Welcome to Fish stock assessment: SAM and TMB

Anders Nielsen & Olav Nikolai Breivik an@aqua.dtu.dk

Welcome!

- Please introduce yourselves
 - Name and Organization
 - Experience (TMB, ADMB, R/C coding)
 - What do you hope to learn
 - Special requests

Outline

Day 1: Intro and basics

- ICES presentation (30m)
- Intro (what is TMB, what is SAM)
- First simple TMB example
- Parameters
- Data
- Basic parametric assessment model (study basic model implementation, add small improvements)

Day 2: SAM basic use and foundation

- Ways to run SAM (basic sam, web, R, git)
- Multivariate normal distribution
- Intro to random effects

Day 3: Processes in SAM

- Recruitment & Survival (a) Explain, (b) Implement, (c) Study SAM configuration
- Fishing mortality (a) Explain, (b) Implement, (c) Study SAM configuration

Day 4: Observations in SAM

- Catches, total catches, Biomass indices
- Surveys, tagging, missing, and correlations

Day 5: Validation and forecast

- Validating assessment models (e.g. observation and process residuals, leave out, retrospective, simulation, prediction based, jit)
- Forecast scenario options

Format adapted for online course

- Course is a mixture of lectures and exercises
- Each day the lecture parts are recorded for participants in different time zones^a
- On days 2-6 the time from 16-17:30 is dedicated to questions mainly from participants in other time zones^b
- All participants are welcome to join all parts.

- Questions can be asked at all times by interrupting please do!
- Questions can also be asked by writing in the chat box

This will be difficult — but we will do our best

^aThe plan is that the participants in very different time zones view the lectures and work on the exercises offline and then join and ask questions online the following day

^bNotice that we are available on Saturday for questions regarding Friday's exercises

TMB is for Non-standard models

- Models where you need to write your own likelihood
- Models you cannot write in one line in R
- non-trivial non-linearities
- complex covariance structures
- complicated couplings between fixed and random effects
- different sources of observations needing different likelihood types
- Standard models are very useful, but should not limit us

Formula interfaces are sometimes frustrating ...

• A useful model for longitudinal data:

```
\begin{array}{lll} & \mathbf{lnc} & \sim & N(\mu,\mathbf{V}), \text{ where} \\ & \mu_i & = & \mu + \alpha(\mathtt{treatm}_i) + \beta(\mathtt{month}_i) + \gamma(\mathtt{treatm}_i,\mathtt{month}_i), \text{ and} \\ & & \left\{ \begin{array}{ll} 0 & , & \text{if } \mathtt{cage}_{i_1} \neq \mathtt{cage}_{i_2} \text{ and } i_1 \neq i_2 \\ \nu^2 + \tau^2 \exp\left\{\frac{-(\mathtt{month}_{i_1} - \mathtt{month}_{i_2})^2}{\rho^2}\right\} & , & \text{if } \mathtt{cage}_{i_1} = \mathtt{cage}_{i_2} \text{ and } i_1 \neq i_2 \\ \nu^2 + \tau^2 + \sigma^2 & , & \text{if } i_1 = i_2 \end{array} \right.
```

• This model is implemented by:

- So many pitfalls and much is hidden. Even difficult to recover model parameters.
- What is τ ? Some hours with manual, but re-implement to be sure...
- Restricted by what someone else has put in there. Giant task to move beyond.

Terbuthylazine

- It is a herbicide
- Free terbuthylazine can be washed into the drinking water
- It can be bound to the soil
- Certain bacterias can mineralize it



$$\frac{dB_t}{dt} = -k_1 B_t + k_2 F_t, B_0 = 0$$

$$\frac{dF_t}{dt} = k_1 B_t - (k_2 + k_3) F_t, F_0 = 100$$

$$\frac{dM_t}{dt} = k_3 F_t, M_0 = 0$$

Simplifying



- The system is closed, so $M_t = 100 (B_t + F_t)$
- Define $X_t = \begin{pmatrix} B_t \\ F_t \end{pmatrix}$
- The simplified system is:

$$\frac{dX_t}{dt} = \underbrace{\begin{pmatrix} -k_1 & k_2 \\ k_1 & -(k_2 + k_3) \end{pmatrix}}_{A} X_t, \qquad X_0 = \begin{pmatrix} 0 \\ 100 \end{pmatrix}$$

• The system is linear, so it can be be solved for instance via the matrix exponential

$$\begin{pmatrix} B_t \\ F_t \end{pmatrix} = e^{At} X_0$$

Observations

• The amount of mineralized terbuthylazine was measured 26 times throughout a year

${f Time}$	${f M}$											
0.77	1.396	-	16 -									
1.69	3.784										0	
2.69	5.948							•	0	0		
3.67	7.717		14 –		,00000	0	0	0	O			
4.69	9.077				00000							
5.71	10.100			00	, 0							
7.94	11.263		12 –	00								
9.67	11.856			0								
11.77	12.251											
17.77	12.699		10 -	0								
23.77	12.869	(%		0								
32.77	13.048	(%) W	0									
40.73	13.222	2	8 –	0								
47.75	13.347											
54.90	13.507		6 -	0								
62.81	13.628		· · ·	O								
72.88	13.804											
98.77	14.087		4 -	0								
125.92	14.185			O								
160.19	14.351											
191.15	14.458		2 -									
223.78	14.756			0								
287.70	15.262		ı						1			
340.01	15.703			0	50	100		150	200	250	300	350
340.95	15.703											
342.01	15.703		Time (days)									
		-										

Simplest statistical model

• The simplest model we can think of would be:

$$M_{t_i} \sim \mathcal{N}\left(100 - (B_{t_i} + F_{t_i}), \sigma^2\right), \text{ independent, and with } \begin{pmatrix} B_{t_i} \\ F_{t_i} \end{pmatrix} = e^{At_i} X_0.$$

```
> library(Matrix)
> nlogL <- function(theta) {</pre>
      k <- exp(theta[1:3])
      sigma <- exp(theta[4])</pre>
      A \leftarrow rbind(c(-k[1], k[2]), c(k[1], -(k[2] + k[3])))
      x0 < -c(0, 100)
      sol <- function(t) 100 - sum(expm(A * t) %*% x0)
      pred <- sapply(dat[, 1], sol)</pre>
      -sum(dnorm(dat[, 2], mean = pred, sd = sigma, log = TRUE))
+ }
> system.time(fit <- optim(c(-2, -2, -2, -2), nlogL, hessian = TRUE))
         system elapsed
   user
 19,409
         0.004 19.428
> fit$value
[1] 19.26905
> fit$convergence
[1] 0
```

• Try some of the different minimizers in R

```
> library(optimx)
> fit<-optimx(c(-2,-2,-2,-2),nlogL,hessian=TRUE,control=list(all.methods=TRUE))
> fit
  fvalues
              method fns grs conv KKT1 KKT2 xtimes
 153.3056
              bobyqa 144 NA
                                O TRUE FALSE 9.629
              Rcgmin 85 50
 102.7661
                                O TRUE FALSE 22.314
 102.7660
                 nlm
                      NA
                          NA
                                   TRUE FALSE 11.865
 102.7660
                BFGS
                          18
                                   TRUE FALSE 15.005
                      79
 102.7660
              Rvmmin 81
                          15
                                   TRUE FALSE 10.517
 102.7660
                  CG 567 101
                                   TRUE FALSE 91.569
91.17466
              newuoa 696
                          NA
                                0 TRUE FALSE 46.063
 19.26905 Nelder-Mead 223
                                O FALSE FALSE 14.837
                          NA
0.9392184
                                         TRUE 14.953
              ucminf 40
                          40
                                O FALSE
0.9392142
                 spg 198
                               0 FALSE TRUE 55.732
                          NA
0.9392142
            L-BFGS-B 85
                          85
                                         TRUE 50.807
                                O FALSE
0.9392142
              nlminb 33 128
                                O TRUE
                                         TRUE 10.729
```

- Difficult because it is non-linear
- Would possibly be helped by accurate gradient info
- Runs in a fraction of a second in TMB (exercise)
- Notice this is a miniature example with only 4 parameters

What is needed to handle a non-standard problem

- A purely parametric assessment model has more than 100 model parameters and it is non-linear
- Code up the negative log likelihood function
- A good function minimizer

AD aided minimizer

• Want to minimize the negative log likelihood w.r.t. $\theta = (\theta_1, \dots, \theta_n)$

$$\widehat{\theta} = \operatorname*{argmin}_{\theta} \ell(y|\theta)$$

- If the dimension of θ is low (say n less than 5) any method can be used (grid search, random search, finite difference approximations, ...)
- We would like to be able to handle much larger problems
- Important for fixed effects models, and even more for random effects models
- A quasi-Newton minimizer aided by automatic differentiation

Quasi-Newton minimizer



Automatic Differentiation Model Builder

- A Newton minimizer is an iterative algorithm
- Each step assumes that the function $\ell(x,\theta)$ can be approximated locally by a quadratic function
- It uses the first ℓ'_{θ} and second ℓ''_{θ} derivatives to find the minimum
- Instead of calculating ℓ''_{θ} at every step, a quasi-Newton minimizer uses successive first derivatives ℓ'_{θ} to approximate ℓ''_{θ}
- So a fast and accurate way to calculate ℓ'_{θ} is needed

Automatic Differentiation

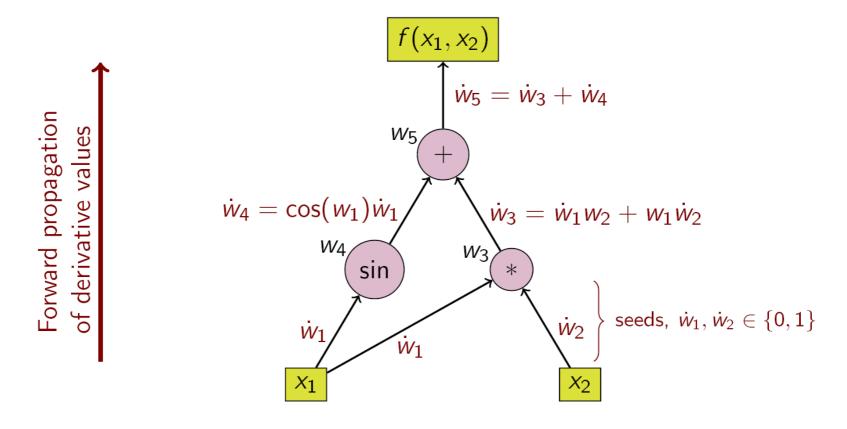
- We need to write a program to compute $\ell(\theta, x)$ anyway
- A computer program is a long list of simple operations: '+', '-', '*', '/', 'exp', 'log', 'sin', 'cos', 'tan', 'sqrt', and so on
- We know how to derive each of these operations
- The chain rule tells us how to combine: (f(g(x)))' = f'(g(x))g'(x)
- So if the computer is instructed to:
 - keep track of all the simple operations used when calculating $\ell(\theta, x)$
 - use the simple derivative formulas and the chain rule
- Then once $\ell(\theta, x)$ is computed, we also have ℓ'_{θ} with a minimum of extra calculations
- This is fast and accurate, and the difficult part is built into TMB(!)
- Alternatives:
 - Finite difference: $(\ell'_{\theta})_i \approx \frac{\ell(\theta_i + \Delta\theta_i, x) \ell(\theta, x)}{\Delta\theta_i}$ Simple, but slow and inaccurate
 - Analytical: Excellent option, but difficult in larger models

```
#include <math.h>
#include <iostream.h>
class result {
  private: double v,d;
 public: result(){v = 0;d= 0;};
          result(double val){v = val; d = 0;};
          result(double val, double der) {v = val; d = der;};
          double Value(){return v;};
          double Der(){return d;};
};
class parameter: public result {
  public: parameter(double pval) : result(pval,1.0) {};
          parameter() : result(0.0,1.0) {};
};
result sin(result n){
  return result(sin(n.Value()), cos(n.Value())*n.Der());
};
result operator*(result n1, result n2){
  return(result(n1.Value()*n2.Value(), n1.Der()*n2.Value() + n2.Der()*n1.Value()));
};
ostream& operator << (ostream& o, result n) {
  o << n.Value() << " (Derative: " << n.Der() << ") ";
  return o;
int main(int argc, char* argv[]){
  parameter theta(2);
  result y;
  v = sin(theta*theta);
  cout << "The result is " << y << endl;</pre>
}
```

cpp/ad.cpp

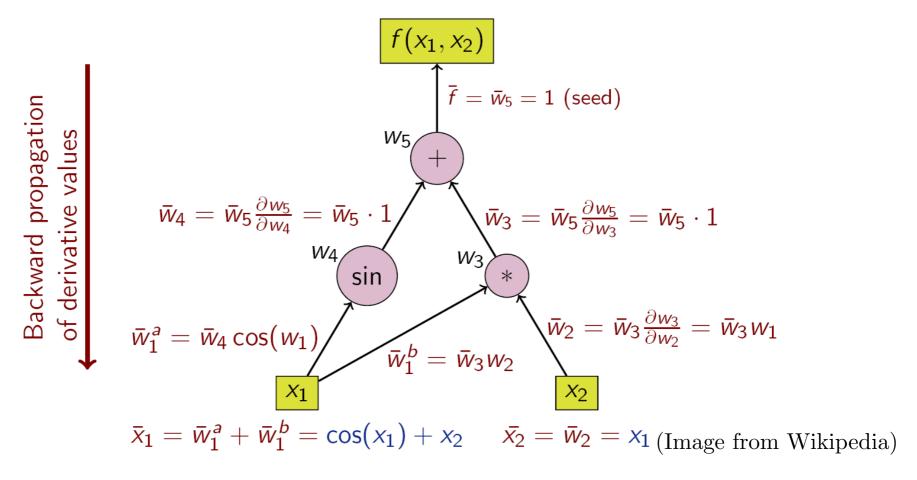
The result is -0.756802 (Derivative: -2.61457)

Forward and reverse mode



(Image from Wikipedia)

- Forward mode is easy to understand and implement
- Not efficient when θ is high dimensional



- Requires recording a stack of all operations
- Efficient in number of operations $(C(\ell'_{\theta}) < 4C(\ell)^{\mathbf{a}})$
- TMB uses reverse mode
- Except for random effects models where a combo of forward and reverse mode is used

^aGriewank, A., 2000. Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation. SIAM, Philadelphia, PA.

Template Model Builder (TMB):

- Developered by Kasper Kristensen (DTU-Aqua)
- ADMB inspired R-package
- Combines external libraries: CppAD, Eigen, CHOLMOD
- Continuously developed since 2009
- Implements Laplace approximation for random effects
- C++ Template based
- Automatic sparseness detection
- Parallelism through BLAS
- Parallel user templates
- Parallelism through parallel package

Example

• Assume that these 15 numbers follow a negative binomial distribution:

13 5 28 28 15 4 13 4 10 17 11 13 12 17 3

• The TMB code becomes

nbin.cpp

```
library(TMB)
compile("nbin.cpp")
dyn.load(dynlib("nbin"))
dat <- list()</pre>
dat $Y \leftarrow c(13, 5, 28, 28, 15, 4, 13, 4,
            10, 17, 11, 13, 12, 17, 3)
par <- list()</pre>
par$logsize <- 0
par$p <- 0.5
obj <- MakeADFun(dat, par, DLL="nbin")</pre>
opt <- nlminb(obj$par, obj$fn, obj$gr)</pre>
summary(sdreport(obj))
```

nbin.R.

Exercise 1:

- Installing TMB on your computer via the instructions on (if you have not already): https://github.com/kaskr/adcomp/wiki/Download
- Try replicating the negative binomial example

State-space assessment models

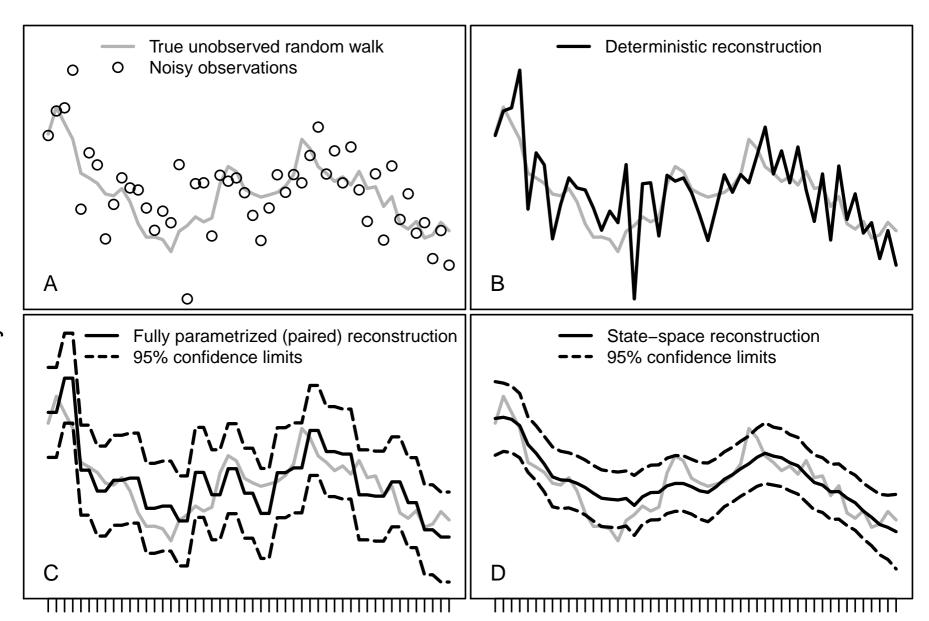
- This model class^a is used in most other quantitative fields
- It is a very useful extension to full parametric statistical models.
- Introduced for stock assessment by Gudmundsson (1987,1994) and Fryer (2001).
- The reason state-space models were not used more frequently for stock assessment in the past was that the software to easily handle these models was not available
- Can give very flexible models with low number of model parameters
- For instance we can include things like:

$$F_{3,y}$$
 is a random walk with yearly variance σ^2

• Importantly σ^2 is a model parameter estimated in the model.

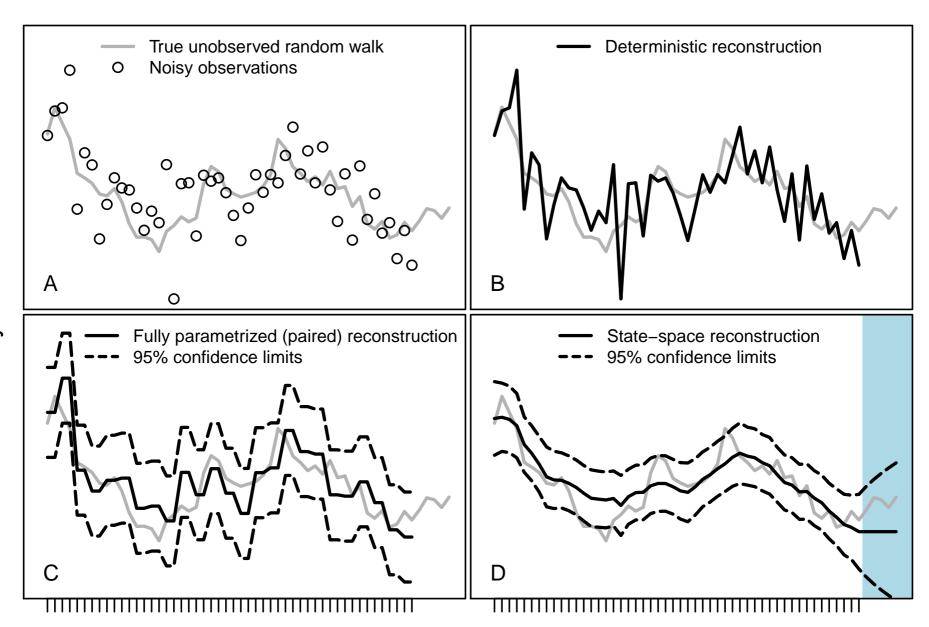
^aa.k.a. random effects models, mixed models, latent variable models, hierarchical models, ...

Illustration of the three types of models



Time

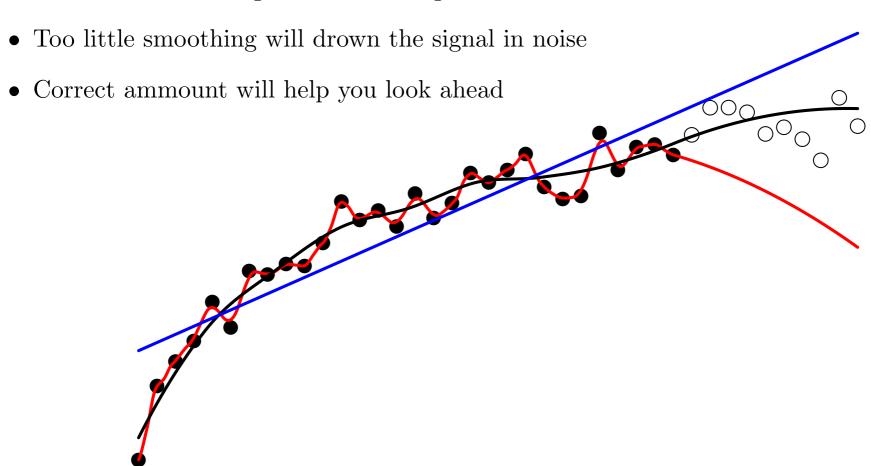
Only one model type can predict



Time

Is smoothing evil?

• Too much smoothing will bias the signal



• Correct amount should not be subjective.

Model

States are the random variables that we don't observe $(N_{a,y}, F_{a,y})$

$$\left(\frac{\log(N_y)}{\log(F_y)} \right) = T \left(\frac{\log(N_{y-1})}{\log(F_{y-1})} \right) + \eta_y$$

Observations are the random variables that we do observe $(C_{a,y}, I_{a,y}^{(s)})$

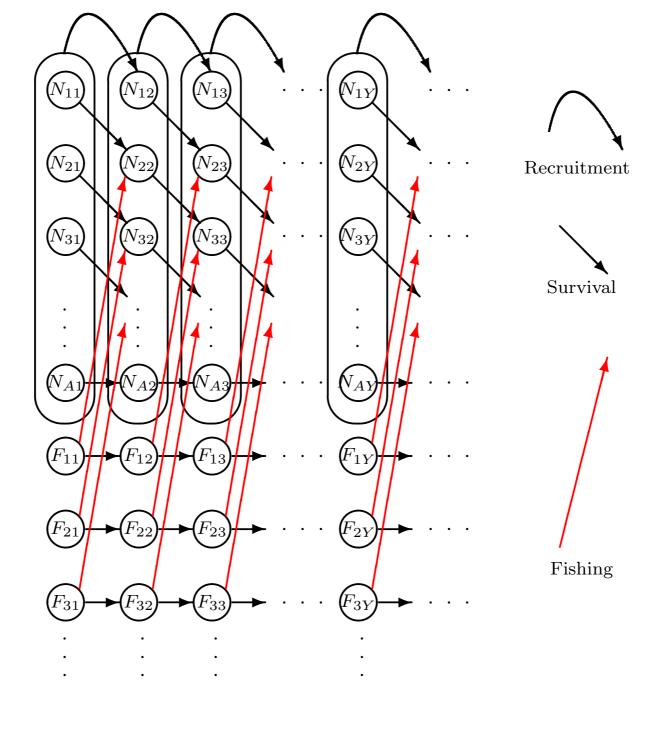
$$\left(\frac{\log(C_y)}{\log(I_y^{(s)})}\right) = O\left(\frac{N_y}{F_y}\right) + \varepsilon_y$$

Model and parameters are what describes the distribution of states and observations through T, O, η_y , and ε_y .

Parameters: Survey catchabilities, S-R parameters, process and observation variances.

All model equation are as expected:

- Standard stock equation
- Standard stock recruitment (B-H, Ricker, or RW)
- Standard equations for total landings and survey indices



Final comments:

- Fisheries research has inspired some tools which are useful for statisticians
- These tools have made the jump from standard to non-standard models smaller
- Writing own models give greater insights
- Read more in:
 - Fournier DA, HJ Skaug, J Ancheta, J Ianelli, A Magnusson, MN Maunder, A Nielsen, J Sibert 2012. AD
 Model Builder: using automatic differentiation for statistical inference of highly parameterized complex nonlinear models. Optimization Methods and Software 27 (2), 233-249
 - Kristensen, K, A. Nielsen, C.W. Berg, H.J. Skaug, B. Bell 2016. TMB: Automatic differentiation and laplace approximation. Journal of Statistical Software 70 (5), 1-21
 - Nielsen, A. and C.W. Berg 2014. Estimation of time-varying selectivity in stock assessments using state-space models. Fisheries Research 158, 96-101
 - Thygesen, U.H., C.M. Albertsen, C.W. Berg, K. Kristensen, and A. Nielsen 2017. Validation of state space models fitted as mixed effects models. (Subm. EES).
 - http://tmb-project.org
 - http://admb-project.org
 - https://github.com/fishfollower/SAM

Exercise 2:

• Install the R-package stockassessment on your computer (if you have not already): This can be done via the line:

```
devtools::install_github("fishfollower/SAM/stockassessment")
```

• Try running the build in example, e.g. with commands like:

```
library(stockassessment)
data(nscodData)
data(nscodConf)
data(nscodParameters)
fit <- sam.fit(nscodData, nscodConf, nscodParameters)
fc<-forecast(fit, fscale=c(1,1,1,1))
ssbplot(fc)</pre>
```