y \odot (X\omega))) + 2\lambda\alpha \frac{\omega}{(1 + \alpha\omega^2)^2}
\end{aligned}$$

66 For the Hessians we first observe two remarks:

67 Remark 2:

$$\begin{aligned}
\sigma(z) &= \frac{1}{1 + e^{-z}} \\
\implies \frac{d}{dz} \sigma(z) &= \frac{d}{dz} (1 + e^{-z})^{-1} = -(1 + e^{-z})^{-2} \cdot (-e^{-z}) = \frac{e^{-z}}{(1 + e^{-z})^2} = \frac{1}{1 + e^{-z}} \cdot \frac{e^{-z}}{1 + e^{-z}} = \sigma(z)(1 - \sigma(z))
\end{aligned}$$

68 Remark 3: By chain rule we have

$$\begin{aligned}
z_i(\omega) &:= -y_i x_i^\top \omega \\
\implies \nabla_\omega z_i(\omega) &= -y_i x_i \\
\implies \nabla_\omega \sigma(z_i(\omega)) &= \sigma'(z_i(\omega)) \nabla_\omega z_i(\omega) \\
&= \sigma(-y_i x_i^\top \omega) (1 - \sigma(-y_i x_i^\top \omega)) (-y_i x_i)
\end{aligned}$$

69 From the gradient we have

$$\nabla_\omega^2 f(\omega) = \nabla_\omega \left(-\frac{1}{n} X^\top (y \odot \sigma(-y \odot (X\omega))) \right) = -\frac{1}{n} X^\top \nabla_\omega (y \odot \sigma(-y \odot (X\omega)))$$

70 Now notice, that

$$y \odot \sigma(-y \odot (X\omega)) = \begin{pmatrix} y_1 \sigma(-y_1 x_1^\top \omega) \\ y_2 \sigma(-y_2 x_2^\top \omega) \\ \vdots \\ y_n \sigma(-y_n x_n^\top \omega) \end{pmatrix}$$

71 and applying Remark 3 yields

$$\begin{aligned}
\nabla_\omega \sigma(-y_i x_i^\top \omega) &= \sigma(-y_i x_i^\top \omega) (1 - \sigma(-y_i x_i^\top \omega)) (-y_i x_i) \\
\implies \nabla_\omega (y_i \sigma(-y_i x_i^\top \omega)) &= - \underbrace{y_i^2}_{=1 \text{ by Remark 1}} \sigma(-y_i x_i^\top \omega) (1 - \sigma(-y_i x_i^\top \omega)) x_i = -\sigma(-y_i x_i^\top \omega) (1 - \sigma(-y_i x_i^\top \omega)) x_i
\end{aligned}$$

$$\begin{aligned}
\Rightarrow \nabla_{\omega}(y \odot \sigma(-y \odot (X\omega))) &= - \begin{pmatrix} \overbrace{\sigma(-y_1 x_1^{\top} \omega)(1 - \sigma(-y_1 x_1^{\top} \omega))}^{=D_{1,1}} x_1 \\ \vdots \\ \underbrace{\sigma(-y_n x_n^{\top} \omega)(1 - \sigma(-y_n x_n^{\top} \omega))}_{D_{n,n}} x_n \end{pmatrix} \\
&= - \begin{bmatrix} D_{1,1} & 0 & \cdots & 0 \\ 0 & D_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & D_{n,n} \end{bmatrix} \begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,d} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,1} & x_{n,2} & \cdots & x_{n,d} \end{bmatrix} \\
&= - \begin{bmatrix} D_{1,1} x_{1,1} & D_{1,1} x_{1,2} & \cdots & D_{1,1} x_{1,d} \\ D_{2,2} x_{2,1} & D_{2,2} x_{2,2} & \cdots & D_{2,2} x_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ D_{n,n} x_{n,1} & D_{n,n} x_{n,2} & \cdots & D_{n,n} x_{n,d} \end{bmatrix} = - \begin{bmatrix} D_{1,1} x_1^{\top} \\ D_{2,2} x_2^{\top} \\ \vdots \\ D_{n,n} x_n^{\top} \end{bmatrix} = -DX
\end{aligned}$$

73 where we factored out the x_i in the last step to rewrite it as matrix-vector product. Deriving the entire
74 expression we conclude:

$$\begin{aligned}
\nabla^2 f(\omega) &= -\frac{1}{n} X^{\top} \nabla_{\omega}(y \odot \sigma(-y \odot (X\omega))) = \frac{1}{n} X^{\top} DX \\
D_{ii} &= \sigma(-y_i x_i^{\top} \omega)(1 - \sigma(-y_i x_i^{\top} \omega))
\end{aligned}$$

75 The hessian of the non-convex regularization term is derived by

$$\begin{aligned}
\nabla_{\omega}^2 r(\omega) &= \nabla_{\omega} \left(2\lambda \alpha \frac{\omega_j}{(1 + \alpha \omega_j^2)^2} \right) \\
\frac{\partial^2}{\partial \omega_j^2} r(\omega) &= 2\lambda \alpha \frac{\partial}{\partial \omega_j} \left(\frac{\omega_j}{(1 + \alpha \omega_j^2)^2} \right) = 2\lambda \alpha \frac{(1 + \alpha \omega_j^2)^2 - 4\alpha \omega_j^2 (1 + \alpha \omega_j^2)}{(1 + \alpha \omega_j^2)^4} = 2\lambda \alpha \frac{1 - 3\alpha \omega_j^2}{(1 + \alpha \omega_j^2)^3} \\
\Rightarrow \nabla^2 r(\omega) &= \text{diag} \left(2\lambda \alpha \frac{1 - 3\alpha \omega_j^2}{(1 + \alpha \omega_j^2)^3} \right)_{j=1, \dots, d}
\end{aligned}$$

76 Combining the steps we derive the Hessian

$$\begin{aligned}
\nabla^2 L_2(\omega) &= \nabla^2 f(\omega) + \nabla^2 r(\omega) = \frac{1}{n} X^{\top} DX + \text{diag} \left(2\lambda \alpha \frac{1 - 3\alpha \omega_j^2}{(1 + \alpha \omega_j^2)^3} \right) \\
D_{ii} &= \sigma(-y_i x_i^{\top} \omega)(1 - \sigma(-y_i x_i^{\top} \omega))
\end{aligned}$$

77 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.

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

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

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

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

80 References

- 81 [1] Jorge Nocedal and Stephen J. Wright. *Numerical Optimization*. Springer, 2nd edition, 2006.
- 82 [2] Konstantin Mishchenko. Regularized newton method with global convergence. *SIAM Journal on*
 83 *Optimization*, 33(3):1440–1462, 2023.
- 84 [3] Slavomír Hanzely, Dmitry Kamzolov, Dmitry Pasechnyuk, Alexander Gasnikov, Peter Richtárik,
 85 and Martin Takáč. A damped newton method achieves global $(o)(\frac{1}{k^2})$ and local quadratic
 86 convergence rate. *Advances in Neural Information Processing Systems*, 35:25320–25334, 2022.
- 87 [4] Kevin P. Murphy. *Machine Learning: A Probabilistic Perspective*. MIT Press, Cambridge, MA,
 88 2012.

89 Checklist

90 The checklist follows the references. Please read the checklist guidelines carefully for information on
 91 how to answer these questions. For each question, change the default **[TODO]** to **[Yes]**, **[No]**, or
 92 **[N/A]**. You are strongly encouraged to include a **justification to your answer**, either by referencing
 93 the appropriate section of your paper or providing a brief inline description. For example:

- 94 • Did you include the license to the code and datasets? **[Yes]** See Section
- 95 • Did you include the license to the code and datasets? **[No]** The code and the data are
 96 proprietary.
- 97 • Did you include the license to the code and datasets? **[N/A]**

98 Please do not modify the questions and only use the provided macros for your answers. Note that the
 99 Checklist section does not count towards the page limit. In your paper, please delete this instructions
 100 block and only keep the Checklist section heading above along with the questions/answers below.

- 101 1. For all authors...
- 102 (a) Do the main claims made in the abstract and introduction accurately reflect the paper’s
 103 contributions and scope? **[TODO]**
- 104 (b) Did you describe the limitations of your work? **[TODO]**
- 105 (c) Did you discuss any potential negative societal impacts of your work? **[TODO]**
- 106 (d) Have you read the ethics review guidelines and ensured that your paper conforms to
 107 them? **[TODO]**
- 108 2. If you are including theoretical results...
- 109 (a) Did you state the full set of assumptions of all theoretical results? **[TODO]**
- 110 (b) Did you include complete proofs of all theoretical results? **[TODO]**
- 111 3. If you ran experiments...
- 112 (a) Did you include the code, data, and instructions needed to reproduce the main experi-
 113 mental results (either in the supplemental material or as a URL)? **[TODO]**
- 114 (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they
 115 were chosen)? **[TODO]**
- 116 (c) Did you report error bars (e.g., with respect to the random seed after running experi-
 117 ments multiple times)? **[TODO]**
- 118 (d) Did you include the total amount of compute and the type of resources used (e.g., type
 119 of GPUs, internal cluster, or cloud provider)? **[TODO]**
- 120 4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
- 121 (a) If your work uses existing assets, did you cite the creators? **[TODO]**

- 122 (b) Did you mention the license of the assets? **[TODO]**
- 123 (c) Did you include any new assets either in the supplemental material or as a URL?
- 124 **[TODO]**
- 125 (d) Did you discuss whether and how consent was obtained from people whose data you're
- 126 using/curating? **[TODO]**
- 127 (e) Did you discuss whether the data you are using/curating contains personally identifiable
- 128 information or offensive content? **[TODO]**
- 129 5. If you used crowdsourcing or conducted research with human subjects...
- 130 (a) Did you include the full text of instructions given to participants and screenshots, if
- 131 applicable? **[TODO]**
- 132 (b) Did you describe any potential participant risks, with links to Institutional Review
- 133 Board (IRB) approvals, if applicable? **[TODO]**
- 134 (c) Did you include the estimated hourly wage paid to participants and the total amount
- 135 spent on participant compensation? **[TODO]**

136 **A Appendix**

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