Lumpkin Foundation - Illinois Bundleflower Final Report

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Introduction and Summary of Work

Materials and Methods

Accession Germination Test

Field Trial Design

Harvesting

Sample Processing

NIR Spectra Sampling

Plant tissues from harvet were ground and filtered using a 1mm sieve \dots and scanned using the NeoSpectra NIR handheld scanner \dots FILL THIS OUT

Wet Chemistry

A total of 75 samples out of the entire population were selected for targeted wet chemistry analysis. Samples were selected out of the entire population using the Kennard Stone algorithm to select samples with the greatest Euclidean distance from each other, ensuring that the samples reflected the available NIR variance in the population. Samples were processed by xyz method, dried and sent to ABC labs for targeted wet chemistry analysis.. FILL THIS OUT

NIR Modeling

A total of ten wet chemistry metrics were selected for modeling. These included forage moisture content (%), forage dry matter content (%), ADF (units), NDF (units), relative feed value (units), total digestible nutrients (units), net energy gain (Mcal/cwt), net energy maintenance (Mcal/cwt), net energy lactation (Mcal/cwt), and forage yield (kg/Ha) all calculated on a dry matter basis. Spectra were presented as the percent reflectance per wavelength measured. Low quality spectra, i.e. low variance among the response values for all wavelengths, were filtered out of the dataset programatically. All spectra were then linearly resampled by wavelength to ensure equal wavelength intervals between each response value. The spectra were smoothed and detrended using a Savitsky-Golay filter by fitting a 5^{th} order polynomial over a window length of 15 frames and taking the second derivative. Standard mean subtraction scaling was applied per wavelength, but were not scaled by the colum variance. Training and testing populations (70% and 30%,

respectively) were selected from the calibration samples by using the Kennard-Stone selection algorithm. A partial least squares regression (PLSR) model was fit to the data for each of the target variables, allowing the number of model components to vary from 1 to 16 total components. Root Mean Squared Error (RMSE) defined below was used to evaluate each models performance on the training and testing populations.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} (y_i - \hat{y}_i)^2}{N}}$$

where y_i represents the ground truth target value of the i^{th} sample and \hat{y}_i represents the model prediction for that sample. The model with the lowest testing population RMSE was selected as the final model.

```
# Example dataset
set.seed(123)
data <- data.frame(</pre>
  Genotype = rep(paste0("G", 1:10), each=10),
  Location = rep(paste0("Loc", 1:5), times=20),
 Year = rep(2019:2020, each=5, times=10),
  Yield = rnorm(100, mean=500, sd=50)
)
# BLUEs: Treat Genotype as a fixed effect
model_blue <- lm(Yield ~ Genotype + Location + Year, data=data)</pre>
blues <- emmeans(model_blue, ~ Genotype)</pre>
blues_df <- as.data.frame(blues)</pre>
print(blues_df)
##
    Genotype
               emmean
                            SE df lower.CL upper.CL
             503.7313 14.7434 85 474.4175 533.0451
##
    G1
    G10
##
             521.8547 14.7434 85 492.5409 551.1685
##
  G2
             510.4311 14.7434 85 481.1173 539.7449
##
   G3
             478.7721 14.7434 85 449.4582 508.0859
             516.1022 14.7434 85 486.7884 545.4161
##
   G4
##
    G5
             499.5642 14.7434 85 470.2504 528.8780
##
   G6
             511.0843 14.7434 85 481.7705 540.3981
##
   G7
             506.1542 14.7434 85 476.8404 535.4680
##
    G8
             481.8541 14.7434 85 452.5403 511.1679
##
             515.6548 14.7434 85 486.3409 544.9686
##
## Results are averaged over the levels of: Location, Year
## Confidence level used: 0.95
# BLUPs: Treat Genotype as a random effect
model_blup <- lmer(Yield ~ Location + Year + (1 | Genotype), data=data)</pre>
## boundary (singular) fit: see help('isSingular')
blups <- ranef(model_blup)$Genotype</pre>
blups_df <- data.frame(Genotype=rownames(blups), BLUP=blups[,1])</pre>
print(blups_df)
##
      Genotype
                         BI.UP
            G1 -3.157477e-11
## 1
```

```
## 2
          G10 6.936893e-10
## 3
          G2 2.365388e-10
## 4
           G3 -1.030394e-09
## 5
           G4 4.634863e-10
## 6
           G5 -1.983323e-10
## 7
           G6 2.626786e-10
## 8
           G7 6.538503e-11
           G8 -9.070564e-10
## 9
## 10
           G9 4.455797e-10
```

BLUE/BLUP

Selection Index

Results

Germination Results

```
germination_data <- fread('../data/lumpkin_ibf_germination_test.csv')
head(germination_data)</pre>
```

```
##
      sample_id germination_test germination_pct hard_pct total_viable_pct
##
        <char>
                         <char>
                                          <num>
                                                   <num>
                                                                   <num>
## 1: IBF-KS-1
                       200 seed
                                           16.0
                                                    15.5
                                                                    31.5
## 2: IBF-KS-2
                       200 seed
                                           18.0
                                                    16.5
                                                                    34.5
## 3: IBF-KS-3
                       200 seed
                                          21.0
                                                    24.0
                                                                    45.0
## 4: IBF-KS-4
                                          16.5
                                                  19.0
                                                                    35.5
                       200 seed
## 5: IBF-KS-5
                       200 seed
                                          18.5
                                                  18.0
                                                                    36.5
## 6: IBF-KS-6
                                                  22.5
                       200 seed
                                          28.0
                                                                    50.5
```

Yield Data

```
## Type III Analysis of Variance Table with Satterthwaite's method
## Sum Sq Mean Sq NumDF DenDF F value Pr(>F)
## trts 224162941 2837506    79 227.06 1.4554 0.01718 *
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

summary(yield_mm)

```
## Linear mixed model fit by REML. t-tests use Satterthwaite's method [
## lmerModLmerTest]
## Formula: forage_yield_kg_ha ~ trts + (1 | block)
      Data: yield_data
##
##
## REML criterion at convergence: 4097
## Scaled residuals:
       Min
                10 Median
                                30
                                       Max
  -2.7993 -0.6403 -0.0022 0.5280
                                    3.2584
##
## Random effects:
   Groups
##
            Name
                         Variance Std.Dev.
  block
             (Intercept) 121474
                                   348.5
## Residual
                         1949644 1396.3
## Number of obs: 310, groups: block, 4
##
## Fixed effects:
                       Estimate Std. Error
##
                                                df t value Pr(>|t|)
## (Intercept)
                         3362.2
                                     719.6
                                            182.9
                                                     4.673 5.75e-06 ***
## trtsID 1006 Year 88
                         1797.0
                                     987.3
                                            227.0
                                                     1.820 0.070066
## trtsID 1007 Year 90
                         2754.6
                                     987.3
                                            227.0
                                                     2.790 0.005720 **
## trtsID 1009 Year 90
                         1025.0
                                     987.3 227.0
                                                     1.038 0.300320
                                     987.3 227.0
## trtsID 1010 Year 88
                          958.4
                                                     0.971 0.332748
                                     987.3 227.0
## trtsID 1014 Year 88
                         2571.1
                                                     2.604 0.009820 **
## trtsID 1015 Year 88
                         2716.2
                                     987.3 227.0
                                                     2.751 0.006419 **
## trtsID 1017 Year 88
                         3191.9
                                     987.3 227.0
                                                     3.233 0.001408 **
## trtsID 103 Year 88
                         2867.7
                                     987.3 227.0
                                                     2.904 0.004042 **
## trtsID 1031 Year 90
                         1668.0
                                    1067.3 227.2
                                                     1.563 0.119482
                         1721.7
## trtsID 1032 Year 89
                                     987.3 227.0
                                                     1.744 0.082548
## trtsID 1037 Year 89
                         1623.1
                                     987.3 227.0
                                                     1.644 0.101569
                                    1067.3 227.2
## trtsID 1040 Year 90
                         1841.6
                                                     1.726 0.085791
## trtsID 1042 Year 89
                         2413.1
                                     987.3 227.0
                                                     2.444 0.015286 *
## trtsID 1043 Year 90
                                     987.3 227.0
                                                     1.110 0.268256
                         1095.7
## trtsID 1045 Year 88
                         1215.5
                                     987.3 227.0
                                                     1.231 0.219561
                                     987.3 227.0
## trtsID 1046 Year 88
                         3352.9
                                                     3.396 0.000807 ***
## trtsID 1047 Year 89
                         1596.3
                                     987.3 227.0
                                                     1.617 0.107304
## trtsID 1056 Year 89
                                     987.3 227.0
                         3949.4
                                                     4.000 8.57e-05 ***
## trtsID 1062 Year 88
                         1733.7
                                     987.3
                                            227.0
                                                     1.756 0.080449
                                     987.3 227.0
## trtsID 1063 Year 88
                         1674.8
                                                     1.696 0.091198
## trtsID 1064 Year 89
                         1971.2
                                     987.3 227.0
                                                     1.996 0.047076 *
## trtsID 1065 Year 90
                                     987.3 227.0
                          996.8
                                                     1.010 0.313742
## trtsID 1067 Year 88
                         2510.6
                                     987.3 227.0
                                                     2.543 0.011661 *
## trtsID 1070 Year 88
                                    1067.3 227.2
                                                     1.221 0.223204
                         1303.5
## trtsID 1071 Year 89
                         1583.8
                                     987.3 227.0
                                                     1.604 0.110086
## trtsID 1075 Year 88
                         2233.0
                                     987.3 227.0
                                                     2.262 0.024668
## trtsID 1076 Year 88
                         2188.4
                                     987.3 227.0
                                                     2.216 0.027652 *
## trtsID 1080 Year 90
                         1317.9
                                    1067.3 227.2
                                                     1.235 0.218149
## trtsID 1081 Year 90
                                    1067.3 227.2
                                                     1.692 0.091968 .
                         1806.1
## trtsID 1095 Year 90
                         1072.0
                                     987.3 227.0
                                                     1.086 0.278735
                          865.2
                                     987.3 227.0
## trtsID 1096 Year 90
                                                    0.876 0.381765
```

```
## trtsID 1097 Year 90
                         2768.0
                                     987.3 227.0
                                                     2.804 0.005492 **
                                                     2.407 0.016895 *
## trtsID 1099 Year 90
                                     987.3 227.0
                         2376.3
## trtsID 1100 Year 90
                         1917.5
                                     987.3 227.0
                                                     1.942 0.053360
## trtsID 1101 Year 90
                                     987.3 227.0
                                                     1.503 0.134205
                         1484.0
## trtsID 1104 Year 90
                          841.5
                                     987.3
                                            227.0
                                                     0.852 0.394972
## trtsID 1107 Year 90
                         2014.4
                                     987.3 227.0
                                                     2.040 0.042482 *
## trtsID 1108 Year 90
                         1863.0
                                     987.3 227.0
                                                     1.887 0.060447 .
## trtsID 1109 Year 90
                         2908.0
                                     987.3 227.0
                                                     2.945 0.003562 **
## trtsID 1110 Year 90
                         1243.6
                                     987.3
                                            227.0
                                                     1.260 0.209111
                                                     1.344 0.180361
## trtsID 1111 Year 90
                         1434.2
                                    1067.3 227.2
## trtsID 1112 Year 90
                          794.6
                                     987.3 227.0
                                                     0.805 0.421760
## trtsID 1114 Year 90
                                     987.3 227.0
                         3767.7
                                                     3.816 0.000175 ***
## trtsID 1115 Year 90
                         2419.3
                                     987.3 227.0
                                                     2.450 0.015027 *
## trtsID 1117 Year 90
                                     987.3 227.0
                         1970.4
                                                     1.996 0.047159 *
## trtsID 1118 Year 90
                                     987.3 227.0
                         2406.3
                                                     2.437 0.015572 *
## trtsID 1119 Year 90
                         2246.3
                                     987.3
                                            227.0
                                                     2.275 0.023833 *
                                     987.3 227.0
## trtsID 1120 Year 90
                         3507.6
                                                     3.553 0.000464 ***
## trtsID 1123 Year 90
                         2175.1
                                     987.3 227.0
                                                     2.203 0.028601 *
## trtsID 1124 Year 90
                                     987.3 227.0
                         2723.3
                                                     2.758 0.006286 **
## trtsID 1125 Year 90
                         1315.4
                                     987.3 227.0
                                                     1.332 0.184111
## trtsID 1126 Year 90
                         1961.5
                                     987.3 227.0
                                                     1.987 0.048162 *
## trtsID 1127 Year 90
                                     987.3 227.0
                                                     3.168 0.001747 **
                         3127.8
## trtsID 1129 Year 90
                                     987.3 227.0
                         2555.3
                                                     2.588 0.010275 *
## trtsID 1130 Year 90
                                            227.0
                         2510.1
                                     987.3
                                                     2.542 0.011677 *
## trtsID 1132 Year 90
                         1221.5
                                     987.3 227.0
                                                     1.237 0.217305
## trtsID 1136 Year 90
                         2720.3
                                     987.3 227.0
                                                     2.755 0.006341 **
## trtsID 1137 Year 90
                         1272.0
                                     987.3 227.0
                                                     1.288 0.198941
## trtsID 1139 Year 90
                         2906.3
                                     987.3 227.0
                                                     2.944 0.003582 **
                                     987.3 227.0
                                                     1.366 0.173250
## trtsID 1140 Year 90
                         1348.8
## trtsID 1141 Year 90
                         1343.3
                                     987.3 227.0
                                                     1.361 0.175015
## trtsID 1143 Year 90
                         1304.2
                                     987.3 227.0
                                                     1.321 0.187842
## trtsID 1144 Year 90
                         4493.5
                                     987.3
                                            227.0
                                                     4.551 8.70e-06 ***
## trtsID 275 Year 88
                         2161.3
                                     987.3 227.0
                                                     2.189 0.029614 *
## trtsID 282 Year 90
                                    1067.3 227.2
                          370.3
                                                     0.347 0.728906
## trtsID 289 Year 88
                         1731.1
                                    1067.3
                                            227.2
                                                     1.622 0.106198
## trtsID 291 Year 90
                                     987.3 227.0
                         2819.8
                                                     2.856 0.004689 **
## trtsID 294 Year 90
                         2450.9
                                     987.3 227.0
                                                     2.482 0.013775 *
## trtsID 360 Year 90
                         1962.2
                                     987.3 227.0
                                                     1.987 0.048080 *
## trtsID 371 Year 88
                         1300.5
                                     987.3 227.0
                                                     1.317 0.189094
## trtsID 377 Year 90
                                     987.3 227.0
                         1552.1
                                                     1.572 0.117339
## trtsID 379 Year 89
                         2630.8
                                     987.3 227.0
                                                     2.665 0.008262 **
## trtsID 382 Year 88
                                     987.3 227.0
                                                     1.339 0.181954
                         1321.9
## trtsID 391 Year 90
                         3226.8
                                     987.3 227.0
                                                     3.268 0.001250 **
## trtsID 393 Year 88
                                     987.3 227.0
                                                     1.515 0.131203
                         1495.7
## trtsID 413 Year 90
                         1845.8
                                     987.3 227.0
                                                     1.870 0.062837
## trtsID 415 Year 89
                                     987.3 227.0
                                                     2.511 0.012744 *
                         2478.9
## trtsKura Clover
                          254.4
                                     987.3 227.0
                                                     0.258 0.796916
## trtsSainfoin
                         1123.7
                                    1211.4 227.4
                                                     0.928 0.354581
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
## Correlation matrix not shown by default, as p = 80 > 12.
## Use print(value, correlation=TRUE)
```

NIR Modeling

Model	Num. Components	Test RMSE	Train RMSE
Forage Yield	6	1331.441	1238.371
NEL	4	3.937	3.050
NEG	2	2.896	2.246
NEM	2	3.142	2.439
TDN	4	1.848	1.559
RFV	5	11.293	8.491
NDF	5	2.889	2.174
ADF	2	4.744	4.029
Crude Protein	2	1.159	1.053
Dry Matter Content	1	2.997	2.557
Moisture Content	1	2.997	2.557