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Original Article

Prediction–variance relation in a state-space fish stock assessment model

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The state-space assessment model (SAM) is extended by allowing a functional relationship between observation variance and the corresponding prediction. An estimated relationship between observation variance and predicted value for each individual observation allows the model to assign smaller (or larger) variance to predicted larger log-observations. This relation is different from the usual assumption of constant variance of log-observations within age groups. The prediction–variance link is implemented and compared to the usual constant variance assumption for the official assessments of North East Arctic cod and haddock. For both of these stocks, the prediction–variance link is found to give a significant improvement.

Keywords: mean–variance relationship, observation variance, SAM.

Introduction

The state-space assessment model (SAM; Nielsen and Berg, 2014) is a frequently used assessment model for species being monitored by the International Council for the Exploration of the Sea (ICES). The model incorporates standard stock equations and includes year- and age-specific fishing mortalities and abundances as latent variables. Several options are available in SAM to accommodate for observation variance structures in data. Variances can be estimated to be independent, correlated in different ways (Berg and Nielsen, 2016), separate or combined across ages. In addition, externally estimated variance/covariance matrices can be assigned. Here, we further expand SAM by allowing a functional relationship between observation variance and its associated prediction to be estimated. The link is similar to the relation that Taylor (1961) found to typically exist in survey data and to the link used in the assessment model Aanes (2016). The main difference is, however, that here the relationship is estimated within the assessment model, rather than being based on external variance estimates.

Log-normal distributions have a quadratic mean-variance relation on natural scale, i.e. the variance is given by

$$v = \alpha\mu^\beta, \quad (1)$$

where $\beta = 2$, μ is the expectation, and α is a dispersion parameter. The relation between prediction and variance Equation (1) is included in several statistical models, e.g. the Tweedie distributions (Jørgensen, 1987; Dunn and Smyth, 2008), are a family of exponential dispersion models with variable β . Also, Kemp (1987) included the mean–variance relation within models for count data. Wood and Fasiolo (2017) introduced a method for estimating Tweedie distributions with spatial components in the power parameter in Equation (1) and applied it in a case study for mackerel egg densities. Observations in fish stock population models may be included as log-normal distributed (Miller *et al.*, 2016; Nielsen and Berg, 2014). However, studies indicate that often is $\beta \neq 2$ for survey index and catch estimates (Taylor, 1961; Brynjarsdóttir and Stefánsson, 2004; Aanes, 2016). The contribution in our research is to

estimate the power relation Equation (1) for log-normal observations within a population dynamic model.

Taylor (1961) illustrated that log-transformed survey indices typically has prediction dependent variance. In this paper, we extend SAM to include the flexible relation between prediction and variance Equation (1) applied in Taylor (1961). The usual assumption of constant log-observation variance implies that the relative uncertainty on natural scale is constant. By estimating a functional relation between observation variance and its associated prediction within SAM, we relax the assumption of constant variance and the model has flexibility to assign a lower (or larger) relative uncertainty to observations as a function of the predicted value. Note that constant log-observation variance is a special case of the prediction-variance link.

North East Arctic (NEA) cod and NEA haddock are commercially important stocks assessed with SAM (ICES, 2020a). It has been observed that occasional large catches have not been predicted well by the model, so these stocks are interesting case studies. The prediction-variance link is tested and compared to the standard options in the assessments of these two stocks. Significant relations between observation variance and associated predictions are detected for both species. Note that prediction-variance link has recently been adopted for the official assessment of NEA haddock (ICES, 2020b).

SAM is open source, and the source code is available at <https://github.com/fishfollower/SAM>. The prediction-variance link is now implemented as a general option in the official version of SAM. Code and data to reproduce all results in this manuscript are available at <https://github.com/OlavNikolaiBreivik/predVarPaperSAM>.

Methods

Model

The applied stock assessment model is an extension of the SAM (Nielsen and Berg, 2014; Berg and Nielsen, 2016). SAM is based on standard stock equations and includes key quantities of interest (fishing mortality and abundance) as latent random effects. Observations are included in SAM as realizations of random variables with densities defined by latent effects and model parameters. An important aspect of SAM is that it automatically weights observations based on how well the corresponding time series fits the assumed population dynamic structure. In this research, we expand the functionality on how observations are weighted in SAM.

We will now define the applied SAM model mathematically. Let $N_{a,y}$ be the abundance at age a in year y , and let $F_{a,y}$ be the corresponding fishing mortality rate. Both these parameters are included as latent random variables, and as in Nielsen and Berg (2014) and Berg and Nielsen (2016), we assume the population dynamic structure as follows:

$$\log N_{1,y} = \log N_{1,y-1} + \eta_{1,y} \tag{2a}$$

$$\log N_{a,y} = \log N_{a-1,y-1} - F_{a-1,y-1} - M_{a-1,y-1} + \eta_{a,y} \quad \text{for } 1 < a < A, \tag{2b}$$

$$\log N_{A,y} = \log (N_{A-1,y-1} e^{-F_{A-1,y-1} - M_{A-1,y-1}} + N_{A,y-1} e^{-F_{A,y-1} - M_{A,y-1}}) + \eta_{A,y}. \tag{2c}$$

Here, $M_{a,t}$ is the assumed known natural mortality rate at age a in year y , and age 1 is recruitment age. It is further assumed that $\eta_{1,y}, \dots, \eta_{A,y}$ are independent mean zero Gaussian distributed, and typically $\eta_{2,y}, \dots, \eta_{A,y}$ are assumed to share the same variance parameter, whereas a separate variance is estimated for $\eta_{1,y}$ (recruitment process). Age group A is included as a plus age group, meaning that it consists of all fish at age A or older.

The fishing mortality vector $\mathbf{F}_y = \{F_{1,y}, \dots, F_{A,y}\}$ is assumed to follow a random walk as in Nielsen and Berg (2014) and Berg and Nielsen (2016) as follows:

$$\log \mathbf{F}_y = \log \mathbf{F}_{y-1} + \boldsymbol{\xi}^F. \tag{3}$$

Here, $\boldsymbol{\xi}^F$ is mean zero Gaussian distributed with a first order autoregressive structure defined in Berg and Nielsen (2016).

The observations included are time series of commercial catch-at-age and indices per age, which enter the model through familiar catch equations. The indices are assumed to be proportional to the true abundance (with noise), where the unknown proportionality constants are unchanged across years. The two observation equations are

$$\log C_{a,y} = \log \left(\frac{F_{a,y}}{F_{a,y} + M_{a,y}} (1 - e^{-F_{a,y} - M_{a,y}}) N_{a,y} \right) + \epsilon_{a,y}^{(c)} \tag{4a}$$

$$\log I_{a,y}^{(s)} = \log (Q_a^{(s)} e^{-(F_{a,y} + M_{a,y}) \text{day}^{(s)} / 365} N_{a,y}) + \epsilon_{a,y}^{(s)}. \tag{4b}$$

Here, $\{Q_a^{(s)}\}_{a=1, \dots, A}$ represents the proportionality factors for survey s , and $\text{day}^{(s)}$ is the number of days into the year when the survey is typically half done. Further are $\epsilon_{a,y}^{(c)}$ and $\epsilon_{a,y}^{(s)}$ mean zero multivariate Gaussian distributed. The ordinary observation correlation structure options available in SAM are elaborated in (Berg and Nielsen, 2016). Note that there is also implemented functionality for including external covariance structures if those are known. Equation (4) defines how data informs the model, observed values are given on the left side, and predicted observations (with uncertainty structures) are provided on the right side. The contribution in this research is an inclusion of a relation between the predicted observation and the corresponding uncertainty within the assessment model.

The focus of this study is a functional relationship between predicted observations and corresponding observation variances. It is only in this part of the model that differs from the model applied in (Berg and Nielsen, 2016). The suggested flexible parametric structure, for each fleet is

$$\sigma_{a,y}^2 = \log (\alpha_a \mu_{a,y}^{\beta_a - 2} + 1). \tag{5}$$

Here, $\sigma_{a,y}^2$ is the variance of a log-observation, i.e. the variance of either $\epsilon_{a,y}^{(c)}$ or $\epsilon_{a,y}^{(s)}$ in Equation (4). Further, $\mu_{a,y}$ is the corresponding prediction on natural scale, and α_a and β_a are model parameters to be estimated within the assessment model. Separate α - and β -parameters may be configured for each age group within each fleet but are assumed constant across years. Equation (5) is obtained by assuming the mean-variance relation [Equation (1)] on natural scale (see Appendix 1 for derivation). This relation was observed by Taylor (1961) to typically exist in survey data. Note that the usual assumption of constant variance is a special case of the prediction-variance link when $\beta = 2$. Furthermore, $\beta < 2$ implies that the variance on log scale decreases with increasing μ , and $\beta = 1$ implies that the variance on natural scale increases linearly with μ . We have chosen to use the median as the predicted observation, and we have investigated that differences are minor if the mean is used in our case studies by scaling the median with $e^{\frac{1}{2} \sigma_{a,y}^2}$.

Table 1. Applied configurations for observation variance.

Species	Model	Observation variance configurations
Cod	1	Variance configurations applied in the official assessment (ICES, 2021).
Cod	2	Prediction variance relation proposed at the recent NEA cod benchmark (ICES, 2021).
Cod	3	Separate time constant variances for all fleets and ages.
Haddock	1	Same constant variance coupling as applied for α in [Equation (5)] in current official assessment.
Haddock	2	Prediction variance relation applied in the official assessment (ICES, 2020a).
Haddock	3	Separate time constant variances for all fleets and ages.

Inference

Maximum likelihood techniques are applied to estimate key quantities of interest (with uncertainty) and to provide knowledge about the investigated population. The model is implemented by using Template Model Builder (TMB) (Kristensen *et al.*, 2016) combined with the optimization function nlminb (Core-Team and contributors worldwide, 2019). TMB is a freely available R-package and is well-suited for performing fast inference with latent Gaussian models when the likelihood can be written as a three times differentiable function. TMB automatically differentiates the likelihood, and utilizes Markov structures to efficiently integrate over latent variables with the Laplace approximation. In our case, the latent variables are log-abundance and log-fishing mortality. The gradient computed by TMB is further utilized by nlminb to effectively optimize the likelihood.

The only new parameters in our research compared to Berg and Nielsen (2016) are the prediction–variance link parameters [Equation (5)]. In our implementation we have assumed that the variance on natural scale increases at least linearly with the expectation, i.e. that $\beta > 1$ in Equation (1). All presented uncertainty intervals are based on standard Gaussian approximations of the log of the quantity of interest.

Results

Case study

As a case study, we investigate how the current assessments of NEA cod and haddock are affected by the prediction–variance link extension. Both of these stocks are currently assessed with SAM (ICES, 2020a, 2021), and the following three different model configurations are compared:

- (1) Standard variance configuration for log-observations (variance of log-observation independent of observation prediction).
- (2) As model 1, but with the prediction–variance link.
- (3) As model 1, but with separate variance parameters for all fleets and ages

Model 3 is included to compare the prediction–variance link with a model which has as much flexibility in the constant variance part as possible. Applied data and model configurations (except for observation variance) are the same as in the corresponding official assessments (ICES, 2020a, 2021).

When applying SAM, the user may specify separate observation variance parameters per age within fleets [Equation (5)], but these parameters are assumed constant across years. It is only the configuration for the observation variance parameters that differs between the three investigated models. The applied observation

Table 2. AIC comparison of the different models for NEA cod and haddock.

Species	Model	Log-likelihood	AIC	Parameters
NEAcod	1	−1 263	2 682	78
NEAcod	2	−1 213	2 584	79
NEAcod	3	−1 203	2 663	128
NEAhaddock	1	−1 176	2 424	36
NEAhaddock	2	−1 028	2 143	43
NEAhaddock	3	−1 056	2 248	68

variance configurations are shortly elaborated in Table 1, and provided in detail in Supplementary Tables S1 and S2.

Table 2 shows the Akaike information criterion (AIC) values obtained with the different models. The favoured AIC values are written in bold. Note that obtained likelihood with model 3 is smaller compared to model 2 for NEA haddock. Thus, no coupling of standard time constant variance parameters exists that would result in a better likelihood compared to using model 2 for this species.

Prediction–variance link parameter estimates with 95% confidence intervals are provided in Table 3. These parameters defines the estimated relation between prediction and variance through Equation (5). Note that $\beta = 2$ implies no relation between prediction and variance. For all data sources with a significant prediction–variance relation, the β -parameters are estimated less than 2, meaning that the corresponding relative uncertainties decrease with respect to predicted values. Supplementary Figures S1 and S2 illustrate the estimated relations for all fleets for both species. Note that the NEA cod prediction variance relation parameters for survey 1 and survey 2 are coupled. This is done because these two time-series are in fact *one* survey, but the survey area was extended from year 2014 and onwards (ICES, 2021), and it was decided to split the survey time-series and assume same observation variance structure before and after the area extension in the official assessment (ICES, 2021).

Figure 1 shows estimated spawning stock biomass (SSB) with the three models. Confidence intervals are only provided for the model favored by the AIC (model 2 in both cases). Figure 2 shows estimated average fishing mortality. Note that the estimated SSBs are not affected much by applying the prediction–variance relation in both case studies. However, the estimated fishing mortality estimates differ in the most recent years for NEA haddock.

Figure 3 shows aggregated catch predictions in tonnes obtained with all three models. We see that the predicted and the observed catches are typically more similar when applying model 2 compared to model 1 or 3 for NEA haddock. A main reason for applying the prediction–variance relation in the current NEA haddock

Table 3. Estimated prediction–variance link parameters with 95% confidence intervals. If no age is provided in the subscript it is the parameter for all ages within the fleet. If no parameter is provided for a fleet, time constant observation variance is assumed.

NEA cod		NEA haddock	
$\alpha_{5-15}^{(c)}$	1.34 (0.77,2.3)	$\alpha_3^{(c)}$	0.94 (0.010, 86.3)
$\alpha_3^{(s1)}$	13.3 (5.0,35.4)	$\alpha_4^{(c)}$	0.22 (0.00083, 59.5)
$\alpha_{4-12}^{(s1)}$	2.96 (1.41,6.2)	$\alpha_{5-13}^{(c)}$	8.51 (4.07, 17.8)
$\alpha_3^{(s2)}$	Coupled with $\alpha_3^{(s1)}$	$\alpha^{(s1)}$	0.51 (0.22, 1.19)
$\alpha_{4-12}^{(s2)}$	Coupled with $\alpha_{4-12}^{(s1)}$		–
$\alpha_3^{(s3)}$	3.08 (1.28,7.4)	$\alpha^{(s2)}$	0.50 (0.28, 0.87)
$\alpha_{4-12}^{(s3)}$	1.56 (0.77,3.18)	$\alpha^{(s3)}$	0.72 (0.45, 1.14)
$\alpha^{(s5)}$	0.32 (0.15, 0.72)	$\alpha^{(s4)}$	0.76 (0.34, 1.71)
$\beta_{5-15}^{(c)}$	1.61 (1.53, 1.70)	$\beta_3^{(c)}$	1.86 (1.47, 2.57)
$\beta^{(s1)}$	1.55 (1.46, 1.66)	$\beta_4^{(c)}$	1.89 (1.46, 2.70)
$\beta^{(s2)}$	Coupled with $\beta^{(s1)}$	$\beta_{5-13}^{(c)}$	1.37 (1.27, 1.51)
$\beta^{(s3)}$	1.65 (1.53,1.79)	$\beta^{(s1)}$	1.84 (1.67, 2.05)
$\beta^{(s5)}$	1.81 (1.69,1.96)	$\beta^{(s2)}$	1.58 (1.44, 1.75)
		$\beta^{(s3)}$	1.53 (1.42, 1.68)
		$\beta^{(s4)}$	1.70 (1.56, 1.88)

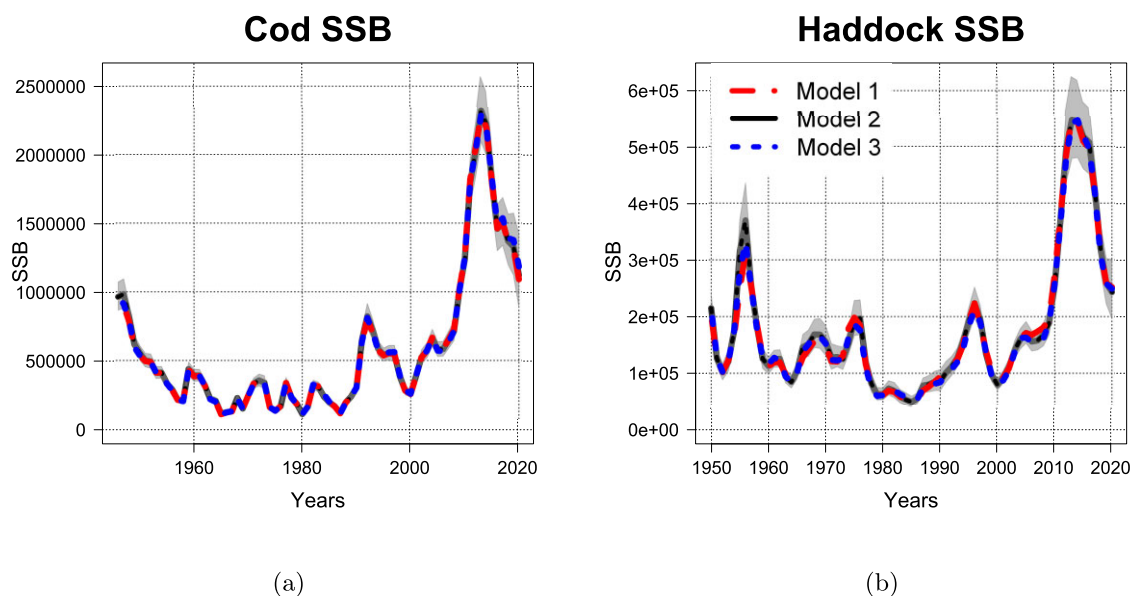


Figure 1. Estimated SSB with the three models, shaded area represents 95% confidence intervals, (a) is for cod, and (b) is for haddock.

assessment is that the obtained historical catch predictions in Figure 3b are believed to be more realistic (ICES, 2020b). Aggregated catch plots are not provided for NEA cod because these are rather similar for all the three models.

Validation

In this subsection, we validate the model including the prediction–variance relation in our case study. The validation is divided into the following three parts: (1) a visual inspection of one-step-ahead (OSA) residuals, (2) a simulation study, and (3) a jitter analysis to confirm that the optimization routine is not affected by starting values.

Conditional independence assumptions are validated by investigating OSA residual patterns (Thygesen *et al.*, 2017). OSA residuals for all three models are illustrated in Supplementary Figures S3 and S4. No clear systematic patterns are observed for haddock. For cod, there are observed patterns within years for the catches with use of all three models. Such patterns within years indicate that there exist correlation structures within the fishing mortality increments [Equation (3)] that are not accommodated for. By allowing our model to include (and estimate) an AR1 structure within the fishing mortality increments these visible patterns are removed, see Supplementary Figure S5.

Figure 4 shows OSA residuals plotted against predicted catch of haddock. From Figure 4a, we observe that smaller predictions are more often associated with larger residuals. When including the

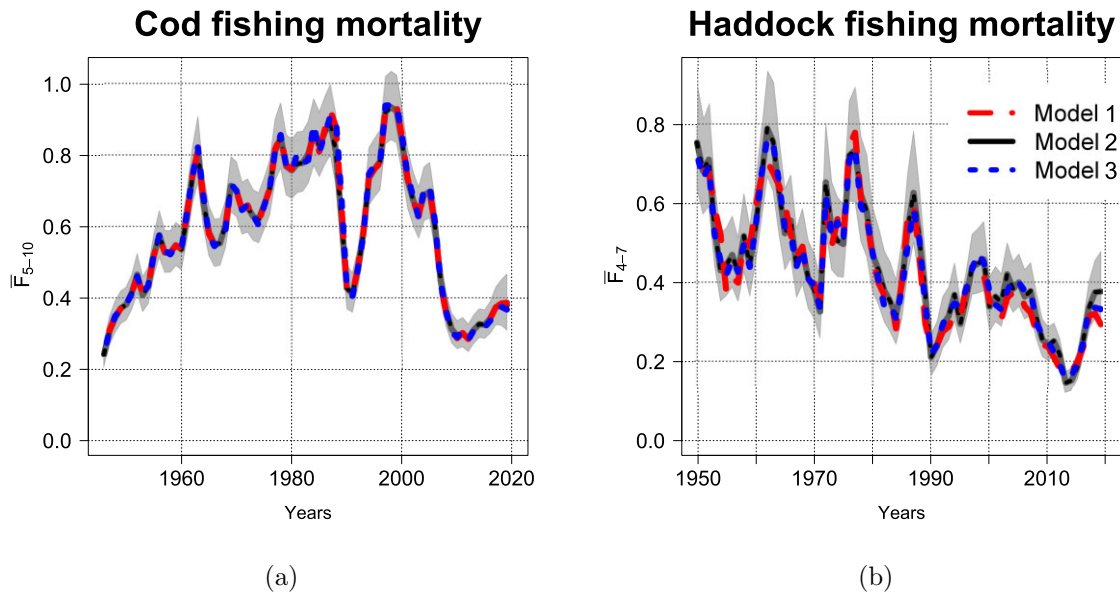


Figure 2. Estimated fishing mortality by the three models, Shaded area represents 95% confidence intervals, (a) shows average fishing mortality for age 5–10 cod, and (b) shows average fishing mortality for age 4–7 haddock.

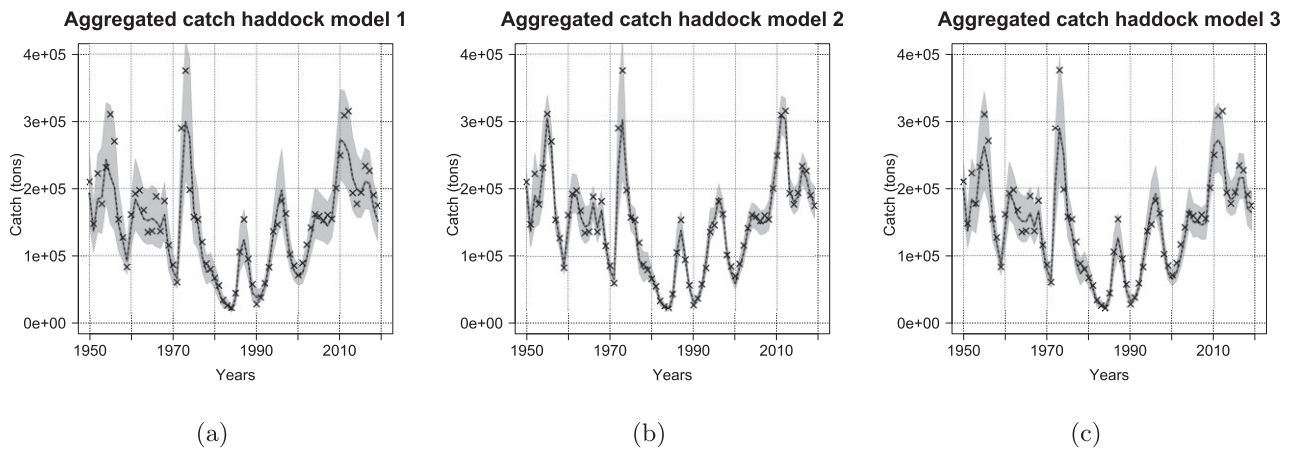


Figure 3. Estimated aggregated catch in tons of NEA haddock with model 1 (a), model 2 (b), and model 3 (c). Shaded area represents 95% prediction intervals and points illustrate the observed values.

prediction–variance relation, such a structure is no longer visible, see Figure 4b. Only residuals associated with age 5 and older are illustrated in Figure 4 because the link is only found significant for catches of those ages. Residuals vs. predictions are not illustrated for NEA cod because no relation between prediction and variance is visible for this species.

A simulation experiment is conducted to verify that the model is identifiable and to investigate consequences of applying the prediction–variance link. Model 2 is used to simulate 200 observation data sets given the estimated abundance and fishing mortality. Supplementary Figures S6 and S7 illustrate estimated SSB and predictions variance link parameters obtained by model 2, and we observe that the model is able to reconstruct the assumed truth.

Inclusion of the prediction–variance relation clearly improved the AIC (see Table 2), which intuitively implies that key quantities are estimated more correctly. To verify our intuition we compare the predicted log SSB and log \bar{F} with the known truth in our simulation experiment. Here, \bar{F} is defined as the average fishing mortality within ages 5–10 and 4–7 for cod and haddock, respectively. Quota advice for these two species are constructed such that \bar{F} attains a certain value dependent on SSB (ICES, 2020a), and these quantities are, therefore, of particular importance to estimate with high precision. Table 4 shows obtained mean absolute differences from the assumed truth, and we observe that the smallest values are obtained when including the prediction–variance relation. Table 4 further provides mean standard deviation for estimated log SSB and log \bar{F} . We observe that the smallest average

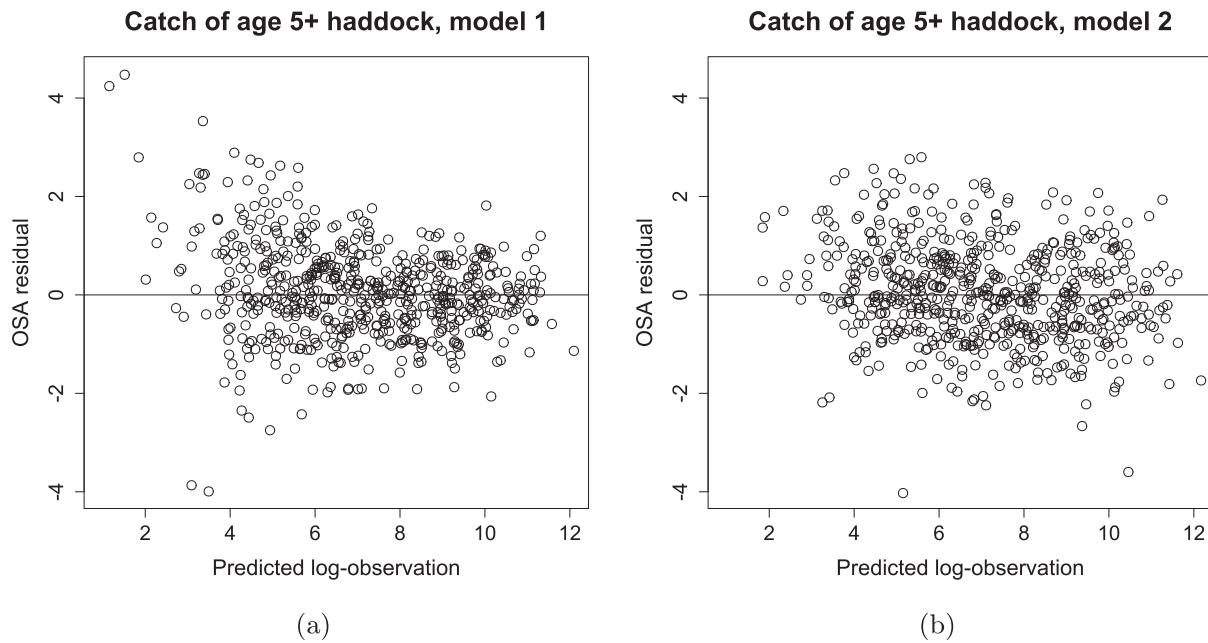


Figure 4. OSA residuals vs. predicted catch of age 5 or older haddock (a) and (b) show residuals obtained with model 1 and 2, respectively.

Table 4. Obtained mean absolute difference between estimated and true log SSB and log \bar{F} in the simulation experiment, and obtained mean estimated standard deviation of log SSB and log \bar{F} . Smallest values are written in bold. Numbers in parenthesis provide the proportion of assumed true values within estimated 95% confidence intervals.

Species	Model	log SSB difference	log \bar{F} difference	Std. log SSB	Std. log \bar{F}
NEAcod	1	0.042	0.040	0.052 (94.0%)	0.054 (96.2%)
NEAcod	2	0.041	0.038	0.048 (92.9%)	0.053 (96.9%)
NEAcod	3	0.043	0.040	0.52 (93.6%)	0.054 (96.4%)
NEAhaddock	1	0.062	0.079	0.096 (98.5%)	0.11 (96.8%)
NEAhaddock	2	0.045	0.060	0.065 (96.7%)	0.090(96.9%)
NEAhaddock	3	0.050	0.065	0.076 (97.8%)	0.094 (97.2%)

standard deviations are obtained when utilizing the assumed true prediction–variance relation, and the corresponding confidence intervals have reasonable coverage. This result indicates that we obtain reduced uncertainty in our stock assessments by utilizing the prediction–variance relation introduced by Taylor (1961). For a few simulation replicates it was not possible to compute standard errors of all estimated quantities, which indicates that there is little to no curvature in the likelihood function in some directions of the parameter-space for these particular replicates. In our simulation experiment, 96.5% and 97% of the runs were reported with confidence intervals for cod and haddock, respectively. Replicates were one or more models did not include confidence intervals were not included in the computed performance metrics shown in Table 4.

Sensitivity to initial values in the optimization routine was investigated by a jitter analysis, i.e. applying several different initial values. Random initial values were constructed by adding an independent $N(0, 0.25^2)$ value to each default initial value. This procedure was conducted 50 times, and the maximum difference between obtained parameters, latent states or log likelihood was less than 10^{-4} for both species. Technically, we have not proven that a global

maximum is obtained, but confidence has been strengthened because of the jitter analysis and the simulation study.

Discussion

The contribution in this research is the inclusion a functional relation between observation variance and its associated prediction in a stock assessment model. Our case studies show that the usual assumption of constant variance for the log-observations is violated, and that the coefficient of variation (on natural scale) is likely to be higher for small observations compared to large ones.

The intuition behind the prediction–variance link is fairly simple. If we predict to observe many fish, the variance of observations on natural scale will typically be large. However, with the commonly used assumption of constant log-observation variance, the model may estimate this variance too large (or too small). In our case studies, we showed that the model was significantly improved when applying the prediction–variance link (Equation 5), which resulted in downscaling of the variance of log-observations associated with larger predictions. We further illustrated that OSA residuals are dependent on predictions when applying constant variance

of log-observations (see Figure 4a). This assumption violation was no longer visible when applying the prediction–variance link (see Figure 4b).

The optimal observation variance configuration in our case study for NEA cod is a mixture of both constant and prediction dependent variances. For NEA haddock, the relation is included for all ages within every fleet even though they are not significant for some ages (see β not significantly different from 2 in Table 3). The inference procedure may become unstable when non-significant parameters are included, and we therefore recommend that the relation is only included for ages where the associated β -parameter is significantly different from 2.

It is possible to include external observation variances and yearly covariance matrices in SAM. External variance estimates can accommodate for time-varying variances unlike our fixed prediction–variance link. However, these estimates are often not available, or their reliability may be questionable. We leave for future research to investigate if assessments are improved by including external variances. However, studies have indicated that accounting for time-varying (co)-variances in survey data is of minor importance (Berg and Nielsen, 2016).

The applied relation between observation variance and prediction is similar to the relation applied in the assessment model Aanes (2016), which is the official assessment model for Norwegian Spring Spawning Herring (ICES, 2020c). A main difference in our application is that we estimate the relationship within the assessment model and not based on external variance estimates. An advantage of estimating the relation within the assessment model is that the uncertainty of the relation parameters are propagated into the uncertainty of key quantities of interest. Another advantage is that data on observation uncertainty is not needed, making the option to include the relation user friendly in practice. An advantage of estimating the relation outside of the assessment model is to reduce the number of parameters within the assessment model by utilizing external variance estimates. We leave for future research to compare results when estimating the prediction–variance relation within or outside of an assessment model.

The prediction–variance relation was chosen to be included in the official assessment of NEA haddock (ICES, 2020b), but not for NEA cod (ICES, 2021). The decision not to include the prediction–variance relation in the official NEA cod assessment was based on that it only provided a small improvement, and the proposal was made too late in the benchmark meeting due to time consuming issues with data sources (ICES, 2021). It was, therefore, decided to not include the relation even though the validation pointed towards a minor improvement (ICES, 2021). Instead, it was recommended to provide a publication of this structure in SAM as a research proposal.

We recommend that all stock assessment models should include a similar prediction–variance link option, and in particular that all SAM assessments explore the consequences of applying this link. At least the assumption of constant coefficient of variation should be checked by plotting residuals vs. predicted values. This is especially important for assessments where there has been large variations in catches and/or indices over time.

Supplementary material

Supplementary material is available at the ICES/JMS online version of the manuscript.

Data availability statement

Code and data to reproduce all results in this manuscript are available at <https://github.com/OlavNikolaiBreivik/predVarPaperSAM>.

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Appendix 1: Prediction-variance relation

The prediction-variance link [Equation (5)] is obtained by assuming a log-linear relation between variance and mean on nat-

ural scale. Let $x \sim N(\xi, \sigma^2)$ and $y = e^x$, and denote μ and ν as the mean and variance of y , respectively. By using the identities $\mu = e^{\xi+0.5\sigma^2}$ and $\nu = (e^{\sigma^2} - 1)e^{2\xi+\sigma^2} = (e^{\sigma^2} - 1)\mu^2$, we obtain that

$$\sigma^2 = \log\left(\frac{\nu}{\mu^2} + 1\right) = \log(\alpha\mu^{\beta-2} + 1), \quad (6)$$

where the last step includes the relation $\nu = \alpha\mu^\beta$.

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