Fitting models via maximum likelihood using RTMB

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Outline

- Demonstrate a mind-blowing advance with AD
- Show a few examples that may be useful
 - Start with equations, move to code
- Talk about debugging via browser()
- Tips and trickery
- Code for all of this available at: https://github.com/QFCatMSU/RTMB/tree/main

What is RTMB?

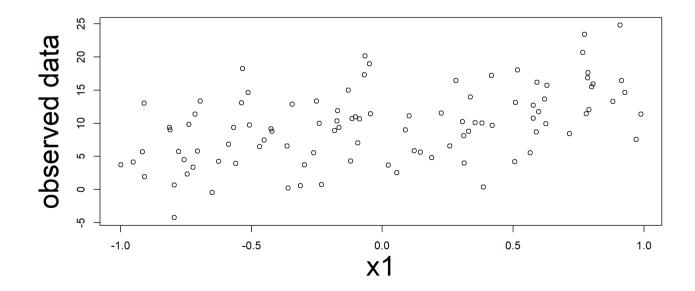
- RTMB is a new package that provides a native R interface for a subset of TMB so you can avoid coding in C++
- See link: https://kaskr.r-universe.dev/RTMB
- No longer need to code a . cpp file to use AD
- All(?) the functionality of TMB
- Easier for others to read the code (no more . cpp files)
- A game changer if you know how to code in R, create an objective f(x) for your model
- Bottom line: less time developing and testing models, more intuitive code

Linear regression

• The math:

$$y_i = eta_0 + eta_1 x_i + \epsilon_i \quad ext{where} \quad \epsilon_i \sim ext{N}(0, \sigma)$$

```
1 par(mar=c(5,6,4,1) + 0.1)
2 plot(y_obs~x1, xlab = "x1", ylab = "observed data", cex.lab = 2.5)
```



```
1  # set up tagged data + parameters lists:
2  data = list(
3    n = n,
4    y_obs = y_obs,
5    x1 = x1
6 )
7
8  pars = list(
9    b0 = 1,
10    b1 = 1,
11    log_sd = log(3)
12 )
```

• see linreg.r

```
library(RTMB)
 3 # write an objective function returning negative log-likelihood
   f = function(pars) {
    getAll(data, pars) # replaces DATA XX, PARAMETER YY
   y pred = b0 + b1 * x1
    nll = -sum(dnorm(y_obs, y_pred, exp(log_sd), log = TRUE))
 8 nll
10
11 obj = MakeADFun(f, pars)
12 obj$fn() # objective function
[1] 777.5154
 1 obj$gr() # gradients
outer mgc: 1051.521
         [,1] [,2] [,3]
[1,] -96.88602 -13.2133 -1051.521
```

Stick to base R

```
1 opt = nlminb(obj$par, obj$fn, obj$gr)
outer mgc:
           1051.521
outer mgc:
           54.72716
outer mgc: 36.6083
outer mgc: 21.88026
outer mgc: 35.7811
           5.686432
outer mgc:
           1.353547
outer mgc:
outer mgc:
           1.508322
           0.08695211
outer mgc:
           0.04554657
outer mgc:
           0.0305969
outer mgc:
           0.002009656
outer mgc:
           1.470605e-05
outer mgc:
```

```
1 sdr = sdreport(obj)

outer mgc: 1.470605e-05

outer mgc: 0.004344401

outer mgc: 0.004344313

outer mgc: 0.001393873

outer mgc: 0.00140084

outer mgc: 0.1997855

outer mgc: 0.2002149
```

We are done.

Access fit

```
1 opt
$par
     b0 b1 log_sd
9.730622 4.775419 1.568146
$objective
[1] 298.7085
$convergence
[1] 0
$iterations
[1] 12
$evaluations
function gradient
```

Access fit

```
1 sdr

sdreport(.) result

Estimate Std. Error

b0 9.730622 0.47978081

b1 4.775419 0.84596427

log_sd 1.568146 0.07071065

Maximum gradient component: 1.470605e-05
```

RTMB scales easily to more complicated models

von Bertalanffy growth model: the math

$$egin{aligned} l_i &= l_\infty \left(1 - e^{-k(a_i - t_0)}
ight) + arepsilon_i \ &arepsilon_i {\sim} \mathrm{N}\left(0, \sigma^2
ight) \end{aligned}$$

RTMB objective f(x) for a von Bertalanffy growth model:

```
1  f = function(pars) {
2    getAll(data, pars)
3    linf = exp(log_linf)
4    vbk = exp(log_vbk)
5    sd = exp(log_sd)
6    l_pred = linf * (1 - exp(-vbk * (age_i - t0)))
7    nll = -sum(dnorm(l_obs_i, l_pred, sd, TRUE))
8    REPORT(linf)
9    REPORT(vbk)
10    ADREPORT(sd)
11    nll
12 }
```

- see vonB.r
- can use REPORT(), ADREPORT()

Poisson GLMM: the math

$$egin{aligned} y_{i,site} &\sim ext{Poisson}\left(\lambda_{i,site}
ight) \ \log(\lambda_{i,site}) &= eta_0 + eta_1 \cdot x_1 + \epsilon_{site} \ \epsilon_{site} &\sim ext{N}(0,\sigma_{site}^2) \end{aligned}$$

- β_0 is global intercept shared among sites
- x_1 is a covariate
- ϵ_{site} is normally distributed random effect

Objective f(x) for a Poisson GLMM:

```
f = function(pars) {
     getAll(data, pars)
    sd site = exp(log_sd_site)
                                                         # back transform
    inll = 0
                                                         # initialize
 4
    jnll = jnll - sum(dnorm(eps_site, 0, sd_site, TRUE)) # Pr(random effects)
    lam i = exp(
                                                         \# exp link f(x)
    Xmat %*% bvec +
                                                         # fixed effects
8
                                                         # random effects
    eps site
 9
10
    jnll = jnll - sum(dpois(yobs, lam i, TRUE)) # Pr(observations)
11
     inll
12 }
```

• see glmm.r

Objective f(x) for a hierarchical normal selectivity model, adapted from Millar and Freyer 1999:

```
1 f = function(pars) {
     getAll(data, pars)
    inll = 0
    jnll = jnll - sum(dnorm(k1 dev, 0, exp(ln sd k1), TRUE))
     jnll = jnll - sum(dnorm(k2 dev, 0, exp(ln sd k2), TRUE))
     k1 = \exp(\ln k1 + k1 \text{ dev})
     k2 = \exp(\ln k2 + k2 \text{ dev})
     sel mat = phi mat = matrix(0, nrow(catches), ncol(catches))
     for (i in 1:nrow(sel mat)) {
9
      for (j in 1:ncol(sel mat)) {
11
          sel mat[i, j] = \exp(-(lens[i] - k1[site[i]] * rel size[j])^2 /
            (2 * k2[site[i]]^2 * rel size[j]^2))
13
14
15
     sel sums = rowSums(sel mat)
16
     for (i in 1:nrow(phi mat)) {
17
       for (j in 1:ncol(phi mat)) {
         phi mat[i, j] = sel mat[i, j] / sel sums[i]
19
20
     jnll = jnll - sum(catches * log(phi mat))
21
      inll
23 }
```

Spatially explicit Poisson GLMM: the math

$$egin{aligned} y_{i,site} &\sim ext{Poisson}\left(\lambda_{i,site}
ight) \ \log(\lambda_{i,site}) &= eta_0 + \epsilon_{site} \ \epsilon_{site} &\sim ext{MVN}(0, \Sigma_{site}) \end{aligned}$$

- where Σ_{site} is calculated via some correlation f(x)

- we'll use exponential

Objective f(x) for a spatially explicit GLMM:

```
f = function(pars) {
   getAll(data, pars)

SIGMA = gp_sigma * exp(-dist_sites / gp_theta)
   jnll = 0

jnll = jnll - sum(dmvnorm(eps_s, SIGMA, TRUE))

y_hat = exp(beta0 + eps_s) # index on site_i in more complex examples

jnll = jnll - sum(dpois(y_obs, y_hat), TRUE)

jnll

jnll

y }
```

- majicks
- see grf.r

Jim Bence's fancy vonB: math

• ?

Objective f(x) for a Bence's fancy vonB:

```
1 f = function(pars) {
     getAll(data, pars)
     Linfmn = exp(logLinfmn)
     logLinfsd = exp(loglogLinfsd)
     Linfs = exp(logLinfs)
     K = \exp(\log K)
     Sig = exp(logSig)
     nponds = length(Linfs)
 8
 9
     nages = length(A)
10
     predL = matrix(0, nrow = nages, ncol = nponds)
     # fill one column (pond) at a time:
11
     for (i in 1:nponds) {
12
      predL[, i] = Linfs[i] * (1 - exp(-K * (A - t0)))
13
14
     nll = -sum(dnorm(x = L, mean = predL, sd = Sig, log = TRUE))
15
     nprand = -sum(dnorm(x = logLinfs, mean = logLinfmn, sd = logLinfsd, log = TRUE))
16
17
     jnll = nll + nprand
18
     inll
19 }
```

• see multilinf.r

Debugging

- Because RTMB is written in R, can use debugging tools (!)
- browser() allows you to step through and check calculations
 - no longer need cout or REPORT() calls to check calculations
- Can also use breakpoints
- Jump to demonstration

Tips

- Talk about advector error messages
 - Often(?) means you are using something that isn't supported by RTMB
- Make sure you are using base R / RTMB f(x)'s
- Hash out each line to find the offending line(s)
- Discuss other oddities

Questions?