From pairs of most similar sequences to phylogenetic best matches

Additional Figures

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Figure S1: Example gene tree (simID 4) with 44 surviving leaves in 20 different species (color-coded).
Statistical properties of the 2000 simulated scenarios

Figure S2: Distribution of the number of leaves in the set of 2000 simulated scenarios: (A) species trees (barplot), (B) (observable part of the) gene trees (histogram, 80 bins), (C) number of genes per species in the whole data set (barplot, log-scale), and (D) average number of genes per species per scenario (in descending order).

Figure S3: Distribution of the number of (A) leaves in the species tree and duplication events, and (B) leaves in the species tree and loss events as color-coded 2-dimensional histograms.
Figure S4: Distribution of the number of duplication and loss events as a color-coded 2-dimensional histogram.

Figure S5: Distribution of the edge lengths in the simulated gene trees (histogram, 200 equal-sized bins, log-scale).

Figure S6: Percentage of gene pairs for with outgroup genes could be found (based on the heuristic that uses outgroup species) among all $n(n-1)/2$ gene pairs per scenario, where $n$ is the number of non-loss leaves. These gene pairs with available outgroups were used to calculate recall and precision for the comparison of the best match inference methods.
Figure S7: Performance comparison of the best match inference from distance data for simulated data (2000 scenarios) and biased noise. Top panel: Median (solid) and 10th percentile (dashed) of recall and precision as a function of noise level $\alpha$, i.e., the contribution of an additive disturbance matrix $D'$ that was built from another tree. For each gene tree and noise level, the final distance matrix was computed as $(1-\alpha)D + \alpha D'$ (see Simulation of measurement noise section). Lower panel: Boxplots of F-measure for different levels of noise superimposed on the additive distance; $\alpha = 0$ refers to perfect data. Orange: $\epsilon$ method, turquoise: explicit construction of the unrooted tree $T$ and midpoint rooting, green: inference of quartets with outgroups chosen in another branch of the root.

Figure S8: Alternative construction of $\Gamma$. In order to further investigate the inaccuracies introduced by unresolved quartets, we considered alternative constructions of the auxiliary graph $\Gamma$. In addition to the default method, we omitted all edges defined for quartets classified as unresolved ($\times$), and we ignored the contribution of outgroups that lead to unresolved and used a majority vote only for the remaining choices of the outgroup. All non-trivial sinks in $\Gamma$ were then interpreted as best matches, i.e., isolated vertices in $\Gamma$ were ignored. Both variants perform worse than the default method. Data are compared for short nucleic acid sequences with rates of sequence divergence scaled by 1 (OR), 1/2 (D2), 1/4 (D4), and 2 (M2).
Figure S9: Inference of best matches from simulated sequence data. Heat map of the fraction of false positive best matches inferred by Quartet Mapping as a function of the number of duplication and loss events in the simulated scenario. Upper panels: absolute number of events; lower panel: number of events normalized by the number of species. Left panels: 200 nt sequences; right panels: 2000 nt sequences.
Figure S10: Inference of best matches from simulated sequence data. Heat map of the F-measure obtained using Quartet Mapping as a function of the number of duplication and loss events in the simulated scenario. Upper panels: absolute number of events; lower panel: number of events normalized by the number of species. Left panels: 200 nt sequences; right panels: 2000 nt sequences.