Tools, tips and tricks for finding a good GLLVM

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Questions so far?



Background

- GLLVMs are complex models
- Convergence can be difficult
- Presenting results can be challenging

Here I present some tips/tricks that can be useful Apologies in advance, it will be a bit all over the place

GLMM FAQ

Need something like Ben Bolker's GLMM FAQ, but for GLLVMs But most (all?) from GLMs and GLMMs also applies to GLLVMs

Outline

Outline: a collection of tools, tips and tricks

Tools

- Confidence intervals
- Information criteria
- Hypothesis testing
- Residuals (and code for DHARMa)
- emmeans and
 MuMIn::dredge
- ightharpoonup Concurrent and r^2
- ordiplot, coefplot, randomCoefPlot
- summary and plot summary (dev)
- Using vegan

Tips or tricks

- LV parameterisation
- Missing response data
- Using a saved gllvm object
- Parallelisation
- Ggplotting a gllvm
- Optimisation and all that
- Starting values
- Small LV values
- Large loadings, small sigma.lv
- (Very) small standard errors
- Predicting/intervals
- Variation partitioning

More?

Information criteria

gllvm provides support for BIC and AIC(c)

- BIC: finds the model closest to the truth
- AIC: finds the model that predicts best
- AICc: penalizes a little stronger than AIC, but was developed for linear models

You can use these, but do so sparingly. They are sensitive to (e.g.,)

- Model misspecification
- Boundary effects (constrained parameters)
- Large sample asymptotics
- Focus issues

Information criteria

Depending on the problem, there are many ways to do selection

- ► The covariates?
- The random effects?
- ► The latent variables?
- Combinations thereof?

Information criteria: example

```
## df AIC
## model1 97 1266.008
## model2 125 1296.065
```

- 1) It seems that the model with 2 LVs is better
- 2) But what if one of the models has poorly converged?

Information criteria

Take-away:

- 1) Apply carefully
- 2) Avoid as much as possible
- 3) Use if necessary

Hypothesis testing

Likelihood ratio test (anova) is a similar story:

- Use carefully
- Mind convergence
- Do not use with a large difference in parameters

The same for wald-tests. Do not stare at any of these results for too long.

Confidence intervals

The confint(.) function provides some (approximate) wald confidence intervals

E.g.,

```
confint(model1, "theta")
```

```
##
                         cilow
                                         ciup
## theta.LV1.1
                   1.00000000
                                  1.00000000
## theta.LV1.2
                  -3.76867965
                                 -0.10240769
## theta.LV1.3
                                  2.28584208
                  -0.71524991
## theta.LV1.4
                  -3.72709274
                                  0.22885264
  theta.LV1.5
                  -0.16512287
                                  3.39603618
## theta.LV1.6
                  -0.35179419
                                  1.11384537
## theta.LV1.7
                  -0.32620856
                                  1.84630923
## theta.LV1.8
                  -2.41193163
                                  1.08913022
## theta.LV1.9
                                  1 01243809
                  -1.65109466
## theta.LV1.10
                  -1.82590399
                                  0.64122960
## theta.I.V1.11
                  -4.84442267
                                  0.08002783
## theta.LV1.12
                  -1.01855572
                                  1 28235696
## theta.LV1.13
                  -1.11480727
                                  2.09461387
## theta.LV1.14
                  -0.48629367
                                  2.65289224
## theta.LV1.15
                  -2.58764458
                                  0.19102795
```

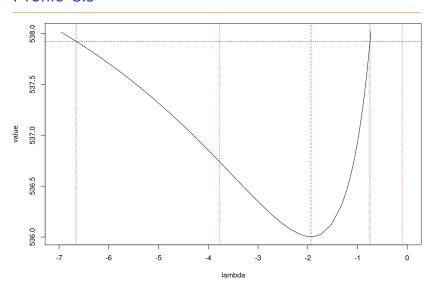
Profile Cls

You can also profile parameters thanks to the TMB R-package. These have better properties, but (very) slow to compute. Finding the right parameter can take some doing (see model\$TMBfn\$par).

For example:

```
prof <- TMB::tmbprofile(model1$TMBfn, which(names(model1$TMBfn$par)=="lamb")</pre>
plot(prof, xlim = c(-7,0))
CIs <- confint(model1);</pre>
abline(v = CIs[grep1("theta",row.names(CIs)),][2,1], col = "red", lty = "d
abline(v = CIs[grep1("theta",row.names(CIs)),][2,2], col = "red", lty = "d"
abline(v=coef(model1, "loadings")[2,1],col="red",lty="dashed")
```

Profile Cls



Using vegan

The vegan R-package has a lot of useful functions. Some of these can be used with GLLVMs:

- procrustes: for comparison of ordinations,
- ordiplot: for plotting, though I have yet to work out how to get it to plot arrows
 - this does require a scores.gllvm function (present on github in a presentation)
- ordisurf? maybe not
- perhaps other functions, I have yet to discover them

scores.gllvm

```
scores_gllvm <- function(x, display ="sites", choices = NULL){
    sol <- list()
    sol | list()
    s
```

Using ordiplot in gllvm

This clashes with vegan's ordiplot, so if it errs..

- Scaling is applied by default: does not always work well with unimodal models or with covariates in the ordination
- Arrows for covariates are relative so you can make them bigger
- Turn pink due to uncertainty (but you can turn it off)
- fac.center is new
- Prediction regions of sites
- By default shows square plots

Ordiplot

For when num.lv, num.lv.c, num.RR are in the model. It is very difficult to create a plotting function that always does well.

- Remember that ordination plots are conditional on other effects in the model
- vegan::ordiplot will clash with gllvm
- biplot adds species coordinates
- Note that ordiplot scales and rotates, so it will not (exactly) be the same
 - But inference should not be affected.

Ordiplot

- Bad scaling can occur for constrained/concurrent ordination
 - Usually due to extreme clustering: species with too few observations
- Bad scaling can occur for unimodal models
 - Optima that are far outside of the estimated gradient mess things up
 - Draw arrows with spp.arrows instead
- Arrows for covariates are drawn from the middle, not from 0
- fac.center to draw categorical effects as points
- type to select which scores to plot for concurrent or hybrid ordination
- predict.region
- use getLV and getLoadings(new) or optima.gllvm to create your own plot

Using ordiplot in vegan

- If you have scores.gllvm you can use vegan's ordiplot
- I have not yet looked into adding the arrows
- It does not do post-hoc scaling or rotation, which is usually needed

Using procrustes

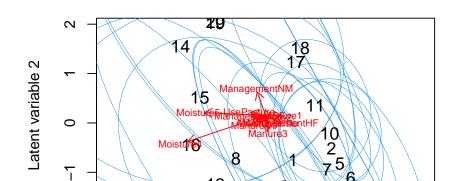
```
vegan::procrustes(gllvm::getLV(model1),
                  vegan::scores(vegan::decorana(Y), choices = 1:2),
                  symmetric = TRUE)
##
## Call:
## vegan::procrustes(X = gllvm::getLV(model1), Y = vegan::scores(vegan::de
##
## Procrustes sum of squares:
## 0.312
```

The procrustes error is very useful if you want to compare ordinations. It is a kind of RMSE that accounts for the different in rotation and scale.

Example with Dune data

```
cnord <- gllvm::gllvm(Y,X, num.lv.c=2,randomB="LV",family="ordinal", seed</pre>
gllvm::ordiplot(cnord, predict.region = TRUE, arrow.ci = FALSE)
```

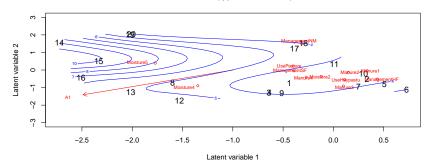
Ordination (type='conditional')



Example with Dune data

```
gllvm::ordiplot(cnord, predict.region = FALSE, fac.center = TRUE, arrow.ci = FALSE, ylim = c(-3,3))
LV = gllvm::getLV(cnord)
rot <- svd(LV)$v
alpha <- 0.5
norms <- sqrt(colSums(LV^2))*sqrt(colSums(gllvm::getLoadings(cnord)^2))
LV <- sweep(LV, 2, (norms^alpha)/sqrt(colSums(LV^2)), "*")%*%rot
vegan::ordisurf(LV, dune.env$A1, add = TRUE, col = "blue")</pre>
```

Ordination (type='conditional')



Residuals and DHARMa

gllvm natively provides randomized quantile residuals. It is possible to use the DHARMa package if preferred, though there is no official support. DHARMa has various tests that can be useful:

- 1) Zero-inflation
- 2) Overdispersion
- 3) Other?

This requires use of createDHARMa

Example

We do simulations and predictions with gllvm:

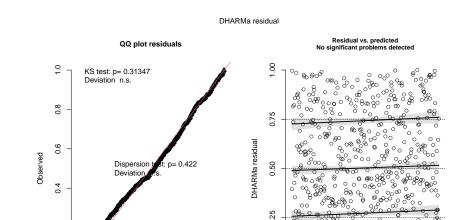
```
# Simulate with model 1000x
sim <- do.call("cbind", replicate(1000,</pre>
         c(as.matrix(gllvm::simulate(cnord, conditional=TRUE))), simplify=F
preds <- c(predict(cnord))</pre>
obs <- c(as.matrix(Y))</pre>
```

Note that these need to be in long format. DHARMa handles the rest:

```
dharma <- DHARMa::createDHARMa(
  simulatedResponse=sim,
  observedResponse=obs,
  integerResponse=TRUE,
 fittedPredictedResponse= preds)
```

Example

plot(dharma)



Residuals and DHARMa

Do not attempt to use the functions that require refitting models.

- GLLVMs (at present) are not suitable for this
- Refitting will take long
- Refitting without monitoring convergence is a recipe for disaster

emmeans

When using categorical variables, R by default uses treatment contrasts. So, the first category is dropped.

A popular choice for inspecting categorical variables is the emmeans package. I recently developed some code to support this (not part yet of gllvm)

- Can be used with JSDM/Residual ordination
- Can be used with constrained ordination (without random slopes)

The functions you need are available on the gllvm github discussions page

Example with Dune data

```
library(emmeans)
coord <- glivm::glivm(Y, X, lv.formula = -Ai-Manure+Moisture+Management, num.RR=2,family="ordinal")
emmeans(coord, -Manure:species, component = "LV")
```

```
## NOTE: A nesting structure was detected in the fitted model:
## Manure %in% species, Moisture %in% species, Management %in% species
```

```
Manure species
                      emmean
                                SE df asymp.LCL asymp.UCL
          Achimill
                    -1.3266 0.325 Inf
                                         -1.9641
          Achimill
                     0.0476 0.327 Inf
                                         -0.5940
                                                  0.6892
          Achimill
                    -0.5447 0.307 Inf
                                                  0.0577
                                         -1.1471
          Achimill
                    -0.6291 0.309 Inf
                                         -1.2352
                                                  -0.0231
          Achimill
                   -1.7443 0.360 Inf
                                        -2.4505
                                                  -1.0381
                    1.6780 0.477 Inf
                                                  2.6125
          Agrostol
                                         0.7435
                   -1.7412 0.997 Inf
          Agrostol
                                         -3.6946
                                                  0.2121
          Agrostol
                    -0.3434 0.580 Inf
                                         -1.4796
                                                  0.7928
## 3
          Agrostol
                    -0.1409 0.539 Inf
                                         -1.1982
                                                   0.9163
## 4
          Agrostol
                    2.5432 0.831 Inf
                                         0.9154
                                                   4.1710
## 0
          Airaprae -22.1585 0.783 Inf -23.6931 -20.6239
          Airaprae -16.6781 2.147 Inf -20.8858 -12.4703
## 2
          Airaprae -22,5258 0,719 Inf -23,9349 -21,1167
          Airaprae -23.2119 0.866 Inf -24.9091 -21.5147
          Airaprae -31.8141 1.817 Inf -35.3763 -28.2519
          Alopgeni
                     0.7223 0.579 Inf
                                         -0.4134
                                                   1.8580
          Alopgeni
                    -3.4468 1.221 Inf
                                         -5.8408
                                                  -1.0527
## 2
          Alopgeni
                    -1.1336 0.565 Inf
                                         -2.2410
                                                  -0.0263
                   -0.8257 0.556 Inf
          Alopgeni
                                         -1.9148
                                                  0.2633
          Alopgeni
                    3.1727 0.924 Inf
                                         1.3615
                                                  4.9840
  0
          Anthodor
                   -1.2340 0.405 Inf
                                         -2.0271
                                                  -0.4410
          Anthodor
                    0.2996 0.689 Inf
                                         -1.0499
                                                  1.6491
          Anthodor
                    -0.3959 0.535 Inf
                                         -1.4446
                                                  0.6529
          Anthodor
                    -0.4936 0.523 Inf
                                         -1.5194
                                                  0.5322
          Anthodor
                    -1.7792 0.591 Inf
                                        -2.9382
                                                  -0.6201
## 0
          Bellpere
                    -1.2009 0.477 Inf
                                         -2.1361
                                                  -0.2657
          Bellpere
                    -0.4086 0.631 Inf
                                        -1.6448
                                                  0.8276
          Bellpere
                    -0.5935 0.479 Inf
                                        -1.5327
                                                   0.3457
```

Dredge

Similar to emmeans very limited functionality is supported for MuMIn::dredge:

- Not for lv.formula type arguments (unless you can figure it out and tell me how)
- not for effects in formula
- Repeated disclaimer: blindly fitting without convergence check is icky
- If you figure out more, let me know!

Example with Dune data

Fixed term is "(Intercept)"

```
fit <- gllvm::gllvm(y = Y, X = X, formula = ~Manure+A1, family = "ordinal"
tab <- MuMIn::dredge(fit,varying=list(num.lv=1:2), rank="AICc")</pre>
```

tab

```
## Global model call: gllvm::gllvm(y = Y, X = X, formula = ~Manure + A1, f
## ---

## Model selection table

## (Intrc) A1 Manur num.lv df logLik AICc delta weight

## 7 + + + 1 218 -442.430 1571.5 0.00 1

## 8 + + + 2 247 -410.604 1663.3 91.78 0

## Models ranked by AICc(x)
```

Example with Dune data

: NA/NaN function evaluation

· NA/NaN function evaluation

These warnings are fine

```
fit <- gllvm:::gllvm(y = Y, X = X, formula = ~Manure+A1, family = "ordinal"
```

- ## Warning in gllvm.iter(y = y, X = X, lv.X = lv.X.design, formula = fo
 ## Can't fit ordinal model if there are species with missing classes. S
 ## 'zeta.struc = `common`'.
- ## Warning in nlminb(objr\$par, objr\$fn, objr\$gr, control = list(rel.tol
- ## warning in nlminb(objispar, objisin, objisgr, control = list(rel.tol
 ## : NA/NaN function evaluation
 ## Warning in nlminb(objr\$par, objr\$fn, objr\$gr, control = list(rel.tol
 - ## Warning in nlminb(objr\$par, objr\$fn, objr\$gr, control = list(rel.tol
 ## : NA/NaN function evaluation
- ## Warning in nlminb(objr\$par, objr\$fn, objr\$gr, control = list(rel.tol
 ## : NA/NaN function evaluation
 ## Warning in nlminb(objr\$par, objr\$fn, objr\$gr, control = list(rel.tol

Variable selection is a very difficult problem. What do we do it for?

- Do not get too obsessed with "a good" model
- Use the magnitude of parameter estimators
- In combination with statistical uncertainties

There is (not quite) one exception: adaptive shrinkage

Adaptive shrinkage

- Fit the full model
- Penalize the parameters
- Let a method work its magic

Random effects kind of do this with their quadratic penalty. This is also what the randomB argument is for.

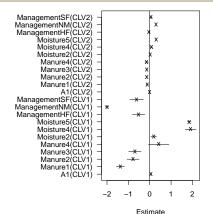
Summary

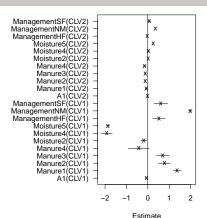
The summary function is a work in progress

- You can plot it (new dev version)
- It shows correlations of the random effects
- Canonical coefficients
- Other parameter estimates
- ▶ But not if there are no standard errors, or for random effects
- It also has a rotate arguments for ordination with covariates; rotates to the same direction as the ordination (which also has rotate)

Summary example

```
plot(summary(coord), mar=c(4,10,2,4))
plot(summary(coord, rotate = FALSE), mar = c(4,10,2,4))
```

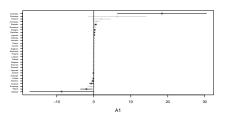




Coefplot

For models with fixed effects

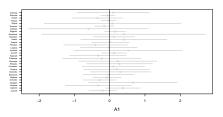
- Makes a "Caterpillar" plot with 95% confidence intervals
- If which.Xcoef does not work, double check names (e.g., categorical covariates have one effect per factor level)
- Grey effects have confidence intervals that cross zero
- Also for constrained/concurrent ordination - effects inside or outside of the ordination



randomCoefplot

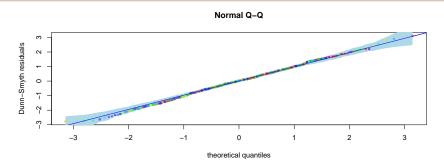
For models with random effects

- Makes a "Caterpillar" plot with 95% prediction intervals
- If which.Xcoef does not work, double check names (e.g., categorical covariates have one effect per factor level)
- Grey effects have prediction intervals that cross zero
- Also for constrained/concurrent ordination - effects inside or outside of the ordination



Residual diagnostic plots in gllvm

plot(coord, which = 2)



- ▶ Always check the residuals and make corrections if needed
- ► Envelopes are included to help check the plots
- ▶ QQ-plot: points should fall in the envelopes (more or less)

NAs in responses

It is possible to have missing data in the responses Y

- Maybe an experiment went wrong
- Perhaps to "trick" the Phylogenetic model into predicting for ancestors
- Or another reason

gllvm will skip the likelihood evaluation and predict the observation instead (i.e., incorporate uncertainty).

Missing data in covariates is not allowed

Using a saved gllvm object

You might want to save a model object when you have finished your analysis. I.e.,:

```
save(cnord,file="cnord.RData")
```

and use it another time:

```
load("cnord.RData")
```

perhaps you ran the model with sd.errors = FALSE (as it is faster) and still need to calculate the standard errors with se.gllvm.

If you try to do that you will be met with this screen:



Start New Session

Using a saved gllvm object

We first need to retape:

```
cnord$TMBfn$retape()
ses <- gllvm:::se(cnord)</pre>
```

And can then safely use the TMB object again.

Parallelisation

Not yet on CRAN, since parallel computation is still very new in gllvm

- Parallel computation: use multiple CPU for model fitting
- Can also slow model fitting down (e.g., small models)
- Creating the TMB object is by default sequential due to memory spikes
 - Can be changed via TMB::config
- It works by setting TMB::openmp(...)
 - ... is the number of CPU to use (see parallel::detectCores())
- Needs to be reset after re-taping

Optimisation and convergence

gllvm uses numerical optimisation. There is no guarantee for finding "the best" solution.

- Switching optimisation routine can help
 - optimizer and optim.method
- Sometimes you need to increase the number of iterations
- Sometimes you need to increase reltol
- Constrained/concurrent ordination has an additional constraint on B
 - This has separate optimisation routines
 - Separate convergence criterium reltol.c
 - If this is not reached, you will get a warning
- Good starting values can make a big difference starting.val
- Fit your model repeatedly with n.init and n.init.max

There are many other control arguments for the

Optimisation and convergence

I am currently trying to find more robust optimisation routines for improved usability.



RESEARCH ARTICLE

Efficient estimation of generalized linear latent variable models

Jenni Niku¹*, Wesley Brooks², Riki Herliansyah³, Francis K. C. Hui⁴, Sara Taskinen 610, David I. Warton 2,500

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Niku et al. article looked into starting values.

Starting values

Generally, repeated fits with different starting values is recommended.

starting.val has three options: zero, random, and res (default):

- zero: Start everything at zero (or 1)
- random: Start at randomly generated values
- res: Start at smartly generated values

jitter.var to add a little noise to res

Multiple starts

n.init: number times to refit the model (and pick best)
n.init.max: n.init exit after this many unsuccessful fits
(defaults quite high)

Small LV values

- It can happen that you get a lot of small values for the LVs
- Usually in NB or binomial models
- Indicates either lack of convergence, or little data
- For NB you can try to switch to method = "EVA" or "LA"
- For EVA you can try to switch to link = "logit", or change method
- ▶ Also repeatedly fit the model with n.init
- If nothing works, omit an LV

Large loadings or small sigma.lv

Usually indicates lack of convergence

- Try reordering the responses: most frequently observed species first
 - Especially for constrained ordination
- Refit the model multiple times
- Sometimes it is normal
- If nothing works, omit an LV

Checking convergence

Checking arrival at the maximum is challenging

- Use gradient.check = TRUE
- Or try hist(model\$TMBfn\$gr()) these should near zero
 - ▶ If not, refit or change model (lack of convergence)
- gllvm might tell you standard errors could not be calculated
 - ▶ This indicates lack of convergence, the model **might** be poor
 - Unclear if a singular Hessian should be accepted
- We could use more checks on the Hessian
 - If you get a warning about the determinant of the Hessian, something is wrong (simplify/refit)

Standard error calculation in gllvm is really quite robust (two fail safes). If it fails, something is wrong

Small standard errors

For a reason that we do not -quite- understand yet the SEs sometimes get very small

Worst case: overfitting

Best case: lack of convergence

Intermediate case: Hessian is being weird

Usually: repeatedly refit the model, change the model, or change method

On the calculation of standard errors: an improvement is coming

Prediction and intervals

The predict function works as with a glm. It is a work in progress, especially for random effects. There are no intervals available (yet).

You can try simulation.

Variance partitioning in gllvms

Jenni Niku is working on this for gllvm, but:

- \blacktriangleright van der Veen et al (2023) has an R^2 for concurrent ordination
- Nakagawa and Schielzeth (2012) can be constructed for GLLVMs
- getResidualCov and getEnvironmentalCov

Citing gllvm

Please cite the software version citation("gllvm").

Always cite the research articles that developed the method. Package development and maintenance is a lot of work that is not otherwise rewarded.

This is good practice for all packages that you use.

Citing gllvm

To cite the 'gllvm' package in publications use:

Niku, J., Brooks, W., Herliansyah, R., Hui, F. K. C., Korhonen, P., Taskinen, S., van der Veen, B., and Warton, D. I. (2023). gllvm: Generalized Linear Latent Variable Models, R package version 1.4.3.

accompanied by any of associated research articles, as applicable:

Niku, J., Hui, F. K. C., Taskinen, S., and Warton, D. I. (2019). gllvm - Fast analysis of multivariate abundance data with generalized linear latent variable models in R. Methods in Ecology and Evolution, 10, 2173-2182.

Niku, J., Hui, F. K. C., Taskinen, S., and Warton, D. I. (2021). Analyzing environmental-trait interactions in ecological communities with fourth-corner latent variable models Environmetrics 32 1-17

van der Veen, B., Hui, F. K. C., Hovstad, K.A., Solbu, E.B., and O'Hara, R.B. (2021). Model-based ordination for species with unequal niche widths. Methods in Ecology and Evolution, 12, 1288-1300.

van der Veen, B., Hui, F. K. C., Hovstad, K.A., and O'Hara, R.B. (2023). Concurrent ordination: simultaneous unconstrained and constrained latent variable modelling. Methods in Ecology and Evolution, 14, 683-695.

Korhonen, P., Hui, F. K. C., Niku, J., and Taskinen, S. (2023). Fast and universal estimation of latent variable models using extended variational approximations. Statistics and Computing, 33, 1-16.

Conclusion

- More points, let me know
- Suggestions to improve usability, let us know
- Questions on github discussions
- ▶ Bug reports on github under issues