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Assimilation of time series data into a dynamic bioeconomic fisheries model An application to the North East Arctic Cod stock

by

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Synopsis

This paper combines the elegant technique of Data Assimilation and a Monte Carlo procedure to analyze time series data for the North East Arctic Cod stock (NEACs). A simple nonlinear dynamic resource model is calibrated to time series data using the variational adjoint parameter estimation method and the Monte Carlo technique. By exploring the efficient features of the variational adjoint technique coupled with the Monte Carlo method, optimal or best parameter estimates with their error statistics are obtained. Thereafter, the weak constraint formulation resulting in a stochastic ordinary differential equation (SODE) is used to find an improved estimate of the dynamical variable, i.e. the stock. Empirical results show that the average fishing mortality imposed on the NEACs is about 16% more than the intrinsic growth rate of the biological species.

Introduction

Two important sources of information to bioeconomists and other researchers are the model on one hand and the data on the other. The model is an embodiment of the scientific beliefs of the researcher. Mathematical or numerical models have been used extensively by economists to gain useful insights in the analysis of natural resource problems (Clark 1990; Hannesson 1993; Sandal and Steinshamn 2001). The other source is the data obtained from field measurements. Unfortunately, this vital source has not been fully exploited thus far. Advanced and efficient techniques of combining these two sources of information need to be developed. This paper employs the technique of data assimilation (Bennett 1992) in which all the available information, i.e., the model and data are used in the analysis of the North East Arctic Cod stock (NEACs). In data assimilation, observations are merged with a dynamical model in order to determine, as accurately as possible, a description of the state of the system. It can be used to estimate the variables of the dynamical model and/or the parameters of the model. It also leads to the resolution of mathematically ill-posed modeling problems (Bennett 1992). In general, there are two forms of assimilation, sequential assimilation and variational assimilation. In sequential assimilation, the model is integrated forward in time and the model solution updated whenever measurements are available. A typical example is the Kalman Filter (Kalman 1960; Gelb 1974) which is an optimal algorithm for linear dynamics.

Variational assimilation, on the other hand aims at globally adjusting a model solution to observations available over the assimilation time interval i.e., the in-sample-period. Two different formalisms exist in variational methods: the method of strong constraint popularly known as the variational adjoint method and the method of weak constraint which is related to the penalty methods (Smedstad and O'Brien 1991). The strong constraint formulation is shown to be the limiting case of the latter where the model is assumed to be perfect. Note that the former is assumed to contain both measurement- and process-error while the latter is assumed to contain only measurement error and is equivalent to the so-called Observation-error estimators in fisheries assessment literature (see Polacheck et al. 1993). In this paper, a variational data assimilation will be employed to estimate the stock and the poorly known input parameter(s) of a bioeconomic fisheries model.

During the last quarter of the century, many important developments have taken place which have affected the structural setup of fisheries management. An important example is the U.N. law of the sea in the late 1970s (United Nations, FAO 1995). The law resulted in the Extended Fisheries Jurisdiction (EFJ) from maximum of 12 to 200 nautical miles, for coastal states. It empowered, for example, Norway to manage the Barent sea cod together with Russia. This calls for annual quotas being determined before each fishing season. This paper aims to address the question of appropriate quota determination. We will however focus our attention on the biomass dynamics models. Data assimilation methods have broad application and a wide range of advantages which is demonstrated by its extensive usage in meteorology, oceanography and other fields. These advantages can be explored in bioeconomics to a great extent. First, it can be used to analyze the data[1] to extract useful information which will lead to important policy implications about the operation of a fishery. Second, the technique can be applied with equal force to both an open access fishery and the sole owner fishery. It is highly suitable for complex and high dimensional problems i.e. large systems of linear or nonlinear models and can be applied to both discrete or continuous models. Multidimensional bioeconmic fisheries models are more realistic as ecosystem effects may be incorporated. In addition, the adjoint technique provides a computationally more efficient method

[1] Note that, by data we mean any information other than the model formulation. This will include prior guesses of the parameters, the estimate of the biomass given by ICES, etc.

of evaluating gradients of the cost function compared to the finite difference approach. Huiskes, (1998) elaborates more on the advantages of the adjoint method. The purpose of this study is threefold. First to introduce the powerful tool of data assimilation in the management of renewable resources such as fisheries. Second, to exploit the elegant and efficient properties of these methods in order to extract the best information from the available measurements. Third, to estimate the parameters of the growth and production relations and thereby estimate the stock.

The remainder of the paper is structured as follows. Section two presents the data assimilation methods. In section three, the estimator is defined and a comprehensive discussion of the methods presented. The least squares method is used to define a scalar objective function emphasizing the link between this technique and the theory of statistical estimation. All technical details are in an Appendix. In the fourth section, a simple bioeconomic model is defined. The biological base is the Schaefer growth function. It is tied to the economics by a catch per unit effort type of production function. A sensitivity analysis of the parameters of the model is also performed. Section five is a historical discussion of the NEACs. Finally, the results are presented in section six with an equilibrium analysis using the estimated parameters.

The Variational Method

In this paper, the variational adjoint technique will be employed to fit the dynamic model to the data. This technique provides a systematic and efficient procedure for estimation of parameters in large and more complex models by comparing forecasts from the model to the real world observations. We then use the estimated parameters in the weak constraint formulation to estimate the stock. In the first problem the control variables are the input parameters. Using the variational adjoint method the gradients of the cost function with respect to the control variables are efficiently calculated through the use of the Lagrange multipliers. The gradients are then used to find the parameters of the model dynamics which best fit the data. In the second case however, the model variables are the control parameters. The gradients of the variables at each grid point are calculated and the values used to search for the minimum of the cost function (see Bennett 1992).

To formulate the problem, a general nonlinear scalar dynamic model together with the initial condition is defined as

$$\frac{dx}{dt} = g(\beta; x) + q_x$$

$$x(0) = u$$

where g is a nonlinear operator, β is a parameter(s) to be estimated. The term q_x is a random white noise term called modeling or process error. The above formulation is referred to as the weak constraint problem (Evensen et al. 1998). That is, the dynamics are approximately satisfied and thus the equality constraint may be violated.

The Least Squares Estimator

In data assimilation, the goal is to find a solution of the model which is as close as possible to the available data. Several estimators exist for fitting models to data. In this paper, we seek residuals that result in model prediction that is in close agreement with the data. Hence the fitting criterion is the least squares cost function. This is given by

$$J = w_q \int_0^{T_f} q(t)^2 dt + \varepsilon^T \varepsilon$$

where w_q is a scalar constant. The weight will reflect our subjective beliefs about the model and the data. They are equally important if w_q is set equal to unity, and if w_q is less than unity, it means that we have more confidence in the data than the model and vice versa.

To derive the strong constraint problem as a special case, define $\lambda = w_q q_x$ where q_x i.e., the equality constraint is exactly satisfied. This is equivalent to assigning infinitely large weight to the dynamics. The cost function reduces to

$$J_s = \varepsilon^T \varepsilon$$

where J_s is the cost function for the strong constraint problem (Ussif et al. 2002 a-b). Inserting λ in (3) we obtain the Lagrange function for the variational adjoint method. The necessary condition for a minimum (local) is that the first variations of the cost function with respect to (wrt) the controls vanish $\partial J = 0$.

There are many efficient algorithms for solving unconstrained optimization problems (Luenberger 1984). The most common are the classical iterative methods such as the gradient descent, the quasi-Newton and the Newton methods. These methods require the derivatives of the cost function and the Hessian for the case of the Newton methods. However, nonconventional methods could be used. For example, methods of optimization without derivatives and statistical methods such as simulated annealing could be used to find the minimum of the cost function at a greater computational cost. Their advantage is that a more general cost function including discontinuous functions could be used. The inherent problem of local solutions in the line search methods is said to be absent in simulated annealing (see Goffe et al. 1992; Matear 1995). In order to make the paper accessible to more readers we avoid the mathematical and computational details but give a comprehensive verbal explanation of the methods. Technical details are relegated to an Appendix.

One approach of solving the data assimilation problem is to derive the Euler-Lagrange (E-L) systems of equations and solve them. This approach is different from the one in Lawson et al. (1995), where the adjoint system is constructed directly from a model description that is close to the computer code. The E-L systems derived from calculus of variations or optimal control theory (see Kamien and Schwartz 1980) are generally coupled and nonlinear and require simultaneous integration of the forward and the adjoint equations. The task easily becomes arduous and very often impractical. Such a procedure is called the integrating algorithm. In the variational adjoint formulation, the assumption of a perfect model leads to the decoupling of the E-L equations. The forward model is then integrated followed by the backward integration of the adjoint equations. For the weak constraint problem, the approach here avoids solving the forward and backward models but uses the gradient information to efficiently search for the control variables that minimize the cost function subject to the constraints. Given the cost function, which is assumed to be continuous wrt the controls, find the derivatives wrt the controls and then use the gradients to find the minimum of the cost function. The second procedure is referred to as the substituting algorithm and is generally efficient in finding the local minimum. In the case of the variational adjoint method, the algorithm is as follows:

- Choose the first guess for the control parameters.
- Integrate the forward model over the assimilation interval.
- Calculate the misfits and hence the cost function.
- Integrate the adjoint equation backward in time forced by the data misfits.

- Calculate the gradient of J with respect to the control variables.
- Use the gradient in a descent algorithm to find an improved estimate of the control parameters which make the cost function move towards a minimum.
- Check if the solution is found based on a certain criterion.[2]
- If the criterion is not met, repeat the procedure until a satisfactory solution is found.

The solution algorithm for the weak constraint problem is similar except that the gradients are not calculated from the backward integration of the adjoint equations but are obtained directly by substitution.

The Bioeconomics

Fisheries management and bioeconomic analysis have been given considerable attention in the last two decades. Fisheries economists have for the past years combined biological and economic theory to understand and address management issues concerning the important resource stocks, such as the commercially valuable fish population. Underlying most bioeconomic analysis is a mathematical model. In this paper we advance a little further by combining information both from the theoretical model of a fishery and the field measurements. In formulating the bioeconomic model, we require a reasonable biological submodel as a basis. Following the tradition in the literature, we propose an aggregated growth model of the Schaefer (1964) type.

Let $x(t)$ denote the total stock biomass and $h(t)$ denote the rate of harvesting from the stock. We represent the dynamics of the stock as

[2] For example, $J \le \delta, \|\Delta J\| \le \delta$ may be appropriate convergence criteria, where δ is a small number such as 0.0001.

$$\frac{dx}{dt} = rx(1 - x / K) - h$$

where r, K are the intrinsic growth rate per unit time and the environmental carrying capacity in 10^3 tons respectively. The growth law for this fishery is assumed to follow the logistic law (Schaefer 1964). The dynamics of the stock depends on the interplay between terms on the right hand side of the equation. The stock will increase if $h(t)$ is less than the growth term and decreases if $h(t)$ is greater. If human predation ceases, i.e., $h = 0.0$ then the stock will increase at a rate equal to the natural growth of the stock, as the stock biomass will increase towards the maximum population size K. The model basically describes the dynamics of an exploited fishery by linking the biological dynamics and the economics through the general production function $h(t)$.

The production function $h(t)$

In this paper the general Cobb-Douglas production function $h(e, x)$ is defined as

$$h = \tilde{q} e^b x^c$$

where e is the fishing effort, $\tilde{q}$, b and c are constants. The production function quantifies the rate of production of the industry and describes how the inputs are combined in the production process. It depends on two important inputs, the stock biomass and the level of effort expended in fishing. In the fisheries economics literature it is often assumed that harvest is linear in effort and stock level, i.e., $b = c = 1$. The harvest function then reduces to $h = \tilde{q} ex$ where $\tilde{q}$ is the catchability coefficient. This results in the catch per unit effort which is proportional to the biomass. Several implicit assumptions underlie the hypothesis including uniform distribution of fish, etc (see Clark 1990). The natural way to link the biology and economics of fishing is through the fishing[3] mortality parameter $f(t)$. Where $f(t) = \tilde{q}e(t)$ is generally a function of time. In this paper we will specialize a bit by assuming that it is a random variable $f(t)$, with mean f and standard error σ_f that will be estimated. If the errors are normally distributed, then the distribution of f is completely specified. That is a constant (average) fishing mortality rate or proportional removal rate of the standing stock policy is applied (see Ussif et al. 2002b). This yields a simple harvest law which can be used by the management authorities to set total allowable catch quotas (TAC). It is important to note that this assumption is equivalent to assuming a constant average effort.

In this case all variation in the harvest is associated with the fluctuation in stock which is in fact more important than the variations in effort. It is also important to note that this assumption makes the r and f directly comparable which has its merits. To understand the nature and kind of policy used in the management of the NEACs, we apply a simple feedback relation to analyze the data. The assumption may be unrealistic, but we still hope that much practical insight will be gained and will lead to better understanding of the fishery.

Thus, the harvest function for the linear case is

$$h = f\,x$$

where f is the unknown, or poorly known economic parameter, to be estimated. Thus, we have the set $\beta = (r, K, f)$ to estimate. This formulation appears quite simple but may be of immense contribution to our understanding of the practical management of the NEACs. It can be considered

[3] That is the instantaneous average fishing mortality.

as a first order linear approximation of the true harvest function. The function proposed is by no means supposed to be the complete and absolute characterization of the feedback specifications but is considered as a useful and practical approximation of the true one. To reiterate, our purpose is to be simple and to construct a model that is tractable which will lead to some important policy implications.

Some remarks about the model

Linking the biology of the exploited species and the simple approximate harvesting or TAC rule above yields

$$\frac{dx}{dt} = rx(1 - x/K) - f\,x$$

put in another form gives

$$\frac{dx}{dt} = \gamma x - \frac{rx^2}{K}$$

where $\gamma = r - f$ is the difference between the intrinsic growth rate and the fishing mortality rate. Let us call this the residual growth rate of the species. The residual growth rate can be positive, zero or negative at least theoretically. If no fishing mortality is imposed on the stock ($\gamma = r, f = 0$) then it grows to its maximum population level K at a rate equal to the natural growth. If f is positive but less than r the population will settle at a level less than K. For the critical scenario where fishing mortality balances the intrinsic growth rate ($\gamma = 0.0$) the population is driven to extinction. This case can be seen mathematically as

$$\frac{dx}{dt} = -\frac{rx^2}{K}$$

It is also the case where f exceeds r and λ becomes negative. The population will be driven to zero even faster. The dynamics are shown as

$$\frac{dx}{dt} = \gamma x - \frac{rx^2}{K}$$

The predictions of this simple model are evident in the case of most commercial fisheries. Many important fisheries have collapsed in recent times. An example is the Norwegian spring spawning herring (Bjorndal and Munro 1998).

Sensitivity analysis

Input parameters of bioeconomic models are crucial in the analysis of the system. To provide good simulations, precise and reasonable parameters are required.

Unfortunately, the values of these parameters are highly uncertain which translate into the output of the models. Sensitivity is a measure of the effect of changes in the given input parameter on a model solution. It quantifies the extent that uncertainties in parameters contribute to uncertainties in the model results (Navon 1997). Several analytical techniques of sensitivity analysis exist.

To quantify the uncertainties of the k^{th} parameter, we define the following sensitivity index IS_k

$$IS_k = \frac{\sum_0^N (z_t - z_t^k)^2}{\sum_0^N z^2{}_t}$$

where N is the time horizon which in this case is 51 time steps, z_t is the original model prediction and the z_t^k is the perturbed prediction. The index is simply a ratio of the sum of the squared deviations due to the variation in the parameters to the sum of the squares of the original solution. Note that the units of r and f are (/year) and the unit of the carrying (average) capacity K is in kilotons. The sensitivity index is a dimensionless quantity.

The parameters are each perturbed to 90 percent of their original values while holding the remaining fixed. The model is then rerun for all the parameters. The results of the sensitivity of the biological and economic parameters are shown in Table 1 below. These parameters are ranked in an increasing order of importance.

Table 1: Sensitivity index of the model parameters

Parameters	Original Values	New Values	IS_k
r	0.450	0.405	1.50
K	6000.0	5400.0	1.68
f	0.400	0.360	5.09

The fourth column indicates the index which measures the sensitivity of the parameters.

The fishing mortality parameter is the most important and the growth rate is the least. The carrying capacity of the species is more sensitive biological parameter which confirms the results of an earlier paper (Ussif et al. 2000a).

The North East Arctic Cod stock

The NEACs is the most important demersal species along the coast of Norway and Northern Russia. This fishery has played an important economic role within the coastal communities for the past thousand years. The NEACs has for the past half century experienced large variations which result in a corresponding variation in the annual harvest quantities.

The stock size fell from its highest level in 1946 of 4.1 million tons to the lowest in 1981 of 0.75 million tons. However, the stock seems to be recovering from the depleted state in the 1990s due to improved management strategies. In this study, a time series from 1946 to 1996 is used. The variables are the annual stock and harvest[4].

In what follows, we present a brief qualitative description of the data (see Anon. 1998). Figure 2, is a plot of the stock and the harvest. The stock and the harvest have a generally downward trend with periodic oscillations. Apart from the first few years the directions of fluctuation in both the stock and the harvest are the same. It may be observed from the graph that there exists some proportional relationship between the harvest rate and the level of stock.

[4]Total international landings as reported in ICES 1998 measured in 10^3 tons

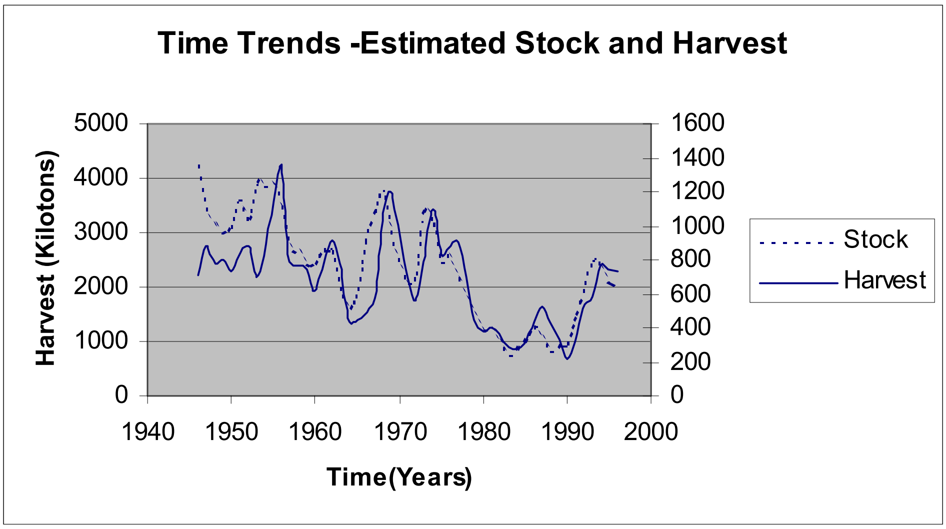

Figure 1: Source: ICES 1998 report. Time series plot of the stock and the actual harvest rate of the NEACs.

Results

The empirical results of the research are discussed and shown in this section. All the results are based on data[5] of the NEACs for the period from 1946 to 1996. The results of the variational adjoint parameter estimation are presented. They are followed by the weak constraint results and then a steady state analysis is performed. Note that twin experiments were performed using both clean and noisy data to test the assimilation algorithm.

Estimation of the growth and yield functions

The combined variational adjoint-Monte Carlo technique was used to fit the bioeconomic model to the data assuming that the fishery is exactly governed by the simple model. The model contains three input parameters: the intrinsic growth, the carrying capacity and the human predation

[5] That is, the data from the ICES.

coefficient. These are all important to a fisheries manager. Estimating all the parameters at the same time for this simplified model may pose a problem of identification. To obviate the bottleneck, the least sensitive parameter in the model is exogenously but randomly selected from a uniform distribution and then the other two, namely the carrying capacity and the fishing mortality rate, are optimally determined using variational adjoint method.

Relying on some physical information from experts, a range of r values between 0.25 and 0.45 is chosen. This subjective information may be interpreted as a Bayesian noninformative prior. A subsample of 3005 was randomly drawned from the population. Using this sample, the variational adjoint method is used to find the optimal estimates of the parameters. The statistic of choice in this paper is the mean even though there are other estimators that are efficient. In table 2, we show the parameter estimates and their standard deviations.

Table 2 : Estimated parameters and their standard deviations.

Parameters	r (/yr)	K (1000 tons)	f (/yr)
Estimates	0.3499	5268.4	0.4076
se	(0.0578)	(868.3)	(0.0579)

The se denotes standard error of the estimates.

These estimates are all reasonable and intuitively appealing. What is interesting is that the model has been able to capture the salient features of the NEACs. The estimated average rate of capture of the stock exceeds the intrinsic growth rate of the species.

State estimation of the stock biomass

Data assimilation can be used to estimate the variables of a dynamical system or the parameters of a dynamical model, using all the available information from the model formulation and the set of observations. The former embodies all the beliefs of the modeler about the system she or he is interested in studying. They may use economic and biological theory as well as intuitive reasoning in order to construct a model that approximately represents the system. In the weak constraint formulation, the model dynamics are assumed to approximately hold.

The fisheries model employed in this paper is quite oversimplified. Many important variables such as the environmental effects and predation from other species are disregarded. The harvest function is also a simple first order approximation. All these factors make the model quite unrealistic. To remedy this, we accept a certain unknown level of error in the model by adding a term that quantifies the errors and their uncertainties.

A cost function measuring the disagreements between the data and the model predictions was defined, and a penalty term appended which penalizes the model misfits. A model prediction that is as close as possible to the data, is sought in a least squares sense. The optimization procedure used in this paper is the classical quasi-Newton method (Gilbert and Lemarechal 1991). The estimation was conducted for two cases. The first case uses the solution of the variational adjoint method as the first guess solution. That is the parameter estimates from the first method were used to solve the model and the solution is taken as the best guess to start the optimization. To show that the algorithm is robust to the initial guess of the solution, a constant equal to the average of the first case is used as the first guess. The results are not shown in this paper.The circles denote data, the broken line is the first guess which is the solution of the strong constraint problem in case 1. Note that the weight $w_q = 0.001$ in this case. This was subjectively chosen to reflect our bias toward the data. As it might be expected, we have more confidence in the data from the ICES than the estimates of our model.

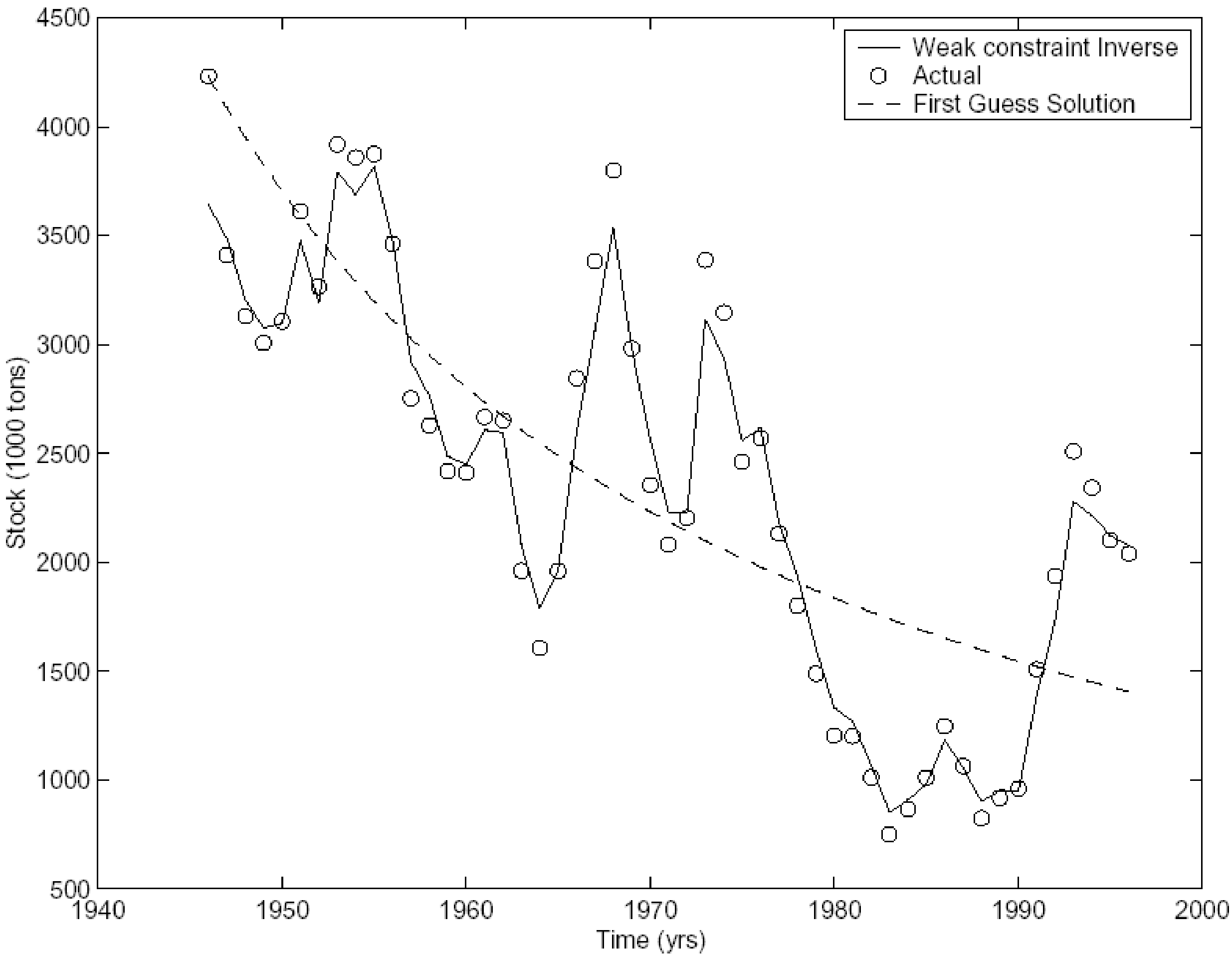

Figure 2: Graph of the stock biomass: case 1 with $w_q = 0.001$. The graphs are the actual ICES stock estimates, the strong constraint and the weak constraint estimates from the models developed above.

The fit of the model is good in general. The coefficient of determination R^2 is about 0.55. The algorithm is also robust and did not depend very much on the initial guesses. However, the convergent rate is slightly affected by the choice of the initial guesses.

Equilibrium analysis using the deterministic model

The use of the population dynamic equation assumes the existence of equilibrium in the model. This section briefly discusses this concept in this application. At the steady state time is no longer important and the stock biomass becomes constant at a level x^*. This implies the time rate of change of the population is identically zero, i.e., the net growth of the stock balances the rate of harvesting

$$\frac{dx}{dt} = 0 \;\; h^* = rx^*(1 - x^* / K)$$

It follows then that for the linear harvest function we have

$$f\, x^* = rx^*(1 - x^* / K)$$

where f is as defined previously. Hence the steady state biomass is

$$x^* = K(1 - f / r)$$

Ideally, the fishing mortality rate should not exceed the intrinsic growth rate of the biological species, i.e, $f < r$ for a stock that is overexploited and is under rehabilitation. If the fishery is unexploited and initial stock is to the right of the maximum sustained biomass level then higher mortality rates may be applied in order to quickly adjust it to the desired optimal state. The equilibrium stock is a function of the biological and economic parameters. It is clear that if the carrying capacity (e.g., the aquatic environment) increases, x^* will increase and vice versa.

The effect of small change in r is similar. However, increasing fishing mortality will result in a decline in the equilibrium biomass. The concept of maximum sustainable yield has been the practical management objective for many fisheries (Clark 1990). The NEACs is not an exception to the rule. For the compensation model used in this paper, the estimated x_{msy}, equals 2634.2 kilotons. Figure 3 below shows the historical state of the NEACs from 1946 to 1996 and the x_{msy}. A careful study of the time series reveals some interesting observations. The stock was at a level of about 80 percent (4231.9 kilotons) of the carrying capacity in 1946. It was fished down to about 50 percent of K (x_{msy}) by 1958. It then remained at about that level forming a window until the late 1970s when the situation got completely out of control.

The state of the stock continued to decline and by 1983 it was at its worst level of less than 20 percent of the carrying capacity. The trend has, however, changed and the 1996 estimate of stock indicates a sign of recovery. Recent observations, however, indicate that the stock is again in deep trouble.

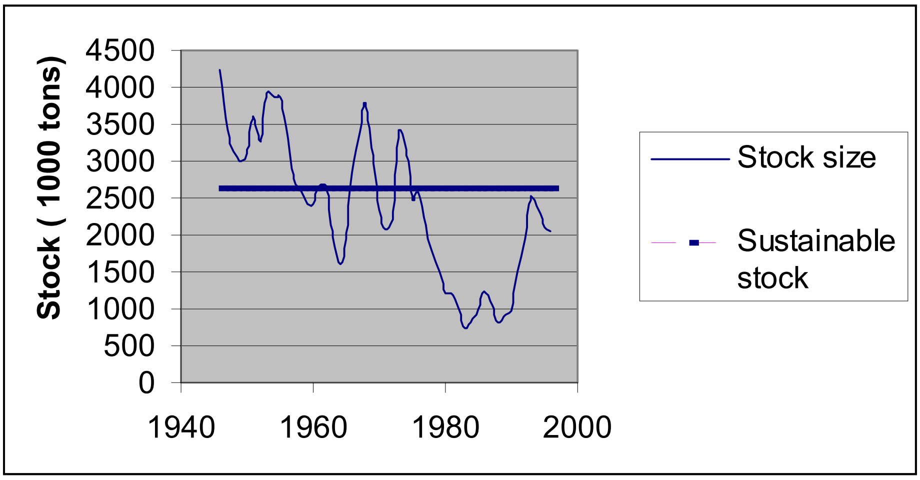

Figure 3: Plot of the stock and estimated sustainable stock (tons) vs. time (yrs).

Conclusion

This paper uses a novel approach of data assimilation into dynamical models to analyze data for the NEACs. To our knowledge no such work has been reported in bioeconomics. For lumped parameter models as well as age-structured models, these methods can be useful technique for the estimation of parameters. The adjoint method has the advantage of efficiently computing the gradients of the cost function. It also provides more reliable parameter estimates (Huiskes 1998) due to the accuracy of the computed gradients. Model parameters were estimated by the variational adjoint technique in combination with a Monte Carlo procedure. The estimates are as expected, the fit to the data is also good with the model capturing the trend in the data but failing to capture the oscillations. This is not surprising because the model is deterministic and does not have the ability to absorb the random events in the system. The weak constraint model however does very well in capturing the stochasticity in the data. Next, we discuss the findings of the research. These are contingent on the hypotheses of the model which is a mathematical approximation to reality. The key results of the paper are that for the NEACs the average intrinsic growth rate is about 0.35 per year and the maximum population that the environment can support is about 5.3 million tons. The fishing mortality rate is about 0.41 per year which is greater than the intrinsic growth rate. This implies the annual harvest or production from the fishery is consistently above the net growth curve. This is intuitively supported by the persistent decline of the stock since 1946. It is important to be reserved in generalizing the findings in this paper. The reason is that the model used in this paper is very simple and does not absolutely represent the fishery. Finally, the assimilation methods have proven very efficient and can be very useful in analyzing, testing and improving resource models.

APPENDIX

Derivation of the adjoint equation

To illustrate the numerical procedure, we use the discrete dynamics

$$x_{n+1} = x_n + g(\vec{\mathrm{P}}; x_n)\, dt \quad ,$$

$$x_0 = u\,,\; 0 \le n \le N-1$$

where N is the number of observations in time, $\vec{\mathrm{P}}$ a vector of parameters to be estimated and dt is the time step. The discretization scheme used is a simple forward difference scheme. The discrete form of the Lagrange functional is constructed as follows

$$L = \sum_{n=1}^{N} (x_n - x_n^{obs})^2 + w_p \sum_{n=1}^{N-1} (p_i - \hat{p}_i)^2$$

$$+ \sum \lambda_n (x_{n+1} - \{x_n + g(\vec{P}; x_n) dt\})$$

From these equations, we obtain

$$x_{n+1} - \{x_n + g(\vec{P}; x_n) dt\} = 0$$

$$\frac{\partial J}{\partial x_n} - \lambda_n (1.0 + dt \frac{\partial g}{\partial x_n}) + \lambda_{n-1} = 0$$

$$\Delta_{p_i} L = \Delta_{p_i J}\, J - \sum \lambda_n dt \frac{\partial g}{\partial p_i}$$

where $\Delta_{p_i} L$ is the derivative with respect to the i^{th} parameter and $\frac{\partial g}{\partial x_n}$ is the tangent linear operator. It is immediately seen that equation (A4) recovers the model dynamics, i.e., the forward model, equation (A5) gives the backward model forced by the model-data misfits and equation (A6) is the gradient with respect to the parameters. To find the model parameters that give model forecasts that are as close as possible to the observations using the classical search algorithms, correct values of the gradients are required. Methods for verifying the correctness of the gradient are available both numerically and analytically where possible (see, Spitz et al. 1998; Smedstad and O'Brien 1991). We have in this paper checked all gradient calculations to ensure reliable parameter estimates.

The optimization procedure used for the minimization is the quasi-Newton procedure developed by Gilbert and Lemarechal (1991).

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