ARB-LLM: ALTERNATING REFINED BINARIZATIONS FOR LARGE LANGUAGE MODELS

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A FIRST-ORDER ARB-X AND ARB-RC

A.1 FIRST-ORDER ARB-X

First-order Alternating Refined Binarization with Calibration Data (ARB-X) is based on the weightactivation quantization error $\mathcal{L} = ||\mathbf{W} \mathbf{X} - \widehat{\mathbf{W}} \mathbf{X}||^2_F.$

Rewritten weight-activation quantization error We first rewrite the quantization error $\mathcal L$ to decouple W and X, reducing the computational cost when calculating the quantization error. We define W as $W = W - \mu$. Then we rewrite the quantization error as

$$
\mathcal{L} = ||\mathbf{W}\mathbf{X} - \widehat{\mathbf{W}}\mathbf{X}||_F^2
$$
 (1)

$$
= ||\mathbf{X}(\widetilde{\mathbf{W}} - \alpha \mathbf{B})^{\top}||_F^2
$$
 (2)

$$
= \sum_{i} \sum_{j} (\sum_{b} \sum_{k} (\mathbf{X}_{b})_{ik} (\widetilde{\mathbf{W}}_{jk} - \alpha_{j} \mathbf{B}_{jk}))^{2}.
$$
 (3)

Then, we define the residual matrix as $\mathbf{R} = \mathbf{W} - \mu - \alpha \mathbf{B}$ and further simplify \mathcal{L} :

$$
\mathcal{L} = \sum_{i} \sum_{j} (\sum_{b} \sum_{k} (\mathbf{X}_{b})_{ik} \mathbf{R}_{jk})^{2}
$$
\n(4)

$$
= \sum_{i} \sum_{j} (\sum_{b} \sum_{k} \sum_{l} (\mathbf{X}_{b})_{ik} (\mathbf{X}_{b})_{il} \mathbf{R}_{jk} \mathbf{R}_{jl})
$$
(5)

$$
= \sum_{k} \sum_{l} (\sum_{b} \sum_{i} (\mathbf{X}_{b})_{ik} (\mathbf{X}_{b})_{il}) (\sum_{j} \mathbf{R}_{jk} \mathbf{R}_{jl}). \tag{6}
$$

After that, we define the matrix S using the following formula:

$$
\mathbf{S}_{kl} = \sum_{b} \sum_{i} (\mathbf{X}_{b})_{ik} (\mathbf{X}_{b})_{il}, \tag{7}
$$

where $k = 1, 2, \ldots, m, l = 1, 2, \ldots, m$. Then we obtain the final simplified $\mathcal L$ as

$$
\mathcal{L} = \langle \mathbf{S}, \mathbf{R}^{\top} \mathbf{R} \rangle_F = \text{Tr}(\mathbf{R} \mathbf{S} \mathbf{R}^{\top}).
$$
\n(8)

Parameter Update We use the quantization error $\mathcal L$ to update μ :

$$
\mathcal{L} = \sum_{k} \sum_{l} \mathbf{S}_{kl} \sum_{j} \mathbf{R}_{jk} \mathbf{R}_{jl} \tag{9}
$$

$$
= \sum_{k} \sum_{l} \mathbf{S}_{kl} \sum_{j} (\widetilde{\mathbf{W}}_{jk} \widetilde{\mathbf{W}}_{jl} - \alpha_j (\mathbf{B}_{jk} \widetilde{\mathbf{W}}_{jl} + \mathbf{B}_{jl} \widetilde{\mathbf{W}}_{jk}) + \alpha_j^2 \mathbf{B}_{jk} \mathbf{B}_{jl})
$$
(10)

$$
= \sum_{k} \sum_{l} \mathbf{S}_{kl} \sum_{j} ((\mathbf{W}_{jk} - \mu_j)(\mathbf{W}_{jl} - \mu_j) - \alpha_j (\mathbf{B}_{jk}(\mathbf{W}_{jl} - \mu_j)) \tag{11}
$$

$$
+\mathbf{B}_{jl}(\mathbf{W}_{jk}-\mu_j))+\alpha_j^2\mathbf{B}_{jk}\mathbf{B}_{jl}).
$$
\n(12)

To obtain the optimal solution for μ , we take the partial derivative of $\mathcal L$ with respect to μ_i , where $j = 1, 2, \ldots, n$:

$$
\frac{\partial \mathcal{L}}{\partial \mu_j} = \sum_k \sum_l \mathbf{S}_{kl} (-\mathbf{W}_{jl} - \mathbf{W}_{jk} + 2\mu_j + \alpha_j \mathbf{B}_{jk} + \alpha_j \mathbf{B}_{jl}).
$$
\n(13)

We set $\frac{\partial \mathcal{L}}{\partial \mu_j} = 0$ to get the optimal solution for μ_j :

$$
\mu_j = \frac{\sum_k \sum_l \mathbf{S}_{kl}(\mathbf{W}_{jk} - \alpha_j \mathbf{B}_{jk} + \mathbf{W}_{jl} - \alpha_j \mathbf{B}_{jl})}{2 \sum_k \sum_l \mathbf{S}_{kl}}, \quad \text{where } j = 1, 2, ..., n. \tag{14}
$$

Then, we define the matrix **P** as:

$$
\mathbf{P}_{kl} = \mathbf{W}_{jk} - \alpha_j \mathbf{B}_{jl}, \text{ where } k = 1, 2, ..., m, l = 1, 2, ..., m.
$$
 (15)

After that, we can simplify μ_j as

$$
\mu_j = \frac{\sum_k \sum_l (\mathbf{S} \odot (\mathbf{P} + \mathbf{P}^\top))_{kl}}{2 \sum_k \sum_l \mathbf{S}_{kl}}, \quad \text{where } j = 1, 2, \dots, n. \tag{16}
$$

Since S is symmetric, we can further simplify the above equation as:

$$
\mu_j = \frac{\sum_k \sum_l (\mathbf{S} \odot \mathbf{P})_{kl}}{\sum_k \sum_l \mathbf{S}_{kl}}, \quad \text{where } j = 1, 2, \dots, n. \tag{17}
$$

We can also express μ in a more compact vector form:

$$
\mu = \frac{\mathbf{1}^\top \mathbf{S} (\mathbf{W} - \alpha \mathbf{B})^\top}{\mathbf{1}^\top \mathbf{S} \mathbf{1}}.
$$
\n(18)

Similarly, we use the same quantization error to update α :

$$
\mathcal{L} = \sum_{k} \sum_{l} \mathbf{S}_{kl} \sum_{j} \mathbf{R}_{jk} \mathbf{R}_{jl} \tag{19}
$$

$$
= \sum_{k} \sum_{l} \mathbf{S}_{kl} \sum_{j} (\widetilde{\mathbf{W}}_{jk} \widetilde{\mathbf{W}}_{jl} - \alpha_j (\mathbf{B}_{jk} \widetilde{\mathbf{W}}_{jl} + \mathbf{B}_{jl} \widetilde{\mathbf{W}}_{jk}) + \alpha_j^2 \mathbf{B}_{jk} \mathbf{B}_{jl}).
$$
 (20)

To obtain the optimal solution for α , we take the partial derivative of $\mathcal L$ with respect to α_j , where $j = 1, 2, \ldots, n$:

$$
\frac{\partial \mathcal{L}}{\partial \alpha_j} = \sum_k \sum_l \mathbf{S}_{kl} (2\mathbf{B}_{jk}\mathbf{B}_{jl}\alpha_j - (\mathbf{B}_{jk}\widetilde{\mathbf{W}}_{jl} + \mathbf{B}_{jl}\widetilde{\mathbf{W}}_{jk})).
$$
\n(21)

We set $\frac{\partial \mathcal{L}}{\partial \alpha_j} = 0$ to get the optimal solution for α_j :

$$
\alpha_j = \frac{\sum_k \sum_l \mathbf{S}_{kl} (\mathbf{B}_{jk}\widetilde{\mathbf{W}}_{jl} + \mathbf{B}_{jl}\widetilde{\mathbf{W}}_{jk})}{2\sum_k \sum_l \mathbf{S}_{kl} (\mathbf{B}_{jk}\mathbf{B}_{jl})}, \quad \text{where } j = 1, 2, \dots, n. \tag{22}
$$

Then, we define the matrix U and V as:

$$
\mathbf{U}_{kl} = \mathbf{B}_{jk}\widetilde{\mathbf{W}}_{jl}, \mathbf{V}_{kl} = \mathbf{B}_{jk}\mathbf{B}_{jl},
$$
\n(23)

where $k = 1, 2, \ldots, m, l = 1, 2, \ldots, m$. After that, we simplify α_j using U and V:

$$
\alpha_j = \frac{\sum_k \sum_l (\mathbf{S} \odot (\mathbf{U} + \mathbf{U}^\top))_{kl}}{2 \sum_k \sum_l (\mathbf{S} \odot \mathbf{V})_{kl}}.
$$
\n(24)

Since S is symmetric, we can further simplify the above equation as

$$
\alpha_j = \frac{\sum_k \sum_l (\mathbf{S} \odot \mathbf{U})_{kl}}{\sum_k \sum_l (\mathbf{S} \odot \mathbf{V})_{kl}}.
$$
\n(25)

We can also express α in a more compact vector form:

$$
\alpha = \frac{\text{diag}(\mathbf{BS}(\mathbf{W} - \mu)^{\top})}{\text{diag}(\mathbf{BSB}^{\top})}.
$$
 (26)

For the detailed pseudocode of first-order ARB-X, see Algorithm [1.](#page-3-1)

func ARB-X ¹ (W, M, X, T)	$\mathbf{S}_{kl} = \sum_{b} \sum_{i} (\mathbf{X}_b)_{ik} (\mathbf{X}_b)_{il}$ 3:
Input: $\mathbf{W} \in \mathbb{R}^{n \times m}$ - full-precision weight	end for 4:
$\mathbf{M} \in \mathbb{R}^{n \times m}$ - group mask	$5:$ end for
$\mathbf{X} \in \mathbb{R}^{B \times L \times m}$ - calibration data	6: return S
T - iteration rounds	func refine_ μ (S, W, B, α , M)
Output: $\mathbf{W} \in \mathbb{R}^{n \times m}$	1: for $i = 1, 2, , n$ do
1: $\mathbf{S} \coloneqq \text{X2S}(\mathbf{X}) \; \mathsf{N} \; \mathbf{S} \in \mathbb{R}^{m \times m}$	for $k = 1, 2, , m; l = 1, 2, , m$ do 2:
2: $\mathbf{W}, \alpha, \mathbf{B}, \mu \coloneqq \text{binary}(\mathbf{W}, \mathbf{M})$	3: $\mathbf{P}_{kl} \coloneqq \mathbf{W}_{ik} - \alpha_i \mathbf{B}_{il} \cdot \mathbf{M}_{il}$
3: for $iter = 1, 2, , T$ do	$4:$ end for
$\mu \leftarrow \text{refine_}\mu(\mathbf{S}, \mathbf{W}, \mathbf{B}, \alpha, \mathbf{M})$ 4:	
$\alpha \leftarrow$ refine_ α (S , W , μ , B , M) 5:	5: $num := \sum_{k} \sum_{l} (\mathbf{S} \odot \mathbf{P})_{kl}$ 6: $den := \sum_{k} \sum_{l} \mathbf{S}_{kl} + \epsilon$
$\mathbf{W} \leftarrow (\alpha \cdot \mathbf{B} + \mu) \odot \mathbf{M}$ 6:	7: $\mu_i \coloneqq \frac{num}{den}$
7: end for	8: end for
8: return W	9: return μ
func binary (\mathbf{W}, \mathbf{M})	func refine_ α (S , W , μ , B , M)
1: $\mu \coloneqq \frac{1}{m} \sum_{i=1}^{m} (\mathbf{W} \odot \mathbf{M})_{.j}$	1: $\mathbf{W} \coloneqq \mathbf{W} - \mu$
2: $\mathbf{W} \coloneqq \mathbf{W} - \mu$	2: for $i = 1, 2, , n$ do
	3: for $k = 1, 2, , m; l = 1, 2, , m$ do
3: $\alpha \coloneqq \frac{1}{m} \sum_{j=1}^{m} (\mathbf{\tilde{W}} \odot \mathbf{M})_{.j} $	4: $\mathbf{U}_{kl} \coloneqq (\mathbf{B}_{ik} \cdot \mathbf{M}_{ik}) \mathbf{W}_{il}$
4: $\mathbf{B} \coloneqq \text{sign}(\mathbf{W} \odot \mathbf{M})$	5: $\mathbf{V}_{kl} \coloneqq (\mathbf{B}_{ik} \cdot \mathbf{M}_{ik}) \mathbf{B}_{il}$
5: $\hat{\mathbf{W}} \coloneqq \alpha \cdot \mathbf{B} + \mu$	end for 6:
6: return $\mathbf{W}, \alpha, \mathbf{B}, \mu$	7: $num \coloneqq \sum_k \sum_l (\mathbf{S} \odot \mathbf{U})_{kl}$
func $X2S(X)$	$den := \sum_{k} \sum_{l} (\hat{\mathbf{S}} \odot \mathbf{V})_{kl} + \epsilon$ 8:
1: for $b = 1, 2, B$ do	$\alpha_i \coloneqq \frac{num}{den}$ 9:
2: for $k = 1, 2, , m; l = 1, 2, , m$ do	10: end for
	11: return α

Algorithm 1 First-Order Alternating Refined Binarization with Calibration Data

A.2 FIRST-ORDER ARB-RC

The first-order ARB-RC is based on the quantization error without calibration data, so in this section, \mathcal{L} is defined as $\mathcal{L} = ||\mathbf{W} - \hat{\mathbf{W}}||_F^2$. We first perform first-order binarization with the row-wise scaling factor α^r and column-wise scaling factor α^c :

$$
\alpha^r = \frac{1}{m} \sum_{j=1}^m |\mathbf{W}_{.j}|, \quad \alpha^c = \frac{1}{n} \sum_{j=1}^n |\frac{\mathbf{W}_{j}}{\alpha_j^r}|, \quad \mathbf{B} = \text{sign}(\mathbf{W}). \tag{27}
$$

where we discard the mean μ in this process. Then we obtain \widehat{W} :

$$
\widehat{\mathbf{W}}_{jk} = \alpha_j^r \alpha_k^c \mathbf{B}_{jk}, \quad \text{where } j = 1, 2, \dots, n, k = 1, 2, \dots, m. \tag{28}
$$

We use the quantization error to update α^r :

$$
\mathcal{L} = ||\mathbf{W} - \widehat{\mathbf{W}}||_{\ell2} \tag{29}
$$

$$
=\sum_{j}\sum_{k}(\mathbf{W}_{jk}-\alpha_{j}^{r}\alpha_{k}^{c}\mathbf{B}_{jk})^{2}
$$
\n(30)

$$
=\sum_{j} \sum_{k} ((\mathbf{W}_{jk})^2 - 2\mathbf{W}_{jk}\alpha_k^c \mathbf{B}_{jk}\alpha_j^r + (\alpha_k^c)^2 \mathbf{B}_{jk}^2 (\alpha_j^r)^2).
$$
 (31)

To obtain the optimal solution for α^r , we take the partial derivative of $\mathcal L$ with respect to α_j^r , where $j = 1, 2, \ldots, n$:

$$
\frac{\partial \mathcal{L}}{\partial \alpha_j^r} = \sum_k (-2\mathbf{W}_{jk} \mathbf{B}_{jk} \alpha_k^c + 2(\alpha_k^c)^2 \mathbf{B}_{jk}^2 \alpha_j^r). \tag{32}
$$

We set $\frac{\partial \mathcal{L}}{\partial \alpha_j^r} = 0$ to get the optimal solution for α_j^r :

$$
\alpha_j^r = \frac{\sum_k \mathbf{W}_{jk} \alpha_k^c \mathbf{B}_{jk}}{\sum_k (\alpha_k^c)^2 \mathbf{B}_{jk}^2}, \quad \text{where } j = 1, 2, \dots, n. \tag{33}
$$

Then we use the same quantization error to update α_c , we take the partial derivative of $\mathcal L$ with respect to α_k^c , where $k = 1, 2, \ldots, m$:

$$
\frac{\partial \mathcal{L}}{\partial \alpha_k^c} = \sum_j (-2\mathbf{W}_{jk} \mathbf{B}_{jk} \alpha_j^r + 2(\alpha_j^r)^2 \mathbf{B}_{jk}^2 \alpha_k^c).
$$
 (34)

We set $\frac{\partial \mathcal{L}}{\partial \alpha_k^c} = 0$ to get the optimal solution for α_k^c :

$$
\alpha_k^c = \frac{\sum_j \mathbf{W}_{jk} \alpha_j^r \mathbf{B}_{jk}}{\sum_j (\alpha_j^r)^2 \mathbf{B}_{jk}^2}.
$$
\n(35)

We can also express α^r and α^c in a more compact vector form:

$$
\alpha^r = \frac{\text{diag}(\mathbf{W}(\alpha^c \mathbf{B})^\top)}{\text{diag}((\alpha^c \mathbf{B})(\alpha^c \mathbf{B})^\top)}, \quad \alpha^c = \frac{\text{diag}(\mathbf{W}^\top (\alpha^r \mathbf{B}))}{\text{diag}((\alpha^r \mathbf{B})^\top (\alpha^r \mathbf{B}))}.
$$
(36)

For the detailed pseudocode of first-order ARB-RC, see Algorithm [2.](#page-4-1)

B SECOND-ORDER ARB, ARB-X, AND ARB-RC

To achieve higher quantization precision for salient weight, we apply the second-order binarization to them. To begin with, we perform a second-order binarization on the full-precision weight matrix W:

$$
\mathbf{W}_1 = \mathbf{W} - \mu_1, \text{ where } \mu_1 = \frac{1}{m} \sum_{j=1}^{m} \mathbf{W}_{.j}.
$$
 (37)

The optimiztion objective for α_1 and \mathbf{B}_1 is:

$$
\alpha_1^*, \mathbf{B}_1^* = \underset{\alpha_1, \mathbf{B}_1}{\arg \min} ||\mathbf{W}_1 - \alpha_1 \mathbf{B}_1||_F^2.
$$
 (38)

We can obtain the optimal solution α_1^* and \mathbf{B}_1^* :

$$
\alpha_1^* = \frac{1}{m} \sum_{j=1}^m |(\mathbf{W}_1)_{.j}|, \quad \mathbf{B}_1^* = \text{sign}(\mathbf{W}_1). \tag{39}
$$

Then, we define the residual matrix \widetilde{W}_1 as $\widetilde{W}_1 = W_1 - \alpha_1^* \cdot B_1^*$. Following the previous steps, we perform binarization on the residual matrix \widetilde{W}_1 :

$$
\mathbf{W}_2 = \widetilde{\mathbf{W}}_1 - \mu_2, \quad \text{where } \mu_2 = \frac{1}{m} \sum_{j=1}^m (\widetilde{\mathbf{W}}_1)_{.j}.
$$
 (40)

$$
\alpha_2^*, \mathbf{B}_2^* = \underset{\alpha_2, \mathbf{B}_2}{\arg \min} ||\mathbf{W}_2 - \alpha_2 \mathbf{B}_2||_F^2.
$$
 (41)

$$
\alpha_2^* = \frac{1}{m} \sum_{j=1}^m |(\widetilde{\mathbf{W}}_2)_{.j}|, \quad \mathbf{B}_2^* = \text{sign}(\mathbf{W}_2). \tag{42}
$$

$$
\mu = \mu_1 + \mu_2. \tag{43}
$$

Then we can achieve the binarized matrix \widehat{W} :

$$
\widehat{\mathbf{W}} = \alpha_1^* \cdot \mathbf{B}_1^* + \alpha_2^* \cdot \mathbf{B}_2^* + \mu. \tag{44}
$$

For a more concise representation of the formula, we adopt the following formula in subsequent calculations:

$$
\mathbf{W} = \alpha_1 \cdot \mathbf{B}_1 + \alpha_2 \cdot \mathbf{B}_2 + \mu. \tag{45}
$$

B.1 SECOND-ORDER ARB

For second-order ARB algorithm, we compute the residual matrix **R** and its row-wise mean δ_{μ} :

$$
\mathbf{R} = \mathbf{W} - \widehat{\mathbf{W}}, \quad \delta_{\mu} = \frac{1}{m} \sum_{j=1}^{m} \mathbf{R}_{.j}.
$$
 (46)

We first use δ_{μ} to refine μ :

$$
\tilde{\mu} = \mu + \delta_{\mu}.\tag{47}
$$

Then, we sequentially update α_1 and α_2 :

$$
\tilde{\alpha}_1 = \frac{\sum_{j=1}^m \left((\mathbf{B}_1) \odot (\mathbf{W} - (\alpha_2 \mathbf{B}_2) - \tilde{\mu}) \right)_{.j}}{\sum_{j=1}^m (\mathbf{B}_1)_{.j}^2},\tag{48}
$$

$$
\tilde{\alpha}_2 = \frac{\sum_{j=1}^m \left((\mathbf{B}_2) \odot (\mathbf{W} - (\tilde{\alpha}_1 \mathbf{B}_1) - \tilde{\mu}) \right)_{.j}}{\sum_{j=1}^m (\mathbf{B}_2)_{.j}^2}.
$$
\n(49)

We can further simplify it into a vectorized form:

$$
\tilde{\alpha}_1 = \frac{1}{m} \operatorname{diag}(\mathbf{B}_1^\top (\mathbf{W} - \tilde{\mu} - \alpha_2 \mathbf{B}_2)), \quad \tilde{\alpha}_2 = \frac{1}{m} \operatorname{diag}(\mathbf{B}_2^\top (\mathbf{W} - \tilde{\mu} - \tilde{\alpha}_1 \mathbf{B}_1)).
$$
 (50)

The optimization objectives for \mathbf{B}_{1}^{*} and \mathbf{B}_{2}^{*} are as follows:

$$
\widetilde{\mathbf{B}}_1, \widetilde{\mathbf{B}}_2 = \underset{\mathbf{B}_1, \mathbf{B}_2}{\arg \min} ||\mathbf{W} - \widetilde{\mu} - \widetilde{\alpha}_1 \mathbf{B}_1 - \widetilde{\alpha}_2 \mathbf{B}_2||_{\ell 1}.
$$
\n(51)

In the implementation, we utilize binary search to optimize them. Then we obtain the refined \widehat{W} :

$$
\widehat{\mathbf{W}}_{\text{refine}} = \widetilde{\alpha}_1 \cdot \widetilde{\mathbf{B}}_1 + \widetilde{\alpha}_2 \cdot \widetilde{\mathbf{B}}_2 + \widetilde{\mu}.\tag{52}
$$

The detailed pseudocode can be found in Algorithm [3.](#page-6-1)

func $\text{ARB}^2(\mathbf{W}, \mathbf{M}, T)$ **Input:** $\mathbf{W} \in \mathbb{R}^{n \times m}$ - full-precision weight $\mathbf{M} \in \mathbb{R}^{n \times m}$ - group mask $T =$ iteration rounds Output: $\widehat{\mathbf{W}} \in \mathbb{R}^{n \times m}$ 1: $\mathbf{W}_1, \alpha_1, \mathbf{B}_1, \mu_1 \coloneqq \text{binary}(\mathbf{W}, \mathbf{M})$ 2: $\mathbf{W}_2, \alpha_2, \mathbf{B}_2, \mu_2 \coloneqq \text{binary}(\mathbf{W} - \mathbf{W}_1, \mathbf{M})$ 3: $\mu := \mu_1 + \mu_2$ 4: $W = W_1 + W_2$ 5: for iter = $1, 2, ..., T$ do 6: $\mathbf{R} \coloneqq \mathbf{W} - \widehat{\mathbf{W}}$ // residual matrix
7: $\delta_{\mu} \coloneqq \sum_i (\mathbf{R} \odot \mathbf{M})_i$ 7: $\delta_\mu \coloneqq \sum_j (\mathbf{R} \odot \mathbf{M})_{.j}$ 8: $\mu \leftarrow \mu + \delta_{\mu}$ // refine mean 9: $\mathbf{W}_1 \coloneqq \mathbf{W} - \alpha_2 \mathbf{B}_2$
10: $\alpha_1 \leftarrow \text{refine_alpha}$ 10: $\alpha_1 \leftarrow$ refine alpha $(\mathbf{B}_1, \mathbf{M}, \mathbf{W}_1, \mu)$
11: $\widetilde{\mathbf{W}}_2 := \mathbf{W} - \alpha_1 \mathbf{B}_1$ 11: $\widetilde{\mathbf{W}}_2 \coloneqq \mathbf{W} - \alpha_1 \mathbf{B}_1$
12: $\alpha_2 \leftarrow \text{refine_alpha}$ 12: $\alpha_2 \leftarrow \text{refine_alpha}(\mathbf{B}_2, \mathbf{M}, \mathbf{W}_2, \mu)$
13: $\mathbf{B}_1, \mathbf{B}_2 \leftarrow \text{refine_B}(\mathbf{W}, \alpha_1, \alpha_2, \mu)$ $\mathbf{B}_1, \mathbf{B}_2 \leftarrow \text{refine_B}(\mathbf{W}, \alpha_1, \alpha_2, \mu)$ 14: $\mathbf{W} \leftarrow \alpha_1 \cdot \mathbf{B}_1 + \alpha_2 \cdot \mathbf{B}_2 + \mu$ 15: end for 16: $return W$ func binary (W, M) 1: $\mu \coloneqq \frac{1}{m} \sum_{j=1}^m (\mathbf{W} \odot \mathbf{M})_{.j}$ 2: $\mathbf{W} \coloneqq \mathbf{W} - \mu$ 3: $\alpha \coloneqq \frac{1}{m} \sum_{j=1}^m |(\widetilde{\mathbf{W}} \odot \mathbf{M})_{\cdot j}|$ 4: $\mathbf{B} \coloneqq \text{sign}(\widetilde{\mathbf{W}} \odot \mathbf{M})$ 5: $\widehat{\mathbf{W}} \coloneqq \alpha \cdot \mathbf{B} + \mu$ 6: return $\hat{\mathbf{W}}, \alpha, \mathbf{B}, \mu$ func refine alpha $(\mathbf{B}, \mathbf{M}, \mathbf{W}, \mu)$ 1: $num \coloneqq \sum_j (\mathbf{B} \odot \mathbf{M} \odot (\mathbf{W} - \mu))_{,j}$ 2: $den := \sum_{j=1}^{m} (\mathbf{B} \odot \mathbf{M})_{.j}^{2} + \epsilon \mathbf{N}$ avoid zerodivision 3: $\alpha \coloneqq \frac{num}{den}$ 4: return α func refine $B(W, \alpha_1, \alpha_2, \mu)$ 1: $\mathbf{v} := [-\alpha_1 - \alpha_2, -\alpha_1 + \alpha_2, \alpha_1 - \alpha_2, \alpha_1 + \alpha_2]$ // ascending order 2: for $i = 1, 2, \ldots, n; j = 1, 2, \ldots, m$ do 3: $x \coloneqq \text{BST}(\mathbf{W}_{ij} - \mu_i, \mathbf{v}_i)$ 4: **switch** (x) 5: case v_1 : 6: $(\mathbf{B}_1)_{ij} = -1, (\mathbf{B}_2)_{ij} = -1$ 7: case v_2 : 8: $(B_1)_{ij} = -1, (B_2)_{ij} = +1$
9: **case v₃:** case v₃: 10: $(B_1)_{ij} = +1, (B_2)_{ij} = -1$
11: **default:** default: 12: $(\mathbf{B}_1)_{ij} = +1, (\mathbf{B}_2)_{ij} = +1$ 13: end switch 14: end for 15: return B_1, B_2 func BST (w, v) 1: $l \coloneqq \text{length}(\mathbf{v})$ 2: if $l == 1$ then 3: return v_1 4: else if $w \ge (v_{m/2} + v_{m/2+1})/2$ then 5: **return** BST $(w, \mathbf{v}_{m/2+1:m})$ 6: else 7: **return** BST $(w, \mathbf{v}_{1:m/2})$ 8: end if

Algorithm 3 Second-Order Alternating Refined Binarization

B.2 SECOND-ORDER ARB-X

Based on the previously discussed second-order binarization process, we can obtain the binarized weights as $\mathbf{W} = \alpha_1 \mathbf{B}_1 + \mu_1 + \alpha_2 \mathbf{B}_2 + \mu_2$. The second-order ARB-X is based on the quantization error $\mathcal L$ with calibration data:

$$
\mathcal{L} = ||\mathbf{W}\mathbf{X} - \widehat{\mathbf{W}}\mathbf{X}||_F^2.
$$
 (53)

Rewritten weight-activation quantization error In this section, we rewrite the quantization error to decouple W and X , reducing the computational cost when calculating the quantization error. We define W as $\mathbf{W} = \mathbf{W} - (\mu_1 + \mu_2)$. Then we rewrite the quantization error:

$$
\mathcal{L} = ||\mathbf{W}\mathbf{X} - \widehat{\mathbf{W}}\mathbf{X}||_F^2
$$
\n(54)

$$
= ||\mathbf{X}(\widetilde{\mathbf{W}} - \alpha_1 \mathbf{B}_1 - \alpha_2 \mathbf{B}_2)^{\top}||_F^2
$$
\n(55)

$$
= \sum_{i} \sum_{j} \left(\sum_{b} \sum_{k} (\mathbf{X}_{b})_{ik} (\widetilde{\mathbf{W}}_{jk} - \alpha_j^{(1)} \mathbf{B}_{jk}^{(1)} - \alpha_j^{(2)} \mathbf{B}_{jk}^{(2)}) \right)^2.
$$
 (56)

We define the residual matrix **as:**

$$
\mathbf{R}_{jk} = \widetilde{\mathbf{W}}_{jk} - \alpha_j^{(1)} \mathbf{B}_{jk}^{(1)} - \alpha_j^{(2)} \mathbf{B}_{jk}^{(2)}, \quad \text{where } j = 1, 2, \dots, n, k = 1, 2, \dots, m. \tag{57}
$$

Then we simplify $\mathcal L$ with residual matrix $\mathbf R$:

$$
\mathcal{L} = \sum_{i} \sum_{j} (\sum_{b} \sum_{k} (\mathbf{X}_{b})_{ik} \mathbf{R}_{jk})^{2}
$$
\n(58)

$$
= \sum_{i} \sum_{j} (\sum_{b} \sum_{k} \sum_{l} (\mathbf{X}_{b})_{ik} (\mathbf{X}_{b})_{il} \mathbf{R}_{jk} \mathbf{R}_{jl})
$$
(59)

$$
= \sum_{k} \sum_{l} (\sum_{b} \sum_{i} (\mathbf{X}_{b})_{ik} (\mathbf{X}_{b})_{il}) (\sum_{j} \mathbf{R}_{jk} \mathbf{R}_{jl}). \tag{60}
$$

After that, we define the matrix S:

$$
\mathbf{S}_{kl} = \sum_{b} \sum_{i} (\mathbf{X}_{b})_{ik} (\mathbf{X}_{b})_{il}, \quad \text{where } k = 1, 2, ..., m, l = 1, 2, ..., m.
$$
 (61)

Then we obtain the final simplified \mathcal{L} :

$$
\mathcal{L} = \langle \mathbf{S}, \mathbf{R}^{\top} \mathbf{R} \rangle_F = \text{Tr}(\mathbf{R} \mathbf{S} \mathbf{R}^{\top}).
$$
 (62)

Parameter Update We use the quantization error $\mathcal L$ to update μ :

$$
\mathcal{L} = \sum_{k} \sum_{l} \mathbf{S}_{kl} \sum_{j} \mathbf{R}_{jk} \mathbf{R}_{jl} \tag{63}
$$

$$
= \sum_{k} \sum_{l} \mathbf{S}_{kl} \sum_{j} (\widetilde{\mathbf{W}}_{jk} - \alpha_j^{(1)} \mathbf{B}_{jk}^{(1)} - \alpha_j^{(2)} \mathbf{B}_{jk}^{(2)}) (\widetilde{\mathbf{W}}_{jl} - \alpha_j^{(1)} \mathbf{B}_{jl}^{(1)} - \alpha_j^{(2)} \mathbf{B}_{jl}^{(2)})
$$
(64)

$$
= \sum_{k} \sum_{l} \mathbf{S}_{kl} \sum_{j} (\widetilde{\mathbf{W}}_{jk} \widetilde{\mathbf{W}}_{jl} - \widetilde{\mathbf{W}}_{jk} \alpha_j^{(1)} \mathbf{B}_{jl}^{(1)} - \widetilde{\mathbf{W}}_{jk} \alpha_j^{(2)} \mathbf{B}_{jl}^{(2)} - \widetilde{\mathbf{W}}_{jl} \alpha_j^{(1)} \mathbf{B}_{jk}^{(1)}
$$
(65)

$$
- \widetilde{W}_{jl}\alpha_j^{(2)}B_{jk}^{(2)} = \sum_k \sum_j S_{kl} \sum_j ((W_{jk} - \mu_j)(W_{jl} - \mu_j) - (W_{jk} - \mu_j)(\alpha_j^{(1)}B_{jl}^{(1)} + \alpha_j^{(2)}B_{jl}^{(2)}) - (W_{jl} - \mu_j)(\alpha_j^{(1)}B_{jk}^{(1)} + \alpha_j^{(2)}B_{jk}^{(2)})).
$$
 (66)

To obtain the optimal solution for μ , we take the partial derivative of $\mathcal L$ with respect to μ_j , where $j = 1, 2, \ldots, n$:

$$
\frac{\partial \mathcal{L}}{\partial \mu_j} = \sum_k \sum_l \mathbf{S}_{kl} (2\mu_j - (\mathbf{W}_{jk} + \mathbf{W}_{jl}) + (\alpha_j^{(1)} \mathbf{B}_{jl}^{(1)} + \alpha_j^{(2)} \mathbf{B}_{jl}^{(2)} + \alpha_j^{(1)} \mathbf{B}_{jk}^{(1)} + \alpha_j^{(2)} \mathbf{B}_{jk}^{(2)})).
$$
 (67)

We set $\frac{\partial \mathcal{L}}{\partial \mu_j} = 0$ to obtain the optimal solution for μ_j :

$$
\mu_j = \frac{\sum_k \sum_l \mathbf{S}_{kl} (\mathbf{W}_{jk} - (\alpha_j^{(1)} \mathbf{B}_{jl}^{(1)} + \alpha_j^{(2)} \mathbf{B}_{jl}^{(2)}) + \mathbf{W}_{jl} - (\alpha_j^{(1)} \mathbf{B}_{jk}^{(1)} + \alpha_j^{(2)} \mathbf{B}_{jk}^{(2)}))}{2 \sum_k \sum_l \mathbf{S}_{kl}},
$$
(68)

where $j = 1, 2, \ldots, n$. We define the matrix **P**:

$$
\mathbf{P}_{kl} = \mathbf{W}_{jk} - (\alpha_j^{(1)} \mathbf{B}_{jl}^{(1)} + \alpha_j^{(2)} \mathbf{B}_{jl}^{(2)}), \text{ where } k = 1, 2, ..., m, l \text{ from 1 to m.}
$$
 (69)

We simplify μ_j using the matrix **P**:

$$
\mu_j = \frac{\sum_k \sum_l (\mathbf{S} \odot (\mathbf{P} + \mathbf{P}^\top))_{kl}}{2 \sum_k \sum_l \mathbf{S}_{kl}}, \quad \text{where } j = 1, 2, \dots, n. \tag{70}
$$

Since S is symmetric, we can further simplify the above equation as:

$$
\mu_j = \frac{\sum_k \sum_l (\mathbf{S} \odot \mathbf{P})_{kl}}{\sum_k \sum_l \mathbf{S}_{kl}}, \quad \text{where } j = 1, 2, \dots, n. \tag{71}
$$

We use the quantization error to sequentially update α_1 and α_2 :

$$
\mathcal{L} = \sum_{k} \sum_{l} \mathbf{S}_{kl} \sum_{j} \mathbf{R}_{jk} \mathbf{R}_{jl} \tag{72}
$$

$$
= \sum_{k} \sum_{l} \mathbf{S}_{kl} \sum_{j} (\widetilde{\mathbf{W}}_{jk} - \alpha_j^{(1)} \mathbf{B}_{jk}^{(1)} - \alpha_j^{(2)} \mathbf{B}_{jk}^{(2)}) (\widetilde{\mathbf{W}}_{jl} - \alpha_j^{(1)} \mathbf{B}_{jl}^{(1)} - \alpha_j^{(2)} \mathbf{B}_{jl}^{(2)}) \tag{73}
$$

To update α_1 , we take the partial derivative of $\mathcal L$ with respect to $\alpha_j^{(1)}$, where $j = 1, 2, \ldots, n$:

$$
\frac{\partial \mathcal{L}}{\partial \alpha_j^{(1)}} = \sum_k \sum_l \mathbf{S}_{kl} (2\mathbf{B}_{jk}^{(1)} \mathbf{B}_{jl}^{(1)} \alpha_j^{(1)} - \mathbf{B}_{jk}^{(1)} \widetilde{\mathbf{W}}_{jl} - \mathbf{B}_{jl}^{(1)} \widetilde{\mathbf{W}}_{jk} + \alpha_j^{(2)} \mathbf{B}_{jk}^{(1)} \mathbf{B}_{jl}^{(2)} + \alpha_j^{(2)} \mathbf{B}_{jl}^{(1)} \mathbf{B}_{jk}^{(2)})
$$
(74)

We set $\frac{\partial \mathcal{L}}{\partial \alpha_j^{(1)}} = 0$ to get the optimal solution for $\alpha_j^{(1)}$:

$$
\alpha_j^{(1)} = \frac{\sum_k \sum_l \mathbf{S}_{kl}(\mathbf{B}_{jk}^{(1)}\widetilde{\mathbf{W}}_{jl} + \mathbf{B}_{jl}^{(1)}\widetilde{\mathbf{W}}_{jk} - \mathbf{B}_{jl}^{(1)}\alpha_j^{(2)}\mathbf{B}_{jk}^{(2)} - \mathbf{B}_{jk}^{(1)}\alpha_j^{(2)}\mathbf{B}_{jl}^{(2)})}{2\sum_k \sum_l \mathbf{S}_{kl}(\mathbf{B}_{jk}^{(1)}\mathbf{B}_{jl}^{(1)})},\tag{75}
$$

where $j = 1, 2, \dots, n$. We define the matrix U_1 and V_1 as:

$$
(\mathbf{U}_{1})_{kl} = \mathbf{B}_{jk}^{(1)} \widetilde{\mathbf{W}}_{jl} - \mathbf{B}_{jk}^{(1)} \alpha_{j}^{(2)} \mathbf{B}_{jl}^{(2)}, \quad (\mathbf{V}_{1})_{kl} = \mathbf{B}_{jk}^{(1)} \mathbf{B}_{jl}^{(1)}, \tag{76}
$$

where $k = 1, 2, \dots, m, l = 1, 2, \dots, m$. Then we simplify $\alpha_j^{(1)}$:

$$
\alpha_j^{(1)} = \frac{\sum_k \sum_l (\mathbf{S} \odot (\mathbf{U}_1 + \mathbf{U}_1^\top))_{kl}}{2 \sum_k \sum_l (\mathbf{S} \odot \mathbf{V}_1)_{kl}}, \quad \text{where } j = 1, 2, \dots, n. \tag{77}
$$

Since S is symmetric, we can further simplify the above equation as

$$
\alpha_j^{(1)} = \frac{\sum_k \sum_l (\mathbf{S} \odot \mathbf{U}_1)_{kl}}{\sum_k \sum_l (\mathbf{S} \odot \mathbf{V}_1)_{kl}}, \quad \text{where } j = 1, 2, \dots, n. \tag{78}
$$

Then we update α_2 , we take the partial derivative of $\mathcal L$ with respect to $\alpha_j^{(2)}$, where $j = 1, 2, \ldots, n$:

$$
\frac{\partial \mathcal{L}}{\partial \alpha_j^{(2)}} = \sum_k \sum_l \mathbf{S}_{kl} (2\mathbf{B}_{jk}^{(2)} \mathbf{B}_{jl}^{(2)} \alpha_j^{(2)} - \mathbf{B}_{jk}^{(2)} \widetilde{\mathbf{W}}_{jl} - \mathbf{B}_{jl}^{(2)} \widetilde{\mathbf{W}}_{jk} + \alpha_j^{(1)} \mathbf{B}_{jk}^{(2)} \mathbf{B}_{jl}^{(1)} + \alpha_j^{(1)} \mathbf{B}_{jl}^{(2)} \mathbf{B}_{jk}^{(1)}).
$$
\n(79)

We set $\frac{\partial \mathcal{L}}{\partial \alpha_j^{(2)}} = 0$ to get the optimal $\alpha_j^{(2)}$:

$$
\alpha_j^{(2)} = \frac{\sum_k \sum_l \mathbf{S}_{kl}(\mathbf{B}_{jk}^{(2)}\widetilde{\mathbf{W}}_{jl} + \mathbf{B}_{jl}^{(2)}\widetilde{\mathbf{W}}_{jk} - \mathbf{B}_{jl}^{(2)}\alpha_j^{(1)}\mathbf{B}_{jk}^{(1)} - \mathbf{B}_{jk}^{(2)}\alpha_j^{(1)}\mathbf{B}_{jl}^{(1)})}{2\sum_k \sum_l \mathbf{S}_{kl}(\mathbf{B}_{jk}^{(2)}\mathbf{B}_{jl}^{(2)})},
$$
(80)

where $j = 1, 2, ..., n$. We define the matrix U_2 and V_2 as:

$$
(\mathbf{U}_2)_{kl} = \mathbf{B}_{jk}^{(2)} \widetilde{\mathbf{W}}_{jl} - \mathbf{B}_{jk}^{(2)} \alpha_j^{(1)} \mathbf{B}_{jl}^{(1)}, \quad (\mathbf{V}_2)_{kl} = \mathbf{B}_{jk}^{(2)} \mathbf{B}_{jl}^{(2)},
$$
(81)

where $k = 1, 2, ..., m, l = 1, 2, ..., m$. We can simplify $\alpha_j^{(2)}$ using U_2 and V_2 :

$$
\alpha_j^{(2)} = \frac{\sum_k \sum_l (\mathbf{S} \odot (\mathbf{U}_2 + \mathbf{U}_2^{\top}))_{kl}}{2 \sum_k \sum_l (\mathbf{S} \odot \mathbf{V}_2)_{kl}}, \quad \text{where } j = 1, 2, \dots, n. \tag{82}
$$

Since S is symmetric, we can further simplify the above equation as:

$$
\alpha_j^{(2)} = \frac{\sum_k \sum_l (\mathbf{S} \odot \mathbf{U}_2)_{kl}}{\sum_k \sum_l (\mathbf{S} \odot \mathbf{V}_2)_{kl}}, \quad \text{where } j = 1, 2, \dots, n. \tag{83}
$$

The detailed pseudocode can be found in Algorithm [4.](#page-9-1)

func ARB-X²(**W**, **M**, **X** ,*T*) **Input:** $\mathbf{W} \in \mathbb{R}^{n \times m}$ - full-precision weight $\mathbf{M} \in \mathbb{R}^{n \times m}$ - group mask $\mathbf{X} \in \mathbb{R}^{B \times L \times m}$ - calibration data T_z iteration rounds Output: $\widehat{\mathbf{W}} \in \mathbb{R}^{n \times m}$ 1: $\mathbf{S} \coloneqq \text{X2S}(\mathbf{X}) \; \mathsf{W}\; \mathbf{S} \in \mathbb{R}^{m \times m}$ 2: $\mathbf{W}_1, \alpha_1, \mathbf{B}_1, \mu_1 \coloneqq \text{binary}(\mathbf{W}, \mathbf{M})$ 3: $\widehat{\mathbf{W}}_2, \alpha_2, \mathbf{B}_2, \mu_2 := \text{binary}(\mathbf{W} - \widehat{\mathbf{W}}_1, \mathbf{M})$ 4: $\mu := \mu_1 + \mu_2$ 5: $\widehat{\mathbf{W}} \coloneqq \widehat{\mathbf{W}}_1 + \widehat{\mathbf{W}}_2$ 6: $B_1 \leftarrow B_1 \odot M$ 7: $B_2 \leftarrow B_2 \odot M$ 8: for $iter = 1, 2, \ldots, T$ do 9: $\mu \leftarrow$ refine $\mu(S, W, B_1, B_2, \alpha_1, \alpha_2)$ 10: $\alpha_1 \leftarrow \text{refine}_{\alpha}(\mathbf{S}, \mathbf{W}, \mu, \mathbf{B}_1, \mathbf{B}_2, \alpha_2)$ 11: $\alpha_2 \leftarrow \text{refine}_{\alpha}(\mathbf{S}, \mathbf{W}, \mu, \mathbf{B}_2, \mathbf{B}_1, \alpha_1)$ 12: $\widehat{\mathbf{W}} \leftarrow (\alpha \cdot \mathbf{B} + \mu) \odot \mathbf{M}$ 13: end for 14: return $\mathbf{\hat{W}}$ func binary (W, M) 1: $\mu \coloneqq \frac{1}{m} \sum_{j=1}^m (\mathbf{W} \odot \mathbf{M})_{.j}$ 2: $\widetilde{\mathbf{W}} := \mathbf{W} - \mu$ 3: $\alpha \coloneqq \frac{1}{m} \sum_{j=1}^m |(\widetilde{\mathbf{W}} \odot \mathbf{M})_{\cdot j}|$ 4: $\mathbf{B} \coloneqq \text{sign}(\mathbf{W} \odot \mathbf{M})$ 5: $\widehat{\mathbf{W}} \coloneqq \alpha \cdot \mathbf{B} + \mu$ 6: return $\widehat{\mathbf{W}}, \alpha, \mathbf{B}, \mu$ func $X2S(X)$ 1: for $b = 1, 2, \ldots, B$ do 2: **for** $k = 1, 2, ..., m; l = 1, 2, ..., m$ do 3: $\mathbf{S}_{kl} = \sum_b \sum_i (\mathbf{X}_b)_{ik} (\mathbf{X}_b)_{il}$ 4: end for 5: end for 6: return S func refine $\mu(S, \mathbf{W}, \mathbf{B}_1, \mathbf{B}_2, \alpha_1, \alpha_2)$ 1: for $i = 1, 2, ..., n$ do 2: **for** $k = 1, 2, ..., m; l = 1, 2, ..., m$ **do** 3: $\mathbf{P}_{kl} = \mathbf{W}_{ik} - (\alpha_i^{(1)} \mathbf{B}_{il}^{(1)} + \alpha_i^{(2)} \mathbf{B}_{il}^{(2)})$ 4: end for 5: $num \coloneqq \sum_k \sum_l (\mathbf{S} \odot \mathbf{P})_{kl}$ 6: $den \coloneqq \sum_k \sum_l \mathbf{S}_{kl} + \epsilon$ 7: $\mu_i \coloneqq \frac{n \overline{u m}}{den}$ 8: end for 9: return μ func refine α (**S**, **W**, μ , **B**, $\tilde{\mathbf{B}}$, $\tilde{\alpha}$) 1: $\widetilde{\mathbf{W}} := \mathbf{W} - \mu$ 2: for $i = 1, 2, ..., n$ do 3: **for** $k = 1, 2, ..., m; l = 1, 2, ..., m$ do 4: $\mathbf{U}_{kl} \coloneqq \mathbf{B}_{ik}\mathbf{W}_{il} - \mathbf{B}_{ik}\widetilde{\alpha}_i\widetilde{\mathbf{B}}_{il}$
5: $\mathbf{V}_{kl} \coloneqq \mathbf{B}_{ik}\mathbf{B}_{il}$ ${\bf V}_{kl}\coloneqq{\bf B}_{ik}{\bf B}_{il}$ 6: end for 7: $num \coloneqq \sum_k \sum_l (\mathbf{S} \odot \mathbf{U})_{kl}$ 8: $den \coloneqq \sum_k \sum_l (\mathbf{S} \odot \mathbf{V})_{kl} + \epsilon$ 9: $\alpha_i \coloneqq \frac{n \overline{u} \overline{m}}{den}$ 10: end for 11: return α

Algorithm 4 Second-Order Alternating Refined Binarization with calibration data

B.3 SECOND-ORDER ARB-RC

We perform second-order binarization under the ARB-RC method:

$$
\alpha_1^r = \frac{1}{m} \sum_{j=1}^m |\mathbf{W}_{.j}|, \quad \alpha_1^c = \frac{1}{n} \sum_{j=1}^n |\frac{\mathbf{W}_{j.}}{(\alpha_1^r)_j}|, \quad \mathbf{B}_1 = \text{sign}(\mathbf{W}). \tag{84}
$$

We define the residual matrix **as:**

$$
\mathbf{R}_{jk} = \mathbf{W}_{jk} - \alpha_j^r \alpha_k^c \mathbf{B}_{jk}, \quad \text{where } j = 1, 2, \dots, n, k = 1, 2, \dots, m. \tag{85}
$$

Then we perform binarization on residual matrix \mathbf{R} :

$$
\alpha_2^r = \frac{1}{m} \sum_{j=1}^m |\mathbf{R}_{.j}|, \quad \alpha_2^c = \frac{1}{n} \sum_{j=1}^n |\frac{\mathbf{R}_{j.}}{(\alpha_2^r)_j}|, \quad \mathbf{B}_2 = \text{sign}(\mathbf{R}). \tag{86}
$$

We can obtain the results of the second-order binarization:

$$
\widehat{\mathbf{W}}_{jk} = (\alpha_1^r)_j (\alpha_1^c)_k (\mathbf{B}_1)_{jk} + (\alpha_2^r)_j (\alpha_2^c)_k (\mathbf{B}_2)_{jk}, \text{ where } j = 1, 2, \dots, n, k = 1, 2, \dots, m. (87)
$$

Then quantization error without calibration data is given by the following formula:

$$
\mathcal{L} = ||\mathbf{W} - \widehat{\mathbf{W}}||_{\ell 2}
$$
\n(88)

$$
= \sum_{j} \sum_{k} (\mathbf{W}_{jk} - ((\alpha_1^r)_j (\alpha_1^c)_k (\mathbf{B}_1)_{jk} + (\alpha_2^r)_j (\alpha_2^c)_k (\mathbf{B}_2)_{jk}))^2.
$$
 (89)

We define \widetilde{W}_1 and \widetilde{W}_2 as:

$$
(\widetilde{\mathbf{W}}_1)_{jk} = \mathbf{W}_{jk} - (\alpha_2^r)_j (\alpha_2^c)_k (\mathbf{B}_2)_{jk}), \quad (\widetilde{\mathbf{W}}_2)_{jk} = \mathbf{W}_{jk} - (\alpha_1^r)_j (\alpha_1^c)_k (\mathbf{B}_1)_{jk}). \tag{90}
$$

where $j = 1, 2, ..., n, k = 1, 2, ..., m$. Then we update α_1^r using the following formulas:

$$
\frac{\partial \mathcal{L}}{\partial (\alpha_1^r)_j} = \sum_k (-2(\widetilde{\mathbf{W}}_1)_{jk} (\mathbf{B}_1)_{jk} (\alpha_1^c)_k + 2(\alpha_1^c)_k^2 (\mathbf{B}_1)_{jk}^2 (\alpha_1^r)_j). \tag{91}
$$

We set $\frac{\partial \mathcal{L}}{\partial (\alpha_1^r)_j} = 0$ to get the optimal solution for $(\alpha_1^r)_j$:

$$
(\alpha_1^r)_j = \frac{\sum_k (\mathbf{W}_1)_{jk} (\alpha_1^c)_k (\mathbf{B}_1)_{jk}}{\sum_k (\alpha_1^c)_k^2 (\mathbf{B}_1)_{jk}^2}, \quad \text{where } j = 1, 2, \dots, n. \tag{92}
$$

We update α_1^c using the following formulas:

$$
\frac{\partial \mathcal{L}}{\partial (\alpha_1^c)_k} = \sum_j (-2(\widetilde{\mathbf{W}}_1)_{jk} (\mathbf{B}_1)_{jk} (\alpha_1^r)_j + 2(\alpha_1^r)_j^2 (\mathbf{B}_1)_{jk}^2 (\alpha_1^c)_k).
$$
(93)

We set $\frac{\partial \mathcal{L}}{\partial (\alpha_1^c)_k} = 0$ to get the optimal solution for $(\alpha_1^c)_k$:

$$
(\alpha_1^c)_k = \frac{\sum_j (\mathbf{W}_1)_{jk} (\alpha_1^r)_j (\mathbf{B}_1)_{jk}}{\sum_j (\alpha_1^r)_j^2 (\mathbf{B}_1)_{jk}^2}, \quad \text{where } k = 1, 2, \dots, m. \tag{94}
$$

We update α_2^r using the following formulas:

$$
\frac{\partial \mathcal{L}}{\partial (\alpha_2^r)_j} = \sum_k (-2(\widetilde{\mathbf{W}}_2)_{jk} (\mathbf{B}_2)_{jk} (\alpha_2^c)_k + 2(\alpha_2^c)_k^2 (\mathbf{B}_2)_{jk}^2 (\alpha_2^r)_j). \tag{95}
$$

We set $\frac{\partial \mathcal{L}}{\partial (\alpha_2^r)_j} = 0$ to get the optimal solution for $(\alpha_2^r)_j$:

$$
(\alpha_2^r)_j = \frac{\sum_k (\mathbf{W}_2)_{jk} (\alpha_2^c)_k (\mathbf{B}_2)_{jk}}{\sum_k (\alpha_2^c)_k^2 (\mathbf{B}_2)_{jk}^2}, \quad \text{where } j = 1, 2, \dots, n. \tag{96}
$$

We update α_2^c using the following formulas:

$$
\frac{\partial \mathcal{L}}{\partial (\alpha_2^c)_k} = \sum_j (-2(\widetilde{\mathbf{W}}_2)_{jk} (\mathbf{B}_2)_{jk} (\alpha_2^r)_j + 2(\alpha_2^r)_j^2 (\mathbf{B}_2)_{jk}^2 (\alpha_2^c)_k). \tag{97}
$$

We set $\frac{\partial \mathcal{L}}{\partial (\alpha_2^c)_k} = 0$ to get the optimal solution for $(\alpha_2^c)_k$:

$$
(\alpha_2^c)_k = \frac{\sum_j (\widetilde{\mathbf{W}}_2)_{jk} (\alpha_2^r)_j (\mathbf{B}_2)_{jk}}{\sum_j (\alpha_2^r)_j^2 (\mathbf{B}_2)_{jk}^2}, \quad \text{where } k = 1, 2, \dots, m. \tag{98}
$$

The objective of optimizing B_1 and B_2 is:

$$
(\mathbf{B}_1)_{jk}, (\mathbf{B}_2)_{jk} = \underset{(\mathbf{B}_1)_{jk}, (\mathbf{B}_2)_{jk}}{\arg \min} ||\mathbf{W}_{jk} - ((\alpha_1^r)_j (\alpha_1^c)_k (\mathbf{B}_1)_{jk} + (\alpha_2^r)_j (\alpha_2^c)_k (\mathbf{B}_2)_{jk})||_{\ell1}, \quad (99)
$$

where $j = 1, 2, \ldots, n$, $k = 1, 2, \ldots, m$. The detailed pseudocode for second-order ARB-RC can be found in Algorithm [5.](#page-11-1)

func ARB-RC²(**W**, **M**, **X**, *T*) **Input:** $\mathbf{W} \in \mathbb{R}^{n \times m}$ - full-precision weight $\mathbf{M} \in \mathbb{R}^{n \times m}$ - group mask $\mathbf{X} \in \mathbb{R}^{B \times L \times m}$ - calibration data T_z iteration rounds Output: $\widehat{\mathbf{W}} \in \mathbb{R}^{n \times m}$ 1: $\widehat{\mathbf{W}}_1, \alpha_1^r, \alpha_1^c, \mathbf{B}_1 \coloneqq \text{binary_rc}(\mathbf{W}, \mathbf{M})$ 2: $\widehat{\mathbf{W}}_2, \alpha_2^c, \alpha_2^c, \mathbf{B}_2 \coloneqq \text{binary_rc}(\mathbf{W}-\widehat{\mathbf{W}}, \mathbf{M})$ 3: $\widehat{\mathbf{W}} = \widehat{\mathbf{W}}_1 + \widehat{\mathbf{W}}_2$ 4: $B_1 \leftarrow B_1 \odot M$ 5: $B_2 \leftarrow B_2 \odot M$ 6: for $iter = 1, 2, \ldots, T$ do 7: **for** $j = 1, 2, ..., n; k = 1, 2, ..., m$ do 8: $(\mathbf{W}_1)_{jk} = \mathbf{W}_{jk} - (\alpha_2^r)_j (\alpha_2^c)_k (\mathbf{B}_2)_{jk}$ 9: $(\mathbf{W}_2)_{jk} = \mathbf{W}_{jk} - (\alpha_1^r)_j (\alpha_1^c)_k (\mathbf{B}_1)_{jk}$ 10: end for 11: α $r_1^r \leftarrow \text{refine}_{\alpha} \alpha^r (\mathbf{W}_1, \mathbf{B}_1, \alpha_1^c)$ 12: $c_1^c \leftarrow \text{refine}_{\alpha} \alpha^c (\mathbf{W}_1, \mathbf{B}_1, \alpha_1^r)$ $13:$ $r_2^r \leftarrow \text{refine}_{\alpha} \alpha^r (\mathbf{W}_2, \mathbf{B}_2, \alpha_2^c)$ 14: $c_2^c \leftarrow \text{refine}_{\alpha} \alpha^c(\mathbf{W}_2, \mathbf{B}_2, \alpha_1^r)$ 15: $\mathbf{B}_1, \mathbf{B}_2 \leftarrow \text{refine_B}(\mathbf{W}, \alpha_1^r, \alpha_2^r, \alpha_1^c, \alpha_2^c)$ 16: **for** $k = 1, 2, ..., n; l = 1, 2, ..., m$ do 17: $\mathbf{\hat{W}}_{kl} \leftarrow ((\alpha_1^r)_k (\alpha_1^c)_l (\mathbf{B}_1)_{kl} +$ $(\alpha_2^r)_k (\alpha_2^c)_l (\mathbf{B}_2)_{kl}) \cdot \mathbf{M}_{kl}$ 18: end for 19: end for $20:$ return W func binary $rc(W, M)$ 1: $\alpha^r \coloneqq \frac{1}{m} \sum_{j=1}^m |(\mathbf{W} \odot \mathbf{M})_{.j}|$ 2: $\alpha^c \coloneqq \frac{1}{n} \sum_{j=1}^n |\frac{(\mathbf{W}\odot\mathbf{M})_{j.}}{\alpha_j^r}|$ 3: $\mathbf{B} \coloneqq \text{sign}(\mathbf{W} \odot \mathbf{M})^{\mathsf{T}}$ 4: for $k = 1, 2, \ldots, n; l = 1, 2, \ldots, m$ do 5: $\widehat{\mathbf{W}}_{kl} \coloneqq \alpha_k^r \alpha_l^c \mathbf{B}_{kl}$ 6: end for 7: return $\widehat{\mathbf{W}}, \alpha^r, \alpha^c, \mathbf{B}$ func refine_ $\alpha^{\rm r}$ (**W**, **B**, α^c) 1: for $j = 1, 2, ..., n$ do 2: $num \coloneqq \sum_k \mathbf{W}_{jk} \alpha_k^c \mathbf{B}_{jk}$ 3: $den := \sum_k (\alpha_k^c)^2 \mathbf{B}_{jk}^2 + \epsilon$ 4: $\alpha_j^r \coloneqq \frac{n \overline{u m}}{den}$ 5: end for 6: **return** α^r func refine $\alpha^c (\mathbf{W}, \mathbf{B}, \alpha^r)$ 1: for $k = 1, 2, ..., m$ do 2: $num := \sum_j \mathbf{W}_{jk} \alpha_j^r \mathbf{B}_{jk}$ 3: $den \coloneqq \sum_j (\alpha_j^r)^2 \mathbf{B}_{jk}^2 + \epsilon$ 4: $\alpha_k^c \coloneqq \frac{num^2}{den}$ 5: end for 6: return α^c func refine_B $(\mathbf{W}, \alpha_1^r, \alpha_2^r, \alpha_1^c, \alpha_2^c)$ 1: for $i = 1, 2, \ldots, n; j = 1, 2, \ldots, m$ do 2: $\mathbf{v} :=$ $\int -(\alpha_1^r)_i(\alpha_1^c)_j - (\alpha_2^r)_i(\alpha_2^c)_j$ $-\left(\alpha_1^{\tilde{r}}\right)_i\left(\alpha_1^{\tilde{c}}\right)_j+\left(\alpha_2^{\tilde{r}}\right)_i\left(\alpha_2^{\tilde{c}}\right)_j$
 $\left(\alpha_1^{\tilde{r}}\right)_i\left(\alpha_2^{\tilde{c}}\right)_j=\left(\alpha_1^{\tilde{r}}\right)_i\left(\alpha_2^{\tilde{c}}\right)_j$ $\overline{1}$ $(\alpha_1^r)_i(\alpha_1^c)_j - (\alpha_2^r)_i(\alpha_2^c)_j$ $(\alpha_1^{\bar{r}})_i(\alpha_1^{\bar{c}})_j+(\alpha_2^{\bar{r}})_i(\alpha_2^{\bar{c}})_j$ $\overline{1}$ 3: $x \coloneqq \text{BST}(\mathbf{W}_{ij}, \mathbf{v})$ 4: **switch** (x) 5: case v_1 : 6: $(\mathbf{B}_1)_{ij} = -1, (\mathbf{B}_2)_{ij} = -1$ 7: case v_2 : 8: $(\mathbf{B}_1)_{ij} = -1, (\mathbf{B}_2)_{ij} = +1$ 9: case v_3 : 10: $(\mathbf{B}_1)_{ij} = +1, (\mathbf{B}_2)_{ij} = -1$ 11: default: 12: $(\mathbf{B}_1)_{ij} = +1, (\mathbf{B}_2)_{ij} = +1$ 13: end switch 14: end for 15: return $\mathbf{B}_1, \mathbf{B}_2$ func BST (w, \mathbf{v}) 1: $l \coloneqq \text{length}(\mathbf{v})$ 2: if $l == 1$ then 3: return v_1 4: else if $w \ge (v_{m/2} + v_{m/2+1})/2$ then 5: **return** BST $(w, \mathbf{v}_{m/2+1:m})$ 6: else 7: **return** BST $(w, \mathbf{v}_{1:m/2})$ 8: end if

Algorithm 5 Second-Order Alternating Refined Binarization along Row-Column Axes

C PROOF OF THEOREM 1

Here we consider a row of the weight matrix $\mathbf{W} \in \mathbb{R}^{1 \times m}$ with single μ and α . In the (τ +1)-th iteration, we update μ by using the following formulas:

$$
\mathbf{R}^{\tau} = \mathbf{W} - \alpha^{\tau} \mathbf{B}^{\tau} - \mu^{\tau},\tag{100}
$$

$$
\delta_{\mu}^{\tau} = \overline{\mathbf{R}^{\tau}},\tag{101}
$$

$$
\mu^{\tau+1} = \mu^{\tau} + \delta_{\mu}^{\tau}.\tag{102}
$$

Then we can compute the specific value of the quantization error reduction after updating μ^{τ} :

$$
||\mathbf{R}^{\tau} - \delta_{\mu}^{\tau}||^2 = ||\mathbf{R}^{\tau}||^2 - 2\langle \mathbf{R}^{\tau}, \delta_{\mu}^{\tau} \rangle + ||\delta_{\mu}^{\tau}||^2
$$
\n(103)

$$
= ||\mathbf{R}^{\tau}||^2 - 2\delta_{\mu}^{\tau} \sum_{k=1}^{m} \mathbf{R}_k^{\tau} + m(\delta_{\mu}^{\tau})^2
$$
 (104)

$$
= ||\mathbf{R}^{\tau}||^2 - m(\delta_{\mu}^{\tau})^2 \tag{105}
$$

$$
\leq ||\mathbf{R}^\tau||^2. \tag{106}
$$

Here we have $m\delta_{\mu}^{\tau^2} = ||\mathbf{R}^{\tau}||^2 - n\sigma^2$. We refine **B** using the following formula: τ

$$
\mathbf{B}^{\tau+1} = \text{sign}(\mathbf{W} - \mu^{\tau} - \delta_{\mu}^{\tau}).
$$
 (107)

The following derivation provides the decrease in quantization error after updating B:

$$
\|\mathbf{R}^{\tau} - \delta_{\mu}^{\tau} + \alpha^{\tau} (\mathbf{B}^{\tau} - \mathbf{B}^{\tau+1})\|^2
$$
\n
$$
\|\mathbf{R}^{\tau} - \delta_{\mu}^{\tau} + \alpha^{\tau} (\mathbf{B}^{\tau} - \mathbf{B}^{\tau+1})\|^2
$$
\n(108)

$$
= ||\mathbf{R}^{\tau} - \delta_{\mu}^{\tau}||^2 + 2\langle (\mathbf{R}^{\tau} - \delta_{\mu}^{\tau}), \alpha^{\tau}(\mathbf{B}^{\tau} - \mathbf{B}^{\tau+1}) \rangle + ||\alpha^{\tau}(\mathbf{B}^{\tau} - \mathbf{B}^{\tau+1})||^2 \tag{109}
$$

$$
= ||\mathbf{R}^{\tau} - \delta_{\mu}^{\tau}||^2 + \alpha^{\tau} \sum_{k} (\mathbf{B}_{k}^{\tau} - \mathbf{B}_{k}^{\tau+1}) (2\mathbf{R}_{k}^{\tau} - 2\delta_{\mu}^{\tau} + \alpha^{\tau} \mathbf{B}_{k}^{\tau} - \alpha^{\tau} \mathbf{B}_{k}^{\tau+1})
$$
(110)

$$
= ||\mathbf{R}^{\tau}||^2 - m\delta_{\mu}^{\tau^2} + \alpha^{\tau} \sum_{k} (\mathbf{B}_k^{\tau} - \mathbf{B}_k^{\tau+1}) (2(\mathbf{W}_k - \mu^{\tau} - \delta_{\mu}^{\tau}) - \alpha^{\tau} (\mathbf{B}_k^{\tau} + \mathbf{B}_k^{\tau+1})) \tag{111}
$$

$$
= ||\mathbf{R}^{\tau}||^2 - m\delta_{\mu}^{\tau 2} + M,
$$
\n(112)

where
$$
M = \alpha^{\tau} \sum_{k} (\mathbf{B}_{k}^{\tau} - \mathbf{B}_{k}^{\tau+1}) (2(\mathbf{W}_{k} - \mu^{\tau} - \delta_{\mu}^{\tau}) - \alpha^{\tau} (\mathbf{B}_{k}^{\tau} + \mathbf{B}_{k}^{\tau+1})).
$$
 (113)

M only has the following conditions:

if
$$
\mathbf{B}_k^{\tau} = \mathbf{B}_k^{\tau+1} \Rightarrow M = 0
$$
,
\nif $\mathbf{B}_k^{\tau} = +1$, $\mathbf{B}_k^{\tau+1} = -1 \Rightarrow \mathbf{W} - \mu^{\tau} - \delta_{\mu}^{\tau} < 0 \Rightarrow M < 0$,
\nif $\mathbf{B}_k^{\tau} = -1$, $\mathbf{B}_k^{\tau+1} = +1 \Rightarrow \mathbf{W} - \mu^{\tau} - \delta_{\mu}^{\tau} > 0 \Rightarrow M < 0$,
\n $\Rightarrow M \le 0$,
\n $\Rightarrow ||\mathbf{R}^{\tau} - \delta_{\mu}^{\tau} + \alpha^{\tau} (\mathbf{B}^{\tau} - \mathbf{B}^{\tau+1})||^2 \le ||\mathbf{R}^{\tau}||^2 - m\delta_{\mu}^{\tau 2}$.

Specifically,

$$
M = 2m(\alpha^{\tau})^2 - 2\alpha^{\tau}\delta_{\mu}^{\tau}\sum_{k} \mathbf{B}_{k}^{\tau} - 2m\alpha^{\tau}\alpha^{\tau+1}
$$
\n(114)

$$
=2m(\alpha^{\tau})^2+2m\delta_{\mu}^{\tau}(\mu^{\tau+1}-\overline{\mathbf{W}})-2m\alpha^{\tau}\alpha^{\tau+1}.
$$
 (115)

Then we refine α and calculate the reduction of quantization error:

$$
\mathbf{R}' = \mathbf{R}^{\tau} - \delta_{\mu}^{\tau} + \alpha^{\tau} (\mathbf{B}^{\tau} - \mathbf{B}^{\tau+1}), \tag{116}
$$

$$
||\mathbf{R}' + (\alpha^{\tau} - \alpha^{\tau+1})\mathbf{B}^{\tau+1}||^2
$$
\n
$$
= ||\mathbf{R}'||^2 + (\alpha^{\tau} - \alpha^{\tau+1})\sum \mathbf{B}^{\tau+1}_{i}(2\mathbf{R}'_{i} + (\alpha^{\tau} - \alpha^{\tau+1})\mathbf{B}^{\tau+1})
$$
\n(118)

$$
= ||\mathbf{R}'||^2 + (\alpha^{\tau} - \alpha^{\tau+1}) \sum_{k} \mathbf{B}_{k}^{\tau+1} (2\mathbf{R}'_{k} + (\alpha^{\tau} - \alpha^{\tau+1}) \mathbf{B}^{\tau+1})
$$
(118)

$$
= ||\mathbf{R}'||^2 + (\alpha^{\tau} - \alpha^{\tau+1}) \sum_{k} \mathbf{B}_{k}^{\tau+1} (2(\mathbf{W}_{k} - \mu^{\tau+1}) - (\alpha^{\tau} + \alpha^{\tau+1}) \mathbf{B}^{\tau+1}) \tag{119}
$$

$$
= ||\mathbf{R}'||^2 + 2m\alpha^{\tau+1}(\alpha^{\tau} - \alpha^{\tau+1}) - m(\alpha^{\tau})^2 + m(\alpha^{\tau+1})^2
$$
\n(120)

$$
= ||\mathbf{R}'||^2 - m(\alpha^\tau - \alpha^{\tau+1})^2
$$
\n(12)

$$
\leq ||\mathbf{R}'||^2. \tag{122}
$$

Combining the results from the above derivation, we can obtain the specific value of the decrease of quantization error after the $(\tau+1)$ -th iteration:

$$
||\mathbf{R}^{\tau+1}||^2 - ||\mathbf{R}^{\tau}||^2 \tag{123}
$$

$$
= -m(\delta_{\mu}^{\tau})^2 + 2m(\alpha^{\tau})^2 + 2m\delta_{\mu}^{\tau}(\mu^{\tau+1} - \mu^0) - 2m\alpha^{\tau}\alpha^{\tau+1} - m(\alpha^{\tau} - \alpha^{\tau+1})^2 \tag{124}
$$

$$
= m((\alpha^{\tau})^2 - (\alpha^{\tau+1})^2 - (\delta_{\mu}^{\tau})^2 + 2\delta_{\mu}^{\tau}(\mu^{\tau+1} - \mu^0))
$$
\n(125)

We can also derive the relationship between the quantization error after the T-th iteration \mathbb{R}^T and the quantization error before iteration \mathbf{R}^0 as

$$
||\mathbf{R}^T||^2 - ||\mathbf{R}^0||^2 = m((\alpha^0)^2 - (\alpha^T)^2 + (\mu^T - \mu^0)^2).
$$
 (126)

D PROOF OF THEOREM 2

 $\mathbf{X} \in \mathbb{R}^{B \times L \times m}$ is the calibration data. $\mathbf{W}, \widehat{\mathbf{W}} \in \mathbb{R}^{n \times m}$ are the full-precision weight matrix and binarized weight matrix, k is the block size, T is theiteration rounds. The quantization error with calibration data \mathcal{L}_1 is shown as follows:

$$
\mathcal{L}_1 = ||\mathbf{W}\mathbf{X} - \widehat{\mathbf{W}}\mathbf{X}||^2
$$
 (127)

$$
= ||\mathbf{X} \cdot (\mathbf{W} - \widehat{\mathbf{W}})^{\top}||^2.
$$
 (128)

We calculate the time complexity of $\mathbf{X} \cdot (\mathbf{W} - \widehat{\mathbf{W}})^{\top}$ as $\mathcal{O}(B \cdot k \cdot L \cdot n)$ since it involves B matrix multiplications, each requiring $(L \cdot n \cdot k)$ multiplications and $(L \cdot n \cdot (k-1))$ additions. The time complexity of squaring all the elements of a matrix and then sums them up is $\mathcal{O}(L \cdot n)$. In each iteration, we need to perform $\frac{m}{k}$ calculations, and there are T iterations in total. Therefore, the overall time complexity is $\hat{T} \cdot \frac{m}{k} \cdot (\hat{\mathcal{O}(B \cdot k \cdot L \cdot n)} + \mathcal{O}(L \cdot n))$, which simplifies to $\mathcal{O}(n \cdot B \cdot L \cdot m \cdot T)$.

$$
\mathcal{L}_2 = \sum_i \sum_j (\mathbf{S} \odot \mathbf{R})_{ij}.
$$
 (129)

We calculate the time complexity of **S** as $\mathcal{O}(B \cdot k^2 \cdot L)$, since **S** contains k^2 elements, and calculating each element involves $(B \cdot L)$ multiplications and $(B \cdot L)$ additions. And we calculate the time complexity of **R** as $\mathcal{O}(n \cdot k^2)$, since **R** contains k^2 elements, and calculating each element involves n multiplications and $(n - 1)$ additions. The time complexity of the element-wise multiplication of S and **R**, as well as the summation of the matrices, is $\mathcal{O}(k^2)$. In each iteration, we need to perform $\frac{m}{k}$ calculations, and there are T iterations in total. It is important to note that the calculation of matrix \tilde{S} does not need to be performed in every iteration of the T iterations; it only needs to be computed once. Therefore, the overall time complexity is $\frac{m}{k} \cdot (\mathcal{O}(B \cdot k^2 \cdot L) + T \cdot (\mathcal{O}(n \cdot k^2) + \mathcal{O}(k^2)))$, which simplifies to $\mathcal{O}(m \cdot k \cdot (B \cdot L + n \cdot T)).$

We define the acceleration ratio η as the quotient of the time complexities of \mathcal{L}_1 and \mathcal{L}_2

$$
\eta = \frac{\mathcal{O}(n \cdot B \cdot L \cdot m \cdot T)}{\mathcal{O}(m \cdot k \cdot (B \cdot L + n \cdot T))}
$$
(130)

$$
\propto \frac{1}{k \cdot \left(\frac{1}{n \cdot T} + \frac{1}{B \cdot L}\right)}.\tag{131}
$$

Typically, we set n to 4096, B to 128, L to 2048, T to 15, and k to 128. Under these circumstances, η is approximately equal to 389.

E MEMORY COMPUTATION

For $\mathbf{W} \in \mathbb{R}^{n \times m}$, block size k, the memory of $\hat{\mathbf{W}}$ after standard row-wise binarization is

$$
\mathcal{M}^{1st} = \overbrace{n \times m}^{\mathbf{B}} + \overbrace{\lceil m/k \rceil}^{multiiple blocks} \times \overbrace{2 \times n \times 16}^{row-wise FP16 \ \alpha \ and \ \mu}
$$
 (132)

Moreover, second-order row-wise binarization can be represented as

$$
\mathcal{M}^{2nd} = \frac{\mathbf{B}_1 \text{ and } \mathbf{B}_2}{2 \times n \times m + \sqrt{m/k}} \times \frac{\text{multiple blocks} \times \text{row-wise FPI6} \alpha_1, \alpha_2, \text{ and } \mu}{3 \times n \times 16}, \tag{133}
$$

since row-wise μ_1 and μ_2 can be combined together as $\mu = \mu_1 + \mu_2$.

Thus, the memory required by BiLLM can be formulated as

$$
\mathcal{M}_{\text{BiLLM}} = \overbrace{2 \times n \times c + \lceil m/k \rceil \times 3n \times 16}^{second-order \, binarization} + \overbrace{n \times (m-c) + \lfloor m/k \rfloor \times 2n \times 16 \times 2}_{2 \, groups}^{first-order \, binarization}
$$
(134)

$$
4 \frac{group\;bitmap}{n \times m} + \frac{salient\;column\;bitmap}{m}, \qquad (135)
$$

where c is the number of salient columns for W .

Similarly, we can formulate the memory occupation of first-order row-column-wise binarization and our ARB-RC as

$$
\mathcal{M}_{\text{row-column-wise}}^{1st} = \overbrace{n \times m}^{\mathbf{B}} + \overbrace{(n+m) \times 16}^{\text{FP16 }\alpha_r \text{ and } \alpha_c} ,
$$
\n
$$
second-order binarization
$$
\n(136)

$$
\mathcal{M}_{ARB-RC} = 2 \times n \times c + (\lceil m/k \rceil \times 2n + 2c) \times 16
$$
\n
$$
first-order binarization
$$
\n(137)

$$
+\overbrace{n \times (m-c) + (\lceil m/k \rceil \times n + (m-c)) \times 16 \times 2}_{2 \text{ groups}}
$$
 (138)

$$
4 \frac{group\;bitmap}{n \times m} + \frac{salient\;column\;bitmap}{m} \tag{139}
$$

In addition, if added CGB, i.e. our refined strategy for the combination of salient column bitmap and group bitmap, the memory requirement slightly increases due to more scaling factors, but still less than BiLLM. The total memory of ARB-RC + CGB is

$$
\mathcal{M}_{ARB-RC+CGB} = 2 \times n \times c + \underbrace{\left(\lceil m/k \rceil \times 2n + 2c\right) \times 16 \times 2}_{2 \text{ groups}} \tag{140}
$$

$$
+ \overbrace{n \times (m-c) + (\lfloor m/k \rfloor \times n + (m-c)) \times 16 \times 2}_{2 \text{ groups}}^{first-order binarization}
$$
\n(141)

$$
4 \frac{group\;bitmap}{n \times m} + \frac{salient\;column\;btmap}{m} \tag{142}
$$

F VISUALIZATION DURING ALTERNATING REFINEMENT

Figure 1: The change of distribution shift (absolute difference between the mean of binarized and fullprecision weights) during alternating refined binarization on LLaMA-7B. Each subfigure represents a block, with iteration 0 corresponding to the BiLLM method.

F.1 DISTRIBUTION SHIFT

As shown in Figure [1,](#page-15-5) our Alternating Refined Binarization progressively reduces the distribution shift with fast convergence, where the initial distribution shift corresponds to BiLLM.

F.2 COLUMN-WISE QUANTIZATION ERROR

As shown in Figure [2,](#page-16-0) We visualize the column-wise quantization error of a block in each layer of the LLM. The results indicate that our ARB-RC method can effectively reduce column-wise quantization error compared to previous row-wise binarization method.

F.3 BINARIZATION PARAMETERS

As shown in Figure [3,](#page-17-0) we visualize the changes of alpha and mean during Alternating Refined Binarization. It is evident that all alpha values increase beyond their initial estimates, as supported by our analysis of quantization error in Equation [\(121\)](#page-12-0). This suggests that alpha was underestimated by previous binarization methods.

G MORE EXPERIMENTAL RESULTS

Comparison on PTB and C4. Due to the page limit, we provide the perplexity comparison on PTB dataset for LLaMA and OPT families in Table [1](#page-18-1) and Table [3](#page-19-0) respectively. Similarly, the comparisons on C4 dataset for LLaMA and OPT families are provided in Table [2](#page-19-1) and Table [4](#page-20-1) respectively.

Comparison on 7 zero-shot QA datasets. We also provide the comparison of 7 zero-shot QA datasets on OPT family, as shown in Table [5.](#page-20-2)

Figure 2: Quantization error comparison between row-wise binarization (red curve) and ARB-RC (blue curve) on LLaMA-7B. We display the error along columns, with each subfigure representing a block. The blue curve is notably lower than the red curve, with the difference being particularly pronounced in the *Gate Project*, *Up Project*, and *Down Project* layers.

Evaluation with other metrics. We conduct additional experiments on LLaMA-7B, measuring the F1 score on the SQuADv2 dataset and chrF on the WMT2014 (En-Fr) dataset. As shown in Table [6,](#page-21-0) our ARB-LLM significantly outperforms previous binarization methods, PB-LLM and BiLLM, in both F1 score and chrF metrics, further demonstrating the effectiveness of our proposed method.

Evaluation on SQuADv2, SWAG, and MMLU College Mathematics datasets. We conduct additional experiments on the long context dataset SQuADv2, math dataset MMLU College Mathematics,

Figure 3: The changes of alpha and mean during alternating refinement on LLaMA-7B, with each subfigure representing a block. The red curve on the left represents the change of alpha, while the blue curve represents the change of mean. All alpha values exceed their initial estimates, indicating that alpha is underestimated in standard binarization.

and reasoning dataset SWAG. As shown in Table [7,](#page-21-1) our ARB-LLM also outperforms the previous binarization methods PB-LLM and BiLLM on these datasets, narrowing the performance gap with FP16, especially on the long-context SQuADv2 dataset.

Comparison on Phi-3 models. We conduct additional experiments by binarizing Phi-3-mini (3.8B) and Phi-3-medium (14B), and evaluate their perplexity (PPL) on WikiText2. As shown in Table [8,](#page-21-2) our ARB-LLM consistently outperforms previous binarization methods, PB-LLM and BiLLM. Moreover, the performance gap between binarized and FP16 models is reasonable. Compared to the binarization of OPT, the results for Phi-3-mini (3.8B) surpass those of OPT (2.7B), and the results for Phi-3-medium (14B) outperform OPT (13B).

Comparison of runtime inference. Evaluating runtime performance is crucial for demonstrating the practical feasibility of our proposed implementation. Unfortunately, previous works such as BiLLM and PB-LLM, did not report runtime performance due to the lack of a CUDA kernel for matrix multiplication between FP activation and 1-bit weights. We use the BitBLAS codebase to benchmark our method and comparable approaches, providing detailed runtime evaluations. We evaluate the runtime inference metrics by measuring the latency (ms) of various linear layers in LLaMA-7B and LLaMA-13B. The sequence length of input tensor X is 2048, and experiments are conducted on an NVIDIA A6000 GPU. As shown in Table [9,](#page-21-3) our method demonstrates significant improvements in inference speed compared to FP16 and PB-LLM. PB-LLM is slower due to the Int8-to-FP16 matrix multiplication. Moreover, both ARB-LLM-X and ARB-LLM-RC achieve a speed similar to BiLLM, while largely improving the performance.

Pareto curve. We present the Pareto curves of binarization methods PB-LLM, BiLLM, and our ARB-LLM (all with CSR compressed bitmap), as well as the low-bit quantization methods GPTQ in Figure [4.](#page-22-0) Among GPTQ models, the 4-bit version achieves the highest accuracy for a given memory budget compared to its 2-bit, 3-bit, and 8-bit counterparts. However, our ARB-LLM still outperforms 4-bit GPTQ on the Pareto curve. Moreover, low-bit quantization methods like GPTQ suffer significant accuracy degradation at extremely low bit levels (e.g., 2-bit). In contrast, our ARB-LLM excels in such scenarios, delivering superior performance while using less memory.

Table 1: Perplexity of RTN, GPTQ, PB-LLM, BiLLM, and our methods on LLaMA family. The columns represent the perplexity results on the PTB dataset with different model sizes. N/A: LLaMA2 lacks a 30B version, and LLaMA3 lacks both 13B and 30B versions. *: LLaMA has a 65B version, while both LLaMA2 and LLaMA3 have 70B versions.

Results of BiLLM. We strictly follow the BiLLM codebase to reproduce the results. However, the experiments were conducted on a different GPU, and some package versions may differ. These slight variations in the experimental environment are likely the primary cause of any discrepancies. As shown in Table [10,](#page-21-4) for these two models, more than half of the reproduced results are better than those reported in the original paper. Whether compared against the original results or the reproduced ones, our ARB-LLM consistently outperforms BiLLM.

H DIALOG EXAMPLES

As shown in Figure [5,](#page-23-0) we provide some dialogue examples of PB-LLM, BiLLM, and our ARB-LLM_{RC} on LLaMA-13B and Vicuna-13B models.

Model	Method	Block Size	Weight Bits	7B/8B*	13B	30 _B	65B/70B*
	Full Precision	$\frac{1}{2}$	16.00	7.34	6.80	6.13	5.81
	RTN	\equiv	3.00	28.24	13.24	28.58	12.76
	GPTQ	128	3.00	9.95	7.16	6.51	6.03
	RTN	\overline{a}	2.00	112668.16	58515.73	27979.50	22130.23
	GPTQ	128	2.00	79.06	18.97	14.86	10.23
LLaMA	RTN	\overline{a}	1.00	194607.78	1288356.88	13556.87	135027.31
	GPTQ	128	1.00	186229.5	108958.73	9584.84	23965.75
	PB-LLM	128	1.70	76.63	40.64	25.16	15.30
	BiLLM	128	1.09	46.96	16.83	12.11	11.09
	$ARB-LLMX$	128	1.09	22.73	13.86	10.93	9.64
	ARB-LLM _{RC}	128	1.09	17.92	12.48	10.09	8.91
	Full Precision	$\overline{}$	16.00	7.26	6.73	N/A	5.71
	RTN	\equiv	3.00	384.02	12.50	N/A	10.03
	GPTQ	128	3.00	7.95	7.06	N/A	5.88
	RTN	\overline{a}	2.00	30843.15	51690.40	N/A	27052.53
	GPTQ	128	2.00	35.27	19.66	N/A	9.55
LLaMA2	RTN	$\overline{}$	1.00	115058.76	46250.21	$\rm N/A$	314504.09
	GPTQ	128	1.00	67954.04	19303.51	N/A	13036.32
	PB-LLM	128	1.70	80.69	184.67	N/A	NAN
	BiLLM	128	1.08	39.38	25.87	N/A	17.30
	$ARB-LLMX$	128	1.08	28.02	19.82	N/A	11.85
	ARB-LLM _{RC}	128	1.08	20.12	14.29	N/A	8.65
	Full Precision	$\overline{}$	16.00	9.45	N/A	N/A	7.17
	RTN	\overline{a}	3.00	566.43	N/A	N/A	12285.45
	GPTQ	128	3.00	17.68	N/A	N/A	10.04
	RTN	\overline{a}	2.00	777230.94	N/A	N/A	447601.09
	GPTQ	128	2.00	394.74	N/A	N/A	122.55
LLaMA3	RTN	$\overline{}$	1.00	1422473.38	N/A	N/A	188916.13
	GPTQ	128	1.00	1118313.13	N/A	N/A	126439.66
	PB-LLM	128	1.70	104.15	N/A	N/A	40.69
	BiLLM	128	1.06	61.04	N/A	N/A	198.86
	$ARB-LLMx$	128	1.06	41.86	N/A	N/A	21.67
	$ARB-LLM_{BC}$	128	1.06	35.70	N/A	N/A	15.44

Table 2: Perplexity of RTN, GPTQ, PB-LLM, BiLLM, and our methods on LLaMA family. The columns represent the perplexity results on the C4 dataset with different model sizes. N/A: LLaMA2 lacks a 30B version, and LLaMA3 lacks both 13B and 30B versions. *: LLaMA has a 65B version, while both LLaMA2 and LLaMA3 have 70B versions.

Table 3: Perplexity of RTN, GPTQ, PB-LLM, BiLLM, and our methods on OPT family. The columns represent the perplexity results on PTB datasets with different model sizes.

Method	Block Size	Weight Bits	1.3B	2.7B	6.7B	13B	30B	66B
Full Precision		16.00	20.29	17.97	15.77	14.52	14.04	13.36
RTN		3.00	8987.17	9054.89	4661.77	2474.14	1043.13	3647.87
GPTO	128	3.00	17.54	15.15	12.86	11.93	11.28	11.42
RTN	$\overline{}$	2.00	8030.18	5969.35	17222.70	72388.19	105760.72	462581.28
GPTQ	128	2.00	110.93	58.38	22.73	17.81	14.19	62.04
RTN	۰	1.00	11062.04	28183.08	11981.09	32157360.00	5435.99	147668.78
GPTO	128	1.00	6524.99	8405.25	5198.99	3444847.25	7158.62	5737.15
PB-LLM	128	1.70	324.62	183.97	169.49	101.00	41.87	45.32
BiLLM	128	1.11	115.94	88.52	69.41	27.16	21.41	18.51
$ARB-LLMX$ $ARB-LLM_{BC}$	128 128	1.11 1.11	71.96 43.34	54.28 31.77	31.23 22.31	23.46 18.81	19.28 16.88	17.64 15.66

Method	Block Size	Weight Bits	1.3B	2.7B	6.7B	13B	30B	66B
Full Precision	$\qquad \qquad -$	16.00	16.07	14.34	12.71	12.06	11.45	10.99
RTN		3.00	5039.85	11165.54	5022.57	2550.72	1030.62	3394.97
GPTO	128	3.00	16.11	14.17	12.29	11.54	10.91	11.05
RTN		2.00	7431.04	7387.40	13192.40	89517.66	61213.64	823566.00
GPTO	128	2.00	63.06	35.81	18.60	16.29	12.92	33.03
RTN		1.00	9999.56	23492.89	9617.07	23436088.00	5041.77	113236.92
GPTO	128	1.00	6364.65	6703.36	5576.82	1799217.88	7971.37	7791.47
PB-LLM	128	1.70	168.12	222.15	104.78	57.84	27.67	27.73
BiLLM	128	1.11	64.14	44.77	42.13	19.83	16.17	14.16
$ARB-LLMx$	128	1.11	47.60	34.97	22.54	17.71	14.71	13.32
$ARB-LLM_{RC}$	128	1.11	28.19	21.46	16.97	15.01	13.34	12.43

Table 4: Perplexity of RTN, GPTQ, PB-LLM, BiLLM, and our methods on OPT family. The columns represent the perplexity results on C4 datasets with different model sizes.

Table 5: Accuracy of 7 QA datasets on OPT family. We compare the results among GPTQ, PB-LLM, BiLLM, $ARB-LLM_X$, and $ARB-LLM_{RC}$ to validate the quantization effect.

Model	Method	Weight Bits				PIQA ↑ BoolQ ↑ OBQA ↑ Winogrande ↑ ARC-e ↑ ARC-c ↑ Hellaswag ↑ Average ↑				
	GPTQ	2.00	59.47	42.66	15.80	50.04	37.21	21.42	30.92	36.79
	PB-LLM	1.70	54.57	61.77	13.00	50.99	28.79	20.56	26.55	36.60
OPT-1.3B BiLLM		1.09	59.52	61.74	14.80	52.17	36.53	17.83	29.64	38.89
	$ARB-LLMX$	1.09	62.84	61.99	13.40	52.17	43.43	18.94	30.86	40.52
	$ARB-LLM_{RC}$	1.09	65.45	60.31	15.40	53.04	48.27	19.37	33.44	42.18
	GPTQ	2.00	61.81	54.43	15.40	52.33	40.15	20.56	32.55	39.60
	PB-LLM	1.70	56.42	62.23	12.80	50.12	31.61	18.60	27.61	37.06
OPT-2.7B BiLLM		1.09	62.57	62.20	15,40	52.57	39.65	19.80	30.88	40.44
	$ARB-LLMX$	1.09	65.61	62.08	14.80	53.59	47.22	19.62	32.57	42.21
	$ARB-LLM_{RC}$	1.09	68.50	61.99	21.60	58.33	52.82	22.27	37.50	46.14
	GPTQ	2.00	69.37	55.05	21.20	55.80	56.06	23.38	41.29	46.02
	PB-LLM	1.70	56.47	55.57	13.20	50.28	29.97	18.69	27.50	35.95
OPT-6.7B BiLLM		1.09	58.60	62.14	13.20	53.12	33.75	18.26	28.83	38.27
	$ARB-LLMx$	1.09	69.75	62.20	17.80	58.64	55.47	24.32	37.78	46.57
	$ARB-LLM_{RC}$	1.09	72.47	62.87	22.20	60.62	59.09	26.79	42.08	49.45
	GPTO	2.00	66.54	56.51	18.60	59.12	48.53	24.06	41.34	44.96
	PB-LLM	1.70	57.29	62.17	12.80	51.22	30.93	20.56	26.83	37.40
OPT-13B BiLLM		1.09	68.72	62.32	18.00	59.91	54.71	26.37	39.02	47.00
	ARB-LLM _x	1.09	71.98	62.57	21.20	61.40	59.72	26.02	41.45	49.19
	$ARB-LLM_{RC}$	1.09	73.56	65.93	24.20	64.25	62.54	29.52	45.14	52.16
	GPTO	2.00	73.88	63.94	24.20	62.19	60.77	28.24	47.88	51.59
	PB-LLM	1.70	66.76	62.29	17.40	51.07	49.33	22.53	36.53	43.70
OPT-30B BiLLM		1.09	72.74	62.35	21.00	60.14	60.69	27.56	42.81	49.61
	$ARB-LLMX$	1.09	74.27	62.39	23.60	64.25	63.51	28.33	46.04	51.77
	$ARB-LLM_{RC}$	1.09	75.08	65.78	26.40	65.43	64.81	29.69	48.59	53.68
	GPTO	2.00	57.62	57.13	13.20	51.85	36.11	21.67	34.01	38.80
	PB-LLM	1.70	72.74	62.54	24.20	63.46	60.10	30.20	43.13	50.91
OPT-66B BiLLM		1.09	75.08	65.26	25.60	65.43	65.66	31.40	47.54	53.71
	$ARB-LLMX$	1.09	75.79	66.27	27.00	66.77	67.51	32.76	49.33	55.06
	$ARB-LLM_{RC}$	1.09	76.88	70.89	28.60	66.22	69.28	33.62	51.23	56.67

I LIMITATIONS

Combination of ARB-X and ARB-RC. We find that it is hard to incorporate the calibration data into the update of column scaling factors. After initializing the row and column scaling factors, we take the derivative of quantization error \mathcal{L}_2 with respect to α^c and set it to zero:

$$
\frac{\partial \mathcal{L}}{\partial \alpha_t^c} = \sum_k \mathbf{S}_{kt} \sum_j (-\alpha_j^r \mathbf{B}_{jt} \mathbf{W}_{jk} + (\alpha_j^r)^2 \alpha_k^c \mathbf{B}_{jt} \mathbf{B}_{jk}) = 0, \text{ where } t = 1, 2, ..., m. \tag{143}
$$

Method	SQuADv2 (F1 score \uparrow)	WMT2014 En-Fr (chrF \uparrow)
FP16	19.45	28.89
PB-LLM	2.78	14.27
BiLLM $ARB-LLMx$	3.55 8.23	17.45 23.90
$ARB-LLM_{RC}$	12.24	19.22

Table 6: Comparison on SQuADv2 (F1 score) and WMT2014 En-Fr (chrF).

Table 8: Perplexity of WikiText2 on Phi-3 models.

Model	Phi-3-mini $(3.8B)$	Phi-3-medium $(14B)$
FP16	5.82	4.02
PB-LLM	377.98	754.27
BiLLM	21.03	10.33
$ARB-LLMx$	18.32	9.31
$ARB-LLM_{RC}$	17.32	8.97

Table 9: Comparison of runtime inference (ms) on LLaMA-1/2-7B and LLaMA-1/2-13B.

Model		$LLaMA-1/2-7B$		$LLaMA-1/2-13B$		
Weight Size	4096×4096	4096×11008	11008×4096	5120×5120	5120×13824	13824×5120
FP16	0.76595	1.63532	1.76949	0.91443	2.68492	2.71254
PB-LLM	0.73363	1.44076	1.69881	0.83148	2.17292	2.19443
BiLLM	0.34201	0.36777	0.37689	0.35948	0.48947	0.49406
$ARB-LLM_{RC}$	0.35974	0.37218	0.37981	0.36312	0.49801	0.50038
ARB-LLM _x	0.33180	0.35539	0.36792	0.35505	0.47788	0.48275

Table 10: Perplexity of WikiText2 on LLaMA-1 and LLaMA-2. ‡We reproduce BiLLM based on their codebase.

We observe that during the process of updating α_t^c , the derivative of the quantization error with respect to α_t^c includes terms involving other α_t^c . This indicates that introducing a calibration set results in coupling between α^c values, complicating their updates. Incorporating calibration data into ARB-RC presents a promising direction for future work.

Figure 4: The Pareto curves of binarization and low-bit quantization methods demonstrate that our ARB-LLM outperforms all other approaches within the same memory constraints. Low-bit methods like GPTQ suffer significant performance degradation at extremely low bit levels (e.g., 2-bit), whereas our method maintains strong performance.

LLaMA-13B

Figure 5: Conversation examples on LLaMA-13B (language supplementary) and Vicuna-13B (Q&A). We compare our best method ARB-LLM_{RC} with PB-LLM and BiLLM. Inappropiate and reasonable responses are shown in corresponding colors.

you rest on Sunday and Monday, and then be ready and full of energy by Tuesday.