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Reducing the model-data misfit in a marine ecosystem model using periodic parameters and Linear Quadratic Optimal Control

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Abstract

This paper presents the application of the *Linear Quadratic Optimal Control (LQOC)* method for a parameter optimization problem in a marine ecosystem model. The ecosystem model simulates the distribution of nitrogen, phytoplankton, zooplankton and detritus in a water column with temperature and turbulent diffusivity profiles taken from a three-dimensional ocean circulation model. We present the linearization method which is based on the available observations. The linearization is necessary to apply the LQOC method on the nonlinear system of state equations. We show the form of the linearized time-variant problems and the resulting two algebraic Riccati Equations. By using the LQOC method, we are able to introduce temporally varying periodic model parameters and to significantly improve – compared to the use of constant parameters – the fit of the model output to given observational data.

1 Introduction

Marine ecosystem models describe biogeochemical processes in the ocean and are used, e.g. for calculating the effect of marine photosynthesis on the global carbon cycle. Typically, such kind of models have several parameters, for example growth and mortality rates for the different species taken into account. Since most of these parameters are not known exactly and difficult to measure, parameter identification or estimation is an important tool to calibrate a model and thereby improve its quality to the extent that reasons other than inappropriate parameter values must be responsible for remaining model deficiencies, see for example Fasham and Evans (1995); Hurtt and Armstromg (1996); Fennel et al. (2001); Prunet et al. (1996). Parameter identification means to perform an optimization in order to minimize the misfit between model output and given data, commonly represented by a least-squares type cost functional. Additionally, uncertainty estimates corresponding to data errors may be computed. The computational effort to perform such kind of optimization runs for the three-dimensional

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coupled system of ocean circulation and marine biogeochemistry is quite high. Thus several simplifications may be used: One of them is to compute the marine biogeochemistry in a so-called *offline mode*, i.e. to solve the transport equations for the tracers with precomputed ocean circulation fields (velocity, temperature, salinity) as forcing or input. The other one is to use models for a single water column only. This simplification is motivated by the fact that most of the ecosystem processes (as for example growth and dying) are happening locally in space and that the main spatial interactions are vertical mixing and sinking of organic matter. Nevertheless, it has been shown that the locally optimized parameters can also be beneficial when used in three-dimensional computations, see Oschlies and Schartau (2005). The work presented in this paper is motivated by results obtained for a typical marine ecosystem model, namely the NPZD model introduced in Oschlies and Garçon (1999). As was reported in several publications with different optimization algorithms, the quality of the model fit to observations was not optimal, and in some cases it was difficult to identify the parameters uniquely, see for example Ward (2009); Ward et al. (2010); Rückelt et al. (2010). In most cases (and in all these studies), the parameters of the marine ecosystem models are assumed to be temporally constant. This reflects the aim to obtain a model that is applicable for arbitrary time intervals. In contrast, in our work we allowed the parameters to vary temporally over the year while remaining periodic over all years of the considered time interval. Our main research question was if such kind of relaxation is able to significantly improve the model-to-data fit. Eknes and Evensen (2002) and Schartau et al. (2001) have examined the possibility of using a sequential data assimilation method for state estimation in a biological model. On the other hand, there are several papers on parameter estimation only, see Schartau et al. (2001); Fasham and Evans (1995); Hurtt and Armstromg (1996); Fennel et al. (2001); Prunet et al. (1996); Matear (1995); Spitz et al. (1998). Work by Losa et al. (2003) combined state and parameter estimation using a sequential weak constraint parameter estimation in an ecosystem model. A good example for time-dependent parameters is introduced in the work by Mattern (2012), they used a statistical emulator technique to estimate time-dependent values

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for two parameters of a 3-dimensional biological ocean model. They demonstrated that emulator techniques are valuable tools for data assimilation and for analyzing and improving biological ocean models. They also allowed for temporally changing parameters in their optimization, but without imposing annual periodicity. We here use the additional annual periodicity constraint on the parameters, which is motivated by the goal to allow for some temporal flexibility of the parameters and at the same time to retain the temporal universality of the optimized model, i.e. allowing for straightforward application to time periods outside the range of observations. Seasonally varying parameters may be interpreted in terms of not properly accounted seasonal processes and may, eventually, lead to improved model parameterizations that can model these variations even with constant model parameters. To achieve these goals, we apply the method of *Linear Quadratic Optimal Control (LQOC)* to the NPZD model. Therein, we allow the parameters to be time-dependent, apply a well-established method for optimal control, and additionally impose the constraint of annual periodicity. This avoids the process of parametrization in the sense that we do not have to know or assume how the above mentioned periodic functions look like. In contrast, the method itself will generate an optimal periodic function for each parameter. Moreover, it allows to balance the two aims that we have: by introducing weight matrices we can choose if it is more important to obtain a very good fit or nearly perfect periodicity. The method requires a reference trajectory at the locations of the data and a reference control, i.e. a reference vector of model parameters. The former can be taken from the measured data, and for the latter we use an initial guess for the parameters which can be the output of an optimization with constant parameters.

The structure of the paper is as follows: in the next section we briefly describe the model, the data used and the cost function to be optimized. In Sect. 3, we present the parameter optimization problem and describe the important parts of the used LQOC method. The application of the LQOC method on the NPZD model is presented in Sect. 3.1. Afterwards, we present our results with respect to the quality of the fit and the periodicity of the parameters and end the paper with some conclusions.

2 Model equation and optimization problem

Marine ecosystem models are coupled systems of partial differential equations (PDEs) consisting of time-dependent advection-diffusion-reaction equations with nonlinear coupling terms. The turbulent diffusivity, temperature and salinity fields are either computed simultaneously or in advance by a physical ocean model. Clearly, the second variant (where the physical ocean model output is used as prescribed forcing for the ecosystem model) that is used in this paper is computationally cheaper but neglects the biology's feedback effects via impacts on the absorption of solar radiation, generally assumed to be small relative to uncertainties in the boundary conditions such as surface heat fluxes, see Oschlies (2004).

2.1 The NPZD model

The model that we use as an example to apply the LQOC method here simulates the interaction of dissolved inorganic nitrogen N, phytoplankton P, zooplankton Z and detritus D. It was developed with the aim of simulating the seasonal cycle of upper-ocean biogeochemical processes in a basin-scale model of the North Atlantic, see Oschlies and Garçon (1999). The dependencies between the four model variables are schematically depicted in Fig. 1. The model uses the ocean circulation and temperature field in an off-line modus, i.e. these are used only as forcing, but no feedback on them is modeled. The model simulates one water column at a given horizontal position, which is motivated by the fact that there have been special time series studies at fixed locations, one of which was used here. In the model, the concentrations (in $\mathrm{mmol\,N\,m^{-3}}$) of N, P, Z, and D are denoted by $\boldsymbol{x} = (x^l)_{l=1,2,3,4}$ are described by the following PDE system:

$$\frac{\partial x^l}{\partial t} = -w^l \frac{\partial x^l}{\partial z} + \frac{\partial}{\partial z}\left(\kappa_\rho \frac{\partial x^l}{\partial z}\right) + q^l(\boldsymbol{x},\boldsymbol{u}), \quad l = 1,2,3,4. \tag{1}$$

$x^l : [0,T] \times [-H,0] \to \mathbb{R}.$

Here z denotes the vertical spatial coordinate, H the depth in the water column, $\boldsymbol{q}^l$

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represents the biogeochemical coupling terms for the four species and $\boldsymbol{u}$ the model parameter. We omitted any additional arguments of the $\boldsymbol{q}_n$ for simplicity. The output taken from the physical ocean model are hourly profiles of the turbulent mixing coefficients κ_ρ and temperature, the latter needed in the biological process parameterizations below. The vertical sinking velocity w^l is a parameter of the biological model that is nonzero only for D, i.e. $w^1 = w^2 = w^3 = 0, w^4 = w_\mathrm{s} > 0$. The biogeochemical coupling (or source-minus-sink) terms $q^l, l = 1,2,3,4$, are given by (see Oschlies and Garçon, 1999):

$$
\begin{aligned}
&\text{for N}: \quad q^1(\boldsymbol{x}) = -\bar{J}(z,t,\mathrm{N})\mathrm{P} + \gamma_2 Z + \mu_\mathrm{D}\mathrm{D},\\
&\text{for P}: \quad q^2(\boldsymbol{x}) = \bar{J}(z,t,\mathrm{N})\mathrm{P} - \mu_p\mathrm{P} - G(\epsilon,g)\mathrm{Z},\\
&\text{for Z}: \quad q^3(\boldsymbol{x}) = \gamma_1 G(\epsilon,g)\mathrm{Z} - \gamma_2\mathrm{Z} - \mu_\mathrm{Z}\mathrm{Z}^2,\\
&\text{for D}: \quad q^4(\boldsymbol{x}) = (1-\gamma_1)G(\epsilon,g)\mathrm{Z} + \mu_\mathrm{Z}\mathrm{Z}^2 + \mu_\mathrm{P}\mathrm{P} - \mu_\mathrm{D}\mathrm{D} - w_\mathrm{s}\tfrac{\partial \mathrm{D}}{\partial z},
\end{aligned}
\tag{2}
$$

where $\bar{J}$ is the daily averaged phytoplankton growth rate as a function of depth z and time t defined in Oschlies and Garçon (1999), and G is the grazing function:

$$
\bar{J}(z,t,\mathrm{N}) = \min\left(\bar{J}(z,t), J_{\max}\tfrac{\mathrm{N}}{K_\mathrm{N}+\mathrm{N}}\right), \qquad G(\epsilon,g) = \frac{g\epsilon \mathrm{P}^2}{g+\epsilon\mathrm{P}^2}.
$$

Table 1 lists the model parameters with their original symbols as in Oschlies and Garçon (1999) which are here summarized in the vector $\boldsymbol{u}$. For more details see Oschlies and Garçon (1999); Schartau and Oschlies (2003a).

2.2 Measurement data and corresponding model output

The observational data used here, denoted by $\boldsymbol{y}^{\mathrm{obs}}$, is taken from the *Bermuda Atlantic Time-series Study* (called BATS; 31° N 64° W). There are five types of measurement data $\boldsymbol{y}^{\mathrm{obs}} = (y_m^{\mathrm{obs}})_{m=1,\dots,5}$, which correspond to aggregated values $\boldsymbol{y}^{\mathrm{mod}} := (y_m^{\mathrm{mod}})_{m=1,\dots,5}$ of the model output. The used data and their corresponding model variables are:

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1. Dissolved inorganic nitrogen (y_1^{obs} = DIN, in mmol m^{-3}), corresponding to variable $y_1^{mod} = x^1$ in the model.
2. Chlorophyll *a* (y_2^{obs} = Chl *a*, in mg m^{-3}) that, with an additional scaling $y_2^{mod} = x^2/1.59$ converts simulated phytoplankton biomass (in mmol N m^{-3}) to chlorophyll (in mg m^{-3}).
3. Vertically integrated mesozooplankton biomass (y_3^{obs} = ZOO, in mmol m^{-2}) that with an additional assumption about the relation of mesozooplankton biomass to total zooplankton biomass according to the formula

   $$\mathrm{ZOO_{total}} \mapsto 1.2344 \cdot \mathrm{ZOO_{meso}} + 0.096504$$

   see also Ward (2009), yields

   $$y_3^{mod} = \int \frac{x^3 - 0.096504}{1.2344}\, dz$$

   with units given in mmol N m^{-3}.
4. Particulate organic nitrogen (y_4^{obs} = PON, in mmol N m^{-3}), corresponding to $y_4^{mod} = \mathrm{P} + \mathrm{Z} + \mathrm{D} = \sum_{l=2}^{4} x^l$.
5. Carbon fixation or primary production as carbon uptake (y_5^{obs}, here abbreviated as PP, in mmol C m^{-3} d^{-1}). As modeled primary production, the temporal mean of the model output P multiplied by the phytoplankton growth rate $J(\mu, u)$P (that itself depends on nutrients and light), over 24 h is taken.

Except for zooplankton, only data in the euphoric zone, i.e. the upper model layers, are considered. If data are not given exactly at the grid points, an additional interpolation has to be performed. For simplicity of notation we will assume that this is already incorporated in the aggregated variables y_m^{mod}, $m = 1, \ldots, 5$.

2.3 The optimization problem

The aim of the optimization is to fit the model output $\boldsymbol{y}^{\text{mod}}$ that was aggregated in the above mentioned way to the given observational data $\boldsymbol{y}^{\text{obs}}$ over a chosen time interval of $j_{\max}$ years. We denote by N_{mj} the number of measurements for y_m^{obs} in year $j \in \{1,\dots,j_{\max}\}$. Note that these numbers may be quite different for the different years j. The i-th measurement in year j of y_l^{obs} is denoted by y_{lji}^{obs}, and the corresponding aggregated model output value by y_{lji}^{mod}. We now firstly compute the annual misfit per model output/ tracer, weighted using the vector

$$\sigma = (\sigma_m)_{m=1,\dots,5} = (0.1, 0.01, 0.01, 0.0357, 0.025) \tag{3}$$

of measurement uncertainties, and by the number N_{mj} of measurements per tracer and year, i.e.

$$F_{mj} := \sum_{i=1}^{N_{mj}} \frac{(y_{mji}^{\text{mod}} - y_{mji}^{\text{obs}})^2}{\sigma_m^2 N_{mj}}, \quad m = 1,\dots,5, j = 1,\dots,j_{\max}. \tag{4}$$

If there are no measurements for a state variable/tracer in a year (i.e. $N_{mj} = 0$), the sum is empty. The overall cost function is then calculated as

$$F = \frac{1}{N_{\text{total}}} \sum_{j=1}^{j_{\max}} \sum_{m=1}^{5} F_{mj}, \tag{5}$$

where N_{total} is the total numbers of non-zero terms F_{mj} actually occurring in the sum. In the usual case we have $N_{\text{total}} = 5 j_{\max}$. If ever $N_{mj} = 0$ and thus $F_{mj} = 0$ for a year and tracer, N_{total} is decreased accordingly.

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3 Finite-Dimensional Linear-Quadratic Optimal Control

Linear-Quadratic Optimal Control (LQOC) is a mathematical technique to compute optimal controls in linear dynamical systems. Usually also the control variables or parameters are time-dependent. The method is widely used in engineering applications and well-studied from the mathematical side, see e.g. Anderson and Moore (1971); Casti (1987); Lunze (1997); Sima (1996). Extensions to non-linear problems are possible, in the first place by linearizing the dynamical system of equations, see Clemens (1993). The main idea of the work presented in this paper is to use this method to introduce time-dependent parameters in marine ecosystem models. Our aim is to allow only for *annual periodicity* of the model parameters that should be optimized to fit the measurement data. We are *not* interested in parameters that vary completely in time over the whole time interval that is taken into account in the cost functional (usually several years), since this would lead to parameters that are very specific for the used time interval. They would lose their generality and their usability for other time periods. Our aim by introducing periodic parameters is to get a rather general extension of the model, such that it can be used for a wide range of scenarios. We moreover want to find out what parameters are sensitive to a variability in time at all, i.e. for which this gives a better fit and – on the other hand – which parameters can be set constant in time without losing any model quality. To enforce periodicity of the model parameters (i.e. the controls in the LQOC setting), we impose appropriate constraints on them. Weighting matrices allow to steer the parameter optimization process such that a balance between

- optimal data fit
- and exactness of periodicity of the parameters/controls

is possible.

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3.1 Application to the NPZD model

In this section we apply the LQOC method to the discretized version of the NPZD model. We present the details of the linearization and enforcement of the periodicity of the parameters/ controls. The NPZD model is forced by output from the OCCAM global circulation model, namely the hourly vertical profiles of temperature T and vertical diffusivity κ_ρ. The vertical grid consists of 66 layers with thickness increasing with depth. The model described by PDE system (1) is solved using an operator splitting method: Given a time-step τ, the discretized scheme reads:

$$\underbrace{\left[I - \tau \mathbf{L}_n^{\mathrm{diff}}\right]}_{:=\mathbf{D}_n} \boldsymbol{x}_{n+1} = \underbrace{\left[I + \tau \mathbf{L}_n^{\mathrm{sink}}\right]}_{:=\mathbf{S}_n} \mathcal{B}_n^q \circ \mathcal{B}_n^q \circ \mathcal{B}_n^q \circ \mathcal{B}_n^q (\boldsymbol{x}_n, \boldsymbol{u}_n),$$

$$n = 1, \ldots, M. \tag{6}$$

Here $\mathbf{D}_n$ and $\mathbf{S}_n$ are the diffusion and sinking matrices, respectively. The time-step τ used in the model is one hour. Note that as in Eq. (1) the state $\boldsymbol{x}_n$ contains all four tracers of the model, i.e. $\boldsymbol{x}_n = (x_n^1, x_n^2, x_n^3, x_n^4)^\top$ and $\boldsymbol{u}_n$ is the control (here the model parameter) vector. In the operator splitting sheme, at first, the nonlinear coupling operators $q_n = (q_n^1, q_n^2, q_n^3, q_n^4)^\top$ are computed at every spatial grid point and integrated by four explicit Euler steps with stepsize $\frac{\tau}{4}$, each of which is described by the operator:

$$\mathcal{B}_n^q(\boldsymbol{x}_n, \boldsymbol{u}_n) := \left[I + \frac{\tau}{4} q_n(\boldsymbol{x}_n, \boldsymbol{u}_n)\right]. \tag{7}$$

Then, an explicit Euler step with full step-size τ is formed for the sinking term, which is spatially discretized by an upstream scheme. This step is summarized in the matrix $\mathbf{L}_n^{\mathrm{sink}}$. This matrix does only depend on the time step n if the sinking velocity w_s is to be optimized. Finally, an implicit Euler step is applied for the diffusion operator, discretized with second order central differences. The resulting matrix $\mathbf{D}_n$ depends on time step n. It is tridiagonal, and the system is solved directly. Note that $\mathbf{D}_n^{\mathrm{diff}}$, $\mathbf{L}_n^{\mathrm{sink}}$ are 4×4 block-diagonal matrices.

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The discrete system can now be written as

$$\begin{aligned} \boldsymbol{x}_{n+1} &= \mathbf{D}_n^{-1}\mathbf{S}_n\mathcal{B}_n^q \circ \mathcal{B}_n^q \circ \mathcal{B}_n^q \circ \mathcal{B}_n^q(\boldsymbol{x}_n, \boldsymbol{u}_n), \\ &=: f(\boldsymbol{x}_n, \boldsymbol{u}_n), \quad n = 1, ..., M-1, \end{aligned} \tag{8}$$

where f is a nonlinear function.

3.2 Linearization

In order to apply the LQOC method to the nonlinear system (8), we can use the linearization method to cope with this nonlinear problem. The linearization is performed around reference trajectories of state $\boldsymbol{x}$ and control $\boldsymbol{u}$. Before discussing a detailed linearization, we will first explain how the approach will be utilized. The idea behind is to apply the LQOC method on the time intervals (called horizon) between two successive observational data separately. Here we only use time instances where observations $(y_m^{\text{obs}})_{m=1,2,3,4}$ are available. From these, reference values for the tracers $(x^l)_{l=1,2,3,4}$ can be obtained. We use the notations:

- N_j is the number of observational data in year $j \in \{1, ..., j_{\max}\}$ obtained in this way,
- $n_{j,i}$ is the time step of the i-th observational data in year j,
- $n_{j,0}$ is the first and n_{j,N_j+1} the last time step in year j.
- $I_{j,i} := [n_{j,i}, n_{j,i+1}], j = 1, \ldots, j_{\max}, i = 0, \ldots, N_j$ is the time horizon on which the same observational data are used.

The linearization is performed around the observational data $(\boldsymbol{x}_{j,i}^{\text{ref}}), j = 1, \ldots, j_{\max}$ and $i = 0, \ldots, N_j$, and a reference parameter trajectory $(\boldsymbol{u}_n^{\text{ref}})_{n=1,\ldots,M}$. The choice of the reference parameter trajectory is described in the Sect. 3.3.

For the first interval $I_{1,0}$, we linearize the model around the first observational data $(\boldsymbol{x}_{1,1}^{\text{ref}})$ and the parameter $(\boldsymbol{u}_n^{\text{ref}})_{n \in I_{1,0}}$. The linearized state equation now reads

$$z_{n+1} = \mathbf{A}_n z_n + \mathbf{B}_n \boldsymbol{v}_n + \boldsymbol{b}_n, \qquad n \in I_{1,0} \tag{9}$$

where

$$
\begin{aligned}
\mathbf{A}_n &= \frac{\partial f}{\partial \boldsymbol{x}}(\boldsymbol{x}_{1,1}^{\mathrm{ref}}, \boldsymbol{u}_n^{\mathrm{ref}}),\\
\mathbf{B}_n &= \frac{\partial f}{\partial \boldsymbol{u}}(\boldsymbol{x}_{1,1}^{\mathrm{ref}}, \boldsymbol{u}_n^{\mathrm{ref}}),\\
\boldsymbol{b}_n &= f(\boldsymbol{x}_{1,1}^{\mathrm{ref}}, \boldsymbol{u}_n^{\mathrm{ref}}) - \boldsymbol{x}_{1,1}^{\mathrm{ref}},\\
\boldsymbol{z}_n &= \boldsymbol{x}_n - \boldsymbol{x}_{1,1}^{\mathrm{ref}}, \quad \boldsymbol{v}_n = \boldsymbol{u}_n - \boldsymbol{u}_n^{\mathrm{ref}}, \quad n \in I_{1,0}.
\end{aligned}
$$

Analogously, we obtain for the second time horizon $I_{1,1}$ by linearization around $(\boldsymbol{x}_{1,2}^{\mathrm{ref}})$ and $(\boldsymbol{u}_n^{\mathrm{ref}})_{n \in I_{1,1}}$:

$$\boldsymbol{z}_{n+1} = \mathbf{A}_n \boldsymbol{z}_n + \mathbf{B}_n \boldsymbol{v}_n + \mathbf{B}_n, \qquad n \in I_{1,1}.$$

At the end we have with $\boldsymbol{z} = (\boldsymbol{z}_n)_{n=1,\ldots,M}$ for all years:

$$\left.\begin{aligned} \boldsymbol{z}_{n+1} &= \mathbf{A}_n \boldsymbol{z}_n + \mathbf{B}_n \boldsymbol{v}_n + \boldsymbol{b}_n, \quad n = 1, \ldots, M \\ &\boldsymbol{z}_1 \text{ (the given initial value).} \end{aligned}\right\} \tag{10}$$

3.3 Choice of the reference parameter trajectory

A main objective of this work is to enforce periodicity of the parameters/controls. We denote the length of a time period – which in our case is one year – measured in time steps by T. We now chose the reference trajectory for the control to be

$$\boldsymbol{u}_n^{\mathrm{ref}} := \begin{cases} \boldsymbol{u}_0, & \text{if } n \le T \\ \boldsymbol{u}_{n-T}, & \text{if } n > T. \end{cases} \tag{11}$$

Here $\boldsymbol{u}_0 \in \mathbb{R}^m$ is an initial guess for the parameters. In our case we took the values from Oschlies and Garçon (1999), compare Table 1. Note that we use these values during the whole first year ($n \le T$).

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As a result, choosing the $R_n \in \mathbb{R}^{p \times p}$ as positive definite matrices and minimizing the quadratic term

$$\boldsymbol{v}_n^{\mathrm{T}} \mathbf{R}_n \boldsymbol{v}_n$$

in Eq. (12) will enforce periodicity of $\boldsymbol{u}_n$ for $n \geq T$. The matrices $\mathbf{R}_n$ can be adapted to weaken or strengthen this enforcement, specifically they can be used to weaken it in the first steps $n \leq T$ where it is not intended to enforce periodicity to the constant reference parameters $\boldsymbol{u}_0$.

3.4 Application of the LQOC theory

We use a discrete *Linear-Quadratic Optimal Control*, i.e. we assume that the dynamical system is already discretized in time, namely at discrete times $t_n, n = 1, \ldots, M$. In the context of the LQOC for discrete linear systems one usually considers a discrete-time system of the form (10), where in every time step n

- $\boldsymbol{z}_n = \boldsymbol{z}(t_n) \in \mathbb{R}^k$ is the state vector (here the model output),
- $\boldsymbol{v}_n = \boldsymbol{v}(t_n) \in \mathbb{R}^p$ is the control (here the model parameter) vector, with the parameter vector from the model (2),
- the matrices $\mathbf{A}_n \in \mathbb{R}^{k \times k}$ and $\mathbf{B}_n \in \mathbb{R}^{k \times p}$ are the system matrix and the input matrix, respectively.

We will use the notations

$$\boldsymbol{z} = (\boldsymbol{z}_n)_{n=1,\ldots,M} \in \mathbb{R}^{M \times k} \cong \mathbb{R}^{Mk},$$

$$\boldsymbol{v} = (\boldsymbol{v}_n)_{n=1,\ldots,M-1} \in \mathbb{R}^{(M-1) \times p} \cong \mathbb{R}^{(M-1)p}$$

for the whole discrete trajectories of state and control vector, respectively. The theory of linear quadratic optimal control gives a formula for the optimal parameter/control

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trajectory $\boldsymbol{u}$ that minimizes the cost function

$$J(\boldsymbol{v}) = \frac{1}{2} z_M^\top \mathbf{Q}_M z_M + \frac{1}{2} \sum_{n=1}^{M-1} z_n^\top \mathbf{Q}_n z_n + \boldsymbol{v}_n^\top \mathbf{R}_n \boldsymbol{v}_n \tag{12}$$

under the constraint Eq. (10). Here for every n

- $\mathbf{Q}_n \in \mathbb{R}^{k\times k}$ is a positive semi-definite diagonal weighting matrix for the state vector,
- $\mathbf{R}_n \in \mathbb{R}^{p\times p}$ is a positive definite diagonal weighting matrix for the control vector.

This formula is given in the following theorem, see e.g. Anderson and Moore (1971); Rugh (1996).

Theorem 1 *If the $\mathbf{Q}_n, n = 1, \ldots, M$, are positive semi-definite and the $\mathbf{R}_n, n = 1, \ldots, M-1$, are positive definite, then there exists a unique solution of the linear quadratic optimal control problem (10), (12). The optimal control is given by the feedback law,*

$$\boldsymbol{u}_n = \begin{cases} \boldsymbol{u}_0 + \mathbf{K}_n z_n + \mathbf{S}_n, & \text{if } n \le T, \\ \boldsymbol{u}_{n-T} + \mathbf{K}_n z_n + \mathbf{S}_n, & \text{if } n > T, \end{cases}$$

where $\mathbf{K}_n$ and $\mathbf{S}_n$ are given by

$$\mathbf{K}_n = -(\mathbf{R}_n + \mathbf{B}_n^\top \mathbf{P}_{n+1} \mathbf{B}_n)^{-1} \mathbf{B}_n^\top \mathbf{P}_{n+1} \mathbf{A}_n, \quad n = 1, \ldots, M-1,$$
$$\mathbf{S}_n = -(\mathbf{R}_n + \mathbf{B}_n^\top \mathbf{P}_{n+1} \mathbf{B}_n)^{-1} \mathbf{B}_n^\top (\mathbf{P}_{n+1} \boldsymbol{b}_n + \boldsymbol{h}_{n+1}), \quad n = 1, \ldots, M-1,$$

and $\mathbf{P}_n$ can be given by

$$\mathbf{P}_M = \mathbf{Q}_M,$$
$$\mathbf{P}_n = \mathbf{Q}_n + \mathbf{A}_n^\top \mathbf{P}_{n+1} \mathbf{A}_n - \mathbf{A}_n^\top \mathbf{P}_{n+1} \mathbf{B}_n (\mathbf{R}_n + \mathbf{B}_n^\top \mathbf{P}_{n+1} \mathbf{B}_n)^{-1} \mathbf{A}_n \mathbf{B}_n^\top \mathbf{A}_n, \quad n = M-1, \ldots, 1,$$

and an additional difference equation for the $\boldsymbol{h}_n$, namely

$$\boldsymbol{h}_M = 0,$$
$$\boldsymbol{h}_n = \mathbf{A}_n^\top (\mathbf{P}_{n+1} \boldsymbol{b}_n + \boldsymbol{h}_{n+1}) - \mathbf{A}_n^\top \mathbf{P}_{n+1} \mathbf{B}_n (\mathbf{R}_n + \mathbf{B}_n^\top \mathbf{P}_{n+1} \mathbf{B}_n)^{-1} \mathbf{B}_n^\top (\mathbf{P}_{n+1} \boldsymbol{b}_n + \boldsymbol{h}_{n+1}), \quad n = M-1, \ldots, 1.$$

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Remark:
During the first time period from 1 to T we have linearized the Eq. (8) around the constant parameter $\boldsymbol{u}_0$. It follows that $\mathbf{A}_n$, $\mathbf{B}_n$, Bb_n are constant over all horizon $I_{1,i}$, for $i = 0, \ldots, N_1$.

3.5 Particular choice of $\mathbf{Q}_n, \mathbf{R}_n$

The weighting matrices $\mathbf{Q}_n$ are taken as constant for all n, namely

$$\mathbf{Q}_n = \mathbf{Q} = \operatorname{diag}\left(\frac{1}{\sigma_l^2}\right)_{l=1,\ldots,5}, \quad n = 1, \ldots, M-1$$

where σ_l are the variances that taken from the original cost function (5). The matrices $\mathbf{R}_n$ are taken as

$$\mathbf{R}_n = \operatorname{diag}(r_i^n)_{i=1,\ldots,p}.$$

They are chosen differently in the first year (on one hand) and in all subsequent years (on the other hand). In all years except the first one (i.e. $n \geq T$), the $\mathbf{R}_n$ are used to enforce periodicity of the parameters. The bigger the r_i^n for these years are, the more perfect periodicity of the parameters is expected. Following this idea, the desired choice for the $\mathbf{R}_n$ in the first year would be just the zero matrices. But by this choice the assumptions of Theorem 1 are not satisfied and the feedback law is not valid. As a consequence, it is desirable to chose the r_i^n for the first year as small as possible. Moreover, the choice of the r_i^n in the first year can be used to keep the parameters in the admissible bounds. For our computations, we thus chose

$$r_i^n = \begin{cases} \dfrac{1}{|(u_{0,i})|^2}, & i = 1, \ldots, p, n = 1, \ldots, T \\ \dfrac{1}{|(u_{n-T,i})|^2}, & i = 1, \ldots, p, n = T+1, \ldots, M, \end{cases} \tag{13}$$

where $\boldsymbol{u}_0$ are the values as listed in Table 1.

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4 Optimization results

In this section we present the results of the parameter optimization performed with the LQOC method described in the last two sections. We show both the obtained fit of the optimized model to the data and the annual periodicity of the parameters.

4.1 Fit of model output to observational data

This section shows a comparison between the optimized model output obtained by the LQOC method with periodic parameters and the observational data. As a reference we also compare the results to those obtained by a direct optimization of the nonlinear model using *constant parameters* with a *Sequential Quadratic Programming (SQP)* method that takes into account parameter bounds. This method was used in Rückelt et al. (2010).

In contrast to these results obtained for constant model parameters, the LQOC method gives a nearly perfect fit of the data. Figure 2 shows the model results, aggregated model output (see Sect. 2.2) $\boldsymbol{y}^{\mathrm{mod}}$ obtained with the LQOC method together with the observational data $\boldsymbol{y}^{\mathrm{obs}}$ for the years 1994 to 1998 in the uppermost layer. The model-data fit for chlorophyll *a* is nearly perfect. Even substantial concentration changes that occur between some neighboring measurement points (e.g. for PON, in 1994, 1995 or 1997) can be captured by the optimized trajectory. There are only some parts of the time interval where the trajectories are slightly farther away from the data, for example in 1996 for zooplankton and in the last two years of the simulated time interval for PON. Figure 4 shows the mismatch between model output and data for all times and depths

We performed the optimization for the years 1994 to 1998, in contrast to the years 1991 to 1996 that were used in Rückelt et al. (2010). The reason for this is that no zooplankton data are available at BATS for the years 1991 to 1993, which would be disadvantageous for the linearization procedure in the LQOC method. In Rückelt et al. (2010) a minimum value of the cost function (5) of $F \approx 70$ was obtained for optimized

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constant parameters for the five year time interval [1991, 1996]. For the time interval [1994, 1998] the value obtained by the SQP method and constant parameters is very similar to the one obtained in Rückelt et al. (2010). Also the quality of the fit – depicted in Fig. 3 – is comparable.

Clearly, the better fit also results in a significantly lower value of the cost function (5) of about $F = 1.35$ compared to $F \approx 70$ obtained by constant parameters and the SQP method, see Rückelt et al. (2010). Results for The other layers are comparable.

4.2 Sensitivity with respect to the weighting matrices $\mathbf{R}_n$

To examine the effect of the weighting matrices $\mathbf{R}_n$ in the first year on the behavior of the parameters and the cost function F, we have additionally performed sensitivity experiments with different entries r_i^n of the weighting matrices $\mathbf{R}_n$ for $n \leq T$. We present two additional experiments with:

$$r_i^n = \begin{cases} \dfrac{1}{|\min(\boldsymbol{u}_i)|^2}, & i = 1, \ldots, m, n = 1, \ldots, T \\ \dfrac{1}{|\max(\boldsymbol{u}_i)|^2}, & i = 1, \ldots, m, n = 1, \ldots, T. \end{cases}$$

The values of $\min(\boldsymbol{u})$ and $\max(\boldsymbol{u})$ are listed in Table 1. The corresponding values of the r_i^n for these two choices and the r_i^n from Eq. (13) (called reference simulation) are shown in Table 2.

The trajectories of the tracers $\mathbf{x}$, the parameters $\mathbf{u}$, and the value of the cost function F depend heavily on the choice of the corresponding entries r_i^n in the matrix $\mathbf{R}_n$. Figure 5 shows the trajectories for three tracers and different r_i^n. All experiment show only minor differences from the reference simulation with the r_i^n from Eq. (13). The results show that a decrease in the entry r_i^n can lead to a small decrease in the cost function. The sensitivities of the parameters with respect to the choice of r_i^n can be seen in Figs. 6, 7, and 8. It is obvious that for smaller values of r_i^n the variability of the parameters is getting larger.

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4.3 Periodicity of the parameters

In this section we show that the above model-to-data fit can be achieved with parameters that are almost periodic with an annual periodicity. Enforcement of periodicity was possible due to an appropriate adjustment of the matrices $\mathbf{R}_n, n = 1, \ldots, M-1$, in the cost function (12) used in the LQOC framework, see Sect. 3.1. It was also possible to keep the parameters in their desired bounds (see Table 1), although the LQOC method does not require to impose these bounds explicitly.

Figures 6, 7, and 8 illustrate the temporal behavior of the ten parameters that were optimized with the LQOC method. These figures show different trajectories for each parameter with the different choices of the r_i^n, compare Table 2. As mentioned above, it is obvious that for a smaller r_i^n, the amplitude of the parameters increases, but it always remains almost periodic.

The parameters controlling growth of phytoplankton, namely the maximum growth rate a and the initial slope of the P-I curve α show in Fig. 6 Both show maximum values in early summer and in winter, with a clear minimum value in spring during the peak of the annual chlorophyll signal (Fig. 7). This is consistent with earlier assimilation studies that, for assumed constant parameters, tended to overestimate plankton production at BATS during the bloom end of winter and, at the same time, tended to underestimate production in oligotrophic summer conditions and in early winter, see Schartau et al. (2001). Such a trend to relatively high values of α has also been found in earlier studies that optimized parameter values by data assimilation, see Fasham and Evans (1995), Schartau et al. (2001). Earlier studies assuming time-independent parameter values have attributed relatively high values of α to the absence of a dial cycle in the turbulent mixing, which might allow for substantial phytoplankton growth even in winter during reduced daytime mixing see Schartau and Oschlies (2003a). This is consistent with the findings of the current study, that also suggests high values of α during the period of deep mixing in winter. In addition, our optimized model predicts even higher values of the initial slope parameters α for late spring and early summer, where the mixed

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layer is usually shallow and growth is limited by nutrients rather than light in the surface mixed layer. A large value of α can, however, help to establish a subsurface chlorophyll maximum in better agreement with the observations. This was also noted by Schartau and Oschlies (2003b). Our results reported here indicate that high values of α may, at BATS, be more important for the establishment of the deep chlorophyll in late spring than for the maintenance of phytoplankton production during periods of deep mixing in winter. Maintenance of high primary production during summer has been difficult to achieve by earlier models run at BATS (Schartau et al., 2001). As nutrient supply to the surface waters is low during the stratified season, models with fixed carbon-to-nutrient stoichiometry and constant model parameters do not seem to be able to reach observed levels of primary production in the surface layer see Schartau and Oschlies (2003b). In the current study, the carbon-to-nutrient factor used to convert simulated (nitrogen-based) primary production to observed (carbon-based) primary production is constant as well. However, the seasonally varying parameters can contribute to maintain high levels of primary production during summer in the absence of substantial inputs of new nutrients. This is realized by enhanced recycling of biomass, evident by high maximum grazing rates, high assimilation efficiencies, high prey capture efficiencies and high zooplankton excretion in late spring and early summer. Similarly, remineralization of detritus is highest in late spring as well. These high rates all contribute to fast recycling of nutrients in the surface ocean, which helps to maintain observed high rates of primary production and thereby reduces the model-data misfit function.

5 Conclusions

In this paper, we successfully applied the method linear quadratic optimal control to the optimization of an one-dimensional marine ecosystem model. The model has to be linearized to fit in the LQOC frame work. The method permits perfect periodic evolution of model parameters and additionally notably improves the fit of the data in comparison with the solution with fixed model parameters. We demonstrated that the LQOC

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optimization is suitable for the considered problem and furthermore have shown that this method provides a very reasonable solution. Even with the available small number of observational data, which is typical to oceanographic time series sites, its quality is very high. Temporal deviations of individual parameters about the annual mean can be analyzed further to help making inferences about processes that the model cannot describe well when constant parameters are used. This latter analysis should contribute to better understanding model deficiencies and, eventually, help to improve marine ecosystem models.

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Table 1. Parameter of the ecosystem model to be optimized with the LQOC method. Here $\boldsymbol{u}_0 = (u_{0,i})_{i=1,\ldots,12}$ is the vector of parameters taken from Oschlies and Garçon (1999), $\min(u_i)$ and $\max(u_i)$ there respective upper and lower bounds used in Schartau and Oschlies (2003a).

parameter	u_i	$u_{0,i}$	units	$\min(u_i)$	$\max(u_i)$
Assimilation efficiency of zooplankton	γ_1	0.75		0.3	0.93
Growth rate parameter	a	0.6	day^{-1}	0.2	1.46
Initial slop of P-I Curve	α	0.025	$\mathrm{m}^2\,\mathrm{W}^{-2}\,\mathrm{d}^{-1}$	0.001	0.256
Zooplankton excretion	γ_2	0.03	day^{-1}	0.01	0.955
Light attenuation by phytoplankton	k_c	0.03	$\mathrm{m}^{-1}(\mathrm{mmol\,m}^{-3})^{-1}$	0.01	0.073
Pry capture efficiency	ϵ	1	$(\mathrm{mmol\,m}^{-3})^{-2}\,\mathrm{d}^{-1}$	0.025	1.6
Maximum grazing rate	g	2	d^{-1}	0.04	2.56
Specific mortality rate	μ_p	0.03	day^{-1}	0.01	0.635
Zooplankton quadratic mortality	μ_z	0.2	$(\mathrm{mmol\,m}^{-3})^{-1}\,\mathrm{d}^{-1}$	0.01	0.955
Remineralization rate parameter of detritus	μ_D	0.05	day^{-1}	0.02	0.146
Sinking velocity of detritus	w_s	5	$\mathrm{m\,day}^{-1}$	1	128
Half-saturation constant for N uptake rate	K_N	0.5	$\mathrm{mmol\,m}^{-3}$	0.1	0.730

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Table 2. The different values of r_i^n for the reference simulation (first row) and the two additional sensitivity experiments.

i	$r_i^n = \dfrac{1}{\lvert(u_{0,i})\rvert^2}$	$r_i^n = \dfrac{1}{\lvert\min(u_i)\rvert^2}$	$r_i^n = \dfrac{1}{\lvert\max(u_i)\rvert^2}$
1	1.77	11	1.15
2	2.77	25	0.469
3	1600	10^4	15.25
4	1111	10^4	1.09
5	1111	10^4	187
6	1	1600	0.39
7	0.25	625	0.152
8	1111	10^4	42.48
9	25	10^4	1.09
10	400	2500	46
11	0.04	1	6.101^{-5}
12	4	100	1.876
cost F see Eq. (4)	1.35	1.9	0.95

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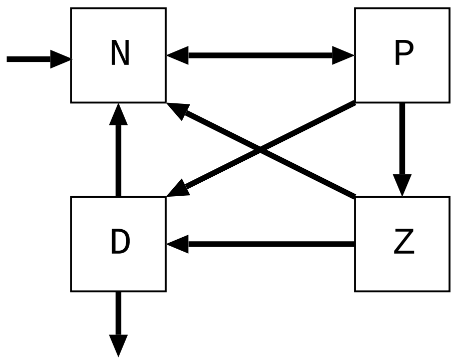

Fig. 1. Schematic description of the coupling between the variables in the NPZD model.

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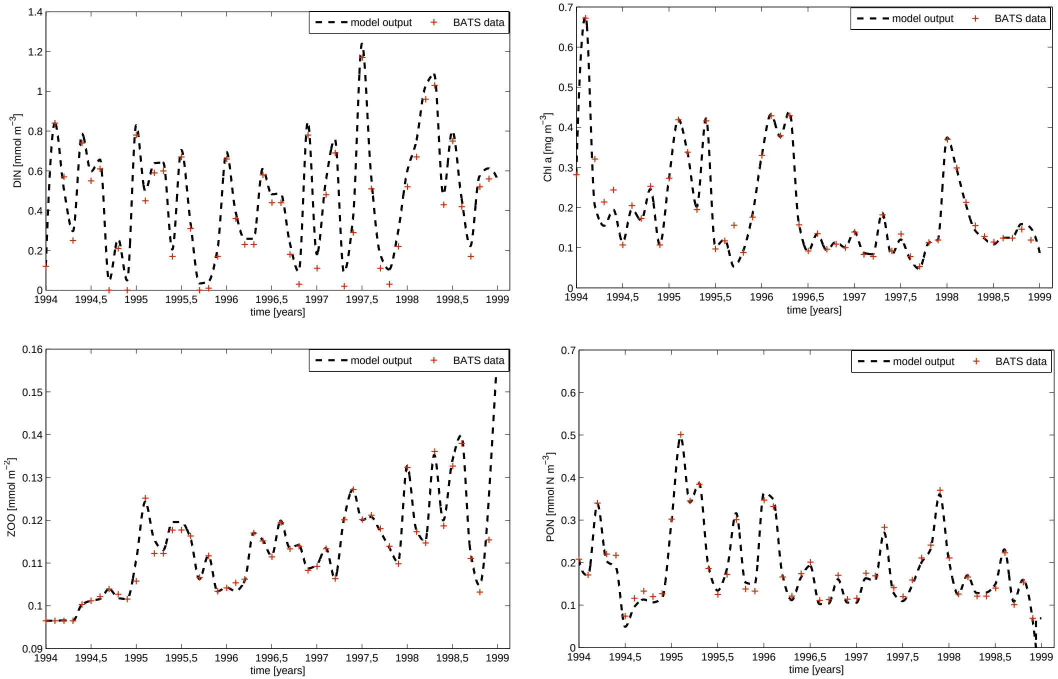

Fig. 2. Observational data $\boldsymbol{y}_m^{\mathrm{obs}}, m = 1,..,4$ and aggregated model trajectories $\boldsymbol{y}_m^{\mathrm{mod}}, m = 1,..,4$, optimized with periodic parameters obtained by the LQOC method. Values are shown for the upper layer (depth less than 5 m) and years 1994–1998.

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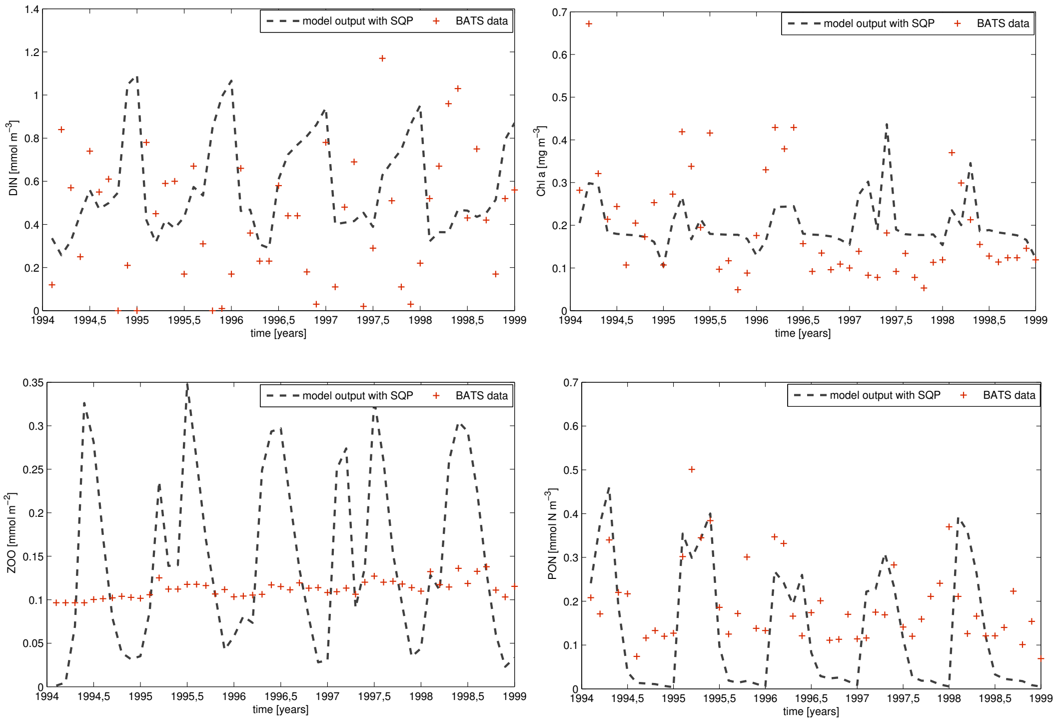

Fig. 3. Observational data $y_m^{\mathrm{obs}}, m = 1, .., 4$ and aggregated model trajectories $\boldsymbol{y}_m^{\mathrm{mod}}, m = 1, .., 4$, optimized with a *Sequential Quadratic Programming (SQP)* method. Values are shown for the upper layer (depth less than 5 m) and years 1994–1998.

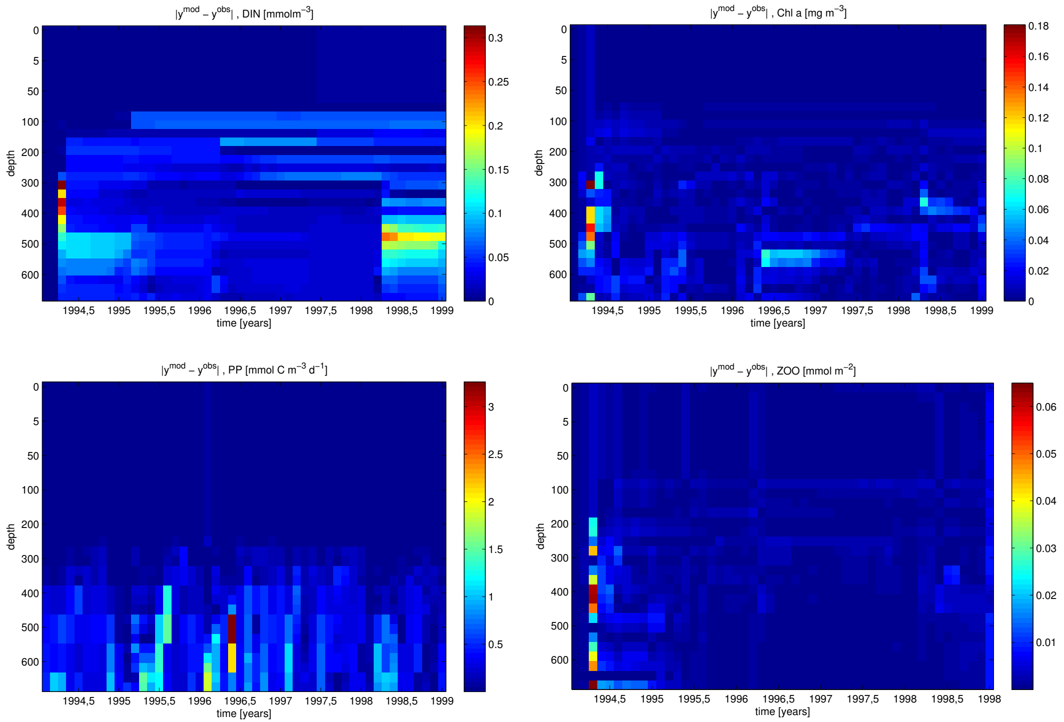

Fig. 4. Model-to-data misfit for three tracers and the primary production with respect to space and time.

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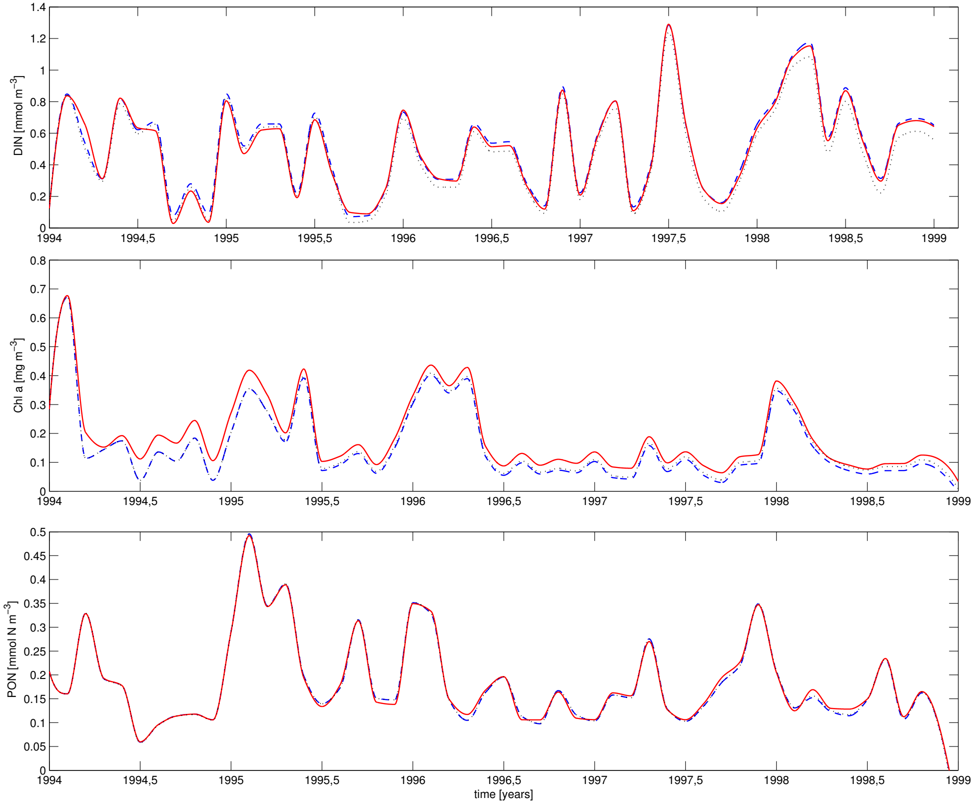

Fig. 5. Model output trajectories with different r_i^n, the reference simulation (dashed), with larger r_i^n (solid) and with smaller r_i^n (dotted) for the upper layer (depth less than 5 m) and years 1994–1998.

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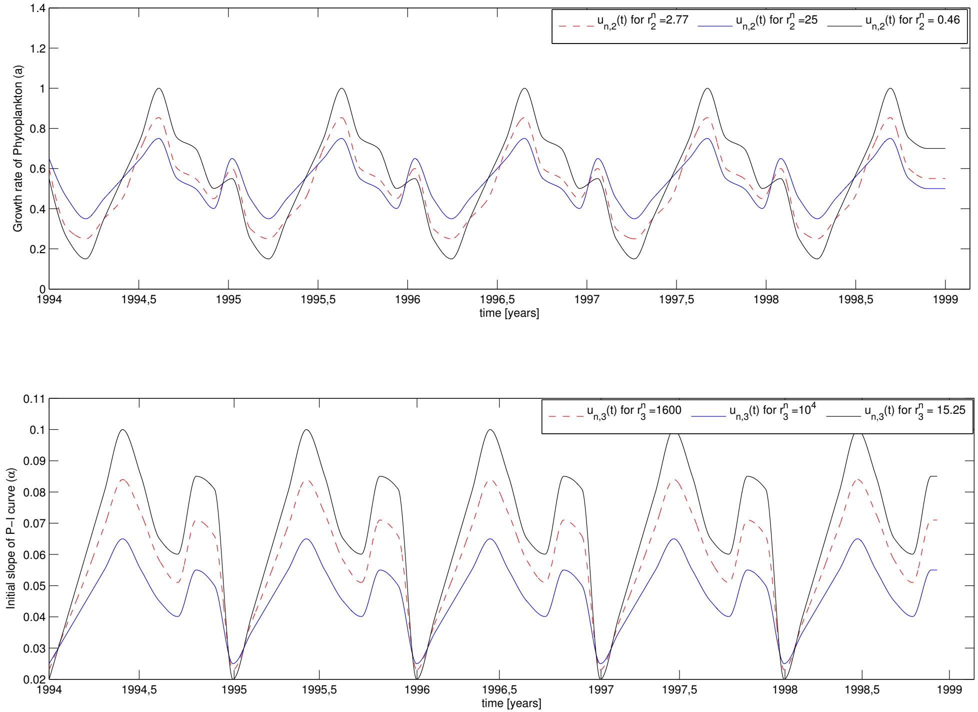

Fig. 6. Periodicity of optimal parameters $u_{n,2} = a$ and $u_{n,3} = \alpha$ obtained by the LQOC method.

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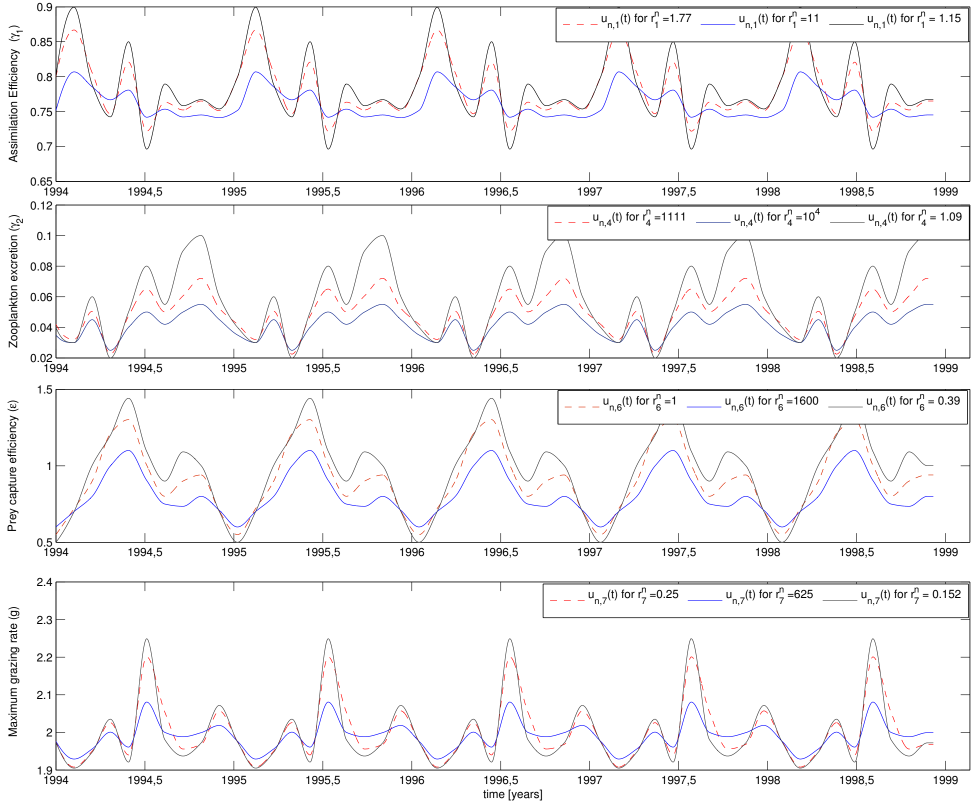

Fig. 7. Periodicity of optimal parameters $u_{n,1} = \gamma_1, u_{n,4} = \gamma_2, u_{n,6} = \epsilon, u_{n,7} = g$ obtained by the LQOC method.

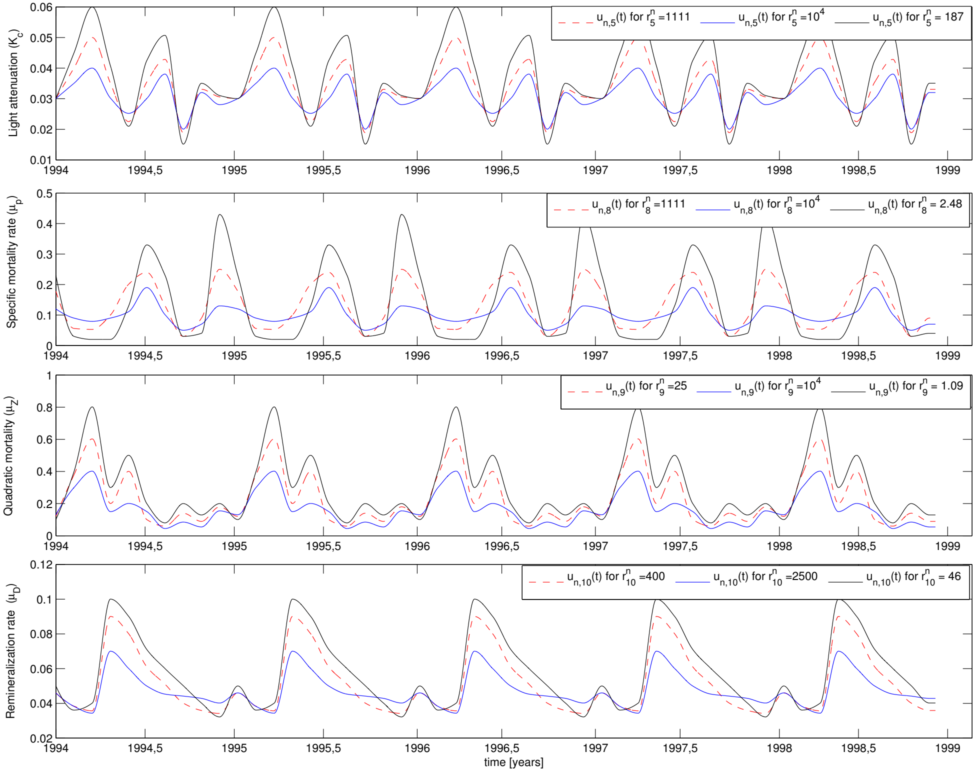

Fig. 8. Periodicity of optimal parameters $u_{n,5} = k_1, u_{n,8} = \mu_p, u_{n,9} = \mu_z, u_{n,10} = \mu_D$ obtained by the LQOC method.

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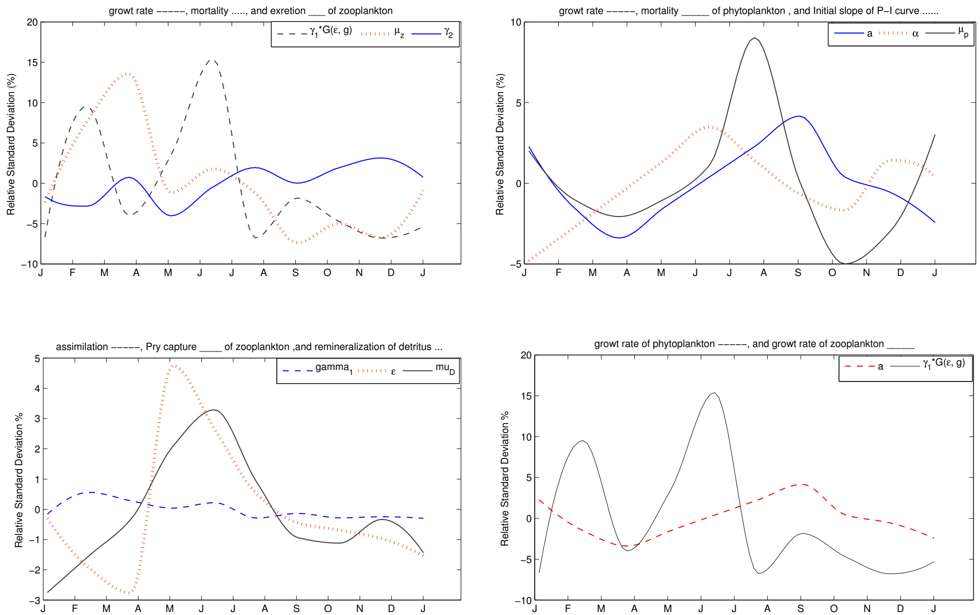

Fig. 9. Relative temporal variations of some of the model parameters in a typical year. Since the periodicity of the parameters is nearly perfect, no difference between the five years is visible.

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