



Maximum  
likelihood  
(ML)  
inconsistency

Patrick Kück,  
Wolfgang  
Wägele

Theory  
Model Violation  
Classes of LBA

Simulations  
LoBraTe  
Topologies  
ML Setup

Results  
Parametric  
Bootstrap  
Likelihood  
Values

Conclusions  
ASRV  
ML Consistency  
LBA I

Gratitute

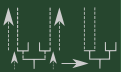
# Maximum likelihood (ML) inconsistency in terms of long branch attraction

Patrick Kück, Wolfgang Wägele

Bioinformatics  
Forschungsmuseum Alexander Koenig

22nd February





# Topological Bias

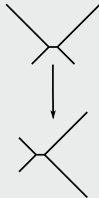
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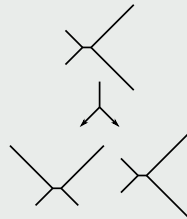
Felsenstein 1978

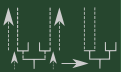
- Phylogenetic methods become inconsistent when model assumptions are **strongly** violated

Felsenstein Zone



Farris Zone

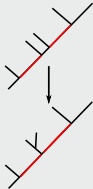




# 3 classes of LBA

Wägele & Mayer 2007

## LBA I (Symplesiomorphy Trap)



- plesiomorphy trap
- synapomorphies substituted
- increase of plesiomorphies / apomorphies ratio
- paraphyletic grouping
- use of more taxa

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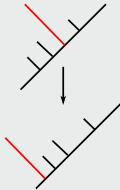
Gratitude



# 3 classes of LBA

Wägele & Mayer 2007

## LBA II (Signal Erosion)



- phylogenetic signal erosion
- shared plesiomorphies with distantly related taxa
- synapomorphies substituted
- long branch slips down
- use of genes with lower rates



# 3 classes of LBA

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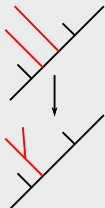
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Wägele & Mayer 2007

## LBA III (Parallel Substitutions)

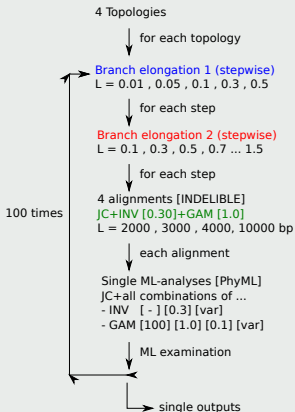


- identical character states evolve independently
- high number of convergent characters
- branches can form nonsense clades

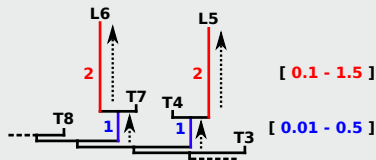


# Long-Branch-Testpipeline (LoBraTe)

## Setup of LoBraTe



## Branch Elongation 1&2

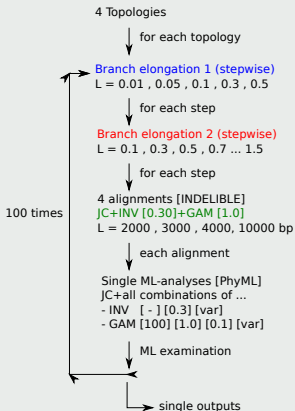


- 768,000 single data sets

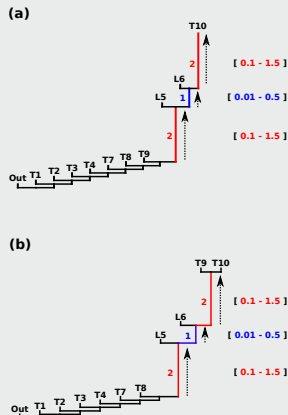


# Long-Branch-Testpipeline (LoBraTe)

## Setup of LoBraTe



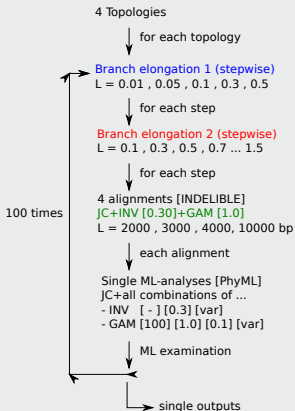
## Topologies for LBA I





# Long-Branch-Testpipeline (LoBraTe)

## Setup of LoBraTe

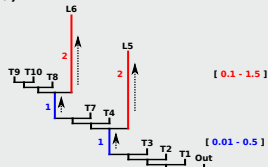


## Topologies for LBA II&III

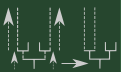
(c)



(d)







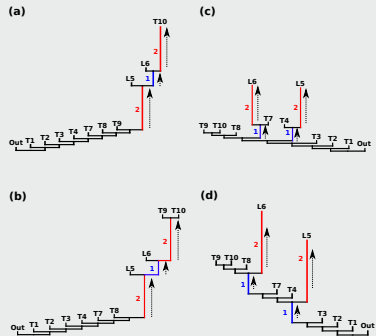
# Model Setup

## PHYML+TBR

### Jukes-Cantor

$\Gamma$		$\rho_{inv}$
$\alpha[0.1]$		
$\alpha[0.1]$	+	$\theta[0.3]$
$\alpha[0.1]$	+	$\theta[var]$
$\alpha[1.0]$		
$\alpha[1.0]$	+	$\theta[0.3]$
$\alpha[1.0]$	+	$\theta[var]$
$\alpha[100]$		
$\alpha[100]$	+	$\theta[0.3]$
$\alpha[100]$	+	$\theta[var]$
$\alpha[var]$		
$\alpha[var]$	+	$\theta[0.3]$
$\alpha[var]$	+	$\theta[var]$

## Topologies





# Model Setup

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LoBraTe  
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## PHYML+TBR

Jukes-Cantor

$\Gamma$

$\rho_{inv}$

$\alpha[1.0] + \theta[0.3]$

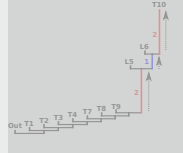
$\alpha[100]$

$\alpha[var]$

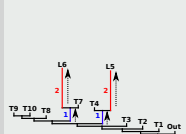
$\alpha[var] + \theta[var]$

## Topologies

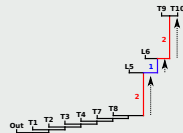
(a)



(c)



(b)



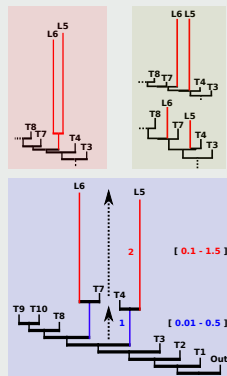
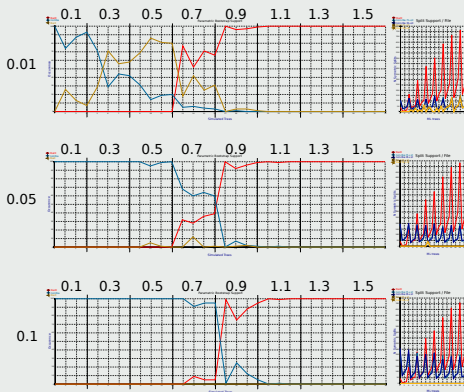
(d)





# LoBraTe output

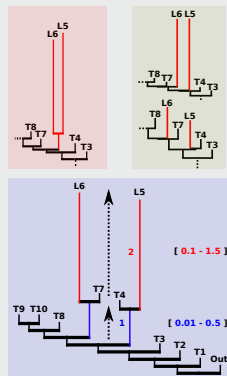
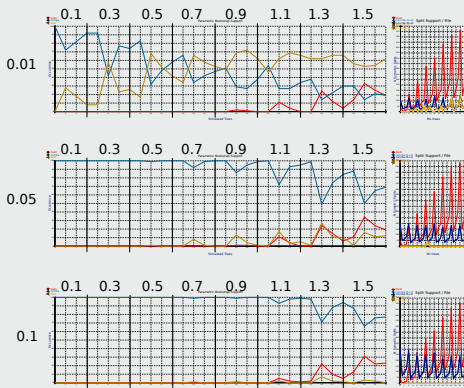
parametric bootstrap|splits (LBA II&III)  $JC + \alpha[100]$





# LoBraTe output

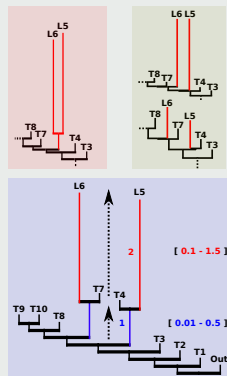
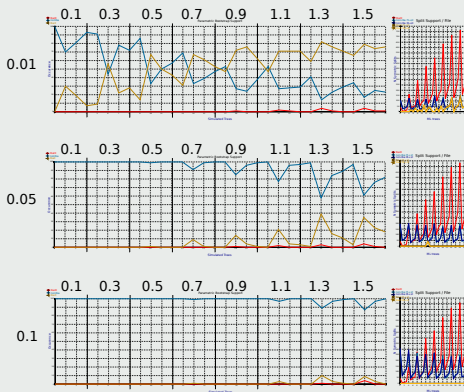
parametric bootstrap|splits (LBA II&III)  $JC + \alpha[var]$





# LoBraTe output

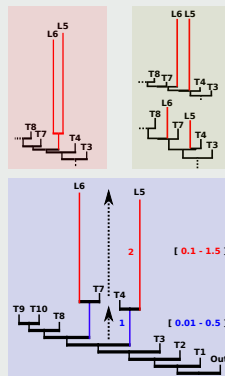
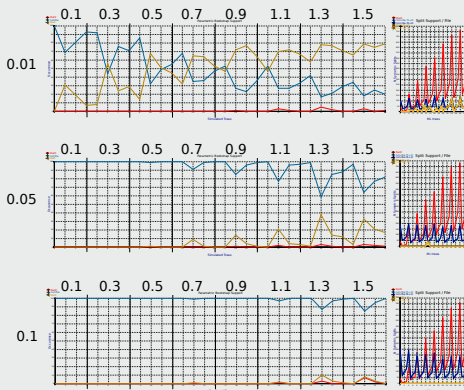
parametric bootstrap|splits (LBA II&III)  $JC + \alpha[var] + \theta[var]$





# LoBraTe output

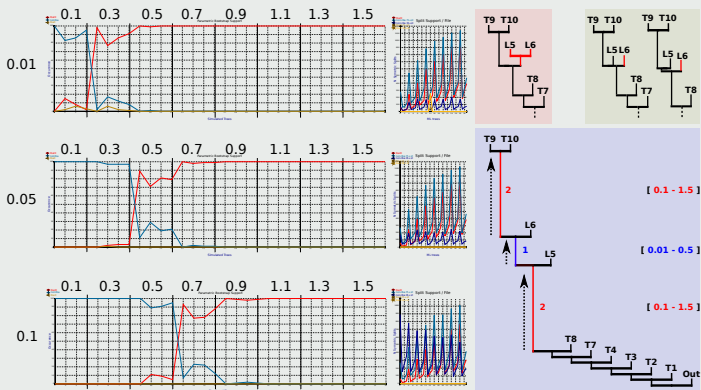
parametric bootstrap|splits (LBA II&III)  $JC + \alpha[1.0] + \theta[0.3]$





# LoBraTe output

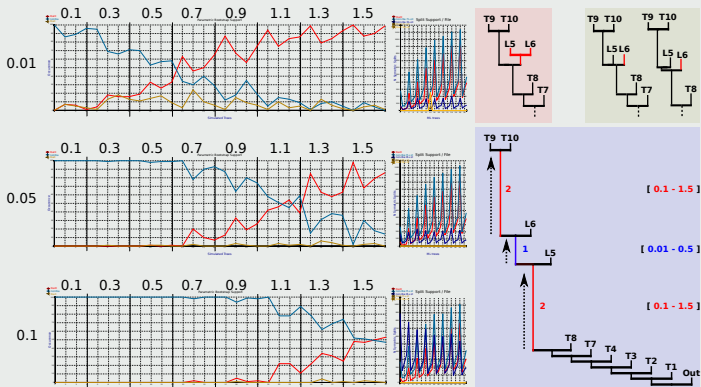
parametric bootstrap|splits (LBA I)  $JC + \alpha[100]$





# LoBraTe output

parametric bootstrap|splits (LBA I)  $JC + \alpha[var]$

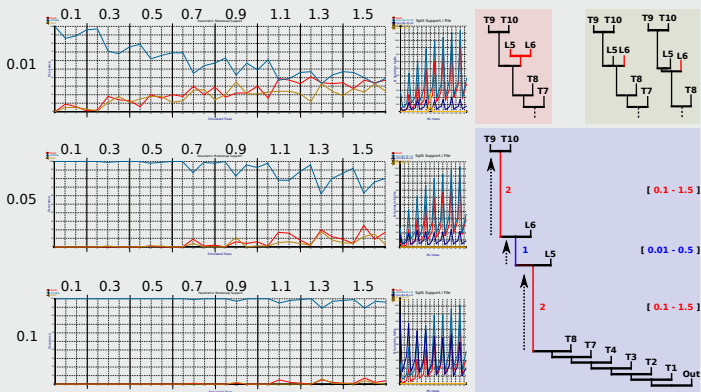






# LoBraTe output

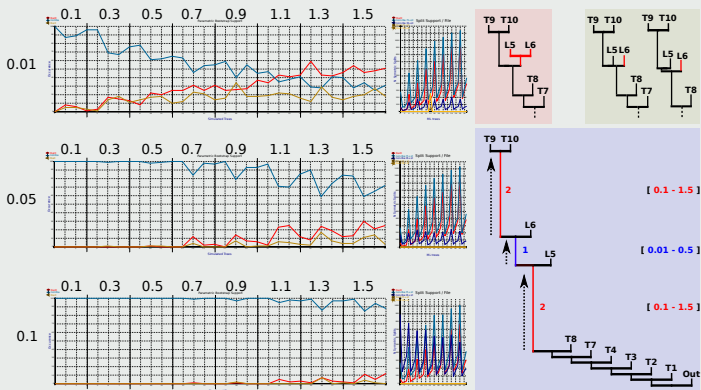
parametric bootstrap|splits (LBA I)  $JC + \alpha[var] + \theta[var]$





# LoBraTe output

parametric bootstrap|splits (LBA I)  $JC + \alpha[1.0] + \theta[0.3]$





# LoBraTe output: Mean Likelihood Values

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LoBraTe  
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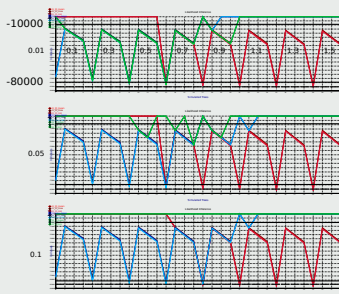
Parametric  
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Conclusions

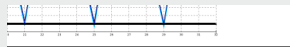
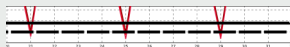
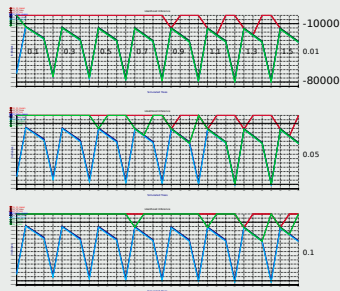
ASRV  
ML Consistency  
LBA I

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LBA II&III  $JC + \alpha[100]$



$JC + \alpha[var] + \theta[var]$





# LoBraTe output: Mean Likelihood Values

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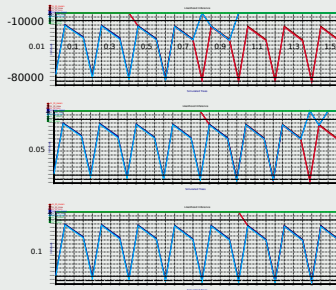
Parametric  
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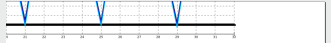
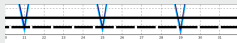
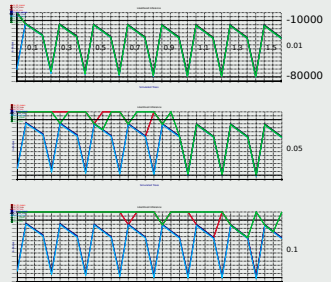
ASRV  
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LBA I  $\text{JC} + \alpha[100]$



$\text{JC} + \alpha[\text{var}] + \theta[\text{var}]$





# Conclusions

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Model Violation  
Classes of LBA

Simulations  
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Topologies  
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Bootstrap  
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Values

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Gratitude

## Among Site Rate Variation (ASRV)

- ML methods are much more robust to LBA if among site rate variation is included
- ASRV including  $\Gamma$  and  $\rho_{inv}$  fit data better than  $\Gamma$  alone
- ASRV leads to improved likelihood scores
- Consistent parameter estimates possible with relative low number of taxa



# Conclusions

## Maximum likelihood (ML) inconsistency

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## Consistency of Maximum Likelihood (ML)

- LBA can afflict ML when models are not/weakly violated
- Large data are not immune to systematic error under correct models
- LBA trees show nearly identic likelihood scores than the true trees
- Near star-like subregions are not choosen at random from the possible resolved topologies



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Model Violation  
Classes of LBA

Simulations

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Topologies  
ML Setup

Results

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## LBA I (symplesiomorphy trap)

- Class I long-branch effects can be shown in simulations
- Long internal branches did not lead to more robust ML estimates



# Acknowledgement

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Topologies  
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Values

Conclusions  
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LBA I

Gratitude

## Best thanks to the...

- ...Forschungsmuseum Koenig, Bonn
  - Bernhard Misof
  - Christoph Mayer
- ...Deutsche Forschungsgemeinschaft DFG
- ...Leibniz Gemeinschaft
- and especially to you !

Deutsche  
Forschungsgemeinschaft  
**DFG**



FORSCHUNGS  
museum  
**KOENIG**



**Leibniz  
Gemeinschaft**