In education, sample characteristics can be complex due to the nested structure of students, teachers, classrooms, schools, and districts. More recently, in the past two decades, education scholars have developed tools to conduct statistical power analysis in multilevel randomized experiments (RE) and regression discontinuity (RD) studies. The purpose of this study is threefold: (i) to derive formulas for various three-level RD studies where discontinuity resides at level 1 and to validate formulas using Monte Carlo (MC) simulations, (ii) to explore consequences of ignoring an intermediate- or top-level when designing such studies, and (iii) to provide a general framework for constrained optimal sample allocation when there are budget and sample size constraints and when treatment and control units are associated with certain costs (equal or unequal). Derived formulas are consistent with the current literature and uses parameters commonly reported in the education studies. MC simulation results confirm validity of the formulas. On the one hand, ignoring an intermediate-level result in underpowered studies, on the other, ignoring a top-level result in inflated power values and Type I error rates. Finally, the general framework for constrained optimal sample allocation allows calculation of sample sizes under budget and sample size constraints for both multilevel RE and RD studies when treatment and control units are associated with certain costs (equal or unequal).