

Phylomania 2011

The UTas theoretical phylogenetics meeting

University of Tasmania, School of Maths and Physics, 10-11 Nov 2011

Program

Thursday, 10 November

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| 8.15am-9:00am | Registration and coffee |
| 9:00am-9:10am | Welcome |
| 9:10am-9:50am | Mike Steel , University of Canterbury, New Zealand <i>'Lassoing' a tree: Phylogenetic theory for sparse patterns of taxon coverage</i> |
| 9:50am-10:30am | Tom Nye , Newcastle University, United Kingdom <i>Distributions and diffusions on tree-space</i> |
| 10:30am-11:00am | Morning tea |
| 11:00am-11:40am | Demos Ellinas , Technical University of Crete, Greece <i>On Quantum Simulation of Phylogenetic Processes</i> |
| 11:40am-12:00pm | Andrew Francis , University of Western Sydney, Australia <i>An algebraic view of bacterial evolution</i> |
| 12:00am-12:20pm | Attila Egri-Nagy , University of Western Sydney, Australia <i>Using group theory to study the inversion distance problem in bacterial genomics</i> |
| 12:20pm-1:40pm | Lunch |
| 1:40pm-2:20pm | Steffen Klaere , University of Otago, New Zealand <i>Hadamard-type Transforms for nonsymmetric models</i> |
| 2:20pm-3:00pm | Jeremy Sumner , University of Tasmania, Australia <i>Lie Markov models: The $\mathbb{Z}_2 \wr \mathbb{Z}_2$ case</i> |
| 3:00pm-3:30pm | Afternoon Tea |
| 3:30pm-3:50pm | Joe Zhu , University of Canterbury, New Zealand <i>Clades and clans probability in Yule trees</i> |
| 3:50pm-4:10pm | Michael Woodhams , University of Tasmania, Australia <i>ADD: Additive Dollo Distances and their friends</i> |
| 4:10pm-4:30pm | Josh Collins , University of Otago, New Zealand <i>Building Phylogenetic Networks</i> |
| 7:30pm | Phylomania 2011 pub dinner: Shipwright Arms |

Friday, 11 November

- 9:00am-9:30am Coffee
- 9:30am-9:50am **Bodie Kaine**, University of Tasmania, Australia
The Effect of Closure on the Estimation of Divergence Times in Phylogenetics
- 9:50am-10:10am **Jonathan Mitchell**, University of Tasmania, Australia
Identifiability of the Convergence of Previously Diverging Taxa
- 10:10am-10:30am **Peter Jarvis**, University of Tasmania, Australia
Lie group structure and Markov invariants for the strand symmetric model
- 10:30am-11:00am Morning tea
- 11:00am-11:40am **Lars Jermiin**, CSIRO Ecosystem Sciences, Canberra, Australia
The role of model misspecification in two recent phylogenetic studies of mitochondrial and nuclear protein-coding genes
- 11:40am-12:20pm **Arndt von Haeseler**, Center for Integrative Bioinformatics, Vienna, Austria
One Step Mutation Matrices: Some Applications
- 12:20pm-1:40pm Lunch
- 1:40pm-2:20pm **James Degnan**, University of Canterbury, New Zealand
Modeling hybridisation: gene trees in species networks
- 2:20pm-3:00pm **Barbara Holland**, University of Tasmania, Australia
Detecting convergent evolution in cormorants and shags
- 3:00pm-3:30pm Afternoon Tea
- 3:30pm-3:50pm **Bojian Zhong**, Massey University, New Zealand
Systematic error in seed plant phylogenomics
- 3:50pm-4:10pm **Iker Irisarri**, CSIRO Ecosystem Sciences, Canberra, Australia
Three key questions in the phylogeny of frogs
- 4:10pm-4:30pm **Chris Burridge**, University of Tasmania, Australia
Reassessing a long-standing biogeographic controversy – the importance of considering ancestral life history and distributional character states
- 4:30pm-6pm Drinks and cheese

Saturday, 12 November

- 12pm- **Phylomania 2011 bushwalk** (details TBA)

Abstracts

Chris Burridge

Institute: University Tasmania, Australia

Reassessing a long-standing biogeographic controversy — the importance of considering ancestral life history and distributional character states

The aim of this study was to determine the contributions of Gondwanan vicariance and marine dispersal to the contemporary distribution of galaxiid fishes. This group has been central in arguments concerning the roles of dispersal and vicariance in the Southern Hemisphere, as some taxa have marine life history stages through which transoceanic dispersal may have been facilitated, yet other galaxiids are entirely restricted to freshwaters. Biogeographic hypotheses of Gondwanan vicariance and marine dispersal were tested using four lines of evidence: (1) concordance of species-area phylogenetic relationships, (2) molecular estimates of lineage divergence times with a priori expectations based on plate tectonics, (3) reconstructions of ancestral dispersal capabilities, and (4) reconstructions of distribution inheritance scenarios (using the dispersal-extinction-cladogenesis model to infer historical ranges and dispersal and extinction events). Phylogenetic relationships were reconstructed from 4531 mitochondrial and nuclear nucleotide characters, and 181 morphological characters, across 53 of the 56 presently recognized species. Phylogenetic relationships were generally well resolved and supported among galaxiids using the combined dataset, and conflicting relationships between molecular and morphological datasets typically received low topological support from either or both datasets. Transoceanic disjunctions were exhibited at 16 nodes, but only three pre-dated relevant continental fragmentation events; furthermore, ancestral distribution inheritance scenarios for two of these nodes reflected cladogenesis within, rather than between, Gondwanan land masses, and ancestral marine dispersal capability could not be rejected for all three. Instead, the four lines of evidence surveyed suggest that Gondwanan vicariance occurred twice, but in both instances was preceded by marine dispersal between land masses, and in at least one instance was initiated by the cessation of marine dispersal subsequent to continental fragmentation. Gondwanan vicariance appears to have been preceded by marine dispersal in the few instances where it may explain contemporary galaxiid distribution, such that these biogeographic mechanisms may sometimes have a synergistic relationship.

Josh Collins

Institute: University of Otago, New Zealand

Building Phylogenetic Networks

Early this year I presented a poster that outlined the basics of an algorithm that would build a phylogenetic network for a set of evolutionary trees. This talk will go into some more depth including the alterations that have since been included to account for some counter examples.

James Degnan

Institute: University of Canterbury, New Zealand

Modeling hybridisation: gene trees in species networks

Probabilities of gene tree topologies given rooted species trees have previously been worked out assuming incomplete lineage sorting as the sole cause of gene tree conflict. There have been several applications, including methods for inferring species trees from gene trees and determining species trees for which methods of species tree inference are potentially misleading. Incomplete lineage sorting is especially likely to happen for closely related populations. However, hybridisation between previously separated populations can also occur in this setting and can lead to different patterns of gene tree conflict than occurs under a pure lineage sorting model. I will talk about different methods for computing probabilities of gene trees when species networks allow for both incomplete lineage sorting and hybridisation.

Attila Egri-Nagy

Institute: University of Western Sydney, Australia

Using group theory to study the inversion distance problem in bacterial genomics

There are efficient combinatorial algorithms for calculating the inversion distance between genomes represented as signed permutations. Here we present a general algebraic framework (group decompositions) in which the different algorithms can be described using a common language. The group decompositions also give structural distance information, a tuple of values instead of a single number. We demonstrate these techniques on the example of a bacterial genome model with fixed terminus, which is not considered by existing algorithms.

Demosthenes Ellinas

Institute: Technical University of Crete, Greece

On Quantum Simulation of Phylogenetic Processes

Joint work with Peter Jarvis.

Phylogenetic processes, such as growth and statistical inference of phylogenetic trees, are formulated along the lines of quantum simulation methodology. Some of the novelties and prospects of the approach are presented.

Andrew Francis

Institute: University of Western Sydney, Australia

An algebraic view of bacterial evolution

Bacteria evolve rapidly in a variety of ways. Segments of DNA can be deleted, relocated, inserted, or inverted, all of which affect the sequence and can be used (theoretically) to measure

evolutionary distance between genomes (useful for phylogeny). At the same time changes to the DNA can occur at a larger scale, in which cutting and rejoining gives rise to knotting of the circular bacterial genome. In this talk I will describe how these seemingly distant processes have connections at both biological and – hopefully – algebraic levels.

Barbara Holland

Institute: University of Tasmania, Australia

Detecting convergent evolution in the cormorants and shags

A phylogenetic tree comprising clades with high bootstrap values or other strong measures of statistical support is usually interpreted as providing a good estimate of the true phylogeny. Convergent evolution acting on groups of characters in concert, however, can lead to highly supported but erroneous phylogenies. Identifying such groups of phylogenetically misleading characters is obviously desirable. Here we present a procedure that uses an independent data source to identify sets of characters that have undergone concerted convergent evolution. We examine the problematic case of the cormorants and shags, for which trees constructed using osteological and molecular characters both have strong statistical support and yet are fundamentally incongruent. We find that the osteological characters can be separated into those that fit the phylogenetic history implied by the molecular data set and those that do not. Moreover, these latter nonfitting osteological characters are internally consistent and form groups of mutually compatible characters or “cliques”, which are significantly larger than cliques of shuffled characters. We suggest, therefore, that these cliques of characters are the result of similar selective pressures and are a signature of concerted convergence.

Iker Irisarri

Institute: CSIRO Ecosystem Sciences, Canberra, Australia

Three key questions in the phylogeny of frogs

Joint work with Diego San Mauro, Miguel Vences, Federico Abascal, Frank Glaw, David M. Green, Annemarie Ohler, and Rafael Zardoya.

Largely due to the contribution of molecular phylogenetic analyses the current picture of the frog Tree of Life has greatly improved in the last years. However, some questions still remain controversial or unanswered (and here we focus on three of them).

The first one involves two relict genera that have been generally considered basal among frogs (*Leiopelma* and *Ascaphus*), but whose precise relative phylogenetic position in the frog Tree of Life awaits resolution. Our phylogenetic analyses unambiguously grouped both genera together, and as sister group to all other frogs. We additionally found a new mitochondrial gene order for *Leiopelma archeyi*, which was convergent with that of other vertebrates. Comparative data on mitochondrial gene order strongly suggested that the 5' end of the control region is a hot spot of gene rearrangement.

Secondly, the limited availability of phylogenetic data for the Pipidae (African clawed frogs and American Surinam toads) led to contentious hypotheses on the phylogenetic position of pipid frogs (and thus of branching order among major anuran lineages), as well as on the internal phylogeny of the family. Using both mitochondrial genomes and a matrix of nine nuclear loci,

we unambiguously recovered the branching order of major lineages of frogs and supported a most likely scenario of internal relationships among pipid genera. Using the recovered robust phylogenetic framework, we studied sound production and associated anatomy of the poorly known genus *Pseudhymenochirus*, and found a reversal to the ancestral non-pipid condition of air-driven mechanism.

The third question focuses on the distribution of substitution rates among lineages of frogs. Previous studies evidenced that modern frogs (*Neobatrachia*) have higher mitochondrial substitution rates, but it was not known whether this trend is general among neobatrachians nor whether nuclear genes showed a similar trend. We added new mitogenomic and nuclear data for basal families within Neobatrachia, which were key to understand such patterns. Our analyses showed that neobatrachian frogs (both basal and derived lineages) have higher mitochondrial substitution rates compared to non-neobatrachians, and using a relaxed molecular clock, we estimated this acceleration to have occurred in the Early-Middle Jurassic. Further examination of the data suggested that purifying selection acting on mitochondrial protein-coding genes relaxed during this period, concluding that this event could account, at least in part, for the observed lineage-specific substitution rates among frogs.

Peter Jarvis

Institute: University of Tasmania, Australia

Lie group structure and Markov invariants for the strand symmetric model

The strand symmetric model of phylogenetic evolution (SSM) posits a six parameter transition matrix consistent with canonical base pairing, for example with equal entries for $A \rightarrow G$ and $T \rightarrow C$, and similar constraints, and generally non-uniform stationary base frequencies which satisfy $\pi_A = \pi_T$, $\pi_C = \pi_G$. Given the multiplicative closure of the SSM, we study the corresponding continuous time model, and the associated Lie group. We identify the structure of the 6 dimensional Lie algebra of rate matrices, and investigate its polynomial representations. Using these results we enumerate Markov invariants for the model, and discuss some low degree examples in detail.

Lars Jermin

Institute: CSIRO Ecosystem Sciences, Canberra, Australia

The role of model misspecification in two recent phylogenetic studies of mitochondrial and nuclear protein-coding genes

In this seminar, I will focus on the role that model misspecification has played in two recent studies of molecular evolution. The first study led to the development of the MtArt model of amino acid substitutions, which often is used in phylogenetic studies of polypeptides encoded by arthropod mitochondrial genomes. The second study led to a clearer understanding of the evolution of pathogenicity and sexual reproduction in eight *Candida* genomes.

A preliminary survey of the amino acid alignment used to estimate the MtArt model of amino acid substitutions indicates that the sequences are unlikely to have evolved under globally stationary, reversible, and homogeneous (SRH) conditions, implying that a critical assumption underlying the use of the MtArt model was violated during its estimation. Using column-and-row permutations of heat maps with the results of matched-pairs tests of symmetry allowed us to

identify a subset of sequences that is consistent with evolution under globally SRH conditions; using this subset, we then inferred a revised MtArt model of amino acid substitutions.

A preliminary survey of the genomic data used to infer the evolutionary relationships among 17 species of yeast disclosed a surprising result: the fit between the data and the optimal tree and substitution model was significantly better for the real data than for data generated on the optimal tree and substitution model. The underlying cause of this disturbing result was assessed using a number of analytical methods, including the parametric bootstrap, matched-pairs test of symmetry, and phylogenetic analysis. We show that the data are unlikely to have evolved under globally SRH conditions, but neither violation of the assumption of evolution under globally SRH conditions nor violation of the assumption of independently distributed processes across sites is able to explain the result. Evidence supporting another explanation is presented.

Bodie Kaine

Institute: University of Tasmania, Australia

The Effect of Closure on the Estimation of Divergence Times in Phylogenetics

The general time-reversible model (GTR) is at the forefront of nucleotide substitution modelling, frequently being used to infer phylogenies (evolutionary trees) and estimate evolutionary rates and divergence times. However the sole basis for the use of this model is the high log-likelihood score it achieves when simulating sequences in model recommendation programs such as MODELTEST, much of which is attributed to its large number of free parameters. But does a high log-likelihood score alone warrant the use of a model? Are there undesirable properties associated with this or other models which arise in certain situations? And to what extent may these undesirable properties lead to incorrect estimations? This presentation will attempt to answer these questions through the analysis and comparison of various models which do or do not feature a potentially important property called closure.

Steffen Klaere

Institute: University of Auckland, New Zealand

Hadamard-type Transforms for nonsymmetric models

Joint work with David Bryant.

The classic Hadamard transform provides a topology-independent bijective relation between relational structure of species and frequency of data. However, the transform only works for very special models. In this talk I will present extensions of the transform to more general models which retain the topology independence. These extensions employ the Random Cluster model and provide some very interesting insights into the likelihood equations. Our extension is not bijective. However we can observe some relationship with linear invariants.

Jonathan Mitchell

Institute: University of Tasmania, Australia

Identifiability of the Convergence of Previously Diverging Taxa

Given a set of taxa, can the model where those taxa evolved independently be identified from the model where convergence of previously diverged taxa occurred? This is a particularly important question because it involves determining whether the case of genetic cross-over (eg. hybridisation) is identifiable from the case of independent lineages evolving. The constraints on the probability distributions arising from the models will be analysed by transforming the distributions into their appropriate basis (i.e. the Hadamard basis for the binary symmetric model). By comparing the set of invariants from the two models it can be determined whether the models are identifiable from each other. I will start by looking at the simplest model, the two taxa binary symmetric model, and show that the two models cannot be identified from each other. I will then show that the three taxa binary symmetric model with convergence is sometimes identifiable from the fully independent case, depending on which taxa interact (the two adjacent taxa versus the two outside taxa). Finally, I will look at more general models.

Tom Nye

Institute: Newcastle University, United Kingdom

Distributions and diffusions on tree-space

Most distributions of trees are analytically intractable and we usually resort to simulating them via bootstrapping or MCMC. This talk describes an approach to constructing analytically tractable distributions based on diffusions on the space of phylogenetic trees. The approach is based on the description of tree-space as a geodesic metric space. The aim is to fit these distributions to samples of trees as a way of giving summary measures, or alternatively to use them to build simplified models.

Mike Steel

Institute: University of Canterbury, New Zealand

'Lassoing' a tree: Phylogenetic theory for sparse patterns of taxon coverage

Phylogenomic data often exhibit partial taxon coverage, whereby each loci is present or sequenced only for some corresponding subset of the species under study. This leads to some interesting mathematical and statistical questions as to whether a fully resolved underlying evolutionary tree for all the taxa can be reconstructed, given perfect phylogenetic estimates from each locus. We first describe the extent to which a pattern of taxon coverage can be 'phylogenetically decisive' in various senses, and provide some applications to data (joint work with Sanderson and McMahon). We then consider tree reconstruction from distance data, in settings where accurate estimates of evolutionary distance exist between only certain pairs of taxa: Does this partial information suffice to pin down or, as we say, 'lasso' the underlying phylogenetic tree? We describe a number of new combinatorial results concerning lassos (joint work with Dress and Huber). We conclude with some open problems.

Jeremy Sumner

Institute: University of Tasmania, Australia

Lie Markov models: The $\mathbb{Z}_2 \wr \mathbb{Z}_2$ case

Joint work with Jesús Fernández-Sánchez, Peter Jarvis and Michael Woodhams.

In recent work we have discussed the importance of closure when considering countinuous-time Markov chain models, as used in phylogenetics. In particular, to ensure closure under multiplication of substitution matrices, it is sufficient that the set of rate-matrices from a model form a Lie algebra. In this talk, I will outline a procedure which generates a complete list of such models given a specific demand of symmetry under nucleotide permutations. Despite being a somewhat crude approach, this is the most systematic method known, with other approaches producing only a subset of the models that we obtain. I will show that our procedure can be applied succesffully to models that are invariant under the group of nucleotide permutations that preserve the purine/pyrimidine groupings; the $\mathbb{Z}_2 \wr \mathbb{Z}_2$ case.

Arndt von Haeseler

Institute: Center for Integrative Bioinformatics, Vienna, Austria

One Step Mutation Matrices: Some Applications

Joint work with Mareike Fischer, Tanja Gesell, Steffen Klaere and Thi Minh Anh Nguyen.

We briefly outline the concept of a one step mutation matrix. Subsequently we will show how it can be used to detect possible deviations of a sequence alignment from an evolutionary model and the underlying inferred phylogenetic tree. The key element to detect such deviations is the computation of the minimal number of substitutions on a tree to convert one alignment pattern into another. We further show that this computation can also be employed to disturb an alignment. Thus, we suggest a method to evaluate the robustness of phylogenetic tree inference. Finally, we will discuss some further generalizations of the one step mutation matrix.

Michael Woodhams

Institute: University of Tasmania, Australia

ADD: Additive Dollo Distances and their friends

We investigate distances on binary (presence/absence) data in the context of a Dollo process, where a trait can only arise once on a phylogenetic tree but may be lost many times. We introduce a novel distance, the Additive Dollo Distance (ADD), and derive it by multiple independent lines of reasoning including an intriguing link to the LogDet distance. Simulations of Dollo data are used to compare a number of binary distances including ADD, LogDet, Nei Li and some simple, but to our knowledge previously unstudied, variations on common binary distances. We apply the ADD in two different contexts. The first application is to a recent Diversity Arrays Technology (DArT) data set to study the phylogeny of *Eucalyptus*. The second application is

to gene family presence/absence on bacteria from the COG database. This data has previously been used in a conditioned genome reconstruction (CGR) approach. We demonstrate that the LogDet distance performs poorly in the context of a Dollo process, which may have implications for use in connection with CGR.

Bojian Zhong

Institute: Massey University, New Zealand

Systematic error in seed plant phylogenomics

Joint work with Bojian Zhong, Oliver Deusch, Vadim V. Goremykin, David Penny, Patrick J. Biggs, Robin A. Atherton and Peter James Lockhart.

Resolving the closest relatives of Gnetales has been an enigmatic problem in seed plant phylogeny. The problem is known to be difficult because of the extent of divergence between this diverse group of gymnosperms and their closest phylogenetic relatives. Here we investigate the evolutionary properties of conifer chloroplast DNA sequences. To improve taxon sampling of Cupressophyta (non-Pinaceae conifers) we report sequences from three new chloroplast (cp) genomes of Southern Hemisphere conifers. We have applied a site pattern sorting criterion to study compositional heterogeneity, heterotachy and the fit of conifer chloroplast genome sequences to a GTR + G substitution model. We show that non-time reversible properties of aligned sequence positions in the chloroplast genomes of Gnetales mislead phylogenetic reconstruction of these seed plants. When these sites are excluded, phylogenetic analyses favour a close evolutionary relationship between the Gnetales and Pinaceae – the Gnepine hypothesis. Our analytical framework provides a useful approach for evaluating the robustness of phylogenomic inferences. Our findings highlight the importance of goodness of fit between substitution model and data for understanding seed plant phylogeny.

Joe Zhu

Institute: University of Canterbury, New Zealand

Clades and clans probability in Yule trees

Joint work with Bojian Zhong, Oliver Deusch, Vadim V. Goremykin, David Penny, Patrick J. Biggs, Robin A. Atherton and Peter James Lockhart.

The Yule model and the coalescent model are two neutral stochastic models for generating trees: a rooted Yule tree describes the speciation from the top of the tree; a coalescent tree models lineages coalesce back in time from bottom of the tree. Although, these two models are quite different, they lead to exactly the same distributions of tree topologies, as well as the probabilities of monophyletic groups (clades). In this project, we extended earlier work, derived exact formulas of computing probabilities of clades in rooted trees, and extended these probabilities for clans in unrooted cases.

List of participants

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