On the dynamics of commercial fishing and parameter identification

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Abstract

This paper has two main objectives. The first is to develop dynamic models of commercial fisheries different from the existing models. The industry is assumed to have a well defined index of performance based on which it either invests or otherwise. We do not however, assume that the industry or firm is efficient or optimal in its operations. The hypotheses in the models are quite general, making the models applicable to different management regimes. The second is that a new approach of fitting model dynamics to time series data is employed to simultaneously estimate the poorly known initial conditions and the parameters of the nonlinear fisheries dynamics. The approach is a data assimilation technique known as the adjoint method. Estimation of the poorly known initial conditions is one of the attractive features of the adjoint method. Unlike the conventional methods, the method employed in this paper, requires relatively less data. Economic parameters were reasonably estimated without cost and price data. The estimated equilibrium biomass is very close to the maximum sustainable biomass which means open access in this case led to economic overfishing but not biological overfishing.

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1 Introduction

The most common approaches of modeling the dynamics of a natural resource system are by the routine application of the sophisticated techniques of the calculus of variations or optimal control theory and dynamic programming (Kamien and Schwartz, 1984; Clark, 1990). The economic theory of an optimally managed fishery has been advanced by many researchers. Clark (1990) discussed various models in some detail. Sandal and Steinshamn (1997a,b,c) made some of the most recent contributions in the area. These frameworks explicitly assume that agents are optimal and efficient. However, most real world fisheries have historically not been optimally managed.

The dynamics of single species models have extensively been studied in the literature of natural resource economics (Sandal and Steinshamn, op. cit.). Extensions have also been made to include ecological effects from other species. The simplest is the predator-prey model (see Clark, 1990).

Commercial models of fisheries have previously been discussed by Crutchfield and Zellner (1962) and Smith (1967). The latter provided a model of theoretical nature which transforms specific patterns of assumptions about cost conditions, demand externalities and biomass growth technology into a pattern of exploitation of the stock. Smith also discussed the three main features of commercial fishing and mentioned the various types of external effects representing external diseconomies to the industry. In two earlier papers, Gordon (1954) and Scott (1955) noted that all of these externalities arise fundamentally because of the unappropriated “common property” character of most ocean fisheries (Smith, 1967).

In this paper, we develop some commercial fishing models that do not necessarily assume optimal behavior of fishers. The goal is to develop models that are quite general and have much wider possible applications. Models of natural resource exploitation consist of two vital components. First, a sound biological base which defines the environmental and ecological constraints is required. Second, an economic submodel that incorporates the basic characteristics of the exploiting firms must be in place. For example, an industry or a firm may be assumed to vary levels of capital investments in proportion to some measurable quantities such as the total profits (Smith, 1967; Clark, 1979).

This paper also focuses on a very important aspect of fisheries management that has largely been ignored. Deacon et al. (1998) noted that much of the information managers need is empirical, i.e., measurements of vital relationships and judgments about various impacts. This area of the economics of fishing has not been adequately explored by economists probably due to lack of data and computational power in the past. Much of the research efforts were used in the search for qualitative answers to management problems.

This paper employs a new and efficient method of advanced data assimilation known as the adjoint technique (Smedstad and O'Brien, 1991) to analyze real fisheries data. In data assimilation, mathematical or numerical models are merged with observational data in order to improve the model itself or to improve the model predictions. The former application is known as model fitting. Using the adjoint technique, in which the model dynamics are often assumed to be perfect, i.e., the dynamical constraints are satisfied exactly (Sasaki, 1970), appropriate initial conditions and parameters of the nonlinear fisheries dynamics are estimated. Nonlinear fisheries dynamics are highly sensitive to the initial conditions and the parameters which are often exogenously given inputs to the system. These inputs are very crucial in simulation studies. Inverse methods and data assimilation are often ill-posed, i.e., they are characterized by nonuniqueness and instability of the identified parameters (Yeh, 1986). It may thus be worthwhile to search for best initial and/or boundary conditions when using these models in analysis. The reader may have noticed that this approach has major advantages compared to conventional methods. It allows us to estimate initial conditions of the model dynamics as additional control variables on equal footing as the model parameters. Thus, treating the initial biomass level and the initial harvest rate as uncertain inputs in the system. Most recent models and traditional approaches consider the initial biomass and harvest amounts as known and deterministic. It also provides an efficient way of calculating the gradients of the loss function with respect to the control variables. Most importantly, data requirements are significantly reduced. In this paper, parameters entering the objective function of the industry have been reasonably estimated without having to use data on prices and costs. Large number of parameters could be estimated with observations on only a subset of the variables.

The structure of the remainder of the paper is as follows. Section 2 is a detailed discussion of the dynamics of the commercial fishing model. It presents a more general model without assuming any optimizing behavior. In section 3, we briefly discuss data assimilation and some basic concepts of the techniques are defined. All technical details are put in an Appendix. Section 4 is an application to the Norwegian cod fishery (NCF). It discusses the results and summarizes the work.

2 Dynamics of Commercial Fishing

The dynamics of the fishing industry are developed and discussed in detail in this section. A fishery resource has one unique characteristic, i.e., the ability to replenish by the laws of natural growth. The dynamics of the stock for a single species are formally described by the simple equation

$$\frac{dx}{dt} = f(x) - y \tag{1}$$

where x is the biomass in weight, dx/dt is the time rate of change of the stock and y is the rate of exploitation by humans. The growth "or natural addition" to the existing stock is represented by the $f(.)$ operator and depend on the current stock. Several forms of the growth model exist. For some species, the empirical law of growth is asymmetric. In this paper, however, we will use the logistic growth law. The Schaefer logistic function takes the form $f = rx(1 - x/K)$, where r is the intrinsic growth rate and K is the maximum growth of the biological species if the population were not exploited. It is symmetric about $K/2$ and has the following properties, $f(0) = f(K) = 0$, $f(K/2)$=max f.

To model the fishing industry, we define the following relationship between the rate of increase or decrease of the exploitation of the fish biomass y and a function $\phi(x, y)$ such that

$$\frac{dy}{dt} = \gamma y \phi(x, y) \tag{2}$$

where $0 < \gamma$ is a constant of proportionality and ϕ is a certain well defined value function to be discussed shortly. The constant of proportionality reflects the rate at which capital is being put in or removed from the industry or firm. For instance, if ϕ is positive one may expect an increase in capital investment in the fishery and a decrease otherwise. The function(s) defined by ϕ can take different parametric forms reflecting our hypotheses about the operation of the industry. It may represent short or long run average costs of fishing vessels, the marginal or average net revenues of a firm, etc. Different forms of the ϕ functions will be discussed in detail. We will first model an industry that is perceived to be a price taker in the output market.

Let p be the unit exvessel price of fish and c be the per unit cost of harvesting. Assume for the first case that costs of fishing are linear in the harvest. Then, the average net revenue is given by

$$\phi(x, y) = p - \frac{c}{x} \tag{3}$$

The average cost of harvesting is assumed to depend explicitly on the size of the stock abundance. This takes into account the stock externalities, i.e., fishing costs decrease as the population of fish increases. The assumption that the total net revenue of the industry is linearly related to the harvest rate may be quite restrictive. We shall slack this assumption of price taking and introduce some relevant nonlinearities in the model. Next we discuss a model in which price depends on the rate of harvesting of the stock. We shall continue to assume that costs are linear in harvest and inversely related to the stock biomass. The average net revenue is defined by

$$\phi(x, y) \quad = \quad P(y) - \frac{c}{x} \tag{4}$$

where $P(y) = a - by$ is the inverse demand function which is assumed to be downward sloping and a, b are positive real constants. From the previous definitions of ϕ and the industry model, equation (2), it is obvious that the rate of harvesting from the stock for the industry is perceived to vary in proportion to the net revenue; that is the difference between total revenues and total costs. Put another way, the output growth rate $\dot{y}/y$ of the industry is proportional to the average or marginal net revenues.

Substituting these functions in equation (2) and combining with the population dynamics model, equation (1), the industry dynamics models are derived. This system of equations (1)-(2) constitute coupled nonlinear ODEs. For the empirical analysis, we will use the following models.

model 1

$$\begin{aligned} \frac{dx}{dt} &= f(x,r,K) - y \\ \frac{dy}{dt} &= \gamma(p - \frac{c}{x})y \end{aligned} \tag{5}$$

In the first model, the term $(py - cy/x)$ is the annual total profit (total revenues minus total costs). Owing to the linearity of the net revenue in the harvest, the average net revenue is equal to the marginal net revenue.

model 2

$$\begin{aligned} \frac{dx}{dt} &= f(x,r,K) - y \\ \frac{dy}{dt} &= \gamma(P(y) - \frac{c}{x})y \end{aligned} \tag{6}$$

In model 2, the demand function is downward sloping, i.e., the output of the industry affects its market price and costs are linear in harvest and inversely related to the stock biomass (Sandal and Steinshamn, 1997b). Hence, the profit function is nonlinear both in the harvest and the biomass. Incorporated in these models are the hypotheses about the costs and the revenues. If the firms were optimizers, they should at least operate at a level where average or marginal profits are positive. In the construction of such behavioral models, an implicit assumption about the harvest rate being proportinal to the number of firms or fishing vessels is made (see simth 1967).

The system of equations contains these input parameters, the biological parameters (r, K) and the economic parameters (γ, p, a, b, c). It is possible to estimate all of the parameters in the models but additional data may be required. To obviate the data problem, we reduce the dimension of the problem by redefining the parameters: $\theta = \gamma p$, $\alpha = \gamma a$, $\beta = \gamma b$, and $\tau = \gamma c$. That is, we now have these parameters $(r, K, \theta, \alpha, \beta, \tau)$ to estimate. Notice here that no data on prices and costs are necessary in order to fit the models. The method enables us to fit the bioeconomic models without using data on economic variables which are often unavailable. These mathematical models of the commercial fishing will be used to analyze real fishery data for the Norwegian cod fishery (NCF) stock.

3 Data Assimilation Methods

Data assimilation methods have been used extensively in meteorology and oceanography to estimate the variables of model dynamics and/or the initial and boundary conditions. These methods include the sequential techniques of Kalman filtering (Kalman, 1960) and the variational inverse approach (Bennett, 1992). The variational adjoint method has been proposed as a tool for estimation of model parameters. It has since proven to be a powerful tool for fitting dynamic models to data (Smedstad and O'Brien, 1991). The methods have recently been used to estimate parameters of the predator-prey equation (Lawson et al., 1995) and also some high dimensional ecosystem models (Spitz et al., 1997 and Matear, 1995). The basic idea is that, given a numerical model and a set of observations, a solution of the model that is as close as possible to the observations is sought by adjusting model parameters such as the initial conditions. The adjoint method has three parts: the forward model and the data which are used to define the penalty function, the backward model derived via the Lagrange multipliers and an optimization procedure. These components and all of the mathematical derivations are discussed in an Appendix. An outline of the technique is also presented for those who may be interested in learning the new and efficient method of data analysis.

4 An Application

The commercial fishing models developed in this paper are used in an application to NCF stock. The fishery has a long history of supporting large part of the Norwegian and Russian coastal populations. Data on catches and estimated stock biomass have been collected since immediately after World War II. Different techniques of stock assessments exist in fisheries management. The data on the NCF are measured using the statistical Virtual Population Analysis (VPA) method. Catch data and biomass estimates obtained by the VPA may be somewhat correlated. This issue will not be dealt with in this paper.

The history of this fishery is not dissimilar from other commercial fisheries elsewhere around the world. It has supposedly been managed based on the common policy of the maximum sustainable yield (MSY) which is the most employed for the most of the last century. The historical data show a decreasing trend for both the stock biomass and the yield. It is also observed that the data are highly fluctuatory which depicts the inherent stochastic feature of a fishery resource. The data available on NCF dates back to 1946 until 1996. It is however intuitive to divide the period into the pre-quota (1946-1977) and the quota (1978-1996) periods which represent different management regimes. The first period may be dubbed the open access period and the second the regulated open access (total allowable catch TAC) period. We will apply our models to analyze the data for the first period. To analyze the second period, additional constraints such as quota restrictions and minimum safe biomass levels Homans and Wilen (1997) which reflect the regulations imposed by the management authorities are required. We shall however concern ourselves about the first period.

In this study, we combine the nonlinear dynamics models developed in the preceding section and the time series of observations to analyze the NCF. The technique in this paper provides a novel and highly efficient procedure of data analysis. Model initial conditions as well as parameters of the dynamics are estimated using the adjoint method. First, artificial data generated from the model itself using known initial conditions and known parameters were used to test the performance of the adjoint code. All the parameters were recovered to within the accuracy of the machine precision. Both clean and noisy data were used to first study the models. The results are not shown in this paper. Next, real data were used to estimate the initial conditions and all the parameters of the model dynamics. Starting from the best guesses of the control variables, the optimization procedure uses the gradient information to find optimal initial conditions and parameters of the model which minimize the penalty function. The procedure is efficient and finds the optimum solution in a matter of a few seconds. The estimated initial conditions and parameters of the two different models are tabulated below.

Parameters	Model 1	Model 2
r	0.3271	0.44305
K	5264.85	5257.55
θ	0.13039	
α		4.1368
β		.00213
τ	309.01	7070.63
$x0$	3902.77	3670.00
$y0$	716.15	770.33

Table 1: Model parameters for the two dynamic models. Blank space means the parameter is not present in that model.

All the estimated parameters are reasonable and as expected. From the table above, the estimated r's are different for the two different models. Model 2 which is more complex than model 1 gives a bigger r value. The maximum population K is about the same for both models. The initial conditions have also been adjusted in both cases. Note that the observed initial values were taken as the best guesses. To further explain the performance of these models, we present some graphics of the time series of the actual observations and the estimated quantities. Figure 1 is a plot of the actual observations (Act. observations) and the models predictions (Est. model 1 and Est. model 2) of the stock biomass using the estimated parameters.

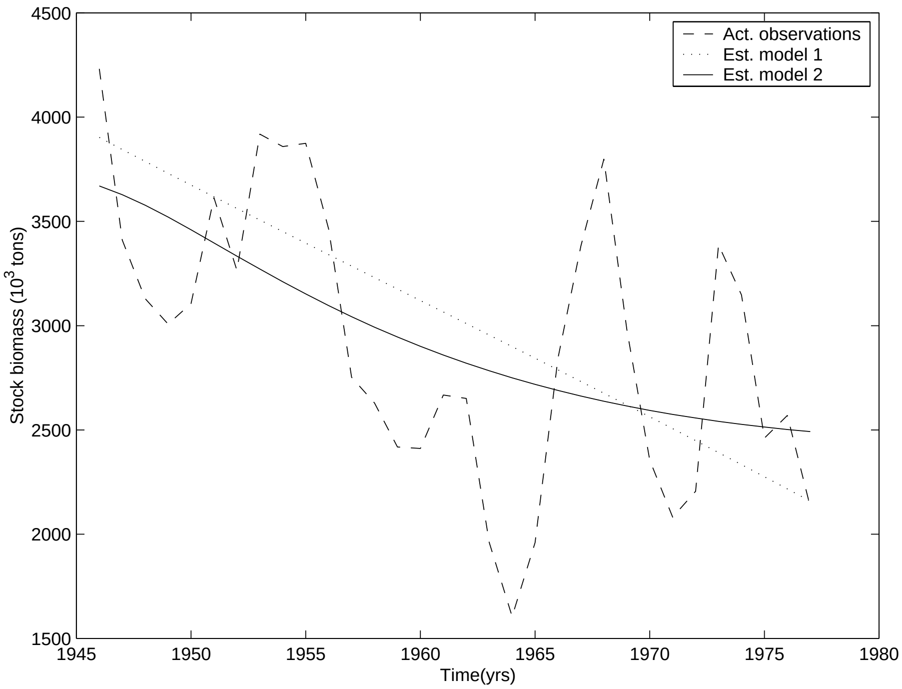

Figure 1: Graphs of the actual and the model estimated stock biomass for the two models

It is observed that, model 1 predicts higher biomass levels and is generally steeper than model 2. The models have both performed well in tracking the downward trend in the data. Model 2 seems to do a little bit better overall and at the tail end of the data. In Figure 2, we have the plot of the actual observations (Act. observations) and the model predictions (Est. model 1 and Est. model 2) of the rate of harvesting.

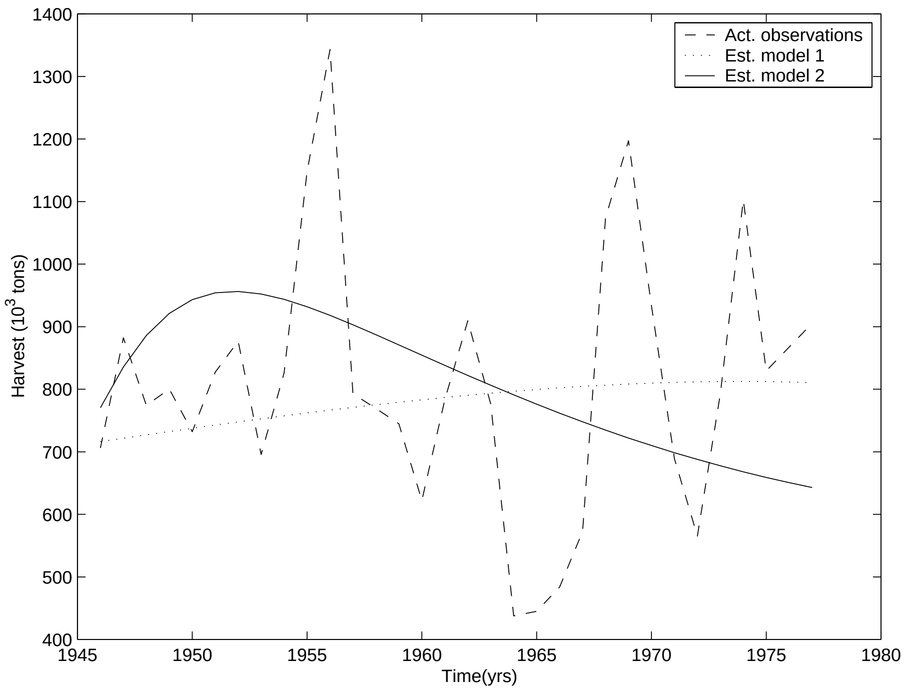

Figure 2: Graphs of the actual and the model estimated harvest for the two models

The fits are in general quite good for both models. Model 1 is more gentle overall. It gives lower estimates initially and then higher afterwards. Model 2 tries to correct for the occasional jumps in the data as shown in the figure. The models have generally performed as expected and have shown some reasonable degree of consistencies with the data. Note however that these data are highly random and may have large measurement errors.

The models we have developed measure the performance of the industry in question using the function $\phi(x, y)$. Industry equilibrium is attained when $\frac{dy}{dt} = 0$. That is, for an open access fishery, industry equilibrium is characterized by zero profits. The parameters of the ϕ function have been estimated using the adjoint method. For the NCF, it will be interesting to look at how the industry performed during the open access regime. To illustrate, we will plot the revenues and the costs versus the stock biomass for each of the two models. The revenue and cost functions are scaled by the parameter γ and the unit of currency is the Norwegian Kroner (NOK).

In figure 3 the total revenues and total costs are graphed. The difference between these represent the net profits. Costs were least when the stock size was largest but increased as the stock decreased. The profits were driven to zero when $x^* = c/p$, i.e., the industry is in a steady state. The industry equilibrium (point where total costs balance total revenues) was reached at the stock level of $x^* = 2370\ 10^3$tons which is the so called open access equilibrium. This is lower but very close to the x_{MSY}=$(K/2)$ level. A further reduction of the stock led to unprofitable investments. Costs exceeded revenues as the stock level fell beyond $x^* = c/p$.

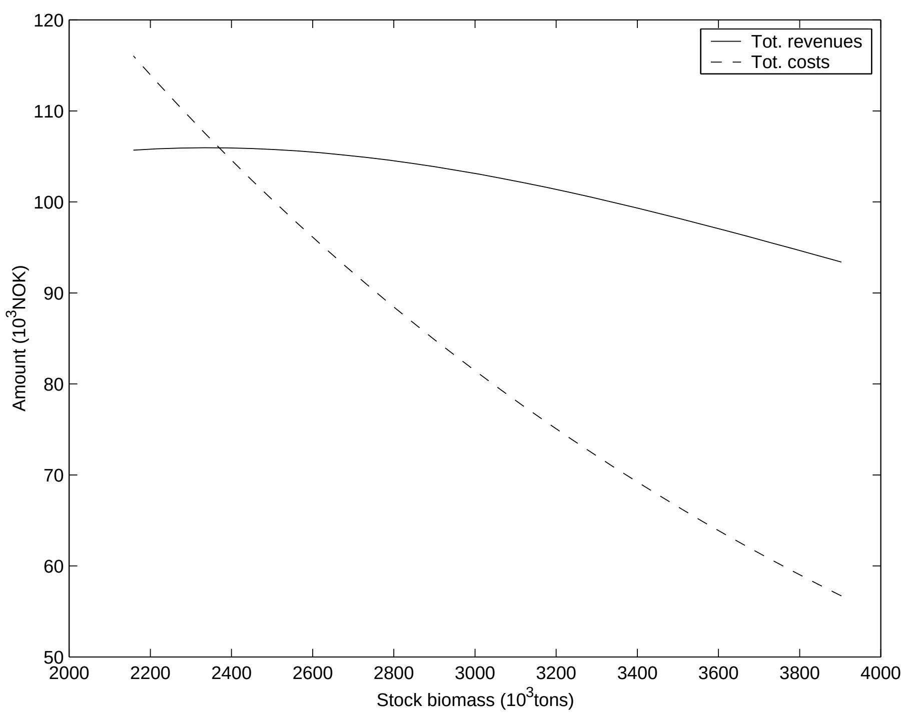

Figure 3: Graphs of the total revenues and the total costs vs. estimated stock biomass for model 1.

Figure 4 is a plot of the revenue and cost functions. The shapes of the functions indicate their level of complexities. The results of model 2 have some similar characteristics to model 1. However, the industry steady state occurred at a higher biomass level of about 3400 Kilo-tons. Extrapolation of the results of model 2 indicate another equilibrium $x^* = 2440\ 10^3$tons close to the one predicted by model 1. This point satisfies the equilibrium conditions $\dot{x} = \dot{y} = 0$. The hypothesis of a large industry whose output affects the market price resulted in a multiple industry equilibria. The first is quite unstable since only the industry reached equilibrium but not the biology. The biological and industry steady state occurred at the second point (extrapolation not shown).

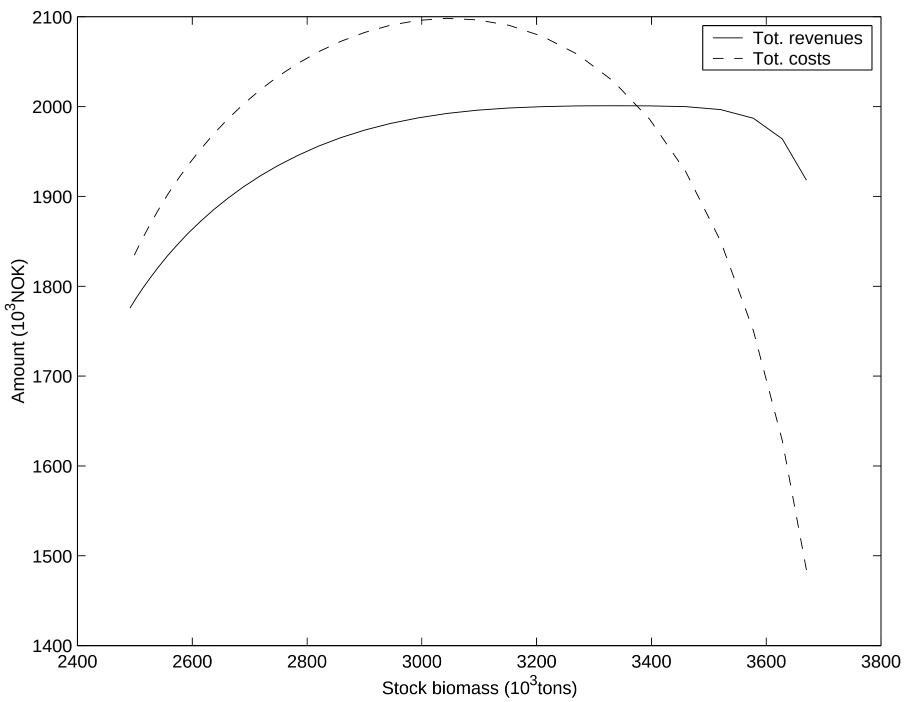

Figure 4: Graphs of the total revenues and the total costs vs. estimated stock biomass for model 2.

In both models, costs are assumed to be inversely related to the stock biomass. This underscores stock externalities in the models which appear to reasonably characterize the NCF. Note that the cod is a demersal species and does not exhibit the schooling characteristics of the species such as herring. Both models will attain bioeconomic steady state at about the same biomass level of little below the MSY biomass level. The question of which of these models is more appropriate for the NCF is still immature to give a definite answer to. More research needs to be done. What is certain is that with more realistic models and data with less errors than the one available, it is possible to operationalize modern fisheries management.

4.1 Summary and conclusion

This paper, unlike most other papers, has addressed two major questions in bioeconomic analysis and fisheries management. It developed simple dynamic fisheries models in a way that is rare in the literature and employs a new and powerful approach of efficiently combining these models with available observations collected over a given time domain. The adjoint method is used to simultaneously estimate the initial conditions and the input parameters of the industry fishing models. An interesting finding of the paper, is that, the steady state without regulation is not too far away from the MSY. Which means that, open access in this case has meant economic overfishing but not necessarily biological overfishing. It is observed that the technique used in this paper has an added virtue compared to the conventional ones used in the literature. Initial conditions of the model dynamics are estimated on equal footing as the model parameters. It is highly versatile that, it enables researchers to include as much information as is available to them. The estimates were all reasonable and as expected for the NCF. The models have quite reasonable explanatory power. However caution must be exercised when interpreting the results due to the inadequacy of the models and the large measurement errors in the data.

It has been demonstrated here that, dynamic resource models can be combined with real data in order to obtain useful insights about real fisheries. Biological parameters such as the carrying capacity and economic parameters entering the objective functions of the industry are identified. These again can be used for dynamic optimization in order to improve the economic performance of the fishery. The adjoint method has proven to be very promising and deserves further research efforts not only in resource economics but economics in general.

APPENDIX A

A.1 Data Assimilation-A Background

This section formulates the parameter estimation problem and presents the mathematical aspects of the adjoint technique. Numerical issues have also been briefly discussed.

A.1.1 The model and the data

The model dynamics are assumed to hold exactly, i.e., the dynamics are perfect. The dynamics are described by the two models above. For the sake of mathematical convenience, we use the compact notation to represent the model dynamics as

$$\frac{d\mathbf{X}}{dt} = F(\mathbf{X}, \mathbf{Q}) \tag{A.1}$$

$$\mathbf{X}(\mathbf{0}) = \mathbf{X}_0 + \hat{\mathbf{X}}_0 \tag{A.2}$$

$$\mathbf{Q} = \mathbf{Q}_0 + \hat{\mathbf{Q}} \tag{A.3}$$

where $\mathbf{X} = (x, y)$ is the state vector, $\mathbf{X}_0$ is the best guess initial condition vector, $\hat{\mathbf{X}}_0$ is the vector of initial misfits, $\mathbf{Q}$ is a vector of parameters and $\hat{\mathbf{Q}}$ is the vector of parameter misfits. The dynamics are assumed to exactly satisfy the constraints while the inputs, i.e., the initial conditions and the parameters are poorly known.

In real world situations, observations are often available for some variables such as the annual catches and fishing efforts. The set of observations are often sparse and noisy and are related to the model counterparts in some fashion. The measurement vector is defined by

$$\hat{\mathbf{X}} = \mathcal{H}[\mathbf{X}] + \epsilon \tag{A.4}$$

where $\hat{\mathbf{X}}$ is the measurement vector, ϵ is the observation error vector and $\mathcal{H}$ is a linear measurement operator. The misfits are assumed to be independent and identically distributed "iid" random deviates. To describe the errors in the initial conditions, the parameters and the data, we require some statistical hypotheses. For our purpose in this paper the following hypotheses will suffice

$$\begin{aligned} \bar{\hat{\mathbf{X}}}_0 = 0, &\qquad \overline{\hat{\mathbf{X}}_0 \hat{\mathbf{X}}_0^T} = \mathbf{W}_{X_0}^{-1} \\ \bar{\epsilon} = 0, &\qquad \overline{\epsilon \epsilon^T} = \mathbf{W}^{-1} \\ \bar{\hat{\mathbf{Q}}} = 0, &\qquad \overline{\hat{\mathbf{Q}} \hat{\mathbf{Q}}^T} = W_{\mathbf{Q}}^{-1} \end{aligned}$$

where the T denotes matrix transpose operator. That is, we are assuming that the errors are normally distributed with zero means and constant variances (homoscedastic) which are ideally the inverses of the optimal weights. For this paper, it will further be assumed that the errors are not serially correlated. This implies that the covariance matrices are now diagonal matrices with the variances along the diagonal. We further assume that the variances are constant.

A.1.2 The loss or penalty function

In adjoint parameter estimation, a loss functional which measures the difference between the data and the model equivalent of the data is minimized by tuning the control variables of the dynamical system. The goal is to find the parameters of the model that lead to model predictions that are as close as possible to the data. A typical penalty functional takes the more general form

$$\begin{aligned}\mathcal{J}[\mathbf{X},\mathbf{Q}] &= \frac{1}{2T_f}\int_0^{T_f}(\mathbf{Q}-\mathbf{Q}_0)^T\mathbf{W}_Q(\mathbf{Q}-\mathbf{Q}_0)dt \\ &+ \frac{1}{2T_f}\int_0^{T_f}(\mathbf{X}(0)-\mathbf{X}_0)^T\mathbf{W}(\mathbf{X}(0)-\mathbf{X}_0)dt \\ &+ \frac{1}{2}\int_0^{T_f}(\mathbf{X}-\hat{\mathbf{X}})^T\mathbf{W}(\mathbf{X}-\hat{\mathbf{X}})dt \end{aligned} \tag{A.5}$$

where the period of assimilation is denoted by T_f and T is the matrix transpose operator. The $\mathbf{W}'s$ are the weight matrices which are optimally the inverses of the error covariances of the observations. They are assumed to be positive definite and symmetric. The first and second terms in the penalty functional represent our prior knowledge of the parameters and the initial conditions, and ensure that the estimated values are not too far away from the first guesses. They may also enhance the curvature of the loss function by contributing positive terms to the Hessian of $\mathcal{J}$ (Smedstad and O'Brien, 1991).

The adjoint technique determines an optimal solution by minimizing the loss function $\mathcal{J}$ which measures the discrepancy between the model predictions and the observations. The loss function is minimized subject to the dynamics. The constrained inverse problem above is efficiently solved by transforming the problem into an unconstrained optimization (Luenberger, 1984). Several algorithms for solving the unconstrained nonlinear programming problem are available (Smedstad and O'Brien, 1991). Statistical methods such as the simulated annealing (Matear, 1995; Kruger, 1992) and the Markov Chain Monte Carlo (MCMC) (Harmon and Challenor, 1997) have recently been proposed as tools for parameter estimation. The most widely used methods are the classical iterative methods such as the gradient descent and the Newton's methods (see Luenberger, 1984).

A.1.3 The adjoint method

Construction of the adjoint code is identified as the most difficult aspect of the data assimilation technique (Spitz et al., 1997). One approach consists of deriving the continuous adjoint equation and then discretizing them (Smedstad and O'Brien, 1991). Another approach is to derive the adjoint code directly from the model code (Lawson et al., 1995; Spitz et al., 1997). To illustrate the mathematical derivation, we use the first approach (see details in Appendix). Formulating the Lagrange function $\mathcal{L}$ by appending the model dynamics as strong constraints, we have

$$\mathcal{L}[\mathbf{X}, \mathbf{Q}] = \mathcal{J} + \frac{1}{2}\int_0^{T_f} \mathbf{M}\frac{dF}{d\mathbf{X}}dt \tag{A.6}$$

where $\mathbf{M}$ is a vector of Lagrange multipliers which are computed in determining the best fit. The original constrained problem is thus reformulated as an unconstrained problem. At the unconstrained minimum the first order conditions are

$$\frac{d\mathcal{L}}{d\mathbf{X}} = 0 \tag{A.7}$$

$$\frac{d\mathcal{L}}{d\mathbf{M}} = 0 \tag{A.8}$$

$$\frac{d\mathcal{L}}{d\mathbf{Q}} = 0. \tag{A.9}$$

It is observed that equation (A.7) results in the adjoint or backward model, equation (A.8) recovers the model equations while (A.9) gives the gradients with respect to the control variables. Using calculus of variations or optimal control theory, the adjoint equation is derived by forming the Lagrange functional via the undetermined multipliers $\mathbf{M}(t)$. The Lagrange function is

$$\mathcal{L} \;=\; \mathcal{J} + \int_0^{T_f} \mathbf{M}(\frac{\partial \mathbf{X}}{\partial t} - F(\mathbf{X}, \mathbf{Q}))\mathbf{dt} \tag{A.10}$$

Perturbing the function $\mathcal{L}$

$$\begin{aligned}\mathcal{L}[\mathbf{X} + \delta\mathbf{X}, \mathbf{Q}] \;&=\; \mathcal{J}[\mathbf{X} + \delta\mathbf{X}, \mathbf{Q}] \\ &+\; \frac{1}{2}\int_0^{T_f} \mathbf{M}(\frac{\partial(\mathbf{X} + \delta\mathbf{X})}{\partial t} - F(\mathbf{X} + \delta\mathbf{X}, \mathbf{Q}))\mathbf{dt}\end{aligned}$$

which implies

$$\begin{aligned}\mathcal{L}[\mathbf{X} + \delta\mathbf{X}, \mathbf{Q}] \;&=\; \mathcal{J} + \Delta_{\mathbf{X}}\mathcal{J}\delta\mathbf{X}^T + \int_0^{T_f} \mathbf{M}(\frac{\partial \mathbf{X}}{\partial t} - F(\mathbf{X}, \mathbf{Q}))\mathbf{dt} \\ &-\; 2\int_0^{T_f} \mathbf{M}(\frac{\partial \delta\mathbf{X}}{\partial t} - \frac{\partial F}{\partial \mathbf{X}}\delta\mathbf{X}^T)dt + O(\delta\mathbf{X}^2)\end{aligned} \tag{A.11}$$

Taking the difference ($\mathcal{L}[\mathbf{X}+\delta\mathbf{X},\mathbf{Q}]-\mathcal{L}[\mathbf{X},\mathbf{Q}]$)

$$\begin{aligned}\delta\mathcal{L} &= \Delta_{\mathbf{X}}\mathcal{J}\delta\mathbf{X}^T \\ &- 2\int_0^{T_f}\mathbf{M}(\frac{\partial\delta\mathbf{X}}{\partial t}-\frac{\partial F}{\partial\mathbf{X}}\delta\mathbf{X}^T)dt+O(\delta\mathbf{X}^2)\end{aligned} \tag{A.12}$$

Requiring that $\delta\mathcal{L}$ be of order $O(\delta\mathbf{X}^2)$ implies

$$\Delta_{\mathbf{X}}\mathcal{J}\delta\mathbf{X}^T-\int_0^{T_f}\mathbf{M}(\frac{\partial\delta\mathbf{X}}{\partial t}-\frac{\partial F}{\partial\mathbf{X}}\delta\mathbf{X}^T)dt=0 \tag{A.13}$$

By integrating the second term of the LHS by parts and rearranging, we have

$$\begin{aligned}\frac{\partial\mathbf{M}}{\partial t}+[\frac{\partial F}{\partial\mathbf{X}}]^T\mathbf{M} &= \mathbf{W}(\mathbf{X}-\hat{\mathbf{X}}) \\ \mathbf{M}(T_f) &= \mathbf{0}\end{aligned} \tag{A.14}$$

which is the adjoint equation together with the boundary conditions and from (A.8) the gradient relation is

$$\Delta_Q\mathcal{J}=-\int_0^{T_f}\mathbf{M}\frac{dF}{d\mathbf{Q}}dt+\mathbf{W}_Q(\mathbf{Q}-\mathbf{Q}_0) \tag{A.15}$$

The term on the RHS of (A.14) is the weighted misfit which acts as forcing term for the adjoint equation. It is worth noting here that we have implicitly assumed that data is continuously available throughout the integration interval. Equations (A.7) and (A.8) above constitute the Euler-Lagrange (E-L) system and form a two-point boundary value problem. The implementation of the adjoint technique on a computer is straightforward. The algorithm is outlined below.

- Choose the first guess for the control parameters.

- Integrate the forward model over the assimilation interval.
- Calculate the misfits and hence the loss function.
- Integrate the adjoint equation backward in time forced by the data misfits.
- Calculate the gradient of $\mathcal{L}$ 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 loss function move towards a minimum.
- Check if the solution is found based on a certain criterion.
- If the criterion is not met repeat the procedure until a satisfactory solution is found.

The optimization step is performed using standard optimization procedures. In this paper, a limited memory quasi-Newton procedure (Gilbert and Lemarechal, 1991) is used. The success of the optimization depends crucially on the accuracy of the computed gradients. Any errors introduced while calculating the gradients can be detrimental and the results misleading. To avoid this incidence from occurring, it is always advisable to verify the correctness of the gradients (see, Smedstad and O'Brien, 1991; Spitz et al., 1997).

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