

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?

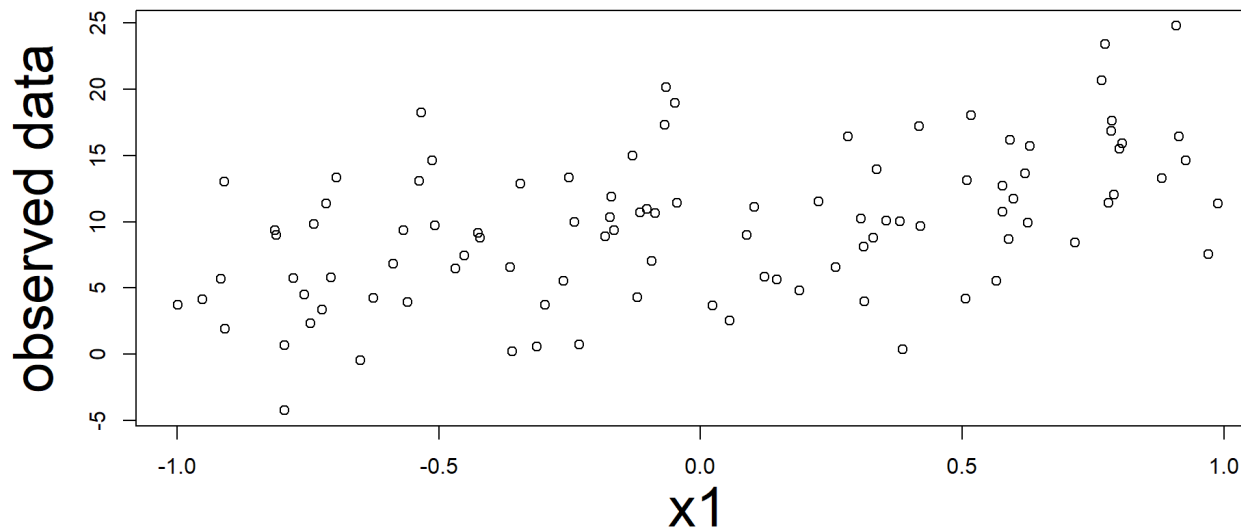
- RTMB is a new package that provides a native R interface for a subset of TMB so you can avoid coding in C++
- See <https://kaskr.r-universe.dev/RTMB>
- In all applications we have tried all TMB functionality was available!
- Because code is all in R, both easier to code and for others to read that code - a game changer!
- A game changer *if* you know how to code in R, create an objective $f(x)$ for your model
- No compiling or compiling errors!
- Bottom line: less time developing and testing models, more intuitive code

Linear regression in RTMB

- The math:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i \quad \text{where} \quad \epsilon_i \sim N(0, \sigma)$$

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



Linear regression (RTMB)

```
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`

Linear regression (RTMB)

```
1 library(RTMB)
2
3 # write an objective function returning negative log-likelihood
4 f = function(pars) {
5   getAll(data, pars) # replaces DATA_XX, PARAMETER_YY
6   y_pred = b0 + b1 * x1
7   nll = -sum(dnorm(y_obs, y_pred, exp(log_sd), log = TRUE))
8   nll
9 }
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

Linear regression (RTMB)

```
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  
outer mgc: 5.686432  
outer mgc: 1.353547  
outer mgc: 1.508322  
outer mgc: 0.08695211  
outer mgc: 0.04554657  
outer mgc: 0.0305969  
outer mgc: 0.002009656  
outer mgc: 1.470605e-05
```

Linear regression (RTMB)

```
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  
      15      10
```

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 to (much)
more complicated models***

von Bertalanffy growth model: the math

$$l_i = l_{\infty} \left(1 - e^{-k(a_i - t_0)}\right) + \varepsilon_i$$

$$\varepsilon_i \sim N(0, \sigma^2)$$

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

$$y_{i,site} \sim \text{Poisson}(\lambda_{i,site})$$

$$\log(\lambda_{i,site}) = \beta_0 + \beta_1 \cdot x_1 + \epsilon_{site}$$

$$\epsilon_{site} \sim \text{N}(0, \sigma_{site}^2)$$

- 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:

```
1 f = function(pars) {
2   getAll(data, pars)
3   sd_site = exp(log_sd_site)           # back transform
4   jnll = 0                             # initialize
5   jnll = jnll - sum(dnorm(eps_site, 0, sd_site, TRUE)) # Pr(random effects)
6   lam_i = exp(                          # link f(x)
7     Xmat %*% bvec +                     # fixed effects
8     eps_site                           # random effects
9   )
10  jnll = jnll - sum(dpois(yobs, lam_i, TRUE)) # Pr(observations)
11  jnll
12 }
```

- see `glmm.r`

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

```
1 f = function(pars) {
2   getAll(data, pars)
3   jnll = 0
4   jnll = jnll - sum(dnorm(k1_dev, 0, exp(ln_sd_k1), TRUE))
5   jnll = jnll - sum(dnorm(k2_dev, 0, exp(ln_sd_k2), TRUE))
6   k1 = exp(ln_k1 + k1_dev)
7   k2 = exp(ln_k2 + k2_dev)
8   sel_mat = phi_mat = matrix(0, nrow(catches), ncol(catches))
9   for (i in 1:nrow(sel_mat)) {
10     for (j in 1:ncol(sel_mat)) {
11       sel_mat[i, j] = exp(-(lens[i] - k1[site[i]] * rel_size[j])^2 /
12         (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)) {
18       phi_mat[i, j] = sel_mat[i, j] / sel_sums[i]
19     }
20   }
21   jnll = jnll - sum(catches * log(phi_mat))
22   jnll
23 }
```


Spatially explicit Poisson GLMM: the math

$$y_{i,site} \sim \text{Poisson}(\lambda_{i,site})$$

$$\log(\lambda_{i,site}) = \beta_0 + \epsilon_{site}$$

$$\epsilon_{site} \sim \text{MVN}(0, \Sigma_{site})$$

- where Σ_{site} is calculated via some correlation $f(x)$
- we'll use exponential

Objective $f(x)$ for a spatially explicit GLMM:

```
1 f = function(pars) {  
2   getAll(data, pars)  
3   SIGMA = gp_sigma * exp(-dist_sites / gp_theta)  
4   jnll = 0  
5   jnll = jnll - sum(dmvnorm(eps_s, SIGMA, TRUE))  
6   y_hat = exp(beta0 + eps_s) # index on site_i in more complex examples  
7   jnll = jnll - sum(dpois(y_obs, y_hat), TRUE)  
8   jnll  
9 }
```

- majicks
- `dist_sites` is a matrix of euclidean distances among sites and is read in as data
- see `grf.r`

Conventional vonB with random L_∞ :

math

$$L_{i,j} = L_{\infty_i} (1 - \exp(-K (a_{i,j} - t_0)) + \varepsilon_{i,j}$$

$$\varepsilon_{i,j} \sim N(0, \sigma^2)$$

$$\log(L_{\infty_i}) \sim N(\log(L_\infty), \sigma_{L_\infty}^2)$$

- Note L_∞ is the median and not mean asymptote among ponds
- Also note, the model code uses likelihood equation with equivalent $L_{i,j} \sim N(\hat{L}_{i,j}, \sigma^2)$

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

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

Tips

- Talk about **advect** 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?

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