Executive Summary

All proofs and the DP formulation are **correct and consistent**. We verify the LOO-CRPS cost formula algebraically and recover exactly $cost(S) = mW/(m-1)^2$. The DP recurrence is standard and provably optimal: $dp[k,j] = \min_{i<j}(dp[k-1,i] + c(i+1,j))$, with correct base cases, ensuring global optimality. Complexity claims hold: Phase 1 is $O(n^2 \log n)$ and Phase 2 is $O(n^2 K)$. Edge cases (bin size $m = 1$ or ties) are handled (by setting $c(i,i) = +\infty$). No unstated assumptions invalidate the results. We recommend clarifying the minimum-bin constraint and explicitly stating the DP recurrence. Below are detailed derivations, proofs, and analysis.

Step-by-Step Verification of LOO-CRPS Formula

Recall $S = \{y_1, \ldots, y_m\}$ sorted responses in one bin. Define

$$d_k \;=\; \sum_{\ell \in S,\ \ell \neq k} |y_\ell - y_k|, \quad D \;=\; \sum_{\ell \neq r,\ \ell,r \in S} |y_\ell - y_r|, \quad W = \sum_{\ell < r} |y_\ell - y_r| = \frac{D}{2}.$$

Each left-out CRPS is (using the identity $\mathrm{CRPS}(F,y) = E_F|X-y| - \frac{1}{2}E_F|X-X'|$ [1]):

$$\mathrm{CRPS}(\hat{F}_{S\setminus\{k\}}, y_k) = \frac{d_k}{m-1} - \frac{1}{2(m-1)^2} \sum_{\substack{\ell \neq r \\ \ell, r \neq k}} |y_\ell - y_r|.$$

Summing over $k = 1, \ldots, m$ gives the total cost:

$$\mathrm{cost}(S) = \sum_{k=1}^{m} \Big[\frac{d_k}{m-1} - \frac{1}{2(m-1)^2}(D - 2d_k)\Big],$$

since $\sum_{\ell \neq r,\, \ell,r \neq k} |y_\ell - y_r| = D - 2d_k$. Simplify each part:

- **First term:** $\sum_k d_k/(m-1) = \frac{1}{m-1}\sum_k d_k = \frac{D}{m-1}$ (because each pair $|y_\ell - y_r|$ appears once in d_ℓ and once in d_r, so $\sum_k d_k = D$).
- **Second term:** $\sum_k \frac{D-2d_k}{2(m-1)^2} = \frac{1}{2(m-1)^2}(mD - 2\sum_k d_k) = \frac{1}{2(m-1)^2}(mD - 2D) = \frac{D(m-2)}{2(m-1)^2}$.

Subtracting:

$$\mathrm{cost}(S) = \frac{D}{m-1} - \frac{D(m-2)}{2(m-1)^2} = \frac{D\big[2(m-1) - (m-2)\big]}{2(m-1)^2} = \frac{mD}{2(m-1)^2}.$$

Finally $D = 2W$, so

$$\boxed{\mathrm{cost}(S) = \frac{m\,W}{(m-1)^2}},$$

matching the claimed formula. Each algebraic step is valid (no cancellation errors). In particular, for $m = 2$ this gives $2W/1^2 = 2|y_1 - y_2|$, which equals the sum of the two LOOCV errors $|y_2 - y_1| + |y_1 - y_2|$. The derivation assumes only finite sums and uses the CRPS identity [1] ; it does *not* assume symmetry beyond absolute values.

DP Recurrence and Optimality

Let $c(i,j) = \mathrm{cost}(\{y_i, \ldots, y_j\})$. The DP fills

$$dp[1][j] = c(1,j), \qquad dp[k][j] = \min_{i=k-1,\ldots,j-1} \big\{\, dp[k-1][i] + c(i+1,j) \big\},$$

with $dp[0][0] = 0$. We prove this finds the optimal K-partition.

Base case (k=1): Putting all points $1..j$ in one bin has cost $c(1,j)$. Hence $dp[1][j] = c(1,j)$ is optimal. (Singleton bins $m = 1$ are forbidden by $c(i,i) = +\infty$.)

Inductive step: Assume $dp[k-1][i]$ is the optimal cost for partitioning $1..i$ into $k-1$ bins. Any optimal k-partition of $1..j$ must split at some $i < j$. Then its cost is $\big(\text{optimal cost of } 1..i\big) + c(i+1,j) = dp[k-1][i] + c(i+1,j)$. Taking $\min_i$ finds the best split.

Optimal substructure: The cost splits additively, so solving subproblems suffices. Standard segmented-DP theory [2] ensures the above recurrence finds the global minimum. No counterexample exists: if an optimal solution had first $k-1$ bins covering $1..i^*$ and last bin $i^* + 1..j$, the recurrence picks i^*.

Mermaid diagram (DP recursion):

```
graph TD
    A[dp[1][j]=c(1,j)] --> B[k=2..K]
    B --> C[j=k..n]
    C --> D{for i=k-1..j-1}
    D --> E[v = dp[k-1][i] + c(i+1,j)]
    E --> F[dp[k][j] = min(dp[k][j], v)]
```

Complexity & Stability Analysis

- **Time complexity:** Phase 1 double loop $i = 1..n,\ j = i..n$ with Fenwick updates takes $O(n^2 \log n)$. Phase 2 triple loop ($k = 1..K,\ j = k..n,\ i < j$) costs $O(Kn^2)$. These match the manuscript's claims.

- **Memory:** The cost matrix $c[i][j]$ is $O(n^2)$ storage. The DP table is $O(Kn)$. Overall $O(n^2)$, as stated.

- **Numerical stability & edge cases:**

- **Bin size $m = 1$:** The algorithm sets $c(i,i) = +\infty$, effectively forbidding a single-point bin. This ensures $m \geq 2$ always, consistent with the formula's domain.
- **Bin size $m = 2$:** Cost $= 2|y_i - y_{i+1}|$ (since $W = |y_i - y_{i+1}|$), which agrees with two CRPS terms.
- **Ties in x or y:** Sorting by x orders ties arbitrarily (doesn't affect correctness). Equal y values give zero distances; all sums remain valid. Fenwick-tree operations handle equal keys by counting occurrences (no break).
- **Degenerate distributions:** If all y are equal, $W = 0$ and every cost is 0; DP still finds trivial bins.
- **Overflow:** Using floating arithmetic, sums of absolute differences may be large ($\sim n^2 \cdot \max|y|$), but double precision should suffice unless n is extremely large. No special optimizations needed beyond careful summation (Fenwick ensures exact integer sums).
- **Conformal coverage:** The DP and CRPS derivation do not depend on probabilistic assumptions. Conformal guarantees (marginal coverage) rely on exchangeability [3]. Here we train on all data and calibrate via leave-one-out CRPS; this is equivalent to the "jackknife+" approach, which is known to give valid marginal coverage [3] under i.i.d. data. There is no hidden extra assumption.

Tables: Claimed vs. Verified

Item	Manuscript Claim	Verified Result
Cost formula	$mW/(m-1)^2$	$mW/(m-1)^2$
Phase 1 complexity	$O(n^2 \log n)$	$O(n^2 \log n)$
Phase 2 complexity	$O(n^2 K)$	$O(n^2 K)$
Memory	$O(n^2)$	$O(n^2)$
LOOCV assumption	i.i.d. data (exchangeable)	Verified exchangeability needed

Recommendations and Questions

- **Clarify bin size restriction:** Explicitly state in text that bins must have $m \geq 2$ (e.g. "set $c(i,i) = +\infty$ to forbid $m = 1$") since it is only in code now.
- **State DP formula:** Include the recurrence and base case in the main text (e.g. $dp[1][j] = c(1,j)$, $dp[k][j] = \min_i\{dp[k-1,i] + c(i+1,j)\}$) for clarity.
- **Tie-breaking:** Note that ties in covariates can be resolved arbitrarily (no effect on outcome).
- **Assumptions:** The proofs assume only i.i.d. exchangeability (for conformal coverage) and finite pairwise sums. Mention these explicitly.
- **Reviewer questions:** How is $c(i,i)$ treated in theory? (It is ∞.) Is there any effect on coverage from using all data in training vs split? (No, Jackknife+ covers it.)

In summary, **no mathematical errors** were found. The derivations are correct under stated assumptions. Minor clarifications (as above) would strengthen the presentation.

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1 Estimation of the Continuous Ranked Probability Score with Limited Information and Applications to Ensemble Weather Forecasts | Mathematical Geosciences | Springer Nature Link
https://link.springer.com/article/10.1007/s11004-017-9709-7

2 Dynamic Programming Algorithm for Segmented Least Squares
https://stackoverflow.com/questions/4084437/dynamic-programming-algorithm-for-segmented-least-squares

3 stat.cmu.edu
https://www.stat.cmu.edu/~ryantibs/papers/conformal.pdf