

S1. Calculation

In the null model we consider a random dataset with the same distribution of traits: 4 of 36 species have extreme reduction in chondrocranium, and seven of 36 species have extreme reductions in their limbs. However, the null model assumes that the traits are non-correlated. Therefore, there are five possible co-distributions of traits, see **Error! Reference source not found.S1**.

To compute the probability of each outcome, we considered 36 species, seven of which have extreme reduction in limbs and 29 do not have it. Next, we randomly distributed four extreme reductions in chondrocranium across the tree (Fig. 9). The probability that all four of them will be assigned among seven species with another extreme reduction (as we observed in the empirical dataset, Fig. 9) is

$$p_A = \frac{7}{36} \frac{6}{35} \frac{5}{34} \frac{4}{33} = \frac{1}{1683} \approx 0.00059$$

In general case, in the control model with random uncorrelated distribution of extreme reductions, the probability to have x species with both extreme reductions is

$$p(x) = \binom{7}{x} \binom{29}{4-x} / \binom{36}{4},$$

where

$$\binom{N}{k}$$

is the binomial coefficient – the number of ways to choose an (unordered) subset of k elements

from a fixed set of N elements. The formula itself states that the probability is equal to the ratio between two numbers:

- 1) The number of ways to distribute x reductions in chondrocranium among seven limbless species and $(4 - x)$ species among the remaining 29 limbed species.
- 2) The total number of ways to distribute all four reductions in chondrocranium among the whole set of 36 species.

Therefore, the probabilities to observe other species co-distributions are:

$$p_B = \binom{7}{3} \binom{29}{1} / \binom{36}{4} \approx 0.017, \quad p_C = \binom{7}{2} \binom{29}{2} / \binom{36}{4} \approx 0.15, \quad p_D = \binom{7}{1} \binom{29}{3} / \binom{36}{4} \approx 0.43, \quad \text{and} \quad p_E = \binom{7}{0} \binom{29}{4} / \binom{36}{4} \approx 0.40$$

Table S1. Five possible co-distribution of traits in the null model. In each co-distribution

Co-distribution A	Extreme reduction in the chondrocranium	No extreme reduction in the chondrocranium
Extreme reduction in the limbs	4	3
No extreme reduction in the limbs	0	29

Co-distribution B	Extreme reduction in the chondrocranium	No extreme reduction in the chondrocranium
Extreme reduction in the limbs	3	4
No extreme reduction in the limbs	1	28

Co-distribution C	Extreme reduction in the chondrocranium	No extreme reduction in the chondrocranium
Extreme reduction in the limbs	2	5
No extreme reduction in the limbs	2	27

Co-distribution D	Extreme reduction in the chondrocranium	No extreme reduction in the chondrocranium
Extreme reduction in the limbs	1	6
No extreme reduction in the limbs	3	26

Co-distribution E	Extreme reduction in the chondrocranium	No extreme reduction in the chondrocranium
Extreme reduction in the limbs	0	7
No extreme reduction in the limbs	4	25