Improving L-BFGS Initialization for Trust-Region Methods in Deep Learning

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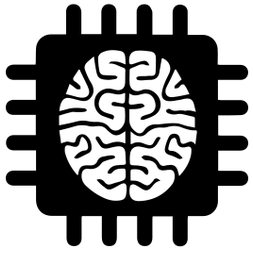


Agenda

- Introduction, Problem Statement and Motivations
- Overview on Quasi-Newton Optimization Methods
- L-BFGS Trust Region Optimization Method
- Proposed Methods for Initialization of L-BFGS
- Application in Deep Learning (Image Classification Task)

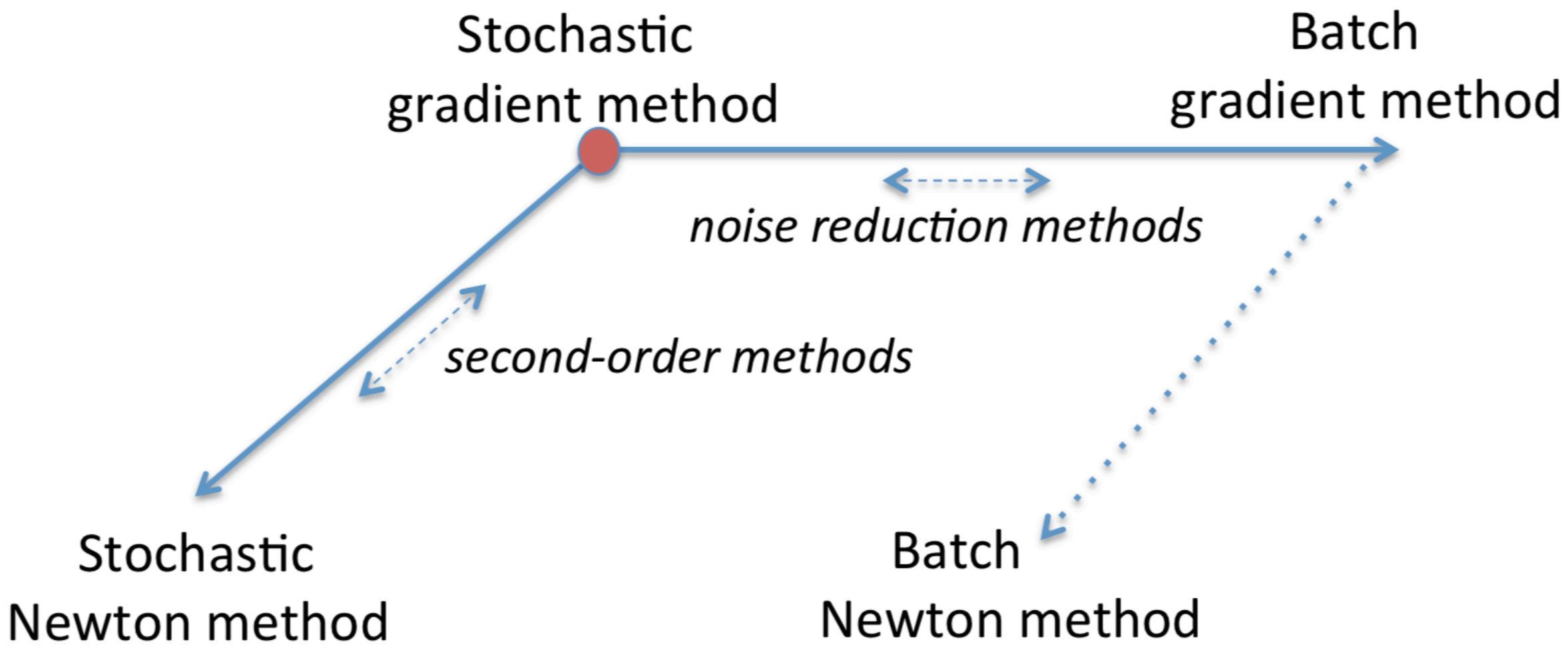
Introduction, Problem Statement and Motivations

Unconstrained Optimization Problem

$$\min_{w \in \mathbb{R}^n} \mathcal{L}(w) \triangleq \frac{1}{N} \sum_{i=1}^{N} \ell_i(w)$$

$$\mathcal{L} : \mathbb{R}^n \to \mathbb{R}$$

Optimization Algorithms



Bottou et al., (2016) Optimization methods for large-scale machine learning, print arXiv:1606.04838

Optimization Algorithms

1. Start from a random point w_0
2. Repeat each iteration, $k = 0, 1, 2, \ldots,$
    3. Choose a search direction p_k
    4. Choose a step size α_k
    5. Update parameters $w_{k+1} \leftarrow w_k + \alpha_k p_k$
6. Until $\|\nabla \mathcal{L}\| < \epsilon$

Properties of Objective Function

$$\min_{w \in \mathbb{R}^n} \mathcal{L}(w) \triangleq \frac{1}{N} \sum_{i=1}^{N} \ell_i(w)$$

- n and N are both large in modern applications.
- $\mathcal{L}(w)$ is a non-convex and nonlinear function.
- $\nabla^2 \mathcal{L}(w)$ is ill-conditioned.
- Computing full gradient, $\nabla \mathcal{L}$ is expensive.
- Computing Hessian, $\nabla^2 \mathcal{L}$ is not practical.

Stochastic Gradient Decent

1. Sample indices $\mathcal{S}_k \subset \{1, 2, \ldots, N\}$

2. Compute *stochastic* (subsampled) gradient

$$\nabla \mathcal{L}(w_k) \approx \nabla \mathcal{L}(w_k)^{(\mathcal{S}_k)} \triangleq \frac{1}{|\mathcal{S}_k|} \sum_{i \in \mathcal{S}_k} \nabla \ell_i(w_k)$$

3. Assign a *learning rate* α_k

4. Update parameters using $p_k = -\nabla \mathcal{L}(w_k)^{(\mathcal{S}_k)}$

$$w_{k+1} \leftarrow w_k - \alpha_k \nabla \mathcal{L}(w_k)^{(\mathcal{S}_k)}$$

H. Robbins, D. Siegmund. (1971). ”A convergence theorem for non negative almost supermartingales and some applications”. Optimizing methods in statistics.

Advantages of SGD

- SGD algorithms are very easy to implement.
- SGD requires only computing the gradient.
- SGD has a low cost-per-iteration.

Bottou et al., (2016) Optimization methods for large-scale machine learning, print arXiv:1606.04838

Disadvantages of SGD

- Very sensitive to the ill-conditioning problem and scaling.
- Requires fine-tuning many hyper-parameters.
- Unlikely exhibit acceptable performance on first try.
- requires many trials and errors.
- Can stuck in a saddle-point instead of local minimum.
- Sublinear and slow rate of convergence.

Bottou et al., (2016). Optimization methods for large-scale machine learning. print arXiv:1606.04838
J. Nocedal and S. J. Wright. (2006). Numerical Optimization. 2nd ed. New York. Springer.

Second-Order Methods

1. Sample indices $\mathcal{S}_k \subset \{1, 2, \ldots, N\}$

2. Compute *stochastic* (subsampled) gradient

$$\nabla \mathcal{L}(w_k) \approx \nabla \mathcal{L}(w_k)^{(\mathcal{S}_k)} \triangleq \frac{1}{|\mathcal{S}_k|} \sum_{i \in \mathcal{S}_k} \nabla \ell_i(w_k)$$

3. Compute Hessian

$$\nabla^2 \mathcal{L}(w_k) \approx \nabla^2 \mathcal{L}(w_k)^{(\mathcal{S}_k)} \triangleq \frac{1}{|\mathcal{S}_k|} \sum_{i \in \mathcal{S}_k} \nabla^2 \ell_i(w_k)$$

Second-Order Methods

4. Compute Newton's direction

$$p_k = -\nabla^2 \mathcal{L}(w_k)^{-1} \nabla \mathcal{L}(w_k)$$

5. Find proper step length

$$\alpha_k = \min_{\alpha} \mathcal{L}(w_k + \alpha p_k)$$

6. Update parameters

$$w_{k+1} \leftarrow w_k + \alpha_k p_k$$

Second-Order Methods Advantages

- The rate of convergence is super-linear (quadratic for Newton method).
- They are resilient to problem ill-conditioning.
- They involve less parameter tuning.
- They are less sensitive to the choice of hyper-parameters.

J. Nocedal and S. J. Wright. (2006). Numerical Optimization. 2nd ed. New York. Springer.

Second-Order Methods Disadvantages

- Computing the Hessian matrix is very expensive and requires massive storage.
- Computing the inverse of Hessian is not practical.

J. Nocedal and S. J. Wright. (2006). Numerical Optimization. 2nd ed. New York. Springer.
Bottou et al., (2016) Optimization methods for large-scale machine learning, print arXiv:1606.04838

Quasi-Newton Methods

1. Construct a **low-rank** approximation of Hessian

$$B_k \approx \nabla^2 \mathcal{L}(w_k)$$

2. Find the search direction by Minimizing the **Quadratic Model** of the objective function

$$p_k = \underset{p \in \mathbb{R}^n}{\operatorname{argmin}} \ \mathcal{Q}_k(p) \triangleq g_k^T p + \frac{1}{2} p^T B_k p^T$$

Quasi-Newton Matrices

- Symmetric
- Easy and Fast Computation
- Satisfies Secant Condition

$$B_{k+1} s_k = y_k$$

$$s_k \triangleq w_{k+1} - w_k$$

$$y_k \triangleq \nabla \mathcal{L}(w_{k+1}) - \nabla \mathcal{L}(w_k)$$

Broyden **F**letcher **G**oldfarb **S**hanno.

J. Nocedal and S. J. Wright. (2006). Numerical Optimization. 2nd ed. New York. Springer.

Broyden **F**letcher **G**oldfarb **S**hanno.

$$B_{k+1} = B_k - \frac{1}{s_k^T B_k s_k} B_k s_k s_k^T B_k + \frac{1}{y_k^T s_k} y_k y_k^T,$$

$$s_k \triangleq w_{k+1} - w_k$$

$$y_k \triangleq \nabla \mathcal{L}(w_{k+1}) - \nabla \mathcal{L}(w_k)$$

$$B_0 = \gamma_k I$$

J. Nocedal and S. J. Wright. (2006). Numerical Optimization. 2nd ed. New York. Springer.

Quasi-Newton Methods Advantages

- The rate of convergence is super-linear.
- They are resilient to problem ill-conditioning.
- The second derivative is not required.
- They only use the gradient information to construct quasi-Newton matrices.

J. Nocedal and S. J. Wright. (2006). Numerical Optimization. 2nd ed. New York. Springer.

Quasi-Newton Methods disadvantages

- The cost of storing the gradient informations can be expensive.
- The quasi-Newton matrix can be dense.
- The quasi-Newton matrix grow in size and rank in large-scale problems.

J. Nocedal and S. J. Wright. (2006). Numerical Optimization. 2nd ed. New York. Springer.

Limited-Memory BFGS

Limited Memory Storage

$$S_k = \begin{bmatrix} s_{k-m} & \cdots & s_{k-1} \end{bmatrix} \qquad Y_k = \begin{bmatrix} y_{k-m} & \cdots & y_{k-1} \end{bmatrix}$$

L-BFGS Compact Representation

$$B_k = B_0 + \Psi_k M_k \Psi_k^T$$

$$B_0 = \gamma_k I$$

where

$$\Psi_k = \begin{bmatrix} B_0 S_k & Y_k \end{bmatrix}, \quad M_k = \begin{bmatrix} -S_k^T B_0 S_k & -L_k \\ -L_k^T & D_k \end{bmatrix}^{-1}$$

$$S_k^T Y_k = L_k + D_k + U_k$$

Limited-Memory Quasi-Newton Methods

- Low rank approximation
- Small memory of recent gradients.
- Low cost of computation of search direction.
- Linear or superlinear Convergence rate can be achieved.

J. Nocedal and S. J. Wright. (2006). Numerical Optimization. 2nd ed. New York. Springer.

Objectives

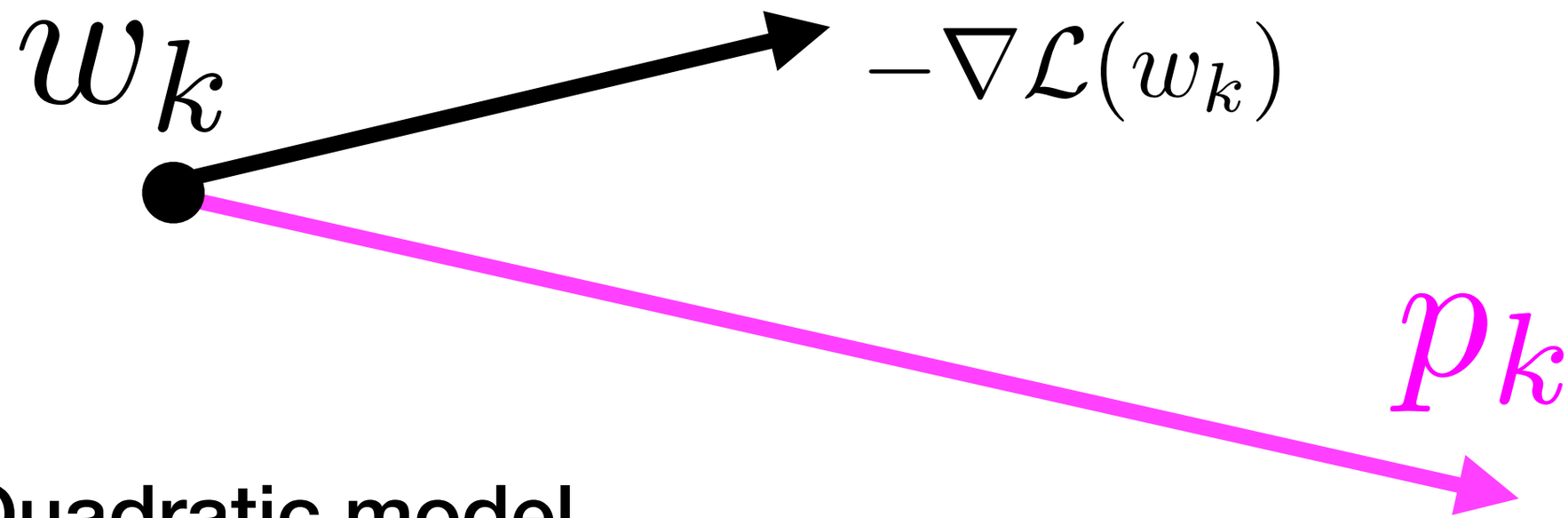
$$B_0 = \gamma_k I$$

$$B_k = B_0 + \Psi_k M_k \Psi_k^T$$

What is the best choice for initialization?

Overview on Quasi-Newton Optimization Strategies

Line Search Method



Quadratic model

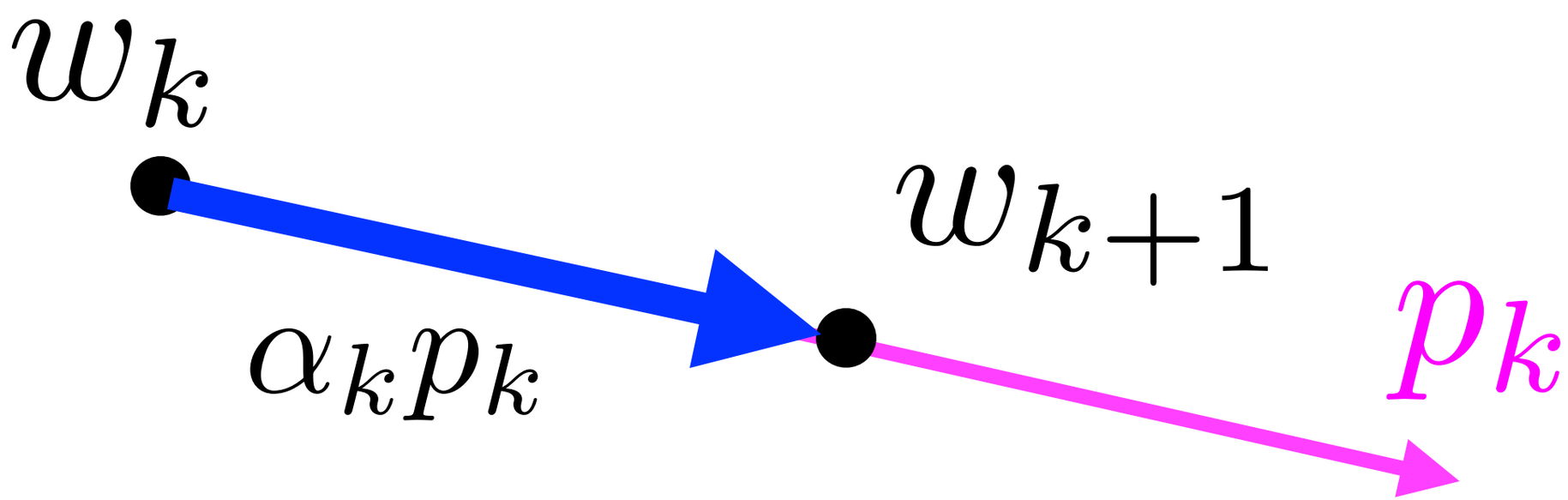
$$p_k = \underset{p \in \mathbb{R}^n}{\operatorname{argmin}} \; \mathcal{Q}_k(p) \triangleq g_k^T p + \frac{1}{2} p^T B_k p^T$$

if B_k is positive definite:

$$p_k = B_k^{-1} g_k$$

J. Nocedal and S. J. Wright. (2006). Numerical Optimization. 2nd ed. New York. Springer.

Line Search Method



Wolfe conditions

$$\mathcal{L}(w_k + \alpha_k p_k) \leq \mathcal{L}(w_k) + c_1 \alpha_k \nabla \mathcal{L}(w_k)^T p_k$$

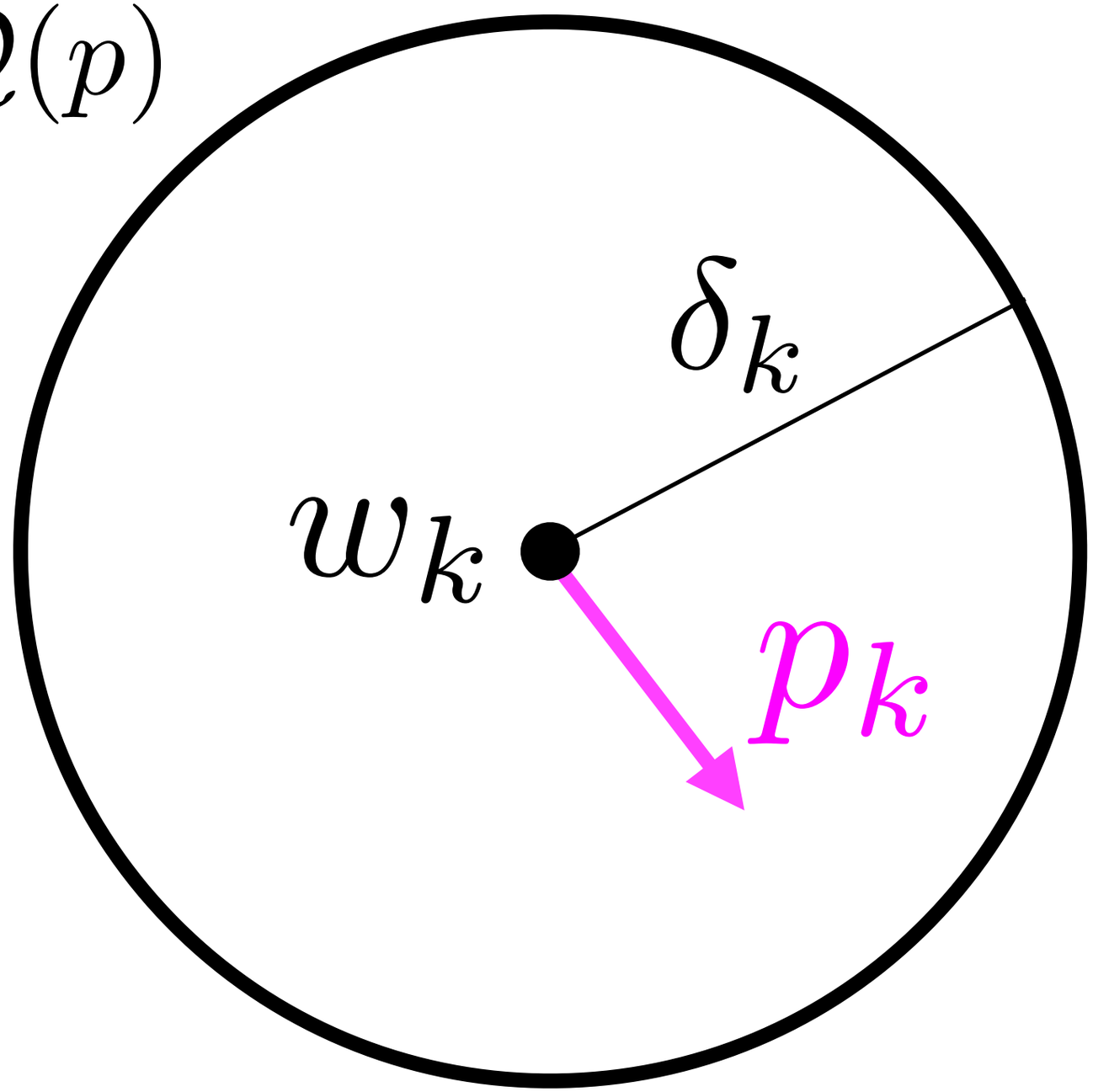
$$\nabla \mathcal{L}(w_k + \alpha_k p_k)^T p_k \geq c_2 \nabla f(w_k)^T p_k$$

J. Nocedal and S. J. Wright. (2006). Numerical Optimization. 2nd ed. New York. Springer.

Trust Region Method

$$p_k = \arg\min_{p \in \mathbb{R}^n} \mathcal{Q}(p)$$

$$\text{s.t. } \|p\|_2 \leq \delta_k$$



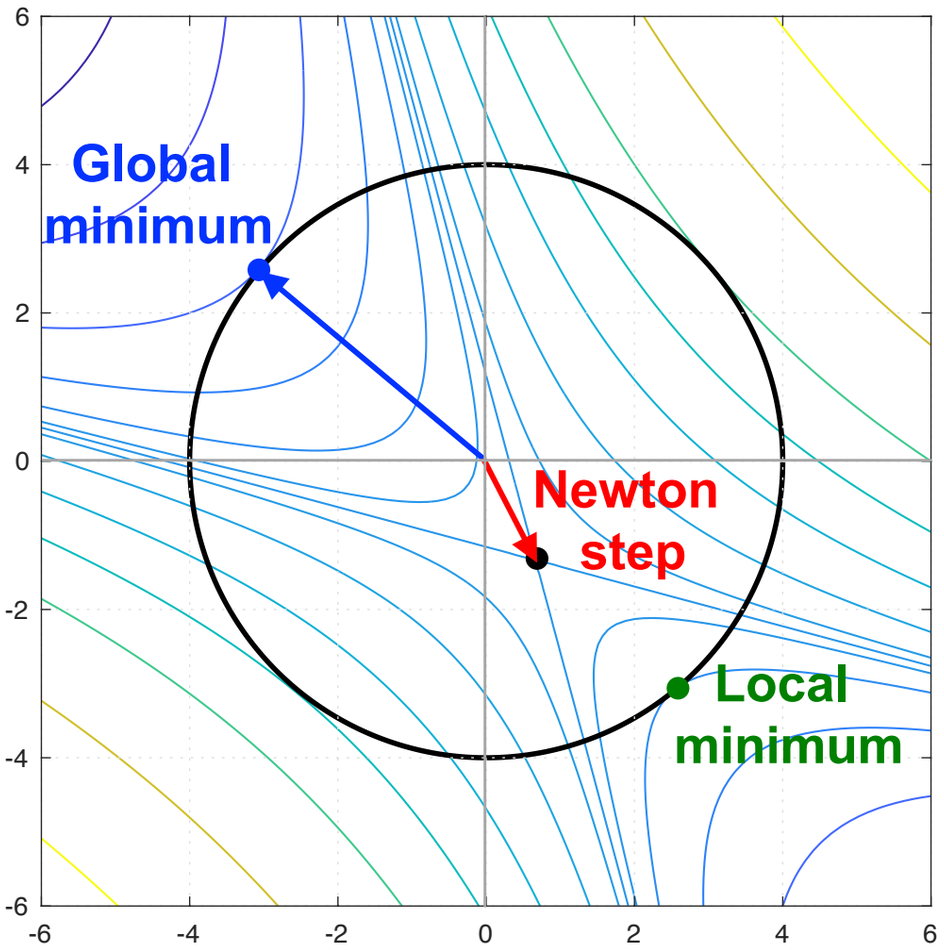
Toint et al. (2000), Trust Region Methods, SIAM.

Trust Region Method

Theorem. Let δ be a positive constant. A vector p^* is a global solution of the trust-region subproblem if and only if $\|p^*\|_2 \leq \delta$ and there exists a unique $\sigma^* \geq 0$ such that $B + \sigma^* I$ is positive semidefinite and

$$(B + \sigma^* I)p^* = -g \quad \text{and} \quad \sigma^*(\delta - \|p^*\|_2) = 0.$$

Moreover, if $B + \sigma^* I$ is positive definite, then the global minimizer is unique.



J. J. Mor´e and D. C. Sorensen, (1984) Newton's method, in Studies in Mathematics, Volume 24. Studies in Numerical Analysis, Math. Assoc., pp. 29–82.

L-BFGS Trust Region Optimization Method

L-BFGS in Trust Region

$$B_k = B_0 + \Psi_k M_k \Psi_k^T$$

Eigen-decomposition

$$B_k = P \begin{bmatrix} \Lambda + \gamma_k I & 0 \\ 0 & \gamma_k I \end{bmatrix} P^T$$

Sherman-Morrison-Woodbury Formula

$$p_k^* = -\frac{1}{\tau^*} \left[I - \Psi_k (\tau^* M_k^{-1} + \Psi_k^T \Psi_k)^{-1} \Psi_k^T \right] g_k,$$

$$\tau^* = \gamma_k + \sigma^*$$

L. Adhikari et al. (2017) “Limited-memory trust-region methods for sparse relaxation,” in Proc.SPIE, vol. 10394.
Brust et al, (2017). “On solving L-SR1 trust-region subproblems,” Computational Optimization and Applications, vol. 66, pp. 245–266.

L-BFGS in Trust Region vs. Line-Search

Trust-Region Minimization Algorithm for Training Responses (TRMinATR): The Rise of Machine Learning Techniques

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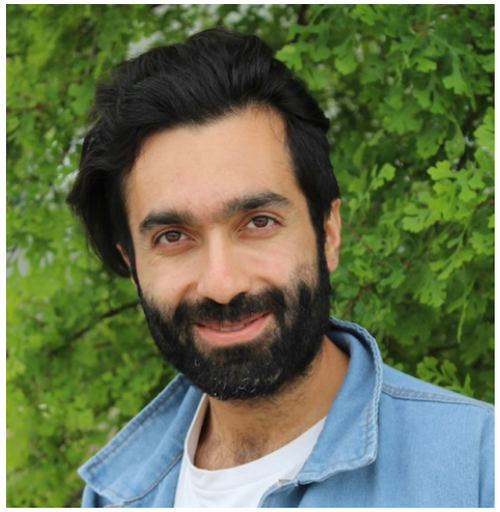


26th European Signal Processing Conference, Rome, Italy. September 2018.

Proposed Methods for Initialization of L-BFGS

Initialization Method I

$$B_0 = \gamma_k I$$

$$B_k = B_0 + \Psi_k M_k \Psi_k^T$$

Spectral estimate of Hessian

$$\gamma_k = \frac{y_{k-1}^T y_{k-1}}{s_{k-1}^T y_{k-1}}$$

$$\gamma_k = \arg\min_{\gamma} \|B_0^{-1} y_{k-1} - s_{k-1}\|_2^2, \quad B_0 = \gamma I$$

J. Nocedal and S. J. Wright. (2006). Numerical Optimization. 2nd ed. New York. Springer.

Initialization Method II

Consider a quadratic function

$$\mathcal{L}(w) = \frac{1}{2} w^T H w + g^T w \qquad \nabla^2 \mathcal{L}(w) = H$$

We have

$$H S_k = Y_k$$

Therefore

$$S_k^T H S_k = S_k^T Y_k$$

Erway et al. (2018). “Trust-Region Algorithms for Training Responses: Machine Learning Methods Using Indefinite Hessian Approximations,” ArXiv e-prints.

Initialization Method II

Since

$$B_k = B_0 + \Psi_k M_k \Psi_k^T \qquad B_0 = \gamma_k I$$

$$\Psi_k = \begin{bmatrix} B_0 S_k & Y_k \end{bmatrix}, \quad M_k = \begin{bmatrix} -S_k^T B_0 S_k & -L_k \\ -L_k^T & D_k \end{bmatrix}^{-1}$$

Secant Condition

$$B_k S_k^T = Y_k$$

We have

$$S_k^T H S_k - \gamma_k S_k^T S_k = S_k^T \Psi_k M_k \Psi_k^T S_k$$

Initialization Method II

$$S_k^T H S_k - \gamma_k S_k^T S_k = S_k^T \Psi_k M_k \Psi_k^T S_k$$

General Eigen-Value Problem

$$(L_k + D_k + L_k^T) z = \lambda S_k^T S_k z$$

Upper bound for initial value to avoid false curvature information

$$\gamma_k \in (0, \lambda_{\min})$$

Initialization Method III

$$B_0 = \gamma_k I \qquad\qquad B_k = B_0 + \Psi_k M_k \Psi_k^T$$

$$S_k^T H S_k - \gamma_k S_k^T S_k = S_k^T \Psi_k M_k \Psi_k^T S_k$$

Note that compact representation matrices contains γ_k

$$\Psi_k = \begin{bmatrix} B_0 S_k & Y_k \end{bmatrix}, \quad M_k = \begin{bmatrix} -S_k^T B_0 S_k & -L_k \\ -L_k^T & D_k \end{bmatrix}^{-1}$$

Initialization Method III

General Eigen-Value Problem

$$A^* z = \lambda B^* z$$

Upper bound for initial values to avoid false curvature information

$$\gamma_k \in (0, \lambda_{\min})$$

$$A^* = L_k + D_k + L_k^T - S_k^T Y_k \tilde{D} Y_k^T S_k - \gamma_{k-1}^2 (S_k^T S_k \tilde{A} S_k^T S_k),$$
$$B^* = S_k^T S_k + S_k^T S_k \tilde{B} Y_k^T S_k^T + S_k^T Y_k \tilde{B}^T S_k^T S_k.$$

Applications in Deep Learning

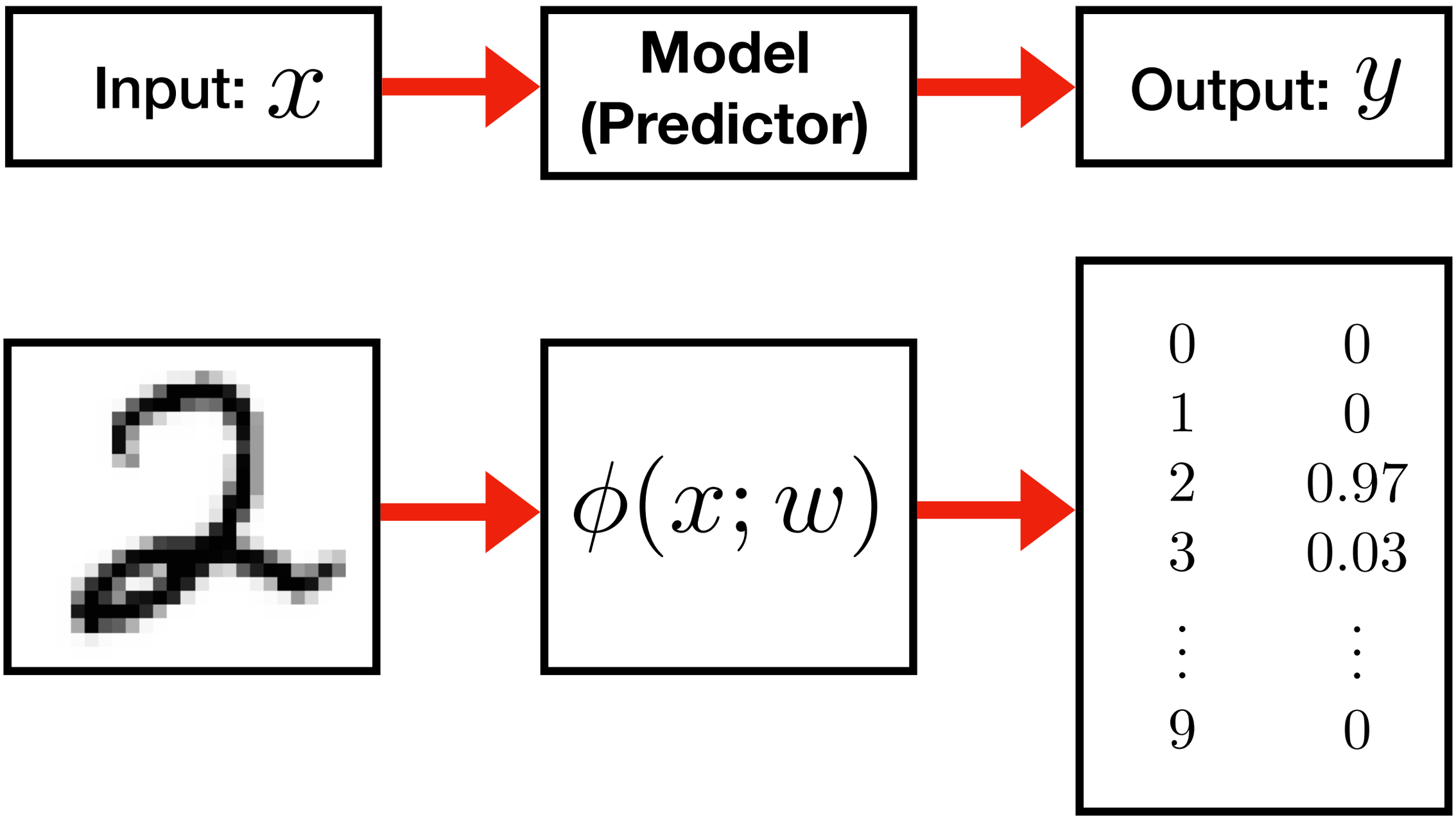
Supervised Learning

Features $X = \{x_1, x_2, \ldots, x_i, \ldots, x_N\}$

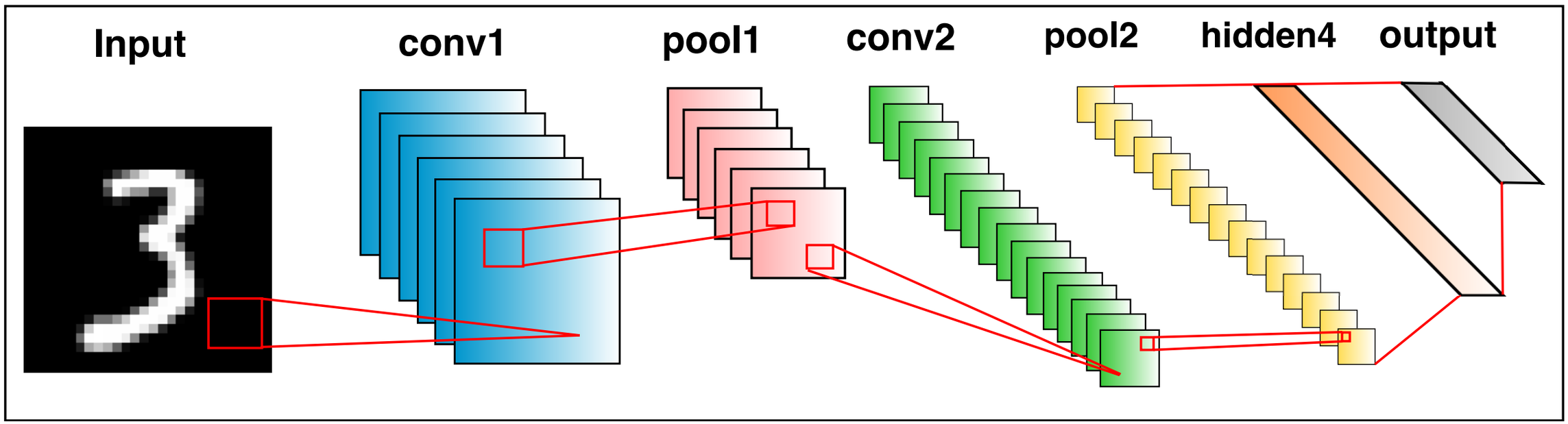
Labels $T = \{t_1, t_2, \ldots, t_i, \ldots, t_N\}$

$$\Phi : X \rightarrow T$$

Supervised Learning



Convolutional Neural Network



$$\phi(x; w)$$

$$n = 413,080$$

Lecun et al. (1998) “Gradient-basedlearning applied to document recognition,” Proceedings of the IEEE, vol. 86, no. 11, pp. 2278–2324.

Loss Function

Target $t = \begin{bmatrix} 0, & 0, & 1, & 0, & \dots, & 0 \end{bmatrix}$

Output $y = \begin{bmatrix} 0, & 0, & 0.97, & 0.03, & \dots, & 0 \end{bmatrix}$

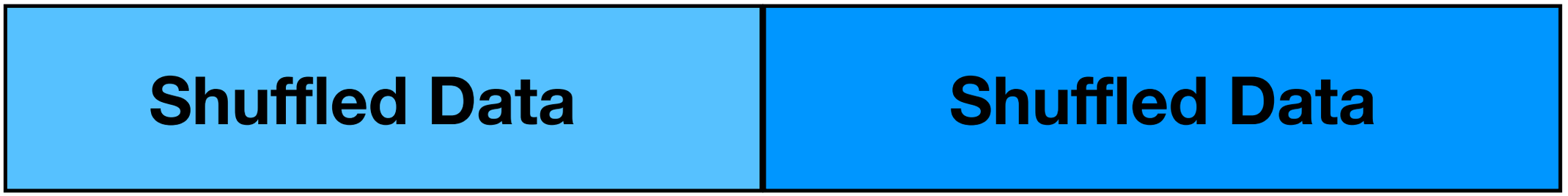
Cross-entropy

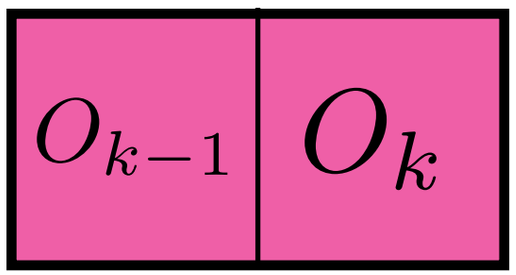
$$\ell(t, y) = -t.\log(y) - (1 - t).\log(1 - y)$$

Empirical Risk

$$\mathcal{L}(w) = \frac{1}{N} \sum_{i=1}^{N} \ell(t_i, \phi(x_i, w))$$

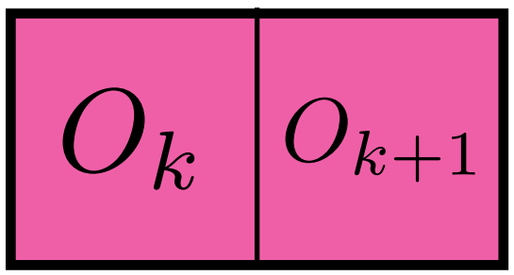
Multi-Batch L-BFGS



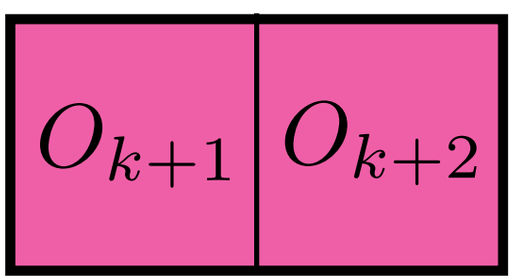


$\mathcal{S}_k$

$O_k = \mathcal{S}_k \cap \mathcal{S}_{k+1}$



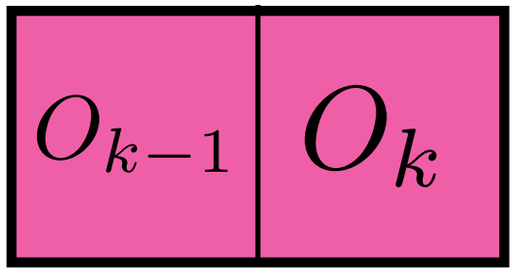
$\mathcal{S}_{k+1}$



$\mathcal{S}_{k+2}$

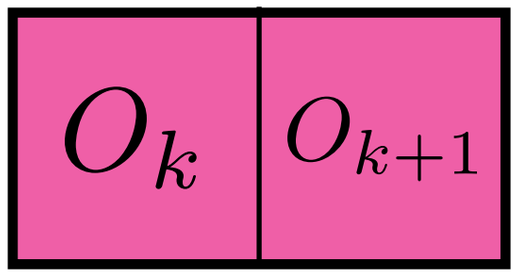
Berahas et al. (2016). “A multi-batch L-BFGS method for machine learning,” in Advances in Neural Information Processing Systems 29, pp. 1055–1063.

Computing gradients



$\mathcal{S}_k$

$O_k = \mathcal{S}_k \cap \mathcal{S}_{k+1}$



$\mathcal{S}_{k+1}$

$$g_k = \nabla \mathcal{L}(w_k)^{(\mathcal{S}_k)} = \frac{1}{|\mathcal{S}_k|} \sum_{i \in J_k} \nabla \mathcal{L}_i(w_k)$$

$$y_k = \nabla \mathcal{L}(w_{k+1})^{(O_k)} - \nabla \mathcal{L}(w_k)^{(O_k)}$$

Berahas et al. (2016). “A multi-batch L-BFGS method for machine learning,” in Advances in Neural Information Processing Systems 29, pp. 1055–1063.

Experiment

Initialization	Source	Formula
Method I	Solve the optimization problem: $\gamma_k = \arg\min_\gamma \|B_0^{-1} y_{k-1} - s_{k-1}\|_2^2$	$\gamma_k = \max\left\{1, \frac{y_{k-1}^T y_{k-1}}{s_{k-1}^T y_{k-1}}\right\}$
Method II	Solve the generalized eigenvalue problem: $(L_k + D_k + L_k^T)z = \lambda S_k^T S_k z$	$\gamma_k = \begin{cases} \max\{1, 0.9\lambda_{\min}\} & \text{if } \lambda_{\min} > 0, \\ \text{Use Method I} & \text{if } \lambda_{\min} \leq 0. \end{cases}$
Method III	Solve the generalized eigenvalue problem: $A^* z = B^* \lambda z$	$\gamma_k = \begin{cases} \max\{1, 0.9\lambda_{\min}\} & \text{if } \lambda_{\min} > 0, \\ \text{Use Method I} & \text{if } \lambda_{\min} \leq 0. \end{cases}$

Trust-Region Algorithm

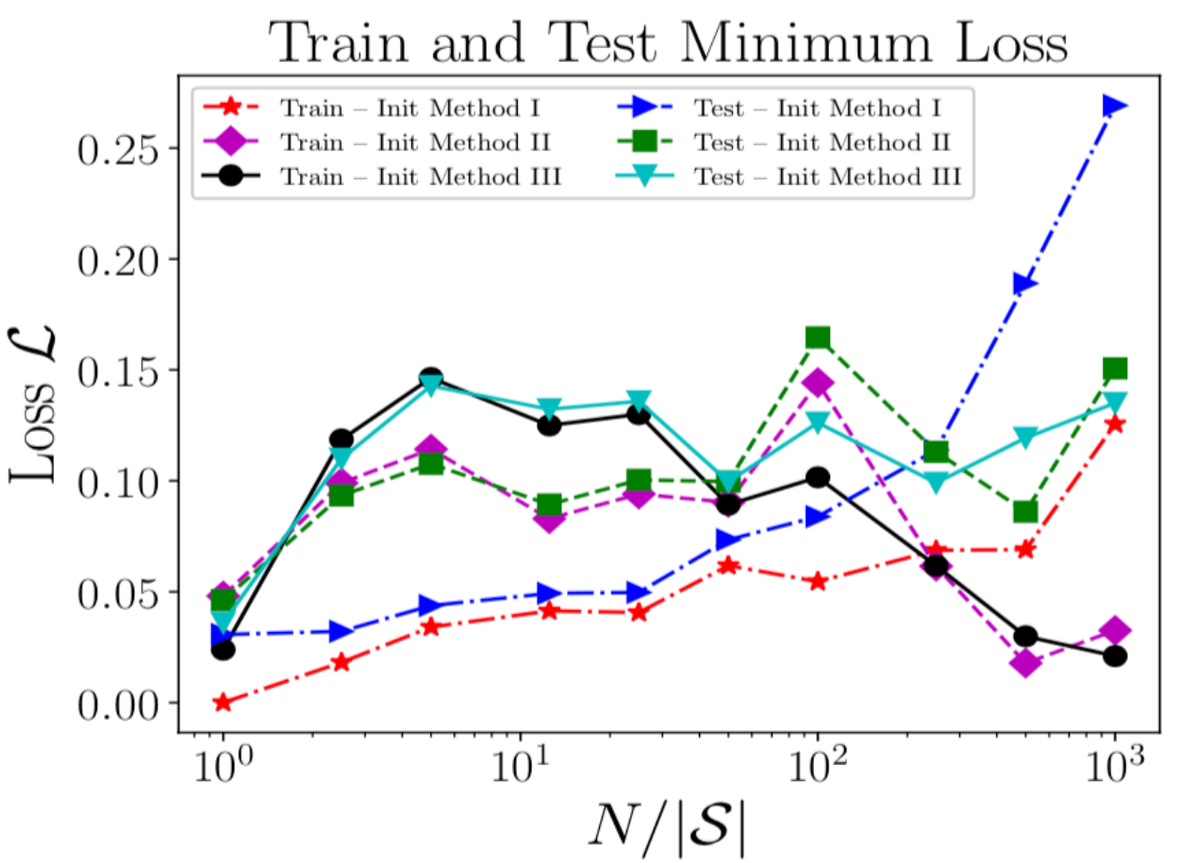
Algorithm Limited-memory BFGS trust-region method.

Input: starting point w_0, tolerance $\epsilon > 0$, δ_0, $\eta < \frac{1}{4}$
Choose initialization **Method I**, **Method II**, or **Method III**

for $k = 0, 1, 2, \ldots$ **do**
  Compute $g_k = \nabla \mathcal{L}(w_k)$
  Compute γ_k to initialize $B_0 = \gamma_k I$
  $\gamma_k \leftarrow \max\{\gamma_k, 1\}$
  Compute Ψ_k and M_k
  Form B_k orthonormal matrices
  Compute search step p_k by solving TR subproblem
  Compute $s_k = p_k$ and $y_k = \nabla \mathcal{L}(w_k + p_k) - \nabla \mathcal{L}(w_k)$
  if $s_k^T y_k > 0$ **then**
    Store $\{s_k, y_k\}$ in storage S_{k+1} and Y_{k+1}
    Discard $\{s_{k-m}, y_{k-m}\}$ from storage if $k > m$
  end if
  $\rho_k \leftarrow (\mathcal{L}(w_k) - \mathcal{L}(w_k + p_k))/(\mathbf{Q}_k(0) - \mathbf{Q}_k(p_k))$
  if $\rho_k > \eta$ **then**
    $w_{k+1} = w_k + p_k$
  else
    $w_{k+1} = w_k$
  end if
  Update trust-region radius δ_{k+1}
  if $\|g\|_2 < \epsilon$ or k reached to maximum episodes **then**
    break
  end if
end for

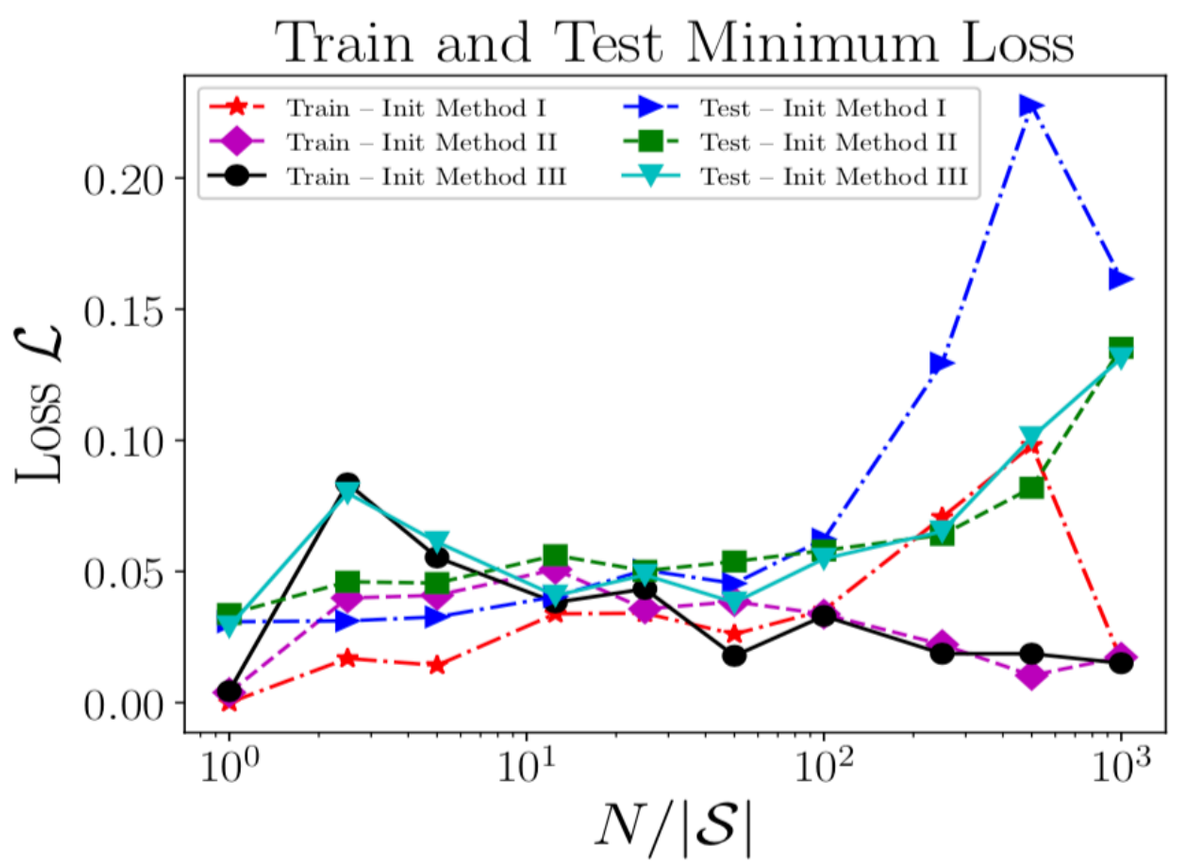
Results - Loss

$m = 10$



Full ⟷ **Stochastic**

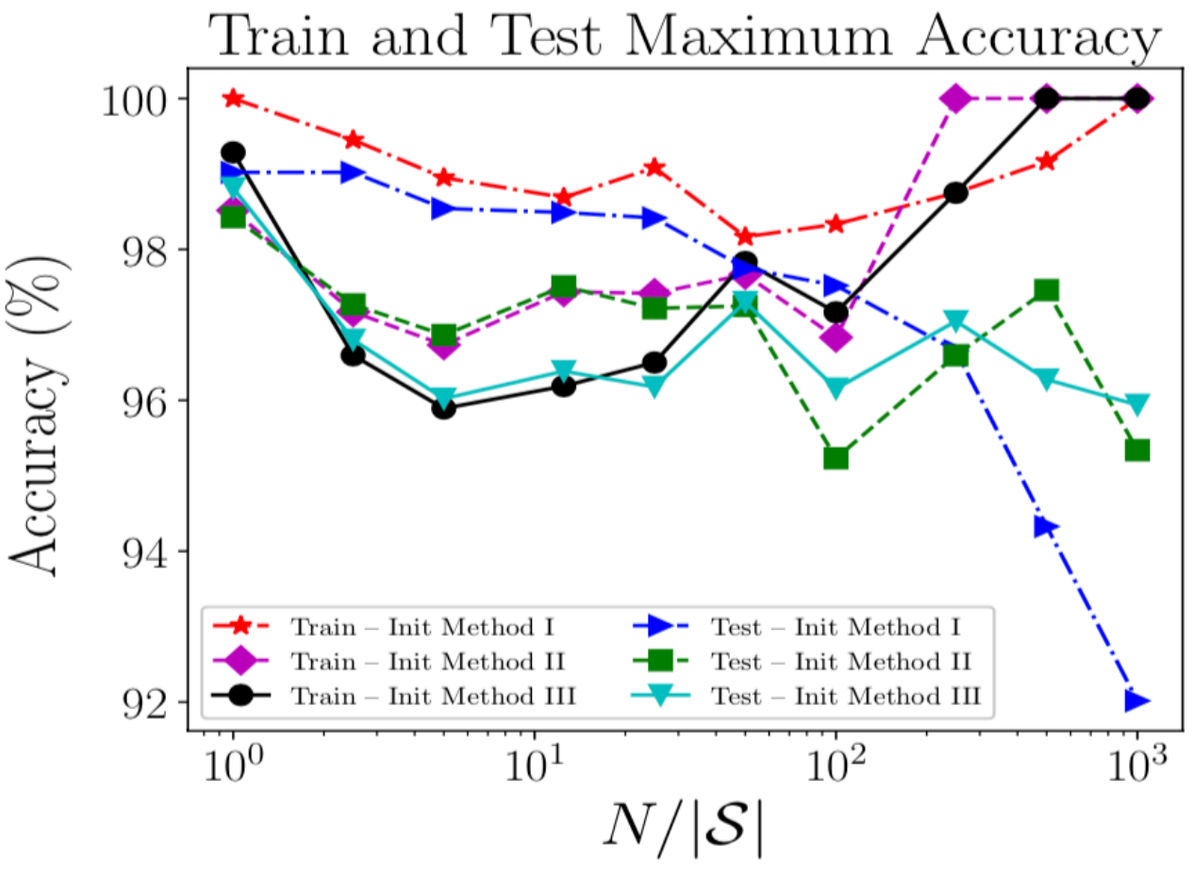
$m = 20$



Full ⟷ **Stochastic**

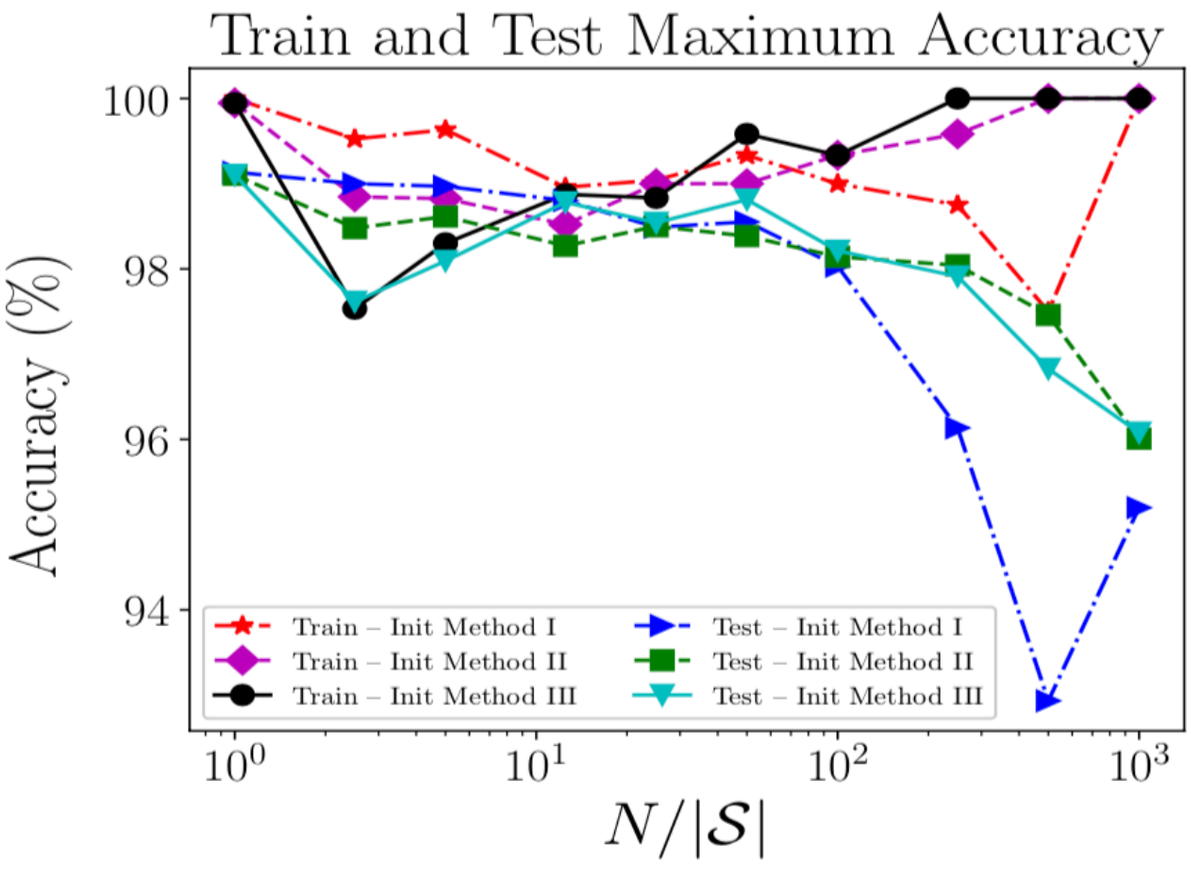
Results - Accuracy

$m = 10$



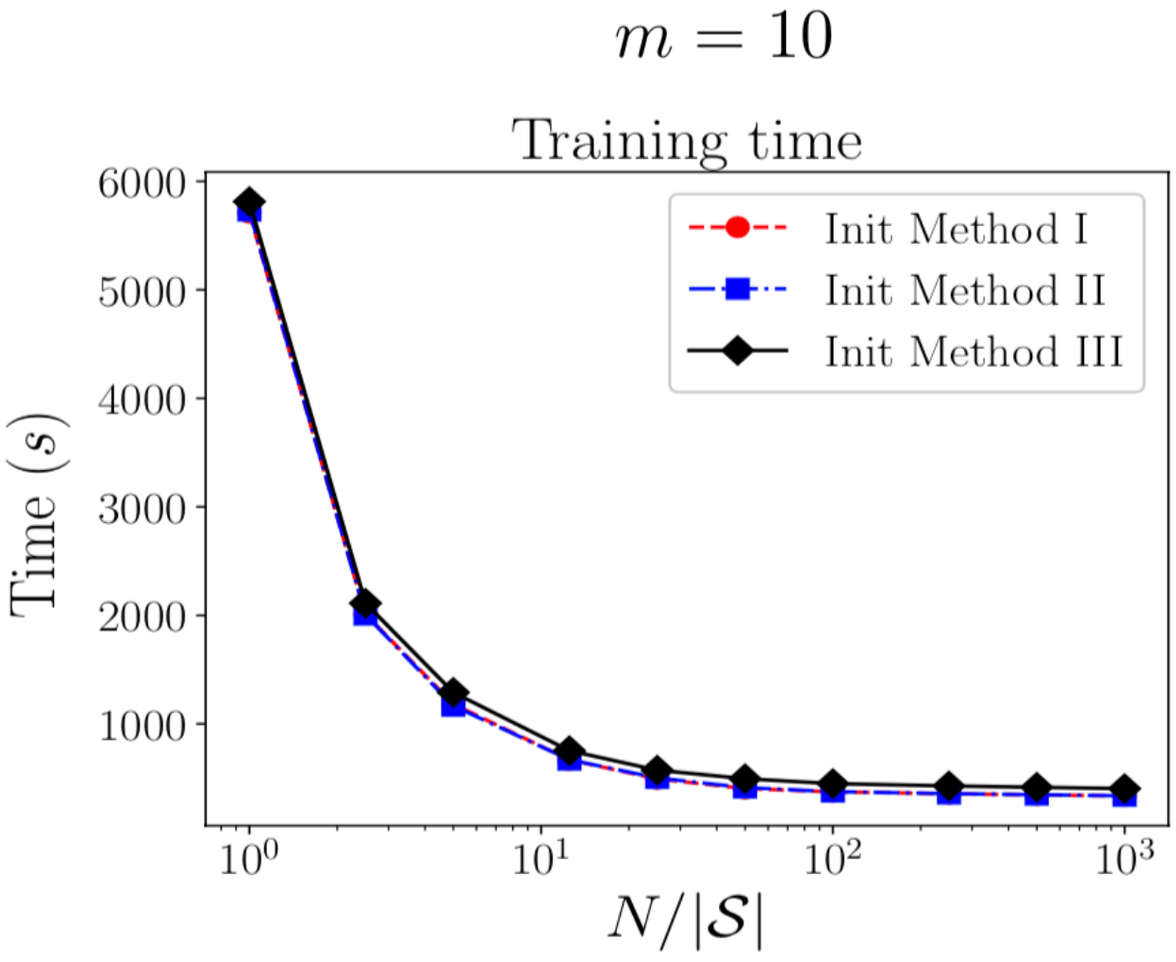
Full ⟷ **Stochastic**

$m = 20$



Full ⟷ **Stochastic**

Results - Training Time



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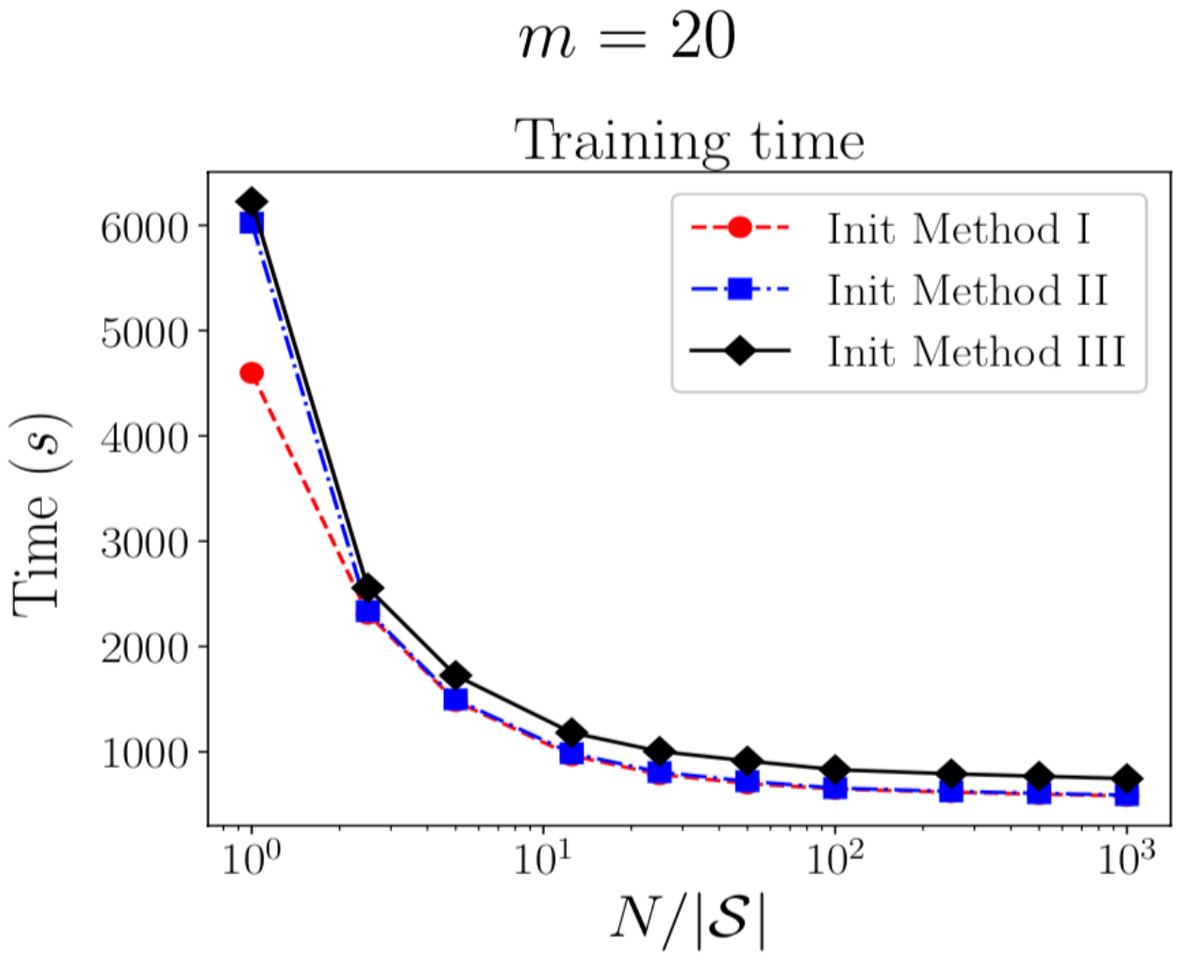

Full ⟷ **Stochastic**

Acknowledgement

Improving L-BFGS Initialization For Trust-Region Methods In Deep Learning

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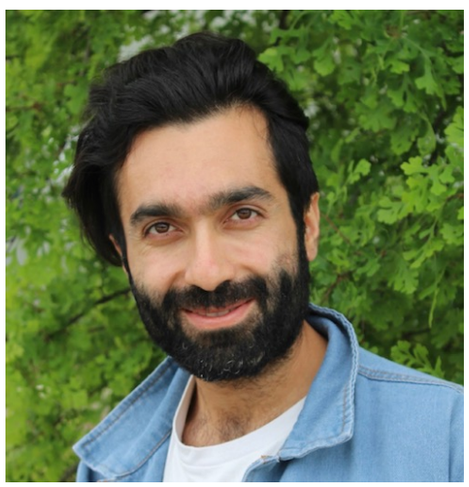

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