Adding complexity...

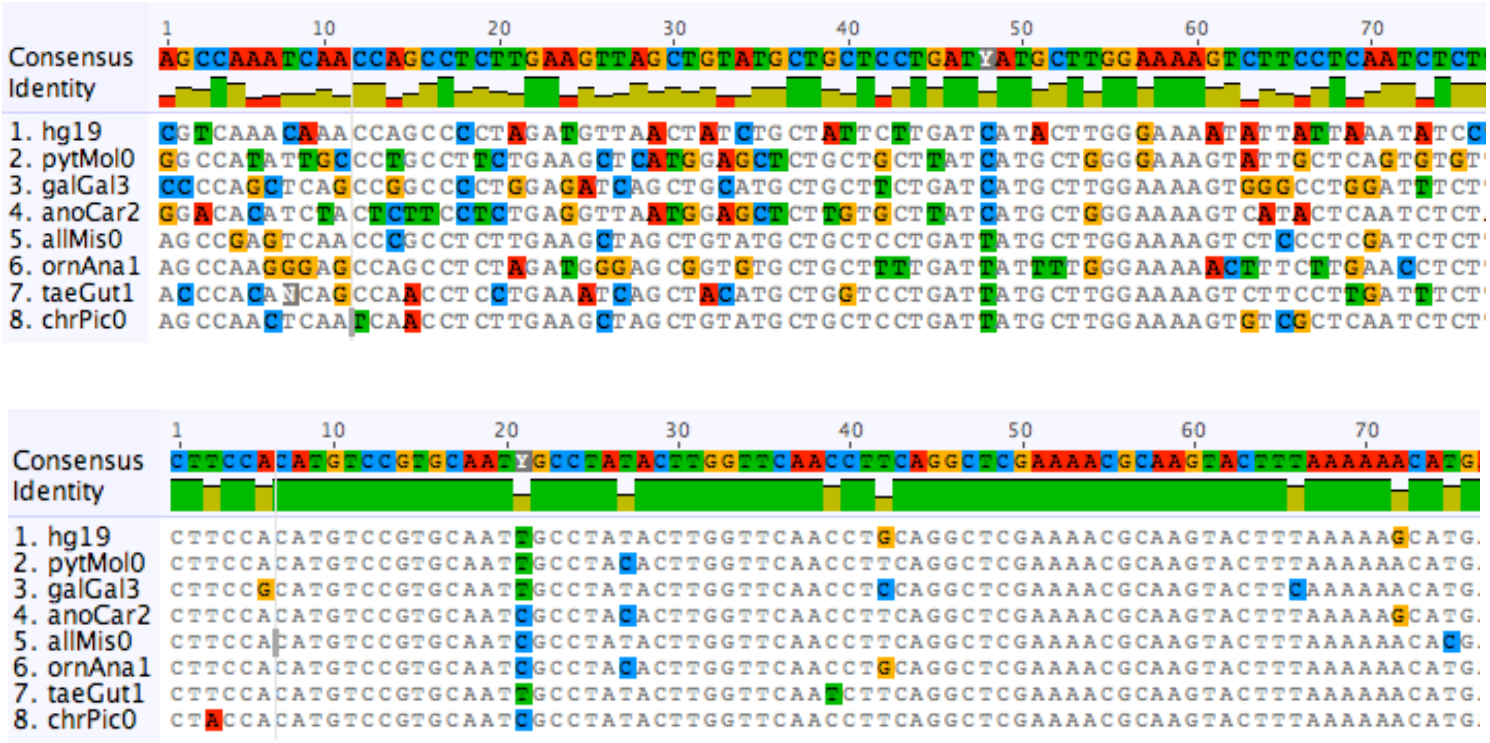
Heterogeneous substitution processes, partitioned models, and mixture models

Bob Thomson

Outline for this session

- Process heterogeneity
- Partitioned-data models
- Challenges & Difficulties
- Tutorial and Activity

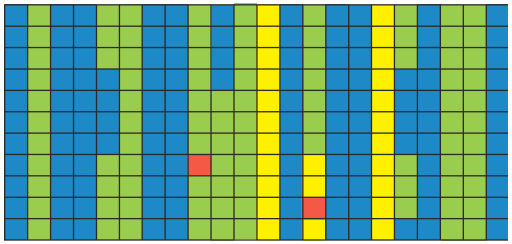
Heterogeneity

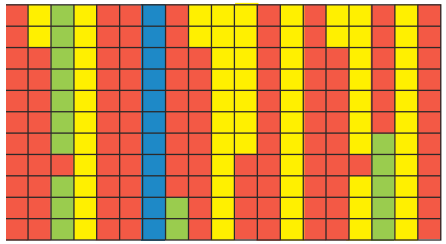


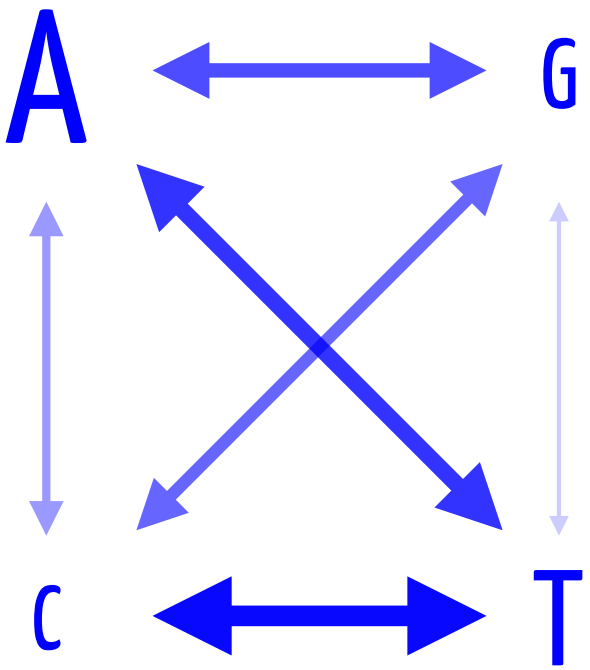
Different Genes, Different Processes

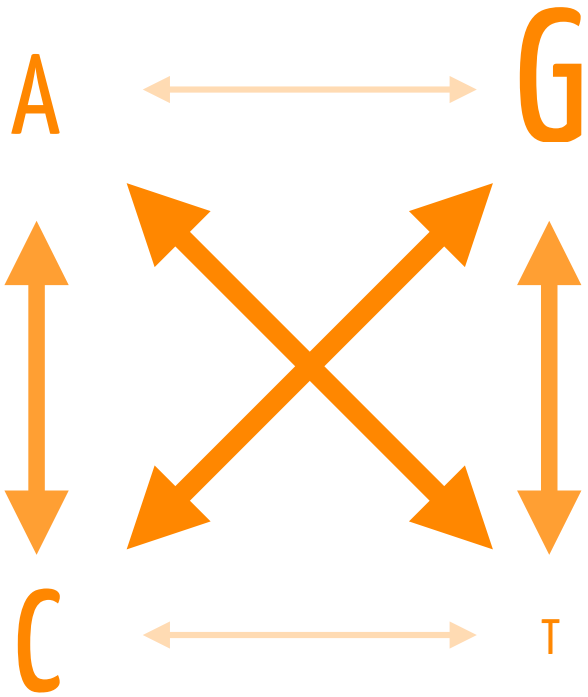
A key distinction...

- Process heterogeneity is distinct from rate heterogeneity





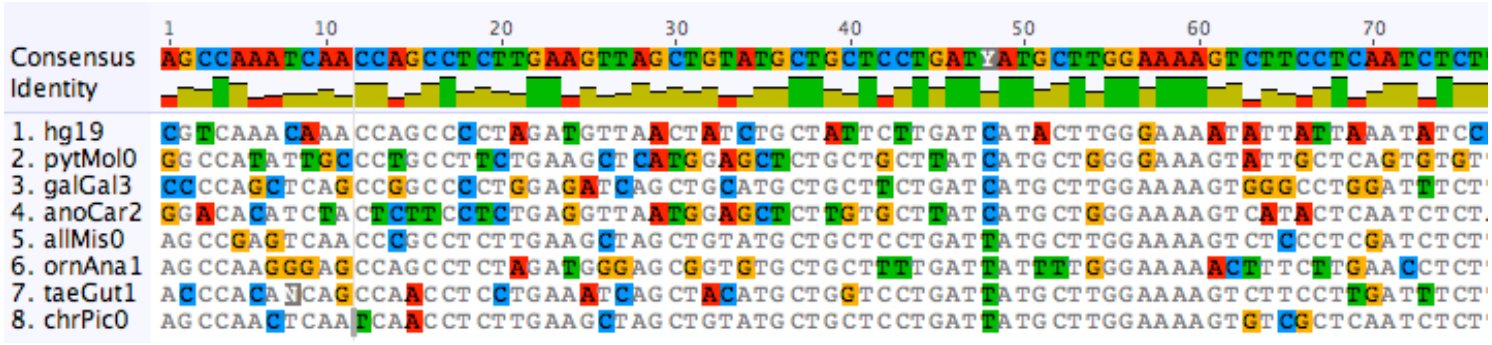


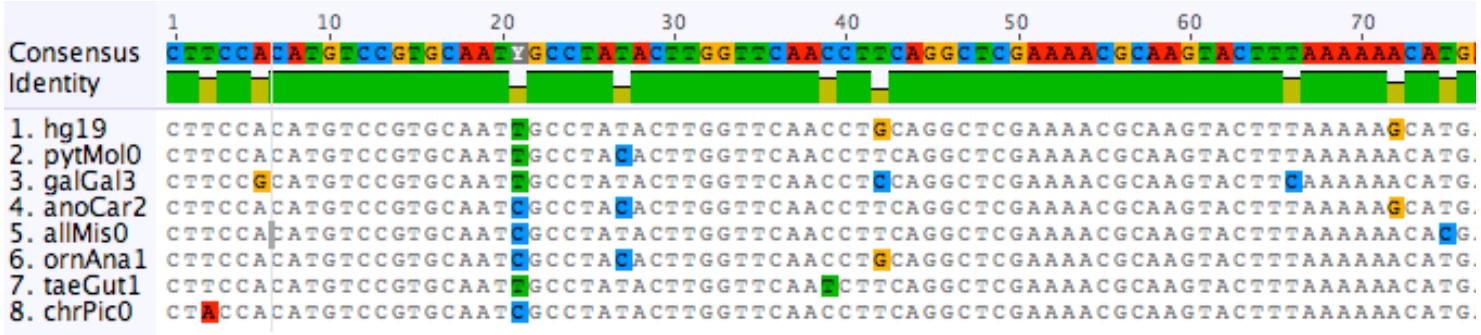


stolen from Jeremy

A key distinction…

- Process heterogeneity is distinct from rate heterogeneity





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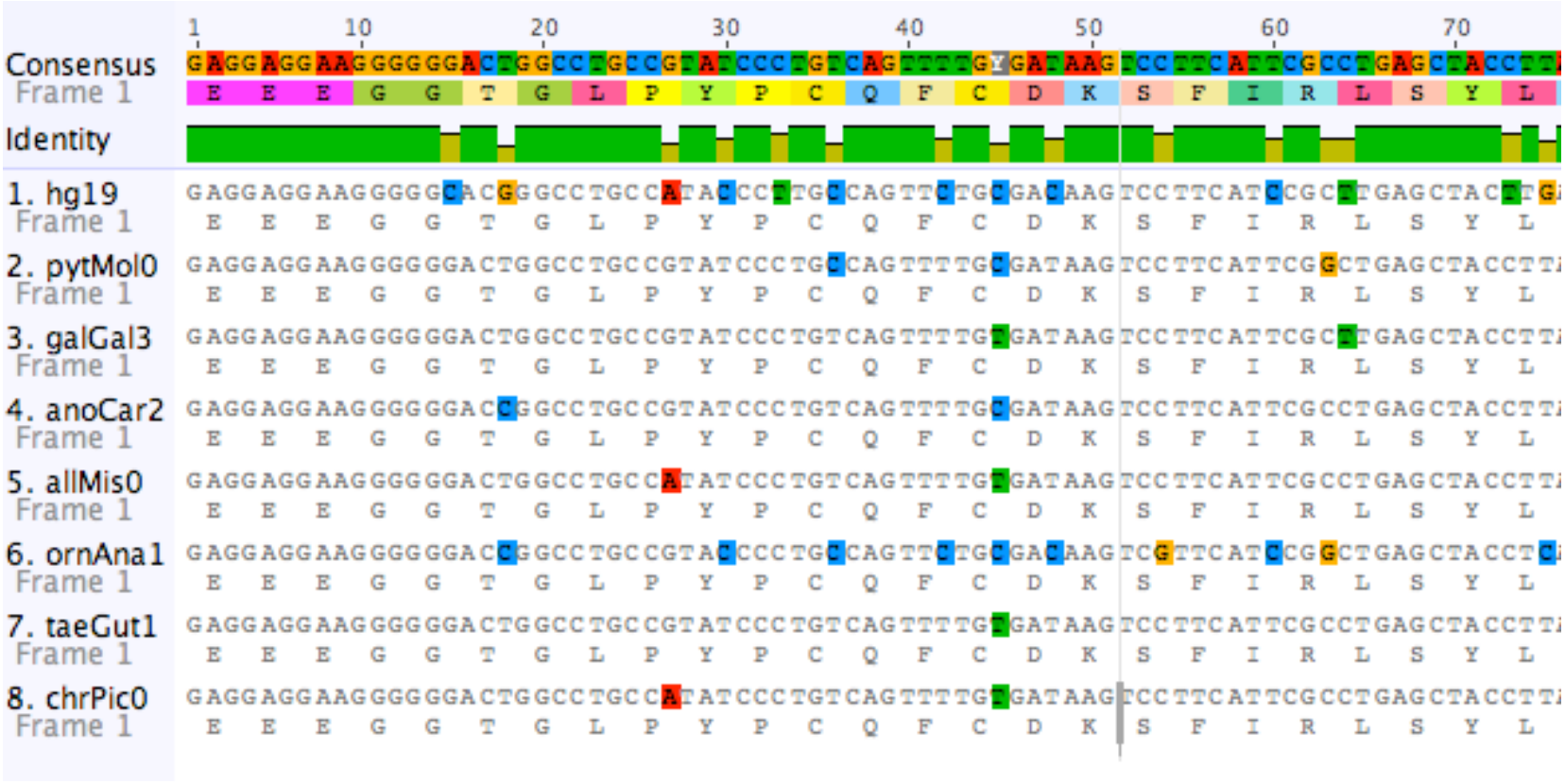
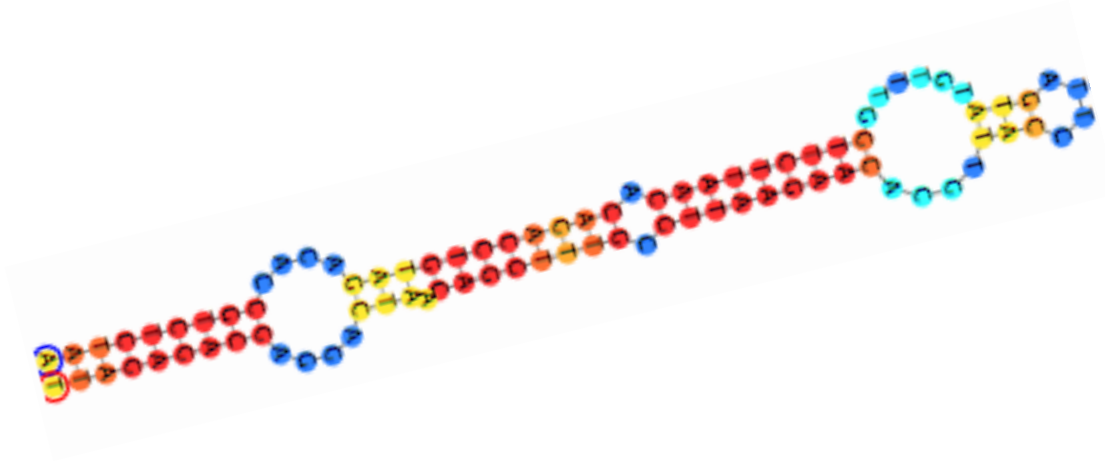
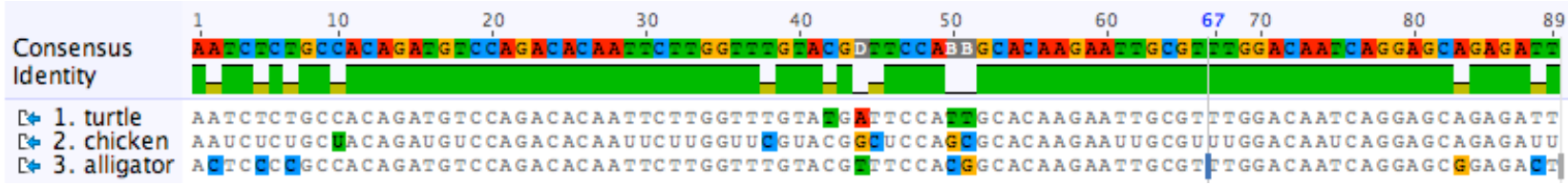
Heterogeneity



Single Gene, Different Processes

Heterogeneity





Single Gene, Different Processes

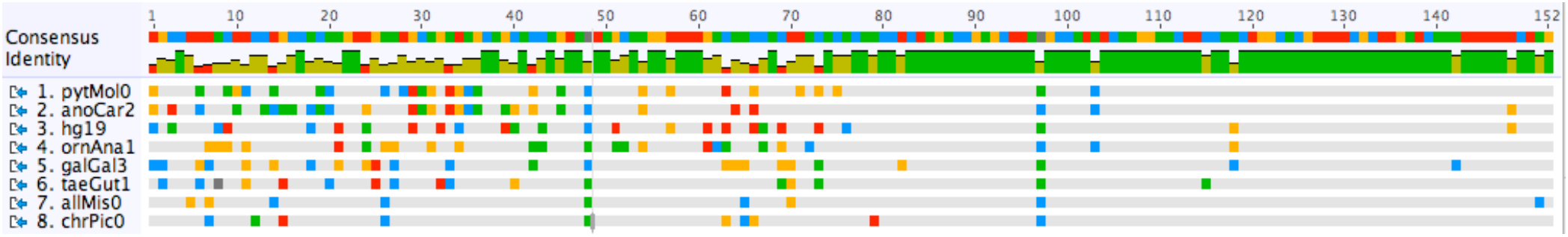
Nucleotide Substitution Models

- Recall (from yesterday) CTMC models for nucleotide substitution make several simplifying assumptions:
  - the rate of the substitution process is constant across sites
  - the nature of the substitution process is constant cross sites
  - sites are independant

For instance, the GTR:

$$Q = q_{ij} = \begin{pmatrix} - & \pi_c r_{ac} & \pi_g r_{ag} & \pi_t r_{at} \\ \pi_a r_{ac} & - & \pi_g r_{cg} & \pi_t r_{ct} \\ \pi_a r_{ag} & \pi_c r_{cg} & - & \pi_t r_{gt} \\ \pi_a r_{at} & \pi_c r_{ct} & \pi_g r_{gt} & - \end{pmatrix} \mu$$

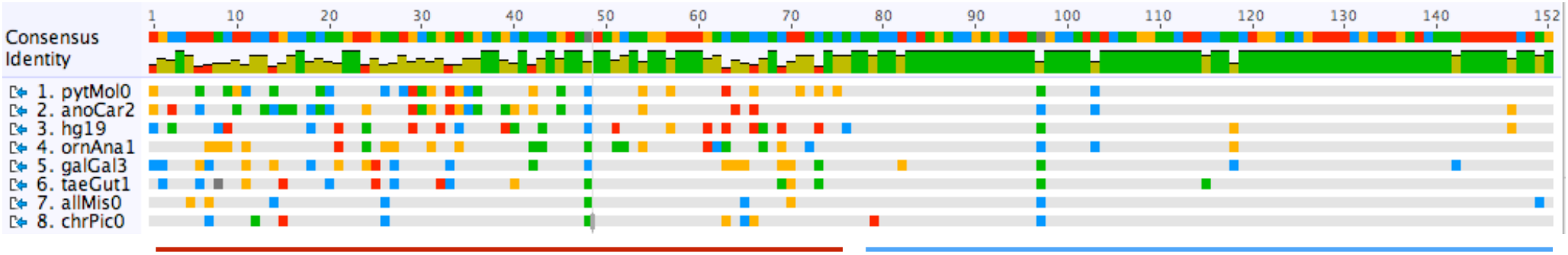
Process Heterogeneity



Class 1

Class 2

Process Heterogeneity



Class 1

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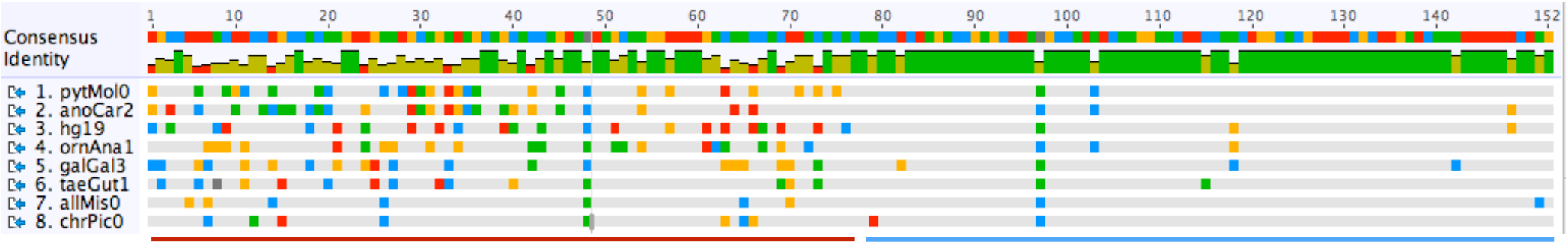
non-partitioned model

Accommodating Heterogeneity



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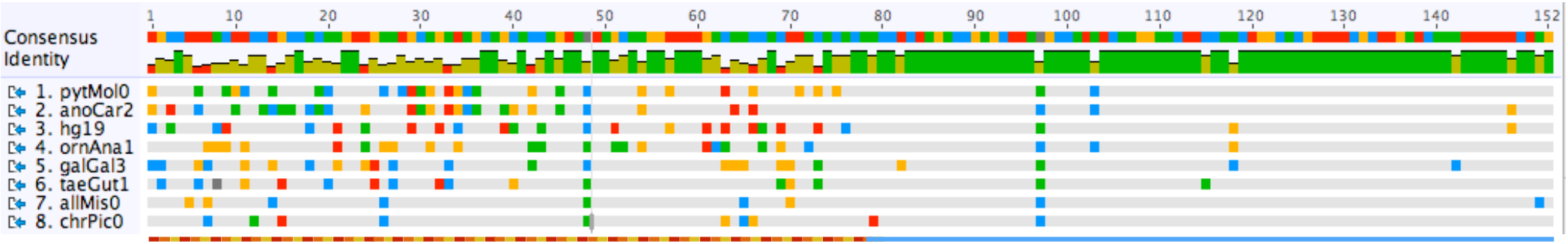
Class 2

$$Q = q_{ij} = \begin{pmatrix} - & \pi_c r_{ac} & \pi_g r_{ag} & \pi_t r_{at} \\ \pi_a r_{ac} & - & \pi_g r_{cg} & \pi_t r_{ct} \\ \pi_a r_{ag} & \pi_c r_{cg} & - & \pi_t r_{gt} \\ \pi_a r_{at} & \pi_c r_{ct} & \pi_g r_{gt} & - \end{pmatrix} \mu$$

Partitioned model

Accommodating Heterogeneity



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$$Q = q_{ij} = \begin{pmatrix} - & \pi_c r_{ac} & \pi_g r_{ag} & \pi_t r_{at} \\ \pi_a r_{ac} & - & \pi_g r_{cg} & \pi_t r_{ct} \\ \pi_a r_{ag} & \pi_c r_{cg} & - & \pi_t r_{gt} \\ \pi_a r_{at} & \pi_c r_{ct} & \pi_g r_{gt} & - \end{pmatrix} \mu$$ Class 2

$$Q = q_{ij} = \begin{pmatrix} - & \pi_c r_{ac} & \pi_g r_{ag} & \pi_t r_{at} \\ \pi_a r_{ac} & - & \pi_g r_{cg} & \pi_t r_{ct} \\ \pi_a r_{ag} & \pi_c r_{cg} & - & \pi_t r_{gt} \\ \pi_a r_{at} & \pi_c r_{ct} & \pi_g r_{gt} & - \end{pmatrix} \mu$$ Class 3

more highly partitioned model

Accommodating Heterogeneity

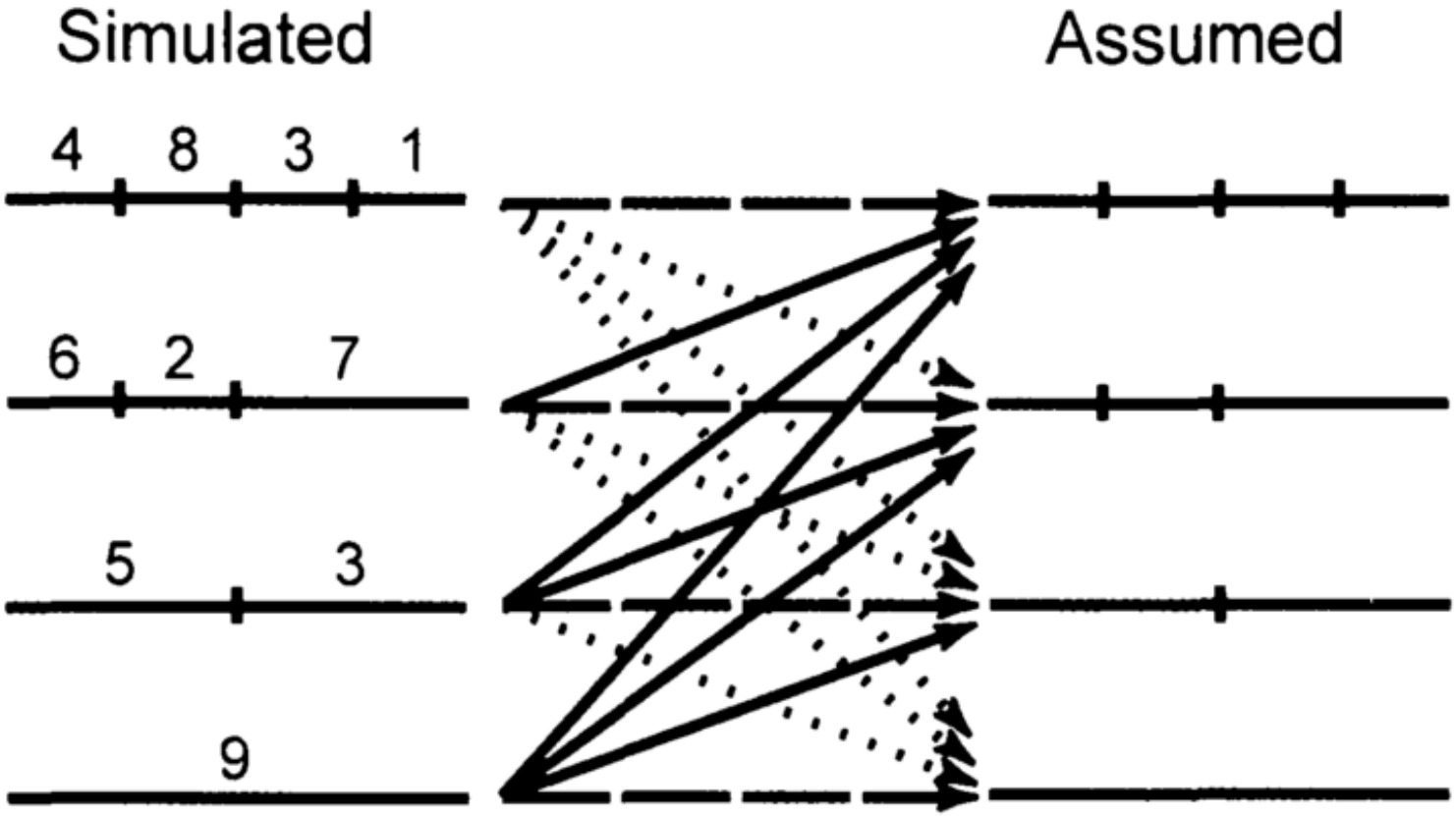
$$L(\tau, \boldsymbol{\nu}, \boldsymbol{\Phi}) = \prod_{i=1}^{n} f(\boldsymbol{x}_i | \tau, \boldsymbol{\nu}, \boldsymbol{\Phi})$$

- Typically (but not necessarily):
  - τ, $\boldsymbol{\nu}$ - shared among data partitions
  - $\boldsymbol{\Phi}$ -independent for each data partition

$$\boldsymbol{r} = (r_{ac}, r_{ag}, r_{at}, r_{cg}, r_{ct}, r_{gt})$$
$$\boldsymbol{\pi} = (\pi_a, \pi_c, \pi_g, \pi_t)$$
$$\alpha$$

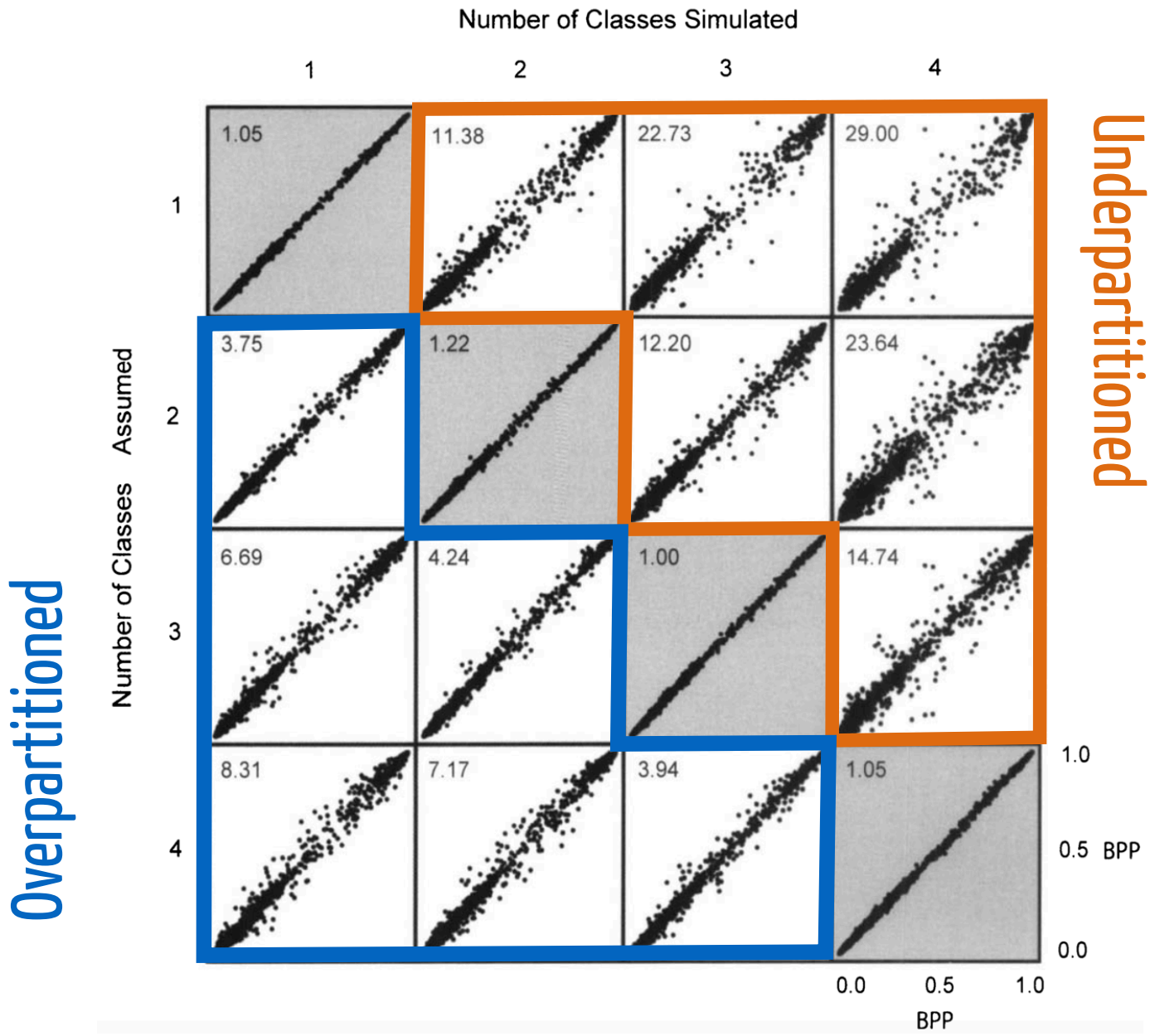
How does this influence inference?

Importance of accommodating process heterogeneity



Brown & Lemmon 2007

Importance of accommodating process heterogeneity



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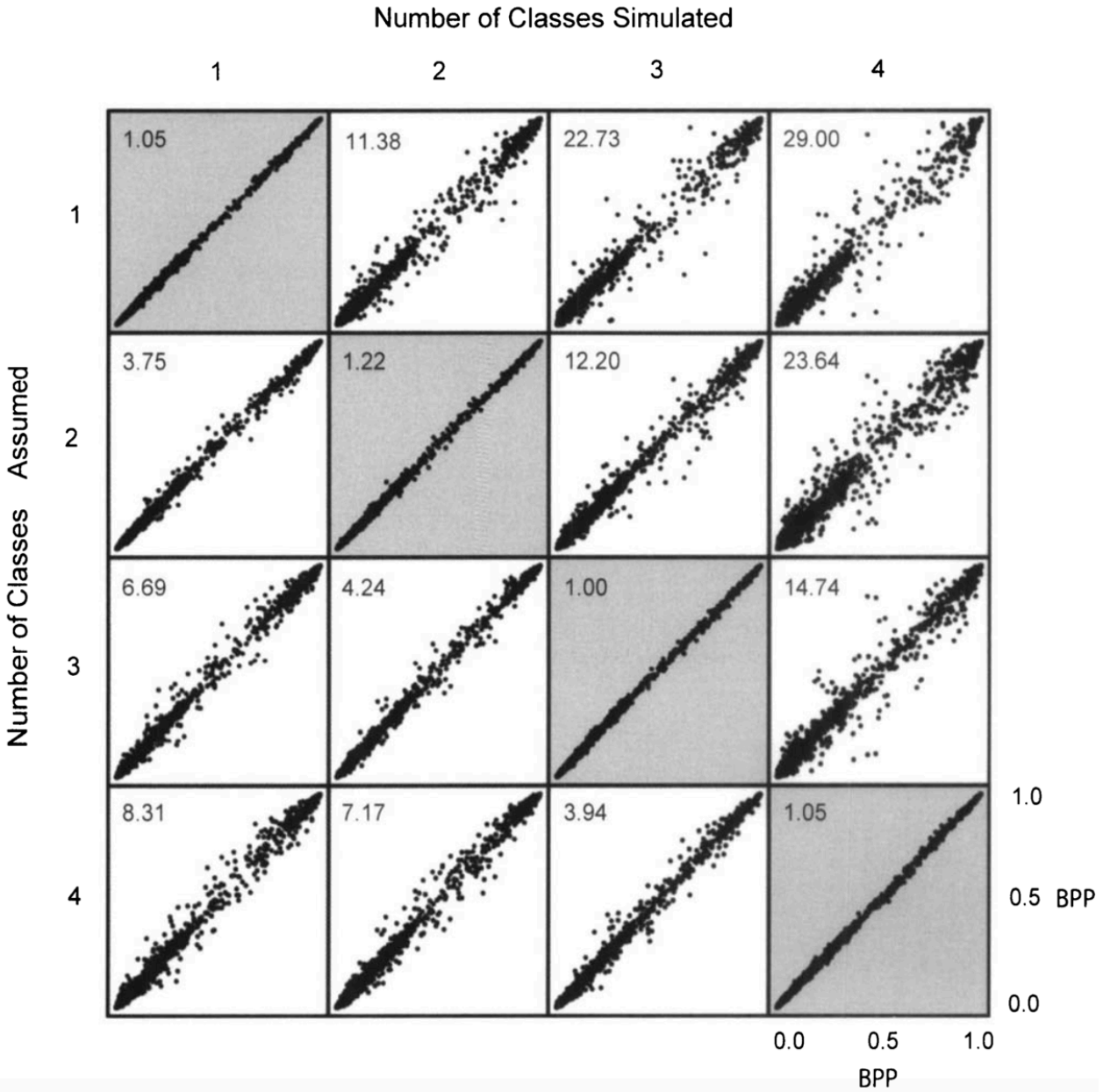
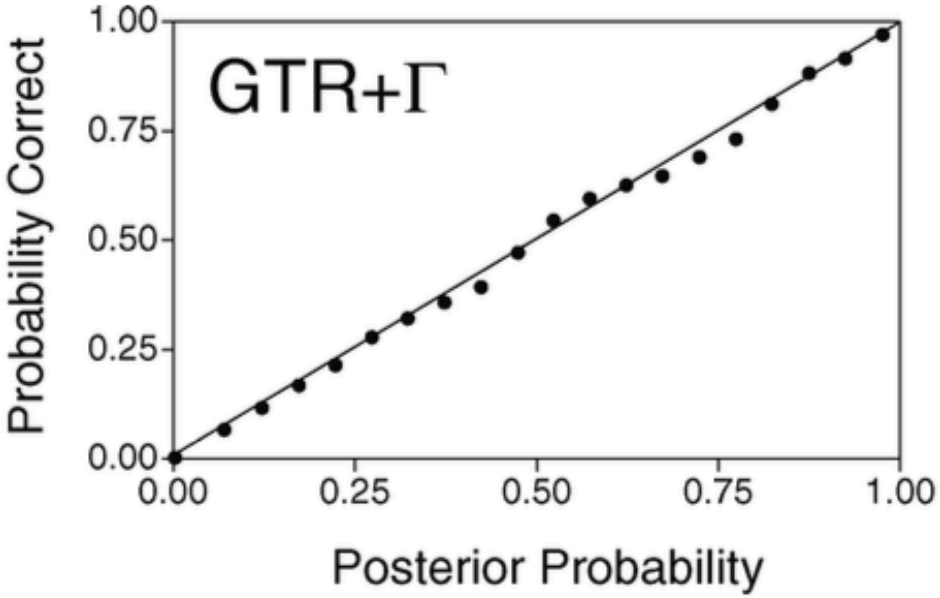
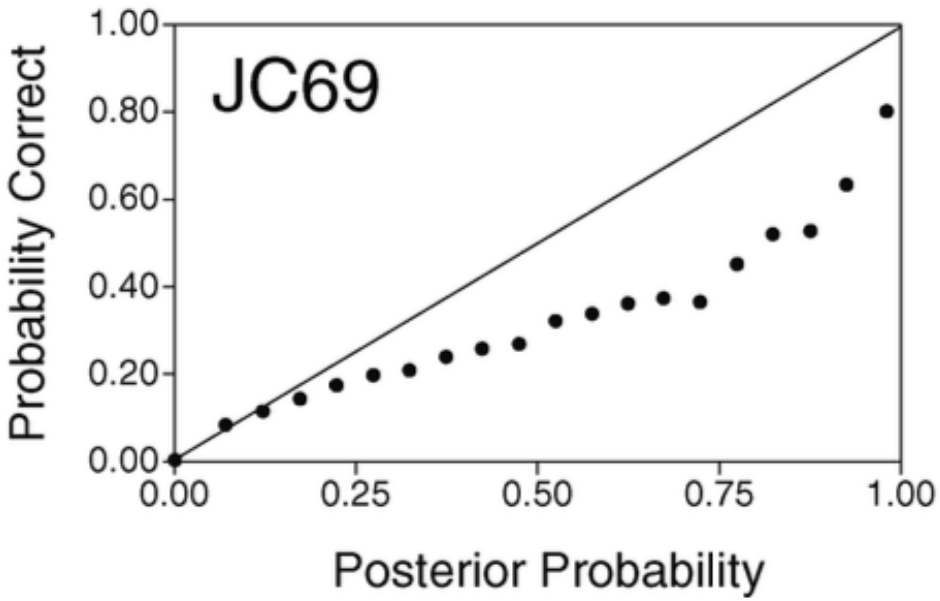


Brown & Lemmon 2007

Underparameterization is often worse than overparameterization

Generating model is GTR+G

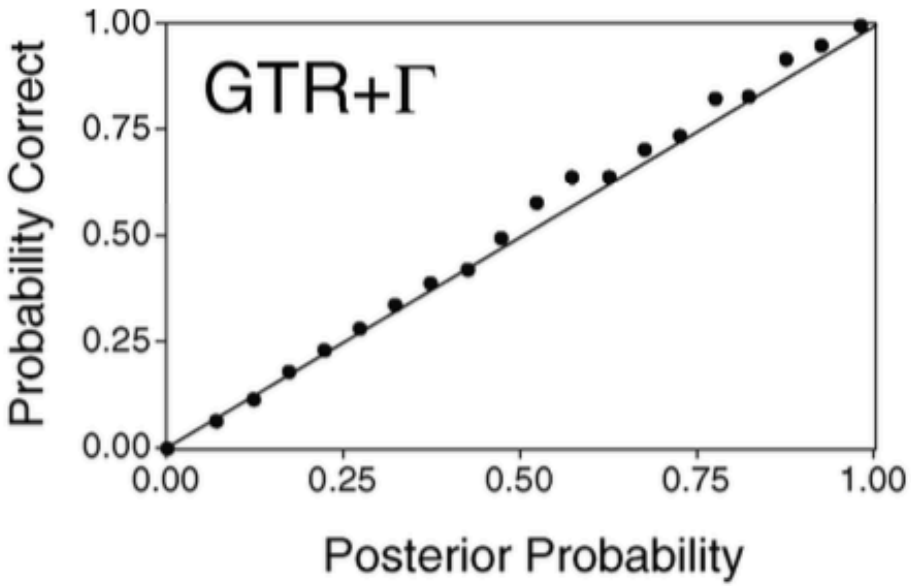


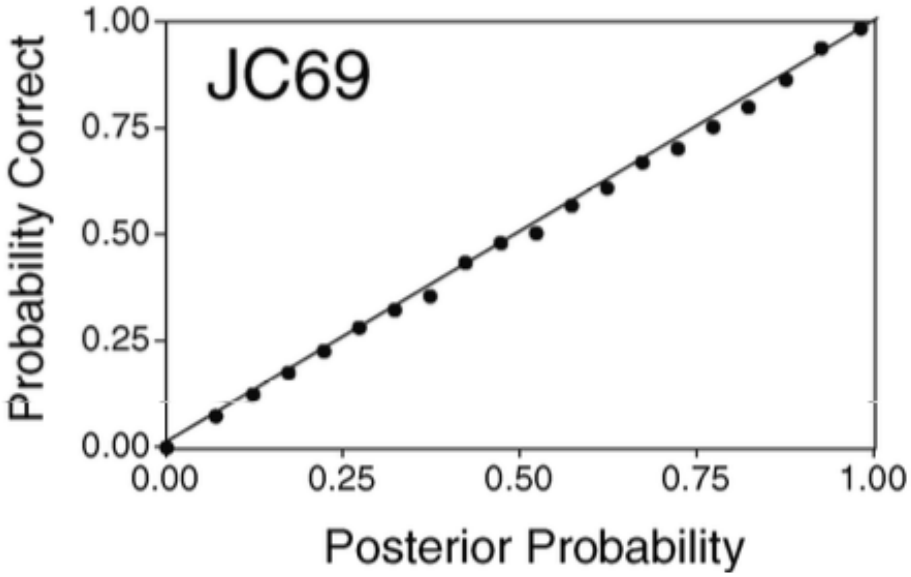


Huelsenbeck & Rannala 2004

Underparameterization is often worse than Overparameterization

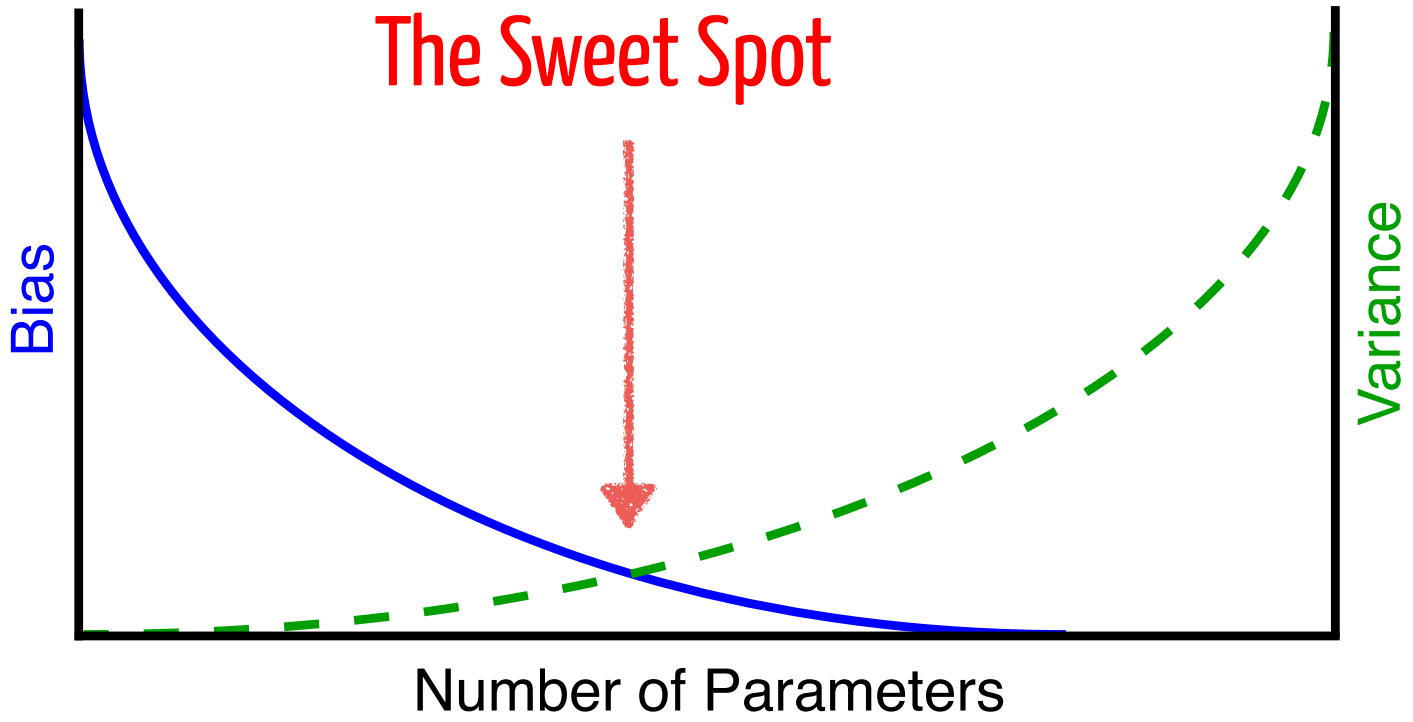
Generating model is JC



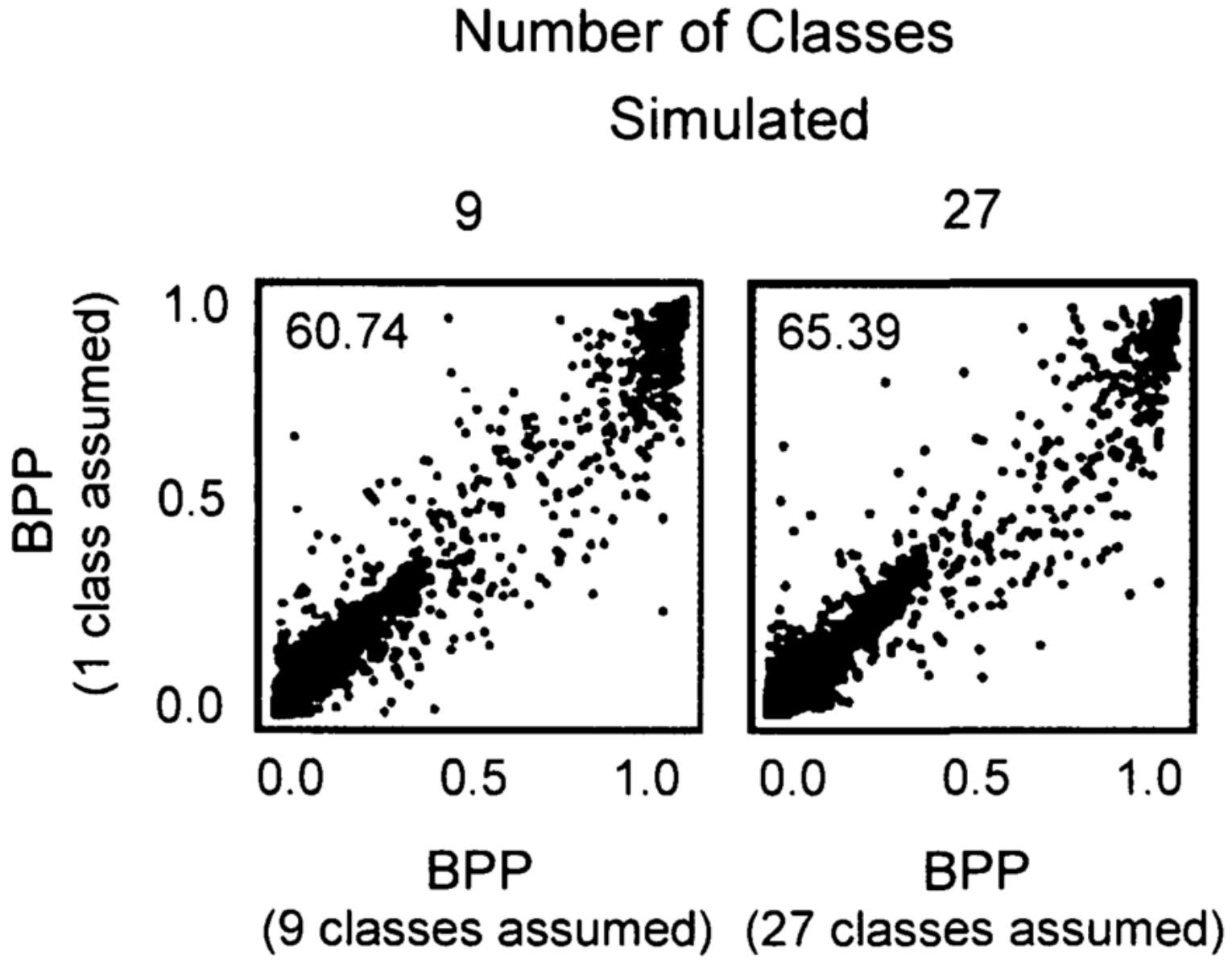


Huelsenbeck & Rannala 2004

From earlier today...



Importance of accommodating process heterogeneity



Brown & Lemmon 2007

Take homes

- abundant empirical evidence that substitution process varies
- models that ignore heterogeneity can give inaccurate estimates of node posteriors
- this effect is worse in large (more heterogenous) datasets

Importance of accommodating process heterogeneity

Data Set	Data Type[a]	Taxa	Sites	Data Blocks	Clade (Latin)	Clade (English)	Study Ref.	Data Set Ref.
Anderson_2013	M	145	3,037	4	Loliginidae	Pencil squids	Anderson et al. (2014)	Anderson et al. (2013)
Bergsten_2013	M,N	38	2,111	8	Dytiscidae	Diving beetles	Bergsten et al. (2013a)	Bergsten et al. (2013b)
Broughton_2013	M,N	61	19,997	61	Osteichthyes	Bony fishes	Broughton et al. (2013b)	Broughton et al. (2013a)
Brown_2012	N	41	1,665	7	Ptychozoon	Asian geckos	Brown et al. (2012b)	Brown et al. (2012a)
Caterino_2001	M,N	37	3,228	9	Papilionidae	Butterflies	Caterino et al. (2001)	Kuo et al. (2001)
Cognato_2001	M,N	44	1,896	7	Scolytinae	Bark beetles	Cognato and Vogler (2001b)	Cognato and Vogler (2001a)
Day_2013	M,N	152	3,586	11	Synodontis	African catfish	Day, Peart, Brown, Friel, et al. (2013)	Day, Peart, Brown, Bills, et al. (2013)
Devitt_2013	M	69	823	4	Ensatina	Salamander	Devitt et al. (2013b)	Devitt et al. (2013a)
Dornburg_2012	M,N	44	5,919	21	Holocentridae	Squirrel fishes	Dornburg et al. (2012b)	Dornburg et al. (2012a)
Dsouli_2011	M,N	39	1,635	7	Muscidae	Flies	Dsouli et al. (2011)	NA
Ekrem_2010	M,N	74	2,701	10	Chironomidae	Midges	Ekrem et al. (2010)	NA
Elias_2009	M,N	143	4,159	12	Nymphalidae	Butterflies	Elias, Joron, Willmott, Silva-Brandão, et al. (2009)	Elias, Joron, Willmott, Kaiser, et al. (2009)
Fishbein_2001	N,C	40	9,005	11	Saxifragales	Core Eudicots	Fishbein et al. (2001b)	Fishbein et al. (2001a)
Fong_2012	N	110	25,919	168	Vertebrata	Vertebrates	Fong et al. (2012b)	Fong et al. (2012a)
Grande_2013	M,N	65	4,027	12	Paracanthopterygii	Fish	Grande et al. (2013a)	Grande et al. (2013b)
Guschanski_2013	M,C	110	17,092	63	Cercopithecini	Monkeys	Guschanski et al. (2013b)	Guschanski et al. (2013a)
Kaffenberger_2011	M,N	54	6,548	26	Gephyromantis	Malagasy frogs	Kaffenberger et al. (2012)	Kaffenberger et al. (2011)
Kang_2013a	N	28	7,276	15	Xiphophorus	Swordtail fish	Kang et al. (2013)	NA
Kang_2013b	M	28	1,239	6	Xiphophorus	Swordtail fish	Kang et al. (2013)	NA
Kawahara_2013	M,N	70	2,238	9	Hyposmocoma	Caterpillar	Kawahara and Rubinoff (2013a)	Kawahara and Rubinoff (2013b)
Lartillot_2012	N	78	15,117	51	Eutheria	Mammals	Lartillot and Delsuc (2012b)	Lartillot and Delsuc (2012a)
Leavitt_2013	M	34	15,404	87	Acridoidea	Grasshoppers	Leavitt et al. (2013)	NA
Li_2008	N	56	7,995	30	Actinopterygii	Fishes	Li et al. (2008)	NA
Murray_2013	M,N	237	3,111	9	Eucharitidae	Wasps	Murray et al. (2013a)	Murray et al. (2013b)
Rightmyer_2013	M,N	94	3,692	25	Hymenoptera	Bee	Rightmyer et al. (2013b)	Rightmyer et al. (2013a)
Sauquet_2011	N,C	51	5,444	10	Nothofagus	Beeches	Sauquet et al. (2012)	Sauquet et al. (2011)
Seago_2011	M	116	2,253	7	Coccinellidae	Ladybirds	Seago et al. (2011b)	Seago et al. (2011a)
Sharanowski_2011	N	139	3,982	11	Braconidae	Wasps	Sharanowski et al. (2011b)	Sharanowski et al. (2011a)
Siler_2013	M,N	61	2,697	7	Lycodon	Wolf snakes	Siler, Oliveros, et al. (2013)	Siler, Brown, et al. (2013)
Tolley_2013	M	203	5,054	16	Chamaeleonidae	Chameleons	Tolley et al. (2013b)	Tolley et al. (2013a)
Unmack_2013	M	139	6,827	25	Melanotaeniidae	Rainbowfish	Unmack et al. (2013b)	Unmack et al. (2013a)
Wainwright_2012	N	188	8,439	30	Acanthomorpha	Fishes	Wainwright, Smith, Price, Tang, Sparks, Ferry, Kuhn, Eytan, et al. (2012)	Wainwright et al. (2012)
Ward_2010	N	54	9,173	27	Dolichoderinae	Ants	Ward et al. (2010)	NA
Welton_2013	M,N	145	4,552	16	Varanus	Lizards	Welton et al. (2013b)	Welton et al. (2013a)

34 real datasets

Kainer and Lanfear 2015

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34 real datasets

4 partitioning schemes

1. unpartitioned
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Kainer and Lanfear 2015

Importance of accommodating process heterogeneity

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Brown_2012	N	41	1,665	7	Ptychozoon	Asian geckos	Brown et al. (2012b)	Brown et al. (2012a)
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Ekrem_2010	M,N	74	2,701	10	Chironomidae	Midges	Ekrem et al. (2010)	NA
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Kawahara_2013	M,N	70	2,238	9	Hyposmocoma	Caterpillar	Kawahara and Rubinoff (2013a)	Kawahara and Rubinoff (2013b)
Lartillot_2012	N	78	15,117	51	Eutheria	Mammals	Lartillot and Delsuc (2012b)	Lartillot and Delsuc (2012a)
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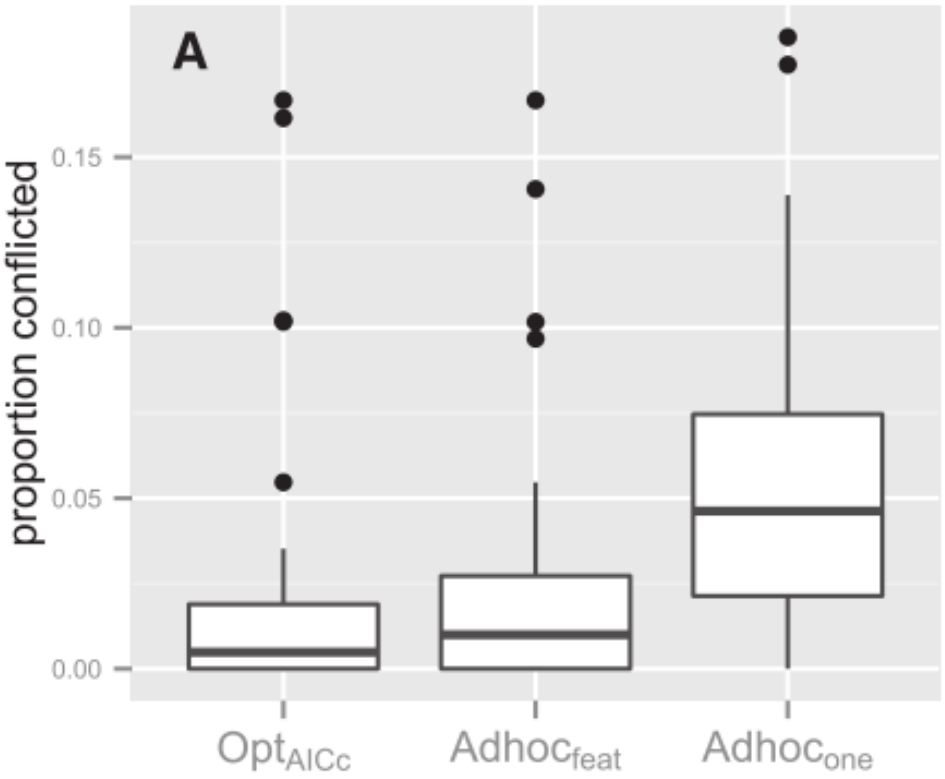
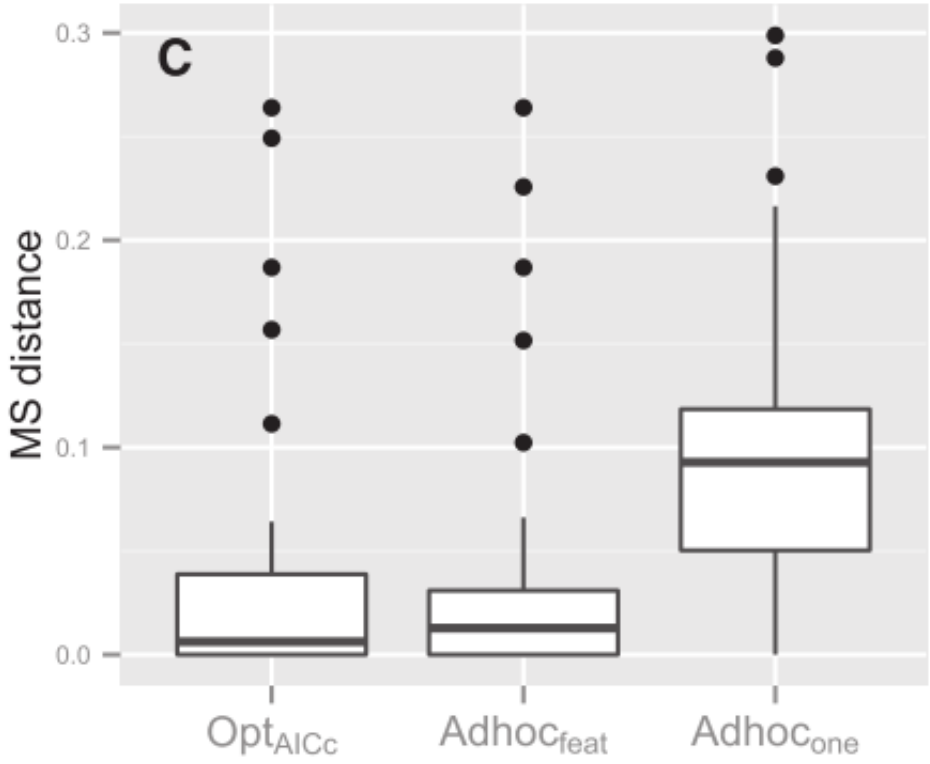
Analyze

Ask what changes

Kainer and Lanfear 2015

Importance of accommodating process heterogeneity





Topology changes

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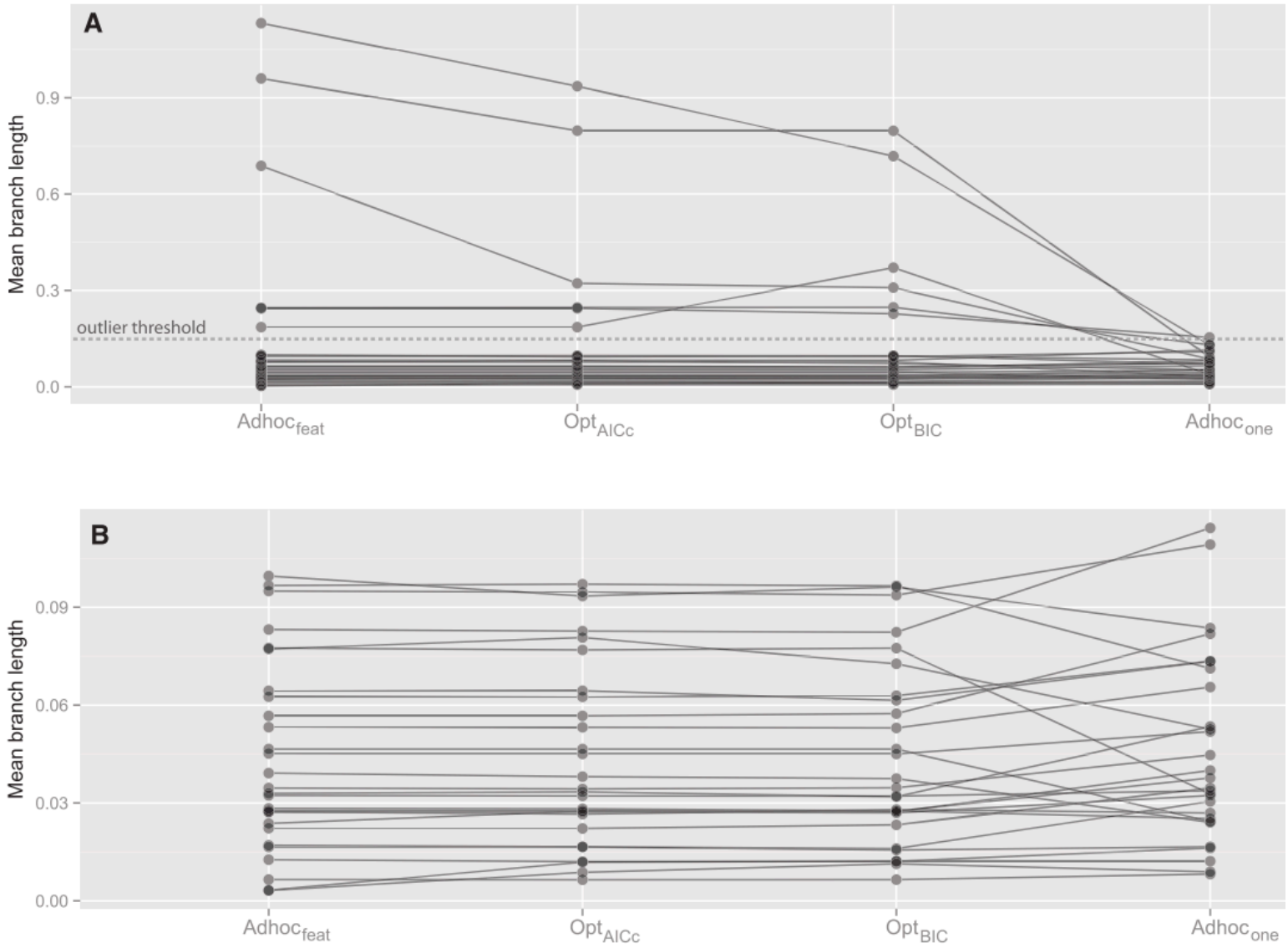
Importance of accommodating process heterogeneity



Branch lengths also change

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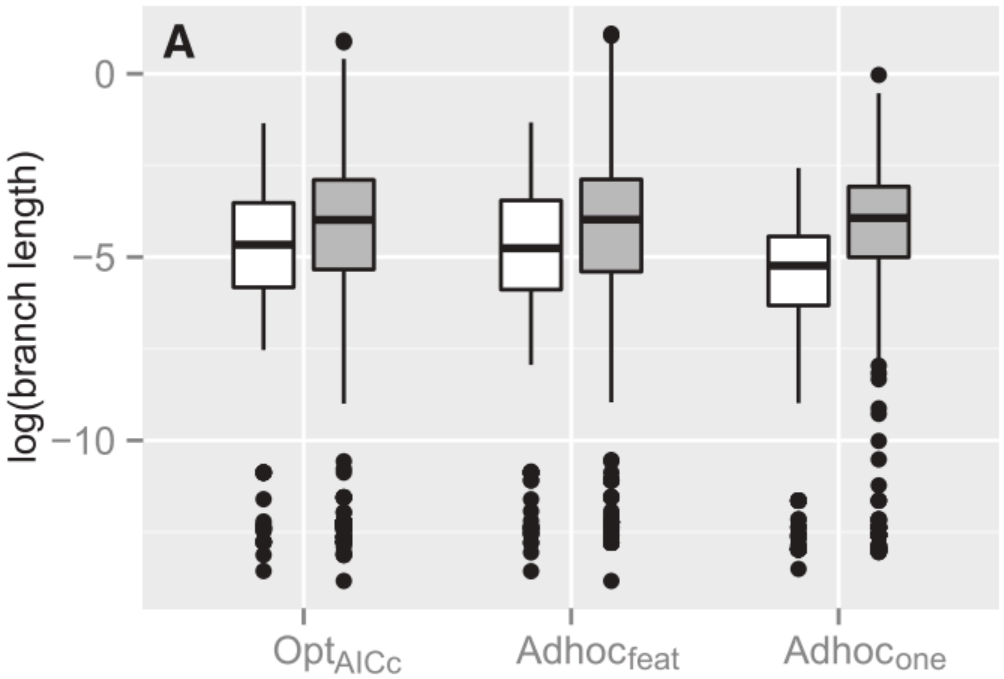
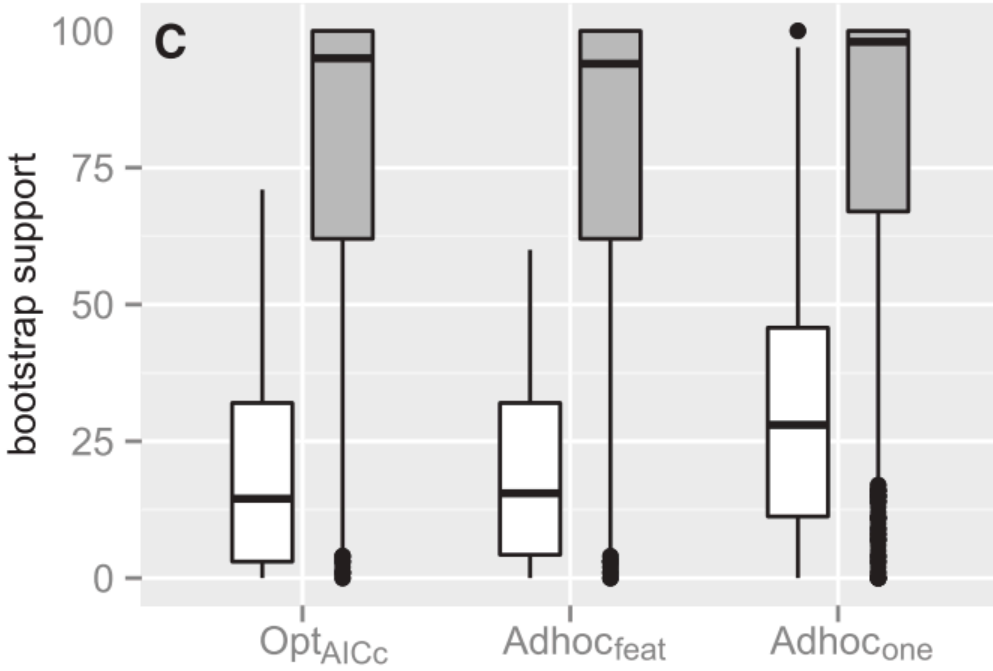
Importance of accommodating process heterogeneity





Nodes subtended by short branch lengths and low support disproportionately effected

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Take homes

- abundant empirical evidence that substitution process varies
- models that ignore heterogeneity can give inaccurate estimates of node posteriors
- this effect is worse in large (more heterogenous) datasets

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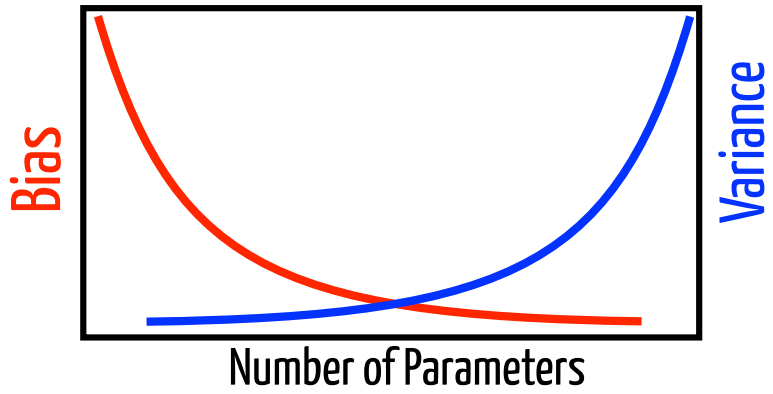
- models that ignore heterogeneity can give inaccurate estimates of node posteriors, and branch lengths, and topologies
- **this effect is worse in large (more heterogenous) datasets**
- **this effect is worse for difficult to resolve nodes**

Precise conditions of 'Big Data' studies

How do we select a partitioning model?

- This is a similar problem to what we covered this morning
  - Seek to capture the relevant variation in the data, balancing the bias-variance tradeoff

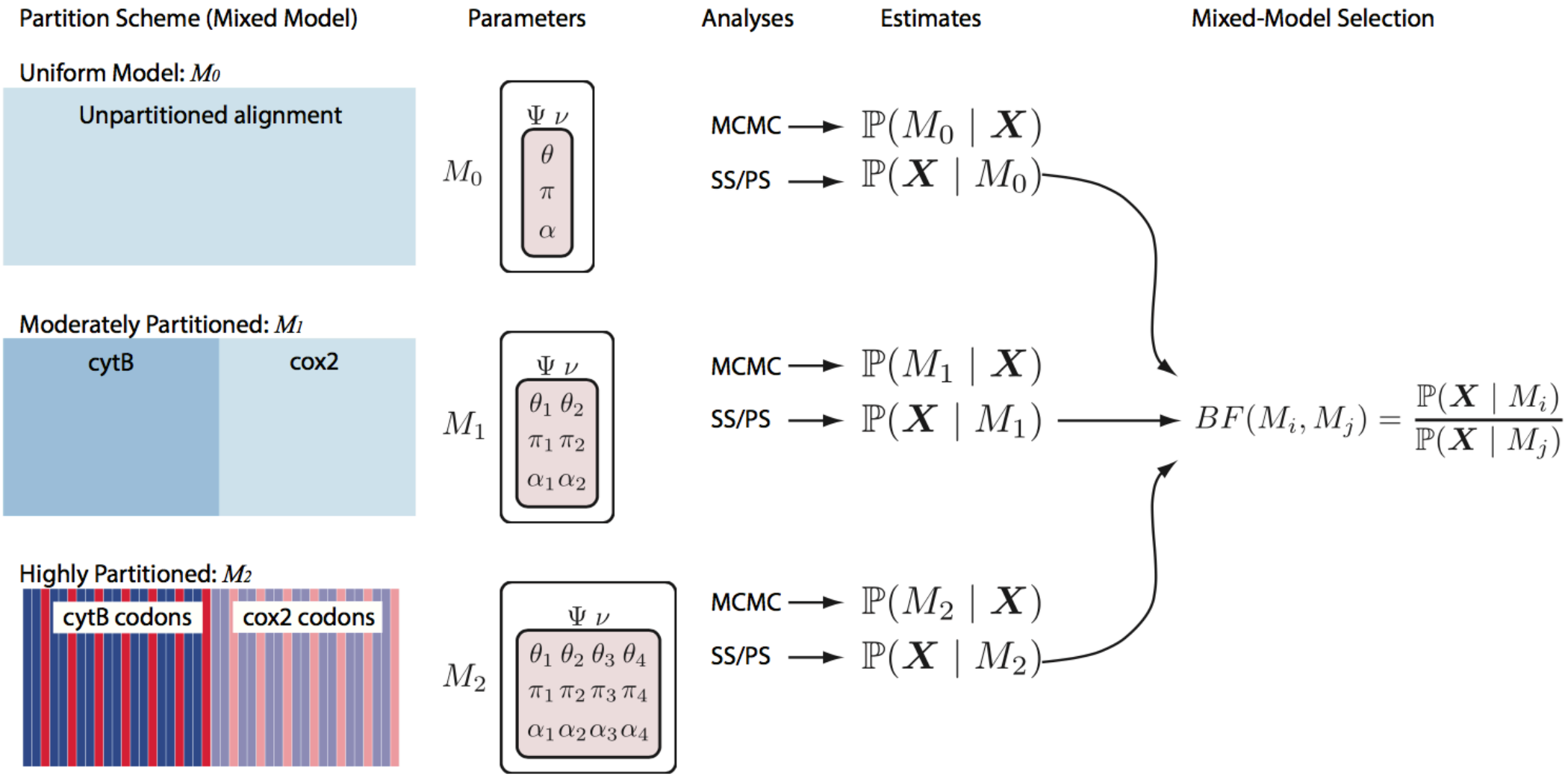


Extreme Underpartitioning

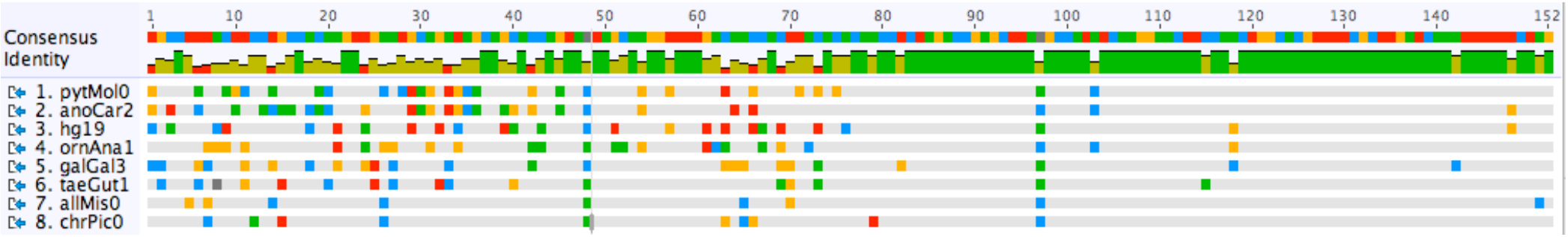
Extreme Overpartitioning

- We can use similar tools as before

How do we select a partitioning model?



Scaling up



- Many possible partition models even for 'small data'.
- **Simple** partitioning by biological features: 2 genes x 3 codon positions:

# of Classes	# of possible models
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total	**203**

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Two issues:

1. This counts only possibilities where the partition model is the same for all parameters

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Phylogenetic Model Parameters

Topology τ

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ASRV Gamma Shape α

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Should we consider other partial partition models?

If so, **many** more models are possible.

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Like many problems in phylogenetics, this doesn’t scale easily

Scaling up: potential solutions

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General approach: Calculate likelihood of data under a particular model, penalize for model complexity via the prior (marginal likelihood) or some penalty term (AIC or BIC). Compare.

Model Selection and Model Averaging

- **Model Selection:** Choose the model that best fits the data.
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Model Selection and Model Averaging

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  - The data are random variables, the parameters are (or are not) random variables, but **the model is fixed.**
- **Model Averaging:** Consider alternative models in proportion to their probability
  - The **model itself is a random variable** with associated uncertainty, so we account for this.

Scaling up: potential solutions

- **Model Averaging:** Treat the partition-model itself as a random variable and use MCMC to marginalize over possible partition models (and other parameters of the joint phylogenetic model)
  - Moore et al. 2014 - AutoParts
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General approach: Model the number of partitions and the assignment of sites or classes to those partitions using the Dirichlet Process

Dirichlet Process

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Dirichlet Process

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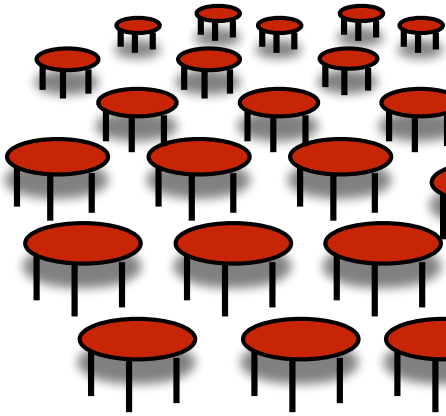
- More simply: A prior probability distribution for clustering problems
  - How many clusters are there?
  - Which observations belong to which clusters?

‘The Chinese Restaurant Process’

- Imagine a restaurant with an infinite number of tables. Customers walk in one at a time and choose a table to sit down at:



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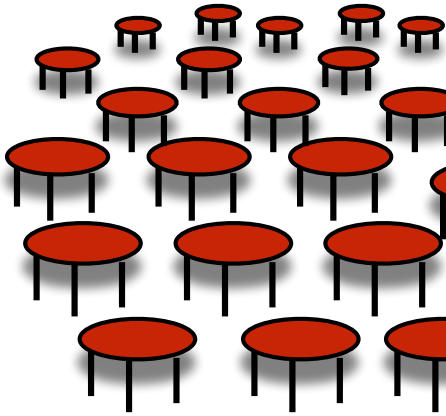

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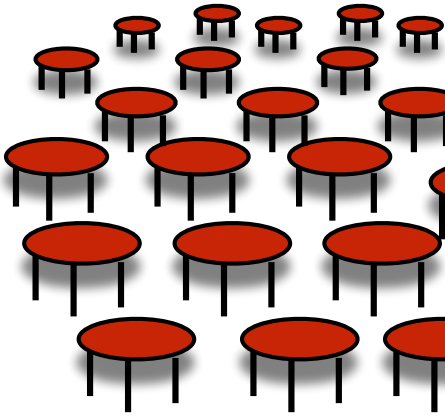

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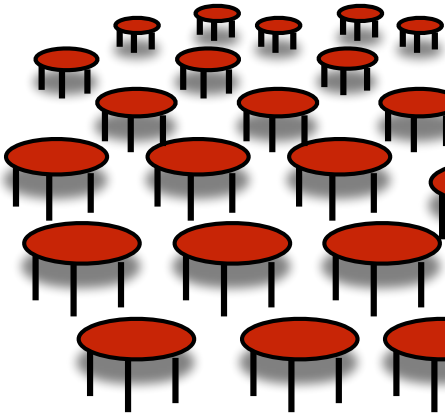
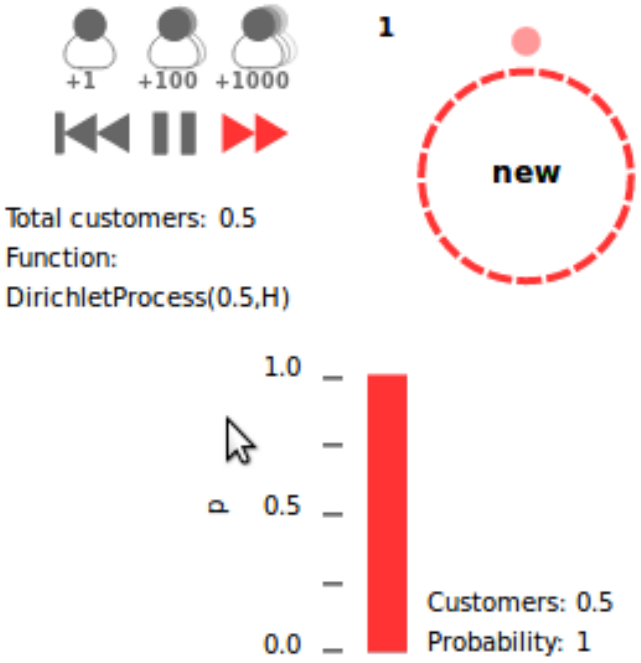


Large alpha - many tables in use

Popular tables stay popular

‘The Chinese Restaurant Process’



Sorts customers into tables

http://topicmodels.west.uni-koblenz.de/ckling/tmt/crp.html

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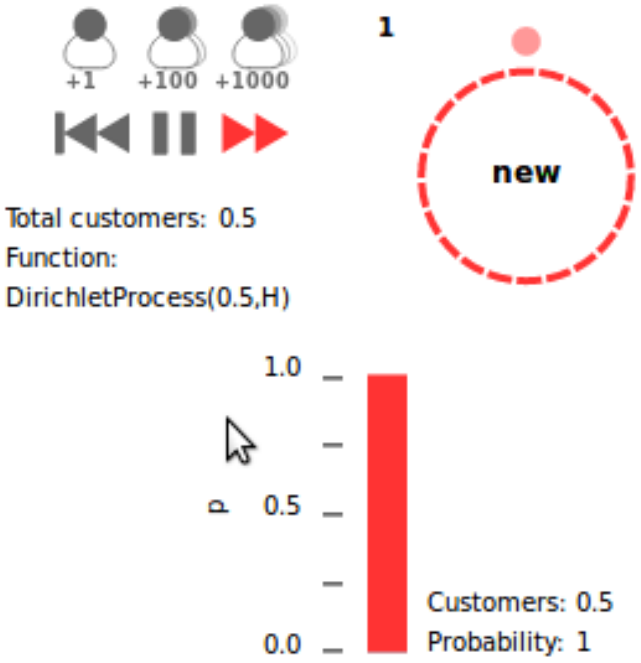

Sorts customers into tables
Sorts observations into clusters

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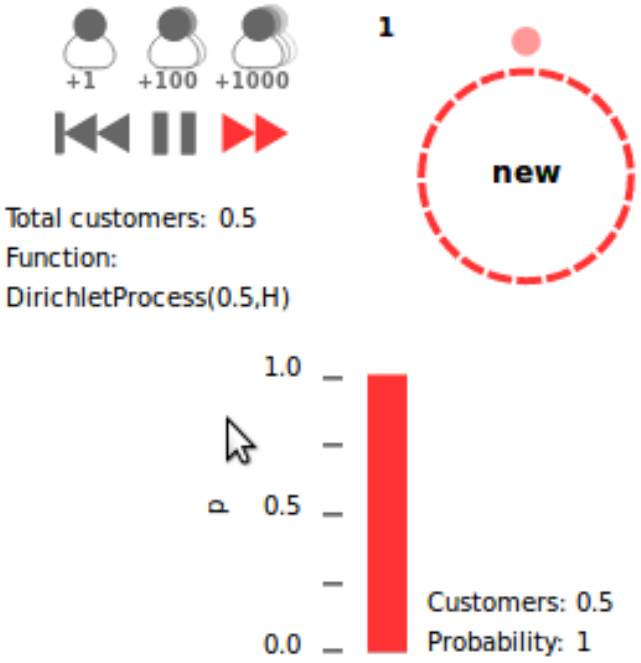


Sorts customers into tables
Sorts observations into clusters
Sorts alignment classes into partitions

http://topicmodels.west.uni-koblenz.de/ckling/tmt/crp.html

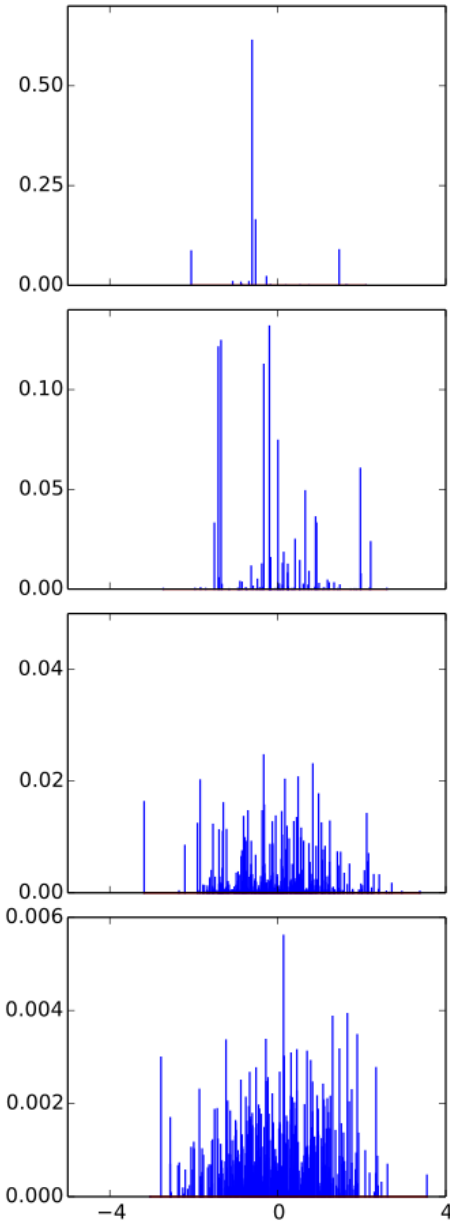
Dirichlet Process Prior

$\alpha = 1$

$\alpha = 10$

$\alpha = 100$

$\alpha = 1000$



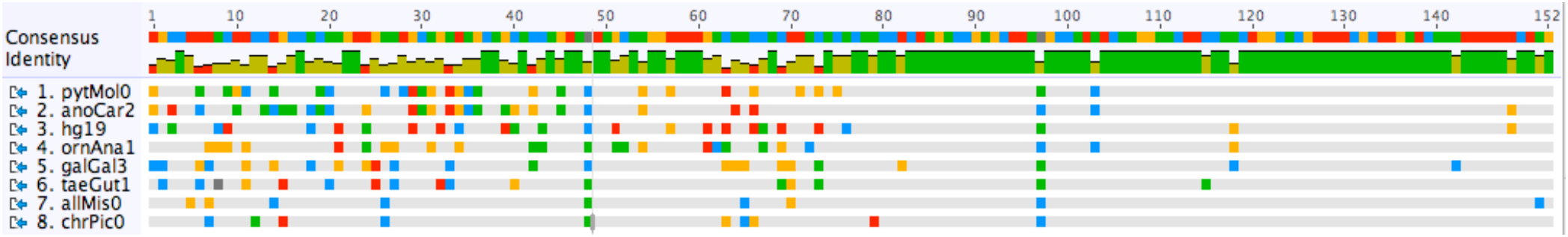
High Prior Probability for **few partitions**

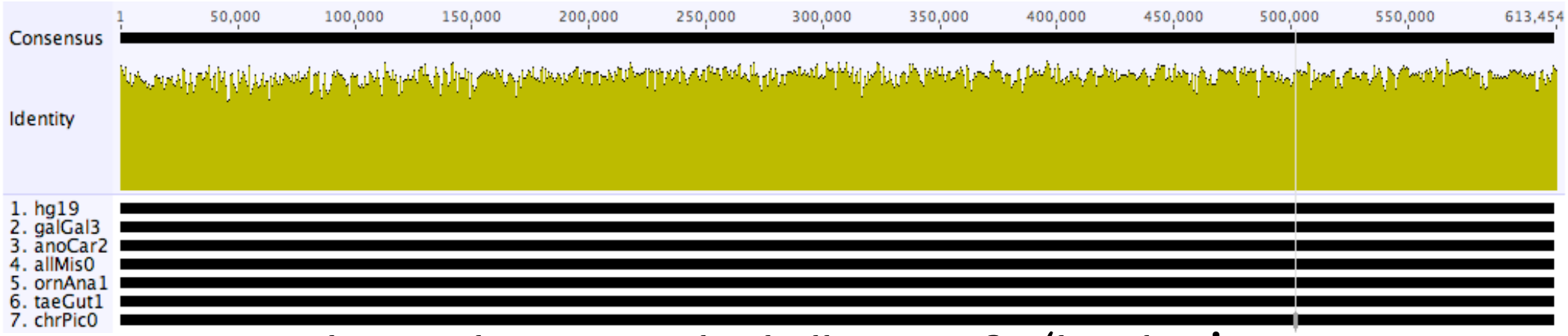
High Prior Probability for **many partitions**

new cluster: $\frac{\alpha}{n-1+\alpha}$

'occupied' cluster: $\frac{c}{n-1+\alpha}$

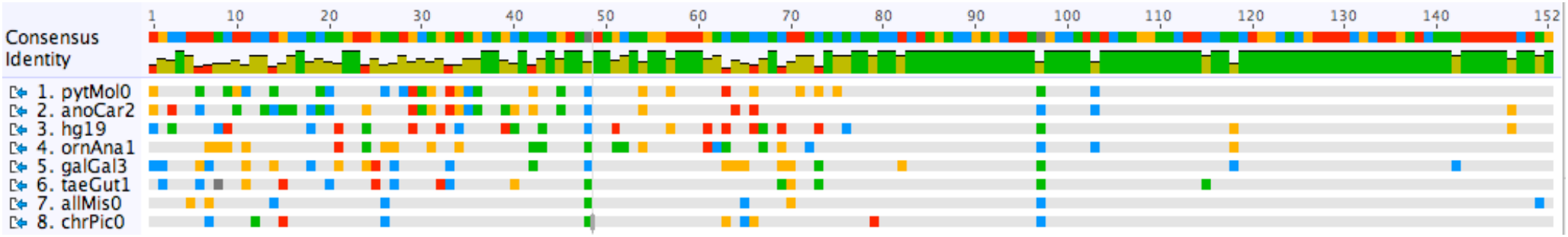
Scaling up

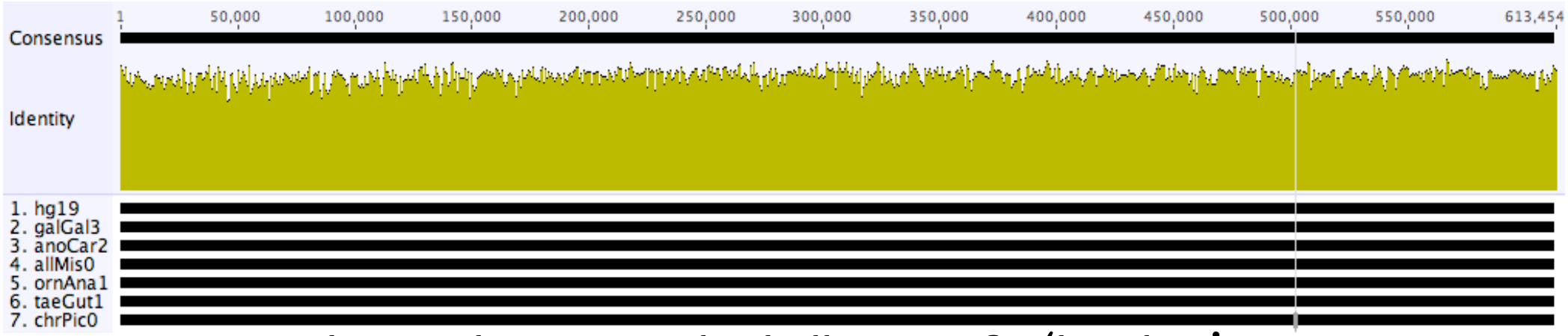




This can be extremely challenging for ‘big data’.

Scaling up



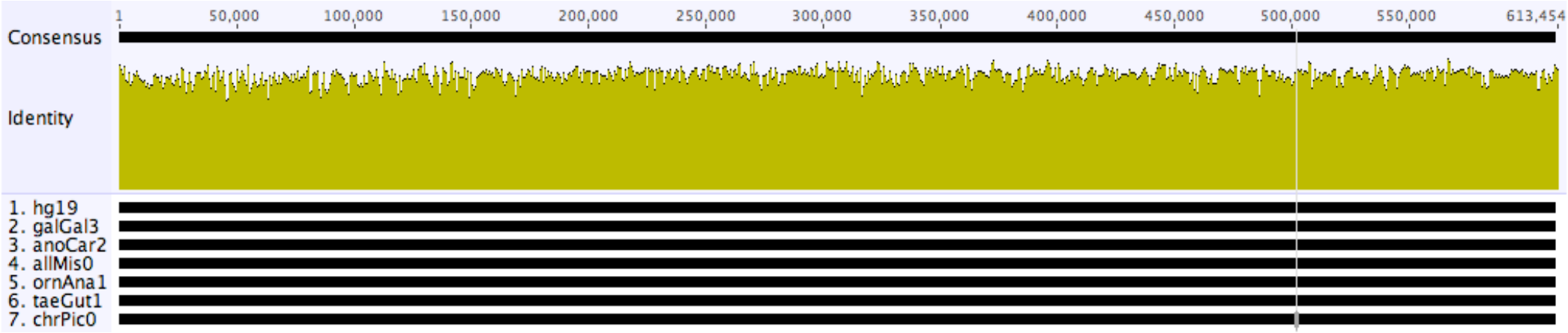


This can be extremely challenging for 'big data'.

e.g. 100 classes:

4758539127676483365879076884138720782636366968682561146661633463755911449789244262267272404421775630695355788256075 1 partition models

Scaling up



Scaling up may also mean that we need to relax this assumption

Phylogenetic Model Parameters

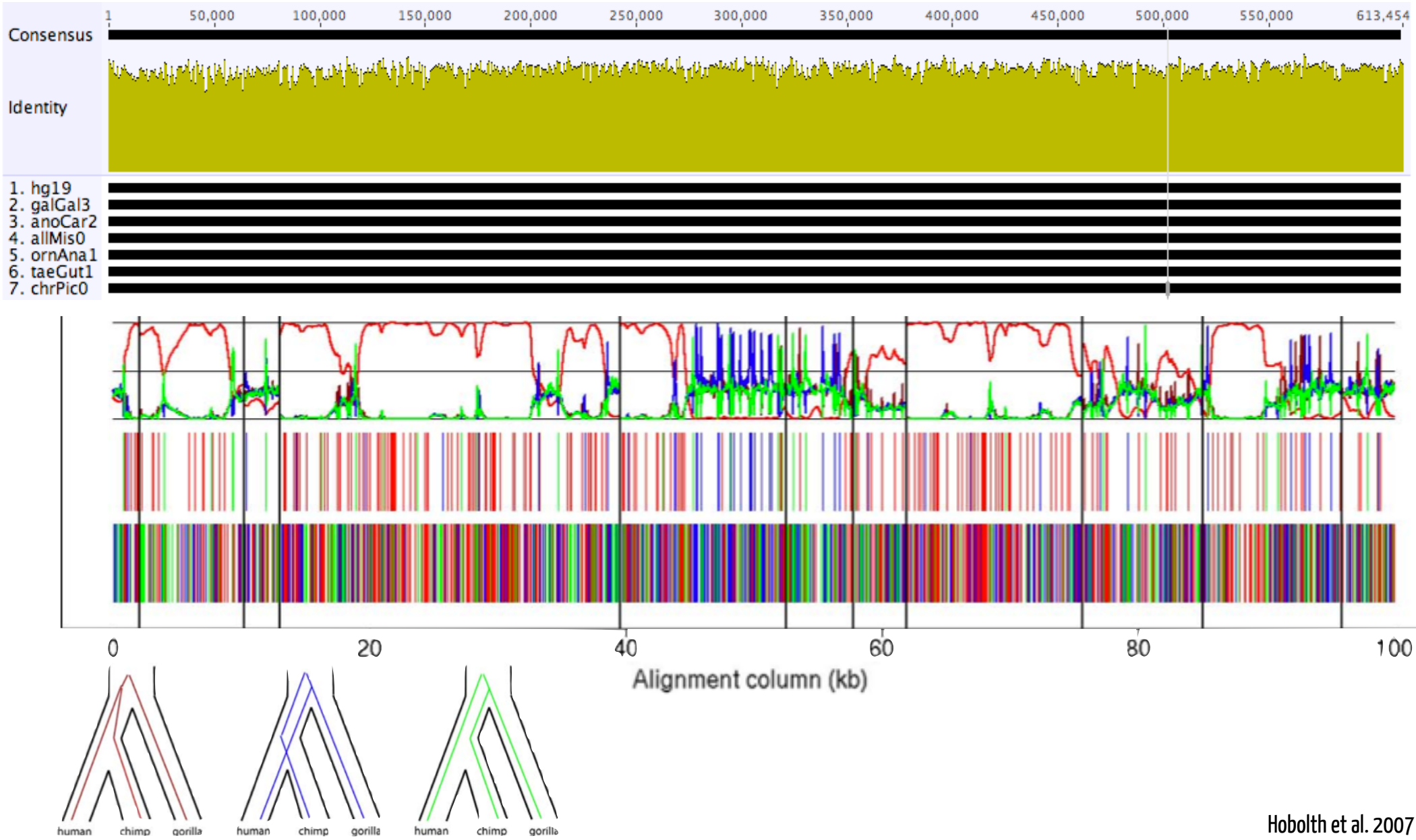
Topology	τ
Branch lengths	$\boldsymbol{\nu}$

Shared across partitions

Exchangeability rates	$\boldsymbol{r} = (r_{ac}, r_{ag}, r_{at}, r_{cg}, r_{ct}, r_{gt})$
Base frequencies	$\boldsymbol{\pi} = (\pi_a, \pi_c, \pi_g, \pi_t)$
ASRV Gamma Shape	α

Independent for each partition

Scaling up



Hobolth et al. 2007

Tutorial

- Partition models in RevBayes
  - **set up** partitioned model
  - run **mcmc**
  - stepping stone integration for **marginal likelihood estimation**

Exercise

- I have supplied data for four 'loci' (sim_locus1.nex,...sim_locus4.nex)
- Choose (**and sign up for**) one partition model of the form (12,34 or 1,2,34 or 1234 or 1,2,3,4)
- GTR + Gamma model for all partitions
- Settings for stepping stone integration:
  - 50 power posteriors (cats=50)
  - burnin=500, tuning interval=200
  - 2000 generations per power posterior
  - add your estimate to the spreadsheet