

DirichletReg: Dirichlet Regression for Compositional Data in R

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Abstract

...

Keywords: Dirichlet regression, Dirichlet distribution, multivariate generalized linear model, rates, proportions, rates, compositional data, simplex, R.

4. Application examples

4.1. The Arctic lake (common parametrization)

```
> library(DirichletReg)
> head(ArcticLake)

  sand   silt   clay depth
1 0.775 0.195 0.030 10.4
2 0.719 0.249 0.032 11.7
3 0.507 0.361 0.132 12.8
4 0.522 0.409 0.066 13.0
5 0.700 0.265 0.035 15.7
6 0.665 0.322 0.013 16.3

> AL <- DR_data(ArcticLake[, 1:3])

> AL[1:6, ]

  sand      silt      clay
1 0.7750000 0.1950000 0.0300000
2 0.7190000 0.2490000 0.0320000
3 0.5070000 0.3610000 0.1320000
4 0.5235707 0.4102307 0.0661986
5 0.7000000 0.2650000 0.0350000
6 0.6650000 0.3220000 0.0130000

> lake1 <- DirichReg(AL ~ depth, ArcticLake)
> lake1

Call:
DirichReg(formula = AL ~ depth, data = ArcticLake)
using the common parametrization
```

```

> par(mfrow = c(2, 1))
> plot(AL, cex = 0.5, a2d = list(colored = FALSE, c.grid = FALSE))
> plot(rep(ArcticLake$depth, 3), as.numeric(AL), pch = 21, bg = rep(c("#E495A5",
+      "#86B875", "#7DB0DD"), each = 39), xlab = "Depth (m)", ylab = "Proportion",
+      ylim = 0:1)

```

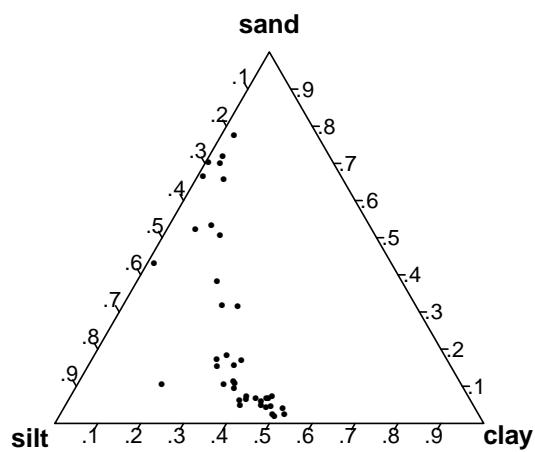


Figure 1: Arctic lake: Ternary plot and depth vs. composition.

```

Log-likelihood: 101.4 on 6 df (54+3 iterations)

-----
Coefficients for variable no. 1: sand
(Intercept)      depth
  0.11662     0.02335
-----
Coefficients for variable no. 2: silt
(Intercept)      depth
 -0.31060     0.05557
-----
Coefficients for variable no. 3: clay
(Intercept)      depth
 -1.1520      0.0643
-----

> coef(lake1)

$sand
(Intercept)      depth
  0.11662480   0.02335114

$silt
(Intercept)      depth
 -0.31059591   0.05556745

$clay
(Intercept)      depth
 -1.15195642   0.06430175

> lake2 <- update(lake1, . ~ . + I(depth^2) | . + I(depth^2) | . + I(depth^2))
> anova(lake1, lake2)

Analysis of Deviance Table

Model 1:
DirichReg(formula = AL ~ depth, data = ArcticLake)
Model 2:
DirichReg(formula = AL ~ depth + I(depth^2) | depth + I(depth^2) | depth + I(depth^2), data = ArcticLake)

      Deviance  N. par  Difference  df      p-value
Model 1    -202.7393      6          -      -        -
Model 2    -217.9937      9       15.25441      3  0.001611655

> summary(lake2)

Call:
DirichReg(formula = AL ~ depth + I(depth^2) | depth + I(depth^2) | depth + I(depth^2), data =
ArcticLake)

Standardized Residuals:
      Min      1Q      Median      3Q      Max
sand -1.7647 -0.7080 -0.1786  0.9598  3.0460
silt -1.1379 -0.5330 -0.1546  0.2788  1.5604
clay -1.7661 -0.6583 -0.0454  0.6584  2.0152

-----
Beta-Coefficients for variable no. 1: sand
      Estimate Std. Error z-Value p-Value
(Intercept) 1.4361967  0.8026814   1.789  0.0736 .

```

```

depth      -0.0072383  0.0329433 -0.220  0.8261
I(depth^2)  0.0001324  0.0002761   0.480  0.6315
-----
Beta-Coefficients for variable no. 2: silt
  Estimate Std. Error z-Value p-Value
(Intercept) -0.0259705  0.7598827 -0.034  0.9727
depth       0.0717450  0.0343089  2.091  0.0365 *
I(depth^2) -0.0002679  0.0003088 -0.867  0.3857
-----
Beta-Coefficients for variable no. 3: clay
  Estimate Std. Error z-Value p-Value
(Intercept) -1.7931487  0.7362293 -2.436 0.01487 *
depth       0.1107906  0.0357705  3.097 0.00195 **
I(depth^2) -0.0004872  0.0003308 -1.473 0.14079
-----
Signif. codes: `***' < .001, `**' < 0.01, `*' < 0.05, `.' < 0.1

Log-likelihood: 109 on 9 df (168+2 iterations)
AIC: -200, BIC: -185.0217
Number of Observations: 39
Link: Log
Parametrization: common

```

4.2. Blood samples (alternative parametrization)

```

> Bld <- BloodSamples
> Bld$Smp <- DR_data(Bld[, 1:4])

> blood1 <- DirichReg(Smp ~ Disease | 1, Bld, model = "alternative", base = 3)
> blood2 <- DirichReg(Smp ~ Disease | Disease, Bld, model = "alternative", base = 3)
> anova(blood1, blood2)

Analysis of Deviance Table

Model 1:
DirichReg(formula = Smp ~ Disease | 1, data = Bld, model = "alternative", base = 3)
Model 2:
DirichReg(formula = Smp ~ Disease | Disease, data = Bld, model = "alternative", base = 3)

      Deviance  N. par  Difference  df      p-value
Model 1 -303.8560    7          -        -        -
Model 2 -304.6147    8     0.7586655    1  0.3837465

> summary(blood1)

Call:
DirichReg(formula = Smp ~ Disease | 1, data = Bld, model = "alternative", base = 3)

Standardized Residuals:
      Min      1Q   Median      3Q      Max
Albumin -2.1310 -0.9307 -0.1234  0.8149  2.8429
Pre.Albumin -1.0687 -0.4054 -0.0789  0.1947  1.5691
Globulin.A -2.0503 -1.0392  0.1938  0.7927  2.2393
Globulin.B -1.8176 -0.5347  0.1488  0.5115  1.3284

MEAN MODELS:
-----
Coefficients for variable no. 1: Albumin
  Estimate Std. Error z-Value p-Value
(Intercept)  1.11639   0.09935 11.237 <2e-16 ***

```

```

> par(mar = c(4, 4, 4, 4) + 0.1)
> plot(rep(ArcticLake$depth, 3), as.numeric(AL), pch = 21, bg = rep(c("#E495A5",
+      "#86B875", "#7DB0DD"), each = 39), xlab = "Depth (m)", ylab = "Proportion",
+      ylim = 0:1, main = "Sediment Composition in an Arctic Lake")
> Xnew <- data.frame(depth = seq(min(ArcticLake$depth), max(ArcticLake$depth),
+      length.out = 100))
> for (i in 1:3) lines(cbind(Xnew, predict(lake2, Xnew)[, i]), col = c("#E495A5",
+      "#86B875", "#7DB0DD")[i], lwd = 2)
> legend("topleft", legend = c("Sand", "Silt", "Clay"), lwd = 2, col = c("#E495A5",
+      "#86B875", "#7DB0DD"), pt.bg = c("#E495A5", "#86B875", "#7DB0DD"), pch = 21,
+      bty = "n")
> par(new = TRUE)
> plot(cbind(Xnew, predict(lake2, Xnew, F, F, T)), lty = "24", type = "l", ylim = c(0,
+      max(predict(lake2, Xnew, F, F, T))), axes = F, ann = F, lwd = 2)
> axis(4)
> mtext(expression(paste("Precision (", phi, ")")), 4, line = 3)
> legend("top", legend = c(expression(hat(mu)[c] == hat(alpha)[c]/hat(alpha)[0])),
+      expression(hat(phi) == hat(alpha)[0])), lty = c(1, 2), lwd = c(3, 2), bty = "n")

```

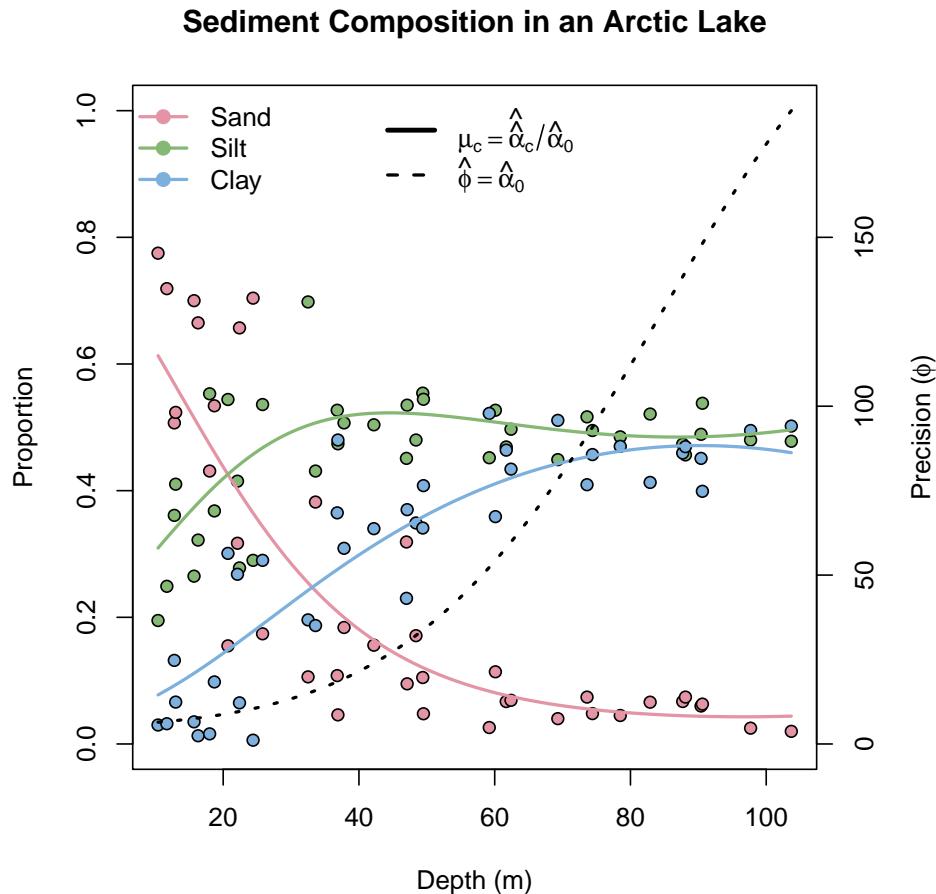


Figure 2: Arctic lake: Fitted values of the quadratic model.

```

> AL <- ArcticLake
> AL$AL <- DR_data(ArcticLake[, 1:3])
> dd <- range(ArcticLake$depth)
> X <- data.frame(depth = seq(dd[1], dd[2], length.out = 200))
> pp <- predict(DirichletReg(AL ~ depth + I(depth^2), AL), X)
> plot(AL$AL, cex = 0.1, reset_par = FALSE)
> points(DirichletReg:::coord.trafo(AL$AL[, c(2, 3, 1)]), pch = 16, cex = 0.5,
+ col = gray(0.5))
> lines(DirichletReg:::coord.trafo(pp[, c(2, 3, 1)]), lwd = 3, col = c("#6E1D34",
+ "#004E42")[2])
> Dols <- log(cbind(ArcticLake[, 2]/ArcticLake[, 1], ArcticLake[, 3]/ArcticLake[, 1]))
> ols <- lm(Dols ~ depth + I(depth^2), ArcticLake)
> p2 <- predict(ols, X)
> p2m <- exp(cbind(0, p2[, 1], p2[, 2]))/rowSums(exp(cbind(0, p2[, 1], p2[, 2])))
> lines(DirichletReg:::coord.trafo(p2m[, c(2, 3, 1)]), lwd = 3, col = c("#6E1D34",
+ "#004E42")[1], lty = "21")

```

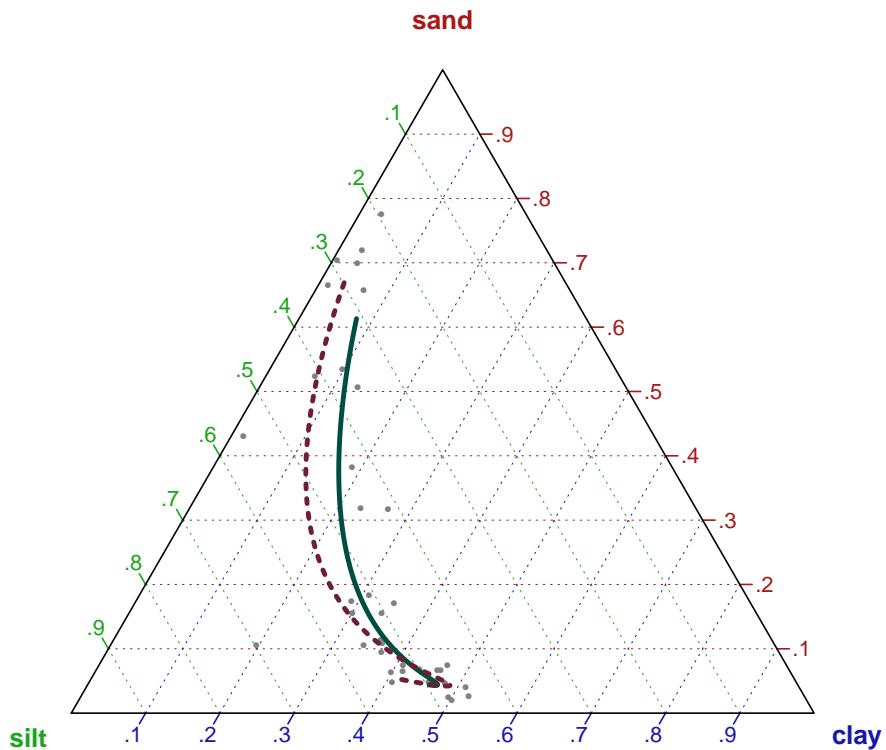


Figure 3: Arctic lake: OLS (dashed) vs. Dirichlet regression (solid) predictions.

```
> par(mfrow = c(1, 4))
> for (i in 1:4) {
+   boxplot(Bld$Smp[, i] ~ Bld$Disease, ylim = range(Bld$Smp[, 1:4]), main = paste(names(Bld)[i]),
+         xlab = "Disease Type", ylab = "Proportion")
+   segments(c(-5, 1.5), unique(fitted(blood2)[, i]), c(1.5, 5), unique(fitted(blood2)[,
+     i]), lwd = 3, lty = 2)
+ }
```

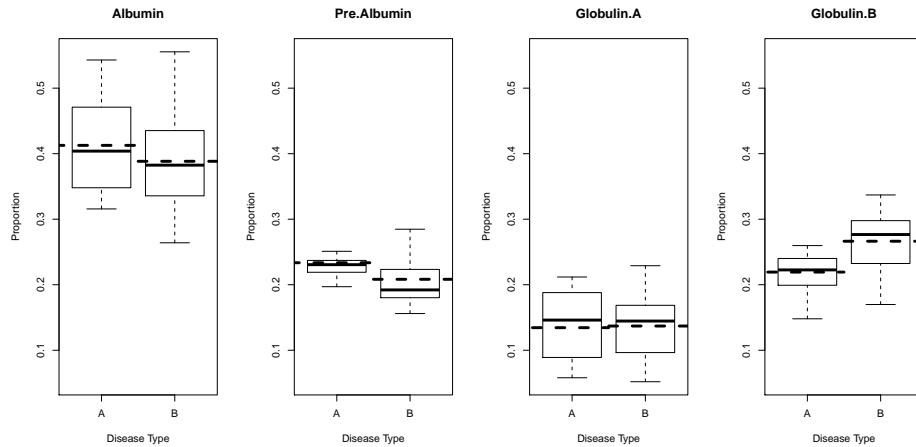


Figure 4: Blood samples: Box plots and fitted values (dashed lines indicate the fitted values for each group).

```
DiseaseB      -0.07002    0.13604   -0.515    0.607
-----
Coefficients for variable no. 2: Pre.Albumin
Estimate Std. Error z-Value p-Value
(Intercept)  0.5490    0.1082   5.076 3.86e-07 ***
DiseaseB     -0.1276    0.1493   -0.855    0.393
-----
Coefficients for variable no. 3: Globulin.A
- variable omitted (reference category) -
-----
Coefficients for variable no. 4: Globulin.B
Estimate Std. Error z-Value p-Value
(Intercept)  0.4863    0.1094   4.445 8.8e-06 ***
DiseaseB     0.1819    0.1472   1.236    0.216
-----
PRECISION MODEL:
-----
Estimate Std. Error z-Value p-Value
(Intercept)  4.2227    0.1475  28.64 <2e-16 ***
-----
Signif. codes: '***' < .001, '**' < 0.01, '*' < 0.05, '.' < 0.1

Log-likelihood: 151.9 on 7 df (56+2 iterations)
AIC: -289.9, BIC: -280.0476
Number of Observations: 30
Links: Logit (Means) and Log (Precision)
Parametrization: alternative
```

```
> alpha <- predict(blood2, data.frame(Disease = factor(c("A", "B"))), F, T, F)
> L <- sapply(1:2, function(i) ddirichlet(DR_data(Bld[31:36, 1:4]), unlist(alpha[i,
+   ])))
```

```
> LP <- L/rowSums(L)
> dimnames(LP) <- list(paste("C", 1:6), c("A", "B"))
> print(data.frame(round(LP * 100, 1), pred. = as.factor(ifelse(LP[, 1] > LP[, 2], "=> A", "=> B"))), print.gap = 2)

      A     B  pred.
C 1 59.4 40.6  ==> A
C 2 43.2 56.8  ==> B
C 3 38.4 61.6  ==> B
C 4 43.8 56.2  ==> B
C 5 36.6 63.4  ==> B
C 6 70.2 29.8  ==> A
```

4.3. Reading skills data (alternative parametrization)

```
> RS <- ReadingSkills
> RS$acc <- DR_data(RS$accuracy)
> RS$dyslexia <- C(RS$dyslexia, treatment)
> rs1 <- DirichReg(acc ~ dyslexia * iq | dyslexia * iq, RS, model = "alternative")
> rs2 <- DirichReg(acc ~ dyslexia * iq | dyslexia + iq, RS, model = "alternative")
> anova(rs1, rs2)
```

Analysis of Deviance Table

```
Model 1:
DirichReg(formula = acc ~ dyslexia * iq | dyslexia * iq, data = RS, model = "alternative")
Model 2:
DirichReg(formula = acc ~ dyslexia * iq | dyslexia + iq, data = RS, model = "alternative")

      Deviance   N. par   Difference   df      p-value
Model 1 -133.4682       8          -         -        -
Model 2 -131.8037       7      1.664453      1  0.1970031
```

```
> a <- RS$accuracy
> logRa_a <- log(a/(1 - a))
> rlr <- lm(logRa_a ~ dyslexia * iq, RS)
> summary(rlr)
```

Call:
`lm(formula = logRa_a ~ dyslexia * iq, data = RS)`

Residuals:

Min	1Q	Median	3Q	Max
-2.66405	-0.37966	0.03687	0.40887	2.50345

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	2.8067	0.2822	9.944	2.27e-12 ***
dyslexiayes	-2.4113	0.4517	-5.338	4.01e-06 ***
iq	0.7823	0.2992	2.615	0.0125 *
dyslexiayes:iq	-0.8457	0.4510	-1.875	0.0681 .

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.2 on 40 degrees of freedom
Multiple R-squared: 0.6151, Adjusted R-squared: 0.5862
F-statistic: 21.31 on 3 and 40 DF, p-value: 2.083e-08

```
> summary(rs2)
```

```

> B2 <- DR_data(BloodSamples[, c(1, 2, 4)])
> plot(B2, cex = 0.001, reset_par = FALSE)
> div.col <- c("#023FA5", "#1A44A4", "#2749A4", "#314DA4", "#3952A5", "#4056A6",
+   "#465BA8", "#4D5FA9", "#5264AA", "#5868AC", "#5D6CAE", "#6371AF", "#6875B1",
+   "#6D79B3", "#727DB5", "#7681B7", "#7B85B8", "#8089BA", "#848DBC", "#8991BE",
+   "#8D95BF", "#9199C1", "#959CC3", "#9AA0C5", "#9EA4C6", "#A2A7C8", "#A5ABCA",
+   "#A9AEBC", "#ADB1CD", "#B1B5CE", "#B4B8D0", "#B8BBB1", "#BBBED2", "#BEC1D4",
+   "#C1C4D5", "#C5C7D6", "#C8CAD8", "#CBCCD9", "#CDCFDA", "#D0D1DB", "#D3D4DC",
+   "#D5D6DD", "#D7D8DE", "#D9DADF", "#DBDCEO", "#DDDEEO", "#DFDFE1", "#E0E0E1",
+   "#E1E1E2", "#E2E2E2", "#E2E1E1", "#E2E0E0", "#E1DFDF", "#E1DDDD",
+   "#E0DBDC", "#E0D9DA", "#DFD6D8", "#DED4D6", "#DDD1D3", "#DCCFD1", "#DBCCCE",
+   "#DBC9CC", "#D9C6C9", "#D8C2C6", "#D7BFC3", "#D6BCC0", "#D5B8BD", "#D4B5BA",
+   "#D2B1B7", "#D1ADB3", "#CFA9B0", "#CEA5AC", "#CCA1A9", "#CB9DA5", "#C999A2",
+   "#C7949E", "#C6909A", "#C48C96", "#C28792", "#C0828E", "#BE7E8A", "#BC7986",
+   "#B97482", "#B76F7E", "#B56A7A", "#B36576", "#B06071", "#AE5A6D", "#AB5569",
+   "#A94F64", "#A64A60", "#A3445B", "#A03E57", "#9D3752", "#9B304E", "#982949",
+   "#952045", "#911640", "#8E063B")
> temp <- (alpha/rowSums(alpha))[, c(2, 4, 1)]
> points(DirichletReg:::coord.trafo(temp/rowSums(temp)), pch = 22, bg = div.col[c(1,
+   100)], cex = 2, lwd = 0.25)
> temp <- B2[1:30, c(2, 3, 1)]
> points(DirichletReg:::coord.trafo(temp/rowSums(temp)), pch = 21, bg = (div.col[c(1,
+   100)][BloodSamples$Disease[1:30]]), cex = 0.5, lwd = 0.25)
> temp <- B2[31:36, c(2, 3, 1)]
> points(DirichletReg:::coord.trafo(temp/rowSums(temp)), pch = 21, bg = div.col[round(100 *
+   LP[, 2], 0)], cex = 1, lwd = 0.5)
> legend("topleft", bty = "n", legend = c("Disease A", "Disease B", NA, "Expected Values"),
+   pch = c(21, 21, NA, 22), pt.bg = c(div.col[c(1, 100)], NA, "white"))

```

- Disease A
- Disease B
- Expected Values

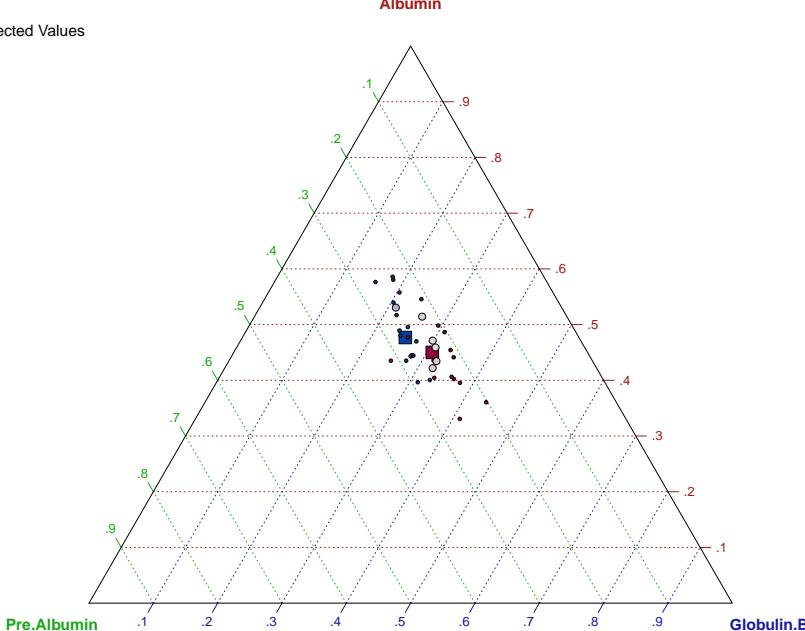


Figure 5: Blood samples: Observed values and predictions

```

Call:
DirichReg(formula = acc ~ dyslexia * iq | dyslexia + iq, data = RS, model = "alternative")

Standardized Residuals:
      Min     1Q   Median     3Q    Max
1 - accuracy -1.5661 -0.8204 -0.5112  0.5211  3.4334
accuracy     -3.4334 -0.5211  0.5112  0.8204  1.5661

MEAN MODELS:
-----
Coefficients for variable no. 1: 1 - accuracy
- variable omitted (reference category) -
-----
Coefficients for variable no. 2: accuracy
  Estimate Std. Error z-Value p-Value
(Intercept)  1.8649    0.2991  6.235 4.52e-10 ***
dyslexiayes -1.4833    0.3029 -4.897 9.74e-07 ***
iq           1.0676    0.3359  3.178 0.001482 **
dyslexiayes:iq -1.1625    0.3452 -3.368 0.000757 ***
-----
PRECISION MODEL:
-----
  Estimate Std. Error z-Value p-Value
(Intercept)  1.5579    0.3336  4.670 3.01e-06 ***
dyslexiayes  3.4931    0.5880  5.941 2.83e-09 ***
iq           1.2291    0.4596  2.674  0.00749 **
-----
Signif. codes: `***' < .001, `**' < 0.01, `*' < 0.05, `.' < 0.1

Log-likelihood: 65.9 on 7 df (37+2 iterations)
AIC: -117.8, BIC: -105.3144
Number of Observations: 44
Links: Logit (Means) and Log (Precision)
Parametrization: alternative

> confint(rs2)

95% Confidence Intervals (original form)

- Beta-Parameters:
Variable: 1 - accuracy
  variable omitted

Variable: accuracy
      2.5%  Est.  97.5%
(Intercept)  1.279  1.86  2.451
dyslexiayes -2.077 -1.48 -0.890
iq           0.409  1.07  1.726
dyslexiayes:iq -1.839 -1.16 -0.486

- Gamma-Parameters
      2.5%  Est.  97.5%
(Intercept)  0.904  1.56  2.21
dyslexiayes  2.341  3.49  4.65
iq           0.328  1.23  2.13

> confint(rs2, exp = TRUE)

95% Confidence Intervals (exponentiated)

- Beta-Parameters:
Variable: 1 - accuracy

```

```

variable omitted

Variable: accuracy
      2.5% exp(Est.) 97.5%
(Intercept)    3.592     6.455 11.601
dyslexiayes    0.125     0.227  0.411
iq             1.506     2.908  5.618
dyslexiayes:iq 0.159     0.313  0.615

- Gamma-Parameters
      2.5% exp(Est.) 97.5%
(Intercept)    2.47      4.75   9.13
dyslexiayes   10.39     32.89 104.12
iq            1.39      3.42   8.41

```

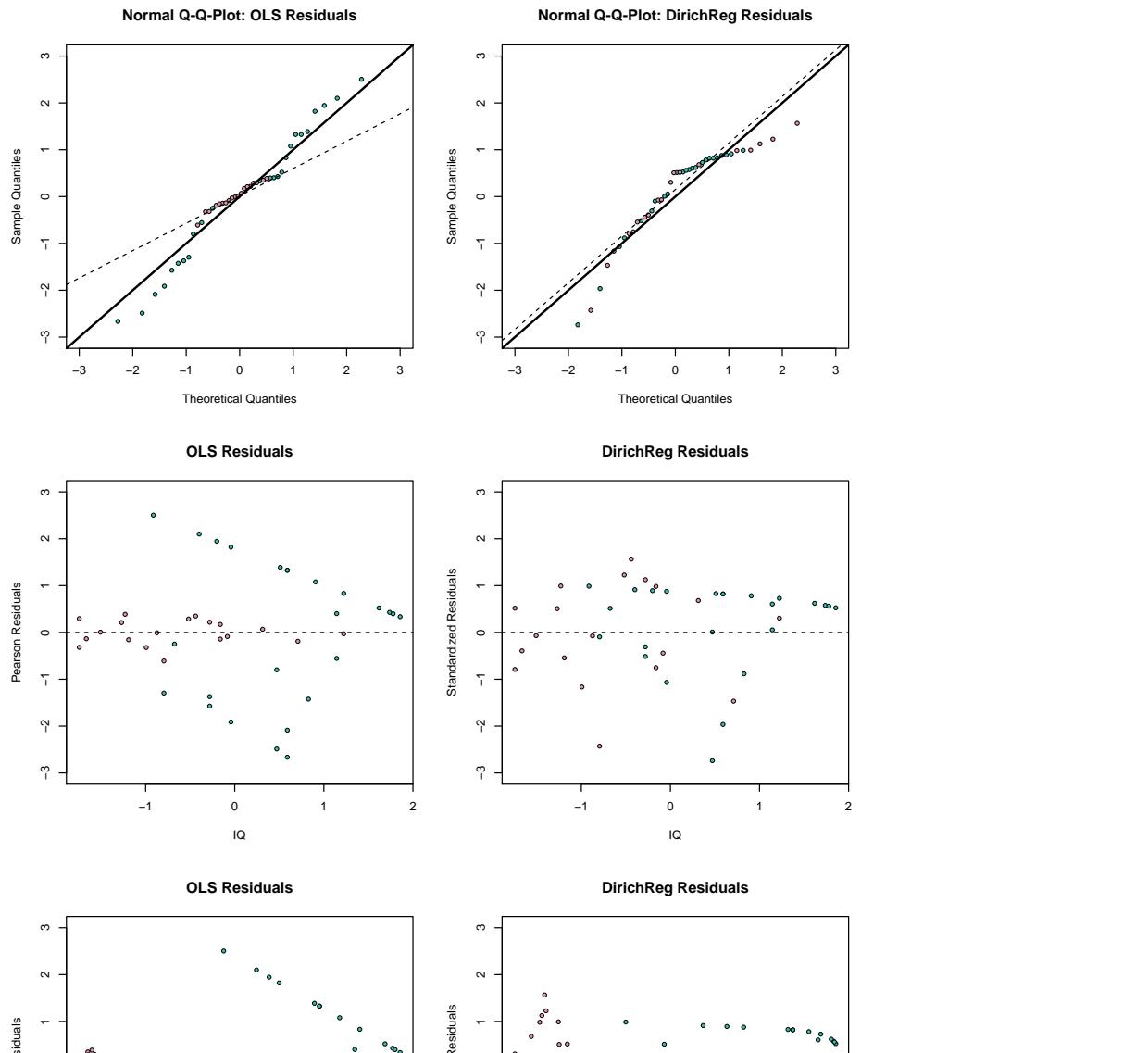
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```

> gcol <- c("#E495A5", "#39BEB1")[3 - as.numeric(RS$dyslexia)]
> tmt <- c(-3, 3)
> par(mfrow = c(3, 2))
> qqnorm(residuals(rlr, "pearson"), ylim = tmt, xlim = tmt, pch = 21, bg = gcol,
+ main = "Normal Q-Q-Plot: OLS Residuals", cex = 0.75, lwd = 0.5)
> abline(0, 1, lwd = 2)
> qqline(residuals(rlr, "pearson"), lty = 2)
> qqnorm(residuals(rs2, "standardized")[, 2], ylim = tmt, xlim = tmt, pch = 21,
+ bg = gcol, main = "Normal Q-Q-Plot: DirichReg Residuals", cex = 0.75, lwd = 0.5)
> abline(0, 1, lwd = 2)
> qqline(residuals(rs2, "standardized")[, 2], lty = 2)
> plot(ReadingSkills$iq, residuals(rlr, "pearson"), pch = 21, bg = gcol, ylim = c(-3,
+ 3), main = "OLS Residuals", xlab = "IQ", ylab = "Pearson Residuals", cex = 0.75,
+ lwd = 0.5)
> abline(h = 0, lty = 2)
> plot(ReadingSkills$iq, residuals(rs2, "standardized")[, 2], pch = 21, bg = gcol,
+ ylim = c(-3, 3), main = "DirichReg Residuals", xlab = "IQ", ylab = "Standardized Residuals",
+ cex = 0.75, lwd = 0.5)
> abline(h = 0, lty = 2)
> plot(fitted(rlr), residuals(rlr, "pearson"), pch = 21, bg = gcol, ylim = c(-3,
+ 3), main = "OLS Residuals", xlab = "Fitted", ylab = "Pearson Residuals",
+ cex = 0.75, lwd = 0.5)
> abline(h = 0, lty = 2)
> plot(fitted(rs2)[, 2], residuals(rs2, "standardized")[, 2], pch = 21, bg = gcol,
+ ylim = c(-3, 3), main = "DirichReg Residuals", xlab = "Fitted", ylab = "Standardized Residuals",
+ cex = 0.75, lwd = 0.5)
> abline(h = 0, lty = 2)

```



```

> g.ind <- as.numeric(RS$dyslexia)
> g1 <- g.ind == 1
> g2 <- g.ind != 1
> par(mar = c(4, 4, 4, 4) + 0.1)
> plot(accuracy ~ iq, RS, pch = 21, bg = c("#E495A5", "#39BEB1")[3 - g.ind], cex = 1.5,
+       main = "Dyslexic (Red) vs. Control (Green) Group", xlab = "IQ Score", ylab = "Reading Accuracy",
+       xlim = range(ReadingSkills$iq))
> x1 <- seq(min(RS$iq[g1]), max(RS$iq[g1]), length.out = 200)
> x2 <- seq(min(RS$iq[g2]), max(RS$iq[g2]), length.out = 200)
> n <- length(x1)
> X <- data.frame(dyslexia = factor(rep(0:1, each = n), levels = 0:1, labels = c("no",
+   "yes")), iq = c(x1, x2))
> pv <- predict(rs2, X, TRUE, TRUE, TRUE)
> lines(x1, pv$mu[1:n], col = c("#E495A5", "#39BEB1")[2], lwd = 3)
> lines(x2, pv$mu[(n + 1):(2 * n)], col = c("#E495A5", "#39BEB1")[1], lwd = 3)
> ols <- 1/(1 + exp(-predict(rlr, X)))
> lines(x1, ols[1:n], col = c("#AD6071", "#00897D")[2], lwd = 3, lty = 2)
> lines(x2, ols[(n + 1):(2 * n)], col = c("#AD6071", "#00897D")[1], lwd = 3, lty = 2)
> par(new = TRUE)
> plot(x1, pv$phi[1:n], col = c("#6E1D34", "#004E42")[2], lty = "11", type = "l",
+       ylim = c(0, max(pv$phi)), axes = F, ann = F, lwd = 2, xlim = range(RS$iq))
> lines(x2, pv$phi[(n + 1):(2 * n)], col = c("#6E1D34", "#004E42")[1], lty = "11",
+       type = "l", lwd = 2)
> axis(4)
> mtext(expression(paste("Precision (", phi, ")")), 4, line = 3)
> legend("topleft", legend = c(expression(hat(mu)), expression(hat(phi)), "OLS"),
+        lty = c(1, 3, 2), lwd = c(3, 2, 3), bty = "n")

```

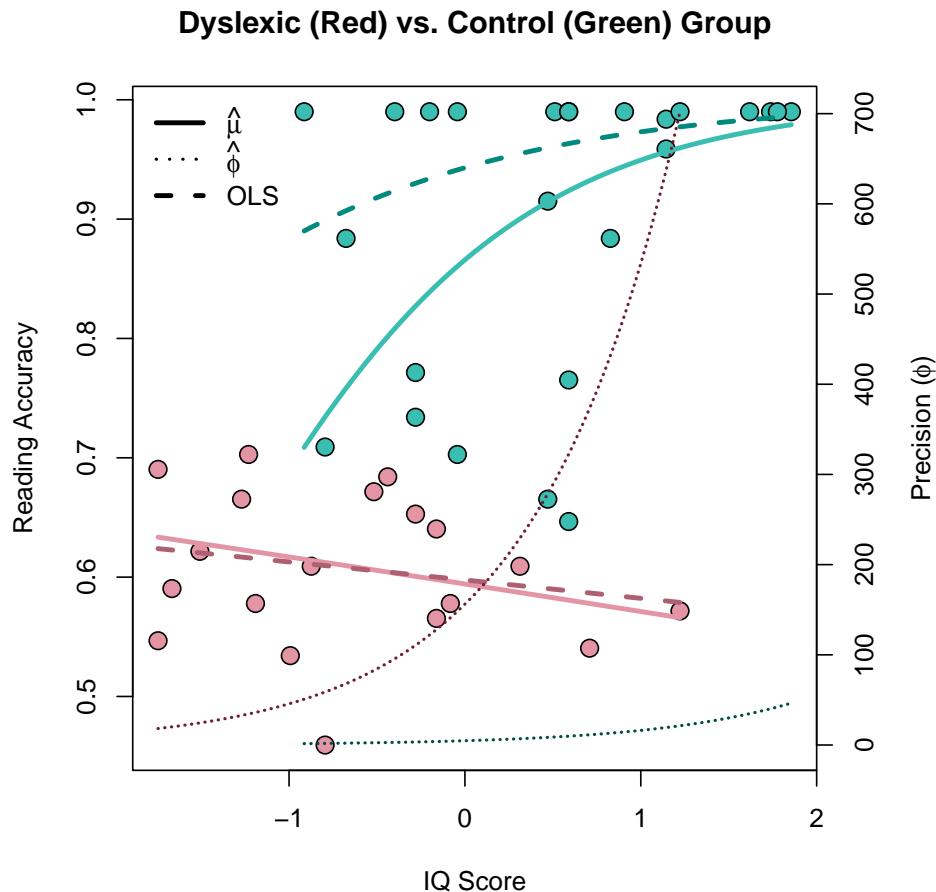


Figure 7: Reading skills: Predicted values of Dirichlet regression and OLS regression.