TESTING THE EFFICACY OF OUR SUPERSPRAY ON THE ORAL MICROBIOME

Team 37

New Mexico Supercomputing Challenge

Final Report

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Team Number: 37

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Executive Summary

TESTING THE EFFICACY OF OUR SUPERSPRAY ON THE ORAL MICROBIOME

Utilizing the information obtained in our research, we outlined our ideal model to be this: first set up two model mouths. Both mouths will start with 10^4 turtles (this represents the total number of good and bad bacteria in the mouth). One mouth will be our control group, and will not receive our spray while the other group will be our experimental group and will receive our spray. We will then set the good bacteria to bad bacteria ratio to 51:49, differentiating the good bacteria with green turtles and the bad bacteria with red turtles. Afterwards, we will set our control group to double every 2 hours, while having the total bacteria decrease by 10% every minute. We will set the total number of bacteria in the experimental group to grow by a factor of 26.67 every two hours and decrease by 1% every minute. We used the wolf-sheep model on netlogo to recreate our ideal outline as best as we could.

Introduction

Problem Statement: Will our hypothetical spray fortify the oral bacteria enough to prevent dysbiosis?

Background Research: In the past, people have proposed eating high fiber foods and doing aerobic exercise, to make the oral microbiota healthier and thereby prevent themselves from contracting strep throat. We inferred that if we could make a super spray that could increase the ratio of good:bad bacteria then, then it would prevent the mouth from dysbiosis (more bad bacteria than good), and thus decrease the chance of a person contracting strep throat or any disease. Some of the variables that influence the problem are: the ratio of good bacteria to bad bacteria (periodontopathic) bacteria, bacterial communal diversity, genetic differences, salivary flow rates, activity of salivary proteins, innate immune factors, oral hygiene, diet, smoking, antibiotics/antimicrobial agents, and diseases, all of which affect how a person's composition of "healthy" microbiota will look to them, with salivary flow rates and activity of salivary proteins contributing the most to maintaining and promoting a healthy oral microbiota.

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In an effort to test the validity of the theoretical framework behind our hypothetical SuperSpray, we simplified the concept of our superspray down to a prototype and decided to see how the computational model of our superspray influenced two variables: salivary flow rate and salivary protein activity.

To solve the problem computationally, we are testing to see if our spray will increase the number of good bacteria. We will link our spray to the salivary flow rate and salivary protein activity, and depending on whether those variables go up or down, the number of good bacteria will remain the same or increase.

Computational Model

Selection: Netlogo

Modification: In code, changed names of wolf to bad bacteria, and changed names of sheep to good bacteria. We also set the starting ratio to 51(good bacteria) to 49) bad bacteria in order to represent a baseline healthy oral microbiota in a person.

Conclusions

Results: Control group: Starting Ratio 51:49

At t=50 end ratio 51983:1850

1019.3 fold increase

Experimental group: At t=50 End Ratio: 68100:61

-1335.3 fold increase.

+316 fold!

Discussion: The pseudo-sample code that chat-gpt generated still had errors because of the limitations that chat-gpt has. Although it has a vast amount of external information to access, the code that it generates often has errors, and even when we ask it to fix the errors in its own code, it often will fix the specific error we mentioned and add a different error, in short, replacing one error with another. This is why the judgment of someone who knows what we want to accomplish and also has domain knowledge in coding is useful for creating a model that we actually like.

We plan on using behavior space to run at least 1000 more iterations on our netlogo model, as well as getting more research on the different ways that people have utilized ChatGPT to do research. From this, we hope to get a more comprehensive demonstration in our data, of how effective our superspray would be at improving the oral microbiome for different people, since we already know that it would be effective in someone who meets baseline oral microbiota standards.

Acknowledgements

-Dr.Ndingsa Fomukong (Phd in Molecular Biology; for further context and explanation of oral microbiota)

-Dr.Anthony(Phd in Computer Science; for updating computer model)

-Justice Code for giving us the support and the resources to do a project like this.

References

--https://www.listerine.com/fresh-breath/good-vs-bad-oral-microbiome-bacteria

-https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5052503/

-https://www.nature.com/articles/sj.bdj.2016.865/tables/1

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5052503/#:~:text=Thenormaldailyproduction of,chewing and other stimulating activities.

Introduction

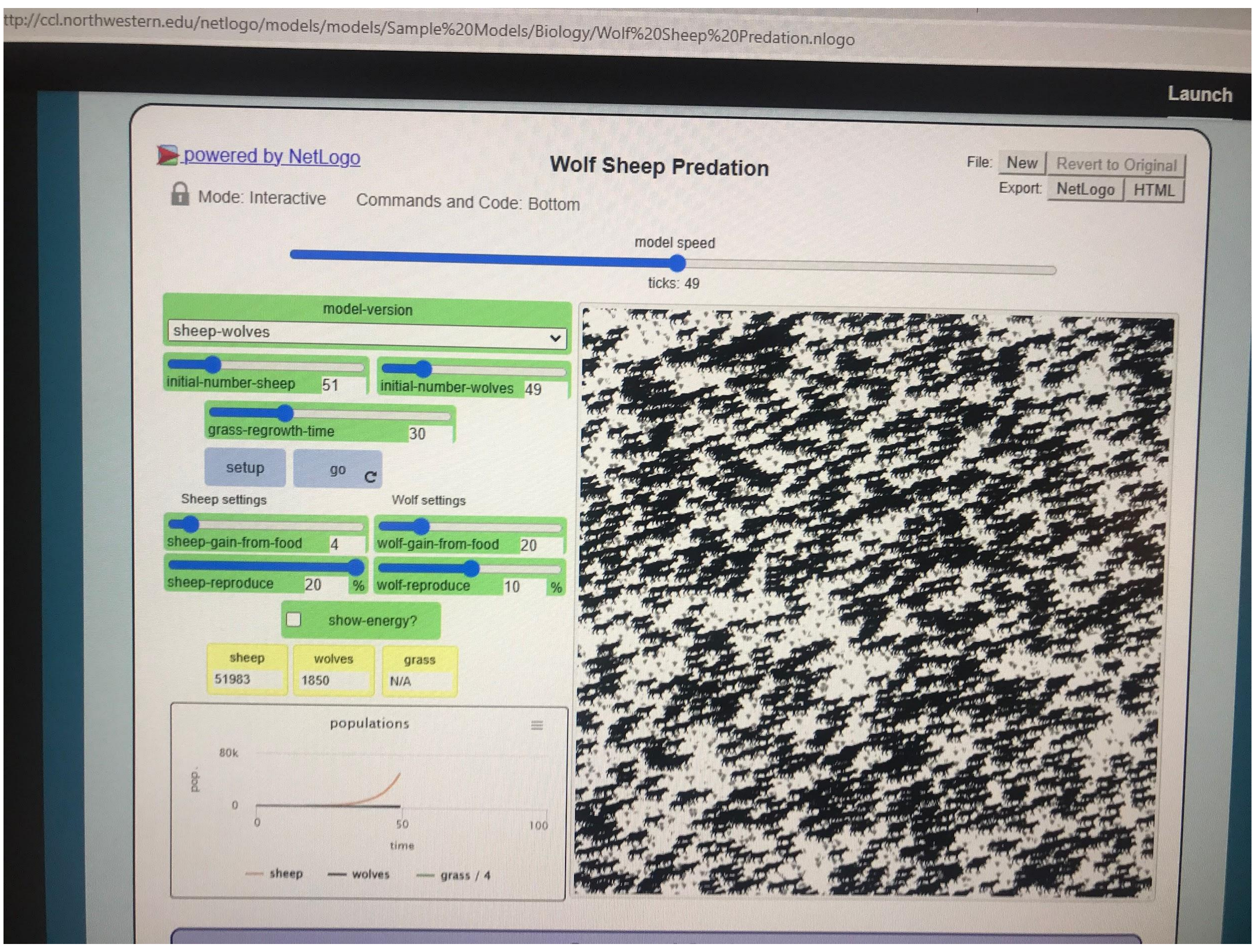
Problem Statement

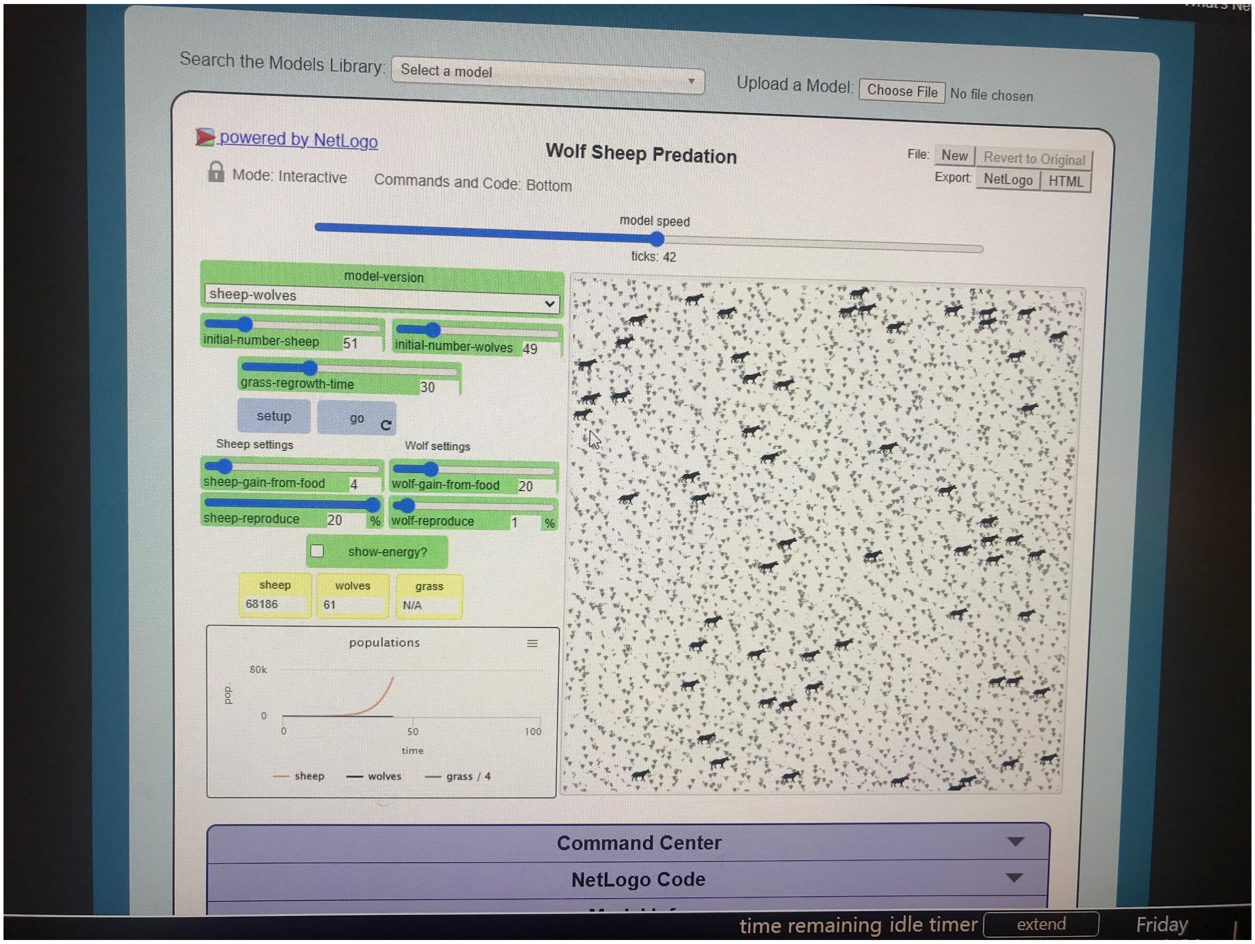
Will our hypothetical spray fortify the oral bacteria enough to prevent dysbiosis?

Computational Model

Selection We utilized netlogo in order to make our functioning computer model

Visualization:





Limitations

Netlogo would not allow us to set rates of increases past 100% which limited our ability to represent what would actually happen in our model of our experimental group, which was supposed to increase by 26.67 every 2 hours, which is much larger than 100%.

Problem Solving Method

Verification: we are yet to verify our computational model and we plan to collaborate with an expert in programming working at Justice code.

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Corroboration

There are sprays like our superspray that actually exist; they are called probiotic sprays. Most of them do not have detailed models of precisely how much they improve the ratio of the oral microbiota, but instead just include different cultures of bacteria that are known to increase the ratio of good bacteria to bad bacteria in varying amounts for different people. For example, there are sprays that include Lactobacillus Reuteri, a lactic acid bacteria that can increase the ratio of good bacteria to bad bacteria.

Conclusion

Results: Results : Control group: Starting Ratio 51:49

At t=50 end ratio 51983:1850

1019.3 fold increase

Experimental group: At t=50 End Ratio: 68100:61

-1335.3 fold increase.

+316 fold!

Future Work

We plan on using behavior space to run at least 1000 more iterations on our netlogo model, as well as getting more research on the different ways that people have utilized chat gpt to do research. From this, we hope to get a more comprehensive demonstration in our data, of how effective our superspray would be at improving the oral microbiome for different people, since we already know that it would be effective in someone who meets baseline oral microbiota standards.

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[https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5052503/#:~:text=The Normal%](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5052503/#:~:text=The%20Normal%) 20daily production of,chewing and other stimulating activities.

Appendix: Code

Netlogo Code

```
Globals [ max-good bacteria ]  ; don't let the good bacteria population grow too large

; good bacteria and wolves are both breeds of turtles
breed [ good bacteria a-good bacteria ]  ; good bacteria is its own plural, so we use
"a-good-bacteria" as the singular
breed [ wolves wolf ]

turtles-own [ energy ]       ; both wolves and good-bacteria have energy

patches-own [ countdown ]    ; this is for the good bacteria-wolves-grass model version

to setup
  clear-all
```

```
  ifelse netlogo-web? [ set max-good bacteria 10000 ] [ set max-good bacteria 30000 ]

  ; Check model-version switch
  ; if we're not modeling grass, then the good bacteria don't need to eat to survive
  ; otherwise each grass' state of growth and growing logic need to be set up
  ifelse model-version = "good bacteria-wolves-grass" [
    ask patches [
      set pcolor one-of [ green brown ]
      ifelse pcolor = green
        [ set countdown grass-regrowth-time ]
      [ set countdown random grass-regrowth-time ] ; initialize grass regrowth clocks randomly for
brown patches
    ]
  ]
  [
    ask patches [ set pcolor green ]
  ]

  Create-good-bacteria initial-number-good bacteria  ; create the good-bacteria, then initialize
their variables
  [
    set shape  "good-bacteria"
    set color white
    set size 1.5  ; easier to see
    set label-color blue - 2
    set energy random (2 * good-bacteria-gain-from-food)
    setxy random-xcor random-ycor
  ]

  create-wolves initial-number-wolves  ; create the wolves, then initialize their variables
  [
    set shape "wolf"
    set color black
    set size 2  ; easier to see
    set energy random (2 * wolf-gain-from-food)
    setxy random-xcor random-ycor
  ]
  display-labels
  reset-ticks
end

to go
  ; stop the model if there are no wolves and no good-bacteria
  if not any? turtles [ stop ]
```

```
  ; stop the model if there are no wolves and the number of good-bacteria gets very large
  if not any? wolves and count good-bacteria > max-good-bacteria [ user-message "The good-bacteria have inherited the earth" stop ]
  ask good-bacteria [
    move

    ; in this version, good-bacteria eat grass, grass grows, and it costs good-bacteria energy to move
    if model-version = "good-bacteria-wolves-grass" [
      set energy energy - 1  ; deduct energy for good-bacteria only if running good-bacteria-wolves-grass model version
      eat-grass  ; good-bacteria eat grass only if running the good-bacteria-wolves-grass model version
      death ; good-bacteria die from starvation only if running the good-bacteria-wolves-grass model version
    ]

    reproduce-good-bacteria  ; good-bacteria reproduce at a random rate governed by a slider
  ]
  ask wolves [
    move
    set energy energy - 1  ; wolves lose energy as they move
    eat-good-bacteria ; wolves eat a good-bacteria on their patch
    death ; wolves die if they run out of energy
    reproduce-wolves ; wolves reproduce at a random rate governed by a slider
  ]

  if model-version = "good-bacteria-wolves-grass" [ ask patches [ grow-grass ] ]

  tick
  display-labels
end

to move  ; turtle procedure
  rt random 50
  lt random 50
  fd 1
end

to eat-grass  ; good-bacteria procedure
  ; good-bacteria eat grass and turn the patch brown
  if pcolor = green [
    set pcolor brown
    set energy energy + good-bacteria-gain-from-food  ; good-bacteria gain energy by eating
```

```
  ]
end

to reproduce-good-bacteria  ; good-bacteria procedure
  if random-float 100 < good-bacteria-reproduce [  ; throw "dice" to see if you will reproduce
    set energy (energy / 2)               ; divide energy between parent and offspring
    hatch 1 [ rt random-float 360 fd 1 ]   ; hatch an offspring and move it forward 1 step
  ]
end

to reproduce-wolves  ; wolf procedure
  if random-float 100 < wolf-reproduce [  ; throw "dice" to see if you will reproduce
    set energy (energy / 2)               ; divide energy between parent and offspring
    hatch 1 [ rt random-float 360 fd 1 ]  ; hatch an offspring and move it forward 1 step
  ]
end

to eat-good-bacteria  ; bad-bacteria procedure
  let prey one-of sheep-here                    ; grab a random sheep
  if prey != nobody  [                          ; did we get one? if so,
    ask prey [ die ]                            ; kill it, and...
    set energy energy + wolf-gain-from-food     ; get energy from eating
  ]
end

to death  ; turtle procedure (i.e. both wolf and sheep procedure)
  ; when energy dips below zero, die
  if energy < 0 [ die ]
end

to grow-grass  ; patch procedure
  ; countdown on brown patches: if you reach 0, grow some grass
  if pcolor = brown [
    ifelse countdown <= 0
      [ set pcolor green
        set countdown grass-regrowth-time ]
      [ set countdown countdown - 1 ]
  ]
end

to-report grass
  ifelse model-version = "sheep-wolves-grass" [
    report patches with [pcolor = green]
  ]
```

```
  [ report 0 ]
end


to display-labels
  ask turtles [ set label "" ]
  if show-energy? [
    ask wolves [ set label round energy ]
    if model-version = "sheep-wolves-grass" [ ask sheep [ set label round energy ] ]
  ]
end


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```

ChatGPT sample code(still adjusting and improving)

```
globals [
  control-group
  experimental-group
]

turtles-own [
  is-good-bacteria?
  energy
]

to setup
  clear-all
  ; create control group of 10,000 turtles
  create-turtles 10000 [
    set is-good-bacteria? random-float 1.0 < 0.51
    ifelse is-good-bacteria? [
      set color green
    ] [
      set color red
    ]
    setxy random-xcor random-ycor
    set heading random-float 360
    set group control-group
    set energy 100
```

```
  ]
  ; create experimental group of 10,000 turtles
  create-turtles 10000 [
    set is-good-bacteria? random-float 1.0 < 0.51
    ifelse is-good-bacteria? [
      set color green
    ] [
      set color red
    ]
    setxy random-xcor random-ycor
    set heading random-float 360
    set group experimental-group
    set energy 100
  ]
  reset-ticks
end

to go
  ask turtles [
    ; perform group-specific actions
    if group = control-group [
      ; double every 2 hours
      if ticks mod 120 = 0 [
        set energy energy * 2
      ]
      ; decrease by 10% every minute
      set energy energy * 0.999
    ] else if group = experimental-group [
      ; increase by factor of 26.67 every 2 hours
      if ticks mod 120 = 0 [
        set energy energy * 26.67
      ]
      ; decrease by 1% every minute
      set energy energy * 0.99
    ]
  ]
  tick
end
```