S01 supplemental methods

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November 03, 2025

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1 Supplemental Methods

This section provides detailed methodological information that supplements Section ??.

1.1 S1.1 Extended Algorithm Variants

1.1.1 S1.1.1 Stochastic Variant

For large-scale problems, we developed a stochastic variant of our algorithm:

$$x_{k+1} = x_k \ _k f_{i_k}(x_k) + _k(x_k \ x_{k1}) \tag{1.1}$$

where i_k is a randomly sampled index from $\{1, , n\}$ at iteration k.

Convergence Analysis: Under appropriate sampling strategies, this variant achieves $O(1/k)$ convergence rate for non-strongly convex problems.

1.1.2 S1.1.2 Mini-Batch Variant

To balance between computational efficiency and convergence speed:

$$x_{k+1} = x_k \ _k \frac{1}{|B_k|} \ _{iB_k} f_i(x_k) + _k(x_k \ x_{k1}) \tag{1.2}$$

where $B_k \ \{1, , n\}$ is a mini-batch of size $|B_k| = b$.

1.2 S1.2 Detailed Convergence Analysis

1.2.1 S1.2.1 Strong Convexity Assumptions

We assume the objective function f satisfies:

$$f(y) \ f(x) + f(x)^T(y \ x) + \frac{}{2}y \ x^2, \quad x, y \ X \tag{1.3}$$

where > 0 is the strong convexity parameter.

1.2.2 S1.2.2 Lipschitz Continuity

The gradient is Lipschitz continuous:

$$f(x) \ f(y) \ Lx \ y, \quad x, y \ X \tag{1.4}$$

The condition number $= L/$ determines the convergence rate: $= 1 \ 1/$.

1.3 S1.3 Additional Theoretical Results

1.3.1 S1.3.1 Worst-Case Complexity Bounds

Theorem S1: Under the assumptions of Lipschitz continuity and strong convexity, the algorithm requires at most $O(\log(1/))$ iterations to achieve -accuracy.

Proof: From the convergence rate (??), we have:

$$x_k \ x \ C^k \quad k \ \frac{\log(C/)}{\log(1/)} = O(\log(1/)) \tag{1.5}$$

since $\log(1/) \ 1/$ for small $1/$. □

1.3.2 S1.3.2 Expected Convergence for Stochastic Variants

For the stochastic variant (1.1):

$$E[x_k \ x^2] \ \frac{C}{k} + {}^2 \tag{1.6}$$

where ^{2} is the variance of the stochastic gradient estimates.

1.4 S1.4 Implementation Considerations

1.4.1 S1.4.1 Numerical Stability

To ensure numerical stability, we implement the following safeguards:

1. Gradient clipping: $f(x_k) \ \min(1, /f(x_k))f(x_k)$
2. Step size bounds: ${}_{\min} \ k \ {}_{\max}$
3. Momentum bounds: $0 \ {}_k \ {}_{\max} < 1$

1.4.2 S1.4.2 Initialization Strategies

We tested three initialization strategies:

1. Random: $x_0 \ N(0, I)$
2. Warm start: $x_0 =$ solution from simpler problem
3. Problem-specific: $x_0 =$ domain knowledge-based initialization

Results show that warm start initialization reduces iterations by approximately 30% for related problem instances.

1.5 S1.5 Extended Mathematical Framework

1.5.1 S1.5.1 Generalized Objective Function

The framework extends to more general objectives:

$$f(x) = \sum_{i=1}^{n} w_i {}_i(x) + \sum_{j=1}^{m} {}_j R_j(x) + \sum_{k=1}^{p} {}_k C_k(x) \tag{1.7}$$

where: - ${}_i(x)$: Data fitting terms - $R_j(x)$: Regularization terms (e.g., ${}_1$, ${}_2$, elastic net) - $C_k(x)$: Constraint terms (penalty or barrier functions)

1.5.2 S1.5.2 Adaptive Weight Selection

Weights w_i can be adapted during optimization:

$$w_i^{(k+1)} = w_i^{(k)} \ \exp\left(\frac{|_i(x_k)|}{|(x_k)|}\right) \tag{1.8}$$

This reweighting scheme gives more emphasis to terms that are harder to optimize.

1.6 S1.6 Convergence Diagnostics

1.6.1 S1.6.1 Diagnostic Criteria

We monitor the following quantities for convergence:

1. Gradient norm: $f(x_k) < {}_g$
2. Step size: $x_{k+1} \ x_k < {}_x$
3. Function improvement: $|f(x_{k+1}) \ f(x_k)| < {}_f$
4. Relative improvement: $|f(x_{k+1}) \ f(x_k)|/|f(x_k)| < {}_r$

All four criteria must be satisfied for declared convergence.

1.6.2 S1.6.2 Failure Detection

Algorithm failure is detected if:

1. Maximum iterations exceeded
2. Step size becomes too small ($_k < {}_{\text{min}}$)
3. NaN or Inf values encountered
4. Objective function increases for consecutive iterations

1.7 S1.7 Parameter Sensitivity

Detailed sensitivity analysis for each parameter:

Parameter	Nominal	Range	Impact on Performance
${}_0$	0.01	[0.001, 0.1]	High (ś30%)
	0.9	[0.5, 0.99]	Medium (ś15%)
	0.001	[0, 0.01]	Low (ś5%)

Table 1. Parameter sensitivity analysis results

The learning rate ${}_0$ has the strongest impact on convergence speed, while regularization primarily affects the final solution quality rather than convergence dynamics.