
Supplemental material

Here we provide the derivation of the results in Section 3.

In Kasza and Forbes¹³, it is shown that if the block exchangeable model is fit to data generated according to the discrete time decay model (with an equal number of participants m in each of K clusters over T periods), then the

following relationships will hold:

$$\begin{aligned} E[\hat{\sigma}_{2\epsilon}^2] &= \sigma_{3\epsilon}^2 \\ E[\hat{\sigma}_\gamma^2] &= \sigma_{3\alpha}^2 \left(\frac{T}{T-1} - \frac{1}{T(T-1)} \sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|} \right) \\ E[\hat{\sigma}_{2\alpha}^2] &= \sigma_{3\alpha}^2 \left(\frac{1}{T(T-1)} \sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|} - \frac{1}{T-1} \right). \end{aligned}$$

Hence, by replacing estimators of variance components with their expected values, the within-period intracluster correlation estimated under the block exchangeable model can be written as:

$$\hat{\rho}_b = \frac{E[\hat{\sigma}_\gamma^2] + E[\hat{\sigma}_{2\alpha}^2]}{E[\hat{\sigma}_\gamma^2] + E[\hat{\sigma}_{2\alpha}^2] + E[\hat{\sigma}_{2\epsilon}^2]} = \frac{\sigma_{3\alpha}^2}{\sigma_{3\alpha}^2 + \sigma_{3\epsilon}^2} = \rho_d.$$

Similarly, the cluster autocorrelation estimated under the block exchangeable model can be written as:

$$\hat{r}_b = \frac{E[\hat{\sigma}_{2\alpha}^2]}{E[\hat{\sigma}_\gamma^2] + E[\hat{\sigma}_{2\alpha}^2]} = \frac{\sigma_{3\alpha}^2 \left(\frac{1}{T(T-1)} \sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|} - \frac{1}{T-1} \right)}{\sigma_{3\alpha}^2} = \frac{1}{T(T-1)} \sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|} - \frac{1}{T-1}.$$

Therefore an estimate of the block-exchangeable r_b can be obtained from the discrete time decay model by the simple arithmetic average of all the off-diagonal elements of the matrix Σ from Equation (3).

To find a value of r_d that is aligned with the estimated value from the block exchangeable model, \hat{r}_b , we thus propose solving the following equation:

$$\sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|} - T(T-1)\hat{r}_b - T = 0$$

The double sum $\sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|}$ is the sum over all elements of the correlation matrix Σ from Equation (3), hence the equation is given by:

$$T + 2(T-1)r_d + 2(T-2)r_d^2 + \dots + 2(T-(T-2))r_d^{T-2} + 2(T-(T-1))r_d^{T-1} - T(T-1)\hat{r}_b - T = 0$$

which, with some minor rearranging, gives the following polynomial in r_d to be solved, yielding Equation (6) in the main text:

$$(T-1)r_d + (T-2)r_d^2 + \dots + 2r_d^{T-2} + r_d^{T-1} - \frac{T(T-1)}{2}\hat{r}_b = 0.$$

In Kasza and Forbes¹³ it is also shown that if the exchangeable model is fit to data generated according to the discrete time decay model (with an equal number of participants m in each of K clusters over T periods), then the following relationships will hold:

$$E[\hat{\sigma}_{1\epsilon}^2] = \sigma_{3\epsilon}^2 + \sigma_{3\alpha}^2 \left(\frac{(K-1)Tm}{KTm - K - T + 1} - \frac{m(K-1)}{T(KTm - K - T + 1)} \sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|} \right)$$

$$E[\hat{\sigma}_{1\alpha}^2] = \sigma_{3\alpha}^2 \left(\frac{Km-1}{T(KTm - K - T + 1)} \sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|} - \frac{K-1}{KTm - K - T + 1} \right).$$

Hence, by replacing estimators of variance components with their expected values, the intracluster correlation estimated under the exchangeable model can be written as:

$$\hat{\rho}_e = \frac{E[\hat{\sigma}_{1\alpha}^2]}{E[\hat{\sigma}_{1\alpha}^2] + E[\hat{\sigma}_{1\epsilon}^2]} = \frac{\sigma_{3\alpha}^2 \left(\frac{Km-1}{T(KTm - K - T + 1)} \sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|} - \frac{K-1}{KTm - K - T + 1} \right)}{\sigma_{3\epsilon}^2 + \sigma_{3\alpha}^2 \left(\frac{(K-1)(Tm-1)}{KTm - K - T + 1} + \frac{m-1}{T(KTm - K - T + 1)} \sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|} \right)}.$$

We will assume that $\sigma_{3\epsilon}^2 + \sigma_{3\alpha}^2 = 1$, so that $\sigma_{3\epsilon}^2 = 1 - \sigma_{3\alpha}^2$, and $\rho_d = \sigma_{3\alpha}^2$. Substituting this into the equation above gives:

$$\hat{\rho}_e = \frac{\rho_d \left(\frac{Km-1}{T(KTm - K - T + 1)} \sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|} - \frac{K-1}{KTm - K - T + 1} \right)}{1 + \rho_d \left(\frac{K+T-Tm}{KTm - K - T + 1} + \frac{m-1}{T(KTm - K - T + 1)} \sum_{t=1}^T \sum_{s=1}^T r_d^{|t-s|} \right)}.$$

Rearranging this equation gives the following polynomial in r_d , which we propose solving to find values of r_d and ρ_d that are aligned with the estimate of the aggregate intracluster correlation $\hat{\rho}_e$, yielding Equation (7) in the main text:

$$(T-1)r_d + (T-2)r_d^2 + (T-3)r_d^3 + \dots + 2r_d^{T-2} + r_d^{T-1} + \frac{T}{2} \left(1 - \frac{\hat{\rho}_e}{\rho_d} \frac{KTm - K - T + 1}{Km - 1 - \hat{\rho}_e m + \hat{\rho}_e} - \frac{(K-1 + \hat{\rho}_e K + \hat{\rho}_e T - \hat{\rho}_e Tm)}{Km - 1 - \hat{\rho}_e m + \hat{\rho}_e} \right) = 0.$$

For this equation to be equivalent to the approximation in Equation (8), we need

$$\frac{KTm - K - T + 1}{Km - 1 - \hat{\rho}_e m + \hat{\rho}_e} - \frac{\rho_d}{\hat{\rho}_e} \frac{(K-1 + \hat{\rho}_e K + \hat{\rho}_e T - \hat{\rho}_e Tm)}{Km - 1 - \hat{\rho}_e m + \hat{\rho}_e}$$

to be approximately equal to T . Rearranging this gives

$$T \frac{Km - 1 - \rho_d + \rho_d m}{Km - 1 - \hat{\rho}_e m + \hat{\rho}_e} + \frac{(1-K)(\hat{\rho}_e + \rho_d) - \rho_d \hat{\rho}_e K}{\hat{\rho}_e (Km - 1 - \hat{\rho}_e m + \hat{\rho}_e)},$$

which will be close to T when Km is large relative to $\rho_d m$, $\hat{\rho}_e m$ and K .

Finally, Kasza and Forbes¹³ shows that if the exchangeable model is fit to data generated according to the block exchangeable model (with an equal number of participants m in each of K clusters over T periods), then the following relationships will hold:

$$E[\hat{\sigma}_{1\epsilon}^2] = \sigma_{2\epsilon}^2 + \sigma_\gamma^2 \frac{(KT - K - T + 1)m}{KTm - K - T + 1}$$

$$E[\hat{\sigma}_{1\alpha}^2] = \sigma_{2\alpha}^2 + \sigma_\gamma^2 \frac{K(m-1)}{KTm - K - T + 1}.$$

Hence, by replacing estimators of variance components with their expected values, the intracluster correlation estimated under the exchangeable model can be written as:

$$\hat{\rho}_e = \frac{E[\hat{\sigma}_{1\alpha}^2]}{E[\hat{\sigma}_{1\alpha}^2] + E[\hat{\sigma}_{1\epsilon}^2]} = \frac{\sigma_{2\alpha}^2(KTm - K - T + 1) + \sigma_\gamma^2 K(m-1)}{KTm - K - T + 1 + \sigma_\gamma^2(m-1)(1-T)}.$$

We will assume that $\sigma_{2\epsilon}^2 + \sigma_{2\alpha}^2 + \sigma_\gamma^2 = 1$, so that $\sigma_{2\alpha}^2 = r_b \rho_b$, and $\sigma_\gamma^2 = \rho_b(1 - r_b)$. Substituting this into the equation above gives Equation 9 in the main text.

References

1. Hemming K, Kasza J, Hooper R, Forbes A, and Taljaard M. A tutorial on sample size calculation for multiple-period cluster randomized parallel, cross-over and stepped-wedge trials using the shiny crt calculator. *International Journal of Epidemiology* 2020; **49**:979–995.
2. Hussey MA and Hughes JP. Design and analysis of stepped wedge cluster randomized trials. *Contemporary Clinical Trials* 2007; **28**:182–191.
3. Girling AJ and Hemming K. Statistical efficiency and optimal design for stepped cluster studies under linear mixed effects models. *Statistics in Medicine* 2016; **35**: 2149–2166.
4. Hooper R, Teerenstra S, de Hoop E and Eldridge S. Sample size calculation for stepped wedge and other longitudinal cluster randomised trials. *Statistics in Medicine* 2016; **35**: 4718–4728.
5. Kasza J, Hemming K, Hooper R, Matthews JNS, and Forbes AB. Impact of non-uniform correlation structure on sample size and power in multiple-period cluster randomised trials. *Statistical Methods in Medical Research* 2019; **28**:703–716.
6. Ouyang Y, Li F, Preisser JS, Taljaard M. Sample size calculators for planning stepped-wedge cluster randomized trials: a review and comparison, *International Journal of Epidemiology* 2022; dyac123, <https://doi.org/10.1093/ije/dyac123>.
7. Korevaar E, Kasza J, Taljaard M, Hemming K, Haines T, Turner EL, Thompson JA, Hughes JP, and Forbes AB Intra-cluster correlations from the CLustered OUtcome Dataset bank to inform the design of longitudinal cluster