Projeto - Rascunho

Modelagem com Apoio Computacional

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The dataset

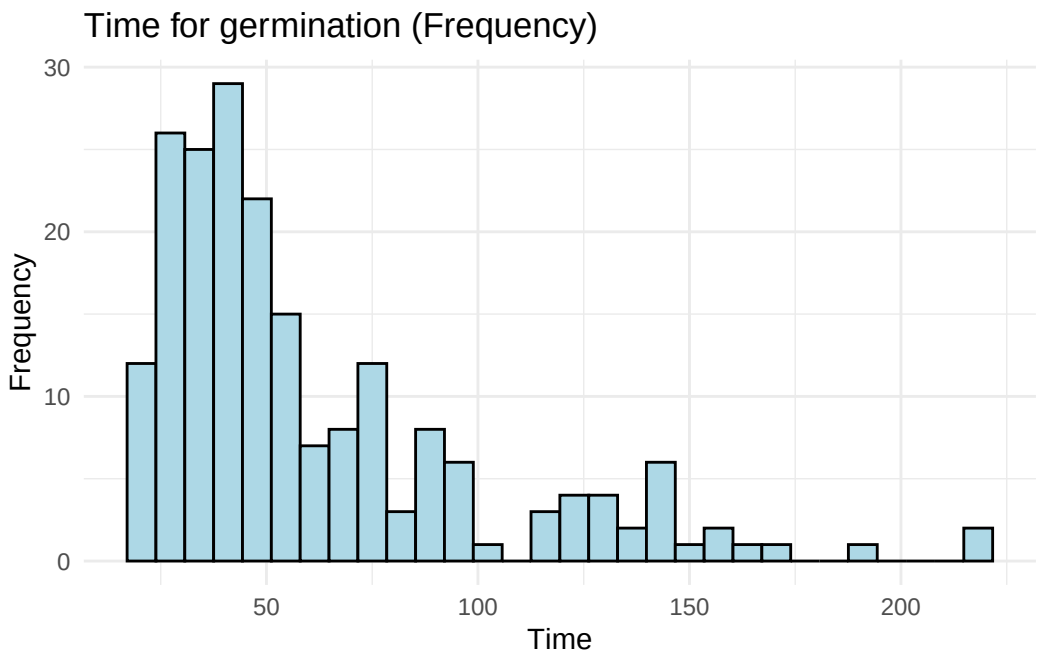
Castor seed germination dataset shared by Doctor Liv Soares Severino from Embrapa Algodão.

Link: Castor seed hydration and germination influenced by temperature and puncture

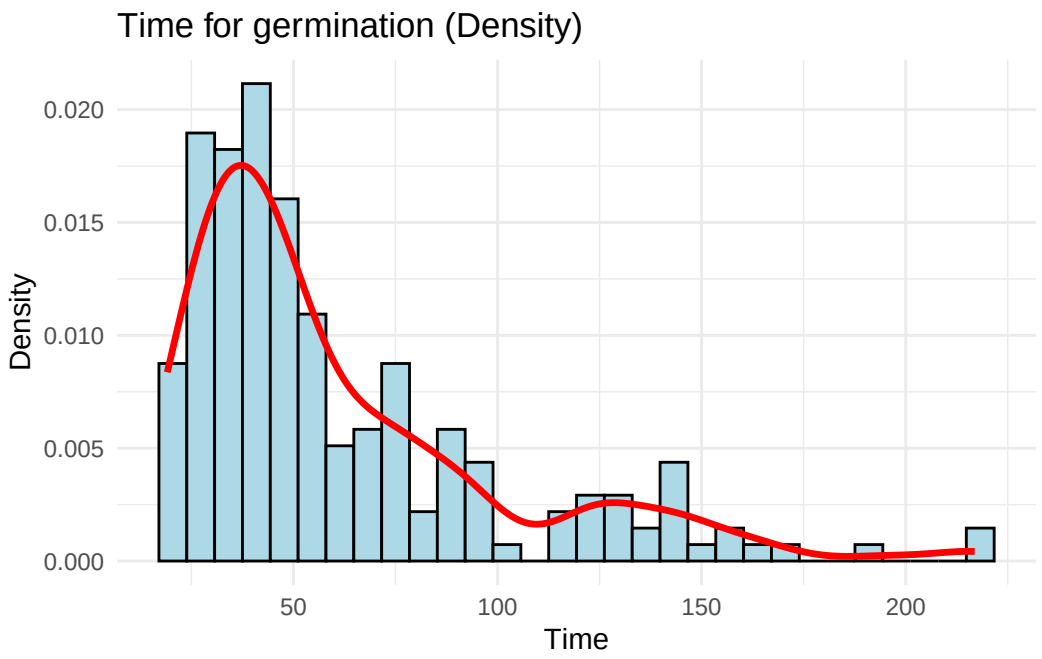
id	puncture	temperature	weight	weight_after_hydration	time_under_hydration	phase	radicle	time
475	Yes	34	0.425	1.342	42	Germinated	10.6	19.10
437	Yes	34	0.483	1.484	41	Germinated	9.9	19.54
390	Yes	31	0.481	1.319	41	Germinated	8.7	20.43
465	Yes	34	0.466	1.434	42	Germinated	9.2	20.93
317	Yes	28	0.384	1.536	41	Germinated	6.9	20.93
401	No	31	0.529	1.606	41	Germinated	8.2	21.37

Exploratory Data Analysis (EDA)

```
#interesse na variável time

ggplot(castor, aes(x = time)) +
  geom_histogram(bins = 30, fill = "lightblue", color = "black") +
  labs(title = "Time for germination (Frequency)", x = "Time", y = "Frequency") +
  theme_minimal()
```




```
  # com a densidade

ggplot(castor, aes(x = time)) +
  geom_histogram(aes(y = after_stat(density)), bins = 30,
                 fill = "lightblue", color = "black") +
  geom_density(color = "red", linewidth = 1.2) +
  labs(title = "Time for germination (Density)", x = "Time", y = "Density") +
  theme_minimal()
```



Birnbaum-Saunders distribution

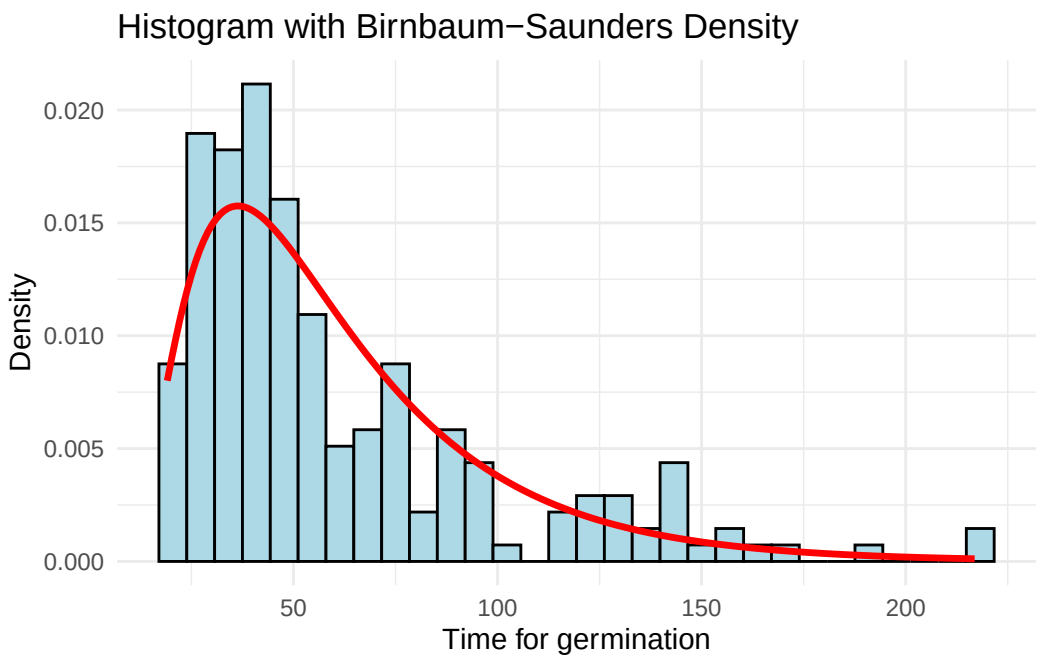
```
#plotar a densidade da distribuição Birnbaum-Saunders em cima do histograma dos dados

fit <- fitdistr(
  castor$time,
  densfun = function(x, alpha, beta) dfatigue(x, alpha = alpha, beta = beta, mu = 0),
  start = list(alpha = 1, beta = mean(castor$time)))
```

```
Warning in cpp_dfatigue(x, alpha, beta, mu, log[1L]): NaNs produced
Warning in cpp_dfatigue(x, alpha, beta, mu, log[1L]): NaNs produced
Warning in cpp_dfatigue(x, alpha, beta, mu, log[1L]): NaNs produced
Warning in cpp_dfatigue(x, alpha, beta, mu, log[1L]): NaNs produced
Warning in cpp_dfatigue(x, alpha, beta, mu, log[1L]): NaNs produced
```

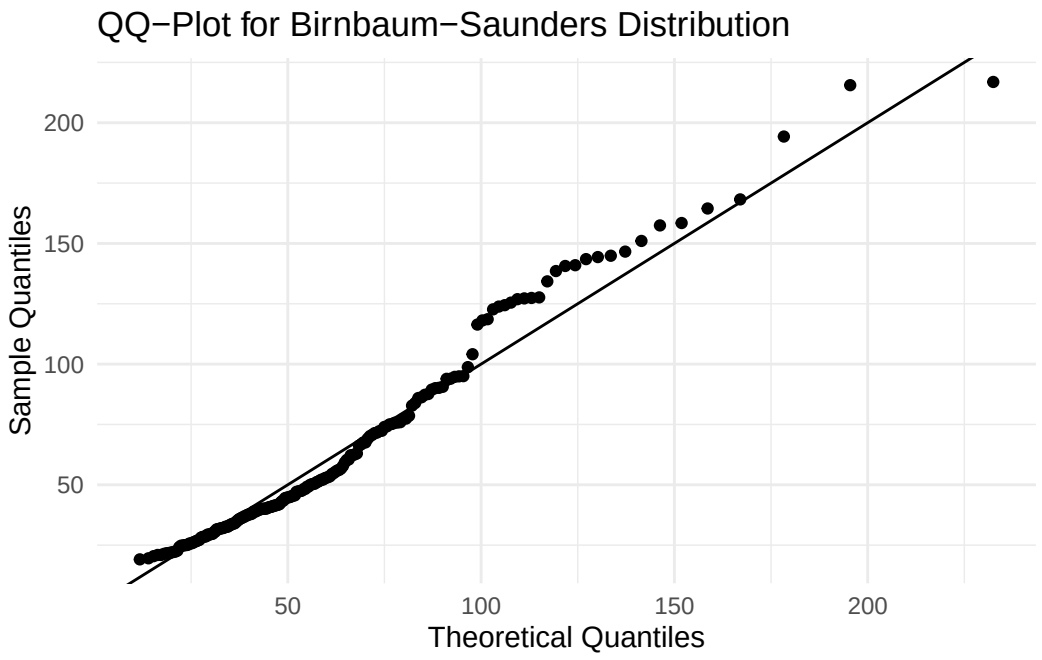
```
fit
```

```
      alpha         beta
  0.58248966   52.22055587
( 0.02905523) ( 2.05433439)
```

```r
alpha0 <- fit$estimate["alpha"]
beta0 <- fit$estimate["beta"]

# grade de valores para a curva
x_grid <- seq(min(castor$time), max(castor$time), length.out = 200)

# densidade BS com esses parâmetros
dens_bs <- dfatigue(x_grid, alpha = alpha0, beta = beta0, mu = 0)

df_bs <- data.frame(x = x_grid, y = dens_bs)

# plot histograma + curva
ggplot(castor, aes(x = time)) +
  geom_histogram(aes(y = after_stat(density)), bins = 30,
                 fill = "lightblue", color = "black") +
  geom_line(data = df_bs, aes(x = x, y = y),
            color = "red", linewidth = 1.2) +
  labs(title = "Histogram with Birnbaum-Saunders Density",
       x = "Time for germination", y = "Density") +
  theme_minimal()
```



```r
theo_quantiles <- qfatigue(ppoints(length(castor$time)), alpha = alpha0, beta = beta0, mu = 0
# quantis amostrais
sample_quantiles <- sort(castor$time)
# data frame para o ggplot
df_qq <- data.frame(Theoretical = theo_quantiles, Sample = sample_quantiles)
# plot QQ
ggplot(df_qq, aes(x = Theoretical, y = Sample)) +
  geom_point() +
  geom_abline(slope = 1, intercept = 0) +
  labs(title = "QQ-Plot for Birnbaum-Saunders Distribution",
       x = "Theoretical Quantiles", y = "Sample Quantiles") +
  theme_minimal()
```



Fitting a Quantile Regression Model based on the Birnbaum-Saunders Distribution

```r
#revised function
#authors: L. Sanchez, V. Leiva
```

```r
bsreg.fit<-function(x, y, link = "log") {
  n<-NROW(x)
  p<-NCOL(x)
  linkobj<-make.link(link)
  linkfun<-linkobj$linkfun
  linkinv<-linkobj$linkinv
  Q.eta<-linkobj$mu.eta
  ystar<-linkfun(y)
  beta<-ginv(t(x) %*% x) %*% t(x) %*% ystar

  xbar<-mean(y)
  vart<-(n/(n-1))*var(y)
  r<-vart / xbar^2
  alphai<-sqrt((2*r-2+2*sqrt(1+3*r))/(5-r))

  if (is.nan(alphai) || is.na(alphai)) { #MUDANÇA
    s1<-mean(y)
    r1<-1/mean(1/y)
    alphai<-sqrt(2*sqrt(s1/r1)-2)
  }

  start<-c(as.vector(beta), alphai) #MUDANÇA

  # função de verossimilhança (log-like)
  fr<-function(vp) {
    betab<-vp[1:p]
    eta<-as.vector(x %*% betab)
    Q<-linkinv(eta)
    alphab<-vp[p+1]    #MUDANÇA: índice corrigido, garantir escalar
    q<-0.5
    zq<-qnorm(q, mean = 0, sd = 1)
    gma_alphab<-alphab * zq + sqrt(alphab^2 * zq^2 + 4)
    vt<-y
    sum(-0.5*log(8*pi*vt) - log(alphab) - log(gma_alphab) - 0.5*log(Q) +
        log(gma_alphab^2/2 + 2*Q/vt) -
        (2*Q/(alphab^2*gma_alphab^2*vt))*(vt*gma_alphab^2/(4*Q) - 1)^2)
  }

  # função gradiente: retorna um vetor NUMÉRICO de comprimento p+1
  grr<-function(vp) {
    betab<-vp[1:p]
    eta<-as.vector(x %*% betab)
```

```r
  Q<-linkinv(eta)
  alphab<-vp[p+1]   # MUDANÇA: garantir escalar
  q<-0.5
  zq<-qnorm(q)
  gma_alphab<-alphab * zq + sqrt(alphab^2 * zq^2 + 4)
  # derivadas auxiliares
  gma_alphabp<-zq + zq^2 * alphab * (1 / sqrt(alphab^2 * zq^2 + 4))
  vt<-y
  z<--0.5*(1/Q) - 2*(1/(alphab^2 * gma_alphab^2 * vt)) +
       gma_alphab^2 * vt * (1/(8 * alphab^2 * Q^2)) +
       4*(1/(vt * gma_alphab^2 + 4*Q))

  b<--(gma_alphab + alphab * gma_alphabp) * (1/(alphab * gma_alphab)) +
       2*vt * gma_alphab * gma_alphabp * (1/(vt * gma_alphab^2 + 4*Q)) -
       (gma_alphab * gma_alphabp * alphab - gma_alphab^2) * vt * (1/(4*Q*alphab^3)) -
       2*(1/(alphab^3)) +
       4*Q*(gma_alphab + alphab * gma_alphabp) * (1/(alphab^3 * gma_alphab^3 * vt))

  # MUDANÇA
  # gradiente em relação a beta (p x 1)
  grad_beta<-as.vector(t(x) %*% (Q.eta(eta) * z))
  # gradiente em relação a alpha (escala)
  grad_alpha<-sum(b)

  # retornar UM VETOR numérico (p+1)
  c(grad_beta, grad_alpha)
}

A<-matrix(c(rep(0,p),1),1,p+1)
B<-0

opt<-maxLik::maxBFGS(fn = fr, grad = grr, start = start,
                     constraints = list(ineqA = A, ineqB = B))

# MUDANÇA: inspeção para debug

if (!is.null(opt$code) && opt$code > 0) warning("optimization failed to converge (opt$code
if (!is.null(opt$convergence) && opt$convergence != 0) warning("optimizer signaled non-zer

estimates<-opt$estimate

# MUDANÇA: garantir que log.lik.est é numérico (NA se não disponível)
```

```
log.lik.est<-if (!is.null(opt$maximum)) opt$maximum else NA

beta<-as.vector(estimates[1:p])
eta<-as.vector(x %*% beta)
Q<-linkinv(eta)
alpha<-estimates[p+1]
q<-0.5
zq<-qnorm(q, mean = 0, sd = 1)

aux<-matrix(1, ncol = 1L, nrow = n)

gma_alpha<-alpha * zq + sqrt(alpha^2 * zq^2+4)
gma_alphap<-zq+alpha*zq^2*(1/sqrt(alpha^2*zq^2+4))
gma_alphapp<-4*zq^2*(1/sqrt(alpha^2*zq^2+4)^3)

par_alpha<-alpha
par_beta <-4*Q/gma_alpha^2

Acal<-((2*gma_alphap+alpha*gma_alphapp)*(alpha*gma_alpha)-(gma_alpha+alpha*gma_alphap)^2)/
        (alpha^2*gma_alpha^2)
Bcal<-8*Q*(gma_alphap^2+gma_alpha*gma_alphapp)
Ccal<-(1/(4*Q*alpha^4))*(alpha^2*gma_alphap^2+alpha^2*gma_alpha*gma_alphapp-alpha*gma_alpha
        3*gma_alpha*gma_alphap*alpha+3*gma_alpha^3)
Dcal<-4*Q*((2*gma_alphap+alpha*gma_alphapp)*alpha*gma_alpha-3*(gma_alpha+alpha*gma_alphap)
        (alpha^4*gma_alpha^4)

if(link == "log"){
    a<-Q
    h1<-Q^2
    h2<--1/(Q^2*(log(Q)^3))}

if(link == "identity"){
    a<-rep(1,n)
    h1<-1
    h2<-0}

if(link == "sqrt"){
    a<-2*sqrt(Q)
    h1<-4*Q
    h2<--1/(4*Q^3)}

  integ.f2<-c()
```

```
  integ.f3<-c()
  integ.f4<-c()
  integ.f5<-c()

f2<-function(u,j){
    return((u/(u*gma_alpha^2+4*Q[j]))^2*dbisa(u, par_beta[j], par_alpha))}

f3<-function(u,j){
    return((u/(u*gma_alpha^2+4*Q[j])^2)*dbisa(u, par_beta[j], par_alpha))}

f4<-function(u,j){
    return((1/(u*gma_alpha^2+4*Q[j])^2)*dbisa(u, par_beta[j], par_alpha))}

f5<-function(u,j){
  return((1/(u*gma_alpha^2+4*Q[j]))*dbisa(u, par_beta[j], par_alpha))}

for(i in 1:n){
    integ.f2[i]<-integrate(f2, lower=0, upper=Inf, j=i)$value
    integ.f3[i]<-integrate(f3, lower=0, upper=Inf, j=i)$value
    integ.f4[i]<-integrate(f4, lower=0, upper=Inf, j=i)$value
    integ.f5[i]<-integrate(f5, lower=0, upper=Inf, j=i)$value}

AIC <- (-2 * log.lik.est + 2 * (p+1))
AICc<- AIC + (2 * (p+1) * ((p+1) + 1)) / (n - (p+1) - 1)
BIC <- (-2 * log.lik.est + log(n) * (p+1))

v<-(-1/(2*Q^2)+16*integ.f4 + (1/(alpha^2*Q^2))*(1+alpha^2/2))*h1-
    (1/(2*Q)+(1/(2*alpha^2*Q))*(1+alpha^2/2)-4*integ.f5)*h2

s<-8*gma_alpha*gma_alphap*integ.f3 -
    ((gma_alpha * gma_alphap * alpha- gma_alpha^2)/(alpha^3*gma_alpha^2*Q^2))*(1+alpha^2/2
    ((gma_alpha +alpha* gma_alphap)/(alpha^3*gma_alpha *Q))*(1+alpha^2/2)

u<-Acal-Bcal*integ.f3 -2*(gma_alpha^3*gma_alphapp-gma_alpha^2*gma_alphap^2)^2*
    integ.f2 + Ccal*(4*Q/gma_alpha^2)*(1+alpha^2/2)-6/alpha^4-
    Dcal*(gma_alpha^2/(4*Q))*(1+alpha^2/2)

kbb<-t(x)%*%diag(as.vector(v))%*%x
kaa<-sum(diag(as.vector(u)))
kba<-t(x)%*%diag(as.vector(a))%*%s

Diag<-function(A){
```

```
    diag.A<-vector()
    for(t in 1:ncol(A)){
      diag.A[t]=A[t,t]
    }
    return(as.vector(diag.A))
  }

  fisher<-cbind(rbind(kbb, t(kba)), rbind(kba, kaa))
  se  <-sqrt(Diag(solve(fisher)))

  hess<-as.matrix(opt$hessian)

  if(p == 1) {
    var.explic<-x
  }  else {
            var.explic<-x[,-1]
          }

  zstatbeta<-beta / se[1:p]
  zstatalpha <-alpha / se[p+1] #MUDANÇA: índice
  pvalorbeta<-2 * pnorm(abs(zstatbeta), lower.tail = F)
  pvaloralpha<-2 * pnorm(abs(zstatalpha), lower.tail = F)

  names(beta)<-colnames(x)

  rval<-list(coefficients=list(beta = beta, alpha = alpha),
              fitted.values.Q=structure(Q, .Names = names(y)),
              n = n, p = p, q = q, eta = eta,
              X = x, y = y,
              # MUDANÇA: garantir hessian é matriz ou NULL
              Hessian=if(!is.null(opt$hessian)) as.matrix(opt$hessian) else NULL,
              matrix.expected.Fisher = fisher,
              loglik = log.lik.est,
              link = list(quantile = linkobj),
              # MUDANÇA: garantir campo 'converged' é TRUE/FALSE/NA
              converged=if(!is.null(opt$code)) (opt$code==0) else NA,
              information.criterions = list(aic = AIC,bic = BIC,aicc=AICc),
              se = se, zstat = list(beta = zstatbeta, alpha = zstatalpha),
              pvalor = list(beta = pvalorbeta, alpha = pvaloralpha))

  return(rval)
}
```

```r
model <- bsreg.fit(
  x = model.matrix(~ temperature + puncture, data = castor),
  y = castor$time,
  link = "log"
)
#summary(model)
model$coefficients
```

```
$beta
(Intercept) temperature punctureYes
 5.30925182 -0.03372853 -0.59352968

$alpha
[1] 0.4911046
```

```r
# resíduos quantilico aleatorizado
```

- introdução
- rev. bibliografica
- modelo
- aplicação