WEEK 2 Research TODO

### Week 1

Broad goal: Fix code.	
✓ Use less filtered dataset	
☐ Distance matrix argument to dist?	
<ul> <li>Need both forms, so may or may not be useful</li> </ul>	
$\square$ Check if phi is correct now, and see how is used	
Figure out large alpha problem	
- Seems the + and one loop beta fixed this?	
☐ Try a different covariate?	
$\square$ Figure out why geem code uses $+$ instead of - on update	
<ul> <li>I think + is correct. At least it converges.</li> </ul>	
$\square$ Identify which covariate is causing the trouble.	
$\hfill\Box$ Try removing the single OTU that seems to be contributing to problem.	
$\square$ Save everything to list correctly to look at later.	
- Saving rho, omega, phi, beta, diff (abs), num iterations	
- Also do residuals. Which residuals? Cross product ones? Squared ones? Standardized sq ones? Probably standardized but not squared. Should be distributed around zero. ?	uared
Plot lists	
<ul> <li>Plotted rhos, omegas, phis, diffs, not sure what else to plot.</li> </ul>	
✓ Remove scalar update.	
– Doesn't work. see journal	
$\square$ Write up algorithm for Yuan to go through? Ask to check.	
$\Box$ Final run through before meeting of graphs and numbers	

### Week 2

Main tasks:

- To-do from sheet
- Prepare presentation

✓ Move timing into function

- $\mathbf{\underline{\checkmark}}$  Include more taxa: more zero-inflation
  - $\bullet$  Not great results. see journal omega = .99, rho = .1
  - runtime of 20 min.
- ✓ Add computation time in model.
- **✓** Make presentation
- **f** Figure out why adding the minus sign changes the code.

WEEK 2 Research TODO

	$ullet$ Pretty sure this is because we are then adding or subtracting the $\lambda I$ incorrectly.
✓	Try changing the minus sign on larger dataset.
	$\bullet$ Either immediate convergence or infinite alpha values on 1st iteration
✓	Set up automatic save outputs along with description
•	Try with a medium sized dataset, like prevalence of .2?
✓	Save test datasets to files for easy loading
•	Only include last beta output?
	Try different covariates (parasite burden/antibiotics/exposure)
	Think about genus level analysis/ phylogenetic tree for taxonomic units
	Choose $\alpha$ automatically (simple line search)
	Write up line-search steps and goals
	Understand how Hessian is calculated and expected values equal zero.
	Run on previous dataset from original paper.
	Rename file with algorithm
	Compare to independence GEE written already geeglm?
	Calculate sandwhich variance estimators for asymptotic significance tests
	See if new shared tree that Tom had is the same?
	Add residuals to output and look at plots
	Change initial value to something different?
	<ul> <li>change initial rho to 10. Changes results (of at least ests of rho and omega)</li> <li>Try previous iterations rho and omega.</li> </ul>
	• See how beta estimates change
	• Run code with initial value of 1 again to compare.
	Read numerical optimization book.
	Save convergence results of nls optim
	Make sure subtraction in $\phi$ is correct

WEEK 3 Research TODO

# Week 3

General
$*\Box$ Read numerical optimization book.
$*\Box$ Understand how Hessian is calculated and expected values equal zero.
$*\Box$ Run on previous dataset from original paper.
$*\Box$ Rename file with algorithm
✓ Take pictures of meeting notes.
$\square$ Figure out how to send jobs to server
Line search
$*\Box$ Choose $\alpha$ automatically (simple line search)
$*\Box$ Write up line-search steps and goals
$\square$ Add condition if infinity or NA to halve gamma
$\Box$ Clean up code for speed and remove redundancy.
$\square$ Look at notes from meeting about (different?) conditions
$\Box$ Code was set up incorrectly. Fix. Shouldnt be updating betas each time, just checking.
$\square$ Save sum of absolute G for each iteration.
Convergence
$*\Box$ Save convergence results of nls optim
$\Box$ Change $\lambda$ to be based on eigenvalues.
$\square$ Save eigenvalues and look at ratio.
$\square$ Test to see difference within iterations of if starting values (eg rho = 10) give different results.
Correlation: Importance of $\rho, \omega$
*□ Compare to independence GEE written already geeglm?
$*\Box$ Calculate sandwich variance estimators for asymptotic significance tests.
$\square$ Keep $\rho$ or $\omega$ the same throughout the algorithm
Other
$*\Box$ See if new shared tree that Tom had is the same?
$*\Box$ Try different covariates (parasite burden/antibiotics/exposure)
$*\Box$ Think about genus level analysis/ phylogenetic tree for taxonomic units
$\Box$ Add condition to make sure $\rho,\omega$ also converge
☐ Email Tom with questions
$\Box$ Think about how hypothesis tests work
□ Read about GEE hypothesis tests

WEEK 4 Research TODO

# Week 4

☐ Writeup meeting notes
$\square$ Email Tom (response to my email) about more information
☐ Look into *resolving nodes*
$\Box$ Select one Genus/Family to only have 10 ish ASVs. Filter dataset, and tree.
Test against identity fixed values of omega and rho

WEEK 5 Research TODO

#### Week 5

✓ Make gamma, lambda values arguments in the functions. ✓ Save final residuals in model. ✓ Convert initilization to one line list. See if weird jump still happens. figure this out. • Seems like jump does not exist anymore. Add model call to result list ✓ Create diagnoistics plot function • Patchwork outputs ✓ Clean up old code ✓ Save beta values again and look at changes. ✓ Run through with bug fixed. See what goes on. Write up results ✓ Figure out a way to compare beta values • Using a line plot across iterations Add GEE values to plot. ✓ Check if gamma = 1 betas are same as gamma = .1 betas • They are not. Figure out how to compare betas across different model runs (probably same line function?) ☐ Think about how to do simulations, since we need to have something to check against.  $\square$  Try to sum up phylogenetic tree and see if there are any problems. ☐ Email Tom about summing up the phylogenetic tree □ Look at residual matrix (cross residuals). See if close to zero.  $\square$  Use data that is just random common taxa. ☐ Try different covariates  $\square$  Consider moving functions to new files  $\square$  Convert all nls functions to matrices to make sure all entries match indeces. ☐ Update roxygen skeletons for functions  $\square$  Add final values of omega, rho and phi to patchwork plot ✓ Try independence  $\square$  Compare independence to geem beta values.  $\square$  Try fixed values of  $\omega, \rho$ Figure out why flavo + 30p dataset stops in 2 iterations

WEEK 5 Research TODO

See how $\lambda$ values change beta values.
Explore convergence of optim loop.
Check variances are correctly between 0 and 1.
Compare beta values with a larger/smaller gamma to $.1$ and see if beta values are different.
Implement line search? maybe will work now that bug is found.

WEEK 6 Research TODO

## Week 6

 $\hfill\Box$  Do simulation WEEK 7 Research TODO

## Week 7

✓ Do better with version control!!!
✓ Split function into multiple parts: b02e5e9
✓ Arrange file structure
Add commits to finished todos.
Make repo public.
✓ Roxygen for all functions. d232743
$\square$ Organize Dirichlet and other simulation files
$\square$ Make sure everything runs with changes
$\square$ Find points in code that were changed in meeting
☐ Simulation:
☐ Get working on just Dirichlet
$\Box$ Fix variance calculated to be true values of alpha.
$\Box$ Check on all instances of making a matrix and if it is the byrow correctly or not!