# Notes for Undergraduate Research Work

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### **General**

### 1 R Notes

Remember: R is 1-indexed. Format of If/Else:

```
if {
}else{
}
```

In R-Studio, you can multiline comment (and uncomment) by pressing CTR + SHIFT + CT

To check current directory in R, type in and execute "getwd()".

### 2 TODOs

- 1. PANSE model implentation:
  - a) PANSEParameter.cpp
  - b) PANSEModel.cpp
  - c) PANSEParameter.h
  - d) PANSEModel.h
  - e) Ask about sigma term Done
  - f) Ask about lambda prime term (is it lambda prime?) check RFP section for how to actually calculate DONE
- 2. Expand Unit Testing:
  - a) Test Cov Matrixes STALLED: Still need final two
  - b) Test MCMC STALLED: Need run, varyInitialConditions, calculateGewekeScore, getLogLikelihoodPosteriorMean, and setRestartFileSettings as well as two test that only functions.
    - Implement other unit testing first
  - c) Parameter In progress
  - d) Test RFP Parameter
  - e) Test Trace
  - f) ...Per class basis
  - g) Eventually, some R scripts to do a short run for each model: Talk to Cedric

#### General

- 3. r
- 4. When working with gene-specific parameters, the openmp statements aren't working (memory is such a mess in the area) break down parallelization, try to find where the issue is. Perhaps start with dynamic arrays, change to vectors. Gabriel thinks the slowdown from vectors in general is made up by better parallelization in avoiding dynamic arrays.
  - —STALLED. Literally can't test speeds of various optimizations and cores right now.
- 5. Documentation

# May 13, 2016 Notes

### 1 PANSE Concepts

$$\sigma_i = \prod_{j=1}^{i} (1 - P_{NSE,j}) \tag{0.1}$$

 $\omega_i$  = pausing for codon i

 $p_n se, i = NSE Pr (probability) for codon i$ 

This is codon-based.

Likelihood of the data given the parameters:  $\mathcal{L}(\vec{x}|P_{NSE},\vec{\omega},\vec{\phi})$ 

Will be a much smaller data set, and with hundreds of calculations rather than thousands.

Randomly select  $\sim 600$  genes instead of 5400

Sigma vector of:  $\sigma_{i+1} = \sigma_i(1 - P_{NSE,i})$ 

Function is of probability of getting there vs waiting time once there

### 2 TODOs

- Getting pausing values with simpler models (ROC)
- First analysis could be just estimating these terms

#### May 13, 2016 Notes

- This would mean creating a simulated data set.
- For simulation:  $P_{NSE} = \frac{b}{\omega + b}$ , where b is on the order of 1/5000 times average omega.  $(b \simeq \frac{1}{5000}\overline{\omega})$  Talk to Jeremy about this, he may have finished this by now.

See the 2015 paper, 2011 paper with primal

# May 19, 2016 Notes

### 1 PANSE Concepts

rfp.model.pdf: Reasoning [for lambda] is that for the sampling the Boltsman coefficient. See the explanation around equation (4) and the Z's and Y's.

Lambda Prime = Lambda.c \*  $\mathbb{Z}$  /  $\mathbb{Y}$ , or call it  $\mathbb{K}$ .

$$\lambda' = \lambda_c * \frac{Z}{V}$$

Z is the overall state space

Y is what is sampled

 $\lambda_c = \lambda' * \frac{C}{K}$ . Let K be a new independent parameter, and keep track of Lambda Prime.

## May 25, 2016 Notes

### 1 PANSE Concepts

Codon-Specific Elongation Rate:  $P_{NSE} = \frac{b}{b+c}$  where b is where it flies off and c is where it continues.

Omega is the odds ratio of  $\frac{P_{NSE}}{1-P_{NSE}}$ . Therefore  $\omega = \frac{b}{c}$  Look at 2006, 2007 papers.

LOOK AT UPDATED PDF: IT'S IN FRAMEWORK

Psi (the symbol which I \*thought\* was Omega) is the ribosome initiation rate: Rate at which ribosomes are jumping onto the mRA. Phi is the rate that they are jumping off at the very end.

If you have 50% chance to get to the end, then Psi is twice as long as Phi Phi = Psi \* Sigma.

Don't redo calculations from scratch, but rather in series.

### 2 Parallelization

- Only 20 AA's Only 20 cores to spread load unto
- AA's with 6 codons of course take more time than those with 2

Gilchrist thinks what is meant by Gene-Specific Parameters is to parallelize at the highest level, i.e. at the gene or amino acid level.

I should check the code; find where the OpenMP statements are etc Mostly something to ask other people about if I want to tackle the problem.

# May 26, 2016 Notes

### 1 Parallelization

#### Cedric's input:

- phi calculation, with mcmc accept/reject
- dynamic arrays
- big loop around everything
- code doesn't work
- couldn't figure out why
- didn't spend that much time

we ended up parallelizing in the model class:

calculateLogLikelihoodRatioPerGene, apparently doesn't do much. Perhaps better to parallelize outside, with the big loop

Run a ROC model, then RFP

I'm running a fasta file that is simulated, so I know that it is true

I kinda need the R side

Get to the point where we suspect memory is the problem

Dynamic Arrays -> Vectors

# May 31, 2016 Notes

- Start 1:21
- break 3:19
- back 3:24
- break 4:55
- return 5:02
- $\bullet$  end 7:02
- 2+1.5+2

### 1 Parallelization

Go ahead and replace dynamic arrays with vectors, first

And then do this barebones calculation of runs to see if it makes it faster, without regards to parallelization.

# June 1, 2016 Notes

- Start 1:30
- Break 3:30
- Return 3:35
- End 7:00

2 + 3.5

### 1 Parallelization

#### From yesterday:

- 0.00621732 10
- 0.00687881 100
- 0.00947537 1000
- 0.00713974 10000
- 0.00785908 10000
- 0.00750889 10

#### For today:

- 0.0572747 10
- 0.0698414 100

...Odd, 10x as long on average

The above was in DEBUG mode. Release mode redos:

A or V	Runs	Modifiers	Avg Time
V	100		0.0141421
A	100		0.0047742
V	10000		0.00850093
A	10000		0.00479609
V	10000	No Deletion	0.00871843
A	10000	No Deletion	0.00491614
V	10000	std::sort	0.00841396
A	10000		0.00598796
A	10000		0.00520682
A	100000		0.00455916
A	100000	std::sort	0.00776886
V	100000		0.00795495
V	100000	std::sort	0.00785736
A	100000	std::sort	0.00383634
A	100000		0.00385638
A	100000	std::sort	0.00392021

Note: Vectors are 2x as long on average now

### **2 PANSE Implementation**

Next step: Make a list of everything PANSE touches and unit test these things (first and foremost before actually writing PANSE)

ALSO: Estimate and track how long, in reality, it takes to do each unit testing PARFP, PTRFP? Just calling it RFP might be misleading.

## June 2, 2016 Notes

- Start 1:01
- Break 3:35
- Return 3:50
- End 6:58

Spent till 4 (3 hours) compiling notes and creating a git directory.

### 1 PANSE Implementation

Expecting to spend 1 hour deciding on what PANSE will need (or, rather, what RFP will need).

Talk with Gilchrist:

So data position feeds into:

- a) data on gene
  - ab) to feed into ROC-RFP
- or b) PANSE-RFP

### 2 Lareau Data

Which file type should I be reading in? RFP or Fasta?

For sample data for PANSE:

Lareau Paper ->GSE ->The untreated replicates 1,2,3. Take one, and even then only a subset of one of them as sample data.

The Lareau material may have undergone more processing that the new Weinberg GSE published Feb 10 2016.

"Start with Lareau paper data" - Gilchrist, 5:33

# June 3, 2016 Notes

- Start 1:35
- Break 4:09
- Return 4:14

### 1 Lareau Data

Decided to start reading the Lareau material. Began by looking directly at definition of data set (I chose untreated replicate 1) and then parse the data to get a smaller subset (file size otherwise is too large at 35MB)

Took longer than expected... When files finally parsed, 5:45.

Now have a data set of size 400 KB: those genes with 11 to 100 (inclusive) codons.

## June 6, 2016 Notes

#### **1 TODOs**

Immediate future goals:

- 1. Generate new Lareau material following specifications of Gilchrist talk, below.
- 2. Just work, from now on, with the labbook class. Don't have to reformat old content.
- 3. Formally write up a list of things TODO with Unit Testing for Parameter
- 4. Unit Test up-to-date with Parameter
- 5. Write up pseudo-code with PANSE itself to prepare for it
- 6. Create and test a function for reading in Lareau material (low priority)
- 7. Parallelization is after the initial PANSE stuff is implemented, very low priority

### 2 Lareau Data

Talk with Gilchrist:

Let's get a randomly distributed set of data rather straight up isolation.

See below for how to randomly distribute; want only 100 genes.

61 Parameters Pausing Time

Lots of gene-specific parameters that scale with each gene.

Let's say average of each gene is 300 AAs.

So 7 observations per gene.

Try to get 2 parameters for a fair amount of information. Calculating at sigma is going increase at gene length.

And of course longer gene sequences take longer to parse.

So probably want a data base for playing around with of 100 genes, between 200 and 400 AAs long

Do we need to test with all 61 parameters? 2-codon AA's are the quickest thing to work with.

So may want to start with 100 genes of 200-400 AAs Estimate these parameters with a small subset of the codons, starting with the 2-codon ones. If they are behaving properly, scale up to 3/4/etc.

Long is de-facto standard Lareau argues that Short is also relevant despite usually being thrown out

Long and short: tell how elongation is at each position. Our model is based on pausing. So how do long and short factor in? Well, we don't know yet.

We could base it on just one or the other or combine the two. For now let's just base it on Long.

After about thirty minutes following the talk with Gilchrist – new subset of data produced via modifying old Perl scripts. Now have the specified data set in the final "finalData.txt" –  $516~{\rm KB}$ .

Interestingly small size – seems like old data set had that many genes of smaller AA length.

Spent an hour afterward reading over labbook documentation and reformatting notes where needed.

## June 7, 2016 Notes

In the course of running an RFP Model, the following functions are called (and have yet to be unit tested).

### **1 TODOs**

- initParameterSet (actually already done... mostly) general parameter
  - test std\_csp changes Done
  - test numAcceptForCodonSpecificParameters changes Done
  - Possibly setNumMutationSelectionValues Ignore for now
  - Possibly initCategoryDefinitions -Ignore for now
  - For the two above Find how to check delM and delEta of category (a vector of Mixture Definitions) – Done
  - Check many final changes at the end of this function Three remaining
- initRFPParameterSet RFP exclusive
- getSelectionCategory general parameter Done
- InitializeSynthesisRate general parameter
  - calculateSCUO
  - quickSortPair
  - quickSort
  - Parameter::randLogNorm
- setParameter RFP model exclusive
- mcmc.run MCMC function on RFP(TODO later?)

### 2 Unit Testing

Going to take it one step at a time, finish up initParameterSet testing...

Finished most of initParameterSet completely. Need to ask Cedric about a duplicate function before finishing the final two functions.

May need to write a function to unit test with the categories variable itself, but all that happens otherwise is it pushes unto the vector of vector of vectors.

Encountering a strange printing bug right before the end. While if statement works correctly, the final confirmation of initParameterSet isn't being printed.

#### Example output:

```
Parameter getMixtureAssignment --- Pass
Parameter setMixtureAssignment --- Pass
Parameter getMutationSelectionState --- Pass
Parameter getNumParam --- Pass
Parameter getNumMixtureElements --- Pass
Parameter getStdDevSynthesisRate --- Pass
Parameter setStdDevSynthesisRate --- Pass
Parameter getCurrentStdDevSynthesisRateProposalWidth --- Pass
Parameter getNumAcceptForStdDevSynthesisRate --- Pass
Parameter getStdCspForIndex --- Pass
Parameter getNumAcceptForCspForIndex --- Pass
Parameter getNumMutationCategories --- Pass
Parameter getNumSelectionCategories --- Pass
Parameter getMutationCategory --- Pass
Parameter getSelectionCategory --- Pass
Parameter getMixtureElementsOfMutationCategory --- Pass
Parameter getMixtureElementsOfSelectionCategory --- Pass
Parameter getCategoryProbability --- Pass
Parameter setCategoryProbability --- Pass
Parameter getSynthesisRate --- Pass
Parameter setSynthesisRate --- Pass
Parameter getSynthesisRateProposalWidth --- Pass
Parameter initParameterSet --- Pass
Process finished with exit code 0
```

vs

```
Parameter getMixtureAssignment --- Pass
Parameter setMixtureAssignment --- Pass
Parameter getMutationSelectionState --- Pass
Parameter getNumParam --- Pass
Parameter getNumMixtureElements --- Pass
Parameter getStdDevSynthesisRate --- Pass
Parameter setStdDevSynthesisRate --- Pass
Parameter getCurrentStdDevSynthesisRateProposalWidth --- Pass
Parameter getNumAcceptForStdDevSynthesisRate --- Pass
Parameter getStdCspForIndex --- Pass
Parameter getNumAcceptForCspForIndex --- Pass
Parameter getNumMutationCategories --- Pass
Parameter getNumSelectionCategories --- Pass
Parameter getMutationCategory --- Pass
Parameter getSelectionCategory --- Pass
Parameter getMixtureElementsOfMutationCategory --- Pass
Parameter getMixtureElementsOfSelectionCategory --- Pass
Parameter getCategoryProbability --- Pass
Parameter setCategoryProbability --- Pass
Parameter getSynthesisRate --- Pass
Parameter setSynthesisRate --- Pass
Parameter getSynthesisRateProposalWidth --- Pass
```

Process finished with exit code 0

## June 8, 2016 Notes

### 1 Unit Testing

Started by writing and testing a function for numAcceptForSynthesisRate.

Printing this statement seems to have fixed the odd print bug mentioned yesterday.

After doing that, I decided to write up on the documentation of Unit Testing I have done so far.

Asked Cedric about getSelectionCategory and getSynthesisRateCategory (paraphrased):

It's related to how we may have delta and Phi values...

We are trying to find out how efficient your codons have to be to reach a production rate assuming cost is constant.

Cost = Benefit \* production rate (Phi)

Switching to a different selection environment: Different cost, different benefit, and therefore different Phi.

If you have 2 selection categories, you have to have two synthesis categories. They are the same even if we don't know them, but it saves renaming it to something more general.

Finally finished initParameterSet besides checking categories matrix itself (minor, to do later).

Continued TODO:

### 2 TODOs

- initRFPParameterSet RFP exclusive
- InitializeSynthesisRate general parameter
  - calculateSCUO
  - quickSortPair
  - quickSort
  - Parameter::randLogNorm
- setParameter RFP model exclusive
- mcmc.run MCMC function on RFP(TODO later?)

Next goals: Do the internal functions for InitializeSynthesisRate related to quickSort. Finish up InitializeSynthesisRate.

## June 9, 2016 Notes

Began by checking github; fixed semicolon error and confirmed package worked correctly.

### **1 TODOs**

To truly finish testing InitializeSynthesisRate, we would need:

- calculateSCUO
- Parameter::randLogNorm
- quickSortPair
  - pivotPair
    - \* swap (doubles)
- quickSort
  - pivot
    - \* swap (ints)

Ask Cedric if it'd be a good idea to just use std::sort instead of quickSort.

The quick sort algorithms are very math-intensive, so Unit Testing them may be lower priority.

For now, I am switching to unit testing RFP-exclusive functions.

- initRFPParameterSet (in RFPParameter.cpp)
  - check currentCodonSpecificParameter
  - check proposedCodonSpecificParameter
  - check lambdaValues (optional currently unused variable)
  - check numParam Done
  - check bias\_csp always set to 0, can ignore for now
  - check std\_csp Done
  - check groupList Done
- setParameter (in RFPModel.cpp) may be untestable, ignore for now

In the course of working on checking RFPParameter, wrote up Unit Testing for all Group List functions in Parameter.cpp

May need a wrapper function for currentCodonSpecificParameter and proposedCodon-SpecificParameter extraction. Talk to Cedric.

Refocusing overall goals:

- 1. Unit Test up-to-date with Parameter
  - initRFPParameterSet
    - -check current Codon Specific Parameter – stalled, ask Cedric
    - check proposedCodonSpecificParameter stalled, ask Cedric
  - $\bullet$  InitializeSynthesisRate
    - calculateSCUO
    - Parameter::randLogNorm
    - quickSortPair
      - \* pivotPair
        - · swap (doubles)
    - quickSort
      - \* pivot
        - · swap (ints)
  - mcmc::run MCMC function on RFP
- 2. Write up pseudo-code with PANSE itself to prepare for it
- 3. Create and test a function for reading in Lareau material (low priority)
- 4. Parallelization is after the initial PANSE stuff is implemented, very low priority

#### TODO tomorrow:

Ask about current/proposed CSP Parameter, quicksort vs std::sort, and how (if) to unit test the more computation-intensive functions.

Finally replace cout statements in my own section of main.

Begin testing with MCMC run while waiting for others to arrive.

## June 10, 2016 Notes

There exists a heirarchy of functions to test before finally testing mcmc.run. Test the subitems first: (NOTE: Testing with RFPModel)

#### • mcmc::run

- mcmc::varyInitialConditions
  - \* model::proposeCodonSpecificParameter wrapper to RFPparameter
  - $*\ model::proposeHyperParameters-parameter::proposeStdDevSynthesisRate$
  - $*\ model::proposeSynthesisRateValues-wrapper\ to\ parameter$
  - \* model::getGroupListSize wrapper to parameter (done?)
  - \* model::getGrouping wrapper to parameter (done?)
  - $*\ model::updateCodonSpecificParameter-wrapper\ to\ RFP parameter$
  - $* \ model::updateAllHyperParameter-just\ calls\ updateStdDevSynthesisRate-Ask$ 
    - · updateStdDevSynthesisRate wrapper to parameter
  - \* model::getNumSynthesisRateCategories wrapper to parameter (done?)
  - \* model::getSynthesisRateCategory wrapper to parameter (done?)
  - \* model::getSynthesisRate wrapper to parameter (done?)
  - \* model::getMixtureAssignment wrapper to parameter (done?)
  - \* model::getStdDevSynthesisRate wrapper to parameter (done?)
  - \* parameter::densityLogNorm
  - \* paramter::randExp
  - \* model::updateSynthesisRate wrapper to parameter
  - \* model::updateGibbsSampledHyperParameters does not do anything
- model::setNumPhiGroupings wrapper to parameter::setNumObservedPhiSets (done?)
- model::initTraces wrapper to RFPparameter initAllTraces
- model::updateTracesWithInitialValues
  - \* parameter::updateSynthesisRateTrace
  - \* parameter::updateMixtureAssignmentTrace
  - \* RFPparameter::updateCodonSpecificParameterTrace
- model::setLastInteration wrapper to parameter (done?)
- model::writeRestartFile wrapper to RFPparameter writeEntireRestartFile

- model::printHyperParameters uneeded to test, just prints
- model::getNumMixtureElements wrapper to parameter (done?)
- mcmc::acceptRejectCodonSpecificParameter
  - \* model::calculateLogLikelihoodRatioPerGroupingPerCategory
  - \* model::updateCodonSpecificParameterTrace
- $-\ model:: adapt Codon Specific Parameter Proposal Width-wrapper\ to\ RFP parameter$
- mcmc::acceptRejectHyperParameter
  - \* model::calculateLogLikelihodRatioForHyperParameters
  - $*\ model::updateHyperParameter--\ parameter::updateStdDevSynthesisRate$
  - \* model::updateHyperParameterTraces
- model::adaptHyperParameterProposalWidths calls adaptStdDevSynthesisProposalWidth, a wrapper to parameter. Uses traces.
- $-\ mcmc:: accept Reject Synthesis Rate Level For All Genes$ 
  - \* model::getMixtureElementsOfSelectionCategory wraps parameter (done?)
  - \* model::calculateLogLikelihoodRatioPerGene
  - \* model::getCategoryProbability wrapper to parameter (done?)
  - \* parameter::randMultinom
  - \* model::setMixtureAssignment wrapper to parameter (done?)
  - \* model::updateSynthesisRateTrace
  - \* model::updateMixtureAssignmentTrace
  - \* model::calculateAllPriors currently does nothing
  - \* parameter::randDirichlet
  - \* model::setCategoryProbability wrapper to parameter (done?)
  - \* model::updateMixtureProbabilitiesTrace
- model::adaptSynthesisRateProposalWidth wrapper to parameter
- mcmc::calculateGewekeScore

#### TODO:

Ask about why it is that Hyper Parameters == StdDevSynthesisRate, always

Don't know if we need to test wrapper functions i.e. those in Model that simply perform a function in its associated Parameter object.

Ask about why dynamic arrays were in code in the first place, i.e. in randMultinom.

New modified list stripping out some things that are more-or-less done (Or those that depend on unimplemented functions or those with random variables):

#### • mcmc::run

- mcmc::varyInitialConditions
- model::initTraces wrapper to RFPparameter initAllTraces
- model::updateTracesWithInitialValues

- \* parameter::updateMixtureAssignmentTrace
- \* RFPparameter::updateCodonSpecificParameterTrace
- model::writeRestartFile wrapper to RFPparameter writeEntireRestartFile
  - \* parameter::writeBasicRestartFile
  - \* writeRFPRestartFile
- mcmc::acceptRejectCodonSpecificParameter
  - \* model::calculateLogLikelihoodRatioPerGroupingPerCategory
  - \* model::updateCodonSpecificParameterTrace
- model::adaptCodonSpecificParameterProposalWidth wrapper to RFPparameter. Uses traces.
- mcmc::acceptRejectHyperParameter
  - \* model::calculateLogLikelihodRatioForHyperParameters
  - $*\ model::updateHyperParameter--\ parameter::updateStdDevSynthesisRate$
  - \* model::updateHyperParameterTraces
- model::adaptHyperParameterProposalWidths calls adaptStdDevSynthesisProposalWidth, a wrapper to parameter. Uses traces.
- mcmc::acceptRejectSynthesisRateLevelForAllGenes
  - $* \ model:: calculateLogLikelihoodRatioPerGene\\$
  - \* model::updateSynthesisRateTrace
  - \* model::updateMixtureAssignmentTrace
  - $* \ model::updateMixtureProbabilitiesTrace\\$
- model::adaptSynthesisRateProposalWidth wrapper to parameter. Uses traces.
- mcmc::calculateGewekeScore

After writing the setNumObservedPhiGroupings and lastIteration unit testing functions and updating these notes, worked on restart file writing.

TODO: Discuss with Cedric how to proceed to unit testing with restart files in the future, i.e. keep in same function or separate.

Next step:

Probably work with traces. Not sure how to proceed with unit testing the most complicated functions re: computation, nor with reading/writing files yet.

# June 11, 2016 Notes

Mostly read documentation. Worked from home, so no benefit of discussing implementation topics. Worked less than planned.

## **June 13, 2016 Notes**

Discussing Unit Testing with Cedric:

OK'd changing quicksort (simple implementation) to std::sort.

Instead of running the higher-level functions that are directly used, probably better to stick to the simple functions and then test mcmc algorithm runs with 100 samples; compare the likelihoods of each model, which should be similar, to detect errors.

For the intense calculations, for now ignore. The calculation unit tests will be summed up (in a general sense) by just doing mcmc algorithm runs.

First, going to change std::sort.

After that was done, decided to clean up some R-side unit testing in preparation of testing mcmc algorithm runs – since in R you can set seed for entire C-side implementation.

### 1 TODOs

- Fix the TODO note in Parameter.cpp under initParameterSet
- Ask Cedric about:
  - Testing restart files: keep in same function or separate unit tests.
  - May need a wrapper function for currentCodonSpecificParameter and proposed-CodonSpecificParameter extraction.
  - How to actually run R-side scripts; weird error messages.
  - What is the inst folder? Can we remove it, since it seems to be old Unit Testing Data stuff?

Still need to look at Trace stuff as next major step without help from Cedric.

Spend at most two more days on Unit Testing at this rate; after, will start thinking solely on PANSE.

## **June 14, 2016 Notes**

Yesterday ended by running memory leak checks in the background on a whim due to debugging some new calls without associated delete calls.

Found a confirmed memory leak with my\_print. Started today by flushing output on both C and R side of code, as well as expanding unit testing for Utility.h.

Spent an hour and a half on this.

Came in late, could not ask Cedric questions.

#### 1 Traces

Order of Trace functions to examine in a typical model run (via MCMC::run):

- model::initTraces(samples + 1, genome.getGenomeSize());
  - RFPparameter-¿initAllTraces
    - \* traces.initializeRFPTrace (RFP-only)
      - $\cdot$  initializeSharedTraces
      - · initCodonSpecificParameterTrace (for both alp and lmPri)
- model::updateTracesWithInitialValues(genome) TO BE EXAMINED
  - parameter::updateSynthesisRateTrace
    - \* traces.updateSynthesisRateTrace
  - parameter::updateMixtureAssignmentTrace
    - \* traces.updateMixtureAssignmentTrace
  - RFPparameter::updateCodonSpecificParameterTrace
    - \* traces.updateCodonSpecificParameterTraceForCodon (for alp and lmPri)
- mcmc::acceptRejectCodonSpecificParameter
  - model::calculateLogLikelihoodRatioPerGroupingPerCategory
  - model::updateCodonSpecificParameter(grouping)
  - model::updateCodonSpecificParameterTrace
- model::adaptCodonSpecificProposalWidth wrapper to RFPparameter. Uses traces
- mcmc::acceptRejectHyperParameter
  - model::calculateLoglIkelihoodRatioForHyperParameters
  - model::updateHyperParameter parameter::updateStdDevSynthesisRate
  - model::updateHyperParameterTraces

- model::adaptHyperParameterProposalWidths calls adaptStdDevSynthesisProposal-Width, a wrapper to parameter. Uses traces.
- $\bullet \ \ mcmc: accept Reject Synthesis Rate Level For All Genes$ 
  - model::calculateLogLikelihoodRatioPerGene
  - model::updateSynthesisRateTrace
  - $-\ model:: update Mixture Assignment Trace$
  - $-\ model::update Mixture Probabilities Trace$
- $\bullet \ \ model :: adapt Synthesis Rate Proposal Width-wrapper\ to\ parameter.\ Uses\ traces.$

This list is still incomplete, but we shall start implementing now for convenience. Need to keep examining functions... Ended before checking model::updateTracesWithInitialValues

## June 15, 2016 Notes

Answers to Cedric questions:

- In general, design of code is up to me. Seems good with whatever.
- DevRScripts are super out-dated. Be careful of what to use, i.e. a lot of functions are using old definitions and need additional arguments.
- Again, for overall unit testing:
  - Do a run, know what the output is.
  - Then repeat that run in the testThat function, compare the two runs. As long as outputs are the same, everything is fine.
- Good scripts to base code off of: allUnique scripts. Specifically allUnique\_kl\_reduced.R, allUnique\_simMod.R
- Bad script: runROCModelFromGoodValues.R

Cedric commented that there was a lot of old and outdated files, so I spent some time trying to clean up the more obvious files.

- Removed inst folder from RibModelFramework.
- Removed cleanSeq() finally
- Cut down on number of my\_print calls; hopefully increases efficiency slightly in either compilation of running phase.

Afterward attempted to learn more about R in order to write scripts to test models with set\_seed.

Testing Restart files:

I think I will create a separate function for each type of file. Basic Parameter, RFP, ROC, etc.

These will be tested by first checking if both read and write work at the same time.

For basic parameter checking, for example, perhaps 1) use initParameter manually, like before.

- 2) Then write the file
- 3) Then read in the file and compare with established, manually set variables.

### **1 TODOs**

For tomorrow:

Unit Test with Restart files. This will help confirm any results.

Continue working with R model unit testing

Cedric will likely not be in for the rest of the week; will continue jumping around with work assignments until after my vacation period.

## June 16, 2016 Notes

Began the day immediately encountering completely unknown errors attempting to run any R scripts that had worked the day before. Problem seems to be with MCMC\_run. As Cedric is not here today, will be much more difficult to check R-side scripts. At the same time, worry that any changes made today may mess up the project as a whole despite the Travis check declaring no errors. Will probably not push any changes made today unless I can debug this.

Decided to clean up the mess of warnings spat out in order to find out how to debug.

To do so, I changed the deprecated Rcpp::loadRcppModules() function to several Rcpp::loadModule() functions, leaving a comment to discuss this change in the future with Cedric

Then, I minorly edited the documentation files to clear up the more obvious errors.

# June 17, 2016 Notes

Continued working on fixing R documentation.

Finishing at 6 after about 4 hours of work and research, I was able to reduce the warnings on my own machine to 4 Warnings and 2 Notes.

The unknown errors and R studio crashing thing has been fixed, but I'm not sure how. I suspect it may have been errors in building/installing the package, but I checked out a fresh copy of all of the files.

Goals for next work days: Restart file testing, model testing, PANSE pseudocode.

Will probably switch to PANSE pseudocode over the vacation period if I have any time to work, so I can discuss any ideas I may have with Dr. Gilchrist once he returns.