

**HIGH PERFORMANCE COMPUTING
IN UNDERGRADUATE RESEARCH**



Sheep breed composition assessment using PCA

Dr. Joel D. Leal-Gutierrez

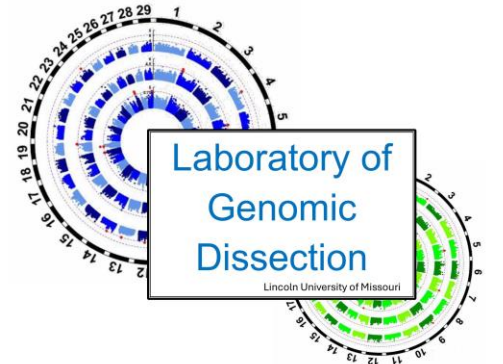
Laboratory of Genomic Dissection

College of Agriculture

Lincoln University of Missouri



College of Agriculture



www.LabOfGenomicDissection.com

Research question: Can I use genomic data to determine the breed composition of individuals in a crossbred sheep population using HPC resources?

www.ocj.com



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CIMUSE



Dr. Joel Leal Gutierrez

Professor of Animal Science

Lincoln University of Missouri

Email

University of Missouri Partners



Mr. Matthew Keeler



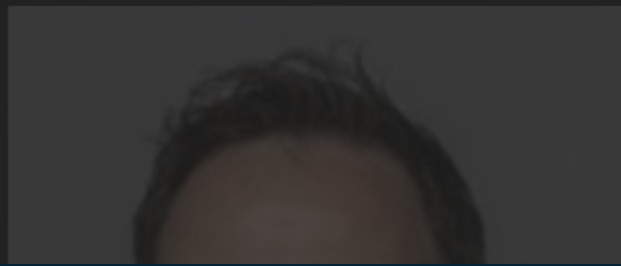
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Mr. Matthew Keeler

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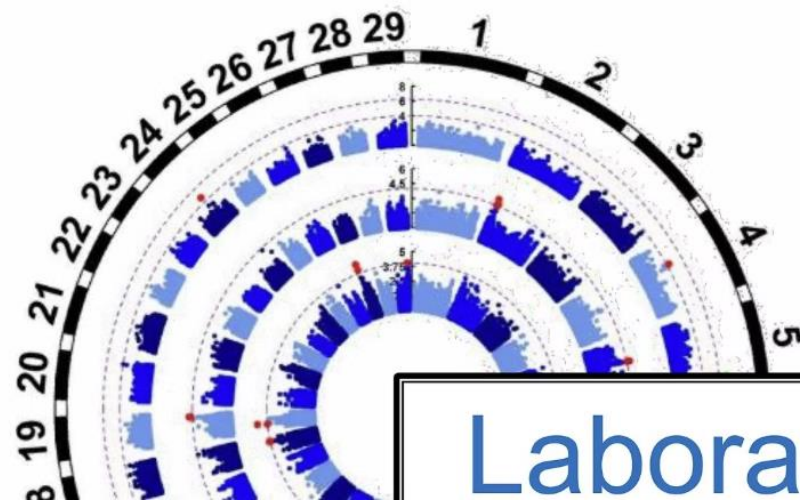
Protocols

Collabs

Grants

Events

Videos



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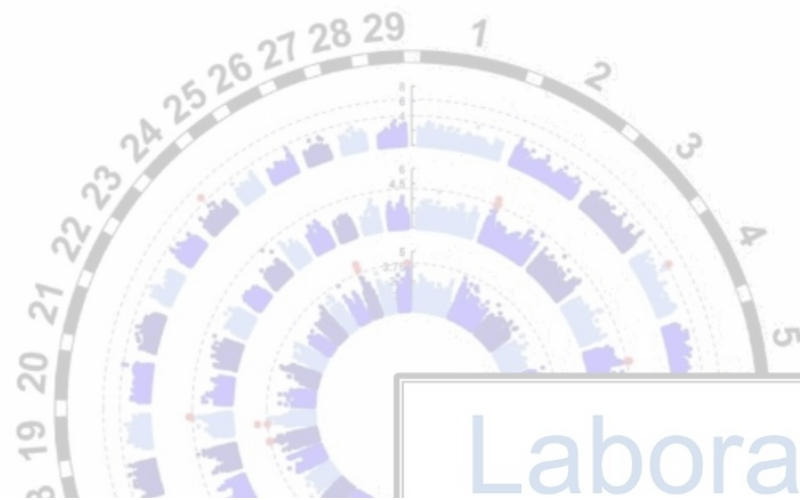
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Wet laboratory protocols

Disclaimer: All protocols are based on the availability of resources in the Laboratory of Genomic Dissection.

[Agarose gel electrophoresis](#)

[Genomic DNA Cleaning & Concentration](#)

[Blood collection](#)

[Primer re-nature and dilution](#)

[Blue Juice 6X loading buffer](#)

[RNA extraction using TRIzol](#)

[DNA extraction Salting-out from blood](#)

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Dry laboratory protocols

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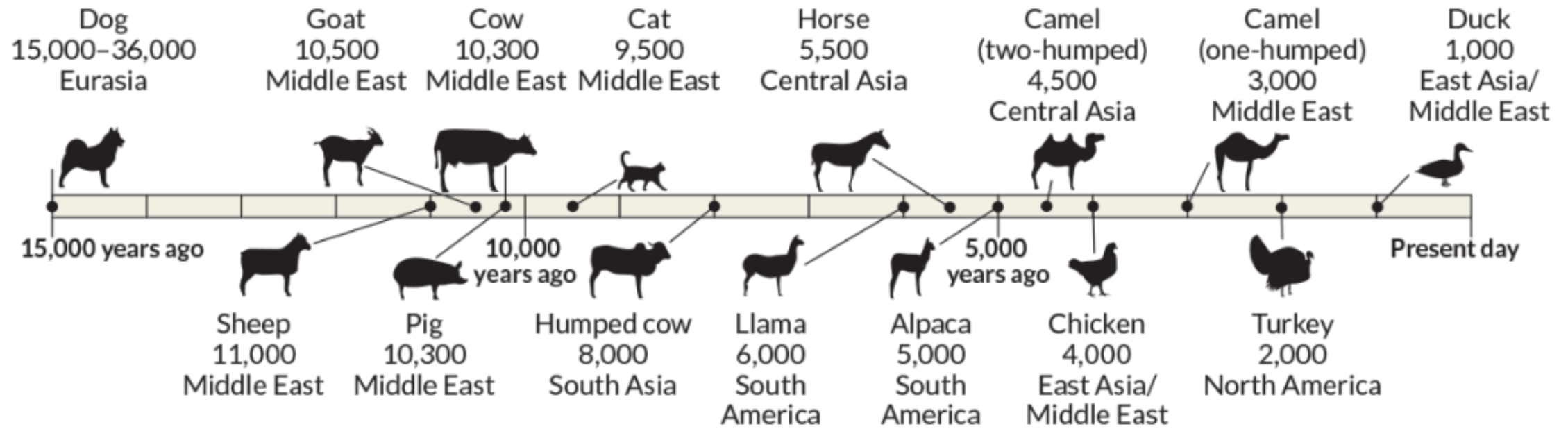
[Swab collection for vaginal microbial assay](#)

Dry laboratory protocols

[Breed composition activity](#)

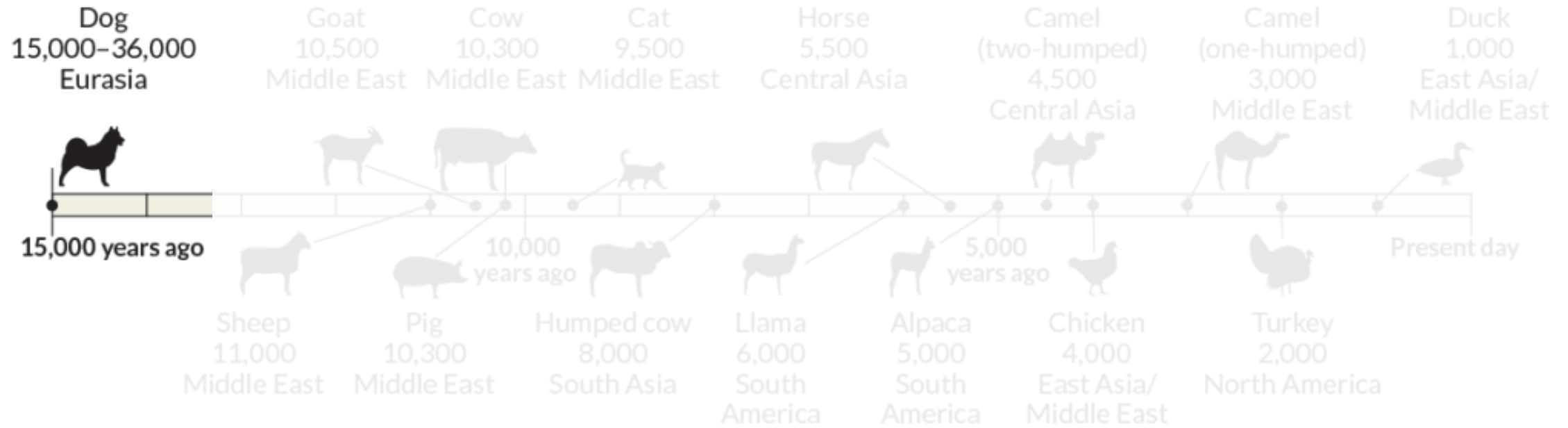
Animal domestication

Approximate time frame of domestication based on archaeology



<https://www.sciencenews.org/article/dna-evidence-rewriting-domestication-origin-stories>

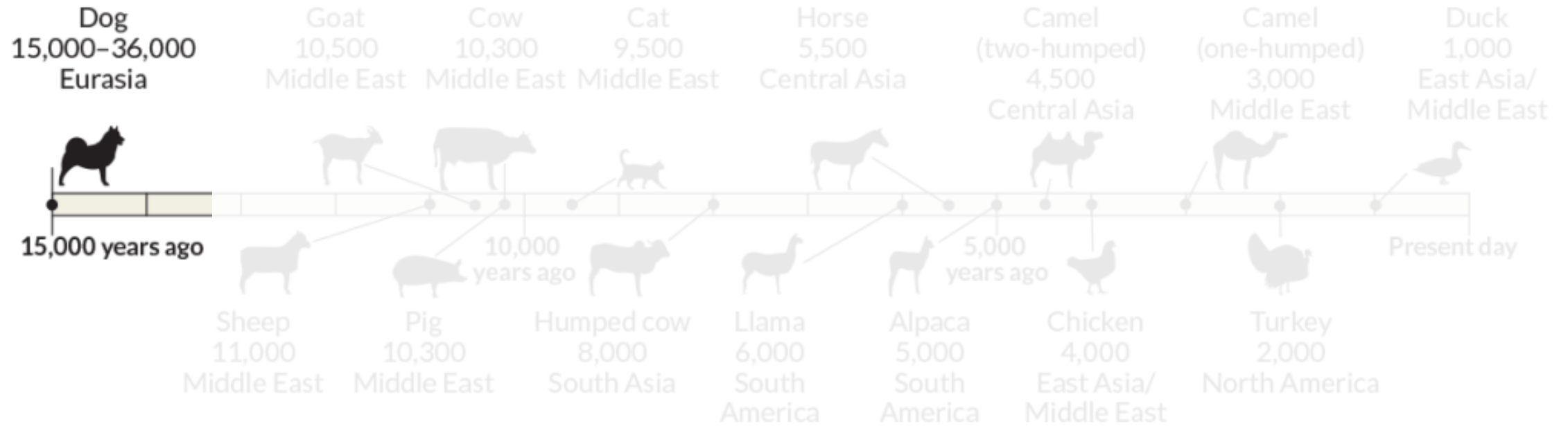
Approximate time frame of domestication based on archaeology



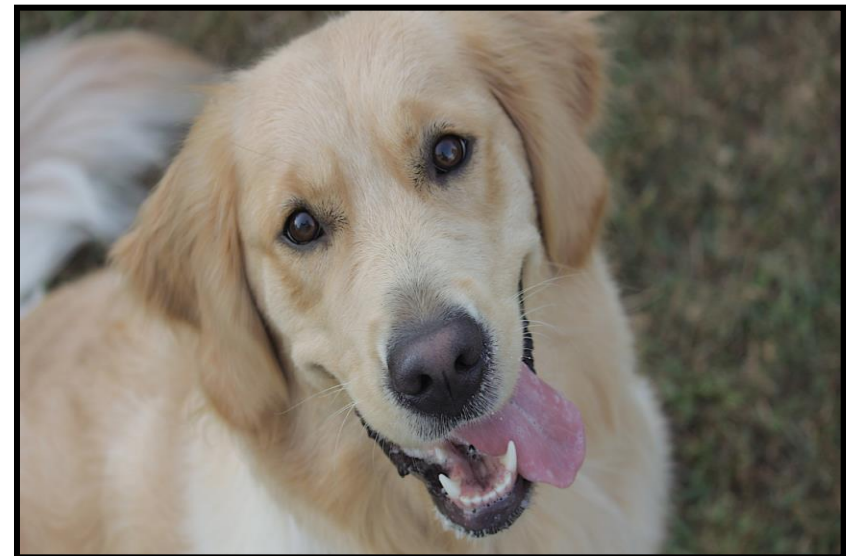
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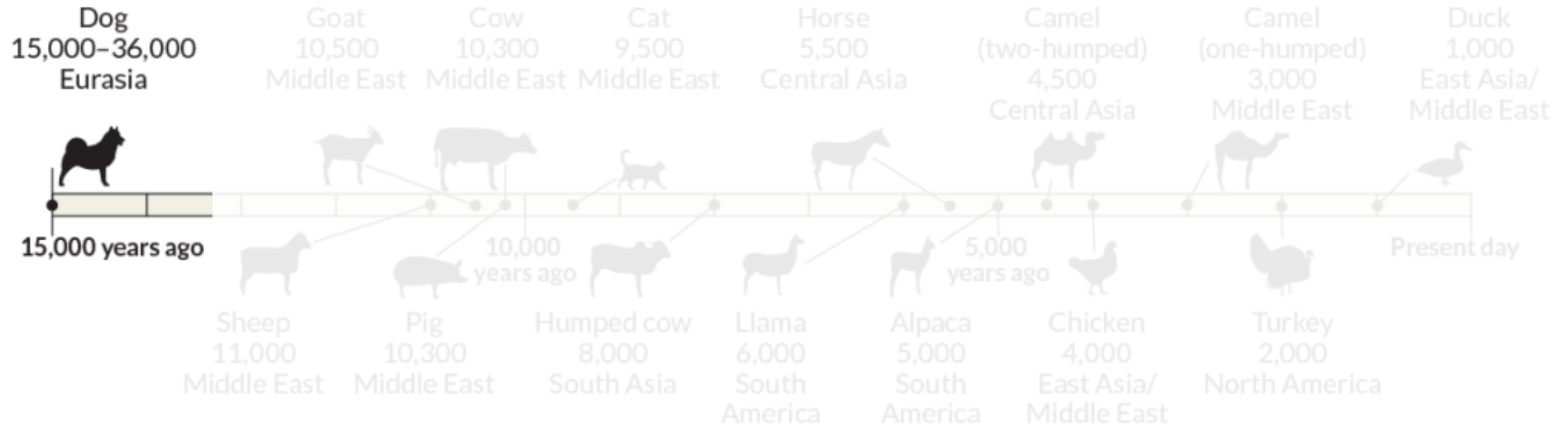
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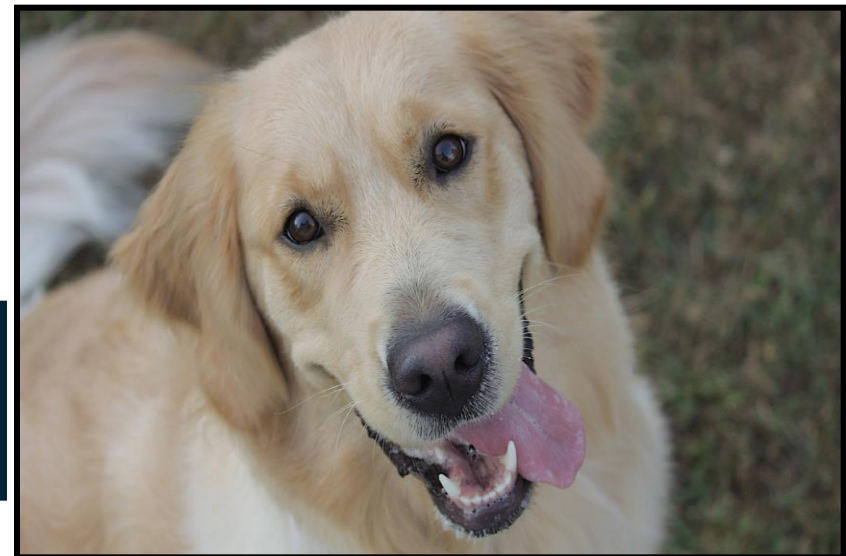
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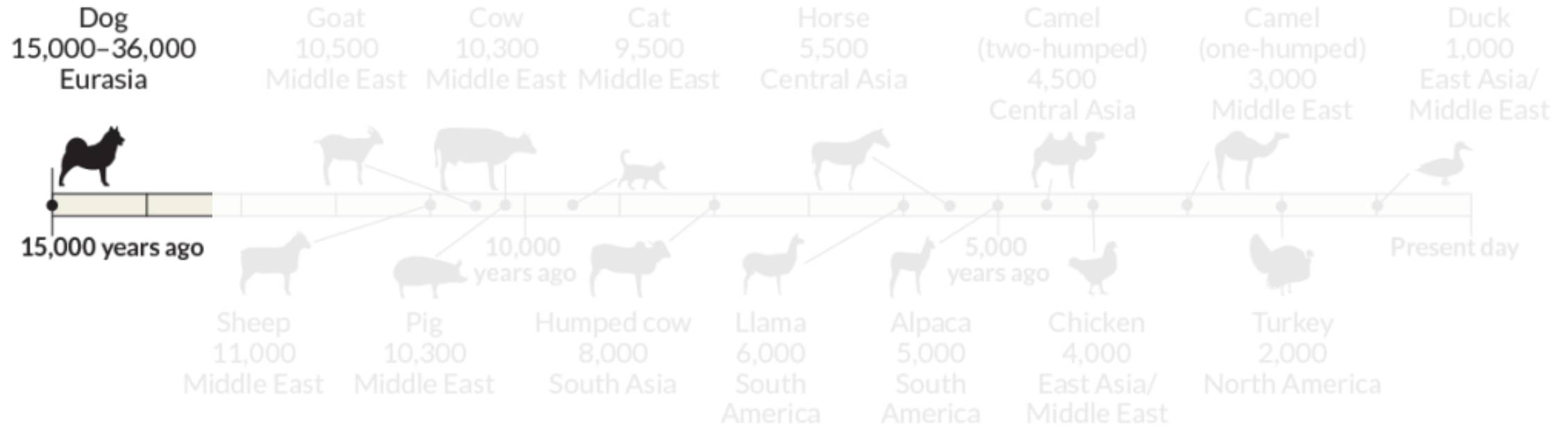
<https://www.sciencenews.org/article/dna-evidence-rewriting-domestication-origin-stories>



Phenotypic selection



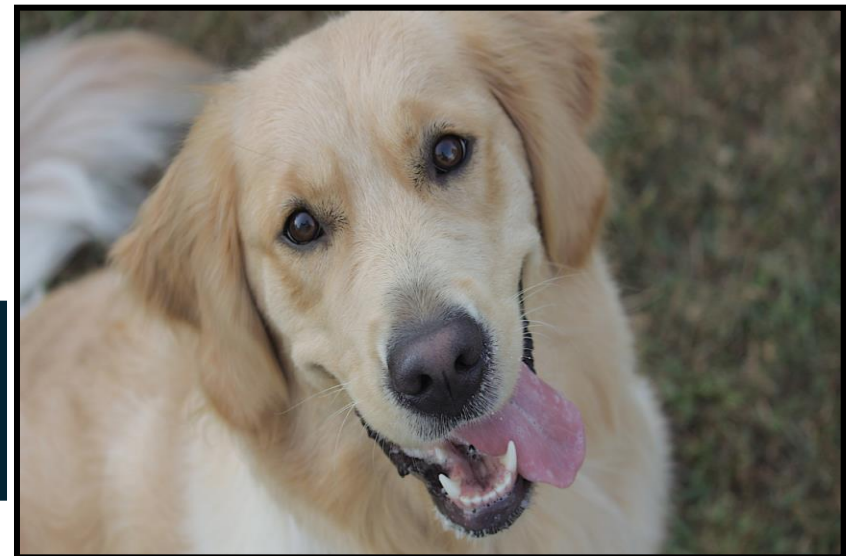
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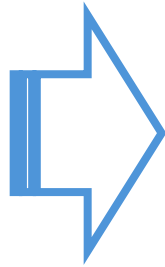


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Genomic
selection

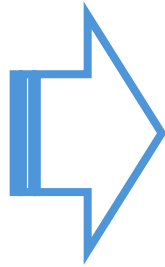




Genomic
selection

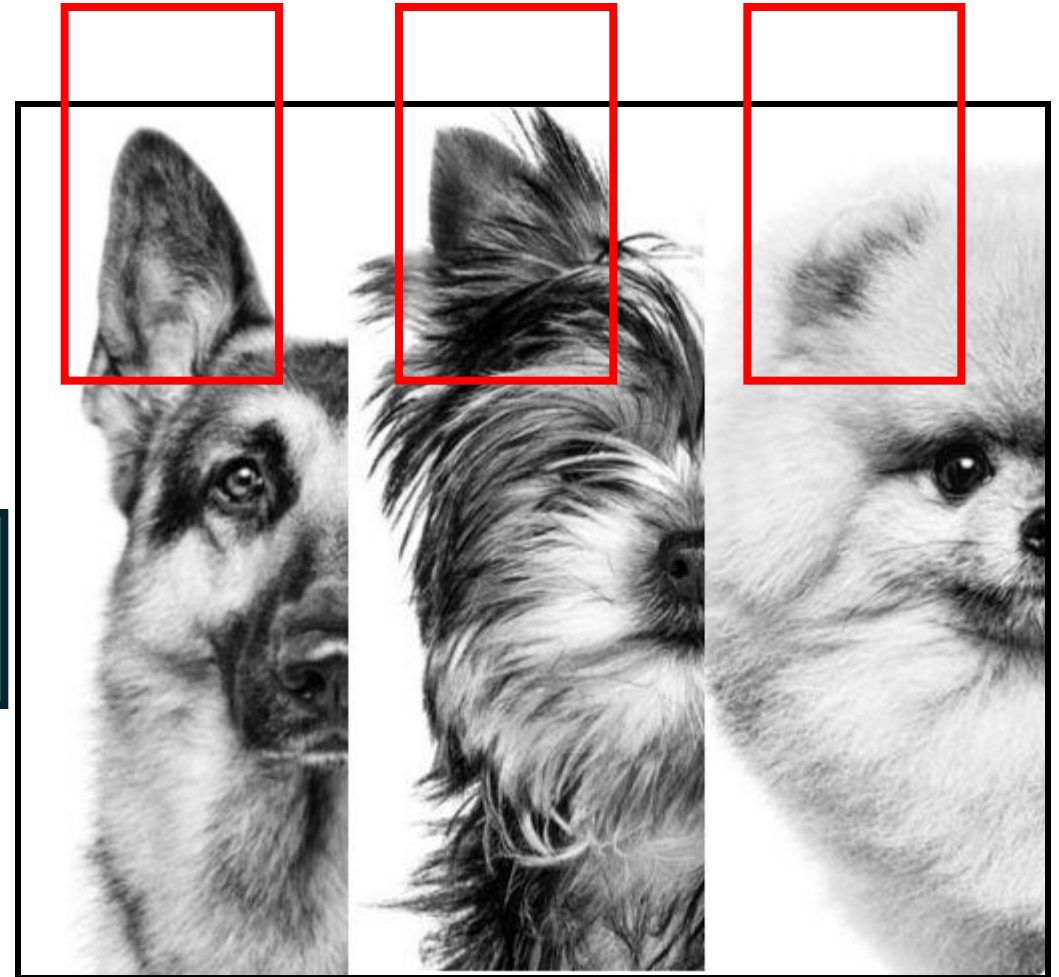


Breeds



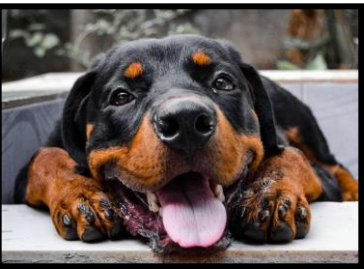
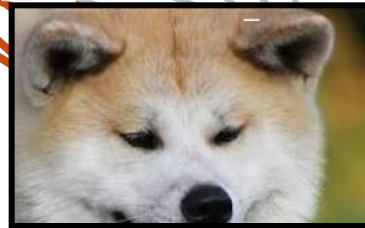
Genomic
selection

Ear shape

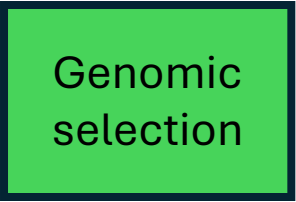


Breeds





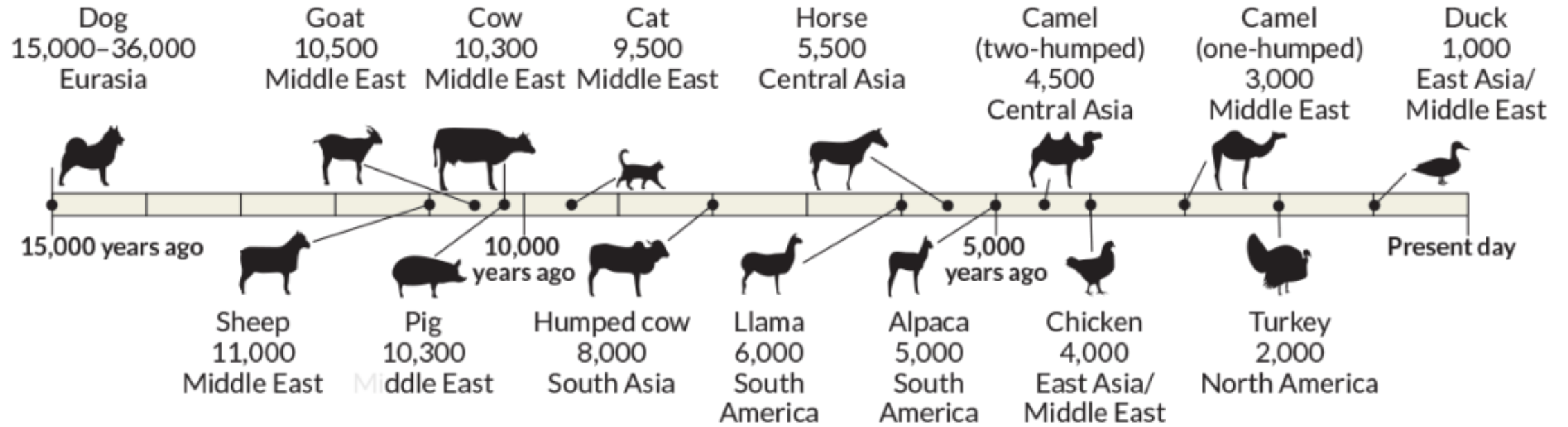
Genomic
selection



Genomic
selection

Genomic variability

Approximate time frame of domestication based on archaeology

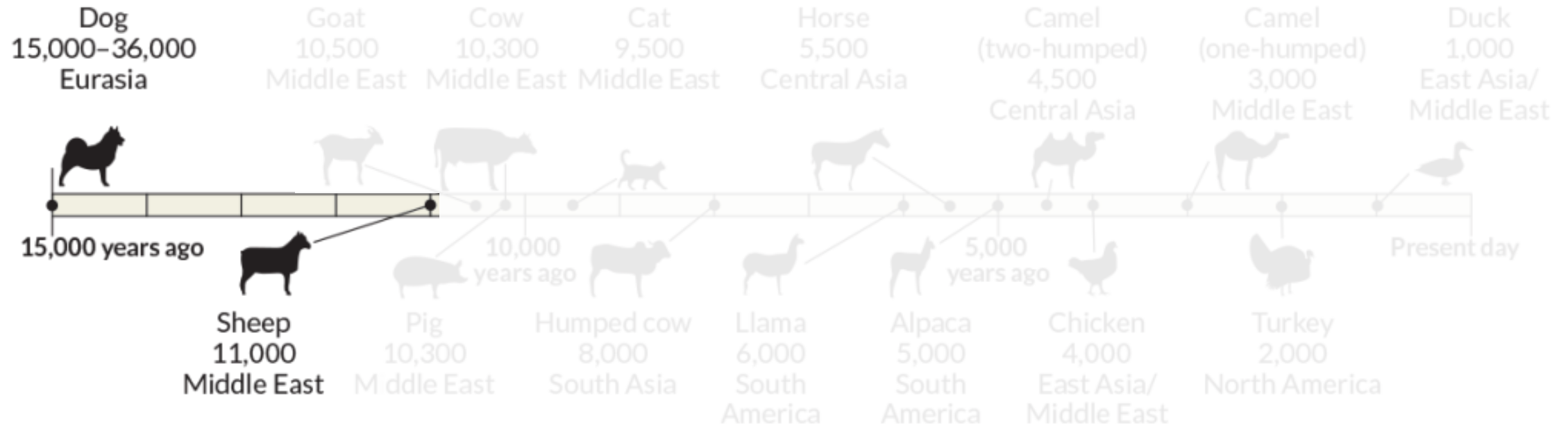


<https://www.sciencenews.org/article/dna-evidence-rewriting-domestication-origin-stories>



Asiatic wild mouflon (*Ovis gmelini*)

Approximate time frame of domestication based on archaeology

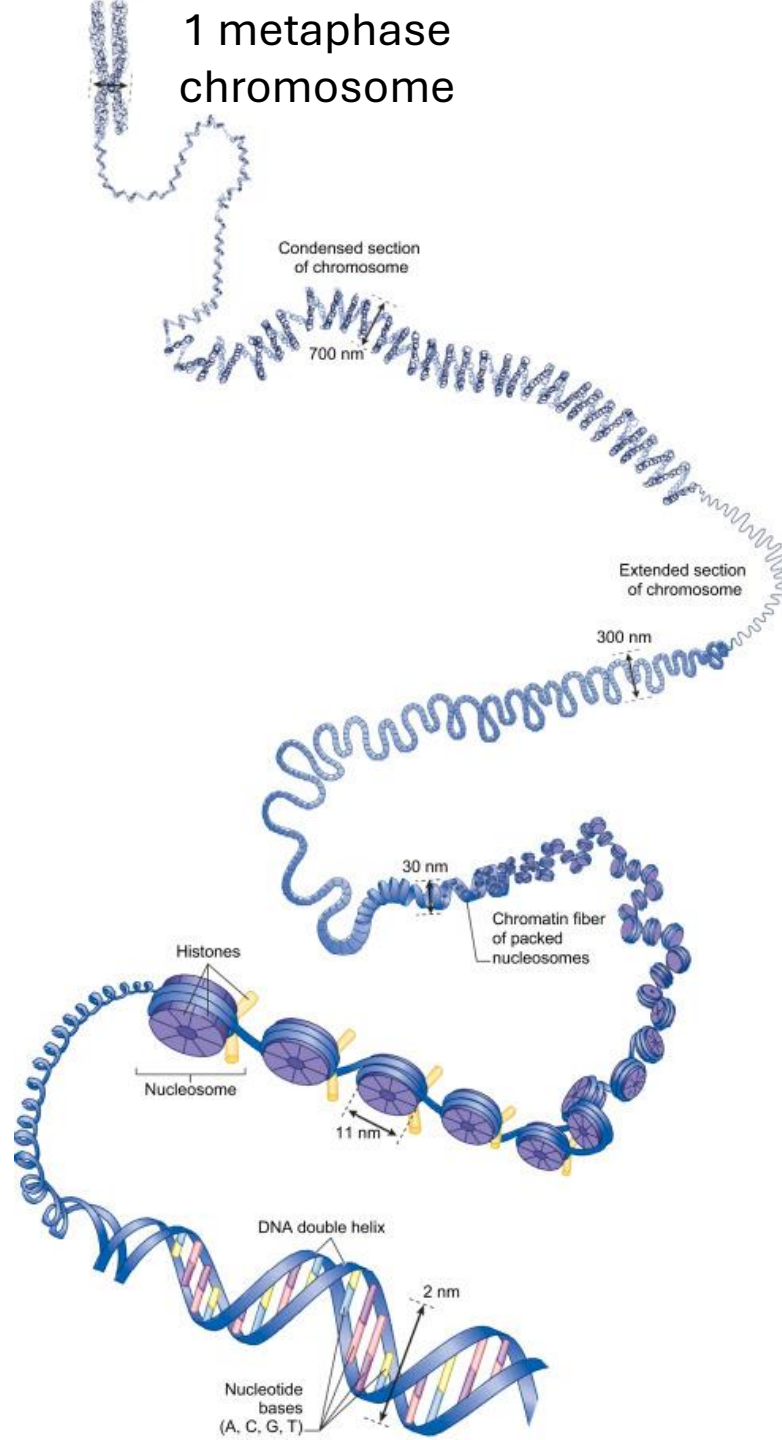


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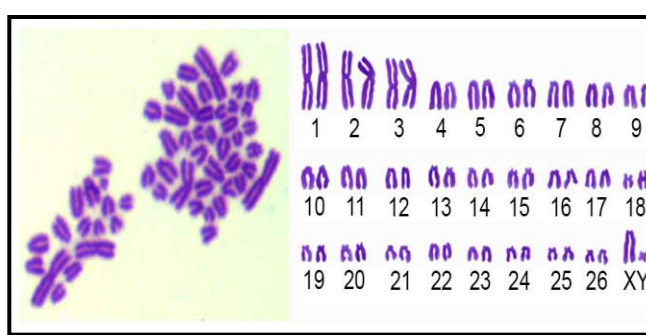
Asiatic wild mouflon (*Ovis gmelini*)

1 metaphase chromosome



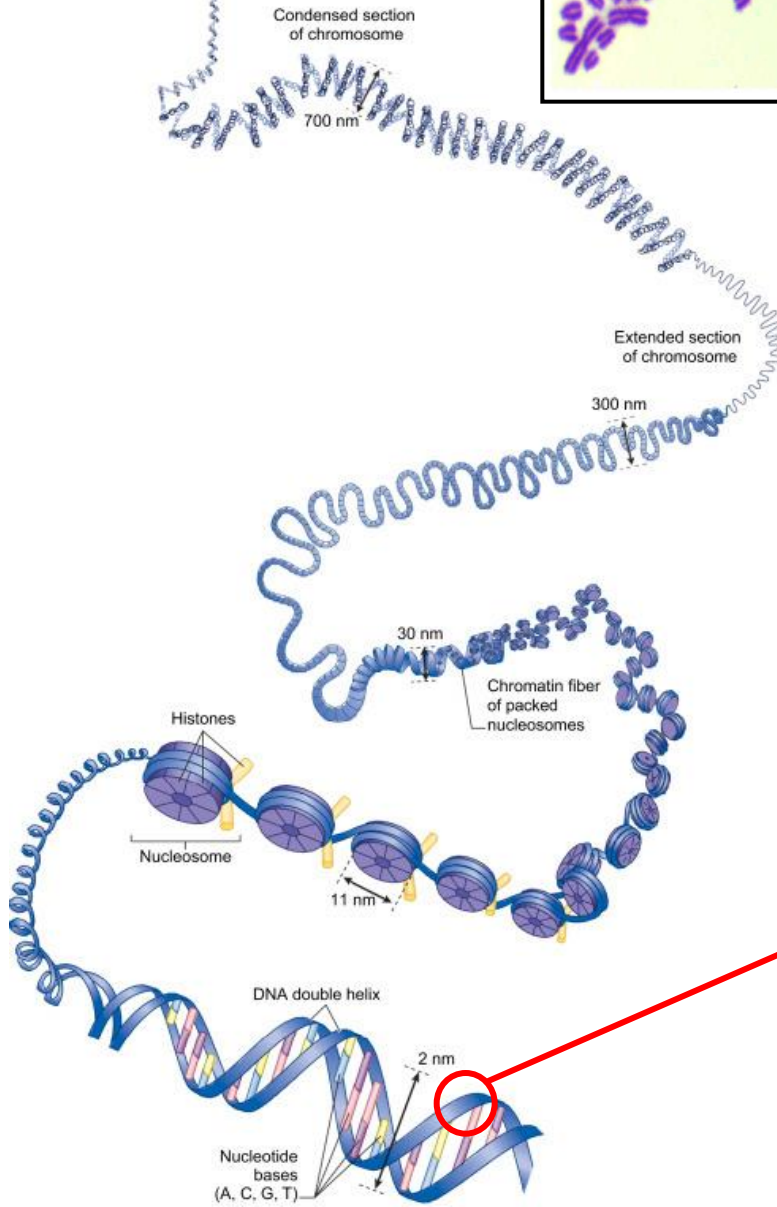
Genomic variability

1 metaphase chromosome

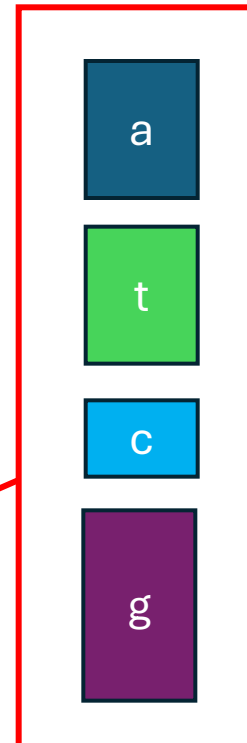


Ji et al., 2016

<https://www.britannica.com/>

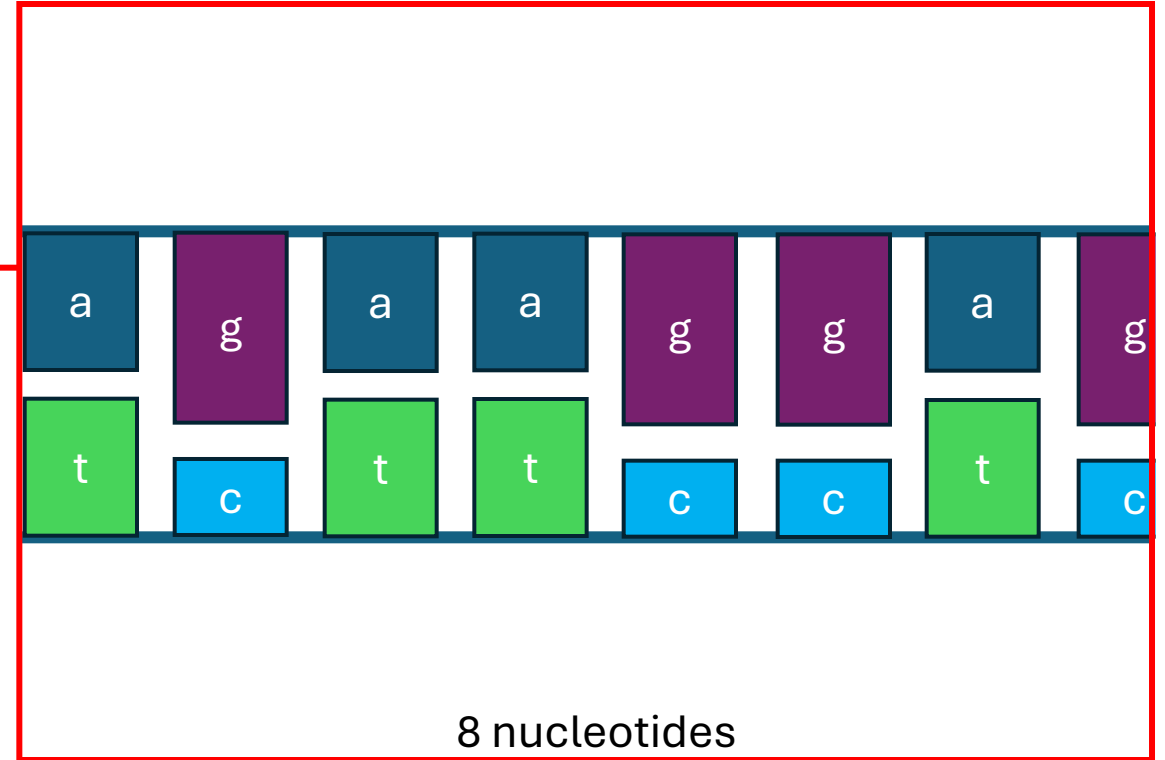
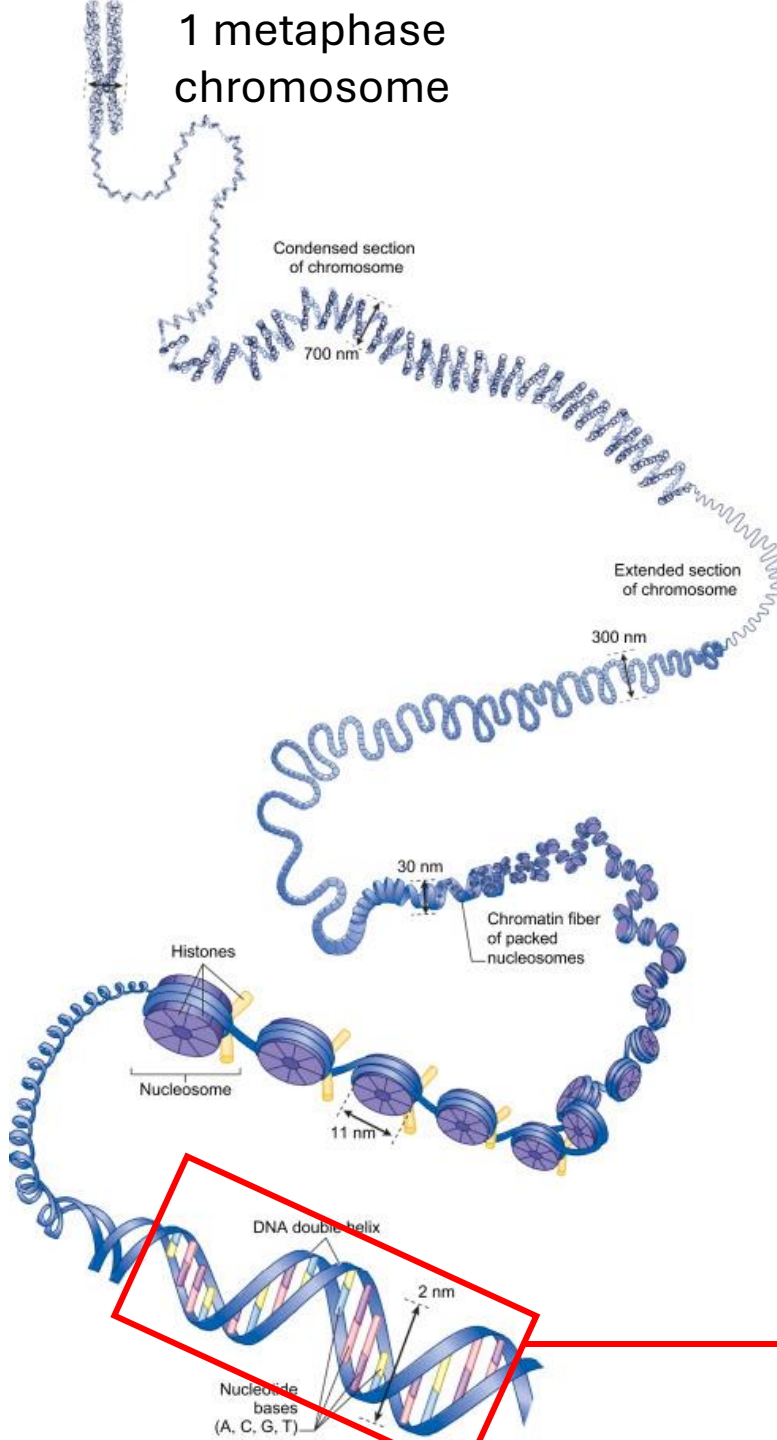


4 nucleotides

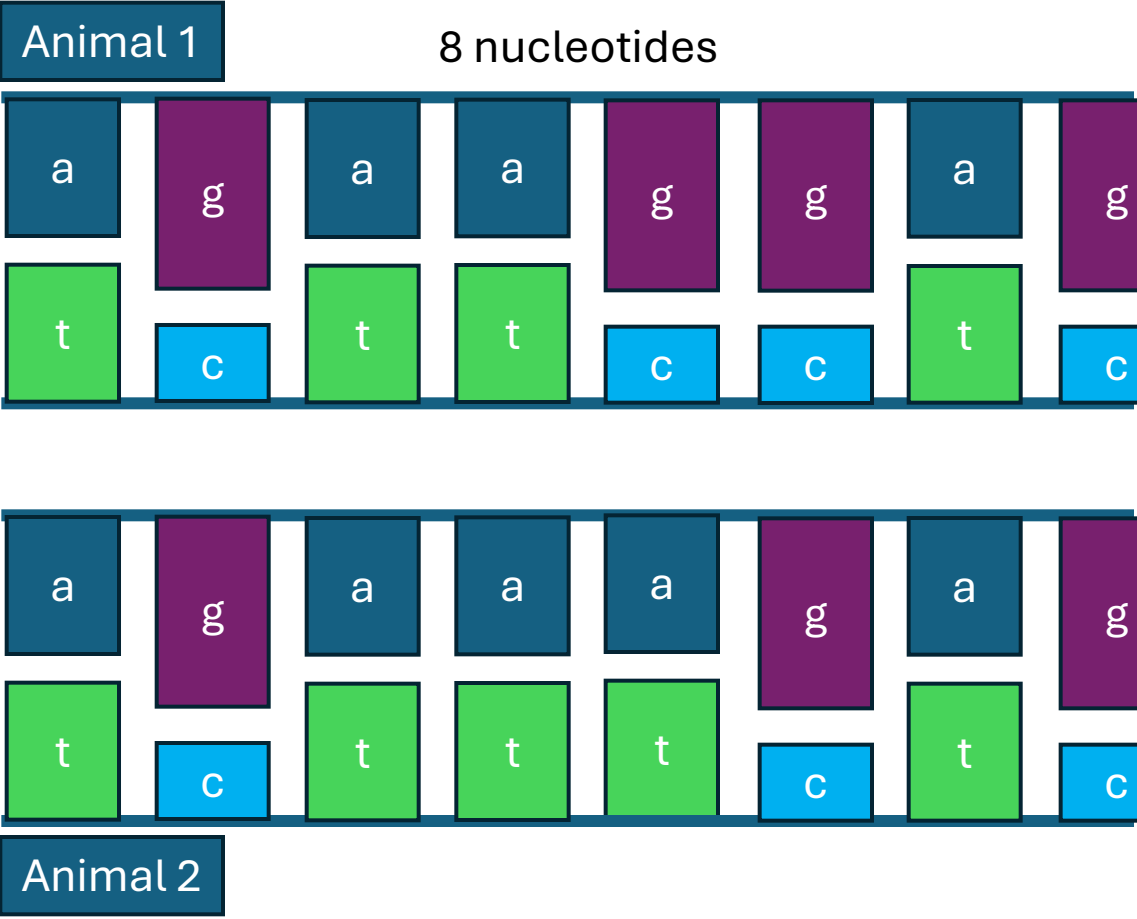


Genomic variability

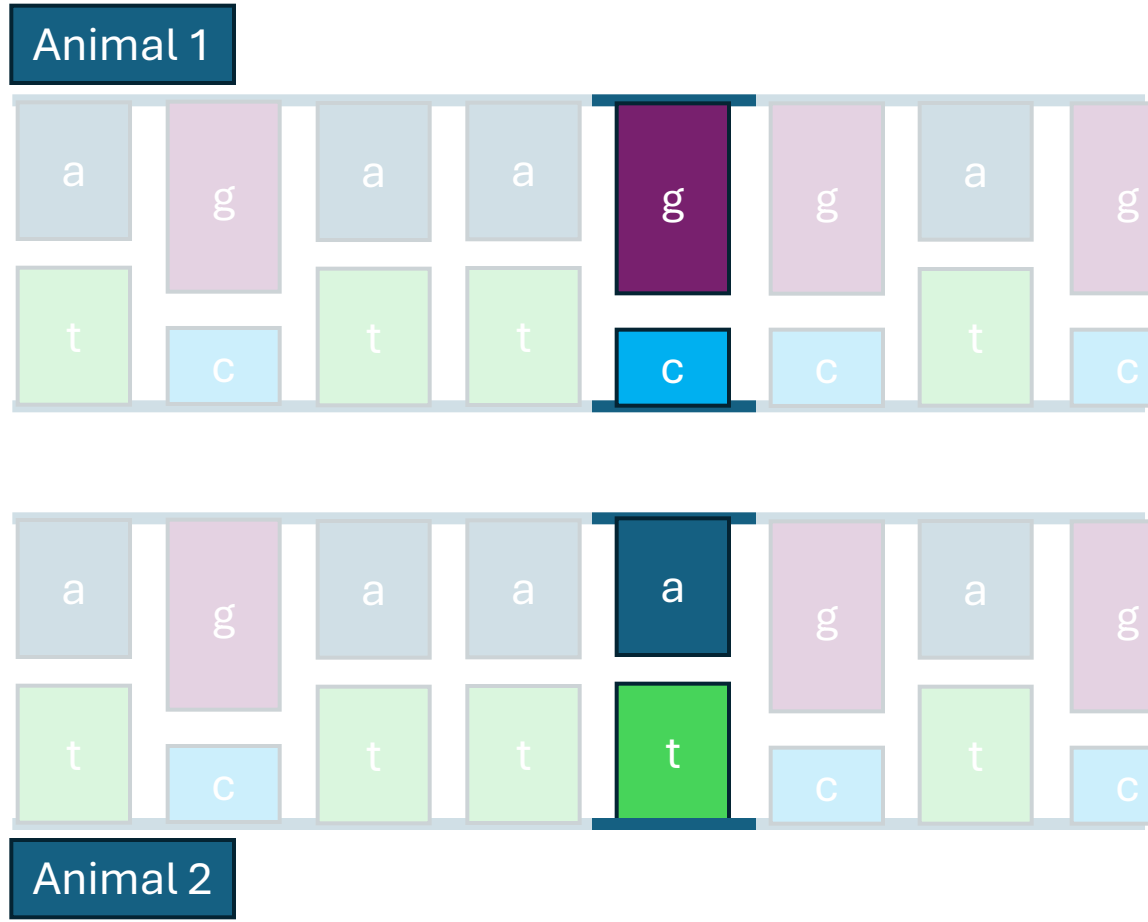
1 metaphase chromosome



Individuals from
the same population

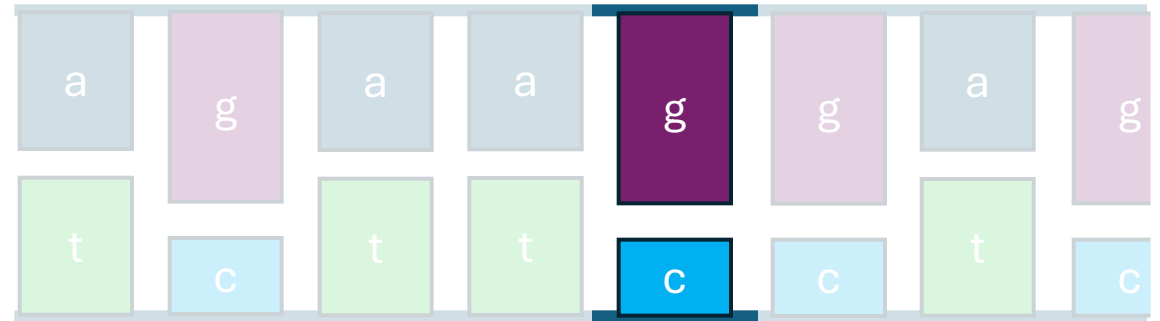


Individuals from
the same population

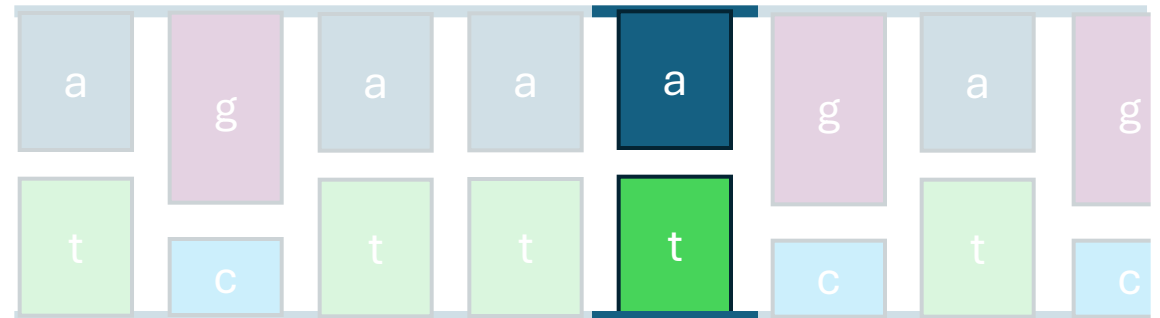


Change G > A in
a known position

Animal 1



Individuals from
the same population



Animal 2



Sheep genome: 2.5 billion bases
distributed into 26 autosomes
and one sex chromosome pair

Individuals from
the same population





Sheep genome: 2.5 billion bases
distributed into 26 autosomes
and one sex chromosome pair

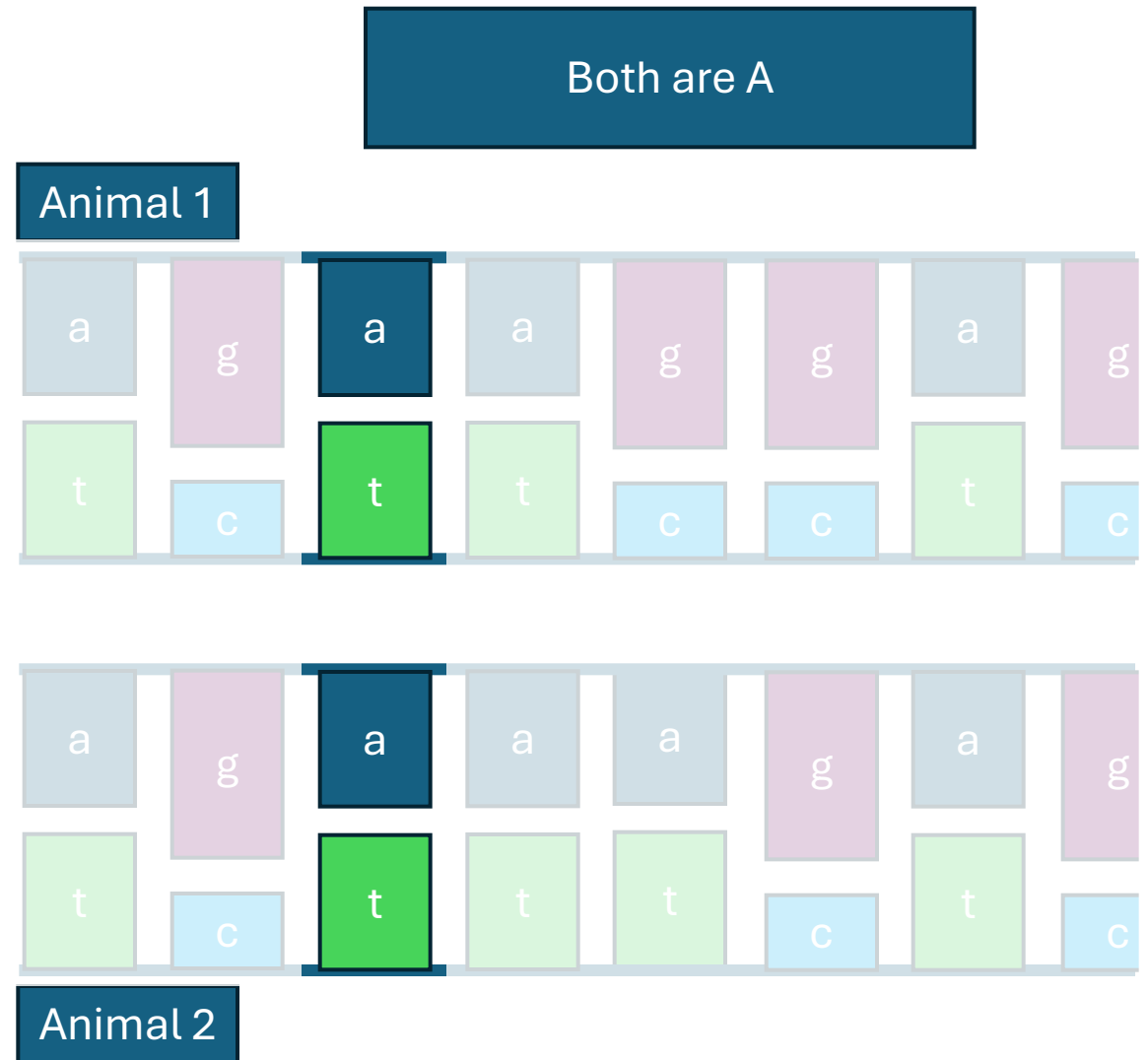
Individuals from
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Sheep genome: 2.5 billion bases
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Individuals from
the same population



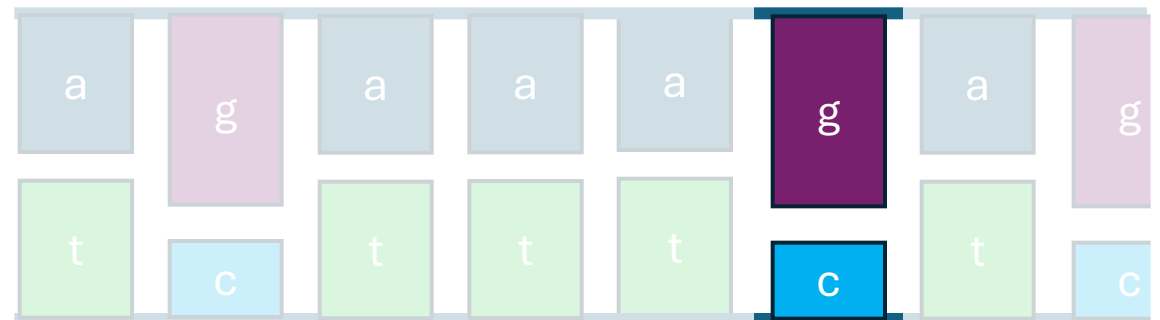
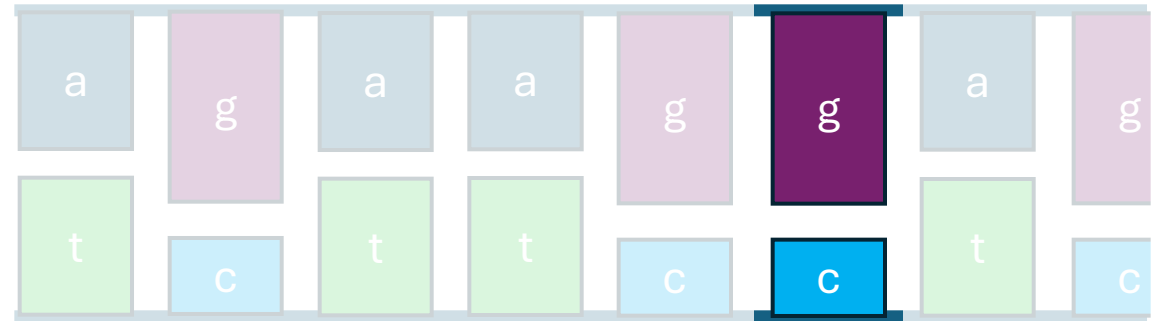


Sheep genome: 2.5 billion bases
distributed into 26 autosomes
and one sex chromosome pair

Individuals from
the same population

Polymorphism?

Animal 1



Animal 2

Specialized sheep breeds for production

Specialized sheep breeds for production



Suffolk sheep



East Friesian sheep

Specialized sheep breeds for production



Suffolk sheep



East Friesian sheep



Specialized sheep breeds for production



Suffolk sheep



East Friesian sheep



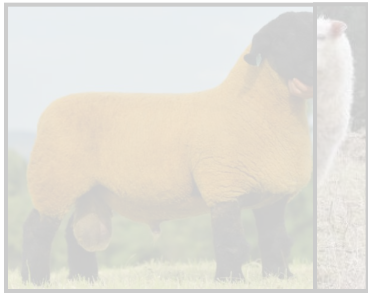
Specialized sheep breeds for production



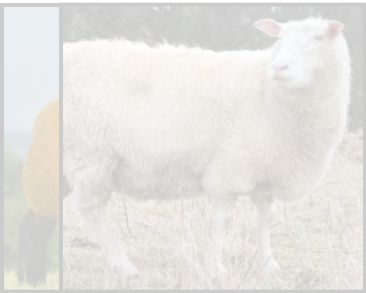
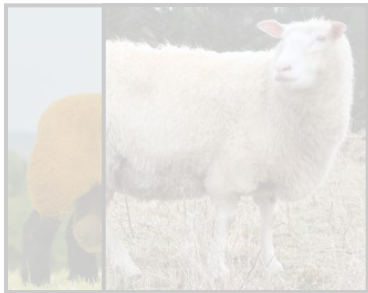
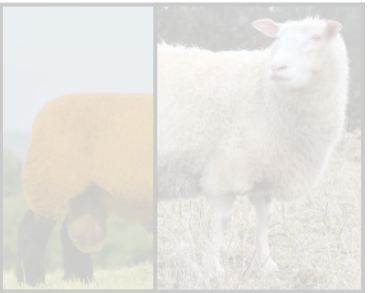
Suffolk sheep



East Friesian sheep



50:50



Specialized sheep breeds for production



Suffolk sheep



East Friesian sheep



- Crossbred:
- 1. Higher productivity
 - 2. Higher resistance
 - 3. Higher prolificacy
 - 4. Double purpose

Specialized sheep breeds for production



Suffolk sheep



East Friesian sheep



- Crossbred:
- 1. Higher productivity
 - 2. Higher resistance
 - 3. Higher prolificacy
 - 4. Double purpose



Breed composition

Files to be used:

Full folder:

<https://figshare.com/s/9148a98043a49e06100e>

Genotypic data filtered:

https://figshare.com/ndownloader/files/65762952?private_link=9148a98043a49e06100e

Breed composition data:

https://figshare.com/ndownloader/files/65762934?private_link=9148a98043a49e06100e

R code:

https://figshare.com/ndownloader/files/65762949?private_link=9148a98043a49e06100e

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 breedComposition	6/19/2026 12:18 P...	Text Document	14 KB
 breedComposition	6/19/2026 12:18 P...	Microsoft Exce...	203 KB
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 genotypicDataFiltered	6/19/2026 10:53 A...	Text Document	176,027 ...
 genotypicDataRecoded	6/18/2026 1:23 PM	Text Document	216,730 ...
 PCA_2PCs	6/19/2026 12:32 P...	Text Document	33 KB
 PCA_Breed_Merged	6/19/2026 12:32 P...	Text Document	42 KB
 populationStructure	6/19/2026 12:14 P...	PNG File	20 KB
 populationStructureCode	6/22/2026 10:03 A...	R File	3 KB

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Raw genotypic data
per animal

2,500,000

Number of animals

700

Provided files:

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Raw genotypic data
per animal

2,500,000

Number of animals

700

Total data points

1,750,000,000

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Genotype

[illegible]

Provided files:

rs1366249228: A/G

$$0/0 = AA$$
$$1/1 = GG$$

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Genotype

[illegible]

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$$0/0 = AA$$

0/1 = ?

1/1 = GG

Genotype

[illegible]

Provided files:

rs1366249228: A/G

$$0/0 = AA$$

0/1 = AG

1/1 = GG

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Genotype

[illegible]

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$$0/0 = AA$$

0/1 = AG

1/1 = GG

$$0/0 = 0$$
$$0/1 = 1$$
$$1/1 = 2$$
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 250KUF	6/18/2026 12:02 P...	vCalendar File	450,554 ...
 breedComposition	6/19/2026 12:18 P...	Text Document	14 KB
 breedComposition	6/19/2026 12:18 P...	Microsoft Exce...	203 KB
 genotypicData	6/18/2026 2:04 PM	Text Document	217,225 ...
 genotypicDataFiltered	6/19/2026 10:53 A...	Text Document	176,027 ...
 genotypicDataRecoded	6/18/2026 1:23 PM	Text Document	216,730 ...
 PCA_2PCs	6/19/2026 12:32 P...	Text Document	33 KB
 PCA_Breed_Merged	6/19/2026 12:32 P...	Text Document	42 KB
 populationStructure	6/19/2026 12:14 P...	PNG File	20 KB
 populationStructureCode	6/22/2026 10:03 A...	R File	3 KB

$$0/0 = AA$$

0/1 = AG

1/1 = GG

$$0/0 = 0$$
 $0/1 = 1$
$$1/1 = 2$$

Exclusion of non-polymorphic markers

[illegible]

Provided files:

rs1366249228: A/G

Name	Date modified	Type	Size
 .Rhistory	6/19/2026 12:33 P...	RHISTORY File	8 KB
 250KUF	6/18/2026 12:02 P...	vCalendar File	450,554 ...
 breedComposition	6/19/2026 12:18 P...	Text Document	14 KB
 breedComposition	6/19/2026 12:18 P...	Microsoft Exce...	203 KB
 genotypicData	6/18/2026 2:04 PM	Text Document	217,225 ...
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 PCA_2PCs	6/19/2026 12:32 P...	Text Document	33 KB
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 populationStructure	6/19/2026 12:14 P...	PNG File	20 KB
 populationStructureCode	6/22/2026 10:03 A...	R File	3 KB

$$0/0 = AA$$

0/1 = AG

1/1 = GG

$$0/0 = 0$$
 $0/1 = 1$
$$1/1 = 2$$

Exclusion of non-polymorphic markers

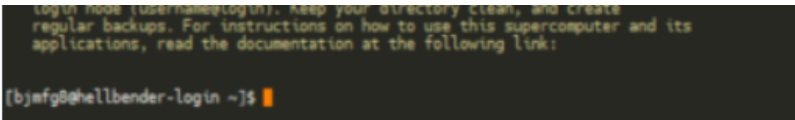


No genomic variability

[illegible]

Run the R script for analysis

- Go to <https://docs.itrss.umsystem.edu/pub/hpc/hellbender>



```
login node (username@login). Keep your directory clean, and create  
regular backups. For instructions on how to use this supercomputer and its  
applications, read the documentation at the following link:  
  
[bjmfg@hellbender-login ~]$
```

Browser

See https://docs.itrss.umsystem.edu/pub/hpc/hellbender#open_ondemand on how to access Hellbender via Open OnDemand.

Open OnDemand

- <https://ondemand.rnet.missouri.edu> - Hellbender Open OnDemand (Researcher)
- <https://hb-classes.missouri.edu> - Hellbender Classes Open OnDemand (Classes)

OnDemand provides an integrated, single access point for all of your HPC resources. The following apps are currently available on Hellbender's Open OnDemand.

- Jupyter Notebook
- RStudio Server
- Virtual Desktop
- VSCode

- Go to <https://docs.itrss.umsystem.edu/pub/hpc/hellbender>

```
login node (username@login). Keep your directory clean, and create
regular backups. For instructions on how to use this supercomputer and its
applications, read the documentation at the following link:

[bjmf9@hellbender-login ~]$
```

Browser

See https://docs.itrss.umsystem.edu/pub/hpc/hellbender#open_ondemand on how to access Hellbender via Open OnDemand.

Open OnDemand

- <https://ondemand.rnet.missouri.edu> - Hellbender Open OnDemand (Researcher)
- <https://hb-classes.missouri.edu> - Hellbender Classes Open OnDemand (Classes)

OnDemand provides an integrated, single access point for all of your HPC resources. The following apps are currently available on Hellbender's Open OnDemand.

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IT Research Support Solutions

University of Missouri

OnDemand provides an integrated, single access point for all of your HPC resources.

Pinned Apps A featured subset of **all available apps**



Code Server

System Installed App



RStudio Server

System Installed App



Jupyter Notebook

System Installed App



Matlab

System Installed App



Hellbender Desktop

System Installed App



VMD

System Installed App



MatLab (Web)

System Installed App



Hellbender Shell Access

System Installed App



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University of Missouri

OnDemand provides an integrated, single access point for all of your HPC resources.

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Code Server

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Matlab

System Installed App



Hellbender Desktop

System Installed App



VMD

System Installed App



MatLab (Web)

System Installed App



Hellbender Shell Access

System Installed App

Interactive Apps	
Desktops	
 Hellbender Desktop	
GUIs	
 Matlab	
 VMD	
Servers	
 Code Server	
 Jupyter Notebook	
 MatLab (Web)	
 RStudio Server	

Hellbender Desktop

This app will launch an interactive desktop on one or more compute nodes. You will have full access to the resources these nodes provide. This is analogous to an interactive batch job.

Account

general

Partition

cimuse-class

Number of hours

1

Maximum of 48 hours

Node Type

CPU

Number of Nodes

1

Number of CPUs

1

Memory (GB)

30

Advanced Options

Enter additional SLURM options.

Enter additional SLURM options.

For example, to run in a reservation use `--reservation=my_reservation`. To run an MPI application use `--ntasks` or `--ntasks-per-node`.

Launch

* The Hellbender Desktop session data for this session can be accessed under the [data root directory](#).



Regular maintenance is scheduled for Tuesday, August 11th 2026, from 8:00 AM to 5:00 PM. The Hellbender cluster will be unavailable at this time.

Session was successfully created.



Home / My Interactive Sessions

Interactive Apps

Desktops

Hellbender Desktop

GUIs

Matlab

VMD

Servers

Code Server

Jupyter Notebook

MatLab (Web)

RStudio Server

Hellbender Desktop (15282851)

Queued

Created at: 2026-07-23 15:46:20 CDT

Cancel

Time Requested: 1 hour

Session ID: 9e57c54b-f4ed-4351-8b5c-a587d8409516

Please be patient as your job currently sits in queue. The wait time depends on the number of cores as well as time requested.

Hellbender Desktop (15281835)

Completed | |

Created at: 2026-07-23 15:06:46 CDT

Delete

Session ID: 4d37fc15-da08-45e1-9ba1-33573a315b2d

For debugging purposes, this card will be retained for 6 more days

Hellbender Desktop (15282851)

1 node

1 core

Running

Host: [_c221.mgmt.hellbender](#)

Cancel

Created at: 2026-07-23 15:46:20 CDT

Time Remaining: 59 minutes

Session ID: [9e57c54b-f4ed-4351-8b5c-a587d8409516](#)

Compression



0 (low) to 9 (high)

Image Quality



0 (low) to 9 (high)

Launch Hellbender Desktop

View Only (Share-able Link)

Hellbender Desktop (15282851)

1 node

1 core

Running

Host: `>_ c221.mgmt.hellbender`

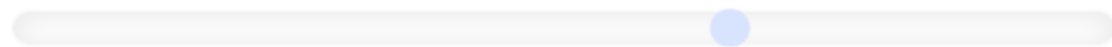
Cancel

Created at: 2026-07-23 15:46:20 CDT

Time Remaining: 59 minutes

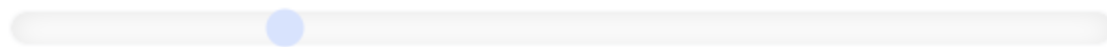
Session ID: 9e57c54b-f4ed-4351-8b5c-a587d8409516

Compression



0 (low) to 9 (high)

Image Quality



0 (low) to 9 (high)

Launch Hellbender Desktop

View Only (Share-able Link)



Applications

All Bookmarks

Thu 23 Jul, 15:48 Joel David Leal Gutierrez



Trash



File System



Home



3:48 PM



Applications

All Bookmarks

Thu 23 Jul, 15:48 Joel David Leal Gutierrez



Trash



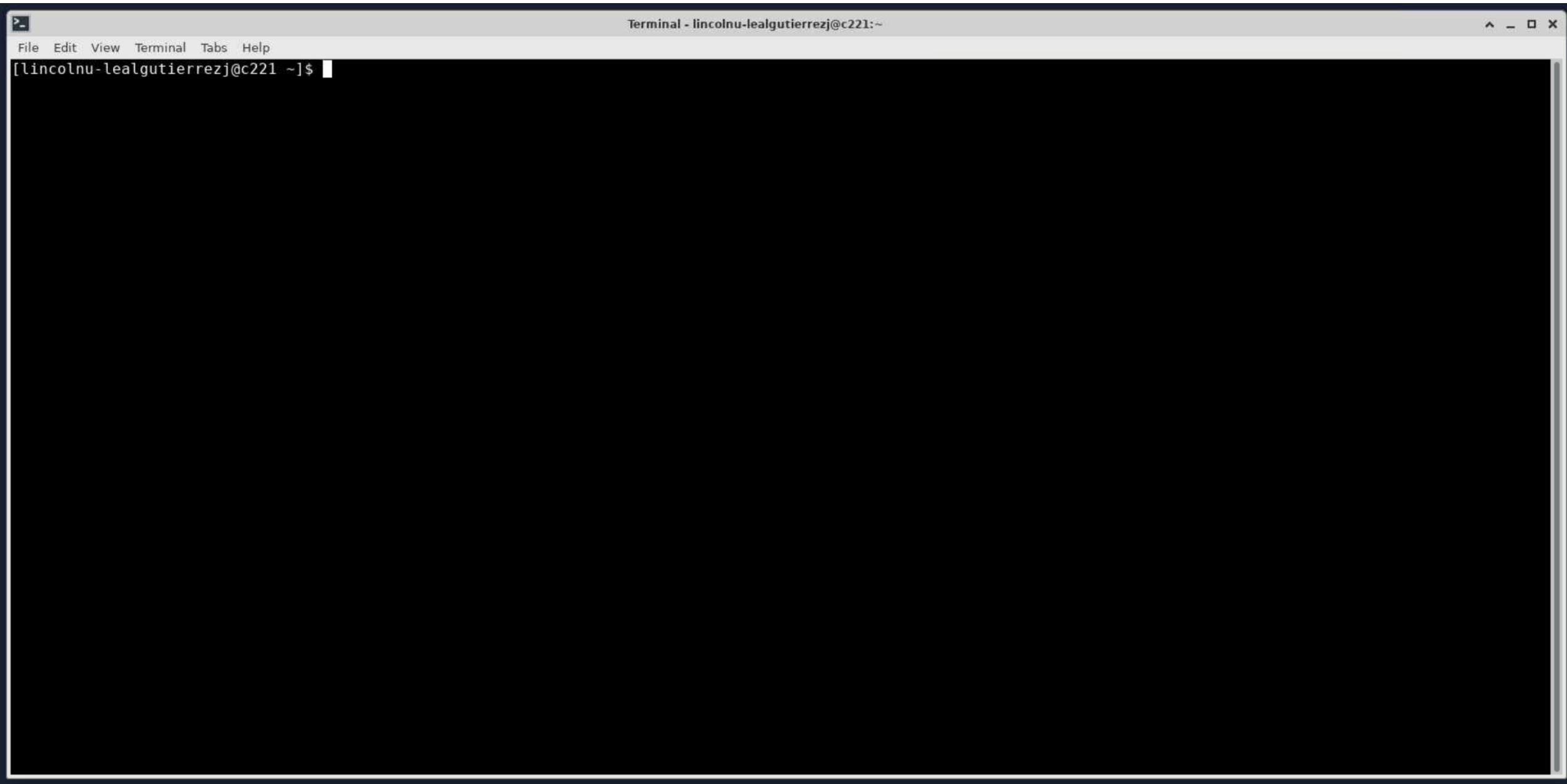
File System

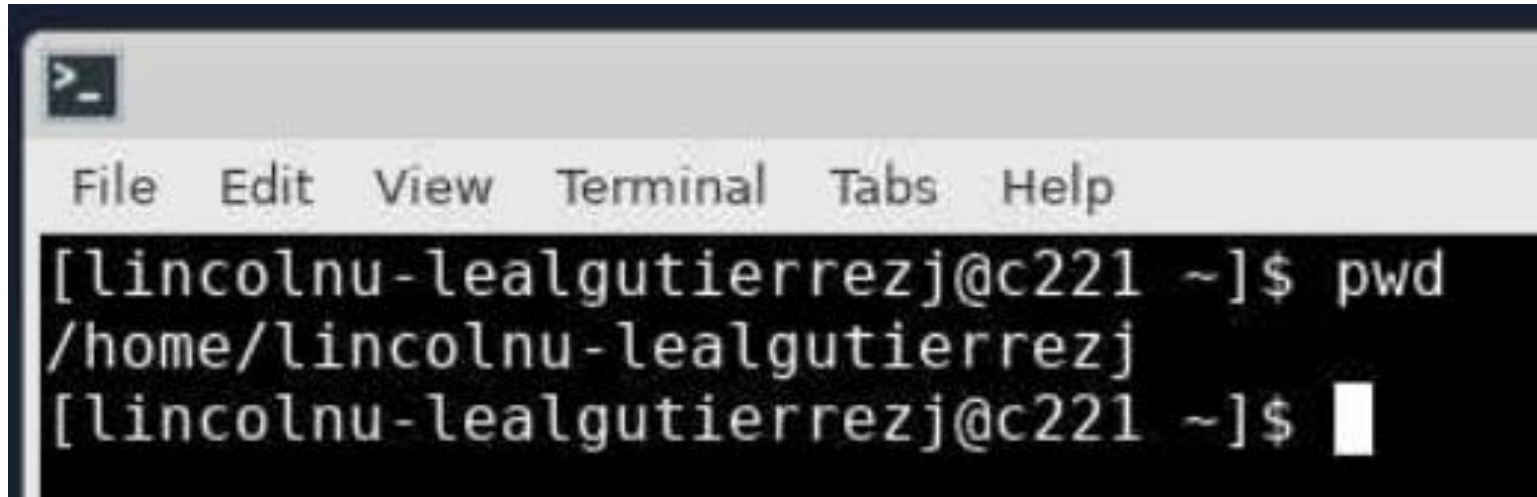


Home



3:48 PM





```
>_  
File Edit View Terminal Tabs Help  
[lincolnu-lealgutierrezj@c221 ~]$ pwd  
/home/lincolnu-lealgutierrezj  
[lincolnu-lealgutierrezj@c221 ~]$
```

```
[lincolnu-lealgutierrezj@c221 ~]$ ls  
cimuseWorkshop  data  Desktop  ondemand  R  
[lincolnu-lealgutierrezj@c221 ~]$
```

```
[lincolnu-lealgutierrezj@c221 ~]$ ls  
cimuseWorkshop  data  Desktop  ondemand  R  
[lincolnu-lealgutierrezj@c221 ~]$
```

We need the folder “cimuseWorkshop”

```
[lincolnu-lealgutierrezj@c221 ~]$ ls  
cimuseWorkshop data Desktop ondemand R  
[lincolnu-lealgutierrezj@c221 ~]$
```

We need the folder “cimuseWorkshop”

```
[lincolnu-lealgutierrezj@c221 ~]$ cp -r /cluster/pixstor/cimuse-workshop/cimuseWorkshop/ .  
[lincolnu-lealgutierrezj@c221 ~]$
```

```
[lincolnu-lealgutierrezj@c221 ~]$ ls  
cimuseWorkshop data Desktop ondemand R  
[lincolnu-lealgutierrezj@c221 ~]$
```

We need the folder “cimuseWorkshop”

```
[lincolnu-lealgutierrezj@c221 ~]$ cp -r /cluster/pixstor/cimuse-workshop/cimuseWorkshop/ .  
[lincolnu-lealgutierrezj@c221 ~]$
```

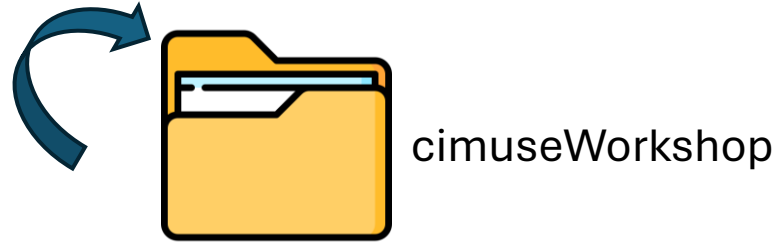
```
[lincolnu-lealgutierrezj@c221 ~]$ ls  
cimuseWorkshop data Desktop ondemand R  
[lincolnu-lealgutierrezj@c221 ~]$
```

```
[lincolnu-lealgutierrezj@c221 ~]$ ls  
cimuseWorkshop data Desktop ondemand R  
[lincolnu-lealgutierrezj@c221 ~]$
```

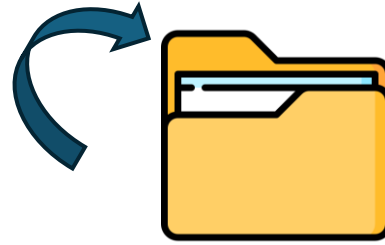
We need the folder “cimuseWorkshop”

```
[lincolnu-lealgutierrezj@c221 ~]$ cp -r /cluster/pixstor/cimuse-workshop/cimuseWorkshop/ .  
[lincolnu-lealgutierrezj@c221 ~]$
```

```
[lincolnu-lealgutierrezj@c221 ~]$ ls  
cimuseWorkshop data Desktop ondemand R  
[lincolnu-lealgutierrezj@c221 ~]$
```



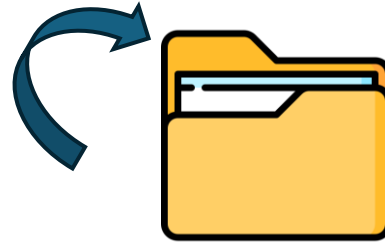
```
[lincolnu-lealgutierrezj@c221 ~]$ cd cimuseWorkshop/
```



cimuseWorkshop

```
[lincolnu-lealgutierrezj@c221 ~]$ cd cimuseWorkshop/
```

```
[lincolnu-lealgutierrezj@c221 cimuseWorkshop]$ ls
250KUF.vcf          genotypicDataFilteredPCARun.txt  PCA_Breed_MergedBuying.txt
breedCompositionBuying.txt  genotypicDataFiltered.txt        PCA_Breed_Merged.txt
breedComposition.txt      genotypicDataRecoded.txt         populationStructureCode.R
breedComposition.xls      genotypicData.txt                populationStructureCode.txt
cimuseWorkshop           PCA_2PCs.txt                     populationStructure.png
[lincolnu-lealgutierrezj@c221 cimuseWorkshop]$
```



cimuseWorkshop

```
[lincolnu-lealgutierrezj@c221 ~]$ cd cimuseWorkshop/
```

```
[lincolnu-lealgutierrezj@c221 cimuseWorkshop]$ ls
250KUF.vcf          genotypicDataFilteredPCARun.txt  PCA_Breed_MergedBuying.txt
breedCompositionBuying.txt  genotypicDataFiltered.txt        PCA_Breed_Merged.txt
breedComposition.txt      genotypicDataRecoded.txt         populationStructureCode.R
breedComposition.xls      genotypicData.txt                populationStructureCode.txt
cimuseWorkshop           PCA_2PCs.txt                    populationStructure.png
[lincolnu-lealgutierrezj@c221 cimuseWorkshop]$
```

```
[lincolnu-lealgutierrezj@c221 cimuseWorkshop]$ ml cimuse_workshop  
[lincolnu-lealgutierrezj@c221 cimuseWorkshop]$ rstudio
```

Console Terminal × Jobs ×

R 4.2.0 . ~/

```
R version 4.2.0 (2022-04-22) -- "Vigorous Calisthenics"
Copyright (C) 2022 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)
```

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

Natural language support but running in an English locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

```
> getwd
function ()
.Internal(getwd())
<bytecode: 0x564cfc2cc6a0>
<environment: namespace:base>
> getwd()
[1] "/home/lincolnu-lealgutierrezj"
Connected to your session in progress, last started 2026-Jul-02 13:28:38 UTC (37 minutes ago)
> |
```

Environment

History

Connections

Tutorial



 Import Dataset ▾
  178 MiB ▾
 
 List ▾
  ▾

R ▾ | Global Environment ▾

Environment is empty

Files Plots Packages Help Viewer

 New Folder  New Blank File  Upload  Delete  Rename  More 

[Home](#)

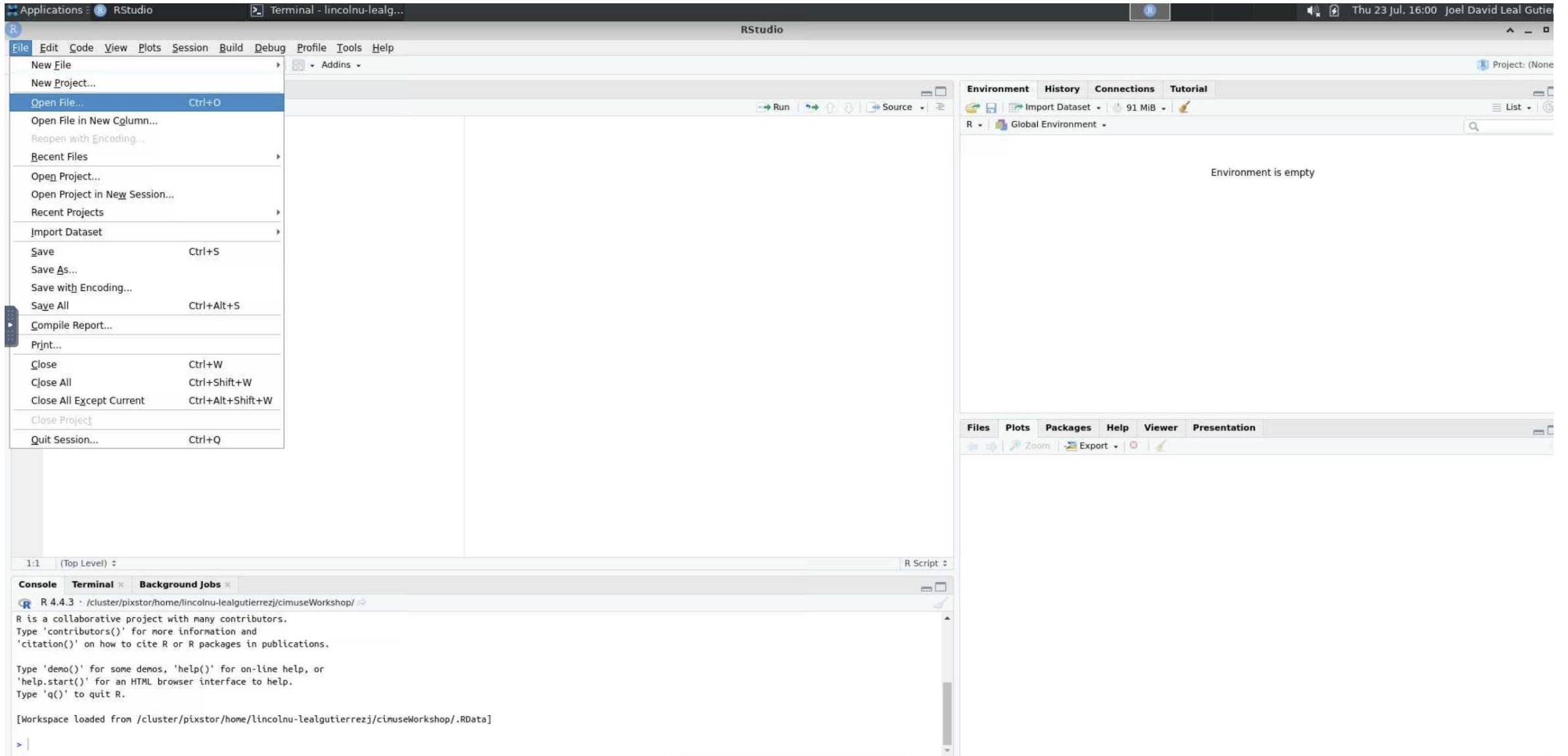
		▲ Name	Size	Modified
--	--	--------	------	----------

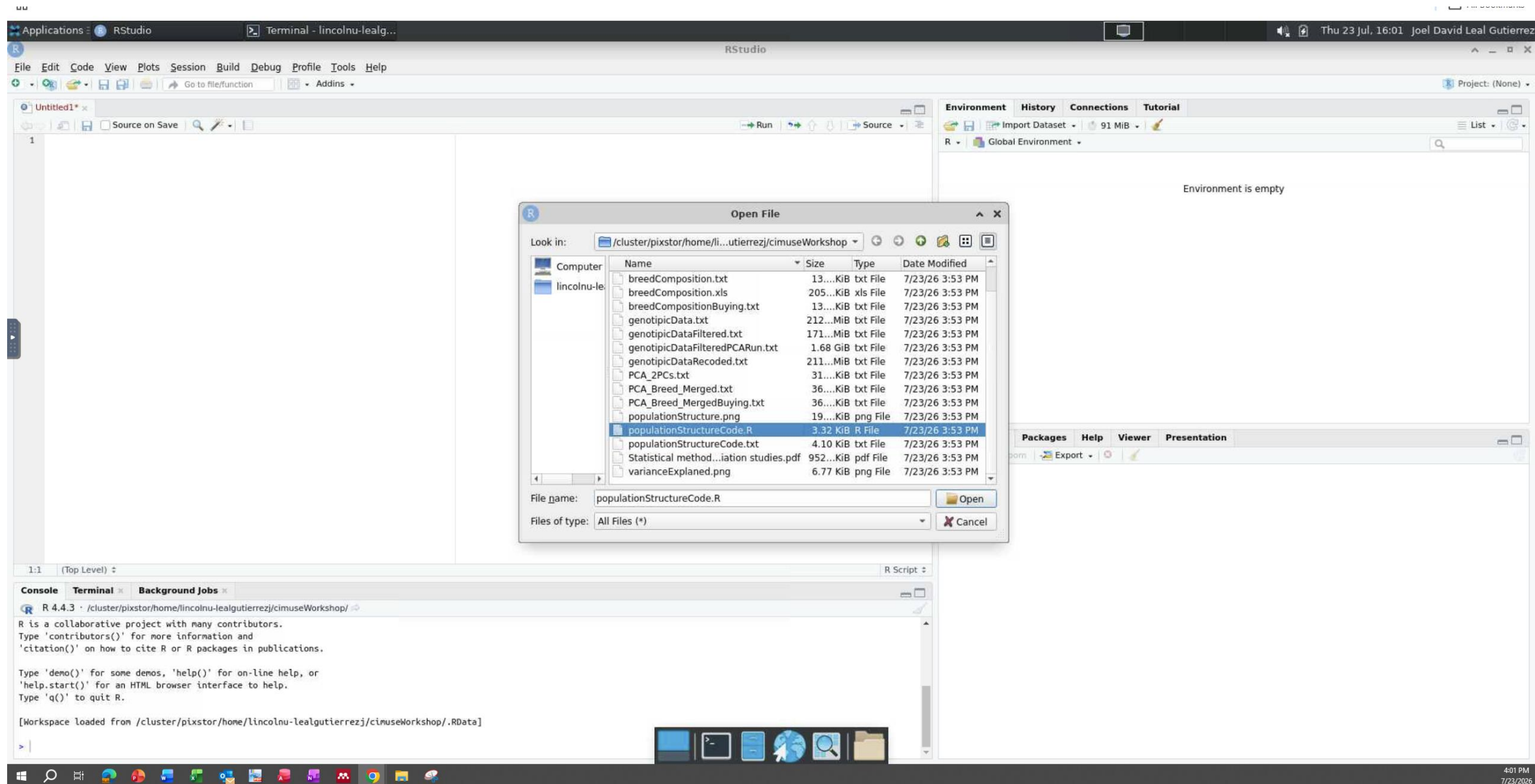
data

ondemand









```
populationStructureCode.R* x
Source on Save
1 # Read tabular data into R
2
3 #setwd("C:/Users/jgut258/Desktop/cimuseWorkshop/")
4
5 # get directory location so you can input this as an string to import and save files
6 directory <- getwd()
7
8 # loading an already installed library to be used downstream, data.table
9 library(data.table)
10
11 # read the file genotypicDataFilteredPCARun.txt, which is available inside directory
12 # it uses tab as delimiter ("\t"), returns a data.frame object and check.names makes names as valid
13 tgeno <- fread(file.path(directory, "genotypicDataFilteredPCARun.txt"),
14               sep = "\t",
15               data.table = FALSE,
16               check.names = FALSE)
17
18 # assigns rownames as the first row
19 rownames(tgeno) <- tgeno[[1]]
20
21 # reads genotypicDataFiltered.txt file, including the header, tab separated
22 # and assign first row as name identifiers
23 tgeno <- read.table(file = file.path(directory, "genotypicDataFiltered.txt"), header = TRUE,
24                   sep = "\t", dec = ".",
25                   row.names=1)
26
27 # invert table tgeno
28 geno<- t(tgeno)
29
30 # Remove markers with zero variance
31 geno <- geno[, apply(geno, 2, var, na.rm = TRUE) > 0]
32
33 # convert to a matrix
34 geno <- as.matrix(geno)
35
36 # Standardize SNPs, from 0, 1 and 2 to -1, 0 and 1
37 geno.scaled <- scale(geno)
38
39 # perform PCA: orthogonal decomposition of variables
40 # PCA takes many correlated variables (such as thousands of SNPs or gene expression values)
41 # and summarizes them into a smaller number of new variables called principal components (PCs).
42 pca <- prcomp(geno.scaled, center = FALSE, scale. = FALSE)
43
44 # Variance explained calculation and plotting
45 # generates orthogonal variables summarizing the original genomic variability
3:2 (Top Level) ↕
```

```
4  
5 # get directory location so you can input this as a string to import and save files  
6 directory <- getwd()  
7
```

```
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5 # get directory location so you can input this as a string to import and save files  
6 directory <- getwd()  
7
```

```
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10
```

```
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7
```

```
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```

```
11  
12 # read the file genotypicDataFilteredPCARun.txt, which is available inside directory  
13 # it uses tab as delimiter ("\t"), returns a data.frame object and check.names makes names as valid  
14 tgeno <- fread(file.path(directory, "genotypicDataFilteredPCARun.txt"),  
15               sep = "\t",  
16               data.table = FALSE,  
17               check.names = FALSE)  
18 tgeno <- tgeno[, -1]
```

```
4  
5 # get directory location so you can input this as a string to import and save files  
6 directory <- getwd()  
7
```

```
8  
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```
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13 # it uses tab as delimiter ("\t"), returns a data.frame object and check.names makes names as valid  
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15               sep = "\t",  
16               data.table = FALSE,  
17               check.names = FALSE)  
18 tgeno <- tgeno[, -1]
```

It will use the value in “directory” as input to find the file needed

```
4  
5 # get directory location so you can input this as a string to import and save files  
6 directory <- getwd()  
7
```

```
8  
9 # loading an already installed library to be used downstream, data.table  
10 library(data.table)
```

```
11 # read the file genotypicDataFilteredPCARun.txt, which is available inside directory  
12 # it uses tab as delimiter ("\t"), returns a data.frame object and check.names makes names as valid  
13 tgeno <- fread(file.path(directory, "genotypicDataFilteredPCARun.txt"),  
14               sep = "\t",  
15               data.table = FALSE,  
16               check.names = FALSE)  
17 tgeno <- tgeno[, -1]
```

It will use the value in “directory” as input to find the file needed
The file needed is “genotypicDataFilteredPCARun.txt”

```
4
5 # get directory location so you can input this as a string to import and save files
6 directory <- getwd()
7
```

```
8
9 # loading an already installed library to be used downstream, data.table
10 library(data.table)
```

```
11 # read the file genotypicDataFilteredPCARun.txt, which is available inside directory
12 # it uses tab as delimiter ("\t"), returns a data.frame object and check.names makes names as valid
13 tgeno <- fread(file.path(directory, "genotypicDataFilteredPCARun.txt"),
14                sep = "\t",
15                data.table = FALSE,
16                check.names = FALSE)
17 tgeno <- tgeno[, -1]
```

It will use the value in “directory” as input to find the file needed
The file needed is “genotypicDataFilteredPCARun.txt”

File name and its location

```
4
5 # get directory location so you can input this as a string to import and save files
6 directory <- getwd()
7
```

```
8
9 # loading an already installed library to be used downstream, data.table
10 library(data.table)
```

```
11 # read the file genotypicDataFilteredPCARun.txt, which is available inside directory
12 # it uses tab as delimiter ("\t"), returns a data.frame object and check.names makes names as valid
13 tgeno <- fread(file.path(directory, "genotypicDataFilteredPCARun.txt"),
14               sep = "\t",
15               data.table = FALSE,
16               check.names = FALSE)
17 tgeno <- tgeno[, -1]
```

It will use the value in “directory” as input to find the file needed
The file needed is “genotypicDataFilteredPCARun.txt”

→ File name and its location

Delete the first column from the genotypic data file. This column included the polymorphism names

```
4  
5 # get directory location so you can input this as an string to import and save files  
6 directory <- getwd()  
7
```

```
8  
9 # loading an already installed library to be used downstream, data.table  
10 library(data.table)
```

```
11  
12 # read the file genotypicDataFilteredPCARun.txt, which is available inside directory  
13 # it uses tab as delimiter ("\t"), returns a data.frame object and check.names makes names as valid  
14 tgeno <- fread(file.path(directory, "genotypicDataFilteredPCARun.txt"),  
15               sep = "\t",  
16               data.table = FALSE,  
17               check.names = FALSE)  
18 tgeno <- tgeno[, -1]
```

```
4
5 # get directory location so you can input this as a string to import and save files
6 directory <- getwd()
7
```

```
8
9 # loading an already installed library to be used downstream, data.table
10 library(data.table)
```

```
11 # read the file genotypicDataFilteredPCARun.txt, which is available inside directory
12 # it uses tab as delimiter ("\t"), returns a data.frame object and check.names makes names as valid
13 tgeno <- fread(file.path(directory, "genotypicDataFilteredPCARun.txt"),
14                sep = "\t",
15                data.table = FALSE,
16                check.names = FALSE)
17 tgeno <- tgeno[, -1]
```

Columns are separated by tabs

The object is not a data.table

It also does not check column names to ensure they are valid during imputation

```
18  
19 # an alternative way to read genotypicDataFilteredPCARun.txt file, including the header, tab separated  
20 # and assign first row as name identifiers  
21 #tgeno <- read.table(file = file.path(directory, "genotypicDataFilteredPCARun.txt"), header = TRUE,  
22 #                               sep = "\t", dec = ".",  
23 #                               row.names=1)  
24
```

```
24  
25 # invert table tgeno  
26 geno<- t(tgeno)  
27
```

Transpose “tgeno” and store the information in a “geno” variable

```

18
19 # an alternative way to read genotypicDataFilteredPCARun.txt file, including the header, tab separated
20 # and assign first row as name identifiers
21 #tgeno <- read.table(file = file.path(directory, "genotypicDataFilteredPCARun.txt"), header = TRUE,
22 #                      sep = "\t", dec = ".",
23 #                      row.names=1)
24

```

```

24
25 # invert table tgeno
26 geno<- t(tgeno)
27

```

Transpose “tgeno” and store the information in a “geno” variable

```

27 |
28 # Remove SNPs with zero variance
29 geno <- geno[, apply(geno, 2, var, na.rm = TRUE) > 0]
30

```

```

30
31 # convert to a matrix
32 geno <- as.matrix(geno)
33

```

```
33  
34 # Standardize SNPs  
35 geno.scaled <- scale(geno)  
36
```

Marker coding:

0

1

2

```
33  
34 # Standardize SNPs  
35 geno.scaled <- scale(geno)  
36
```

Marker coding:

0

1

2



Standardized
marker coding:

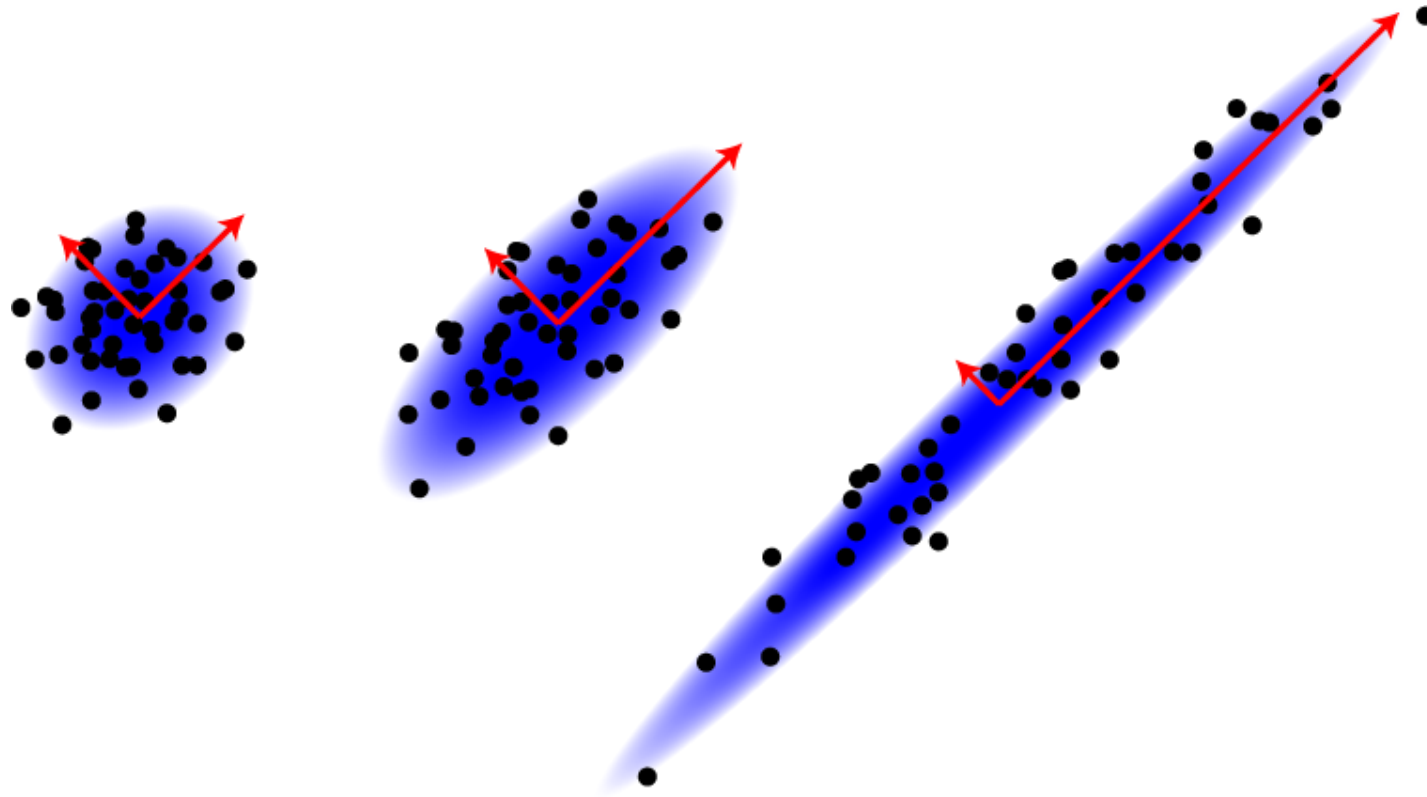
-1

0

1

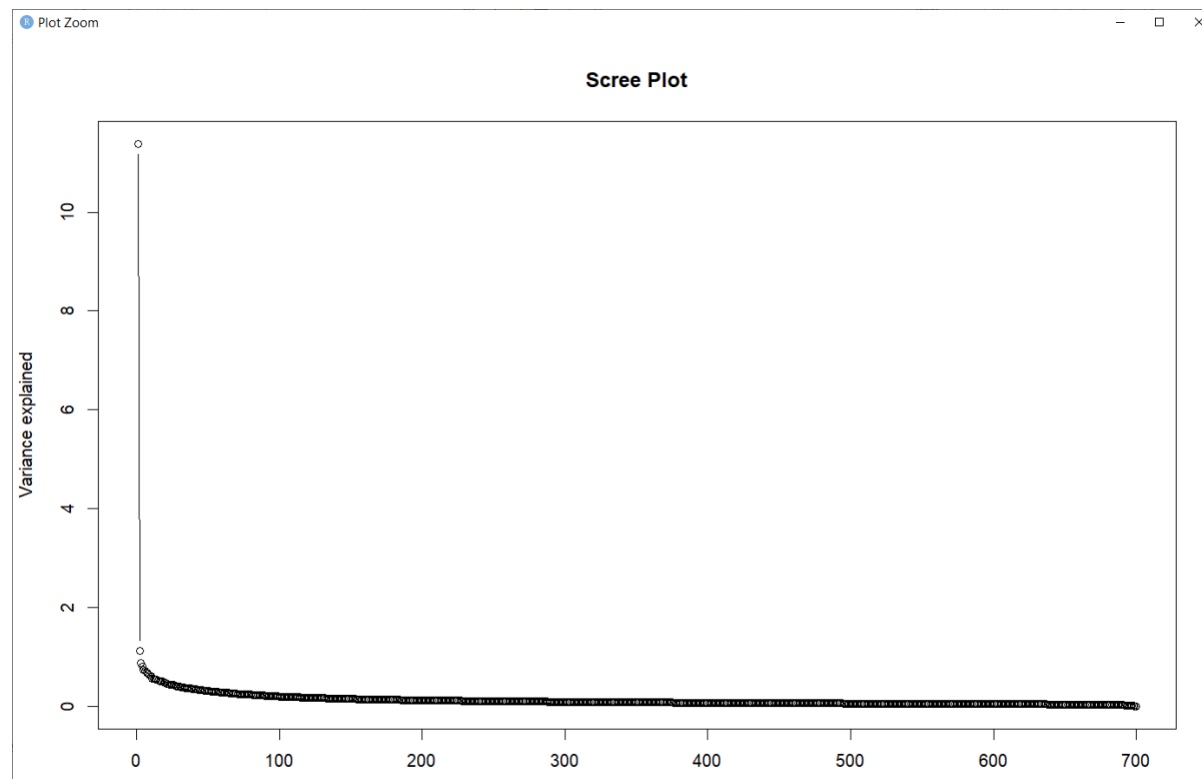
```
36  
37 # perform PCA: orthogonal decomposition of variables  
38 # PCA takes many correlated variables (such as thousands of SNPs or gene expression values)  
39 # and summarizes them into a smaller number of new variables called principal components (PCs).  
40 pca <- prcomp(geno.scaled, center = FALSE, scale. = FALSE)  
41
```

```
30  
37 # perform PCA: orthogonal decomposition of variables  
38 # PCA takes many correlated variables (such as thousands of SNPs or gene expression values)  
39 # and summarizes them into a smaller number of new variables called principal components (PCs).  
40 pca <- prcomp(geno.scaled, center = FALSE, scale. = FALSE)  
41
```



```
41  
42 # Variance explained calculation and plotting  
43 # generates orthogonal variables summarizing the original genomic variability  
44 var.exp <- (pca$sdev^2) / sum(pca$sdev^2) * 100  
45 plot(var.exp, type = "b",  
46       xlab = "Principal Component",  
47       ylab = "Variance explained",  
48       main = "Scree Plot")  
49
```

```
41  
42 # Variance explained calculation and plotting  
43 # generates orthogonal variables summarizing the original genomic variability  
44 var.exp <- (pca$sdev^2) / sum(pca$sdev^2) * 100  
45 plot(var.exp, type = "b",  
46       xlab = "Principal Component",  
47       ylab = "Variance explained",  
48       main = "Scree Plot")  
49
```



```
49
50 # Create output table
51 pca.out <- data.frame(
52   ID = rownames(geno),
53   pca$x
54 )
55
56 # Create data frame with ID, PC1, and PC2
57 pca2 <- data.frame(
58   ID = rownames(geno),
59   PC1 = pca$x[,1],
60   PC2 = pca$x[,2]
61 )
62
63 # Save to tab-delimited text file using the original directory variable as input
64 write.table(
65   pca2,
66   file = file.path(directory, "PCA_2PCs.txt"),
67   sep = "\t",
68   quote = FALSE,
69   row.names = FALSE
70 )
71
```

```
49
50 # Create output table
51 pca.out <- data.frame(
52   ID = rownames(geno),
53   pca$x
54 )
55
56 # Create data frame with ID, PC1, and PC2
57 pca2 <- data.frame(
58   ID = rownames(geno),
59   PC1 = pca$x[,1],
60   PC2 = pca$x[,2]
61 )
62
63 # Save to tab-delimited text file using the original directory variable as input
64 write.table(
65   pca2,
66   file = file.path(directory, "PCA_2PCs.txt"),
67   sep = "\t",
68   quote = FALSE,
69   row.names = FALSE
70 )
71
```

Creates a data frame, keeping row names and including their corresponding PCA1 and PCA2

```

49
50 # Create output table
51 pca.out <- data.frame(
52   ID = rownames(geno),
53   pca$x
54 )
55
56 # Create data frame with ID, PC1, and PC2
57 pca2 <- data.frame(
58   ID = rownames(geno),
59   PC1 = pca$x[,1],
60   PC2 = pca$x[,2]
61 )
62
63 # Save to tab-delimited text file using the original directory variable as input
64 write.table(
65   pca2,
66   file = file.path(directory, "PCA_2PCs.txt"),
67   sep = "\t",
68   quote = FALSE,
69   row.names = FALSE
70 )
71

```

Creates a data frame, keeping row names and including their corresponding PCA1 and PCA2
 Write “pca2” in a file using the “directory” path

```
71
72 # Read file PCA_2PCs.txt using the original directory variable as input
73 pca <- read.table(file.path(directory,"PCA_2PCs.txt"),
74                   header = TRUE,
75                   sep = "\t",
76                   stringsAsFactors = FALSE)
77
78 # Read file BreedComposition.txt using the original directory variable as input
79 breed <- read.table(file.path(directory,"breedComposition.txt"),
80                    header = TRUE,
81                    sep = "\t",
82                    stringsAsFactors = FALSE)
83
84 # Merge by animal ID
85 merged <- merge(pca,
86                breed,
87                by = "ID")
88
89 # Save merged file, PCA_Breed_Merged.txt, using the original directory variable as input
90 write.table(merged,
91            file = file.path(directory,"PCA_Breed_Merged.txt"),
92            sep = "\t",
93            quote = FALSE,
94            row.names = FALSE)
95
```

```
71  
72 # Read file PCA_2PCs.txt using the original directory variable as input  
73 pca <- read.table(file.path(directory,"PCA_2PCs.txt"),  
74                   header = TRUE,  
75                   sep = "\\t",  
76                   stringsAsFactors = FALSE)  
77  
78 # Read file BreedComposition.txt using the original directory variable as input  
79 breed <- read.table(file.path(directory,"breedComposition.txt"),  
80                    header = TRUE,  
81                    sep = "\\t",  
82                    stringsAsFactors = FALSE)  
83  
84 # Merge by animal ID  
85 merged <- merge(pca,  
86                breed,  
87                by = "ID")  
88  
89 # Save merged file, PCA_Breed_Merged.txt, using the original directory variable  
90 write.table(merged,  
91            file = file.path(directory,"PCA_Breed_Merged.txt"),  
92            sep = "\\t",  
93            quote = FALSE,  
94            row.names = FALSE)  
95
```



```
71  
72 # Read file PCA_2PCs.txt using the original directory variable as input  
73 pca <- read.table(file.path(directory,"PCA_2PCs.txt"),  
74                   header = TRUE,  
75                   sep = "\\t",  
76                   stringsAsFactors = FALSE)  
77  
78 # Read file BreedComposition.txt using the original directory variable as input  
79 breed <- read.table(file.path(directory,"breedComposition.txt"),  
80                    header = TRUE,  
81                    sep = "\\t",  
82                    stringsAsFactors = FALSE)  
83  
84 # Merge by animal ID  
85 merged <- merge(pca,  
86                breed,  
87                by = "ID")  
88  
89 # Save merged file, PCA_Breed_Merged.txt, using the original directory variable  
90 write.table(merged,  
91            file = file.path(directory,"PCA_Breed_Merged.txt"),  
92            sep = "\\t",  
93            quote = FALSE,  
94            row.names = FALSE)  
95
```



```
71
72 # Read file PCA_2PCs.txt using the original directory variable as input
73 pca <- read.table(file.path(directory,"PCA_2PCs.txt"),
74                   header = TRUE,
75                   sep = "\t",
76                   stringsAsFactors = FALSE)
77
78 # Read file BreedComposition.txt using the original directory variable as input
79 breed <- read.table(file.path(directory,"breedComposition.txt"),
80                    header = TRUE,
81                    sep = "\t",
82                    stringsAsFactors = FALSE)
83
84 # Merge by animal ID
85 merged <- merge(pca,
86                breed,
87                by = "ID")
88
89 # Save merged file, PCA_Breed_Merged.txt, using the original directory variable
90 write.table(merged,
91            file = file.path(directory,"PCA_Breed_Merged.txt"),
92            sep = "\t",
93            quote = FALSE,
94            row.names = FALSE)
95
```



```
71
72 # Read file PCA_2PCs.txt using the original directory variable as input
73 pca <- read.table(file.path(directory,"PCA_2PCs.txt"),
74                   header = TRUE,
75                   sep = "\t",
76                   stringsAsFactors = FALSE)
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79 breed <- read.table(file.path(directory,"breedComposition.txt"),
80                    header = TRUE,
81                    sep = "\t",
82                    stringsAsFactors = FALSE)
83
84 # Merge by animal ID
85 merged <- merge(pca,
86                breed,
87                by = "ID")
88
89 # Save merged file, PCA_Breed_Merged.txt, using the original directory variable
90 write.table(merged,
91            file = file.path(directory,"PCA_Breed_Merged.txt"),
92            sep = "\t",
93            quote = FALSE,
94            row.names = FALSE)
95
```



```
95
96 # loading an already installed library to be used downstream, ggplot2
97 library(ggplot2)
98
99 # Use library ggplot to create a figure
100 ggplot(merged, aes(x = PC1, y = PC2, color = percentage)) + scale_color_manual(values = c(
101   "B_100-96" = "blue4", "B_95-75" = "lightseagreen", "B_74-51" = "slateblue1", "B_50" = "purple",
102   "B_49-25" = "hotpink4", "B_24-5" = "hotpink1", "B_4-0" = "magenta1")) +
103   geom_point(size = 3) + theme_minimal()
104
```

```
95  
96 # loading an already installed library to be used downstream, ggplot2  
97 library(ggplot2)  
98  
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100 ggplot(merged, aes(x = PC1, y = PC2, color = percentage)) + scale_color_manual(values = c(  
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102   "B_49-25" = "hotpink4", "B_24-5" = "hotpink1", "B_4-0" = "magenta1")) +  
103   geom_point(size = 3) + theme_minimal()  
104
```

Loads a library named “ggplot”

```

95
96 # loading an already installed library to be used downstream, ggplot2
97 library(ggplot2)
98
99 # Use library ggplot to create a figure
100 ggplot(merged, aes(x = PC1, y = PC2, color = percentage)) + scale_color_manual(values = c(
101   "B_100-96" = "blue4", "B_95-75" = "lightseagreen", "B_74-51" = "slateblue1", "B_50" = "purple",
102   "B_49-25" = "hotpink4", "B_24-5" = "hotpink1", "B_4-0" = "magenta1")) +
103   geom_point(size = 3) + theme_minimal()
104

```

Loads a library named “ggplot”

Function to create a plot

```
95
96 # loading an already installed library to be used downstream, ggplot2
97 library(ggplot2)
98
99 # Use library ggplot to create a figure
100 ggplot(merged, aes(x = PC1, y = PC2, color = percentage)) + scale_color_manual(values = c(
101   "B_100-96" = "blue4", "B_95-75" = "lightseagreen", "B_74-51" = "slateblue1", "B_50" = "purple",
102   "B_49-25" = "hotpink4", "B_24-5" = "hotpink1", "B_4-0" = "magenta1")) +
103   geom_point(size = 3) + theme_minimal()
104
```

```

95
96 # loading an already installed library to be used downstream, ggplot2
97 library(ggplot2)
98
99 # Use library ggplot to create a figure
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101   "B_100-96" = "blue4", "B_95-75" = "lightseagreen", "B_74-51" = "slateblue1", "B_50" = "purple",
102   "B_49-25" = "hotpink4", "B_24-5" = "hotpink1", "B_4-0" = "magenta1")) +
103   geom_point(size = 3) + theme_minimal()
104

```

It will plot variable PC1 versus variable PC2

```

95
96 # loading an already installed library to be used downstream, ggplot2
97 library(ggplot2)
98
99 # Use library ggplot to create a figure
100 ggplot(merged, aes(x = PC1, y = PC2, color = percentage)) + scale_color_manual(values = c(
101   "B_100-96" = "blue4", "B_95-75" = "lightseagreen", "B_74-51" = "slateblue1", "B_50" = "purple",
102   "B_49-25" = "hotpink4", "B_24-5" = "hotpink1", "B_4-0" = "magenta1")) +
103   geom_point(size = 3) + theme_minimal()
104

```

It will plot variable PC1 versus variable PC2

Each dot will be colored by the variable “percentage”

```

95
96 # loading an already installed library to be used downstream, ggplot2
97 library(ggplot2)
98
99 # Use library ggplot to create a figure
100 ggplot(merged, aes(x = PC1, y = PC2, color = percentage)) + scale_color_manual(values = c(
101   "B_100-96" = "blue4", "B_95-75" = "lightseagreen", "B_74-51" = "slateblue1", "B_50" = "purple",
102   "B_49-25" = "hotpink4", "B_24-5" = "hotpink1", "B_4-0" = "magenta1")) +
103   geom_point(size = 3) + theme_minimal()
104

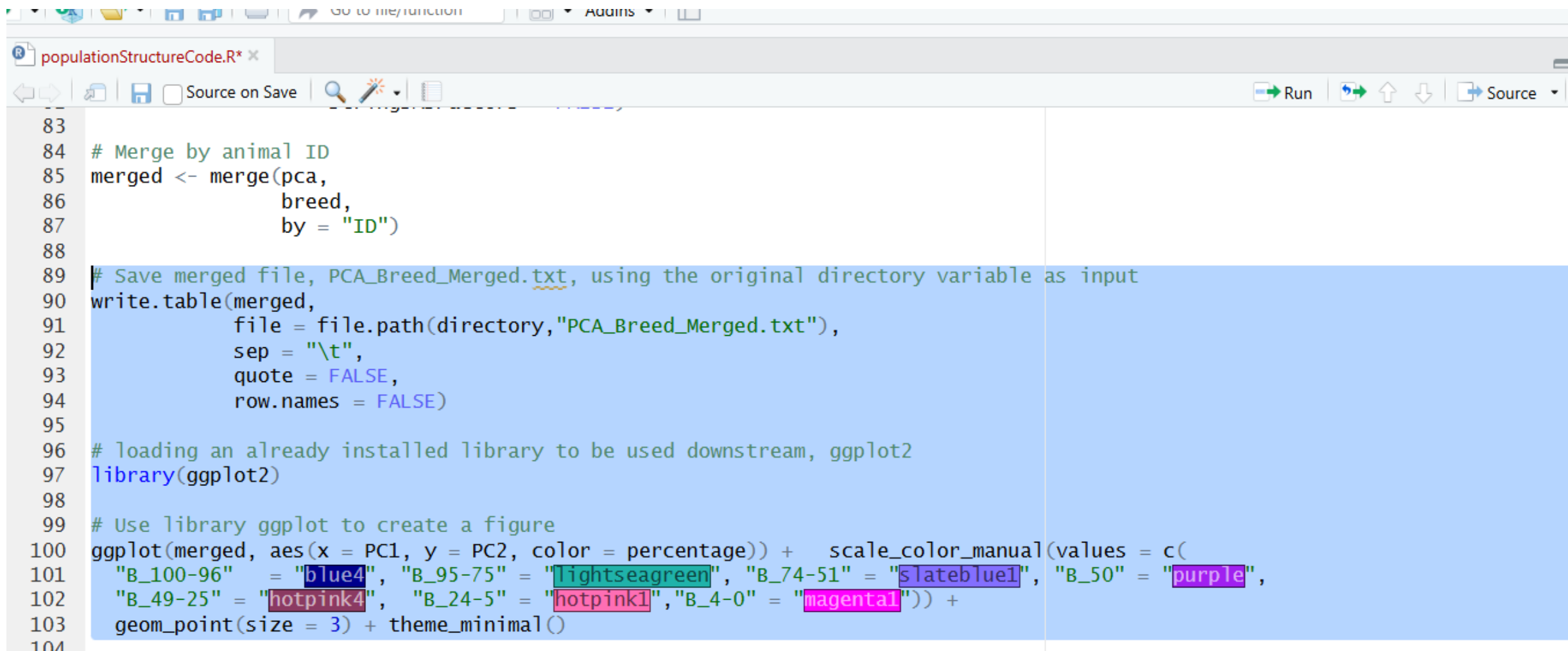
```

It will plot variable PC1 versus variable PC2

Each dot will be colored by the variable “percentage”

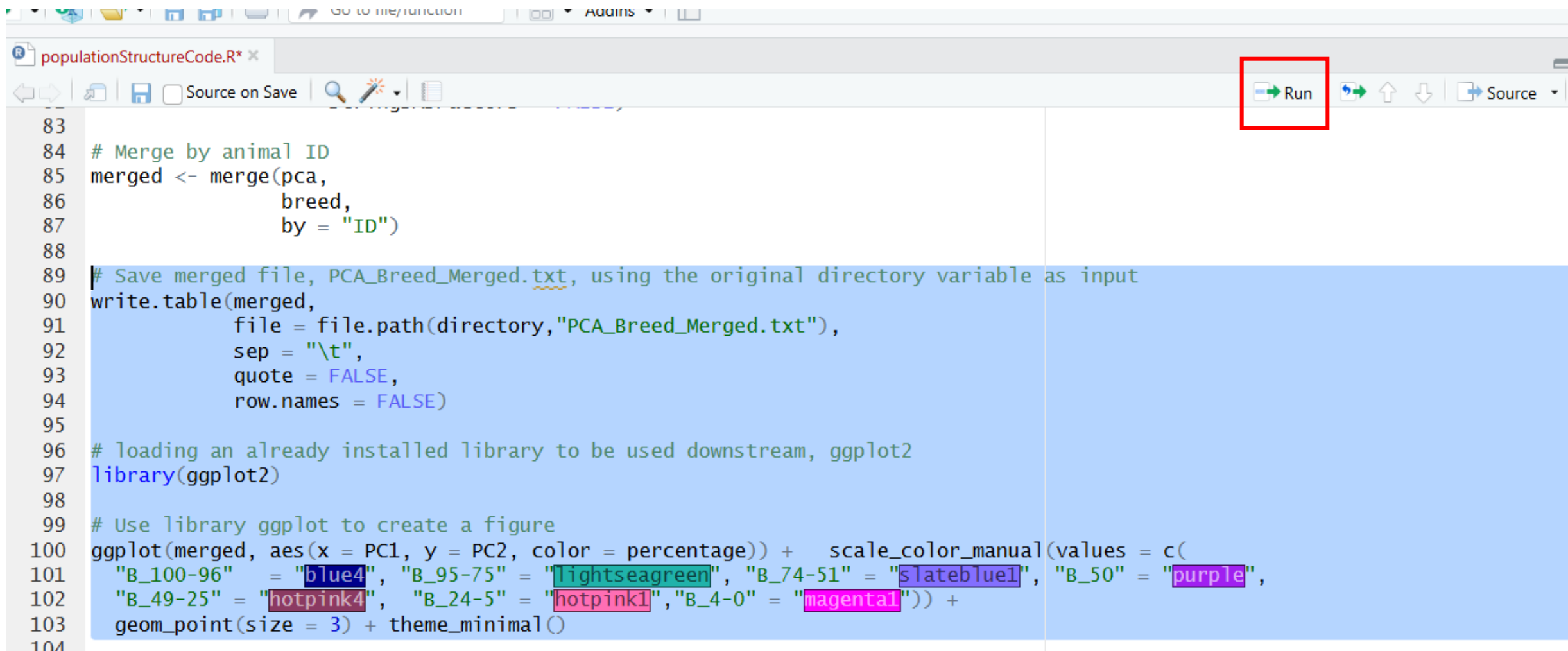
Palette of colors to be used

Run the code



The image shows a screenshot of an RStudio editor window. The title bar at the top reads "populationStructureCode.R* x". Below the title bar is a toolbar with icons for navigation, saving, and running code. The main editor area contains R code with line numbers 83 through 104. The code performs a merge operation, saves a table, loads the ggplot2 library, and creates a scatter plot with points colored by group. A blue highlight covers the code from line 89 to 104. A blue arrow on the left points upwards.

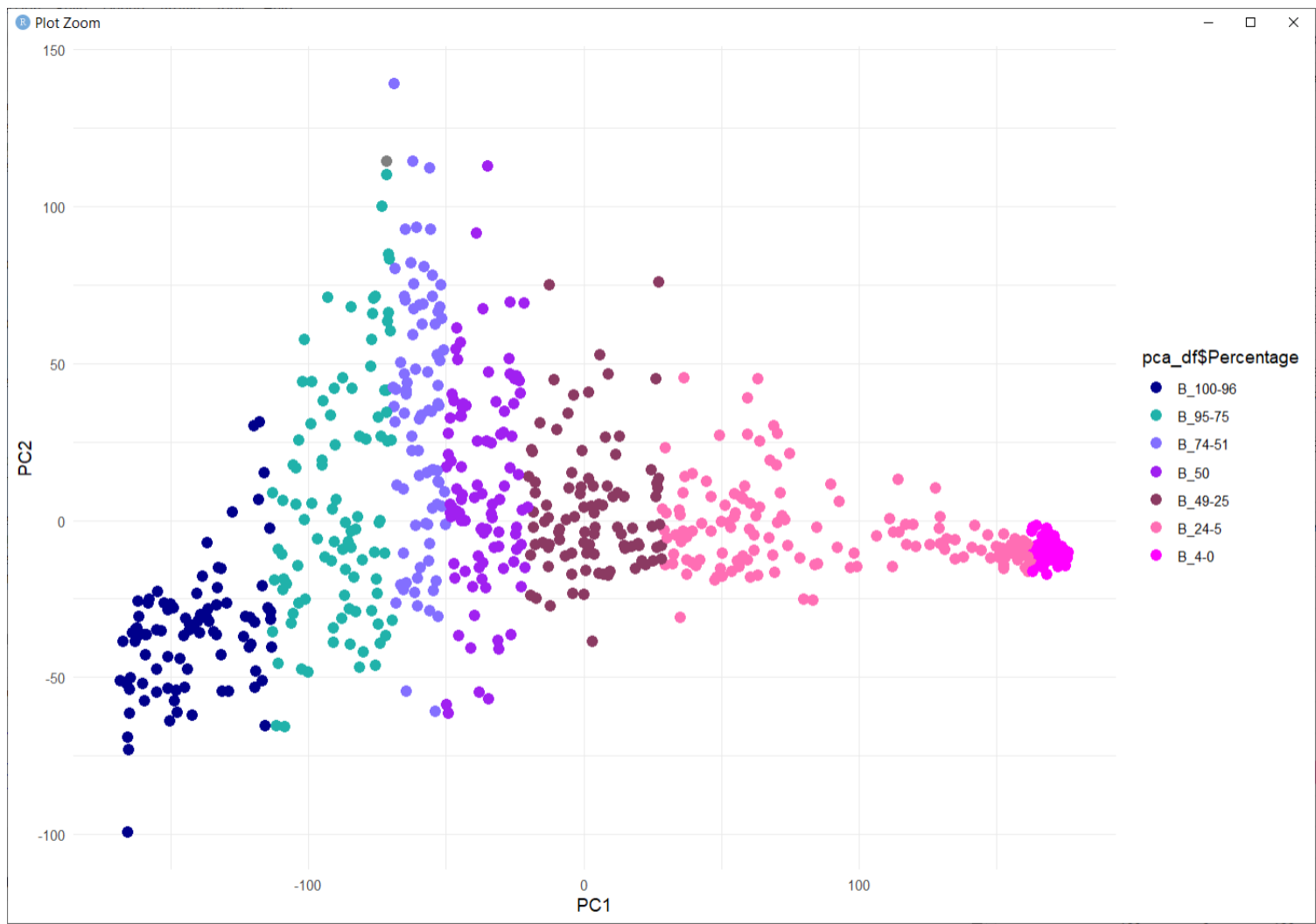
```
83
84 # Merge by animal ID
85 merged <- merge(pca,
86                 breed,
87                 by = "ID")
88
89 # Save merged file, PCA_Breed_Merged.txt, using the original directory variable as input
90 write.table(merged,
91             file = file.path(directory, "PCA_Breed_Merged.txt"),
92             sep = "\t",
93             quote = FALSE,
94             row.names = FALSE)
95
96 # loading an already installed library to be used downstream, ggplot2
97 library(ggplot2)
98
99 # Use library ggplot to create a figure
100 ggplot(merged, aes(x = PC1, y = PC2, color = percentage)) + scale_color_manual(values = c(
101   "B_100-96" = "blue4", "B_95-75" = "lightseagreen", "B_74-51" = "slateblue1", "B_50" = "purple",
102   "B_49-25" = "hotpink4", "B_24-5" = "hotpink1", "B_4-0" = "magenta1")) +
103   geom_point(size = 3) + theme_minimal()
104
```



The image shows the RStudio interface with a script editor open. The script is named "populationStructureCode.R*" and contains R code for merging data, saving it, and creating a plot. A red box highlights the "Run" button in the top right toolbar. A blue arrow on the left points upwards, indicating the execution flow from line 104 to line 83.

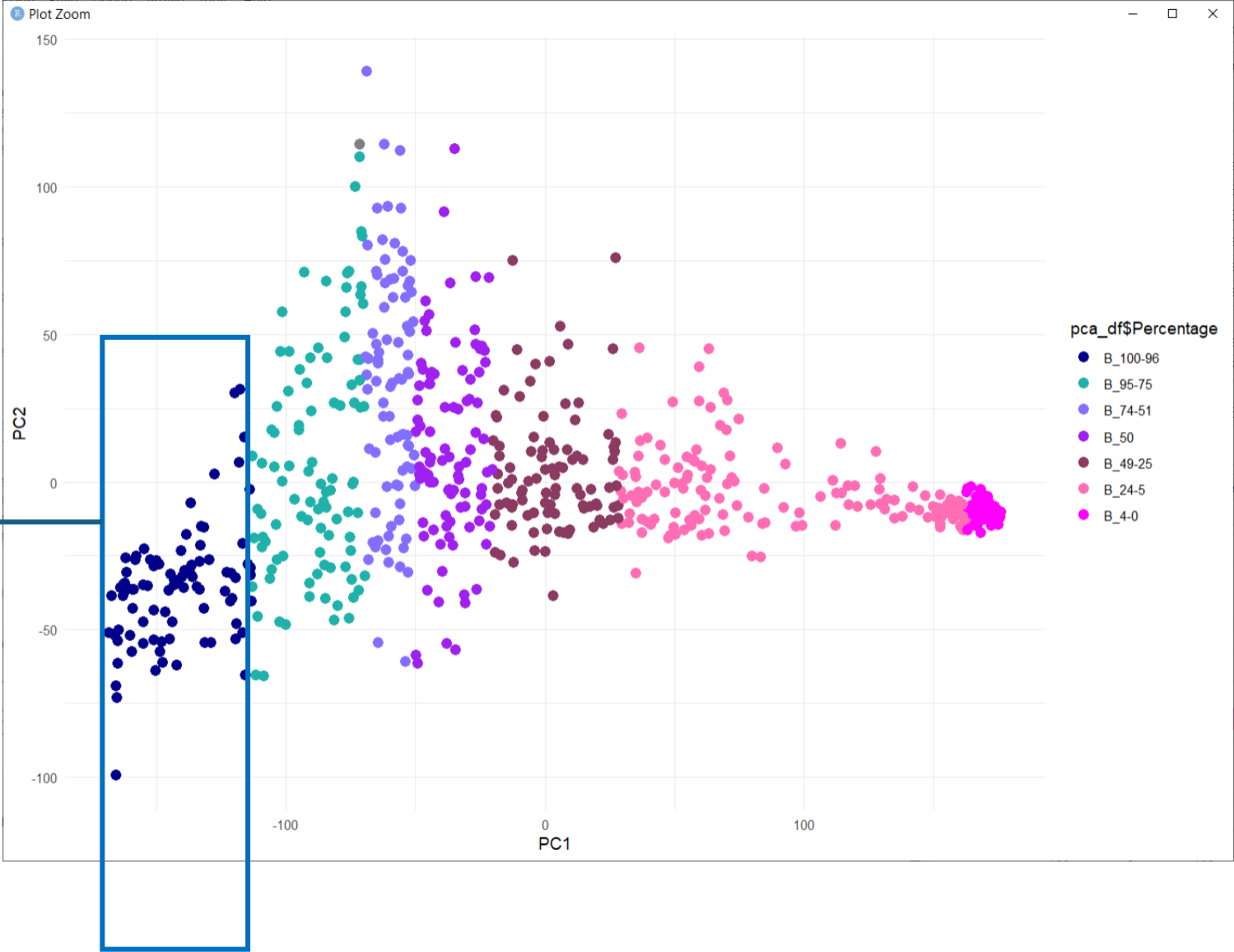
```
83
84 # Merge by animal ID
85 merged <- merge(pca,
86                 breed,
87                 by = "ID")
88
89 # Save merged file, PCA_Breed_Merged.txt, using the original directory variable as input
90 write.table(merged,
91             file = file.path(directory, "PCA_Breed_Merged.txt"),
92             sep = "\t",
93             quote = FALSE,
94             row.names = FALSE)
95
96 # loading an already installed library to be used downstream, ggplot2
97 library(ggplot2)
98
99 # Use library ggplot to create a figure
100 ggplot(merged, aes(x = PC1, y = PC2, color = percentage)) + scale_color_manual(values = c(
101   "B_100-96" = "blue4", "B_95-75" = "lightseagreen", "B_74-51" = "slateblue1", "B_50" = "purple",
102   "B_49-25" = "hotpink4", "B_24-5" = "hotpink1", "B_4-0" = "magenta1")) +
103   geom_point(size = 3) + theme_minimal()
104
```

Results



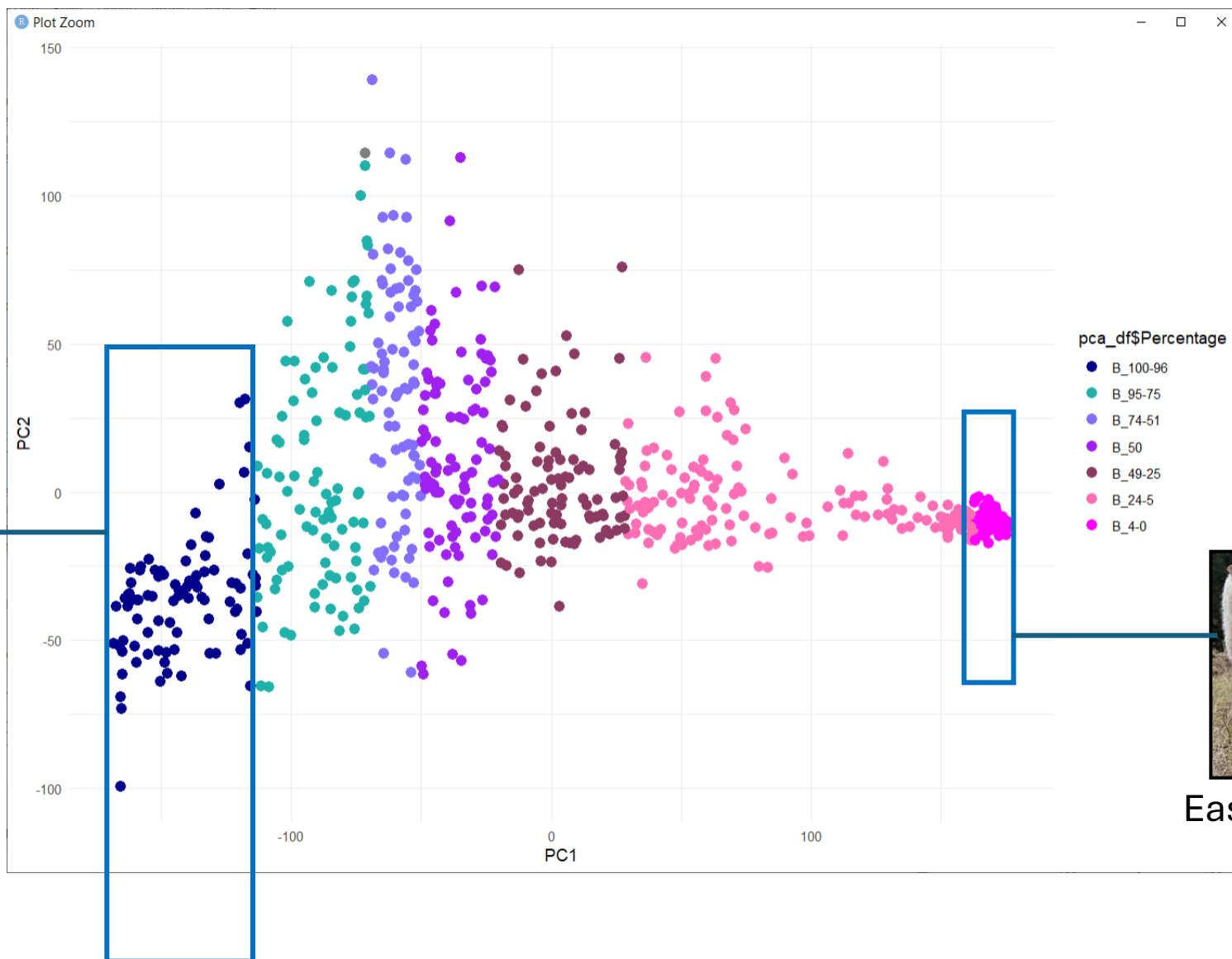


Suffolk sheep





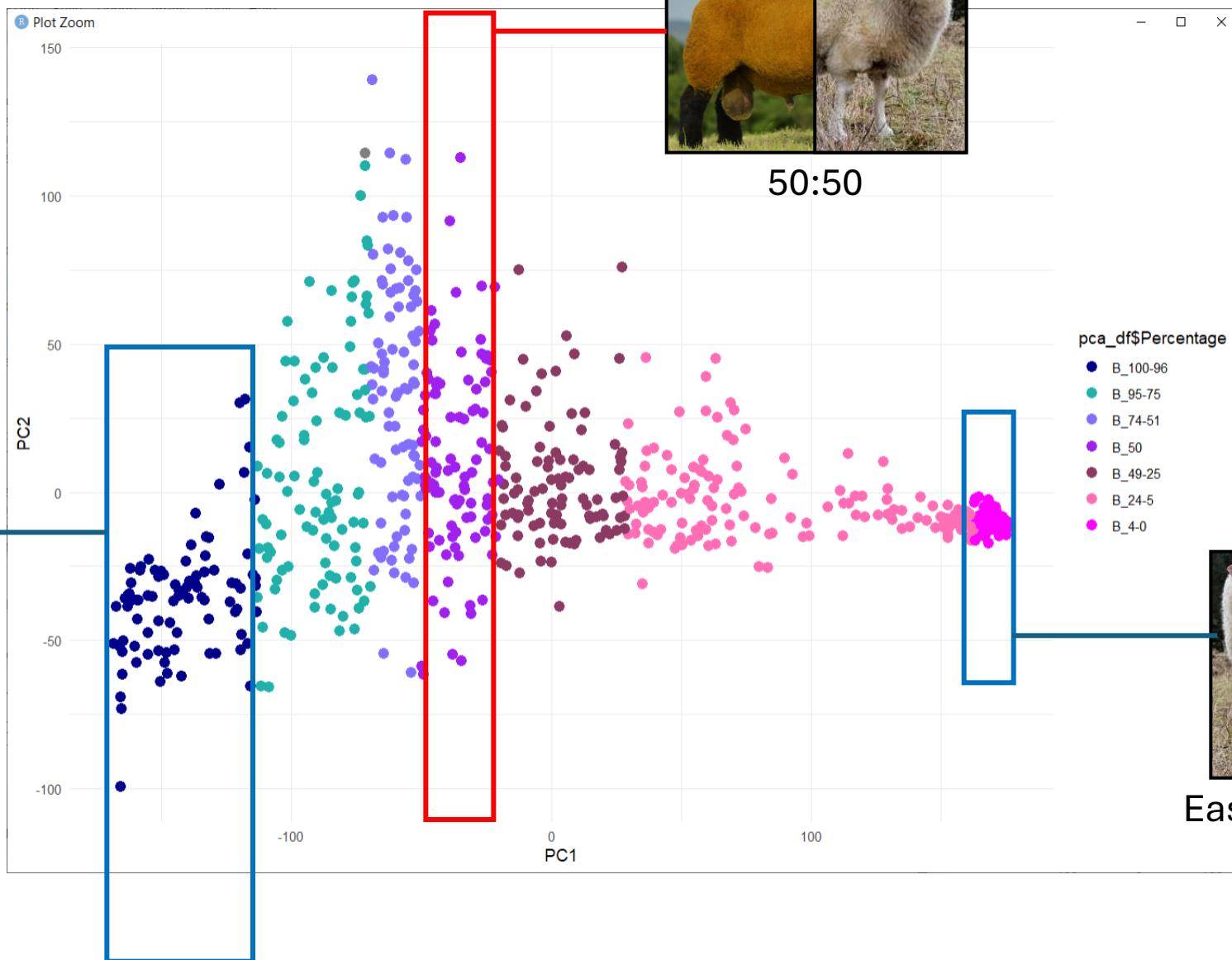
Suffolk sheep



East Friesian sheep



Suffolk sheep



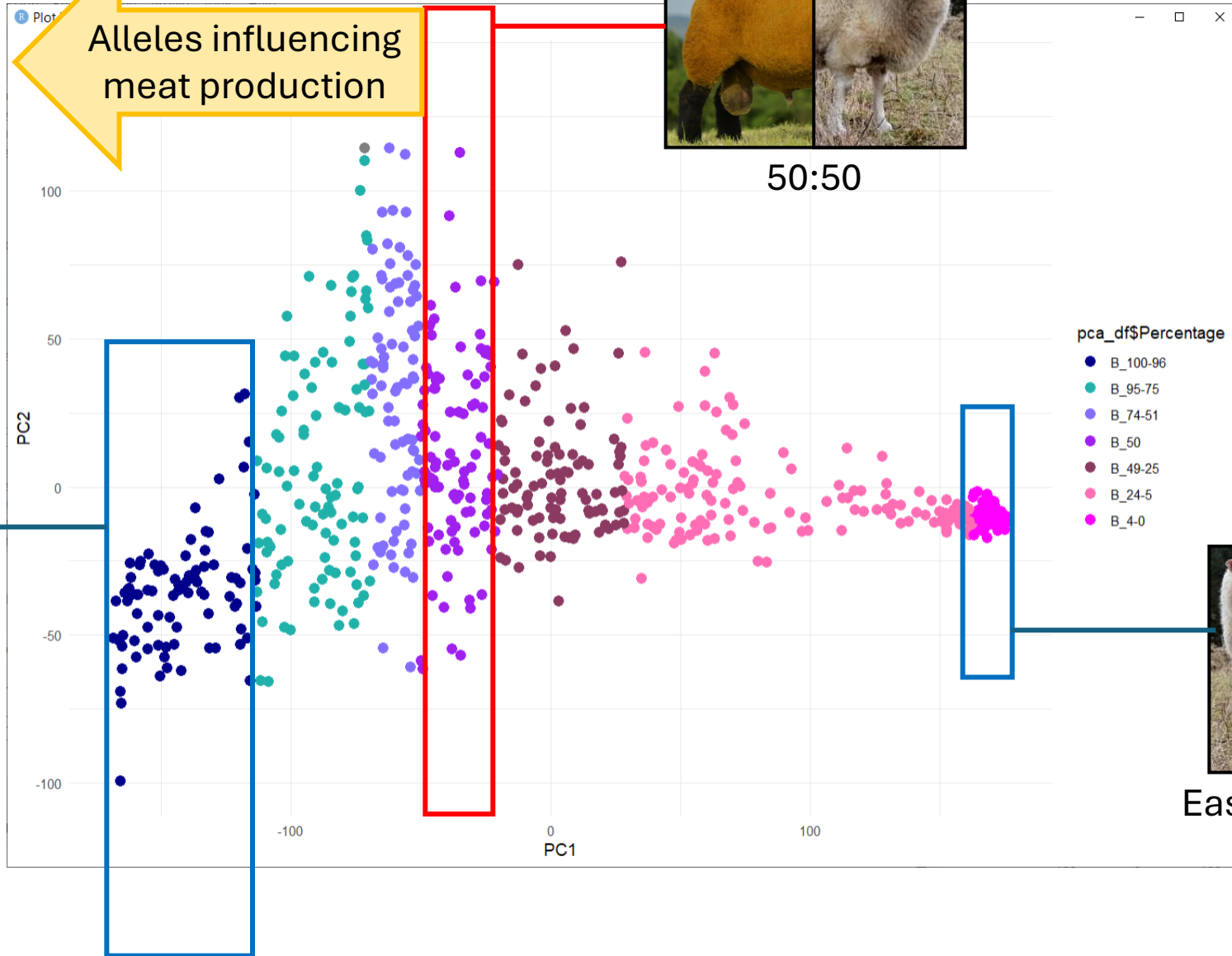
50:50



East Friesian sheep



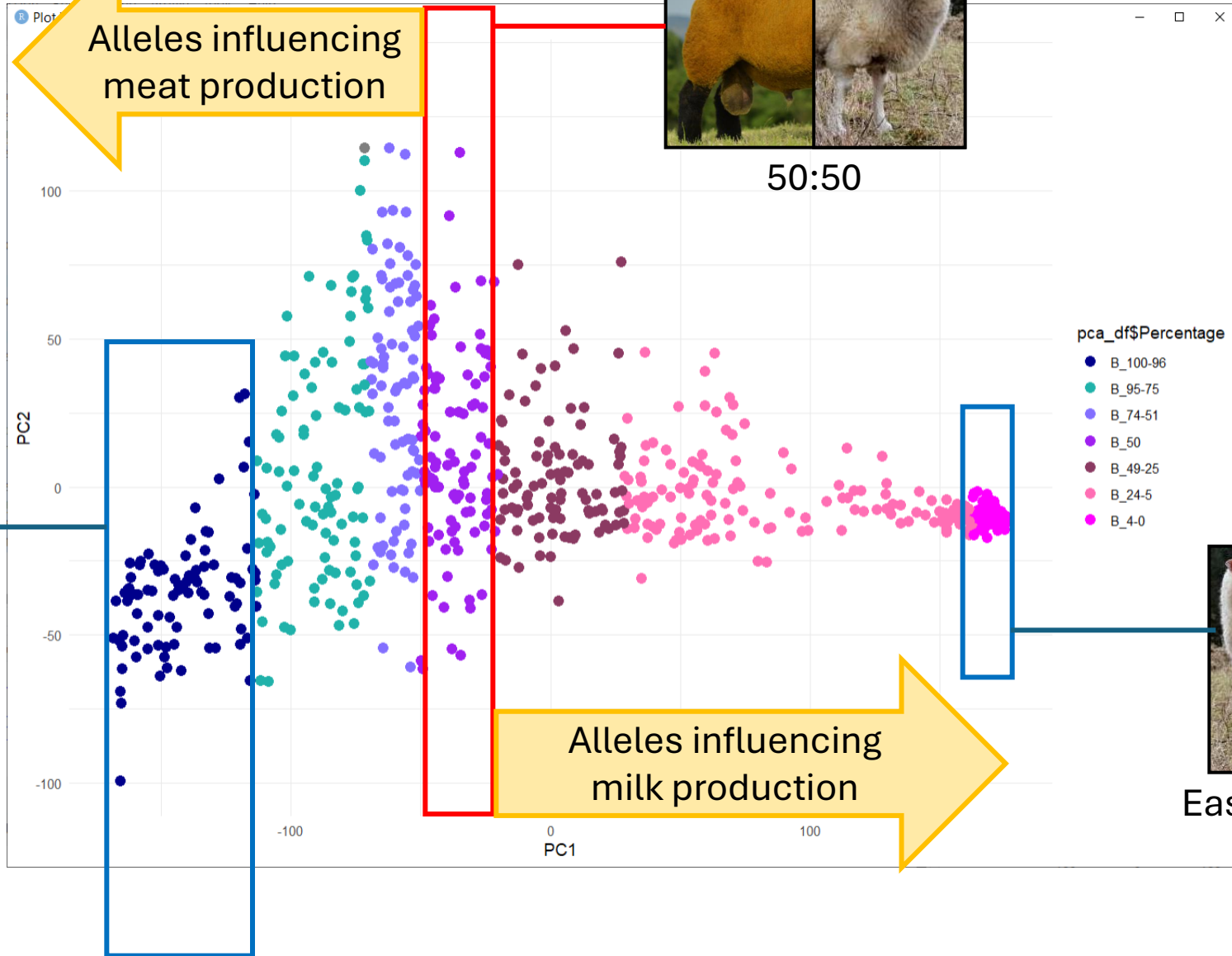
Suffolk sheep



East Friesian sheep



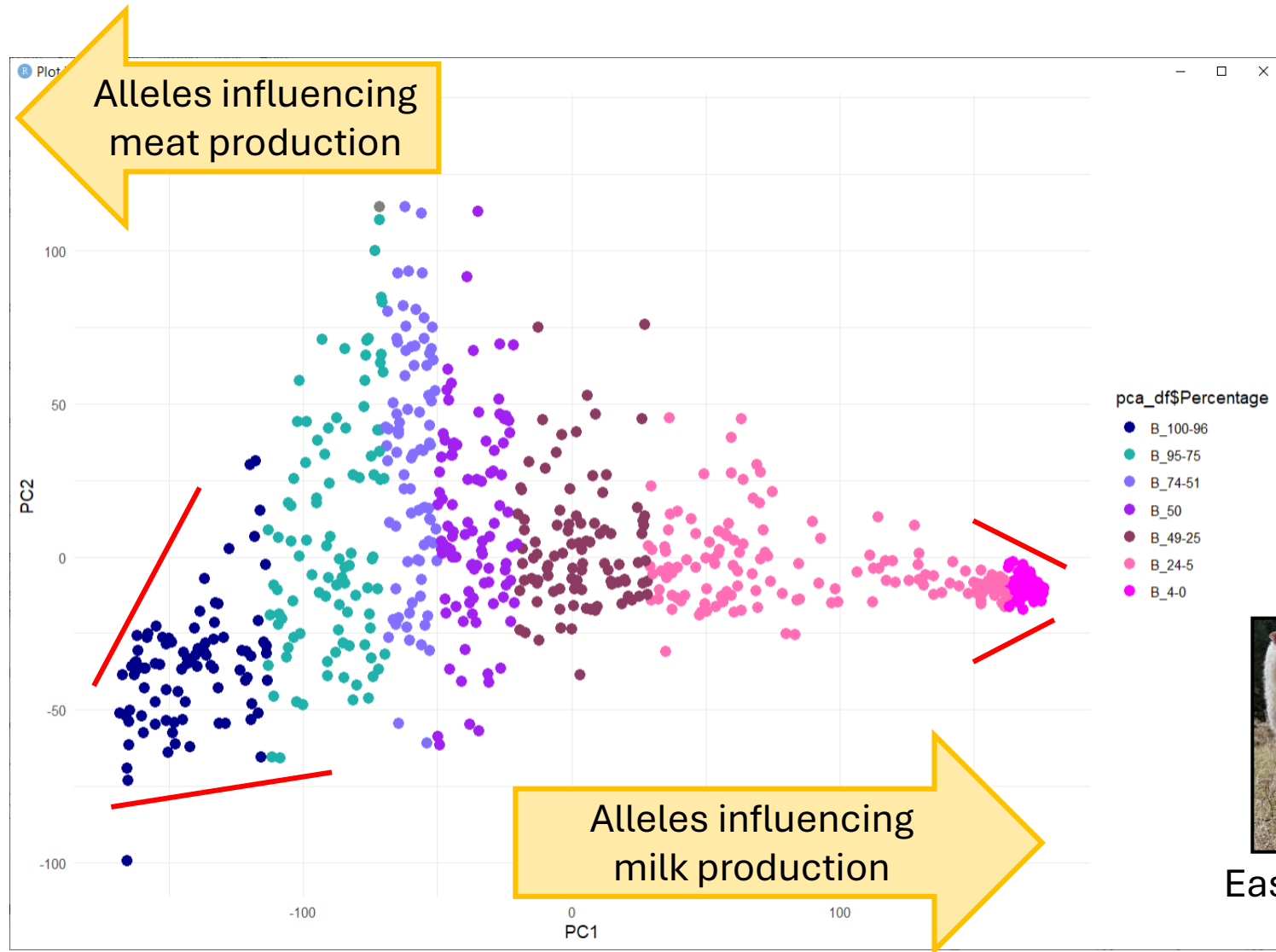
Suffolk sheep



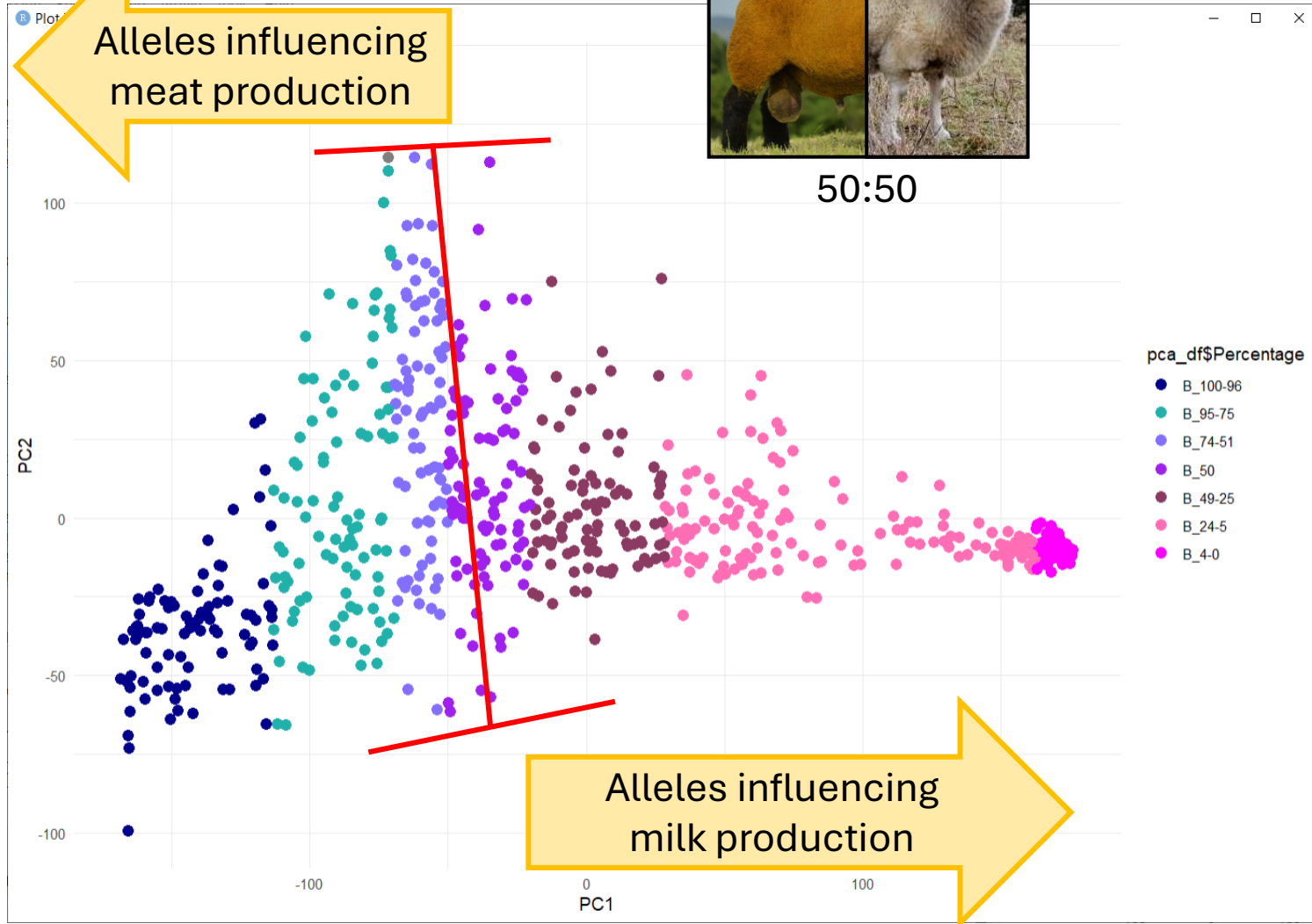
East Friesian sheep



Suffolk sheep



East Friesian sheep



Activities:

1. Verify the breed composition of an animal for a producer interested in high-performance dairy females.
2. Create a grayscale figure for the original breed composition analysis using the provided code.
3. Create a plot using PC2 vs PC3 instead of the original PC1 vs PC2

Activities:

1. Verify the breed composition of an animal for a producer interested in high-performance dairy females.
2. Create a grayscale figure for the original breed composition analysis using the provided code.
3. Create a plot using PC2 vs PC3 instead of the original PC1 vs PC2

- A dairy producer wants to buy an animal from this crossbred/purebred population. They selected Oa_3120065 and were told she was a suitable purebred for their system.



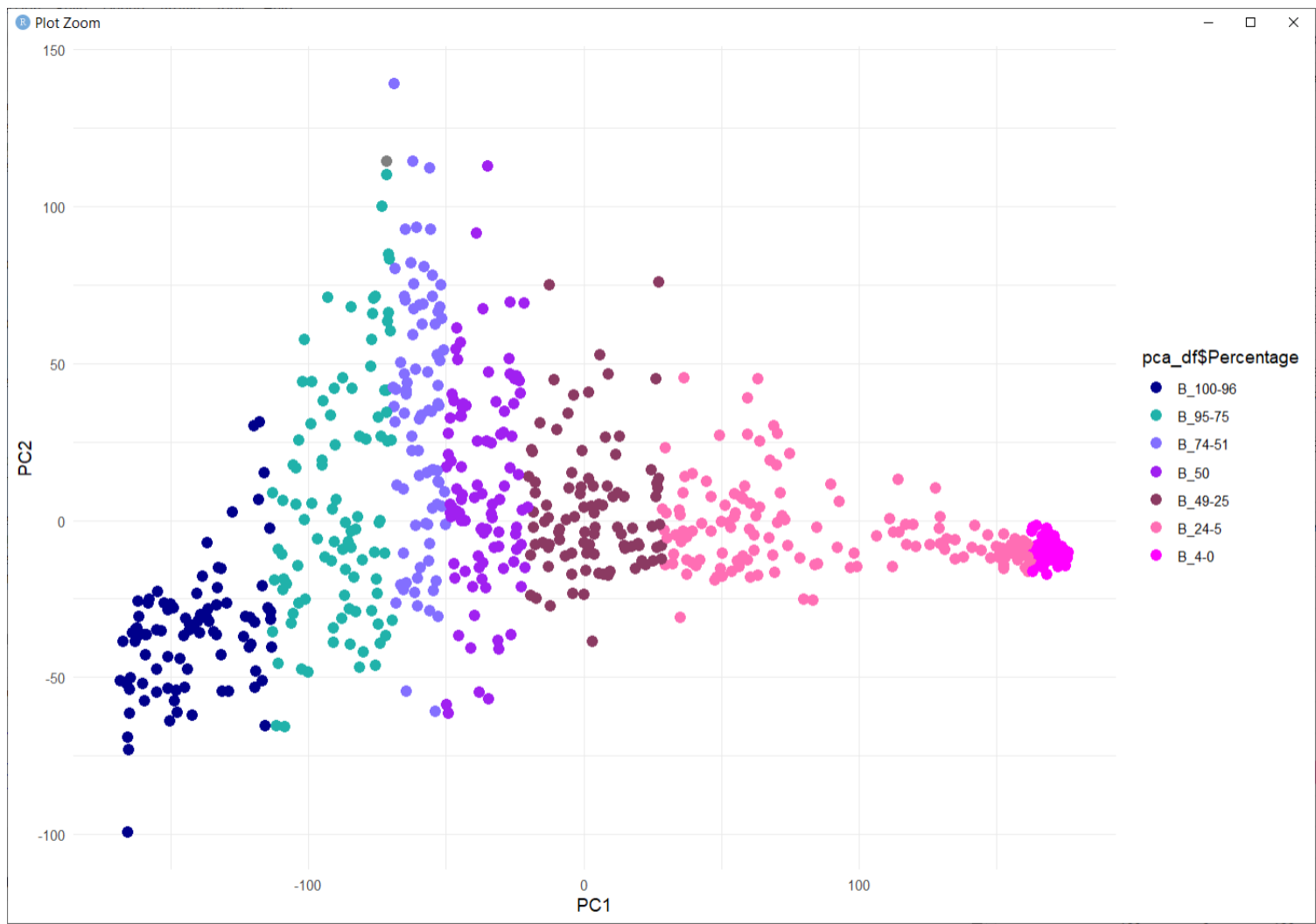
- A dairy producer wants to buy an animal from this crossbred/purebred population. They selected Oa_3120065 and were told she was a suitable purebred for their system. **Is this the case based on the breed composition analysis performed?**



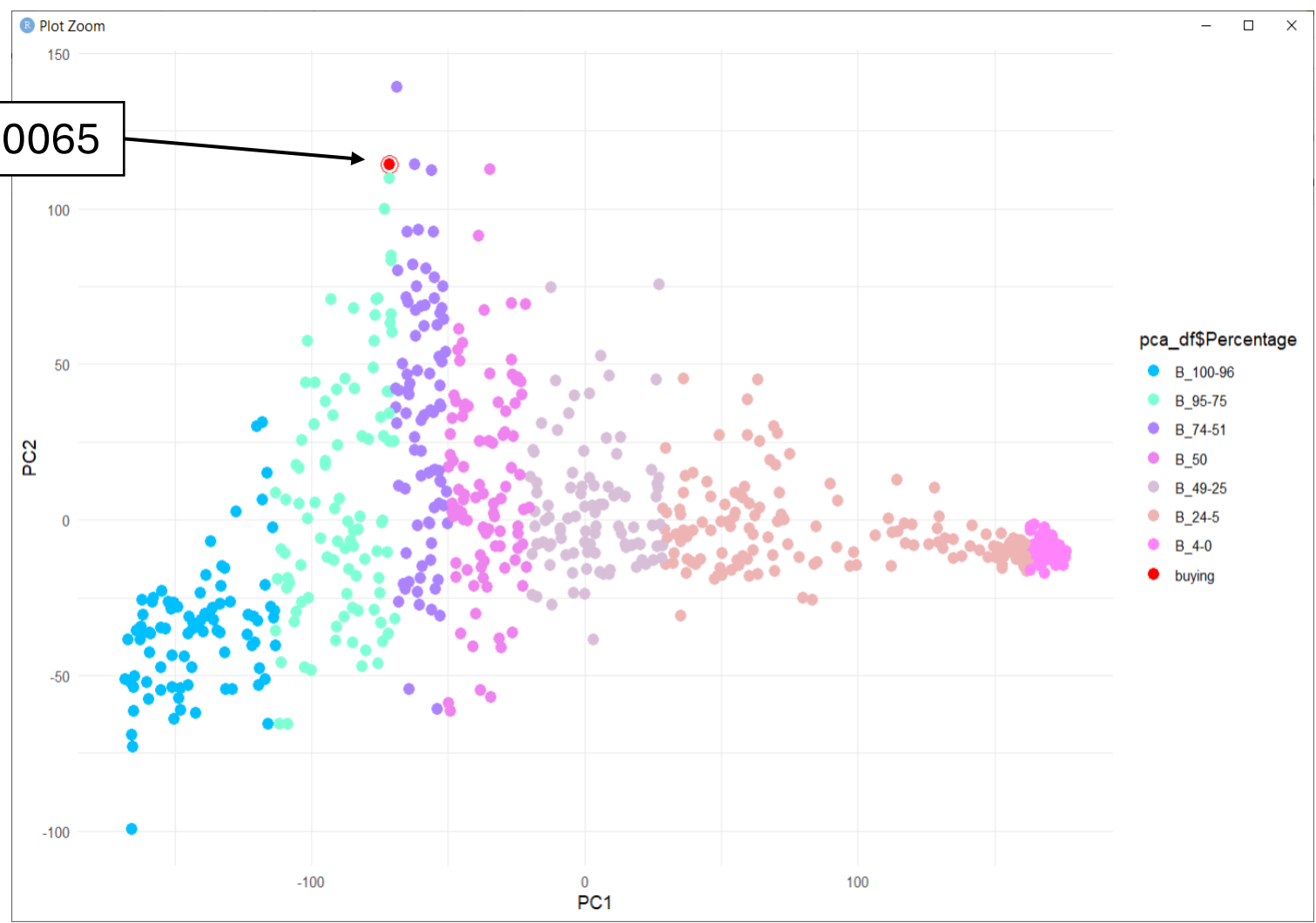
```

104
105 ▾ #####
106 ▾ ##### Activities #####
107 ▾ #####
108
109 ▾ #####
110 ▾ #####      1      #####
111 ▾ #####
112
113 # Objective: Verify the breed composition of an animal for a producer interested in high performance dairy females
114
115 # Read file breedCompositionBuying.txt using the original directory variable as input
116 breed <- read.table(file.path(directory,"breedCompositionBuying.txt"), header = TRUE,
117                     sep = "\t", stringsAsFactors = FALSE)
118
119 # Merge by animal ID objects pca and breed using animal ID
120 merged <- merge(pca, breed, by = "ID")
121
122 # Save merged file using the original directory variable as input
123 write.table(merged, file = file.path(directory,"PCA_Breed_MergedBuying.txt"), sep = "\t", quote = FALSE, row.names = FALSE)
124
125 # Use library ggplot to create a figure
126 ggplot(merged, aes(x = PC1, y = PC2, color = percentage)) +
127   scale_color_manual(values = c("B_100-96" = "deepskyblue", "B_95-75" = "aquamarine1", "B_74-51" = "mediumpurple1",
128     "B_50" = "violet", "B_49-25" = "thistle", "B_24-5" = "rosybrown2", "B_4-0" = "orchid1",
129     "buying" = "red")) +
130   geom_point(data = subset(merged, ID == "0a_3120065"), color = "red", shape = 21, size = 5) +
131   geom_point(size = 3) + theme_minimal()
132

```



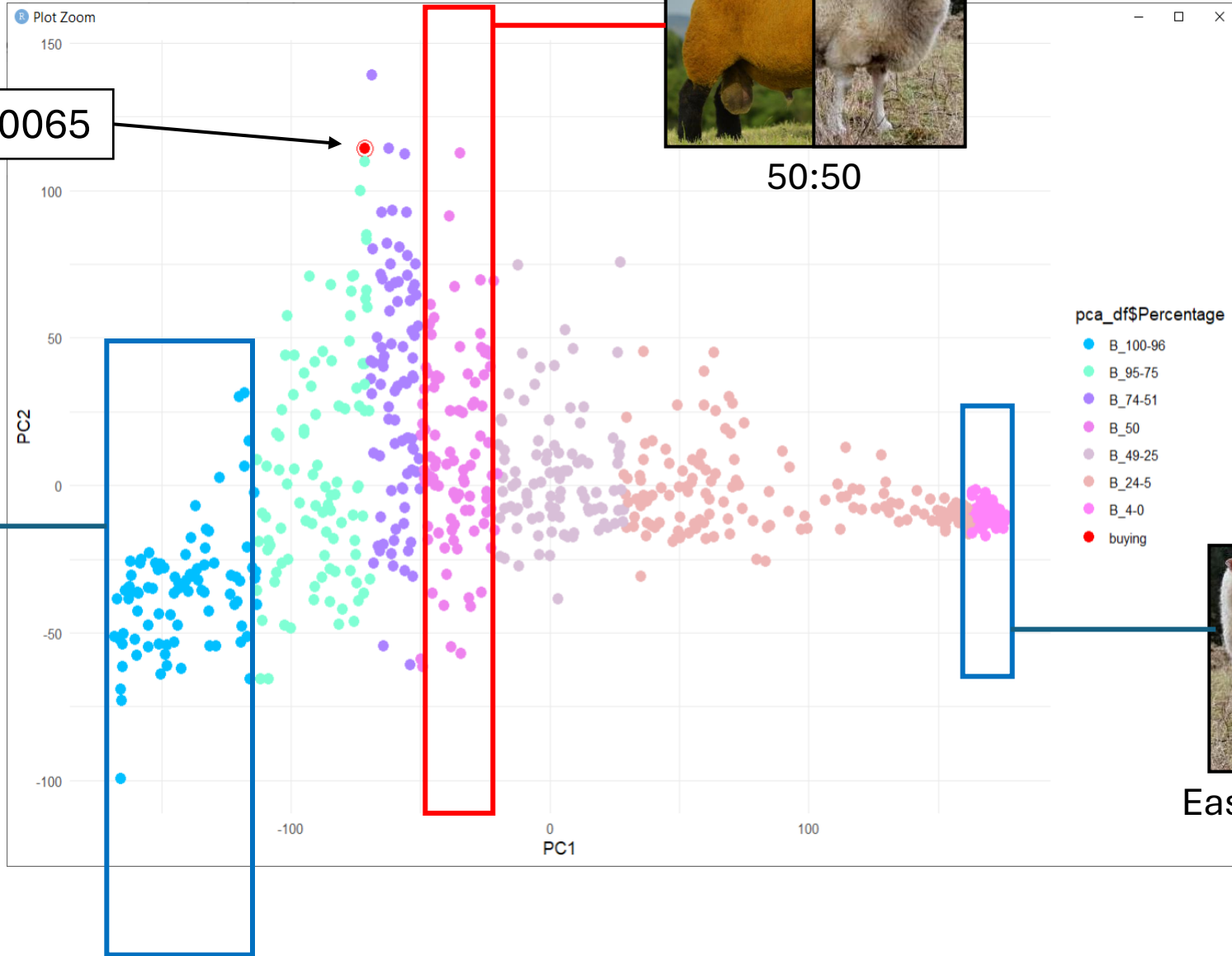
Oa_3120065





Suffolk sheep

Oa_3120065



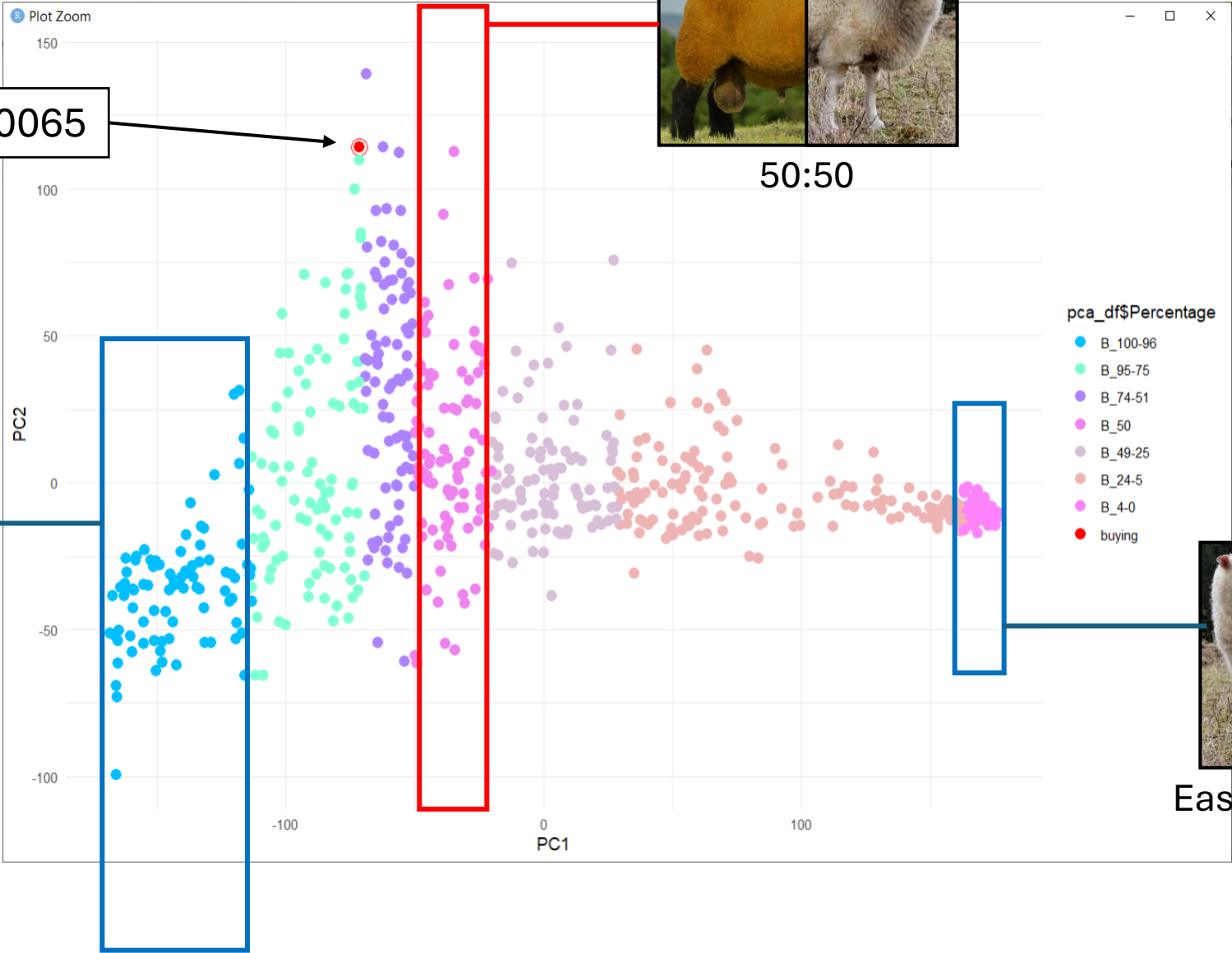
East Friesian sheep

Is this animal suitable for a dairy production system?



Suffolk sheep

Oa_3120065



50:50



East Friesian sheep

Activities:

1. Verify the breed composition of an animal for a producer interested in high-performance dairy females.
2. Create a grayscale figure for the original breed composition analysis using the provided code.
3. Create a plot using PC2 versus PC3

```

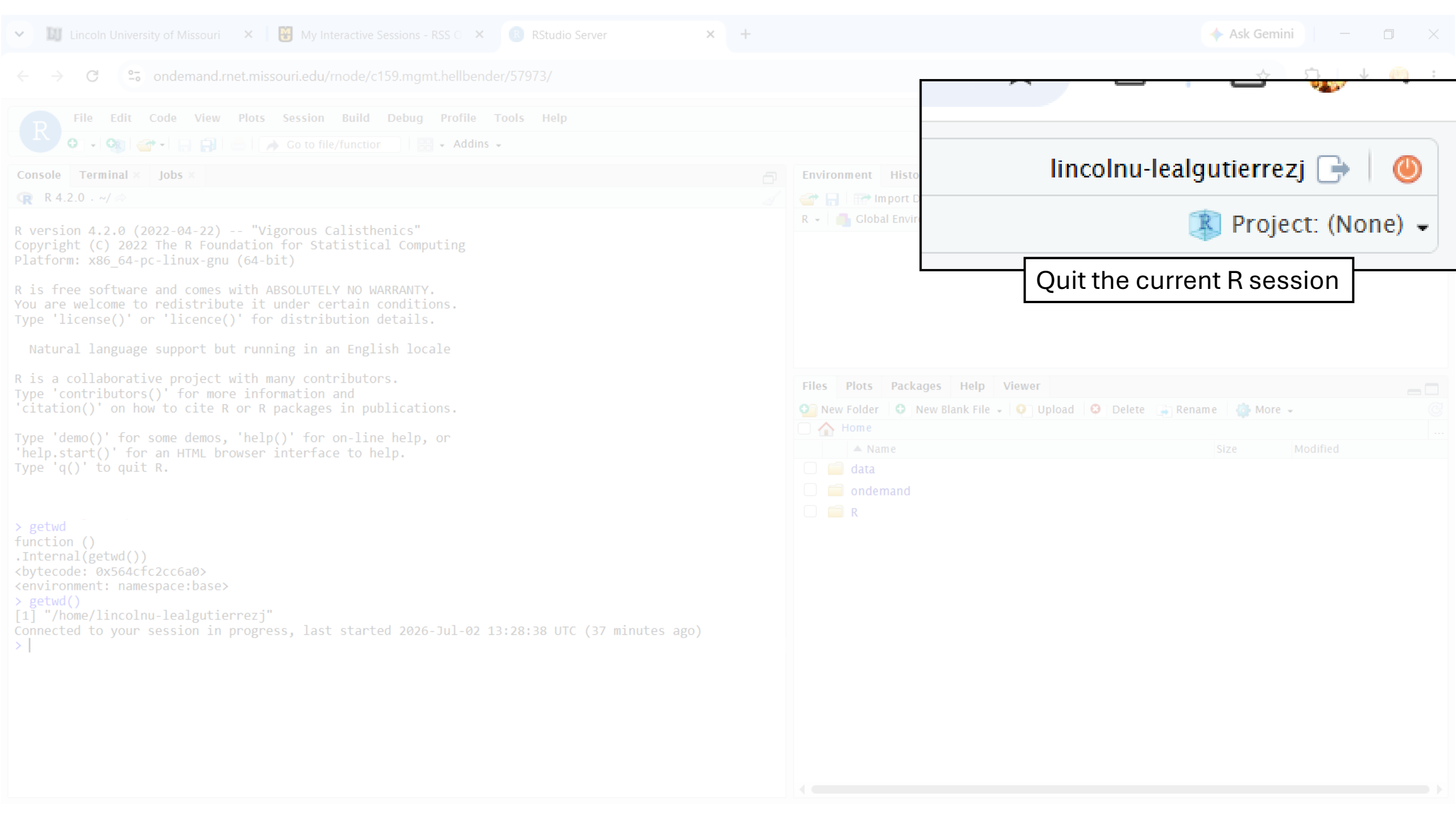
132
133 ▾ #####
134 ▾ #####      2      #####
135 ▾ #####
136
137 # Objective: Create a figure in gray scale using the following code
138
139 # Use library ggplot to create a figure
140 ggplot(merged, aes(x = PC1, y = PC2, color = percentage)) +
141   scale_color_manual(values = c("B_100-96" = "deepskyblue", "B_95-75" = "aquamarine1", "B_74-51" = "mediumpurple1",
142     "B_50" = "violet", "B_49-25" = "thistle", "B_24-5" = "rosybrown2", "B_4-0" = "orchid1",
143     "buying" = "red")) +
144   geom_point(data = subset(merged, ID == "0a_3120065"), color = "red", shape = 21, size = 5) +
145   geom_point(size = 3) + theme_minimal()
146

```

Activities:

1. Verify the breed composition of an animal for a producer interested in high-performance dairy females.
2. Create a grayscale figure for the original breed composition analysis using the provided code.
3. Create a plot using PC2 versus PC3

```
146
147 ▾ #####
148 ▾ #####      3      #####
149 ▾ #####
150
151 # Objective: Create a plot using PC2 versus PC3
152
```

lincolnu-lealgutierrezj

Project: (None)

Quit the current R session

Interactive Apps	
Desktops	
	Hellbender Desktop
GUIs	
	Matlab
	VMD
Servers	
	Code Server
	Jupyter Notebook
	MatLab (Web)
	RStudio Server

Hellbender Desktop (15283304)		Completed  
Created at: 2026-07-23 16:08:33 CDT		 Delete
Session ID: 7662a6b1-f81c-465d-9652-c6e9606845fc		
For debugging purposes, this card will be retained for 6 more days		

RStudio Server (15283292)		Completed  
Created at: 2026-07-23 16:06:53 CDT		 Delete
Session ID: 4aa70e52-4190-49d0-9e63-73e3b0c2e0b7		

Conclusions

We presented an example of how HPC resources can be applied to address complex genomic questions.

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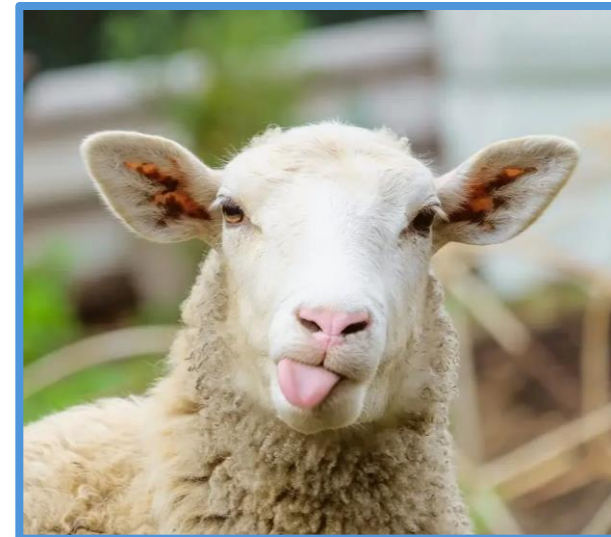
We presented an example of how HPC resources can be applied to address complex genomic questions. Can I determine the breed composition of individuals in a crossbred sheep population?

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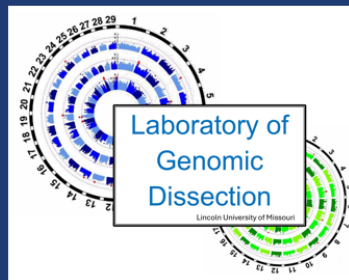


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Questions??