IQ-TREE: Fast and Accurate Phylogenetic Tree Interference

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A Fast and Effective Stochastic Algorithm for Estimating Maximum-Likelihood (ML) Phylogenies

- Open Source software for building phylogenetic trees using Maximum Likelihood
- Designed for speed, accuracy and usability
- · Widely used in bioinformatics, especially for analyzing DNA, RNA, or protein sequence alignments to infer evolutionary relationships between species, genes, or proteins
- Works with aligned sequences (alignment needs to be run with e.g. MAFFT)
- Different evolutionary models can be used (DNA-, Protein-, Codon-Models...)
- Output data can be visualized into trees (FIGTree, StudioR)

IQ-Tree vs RAxML/PhyML

- · Higher likelihoods between 62.2% and 87.1% of the studied alignments (same CPU time)
- · Fast performance on large scale datasets
- Built in ModelFinder and Ultrafast Bootstrap
- User-friendly and widely cited

Core Features

- ModelFinder (automatic model selection)
- Ultrafast Bootsrap (UFBoot)
- Partitioned analysis
- Multiple data types supported
- Highly parallelized (multithreading)

Data formats

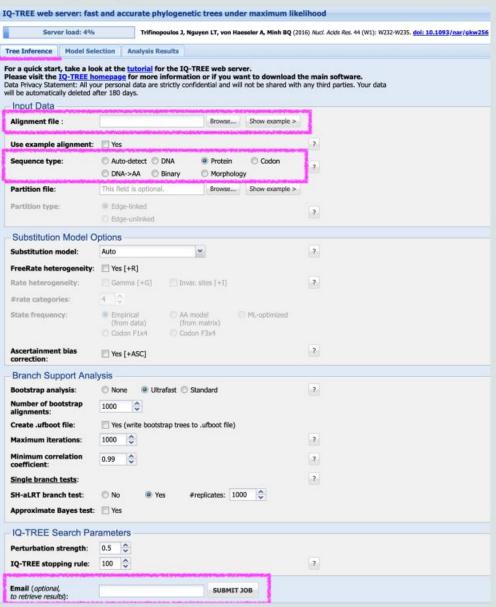
- Input: FASTA, NEXUS, PHYLIP, CLUSTAL
- Output: .iqtree (main report file); .treefile (ML in NEWICK format); .log (logfiles of the entire run, reports, bugs)

Applications

- Evolutionary Biology: Investigating the evolutionary relationships amongst species
- Comparative Genomics: comparing genetic material across different organisms to understand evolutionary processes
- Functional Genomics: exploring the function and evolution of genes and proteins

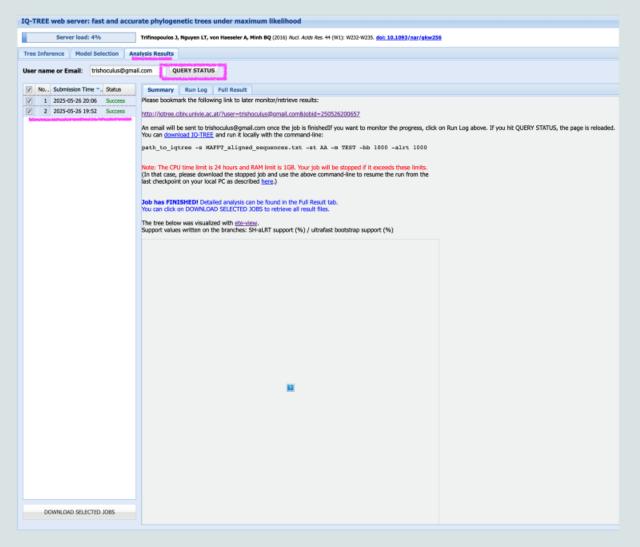
Running IQ-TREE Online: Creating a Phylogenetic Tree

- Visit: http://iqtree.cibiv.univie.ac.at
- Click on Tab "Tree Inference":
 - In the Input Data window, upload Alignment file (FASTA format)
 - For Sequence type, choose Protein
 - (Optional) Add your email to get notified when the job is done
 - Click Submit Job



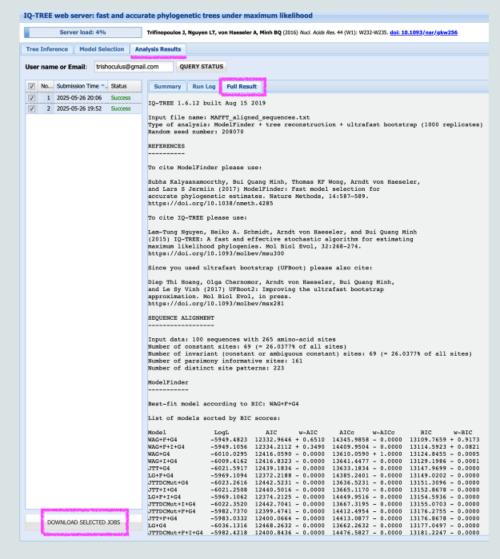
Running IQTREE Online: Where to Find Your Tree?

- Click on Tab "Analysis Results":
 - Click on "Query Status" until the job status changes to "Success"



Running IQTREE Online: Where to Find Your Tree?

- After the job status changes to "Success", go to "Full Result" Tab in order to obtain results and see the tree
- To get the output files, click on "Download Selected Jobs"
- From the downloaded folder, use .treefile file for tree visualization in RStudio



Running IQ-TREE Locally on Your Computer



- Visit iqtree.org in order to download the latest version of IQ-TREE
- Unzip the downloaded folder
- Place your aligned FASTA file in the same folder as the IQ-TREE executable
- Open Terminal (Mac/Linux) or Command (Windows)
- Run following command to start the analysis:

```
(base) trisha@Trivunas-MacBook-Pro iqtree-3.0-2.1-macOS % cd bin

(base) trisha@Trivunas-MacBook-Pro bin % ls

iqtree3
(base) trisha@Trivunas-MacBook-Pro bin % ./iqtree3 -s ../MAFFT_aligned_sequences.txt -st AA -m TEST -bb 1000 -alrt 1000

IQ-TREE version 3.0.1 for MacOS Intel 64-bit built May 5 2025

Developed by Bui Quang Minh, Thomas Wong, Nhan Ly-Trong, Huaiyan Ren
Contributed by Lam-Tung Nguyen, Dominik Schrempf, Chris Bielow,
Olga Chernomor, Michael Woodhams, Diep Thi Hoang, Heiko Schmidt
```

Running IQ-TREE Locally on your Computer - Output

- Four Output files created and saved in same folder where Input file is located:
 - .treefile: the phylogenetic tree
 - .iqtree: summary of results and settings
 - .log: full command-line log
 - .mldist: matrix showing pairwise sequence differences
 - If you want to re-run the same file, add redo at the end of your command to overwrite the old results

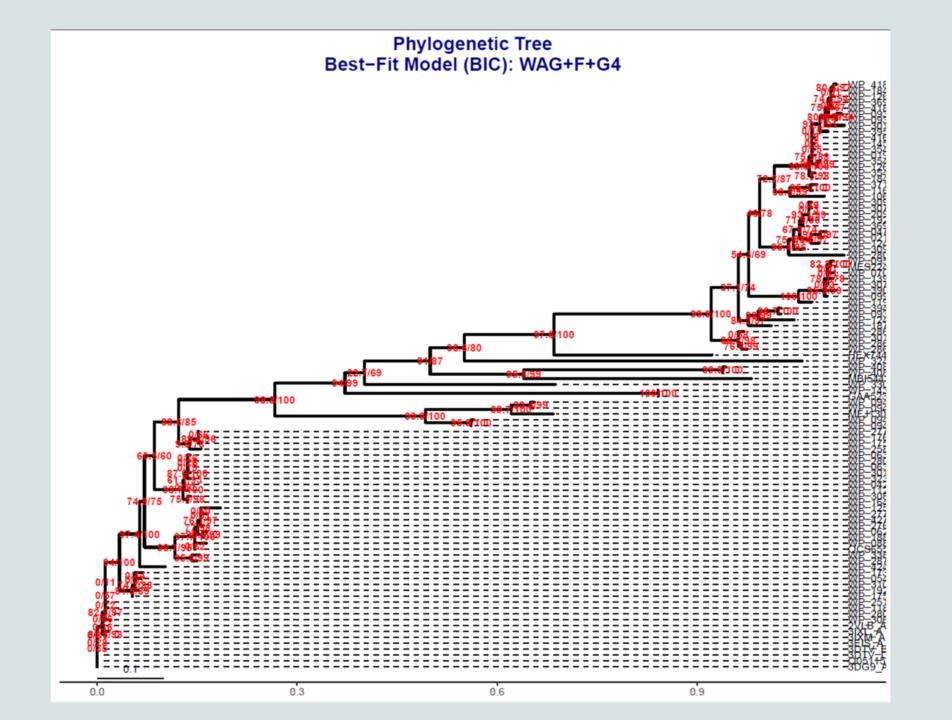
```
FINALIZING TREE SEARCH
Performs final model parameters optimization
Estimate model parameters (epsilon = 0.010)
1. Initial log-likelihood: -5931.587
Optimal log-likelihood: -5931.586
Proportion of invariable sites: 0.149
Gamma shape alpha: 1.242
Parameters optimization took 1 rounds (0.126 sec)
BEST SCORE FOUND : -5931.586
Testing tree branches by SH-like aLRT with 1000 replicates...
Creating bootstrap support values...
Split supports printed to NEXUS file ../MAFFT_aligned_sequences.txt.splits.nex
Total tree length: 5.439
Total number of iterations: 150
CPU time used for tree search: 168.453 sec (0h:2m:48s)
Wall-clock time used for tree search: 169.442 sec (0h:2m:49s)
Total CPU time used: 215.835 sec (0h:3m:35s)
Total wall-clock time used: 217.063 sec (0h:3m:37s)
Computing bootstrap consensus tree...
Reading input file ../MAFFT_aligned_sequences.txt.splits.nex...
100 taxa and 694 splits.
Consensus tree written to ../MAFFT_aligned_sequences.txt.contree
Reading input trees file ../MAFFT_aligned_sequences.txt.contree
Log-likelihood of consensus tree: -5931.606
Analysis results written to:
  IQ-TREE report:
                                 ../MAFFT_aligned_sequences.txt.iqtree
  Maximum-likelihood tree:
                                 ../MAFFT_aligned_sequences.txt.treefile
  Likelihood distances:
                                 ../MAFFT_aligned_sequences.txt.mldist
 Ultrafast bootstrap approximation results written to:
  Split support values:
                                 ../MAFFT_aligned_sequences.txt.splits.nex
  Consensus tree:
                                 ../MAFFT aligned sequences.txt.contree
  Screen log file:
                                 ../MAFFT_aligned_sequences.txt.log
Date and Time: Mon May 26 21:17:57 2025
(base) trisha@Trivunas-MacBook-Pro bin % 🖥
```

Visualization with RStudio

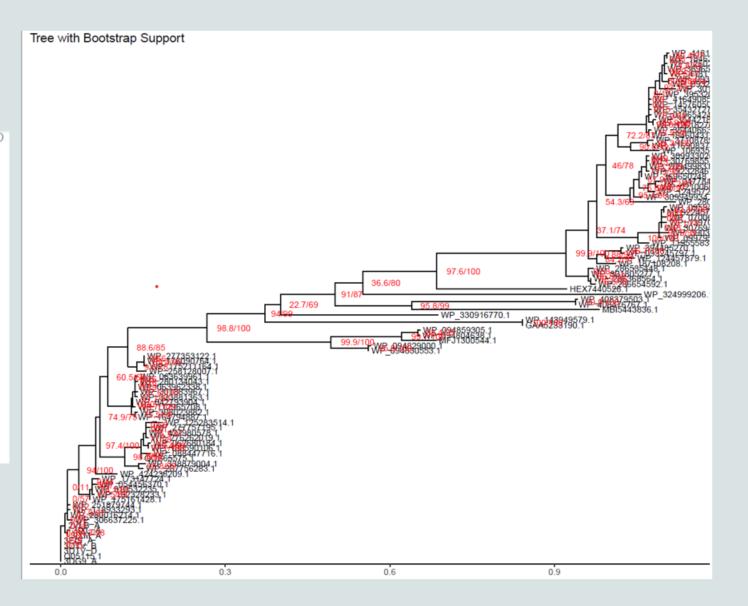
Read is generated through .treefile into Rstudio

Best-fit model according to BIC: WAG+F+G4

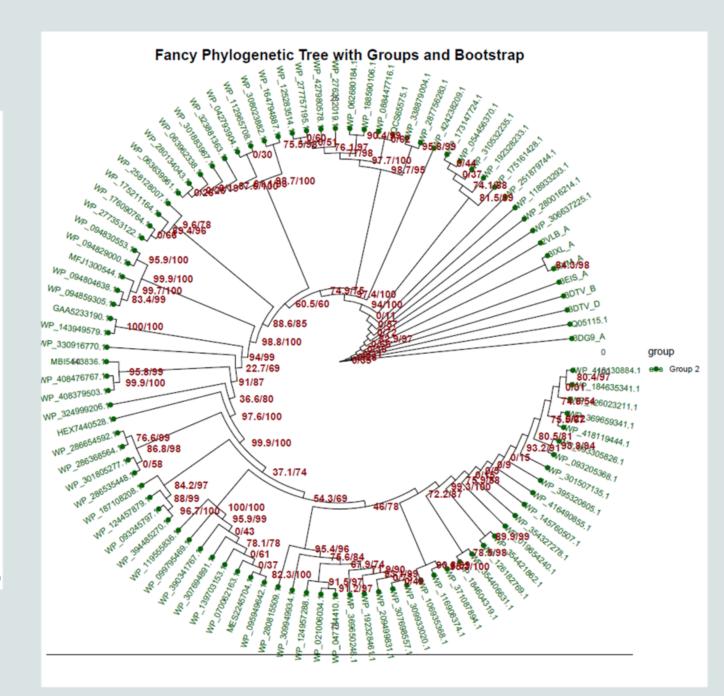
```
if (!requireNamespace("BiocManager", quietly=TRUE)) install.packages("BiocManager")
if (!requireNamespace("ggtree", quietly=TRUE)) BiocManager::install("ggtree")
if (!requireNamespace("ape", quietly=TRUE)) install.packages("ape")
library(ape)
library(ggtree)
library(ggplot2)
tree <- read.tree("C:/Users/andre/Downloads/MAFFT_aligned_sequences.txt.treefile")</pre>
tree <- ladderize(tree)
best_fit_tree_plot <- ggtree(tree, branch.length="branch.length") +</pre>
  geom_tree(linewidth=1) +
  geom_tiplab(size=3, align=TRUE, linetype="dashed", linesize=0.5) +
  geom_text2(aes(subset=!isTip, label=label), color="red", size=3, fontface="bold") +
  theme_tree2() +
  ggtitle("Phylogenetic Tree\nBest-Fit Model (BIC): WAG+F+G4") +
  theme(plot.title=element_text(hjust=0.5, size=16, face="bold", color="darkblue"),
        panel.background=element_rect(fill="White"),
        legend.position="none") +
  geom_treescale(x=0, y=-1, offset=1, fontsize=3)
print(best_fit_tree_plot)
ggsave("C:/Users/andre/Downloads/tree_with_WAGF_G4_model.pdf", best_fit_tree_plot,
       width=10, height=8, dpi=300)
```



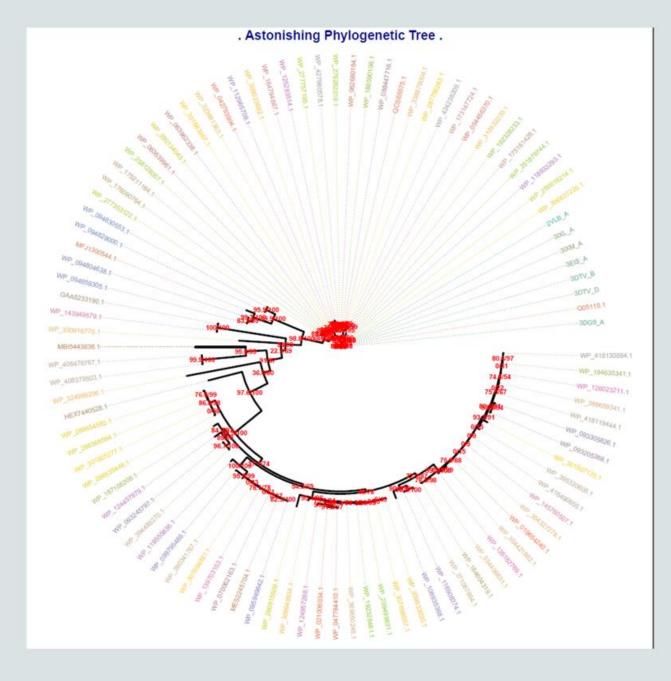
```
if (!requireNamespace("BiocManager", quietly = TRUE)) install.packages("BiocManager")
if (!requireNamespace("ggtree", quietly = TRUE)) BiocManager::install("ggtree")
if (!requireNamespace("ape", quietly = TRUE)) install.packages("ape")
library(ape)
library(ggtree)
library(ggplot2)
tree <- read.tree("C:/Users/andre/Downloads/MAFFT_aligned_sequences.txt.treefile")</pre>
plot(tree, main="Simple Tree")
fancy_plot <- ggtree(tree) +
 geom_tiplab(size=3) +
  geom_tree() +
  theme_tree2() +
  ggtitle("Phylogenetic Tree from IQ-TREE")
print(fancy_plot)
fancy_plot_with_bootstrap <- fancy_plot +</pre>
 geom_text2(aes(subset=!isTip, label=label), hjust=-0.3, size=3, color="red") +
 ggtitle("Tree with Bootstrap Support")
print(fancy_plot_with_bootstrap)
ggsave("my_tree_plot.pdf", fancy_plot_with_bootstrap, width=10, height=8)
```



```
if (!requireNamespace("BiocManager", quietly = TRUE)) install.packages("BiocManager")
if (!requireNamespace("ggtree", quietly = TRUE)) BiocManager::install("ggtree")
if (!requireNamespace("ape", quietly = TRUE)) install.packages("ape")
library(ape)
library(ggtree)
library(ggplot2)
tree <- read.tree("C:/Users/andre/Downloads/MAFFT_aligned_seguences.txt.treefile")
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fancv_plot <- ggtree(tree) +
 geom_tiplab(size=3) +
  geom_tree() +
  theme_tree2() +
  ggtitle("Phylogenetic Tree from IQ-TREE")
print(fancy_plot)
fancy_plot_with_bootstrap <- fancy_plot +
 geom_text2(aes(subset=!isTip, label=label), hjust=-0.3, size=3, color="red") +
  ggtitle("Tree with Bootstrap Support")
print(fancy_plot_with_bootstrap)
ggsave("my_tree_plot.pdf", fancy_plot_with_bootstrap, width=10, height=8)
library(ape)
library(ggtree)
library(ggplot2)
tree <- read.tree("C:/Users/andre/Downloads/MAFFT_aligned_seguences.txt.treefile")
tip_groups <- data.frame(
  label = tree$tip.label,
  group = ifelse(grepl("group1_pattern", tree$tip.label), "Group 1", "Group 2")
fancy_plot <- ggtree(tree, branch.length='none', layout='circular') +
  geom_tiplab(aes(color=group), size=3, align=TRUE, linetype='dashed') +
  geom_tippoint(aes(color=group), size=2) +
  geom_text2(aes(subset = !isTip, label=label), hjust=-0.3, size=4, color="darkred",
             fontface="bold") +
  theme_tree2() +
 scale_color_manual(values = c("Group 1" = "blue", "Group 2" = "darkgreen")) +
  ggtitle("Fancy Phylogenetic Tree with Groups and Bootstrap") +
    legend.position = "right".
    plot.title = element_text(hjust = 0.5, size=16, face="bold")
fancy_plot <- fancy_plot %<+% tip_groups
print(fancv_plot)
ggsave("C:/Users/andre/Downloads/fancy_tree_plot.pdf", fancy_plot, width=10, height=10)
```



```
if (!requireNamespace("BiocManager", quietly=TRUE)) install.packages("BiocManager")
if (!requireNamespace("ggtree", quietly=TRUE)) BiocManager::install("ggtree")
if (!requireNamespace("ape", quietly=TRUE)) install.packages("ape")
if (!requireNamespace("RColorBrewer", quietly=TRUE)) install.packages("RColorBrewer")
library(ape)
library(ggtree)
library(ggplot2)
library(RColorBrewer)
tree <- read.tree("C:/Users/andre/Downloads/MAFFT_aligned_sequences.txt.treefile")
tree <- ladderize(tree)
num_tips <- length(tree$tip.label)</pre>
tip_colors <- colorRampPalette(brewer.pal(8, "Set2"))(num_tips)</pre>
astonishing_tree <- ggtree(tree, layout="circular", branch.length="branch.length") +
  geom_tree(linewidth=1.2, color="black") +
  geom_tiplab2(aes(color=label), size=3, offset=0.5, align=TRUE, linesize=0.4) +
  scale_color_manual(values=tip_colors) +
  geom_text2(aes(subset=!isTip, label=label), color="red", size=3, fontface="bold") +
  geom_treescale(x=0, y=-2, offset=1, fontsize=3) +
  theme(plot.title=element_text(hjust=0.5, size=18, face="bold", color="darkblue"),
        panel.background=element_rect(fill="White"),
        panel.grid=element_blank(),
        legend.position="none") +
  print(astonishing_tree)
ggsave("C:/Users/andre/Downloads/astonishing_tree.pdf", astonishing_tree, width=12,
       height=12, dpi=300)
```



THANK YOU FOR YOUR ATTENTION!