| Assembly accession | bioproject | biosample   | taxid   | Organism name                              | Infraspecific name | isolate       |
|--------------------|------------|-------------|---------|--------------------------------------------|--------------------|---------------|
| GCA_000258425.1    | PRJNA91117 | SAMN02603095 | 1163730 | Fervidicoccus fontis Kam940                | strain=Kam940      |               |
| GCA_001871415.1    | PRJNA297582 | SAMN04328224 | 1805424 | Candidatus Woesearchaeota archaeon          | CG1_02_57_44       |               |
| GCA_002779065.1    | PRJNA362739 | SAMN06659264 | 1974404 | Candidatus Diapherotrites archaeon          | CG08_land_8_20_14_0_20_34_12 |               |
| GCA_000349645.1    | PRJNA168253 | SAMN02261087 | 1198116 | Thermoplasmatales archaeon SCGC AB-539-N05 | SCGC_AB-539-N05    |               |
| GCA_000015945.1    | PRJNA17449 | SAMN02598390 | 399550  | Staphylothermus marinus F1                 | strain=F1          |               |
| GCA_003144275.1    | PRJNA383916 | SAMN07236661 | 2012493 | Candidatus Heimdallarchaeota archaeon       | B3_Heim            |               |
| GCA_000145985.1    | PRJNA33361 | SAMN00016987 | 583356  | Ignisphaera aggregans DSM 17230            | strain=DSM 17230   |               |
| GCA_000011185.1    | PRJNA206   | SAMD00061089 | 273116  | Thermoplasma volcanium GSS1                | strain=GSS1        |               |
| GCA_000025685.1    | PRJNA12524 | SAMN02604027 | 309800  | Halofex volcanii DS2                      | strain=DS2         |               |
| GCA_000018305.1    | PRJNA17421 | SAMN00623034 | 397948  | Caldivirga maquilingensis IC-167           | strain=IC-167      |               |
| GCA_000009965.1    | PRJNA13213 | SAMD00061071 | 69014   | Thermococcus kodakarenis KOD1              | str=KOD1           |               |
| GCA_003345545.1    | PRJNA406094 | SAMN08287972 | 2053491 | Candidatus Thorarchaeota archaeon           | OWC2               |               |
| GCA_000200715.1    | PRJNA202   | SAMN02744041 | 414004  | Cenarchaeum symbiosum A                    |                   |               |
| GCA_000008645.1    | PRJNA289   | SAMN02603244 | 187420  | Methanothermobacter thermautotrophicus str. Delta H | strain=Delta H    |               |
| GCA_000007065.1    | PRJNA300   | SAMN02603290 | 192952  | Methanosarcina mazei Go1                  | str=Go1            |               |
| GCA_000008665.1    | PRJNA104   | SAMN02603985 | 224325  | Archaeoglobus fulgidus DSM 4304            | str=DSM 4304       |               |
| GCA_000007225.1    | PRJNA172   | SAMN02604075 | 178306  | Pyrobaculum aerophilum str. IM2            | str=IM2            |               |
| GCA_000019605.1    | PRJNA16525 | SAMN02598368 | 374847  | Candidatus Korarchaeum cryptofilum OPF8     |                   |               |
| Accession   | Project   | SampleID   | SequenceLength | Organism Description                                                                 | Strain          |
|------------|-----------|------------|----------------|-------------------------------------------------------------------------------------|-----------------|
| GCA_005223125.1 | PRJNA383916 | SAMN07236659 | 2012491       | Candidatus Lokiarchaeota archaeon                                                      | Loki_b32        |
| GCA_000015145.1 | PRJNA208 | SAMN02604082 | 415426        | Hyperthermus butylicus DSM 5456                                                      | strain=DSM 5456 |
| GCA_0000303155.1 | PRJNA60505 | SAMN02603264 | 1237085       | Candidatus Nitrosophaera gargensis                                                    | enrichment culture Ga9.2 |
| GCA_000017945.1 | PRJNA13914 | SAMN02598324 | 453591        | Ignicoccus hospitalis KIN4/I                                                         | strain=KIN4/I   |
| GCA_011364945.1 | PRJNA495098 | SAMN10218972 | 2026747       | Candidatus Heimdallarchaeota archaeon                                                  |                 |
| GCA_000007185.1 | PRJNA294 | SAMN02603235 | 190192        | Methanopyrus kandleri AV19                                                           | strain=AV19     |
| GCA_013343275.1 | PRJNA588232 | SAMN13231772 | 2594798       | Nanohaloarchaeae archaeon                                                             | strain=M3_22    |
| GCA_000011125.1 | PRJNA211 | SAMD00061092 | 272557        | Aeropyrum pernix K1                                                                  |                 |
| GCA_000025665.1 | PRJNA38403 | SAMN02598523 | 439481        | Aciduliprodufum boonei T469                                                          | strain=T469     |
| GCA_000011005.1 | PRJDA20361 | SAMD00060931 | 304371        | Methanocella paludicola SANAE                                                        | strain=SANAE    |
| GCA_000270325.1 | PRJDA49157 | SAMD00016619 | 311458        | Candidatus Caldiarchaeum subterraneum                                                 |                 |
| GCA_000018465.1 | PRJNA19265 | SAMN00000302 | 436308        | Nitrosopumilus maritimus SC1                                                         | strain=SC1      |
| GCA_013375405.1 | PRJNA599172 | SAMN14414634 | 2719382       | Candidatus Helarchaeota archaeon                                                      | CR_Bin_291     |
| GCA_000007305.1 | PRJNA287 | SAMN02604284 | 186497        | Pyrococcus furiosus DSM 3638                                                         | strain=DSM 3638 |
| GCA_009911715.1 | PRJNA258248 | SAMN02991093 | 1535962       | Methanomassiliicoccales archaeon                                                      | strain=DOK      |
| GCA_000015225.1 | PRJNA16331 | SAMN02598366 | 368408        | Thermofilum pendens Hrk 5                                                            | strain=Hrk 5    |
| GCA_008000775.1 | PRJNA557562 | SAMN12405820 | 2594042       | Candidatus Prometheoarchaeum syntrophicum                                            | strain=MK-D1    |
| GCA_000011085.1 | PRJNA105 | SAMN02603385 | 272569        | Haloarcula marismortui ATCC 43049                                                    | strain=ATCC 43049 |
| GCA_008080735.1 | PRJNA521734 | SAMN10909897 | 2053489       | Candidatus Lokiarchaeota archaeon                                                    | BC3             |
| GCA_000008085.1 | PRJNA9599 | SAMN02603208 | 228908        | Nanoarchaeum equitans Kin4-M                                                         |                 |
| GCA_000013445.1 | PRJNA13015 | SAMN02598287 | 323259        | Methanospirillum hungatei JF-1                                                       | strain=JF-1     |
| GCA_001940655.1 | PRJNA288027 | SAMN04958229 | 1849166       | Candidatus Lokiarchaeota archaeon                                                    | CR_4            |
| Accession     | Project ID | Sample ID | Length | Organism                          | Strain       |
|--------------|------------|-----------|--------|-----------------------------------|--------------|
| GCA_000091665.1 | PRJNA102   | SAMN02603984 | 243232 | Methanocaldococcus jannaschii DSM 2661 | strain=DSM 2661 |
| GCA_000349625.1 | PRJNA168252 | SAMN02261086 | 1198115 | Thaumarchaeota archaeon SCGC AB-539-E09 | SCGC AB-539-E09 |
Table S2
Network robustness estimates using distinct $I_{ES}$ thresholds, from coarse (0.3 edge weight threshold) to fine-grained (0.9 edge weight threshold), in increments of 0.05. Robustness of resulting networks are measured by calculating Variation of Information (VI) and Normalized Mutual Information (NMI) between clusters obtained using consecutive $I_{ES}$ threshold. Stable threshold values are expected to produce network clusters resistant to further increase in threshold stringency.

| $I_{ES}$ threshold | Compared $I_{ES}$ threshold | VI     | NMI    | cluster modularity | edge count |
|--------------------|-----------------------------|--------|--------|--------------------|------------|
| 0.3                | 0.35                        | 1.0134 | 0.622  | 0.1008             | 352603     |
| 0.35               | 0.4                         | 1.3584 | 0.4994 | 0.1293             | 231194     |
| 0.4                | 0.45                        | 1.7815 | 0.3842 | 0.1503             | 141248     |
| 0.45               | 0.5                         | 1.5218 | 0.566  | 0.1774             | 81638      |
| 0.5                | 0.55                        | 2.0925 | 0.5957 | 0.1961             | 45268      |
| 0.55               | 0.6                         | 1.916  | 0.7476 | 0.2221             | 23550      |
| 0.6                | 0.65                        | 1.4829 | 0.8493 | 0.252              | 11558      |
| 0.65               | 0.7                         | 0.9883 | 0.9141 | 0.2777             | 5300       |
| 0.7                | 0.75                        | 0.7833 | 0.9386 | 0.3453             | 2142       |
| 0.75               | 0.8                         | 0.4126 | 0.9699 | 0.4147             | 618        |
| 0.8                | 0.85                        | 0.1398 | 0.9901 | 0.5479             | 157        |
| 0.85               | 0.9                         | 0.0397 | 0.9972 | 0.6846             | 30         |
Fig. S1: Similarities between evolutionary histories of gene families as sampled taxa randomly decrease. wODR $R^2$ (orange) tends to increase as taxa representing deviations between evolutionary histories are randomly removed. Bray-Curtis (blue) and $I_{ES}$ (green) both show steady decreases as differential gene losses accumulate between gene families, with $I_{ES}$ initially at a slower pace than Bray-Curtis. Both gene families initially contain 50 taxa, and their phylogenies diverge from each other by 5 SPR transformations.
Fig S2: OLS regression of the number of phylogenetic perturbations and estimated dissimilarities between perfectly aligned simulated gene families. All scatterplots display the number of phylogenetic perturbations between two trees in the X-axis, while varying the method to quantify shared evolution displayed in the Y-axis. OLS regressions are fitted in each scatterplot, with fixed Y-axis intercepts through the origin. The OLS coefficient of determination ($R^2$) shows the association between number of perturbations and estimated difference between evolutionary histories. Low $R^2$ values represent a poor estimation of distance between evolutionary histories based on the number of perturbations, and $R^2 < 0$ occur as estimate distances fail to reflect the number of perturbations between trees. Each subfigure contains ten replicates from trees simulated using weak perturbations (a, random SPR moves within the 10% closest branches); medium (b, random SPR moves within the 50% closest branches); and strong (c, random SPR moves to any branch in the tree). $I_{ES}$ in blue, $D_{geo}$ in red, RF in green, $D_{ms}$ in pink, and $D_{qe}$ in brown.
Fig. S3b

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Fig S3: OLS regression of the number of phylogenetic perturbations and estimated dissimilarities between realigned simulated gene families reconstructed using JTT. All scatter plots display the number of phylogenetic perturbations between two trees in the X-axis, while varying the evolution similarity metric displayed in the Y-axis. OLS regressions are fitted between axes in each scatterplot, with fixed Y-axis intercepts: one for $I_{ES}$ and zero for tree-based methods. OLS coefficient of determination ($R^2$) is depicted the association between number of perturbations and estimated distance between evolutionary histories. Low $R^2$ represent a poor estimation of distance between evolutionary histories based on the number of perturbations, and $R^2 < 0$ occur as estimate distances fail to reflect the number of perturbations between trees. Each subfigure contains ten replicates from trees simulated using weak perturbations (a, random SPR moves within the 10% closest branches); medium (b, random SPR moves within the 50% closest branches); and strong (c, random SPR moves to any branch in the tree). $I_{ES}$ in blue, $D_{geo}$ in red, RF in green, $D_{ms}$ in pink, and $D_{qt}$ in brown.
Fig S4: Shared evolution estimates from realigned simulated gene families. Each set of grouped boxplots shows OLS $R^2$ values for simulated gene families using varying ranges of SPR moves (10%, 50%, and 100%). Each dataset was replicated ten times, and scatterplot and fitted OLS regressions are available in Supplementary Fig. S2. Negative $R^2$ occur as fitted linear regressions do not explain the association between variables, and in this scenario reflect strong saturation of evolutionary similarity measurements. Gene trees were reconstructed using the JTT substitution model.
Fig S5: Impact of alignment and evolutionary model errors to the accuracy of shared evolution estimates. Comparisons of OLS $R^2$ displayed in Fig. 2 and Supplementary Fig. S3, assessing the impact of multiple sequence alignment errors and suboptimal evolutionary model to estimates from each method; using distributions of OLS $R^2$ between shared evolution estimates against number of simulated phylogenetic perturbations as benchmark. Low OLS $R^2$ reflect weak predictive power of a methods estimate, likely caused by loss of resolution as numbers of perturbations increase. Differences between distributions of OLS $R^2$ values obtained using perfectly aligned and realigned gene families was evaluated using Wilcoxon non-parametric test ($p$) and Common Language Effect Size ($f$).
Fig S6a: Clustered heatmap of $I_{ES}$ values between pairs of archaeal gene families. Pairs of gene families with low $I_{ES}$ are colored in blue, while pairs of gene families with high $I_{ES}$ are colored red. Complete linkage clustering was performed using correlation distances.
Fig 6b: Clustered heatmap of $I_{ES}$ values between pairs of archaeal gene families. Pairs of gene families with low $I_{ES}$ are colored in blue, while pairs of gene families with high $I_{ES}$ are colored red. Complete linkage clustering was performed using euclidean distances between average genetic distances between gene families.
Fig S7: Decrease in the proportion of co-evolving over non-co-evolving gene pairs as genomic window size increases. The approximation of a log-log linear relationship suggests a power-law decrease in the predictive power of gene co-evolution from genomic linkage.
Fig S8: Representation of cluster robustness metrics. A) Closeness centrality distributions calculated from subgraphs comprised by nodes from each co-evolving cluster independently. B) Average weighted degree centrality, a.k.a. strength, calculated from cluster specific subgraphs. In order, boxplots represent values estimated from cluster#3, cluster#4, cluster#2, cluster#0, cluster#5, cluster#8, cluster#1, and cluster#15.
Fig. S9: Phylogenetic trees reconstructed from concatenations of genes from each co-evolving cluster. Genomes missing more than 25% of concatenated sites were removed before phylogenetic reconstruction. Leaf names are colored in the same structure as Fig. 7. Trees were reconstructed using LG+F+G+C60 evolutionary model. Trees from each co-evolving cluster were independently rooted using MAD [1].
Fig. S10: wODR between pairwise distances for concatenated sequences from CES cluster#4 and CES cluster#1. Datapoints corresponding to intra and inter-phylum distances were assigned weights ten and one, respectively. This weighting scheme was used to anchor the regression model using intra-phylum pairwise distances, which better reflect the estimated vertical signal, and evaluate how inter-phyla distances fit the expected linear association.
Fig. S11: Distribution of intra-phylum distances for cluster#4 and cluster#1. Pairwise distances were calculated using concatenated sequences from each CES cluster. Intra-phylum (blue) and inter-phyla (orange) distances show a greater difference in cluster#4 than in cluster#1. The smaller difference between intra and inter-phyla distances in cluster#1 is likely due horizontal exchange of its constituent genes between Euryarchaeota and Thaumarchaeota.
Fig. S12: wODR between pairwise distances calculated from concatenated sequences from CES cluster#4 and CES cluster#0. Datapoints corresponding to intra and inter-phylum distances were assigned weights ten and one, respectively. This weighting scheme was used to anchor the regression model using intra-phylum pairwise distances, which better reflect the estimated vertical signal, and evaluate how inter-phyla distances fit the expected linear association.
Fig. S13: Distribution of wODR residuals between cluster#4 and cluster#0 distance matrices. Residuals were estimated from wODR fitted using intra and inter-phylum distances weights of ten and one, respectively. Using Common Language effect size statistics, Crenarchaeota-Euryarchaeota displayed very similar residuals to intra-phylum residuals ($f = 0.62$), while Euryarchaeota-Thaumarchaeota and Crenarchaeota-Thaumarchaeota displayed much larger residuals ($f = 0.97$ and $f = 0.90$, respectively).
Fig. S14: wODR between pairwise distances calculated using concatenated sequences from CES cluster#8 and CES cluster#0. Datapoints corresponding to intra and inter-phylum distances were assigned weights ten and one, respectively. This weighting scheme was used to anchor the regression model using intra-phylum pairwise distances, which better reflect the estimated vertical signal, and evaluate how inter-phyla distances fit the expected linear association.
Fig. S15: wODR between pairwise distances calculated using concatenated sequences from CES cluster#8 and CES cluster#0. Datapoints corresponding to intra and inter-phylum distances were assigned weights ten and one, respectively. This weighting scheme was used to anchor the regression model using intra-phylum pairwise distances, which better reflect the estimated vertical signal, and evaluate how inter-phyla distances fit the expected linear association.
Fig. S16: Frequency with which the most frequent gene copy was selected as best representing the shared evolution between two gene families in the same CES cluster. Empirical values observed in 237 occasions in which a gene family occurred in multiples within a genome (blue). Expected null distribution assuming that each copy among the multiples within a genome had the same chance of been selected (orange).
References
1. Tria FDK, Landan G, Dagan T. Phylogenetic rooting using minimal ancestor deviation. Nat Ecol Evol. 2017;1: 0193. doi:10.1038/s41559-017-0193