

Supplementary Information to "Co-Repressive Interaction and Clustering of Degradable-and-Fire Oscillators"

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I. PROOF OF LEMMA 1

For completeness, we start by recalling the statement of Lemma 1.

Lemma 1 $R_{\{n_k\}} \mathcal{T}_{\{n_k\}} \subset \mathcal{T}_{\{n_{k+1}\}}$ for all $k = 1, \dots, K_{per}$ iff

$$\epsilon_\eta \leq \min_{k=1, \dots, K_{per}} \frac{N}{N - n_k - n_{k+1}} \quad (1)$$

Proof. We first prove that (1) is a sufficient condition. Assume that initially $\{x_k\}_{k=1}^K \in \mathcal{T}_{\{n_k\}}$. Prior to firing, we have $\chi_1(t) = (1 - \epsilon)x_1 + \frac{\epsilon}{N} \sum_{k=1}^K n_k x_k - t$. Accordingly, the quantity χ_1 reaches η at time t_f defined by

$$t_f := \chi_1(0) - \eta = x_1 + \frac{\epsilon}{N} \sum_{k=2}^K n_k (x_k - x_1) - \eta.$$

The quantity t_f is the actual firing time provided that $x_1(t_f) \geq 0$, viz. $t_f \leq x_1$. The latter is equivalent to

$$\epsilon_\eta \sum_{k=2}^K n_k (x_k - x_1) \leq N \quad (2)$$

Using that $0 \leq x_k - x_1 \leq 1$ for state configurations in $\mathcal{T}_{\{n_k\}}$, a sufficient condition for this inequality is $\epsilon_\eta \leq \frac{N}{N - n_1}$. Applying cyclic permutations, we conclude that, for every configuration in any of the $\mathcal{T}_{\{n_{k+\ell}\}}$, the lowest cluster of oscillator fires before (or exactly when) it reaches 0 if

$$\epsilon_\eta \leq \min_{i=1, \dots, K} \frac{N}{N - n_i} \quad (3)$$

When this condition is violated, cluster configurations with all coordinates x_k , $k \geq 2$, sufficiently close to 1 and x_1 sufficiently close to 0 satisfy the inequality $\chi_1(x_1) = \frac{\epsilon}{N} \sum_{k=2}^K n_k (x_k - x_1) \geq \eta$. Accordingly, the concentration x_1 reaches 0 before χ_1 reaches η and, to prevent clustering we have to make sure that $\chi_2(t_f) > \eta$ i.e. $t_f < x_2$ if t_f still denotes the time when x_1 fires. For $t \geq x_1$, we have $\chi_1(t) = \frac{\epsilon}{N} \sum_{k=2}^K n_k (x_k - t)$. The condition $\chi_1(t_f) = \eta$ defines the firing time as follows $t_f = \frac{1}{N - n_1} \left(\sum_{k=2}^K n_k x_k - N\eta_\epsilon \right)$ where $\eta_\epsilon = \frac{\eta}{\epsilon}$. Now, the inequality $t_f < x_2$ turns out to be equivalent to

$$\sum_{k=3}^K n_k x_k - N\eta_\epsilon < (N - n_1 - n_2) x_2 \quad (4)$$

which is certainly satisfied when $\sum_{k=3}^K n_k x_k - N\eta_\epsilon \leq 0$. Solving this inequality for all permutations $\{n_{k+\ell}\}$ gives the desired condition (1) on the coupling parameter.

We now show that $R_{\{n_k\}}$ maps $\mathcal{T}_{\{n_k\}}$ into $\mathcal{T}_{\{n_{k+1}\}}$ when (1) holds. This consists in checking three conditions.

- First, we have $x_2 - t_f > 0$ either because $x_1 - t_f \geq 0$ and $x_2 > x_1$ or simply because of (4) when (3) fails.
- Then, the strict ordering $x_2 < \dots < x_{K-1} < 1$ implies a similar ordering for the coordinates of $R_{\{n_k\}}x$ where $x = (x_1, \dots, x_K)$.

• Finally, we have

$$\begin{aligned}
(1 - \epsilon)(R_{\{n_k\}}x)_1 + \frac{\epsilon}{N} \sum_{k=1}^K n_{k+1}(R_{\{n_k\}}x)_k &= (1 - \epsilon)(x_2 - t_f) + \frac{\epsilon}{N} \left(\sum_{k=1}^{K-1} n_{k+1}(x_{k+1} - t_f) + n_1 \right) \\
&= (1 - \epsilon)(x_2 - t_f) + \frac{\epsilon}{N} \left(\sum_{k=2}^K n_k(x_k - t_f) + n_1 \right) \\
&> (1 - \epsilon)(x_1 - t_f) + \frac{\epsilon}{N} \sum_{k=1}^K n_k(x_k - t_f) = \eta
\end{aligned}$$

where we used $x_2 > x_1$ and $1 \geq x_1 - t_f$ to obtain the inequality. Thus the last inequality in the definition of $\mathcal{T}_{\{n_{k+1}\}}$ is satisfied for $R_{\{n_k\}}x$ and the proof is complete.

Finally, that (1) is a necessary condition is easy to check. Indeed, when $\epsilon_\eta > \frac{N}{N - n_1 - n_2}$, initial conditions in $\mathcal{T}_{\{n_k\}}$ with x_1 and x_2 sufficiently close to 0 and the other x_i close enough to 1 simultaneously violate (2) and (4). Accordingly, the clusters n_1 and n_2 fire simultaneously and a K' -cluster population results with $K' \leq K - 1$. In particular, the image $R_{\{n_k\}}x$ cannot belong to $\mathcal{T}_{\{n_{k+1}\}}$. The proof is complete.

II. PROOF OF LEMMA 2

Lemma 2 *For every $\{n_k\}_{k=1}^K$ and $0 < \epsilon \leq 1$, there is a norm in \mathbb{R}^{K-1} for which $R_{\{n_{k+K_{per}-1}\}}^* \circ \dots \circ R_{\{n_{k+1}\}}^* \circ R_{\{n_k\}}^*$ is a contraction.*

Proof. We begin to prove contraction for the individual map $R_{\{n_k\}}^*$. Its expression depends upon whether the initial condition $x = (x_1, \dots, x_K)$ satisfies (2) or not.

Stability in the domain where x satisfies (2). When only considering the first $K - 1$ coordinates, we obtain

$$(R_{\{n_k\}}^*x)_k = x_{k+1} - t_f = \eta + x_{k+1} - x_1 - \frac{\epsilon}{N} \sum_{\ell=2}^K \alpha_\ell(x_\ell - x_1), \quad k = 1, \dots, K - 1$$

Applying the change of variable $x \mapsto y$ defined by

$$y_k = \begin{cases} x_k - x_{k+1} & \text{if } k = 1, \dots, K - 2 \\ x_{K-1} & \text{if } k = K - 1 \end{cases} \iff x_k = \sum_{\ell=k}^{K-1} y_\ell, \quad \ell = 1, \dots, K - 1$$

the linear part of the previous expression becomes $y \mapsto L_{\{n_k\}}y$ where

$$(L_{\{n_k\}}y)_k = \begin{cases} y_{k+1} & \text{if } k = 1, \dots, K - 2 \\ -\sum_{\ell=1}^{K-1} y_\ell \left(1 - \frac{\epsilon}{N} \sum_{j=\ell+1}^K n_j\right) & \text{if } k = K - 1 \end{cases}$$

(We have used $\sum_{j=2}^{K-1} n_j \sum_{\ell=1}^{j-1} y_\ell = \sum_{\ell=1}^{K-2} y_\ell \sum_{j=\ell+1}^{K-1} n_j$.) The corresponding $(K - 1) \times (K - 1)$ -matrix $L_{\{n_k\}}$ is a companion matrix whose characteristic polynomial $P_{\{n_k\}}$ immediately follows by reading the bottom line, namely

$$P_{\{n_k\}}(\lambda) = \sum_{\ell=0}^{K-1} \lambda^\ell \left(1 - \frac{\epsilon}{N} \sum_{j=\ell+2}^K n_j\right)$$

The polynomial coefficients $1 - \frac{\epsilon}{N} \sum_{j=\ell+2}^K n_j$ are positive and decaying (as ℓ decreases) when $0 < \epsilon \leq 1$. By a classical result in numerical analysis (see eg. p. 116 in [1]), this property implies that $P_{\{n_k\}}$ is Schur stable, viz. all its roots lie inside the unit disk.

Stability in the domain where x does not satisfy (2). In this case, the return map writes

$$(R_{\{n_k\}}^*x)_k = x_{k+1} - \frac{N}{N - n_1} \left(\sum_{\ell=2}^K n_\ell x_\ell - \eta_\epsilon \right), \quad k = 1, \dots, K - 1$$

and the corresponding linear part becomes after applying the same change of variable as before

$$(L'_{\{n_k\}}y)_k = \begin{cases} y_{k+1} & \text{if } k = 1, \dots, K-2 \\ -\frac{1}{N-n_1} \sum_{\ell=2}^{K-1} y_\ell \sum_{j=2}^\ell n_j & \text{if } k = K-1 \end{cases}$$

now based on $\sum_{j=2}^{K-1} n_j \sum_{\ell=j}^{K-1} y_\ell = \sum_{\ell=2}^{K-1} y_\ell \sum_{j=2}^\ell n_j$. The associated characteristic polynomial in this case writes

$$P'_{\{n_k\}}(\lambda) = \frac{1}{N-n_1} \sum_{\ell=1}^{K-1} \lambda^\ell \sum_{j=2}^{\ell+1} n_j$$

Similarly to as before, the polynomial $\frac{P'_{\{n_k\}}(\lambda)}{\lambda}$ has positive and decaying coefficients; hence all roots of $P'_{\{n_k\}}(\lambda)$ lie inside the unit disk.

Proof that the return maps are contractions. Given that both spectral radii $r(L_{\{n_k\}})$ and $r(L'_{\{n_k\}})$ are less than 1, the end of the proof is quite standard. Take any norm $|\cdot|$ in \mathbb{R}^{K-1} . We have $r(L_{\{n_k\}}) = \lim_{t \rightarrow \infty} |L_{\{n_k\}}^t|^{\frac{1}{t}}$ (see e.g. [2]). Take $\delta > 0$ sufficiently small so that $r(L_{\{n_k\}}) + \delta < 1$ and let t_δ be large enough so that

$$|L^t|^{\frac{1}{t}} \leq r(L_{\{n_k\}}) + \delta, \quad \forall t \geq t_\delta$$

Consider the analogous t'_δ for the operator $L'_{\{n_k\}}$ and take $s_\delta = \max\{t_\delta, t'_\delta\}$ (this requires electing δ so that both inequalities $r(L_{\{n_k\}}) + \delta < 1$ and $r(L'_{\{n_k\}}) + \delta < 1$ simultaneously hold). By choosing $\|x\| := |x^{s_\delta}|^{\frac{1}{s_\delta}}$ in \mathbb{R}^{K-1} , we easily conclude that the linear parts of $R_{\{n_k\}}^*$ have norm $\|\cdot\|$ less than 1, viz. $R_{\{n_k\}}^*$ is a global contraction.

Finally, the composed return map $R_{\{n_{k+K_{\text{per}}-1}\}}^* \circ \dots \circ R_{\{n_{k+1}\}}^* \circ R_{\{n_k\}}^*$ will be contracting for the norm $\|x^s\|^{\frac{1}{s}}$ where s is any integer larger than each s_δ of the $R_{\{n_{k+\ell}\}}^*$ and δ is such that all these maps are contracting. The proof is complete.

III. PROOF OF LEMMA 3

Lemma 3 *The periodic orbit passing $\mathcal{T}_{\{n_k\}}$ exists iff*

$$\epsilon_\eta < \zeta(\{n_k\}) := \frac{2N^2}{N^2 - \sum_k n_k^2} \frac{1}{1 - \min_k \frac{n_k}{N-n_{k+1}}} \quad (5)$$

Proof. Without loss of generality, we study the solution in $\mathcal{T}_{\{n_k\}}$ of the equation

$$R_{\{n_{k+K-1}\}} \circ \dots \circ R_{\{n_{k+1}\}} \circ R_{\{n_k\}}(x) = x \quad (6)$$

for any K -cluster configuration $\{n_k\}_{k=1}^K$. For the sake of notation, we use the symbol R^ℓ instead of $R_{\{n_{k+\ell-1}\}} \circ \dots \circ R_{\{n_{k+1}\}} \circ R_{\{n_k\}}$ and $R^0 = \text{Id}$.

Periodic orbits have a property that remarkably simplifies their analysis; namely all coordinates fire from the same value. In particular, this implies that they either all fire before reaching 0 or all reach 0 before firing. To see this, recall that $t_f(x)$ denotes the firing time for x . Using the return map's definition, a moment reflection gives

$$(R^K x)_k = 1 - \sum_{\ell=k}^{K-1} t_f(R^\ell x), \quad k = 1, \dots, K. \quad (7)$$

Together with the periodicity assumption $R^K x = x$ and the return map's definition, this expression implies

$$(Rx)_1 - t_f(Rx) = (R^K x)_2 - t_f(Rx) - t_f(x) = (R^K x)_1 - t_f(x) = x_1 - t_f(x).$$

By induction, we conclude that successive firing levels $(R^\ell x)_1 - t_f(R^\ell x)$ do not depend on $\ell = 0, \dots, K-1$ and the announced alternative follows. To proceed, we consider each case separately.

Analysis when all coordinates fire before reaching 0. In this case, we assume that $t_f(R^\ell x) \leq (R^\ell x)_1$ for $\ell = 0, \dots, K-1$ and we accordingly solve the equation (6), i.e. $R^K(x) = x$.

Letting $\tau_k = x_{k+1} - x_k$ for $k = 0, \dots, K-1$, it turns out convenient to rewrite the periodic orbit coordinates as follows

$$x_k = 1 - \sum_{\ell=k}^{K-1} \tau_\ell, \quad k = 1, \dots, K$$

which in particular confirms that $x_K = 1$. In addition, relation (7) and the periodicity condition (6) easily imply

$$t_f(R^k x) = \tau_k, \quad k = 1, \dots, K-1 \quad (8)$$

To proceed, we use the assumption $t_f(x) \leq x_1$ to rewrite $t_f(x) = x_1 + \frac{\epsilon}{N} \sum_{\ell=2}^K n_\ell(x_\ell - x_1) - \eta$ as follows

$$t_f(x) = 1 - \sum_{\ell=1}^{K-1} \tau_\ell - \Delta_0 \quad \text{where} \quad \Delta_k = \eta - \frac{\epsilon}{N} \sum_{\ell=2}^K n_{\ell+k}((R^k x)_\ell - (R^k x)_1), \quad k = 0, \dots, K-1.$$

Accordingly, the definition of the return map implies $(Rx)_k = x_{k+1} - t_f(x) = \sum_{\ell=1}^k \tau_\ell + \Delta_0$ for $k = 1, \dots, K-1$ and then $t_f(Rx) = (Rx)_1 + \frac{\epsilon}{N} \sum_{\ell=2}^K n_{\ell+1}((Rx)_\ell - (Rx)_1) - \eta = \tau_1 + \Delta_0 - \Delta_1$ since we are assuming $t_f(Rx) \leq (Rx)_1$. Repeating this argument inductively, we obtain

$$(R^\ell x)_k = \sum_{j=\ell}^{k+\ell-1} \tau_j + \Delta_{\ell-1}, \quad k = 1, \dots, K-\ell \quad \text{and} \quad t_f(R^\ell x) = \tau_\ell + \Delta_{\ell-1} - \Delta_\ell, \quad \ell = 1, \dots, K-1 \quad (9)$$

Form equation (8), it results that $\Delta_{\ell-1} = \Delta_\ell$ for $\ell = 1, \dots, K-1$ which is equivalent to

$$\sum_{j=2}^K n_{j+\ell-1}((R^{\ell-1}x)_j - (R^{\ell-1}x)_1) = \sum_{j=2}^K n_{j+\ell}((R^\ell x)_j - (R^\ell x)_1)$$

. Using again the return map definition we have

$$(R^\ell x)_k = \begin{cases} (R^{\ell-1}x)_{k+1} - t_f(R^{\ell-1}x) & \text{if } k = 1, \dots, K-1 \\ 1 & \text{if } k = K \end{cases}$$

and, together with the relation $\sum_{j=1}^K n_{j+\ell-1} = N$, the previous relation thus simplifies to

$$N((R^\ell x)_2 - (R^\ell x)_1) = n_{\ell+1}(1 - (R^\ell x)_1 + t_f(R^\ell x)), \quad \ell = 0, \dots, K-2$$

For $\ell = 1, \dots, K-2$, we can use relation (9) to get $(R^\ell x)_2 - (R^\ell x)_1 = \tau_{\ell+1}$ and $(R^\ell x)_1 = \tau_\ell + \Delta_{\ell-1}$. Accordingly, the previous relation results in

$$\tau_\ell = \frac{n_\ell}{N}(1 - \Delta_\ell), \quad \ell = 2, \dots, K-1.$$

For $\ell = 0$, using the expressions of x_1 and $t_f(x)$ the previous equality becomes

$$\tau_1 = \frac{n_1}{N}(1 - \Delta_0)$$

Since all the $\Delta_\ell = \Delta$ are equal, we finally get the condensed expression $\tau_\ell = \frac{n_\ell}{N}(1 - \Delta)$ for $\ell = 1, \dots, K-1$.

In order to compute Δ we introduce the latter into the definition of Δ_0 via the coordinates x_k . This gives a first order equation for Δ whose solution is

$$\Delta = \frac{\eta - \epsilon \Sigma_K}{1 - \epsilon \Sigma_K},$$

where $\Sigma_K = \frac{1}{N^2} \sum_{k=2}^K n_k \sum_{\ell=1}^{k-1} n_\ell$. Direct combinatorics implies

$$N^2 = \sum_{k=1}^K n_k \sum_{\ell=1}^K n_\ell = 2N^2 \Sigma_K + \sum_{k=1}^K n_k^2$$

showing that $\Sigma_K = \frac{N^2 - \sum_k n_k^2}{2N^2}$. Notice that Δ is well-defined when $\epsilon < 1$ since $\Sigma_K < 1$. Moreover, we have $\Delta < 1$ when $\eta < 1$. From the expression of Δ , we immediately get $\tau_k = \frac{n_k(1-\eta)}{N(1-\epsilon\Sigma_K)}$.

To conclude the analysis in the present case, it remains to check the conditions on parameters for which we have

$$t_f(x) \leq x_1 \quad \text{and} \quad R^\ell x \in \mathcal{T}_{\{n_{k+\ell}\}}, \quad \ell = 0, \dots, K-1.$$

Using (9), the first inequality amounts to $\Delta > 0$, viz. $\epsilon_\eta \leq \frac{1}{\Sigma_K}$. As for the second conditions, the only non trivial restriction is $(R^\ell x)_1 > 0$ for $\ell = 0, \dots, K-1$, since the other ones are automatically satisfied from the definition of R and the non-clustering assumption. Again, (9) shows that $(R^\ell x)_1 = \tau_\ell + \Delta > 0$ for $\ell = 1, \dots, K-1$. For $\ell = 0$, we have $\sum_{k=1}^{K-1} \tau_k = (1 - \frac{n_K}{N})(1 - \Delta) < 1$, i.e. $x_1 > 0$. Summarizing, the periodic orbit passing $\mathcal{T}_{\{n_k\}}$ exists with all coordinate firing before they reach 0 iff

$$\epsilon_\eta \leq \frac{1}{\Sigma_K} = \frac{2N^2}{N^2 - \sum_k n_k^2}$$

Analysis when all coordinates reach 0 before firing. This case can only occur when $\epsilon_\eta > \frac{1}{\Sigma_K}$. We claim that the solution writes

$$x_k = \frac{1}{N} \left(\sum_{\ell=0}^{k-1} n_\ell - \left(1 - \frac{\eta_\epsilon}{\Sigma_K}\right) \sum_{\ell=k+1}^K n_\ell \right), \quad k = 1, \dots, K-1 \quad (10)$$

and obviously $x_K = 1$. To check this assertion, according to (7), it suffices to verify that

$$t_f(R^\ell x) = \frac{1}{N} \left(n_\ell + \left(1 - \frac{\eta_\epsilon}{\Sigma_K}\right) n_{\ell+1} \right), \quad \ell = 1, \dots, K-1.$$

We shall indeed show by induction that this relation holds for $k = 0, \dots, K-1$. Since we now assume that $t_f(x) > x_1$ we have $t_f(x) = \frac{1}{N-n_1} \left(\sum_{k=2}^K n_k x_k - N\eta_\epsilon \right)$. Using (10) and the definition of Σ_K , we successively obtain

$$\begin{aligned} N \left(\sum_{k=2}^K n_k x_k - N\eta_\epsilon \right) &= \sum_{k=2}^K n_k \sum_{\ell=0}^{k-1} n_\ell - \sum_{k=2}^K n_k \sum_{\ell=k+1}^K n_\ell + \left(\frac{\sum_{k=2}^K n_k \sum_{\ell=k+1}^K n_\ell}{\Sigma_K} - N^2 \right) \eta_\epsilon \\ &= \sum_{k=2}^K n_k \sum_{\ell=0}^{k-1} n_\ell - \sum_{k=3}^K n_k \sum_{\ell=2}^{k-1} n_\ell + \left(\frac{\sum_{k=3}^K n_k \sum_{\ell=2}^{k-1} n_\ell - \sum_{k=2}^K n_k \sum_{\ell=1}^{k-1} n_\ell}{\Sigma_K} \right) \eta_\epsilon \\ &= (N - n_1)(n_0 + n_1 - \frac{n_1}{\Sigma_K} \eta_\epsilon) \end{aligned}$$

which gives the desired result for $k = 0$. The other cases proceed similarly by induction.

The existence conditions now become

$$x_1 < t_f(x), \quad t_f(R^\ell x) \leq (R^\ell x)_2 \quad \text{and} \quad R^\ell x \in \mathcal{T}_{\{n_{k+\ell}\}}, \quad \ell = 0, \dots, K-1.$$

The inequalities $x_k < x_{k+1}$ for $k = 1, \dots, K-1$ are equivalent to the following ones

$$\eta_\epsilon < \left(1 + \frac{n_k}{n_{k+1}}\right) \Sigma_K, \quad k = 1, \dots, K-1$$

which certainly hold when $\epsilon_\eta > \frac{1}{\Sigma_K}$. Moreover, $x_1 > 0$ is equivalent to $\eta_\epsilon > (1 - \frac{n_K}{N-n_1}) \Sigma_K$ and naturally, we obtain $x_1 < t_f(x)$ iff $\eta_\epsilon < \Sigma_K$.

For $\ell > 0$, the only non trivial constraint in $R^\ell x \in \mathcal{T}_{\{n_{k+\ell}\}}$ is $(R^\ell x)_1 > 0$, i.e. $(R^{\ell-1}x)_2 > t_f(R^{\ell-1}x)$, since all other constraints follow from the definition of the return map and the non-clustering assumption. Therefore, all what remains to be checked is $t_f(R^\ell x) \leq (R^\ell x)_2$ for $\ell = 0, \dots, K-1$.

By induction we easily get $(R^\ell x)_2 - t_f(R^\ell x) = x_{\ell+2} - \sum_{j=0}^{\ell} t_f(R^j x)$. Using the explicit expression above, it follows that

$$(R^\ell x)_2 - t_f(R^\ell x) = -(N - n_{\ell+2} - n_{\ell+1}) + \frac{\eta_\epsilon}{\Sigma_K}(N - n_{\ell+2}), \quad \ell = 0, \dots, K-1.$$

Altogether, we conclude that the existence condition in the present case reduces to

$$\frac{1}{\Sigma_K} < \epsilon_\eta < \min_{k=1, \dots, K} \frac{1}{\Sigma_K} \frac{N - n_k}{N - n_k - n_{k+1}} = \frac{2N^2}{N^2 - \sum_k n_k^2} \frac{1}{1 - \min_k \frac{n_k}{N - n_{k+1}}}$$

IV. MAXIMISING CONFIGURATIONS

We first formally state the statement to prove.

Lemma 4 *Given $K \geq 3$ and $N \geq K$ (and $N \neq 6$ if $K = 3$), the K -cluster configuration that maximizes the critical value $\zeta(\{n_k\})$ is the one defined by*

$$n_k = \begin{cases} 1 & \text{if } k = 1, \dots, K-1 \\ N - K + 1 & \text{if } k = K \end{cases} \quad (11)$$

This result is not as obvious as it may first appear. Indeed, the action of collapsing extensive clusters together and of splitting off unitary clusters in a way to keep the total number K constant, increases the left term in the expression of $\zeta(\{n_k\})$ but simultaneously decreases the right term; so the overall shift of the critical value needs to be carefully evaluated. In addition, Lemma 4 does not hold in the case $K = 3$ and $N = 6$ since one can check that $\zeta(\{1, 1, 4\}) < \zeta(\{2, 2, 2\})$.

Proof. To show that the configuration (11) minimizes the denominator in $\zeta(\{n_k\})$, we can assume without loss of generality that $\{n_k\}$ is a permutation of the configuration $\{q_k\}_{k=1}^K$ where $1 \leq q_k \leq q_{k+1}$ and $\sum_{k=1}^K q_k = N$. Let $\ell \leq K-1$ be the largest index for which $q_k = 1$. We separate the cases $\ell \geq \lfloor \frac{K}{2} \rfloor + 1$ and $\ell \leq \lfloor \frac{K}{2} \rfloor$.

If $\ell \geq \lfloor \frac{K}{2} \rfloor + 1$, then we have $\ell > K - \ell$, i.e. the configuration $\{q_k\}$ has more clusters with a single unit than it has clusters with more than 1 unit. Thus every permutation $\{n_k\}$ must have two consecutive clusters with a single unit. In this case, the quantity

$$S = \min_{k=1, \dots, K} \frac{n_k}{N - n_{k+1}} = \frac{1}{N - 1}$$

reaches its global maximum. Moreover, adding units to the largest cluster q_K by taking off units from smaller clusters q_k has the effect to increase the quantity $\sum_k q_k^2$. Thus the configuration (11) minimizes the denominator in $\zeta(\{n_k\})$ over all permutations of increasing configurations $\{q_k\}$ with $\ell \geq \lfloor \frac{K}{2} \rfloor + 1$. The corresponding minimum is

$$Q = (K-1)(2N-K) \frac{N-2}{N-1}$$

To deal with the case $\ell \leq \lfloor \frac{K}{2} \rfloor$, we begin to show that for every K -cluster configuration, we have $1 - S \geq \frac{K-2}{K-1}$. Consider the following alternative. Either all $n_k \leq \lceil \frac{N}{K} \rceil$ or there is a pair (n_k, n_{k+1}) for which $\max\{n_k, n_{k+1}\} > \lceil \frac{N}{K} \rceil$. In the second case, by contradiction there must be another pair $(n_{k'}, n_{k'+1})$ where $\min\{n_{k'}, n_{k'+1}\} < \lceil \frac{N}{K} \rceil$ (otherwise we would have $\sum_k n_k > N$ which is impossible) implying that

$$S \leq \frac{\lceil \frac{N}{K} \rceil - 1}{N - \lceil \frac{N}{K} \rceil} \leq \frac{1}{K-1}$$

In the first case, if $\lceil \frac{N}{K} \rceil = \frac{N}{K}$, then we have

$$S \leq \frac{\frac{N}{K}}{N - \frac{N}{K}} = \frac{1}{K-1}.$$

Otherwise there must be k such that $n_k \leq \lceil \frac{N}{K} \rceil - 1$ (otherwise we would again have $\sum_k n_k > N$) and then again

$$S \leq \frac{\lceil \frac{N}{K} \rceil - 1}{N - \lceil \frac{N}{K} \rceil} \leq \frac{1}{K-1}$$

Thus in all cases, we have $S \leq \frac{1}{K-1}$ which implies the desired inequality.

Still for $\ell \leq \lfloor \frac{K}{2} \rfloor$, the configuration that maximizes the sum $\sum_k q_k^2$ is

$$q_k = \begin{cases} 1 & \text{if } k = 1, \dots, \ell \\ 2 & \text{if } k = \ell + 1, \dots, K-1 \\ N - 2(K-1) + \ell & \text{if } k = K \end{cases}$$

(Notice that the assumption that $\{q_k\}_{k=1}^K$ has exactly ℓ sites for which $q_k = 1$ implies that $N - 2(K-1) + \ell \geq 2$.) Altogether we conclude that when $\ell \leq \lfloor \frac{K}{2} \rfloor$, the denominator of $\zeta(\{n_k\})$ is certainly not smaller than

$$Q_\ell = [(2(K-1) - \ell)(2N - 2(K-1) + \ell) - 4(K-1) + 3\ell] \frac{K-2}{K-1}, \quad \ell = 0, \dots, \lfloor \frac{K}{2} \rfloor.$$

Now, the quantity $Q_\ell - (K-1)(2N - K)$ increases with N provided that $(2(K-1) - \ell) \frac{K-2}{K-1} \geq K-1$. This inequality holds for every $\ell \leq \lfloor \frac{K}{2} \rfloor$ when $K \geq 5$. Moreover, the quantity $(K-1) \frac{2N-K}{N-1}$ also increases with N for $K \geq 2$. Thus the quantity $Q_\ell - Q$ increases with N and to ascertain that Q is a global minimum, it suffices to check that each $Q_\ell - Q$ is non-negative for $N = 2K - \ell$. This amounts to verify that the following inequalities hold

$$2K(K-1)(2(2K-1) - 3 \frac{(K-1)^2}{K-2}) \geq \ell(c(K) + b(K)\ell + \ell^2), \quad \ell = 0, \dots, \lfloor \frac{K}{2} \rfloor$$

where

$$c(K) = 12K^2 - 14K + 3 - \frac{(K-1)^2}{K-2}(7K-4) \quad \text{and} \quad b(K) = 2(\frac{(K-1)^2}{K-2} - 3K + 2);$$

The RHS in the inequality above is a third order polynomial in ℓ that is decreasing between 0 and $\lfloor \frac{K}{2} \rfloor$ when $K \geq 5$. Moreover, it is easy to check that

$$2(2K-1) - 3 \frac{(K-1)^2}{K-2} \geq 0$$

for every $K \geq 4$, i.e. we indeed have $Q_\ell \geq Q$ for every $\ell \leq \lfloor \frac{K}{2} \rfloor$ when $K \geq 5$.

For the cases $K = 4$ and $K = 3$, the proof needs to be improved because the quantity $Q_{\lfloor \frac{K}{2} \rfloor} - Q$ actually decreases with N when this integer is large. We begin with assuming $K = 4$ and check separately each case $j = 0, 1$ and 2.

For $K = 4$ and $j = 0$, the inequality $2(K-2) \geq K-1$ shows that $Q_0 - Q$ increases with N . Moreover, we have just checked in the general case that $Q_0 \geq Q$ for all $N \geq 2K$ when $K = 4$; thus Q is also a global minimum in this case.

For $K = 4$ and $j = 1$, since $(2(K-1) - 1) \frac{K-2}{K-1} \geq K-1$, we still have $Q_1 - Q$ increases with N . By numerically computing the values Q_1 and Q for $N = 7 = 2K - 1$, we conclude that Q remains a global minimum in this case.

Case $K = 4$ and $j = 2$. We claim that given an increasing configuration $(1, 1, q, N - q - 2)$ with $2 \leq q \leq \lfloor \frac{N}{2} \rfloor - 1$, the minimum S is maximal for the permutation $(1, N - q - 2, 1, q)$. Indeed, up to a cyclic permutation, there are 3 distinct permutations and $(1, N - q - 2, 1, q)$ is the only one that has non consecutive '1'. For $(1, N - q - 2, 1, q)$, we have $S = \frac{1}{N-q}$ thanks to the assumptions on q and the corresponding denominator of $\zeta(\{n_k\})$ writes

$$2(N(q+2) - q^2 - 2q - 3) \frac{N - q - 1}{N - q}$$

This quantity is convex in the domain q between 2 and $\lfloor \frac{N}{2} \rfloor - 1$ (as a product of two positive functions, one being increasing with decreasing derivative and the other one being decreasing with decreasing derivative). Thus we only have to check that the values for $q = 2$ and $q = \lfloor \frac{N}{2} \rfloor - 1$ are not smaller than the value for $q = 1$. Direct calculations reveal that the former quantity eventually growth with N faster than the latter one when N is large enough. A numerical check shows that these values for $q = 2$ and $q = \lfloor \frac{N}{2} \rfloor - 1$ are not smaller than the value for $q = 1$ provided that $N \geq 6$ (which is the minimal N for $j = 2$) and the proof is complete for $K = 4$.

For $K = 3$, there are two types of configurations to consider, namely the ordered ones (q_1, q_2, q_3) and those of the form (q_1, q_3, q_2) . For (q_1, q_2, q_3) , thanks to the assumption $q_i \leq q_{i+1}$, the minimum S is given by $S = \frac{q_1}{N-q_2}$. For (q_1, q_3, q_2) , depending on the sign of $q_2^2 - q_1 q_3$, the minimum S is either $\frac{q_2}{N-q_1}$ or $\frac{q_1}{N-q_3}$. Since both these quantities are never smaller than $\frac{q_1}{N-q_2}$, the non-ordered configuration always minimizes the denominator of $\zeta(\{n_k\})$.

Using that $S \leq \frac{q+p}{N-q}$ for the configuration $(q, N-2q-p, q+p)$ (where $0 \leq p \leq \lfloor \frac{N-3q}{2} \rfloor$ and $1 \leq q \leq \lfloor \frac{N}{3} \rfloor$), we get that the denominator of the critical value is at least

$$(2N(2q+p) - (2q+p)^2 - (q+p)^2 - q^2) \frac{N-2q-p}{N-q} \quad (12)$$

Using similar arguments as above, one concludes that this quantity is convex for p between 0 and $\lfloor \frac{N-3q}{2} \rfloor$. Therefore, it reaches its minimum at the boundaries of this interval.

For $p = 0$, the quantity (12) becomes

$$2q(2N-3q) \frac{N-2q}{N-q}$$

which is again convex with q between 1 and $\lfloor \frac{N}{3} \rfloor$. Moreover, the value for $q = \lfloor \frac{N}{3} \rfloor$ grows faster with N than the value for $q = 1$ does. A numerical investigation reveals that the former is not smaller than the latter provided that $N \geq 7$, i.e. $\zeta(1, N-2, 1) \leq \zeta(q, N-2q, q)$ for all $q \leq \lfloor \frac{N}{3} \rfloor$ when $N \geq 7$.

For $p = \lfloor \frac{N-3q}{2} \rfloor$, (12) becomes

$$\left(2N \lfloor \frac{N+q}{2} \rfloor - \lfloor \frac{N+q}{2} \rfloor^2 - \lfloor \frac{N-q}{2} \rfloor^2 - q^2 \right) \frac{\lfloor \frac{N-q}{2} \rfloor}{N-q}$$

Using once again a convexity argument, we get that this quantity reaches its minimum for either $q = 1$ or $q = \lfloor \frac{N}{3} \rfloor$. In the first case we want to check the inequality

$$\left(2N \lfloor \frac{N+1}{2} \rfloor - \lfloor \frac{N+1}{2} \rfloor^2 - \lfloor \frac{N-1}{2} \rfloor^2 - 1 \right) \frac{\lfloor \frac{N-1}{2} \rfloor}{N-1} \geq 2(2N-3) \frac{N-2}{N-1}$$

Again, as N increases, the LHS grows faster than the RHS and numerics reveal that the inequality holds provided that $N \geq 10$. For $q = \lfloor \frac{N}{3} \rfloor$, one can prove that the corresponding inequality holds for $N \geq 7$. Therefore, we have shown that $(1, 1, N-2)$ maximizes $\zeta(n_1, n_2, N-n_1-n_2)$ provided that $N \geq 10$. For N between 4 and 9, we have listed all 3-cluster configurations and checked that the property remains valid, except for $N = 6$ as announced above.

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