

EVALUATION OF EXPERIMENTS FOR ESTIMATION OF DYNAMICAL CROP MODEL PARAMETERS

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Abstract: Planned experiments are usually expected to provide maximal benefits within limited costs. However there are known difficulties in optimal design of experiments. They are related to the case when only limited number of parameters could be estimated, because available experiments are the non-informative. The useful method for this case is considered based on the dominant parameters selection procedure (DPS). The methodology is illustrated here with data from five planned experiments related to the NICOLET lettuce growth model. The maximal number and the list of estimated parameters are determined while the conditional number of the information Fisher matrix (modified E-criterion) is kept below a given upper constraint. *Copyright*© 2005 IFAC.

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1. INTRODUCTION

The model-based control of dynamical processes often strongly depends on the reliability of the involved models. The costly experiments are carried in order to provide data for the proper calibration of the models, it means, to estimate its parameters. The known approach to optimize this process is an optimal design of experiments, by finding appropriate inputs, see Kalaba and Springarn (1971), Fedorov (1971), Goodwin and Payne (1977), Munack and Posten (1989), and others. Clearly this method is demonstrated in Kalaba and Springarn (1973), using one-dimensional dynamical system. The criterion maximized is an integral of the difference between of the square of the parameter sensitivity (information content) and the integrated cost of the control during experiment. The model of dynamical system is

$$\frac{dx}{dt} = f(x, y, p, t) \quad (1)$$

where x is a state variable, u is control input, p is system parameter, and t is time. The sensitivity of the state variable x to parameter p along the trajectory is $S(t) = \frac{\partial x}{\partial p}$, and

$$\frac{dS}{dt} = \frac{\partial f}{\partial x} S + \frac{\partial f}{\partial p}. \quad (2)$$

This sensitivity is an additional state variable in the problem of the optimal design of experiment. According to the Optimal Control Theory (OCP) additional equations for correspondent costate variables must be added to the state variable equations. In performing the experiment it is desired to obtain maximum benefit from the observations. The input to the system must be such that it maximizes the sensitivity of the state variable to the parameter. The magnitude of the input should be constrained so that it varies within feasible region and also its cost will be limited. The objective function is taken as

$$I = \int_{t_0}^T (S^2 - gu^2) dt, \quad (3)$$

where g is a weighting coefficient, and the first term is an one-dimensional simplification for the Fisher information matrix. The multidimensional cases are considered *e.g.* in Vereecken and Van Impe (1998), Van Impe and Versyck (2000). A very smart techniques and interesting results are shown in Keesman and Stigter (2002), and Stigter and Keesman (2004). In these works some scalar function of the Fisher information matrix (usually a modified E-criterion: ratio of the maximal to the minimal eigenvalue) is used as an indication of good performance of the experiment. The performance have to be understood in the sense of the ability to estimate the model parameters. This approach however leads to a multidimensional optimal control problem, where the control inputs to the system must be found together with state variables and their sensitivities to all parameters. Let say there are n state variables and m parameters. The dimensionality of the problem then will be $n + n \times m$. In the papers mentioned the problems are related to biotechnology and the optimal control problems are of low dimensionality and the Fisher matrix is nonsingular. This is not the case for the range of biological and environmental models, see Klepper (1971), and many crop growth models. Calibration of crop growth models is a very costs and time consuming operation and it is highly desirable to know in advance what information will be possible to extract from the limited set of available experiments. More definitely the question is: which parameters it will be possible to estimate. Often not all model parameters can be successively identified and a try and error procedure is used to find a reasonable subset of identifiable parameters. One also must notice that there arise essential difficulty in the optimal experiment design when Fisher matrix is singular. When a subset of parameters can be found such that the Fisher matrix is nonsingular, then the method of the optimal design of experiment can be proceeded for this subspace. It will be shown below how the Dominant Parameter Selection (DPS) procedure, Ioslovich *et al.* (2004), can solve this problem and the evaluation of experiments for the lettuce growth model NICOLET will be demonstrated.

2. DPS PROCEDURE

The problem of dynamical models identification is treated in many books and papers, see *e.g.* Nelles (2001), Ljung (1999), Goodwin and Payne (1977), Fedorov (1971). A more general statistical framework can be found in Draper and Smith (1981).

The DPS procedure is described in Ioslovich *et al.* (2004), in all details. Let us consider the dynamical system described by differential equations (1), where x is now a multidimensional state variable vector, u is a control vector (including controlled climate) and p is a vector of parameters. The measurable model outputs $Y_k(t, x, P)$, $k = 1, \dots, r$ are considered along the nominal trajectory $x(t)$ with nominal values of the system parameters p and given control inputs u . The column vector $S_k^j(t_i) = \frac{\partial Y_k(t_i)}{\partial p_j}$ is the sensitivity vector of the model output Y_k to parameter p_j at the moments t_i when the measurements are planned. These sensitivities can be found by solving the correspondent linearized time-dependent equations along the nominal trajectory of the dynamical system (model), or can be found numerically. The components of the vector are multiplied by the weights ω_{ik} , which can be chosen in a different way. Often the time-related index i can be omitted and weights ω_k can be used instead. This is a usual substitution for unknown inverse covariance matrix of the measured errors, see Munack and Posten (1989), Munack (1991). The column vector S_j will then be a notation for concatenation of the vectors $\omega_k S_k^j$. The matrix \mathbf{S} is defined as a horizontal concatenation of the column vectors S^j . The Fisher matrix can be written as

$$\mathbf{F} = S' * S. \quad (4)$$

The rank of the Fisher matrix indicates if the matrix is degenerate and the condition number (ratio of maximal to the minimal eigenvalue) will indicate if it is ill conditioned. This means that some of parameters are correlated or almost correlated. Then the optimization search for the best fit over the set of parameters will follow the ridge (submanifold) where the different values of parameters will give the same or almost the same values of objective. This can occur when sensitivities are linearly dependent, *e.g.* only a combination of parameters can be extracted from the calibration in the conditions of the experiment. According to DPS a subset of parameters for the model calibration must be chosen from the most sensitive (dominant) and independent parameters. From the eigenvalues of the Fisher matrix the dimensionality of this subspace can be found as follows. First an upper threshold α_1 for condition number of the submatrix is selected. Next, the normalized Fisher matrix is formed according to the rule

$$S_n^j = \frac{S^j}{\sqrt{(S^j)'(S^j)}} \\ \mathbf{F}_n = S_n' * S_n, \quad (5)$$

where \mathbf{F}_n is called the normalized Fisher matrix. Its elements are just cosines of angles between

the normalized sensitivity vectors. Thus each off-diagonal element of the normalized Fisher matrix is just a scalar product of the correspondent normalized sensitivities. The second upper threshold α_2 is settled to the values of these elements. Among all correlated pairs for which the correspondent off-diagonal term of the matrix has absolute value more then α_2 only one parameter of each pair can be estimated. The candidate parameters are chosen from the list of parameters, sorted in decreasing order according to their squared sensitivities, means according to the values of the diagonal elements of the Fisher matrix, \mathbf{F} . When element is examined for inclusion in the subset, it is first checked if it is correlated with one of the elements, already included (according to the normalized Fisher matrix). Then the subset of chosen candidate parameters must be checked for the multiple correlation. The correspondent sub-matrix of the Fisher matrix must be formed and the eigenvalues are computed. If the condition number of the sub-matrix is too large according to the established threshold (*i.e.* $cond > \alpha_1$), then the least sensitive parameter is excluded and the most sensitive among remaining parameter is included, unless the list of sensitive parameters will be empty. In this way the maximal parameter subset is found with upper constraint on the conditional number of the Fisher submatrix. For crop growth models a logarithmic Least square Estimation is often used which provide some normalization for data of different age of the exponentially growing crop. In this case the relative sensitivities

$$s_k^j = \frac{p_j}{Y_k} \left(\frac{\partial Y_k}{\partial p_j} \right) \quad (6)$$

can be used for the same purpose. The vector s_j is determined in the same way (as concatenation of the weighted vectors), as the vector S^j , and matrix \mathbf{s} is formed as the horizontal concatenation of the vectors of the column vectors s^j . The product $\mathbf{s}' * \mathbf{s}$ will be the modified Fisher matrix \mathbf{F}_m . The advantage of the relative sensitivity is that it is dimensionless. The normalized matrix also must be calculated in the same way for modified Fisher matrix and the same selection procedures must be hold. We shall demonstrate this approach with the NICOLET lettuce growth model and evaluation of the available set of experiments. This procedure was also used for calibration of different dynamical models, see Ioslovich *et al.* (2002), De Graaf *et al.* (2004), Bortolin *et al.* (2002), Linker and Johnson-Rutzke (2004), *etc.*

3. THE NICOLET MODEL-SHORT DESCRIPTION

NICOLET lettuce growth model, Seginer *et al.* (1998, 1999), is based on the complementary properties of nitrate and carbon in the vacuoles. The calibration of the model was considered in Van Straten *et al.* (1999). Several studies with lettuce produced clear negative linear correlations between sugar and nitrate in the cell sap. The model is used for the lettuce growth optimization and quality control (in terms of the nitrate content). Several basic assumptions have been done. The volume occupied by the vacuoles is a fixed fraction of the total volume of the plant. The nitrogen-to-carbon ratio in the structure is also fixed. The ratio in the vacuoles is variable and constrained by the need to maintain a constant turgor pressure. Respiration and growth are assumed to depend on temperature. The nitrate flow into the vacuoles is calculated from the demand to support growth and to maintain turgor. The model has two state variables, the carbon content of the vacuoles and the carbon content of the structure, M_{Cv} and M_{Cs} , respectively. Other components, like nitrate content in the vacuoles and in the structure, can be expressed in terms of these state variables. The state equations of the model are

$$\begin{aligned} \frac{dM_{Cv}}{dt} &= F_{Cav} - F_{Cm} - F_{Cg} - F_{Cvs}, \\ \frac{dM_{Cs}}{dt} &= F_{Cvs}, \end{aligned} \quad (7)$$

where F_{Cav} is the photosynthetically generated carbon flux (subscript C) from the atmosphere (a) to the vacuoles (v); F_{Cm} and F_{Cg} are the maintenance (m) and growth (g) respiration fluxes; and F_{Cvs} is the flux of carbon from the vacuoles into the structure (s), namely growth. The photosynthesis flux, F_{Cav} , and the growth flux, F_{Cvs} , are modelled as products of three factors: (i) The uninhibited flux for a closed-canopy crop, (ii) a measure of light interception (surface cover) by the canopy, and (iii) an inhibition function. Thus,

$$\begin{aligned} F_{Cav} &= p\{I, C_{Ca}\} f\{M_{Cs}\} h_p\{\Gamma_{Cv}\}, \\ p\{I, C_{Ca}\} &= \frac{\epsilon I \sigma C_{Ca}}{\epsilon I + \sigma C_{Ca}}, \\ F_{Cvs} &= g\{T\} f\{M_{Cs}\} h_g\{T\}, \\ g\{T\} &= \nu e\{T\}, \end{aligned} \quad (8)$$

where $p\{I, C_{Ca}\}$ is the gross-photosynthesis rate, determined by light, I , and by atmospheric (or greenhouse) CO_2 concentration, C_{Ca} ; $g\{T\}$ is the potential growth rate, which is a function of temperature, T ; $f\{M_{Cs}\}$ is a measure of light interception,

$$f\{M_{Cs}\} = 1 - \exp\{-aM_{Cs}\}, \quad (9)$$

which approaches one as the canopy closes; and $h_p\{\Gamma_{Cv}\}$ and $h_g\{\Gamma_{Cv}\}$ are, respectively, dimensionless photosynthesis and growth inhibition functions, which in the uninhibited state are equal to one. h_p depends on parameters b_p and s_p , and h_g depends on parameters b_g and s_g respectively. The first approaches zero for high values of the normalized carbon (sugar) concentration in the vacuoles, Γ_{Cv} , while the second approaches zero for low values of Γ_{Cv} . The respiration fluxes were formulated as

$$\begin{aligned} F_{Cm} &= f\{M_{Cs}\}e\{T\}, \quad e\{T\} = \text{keexp}\{c(T - T^*)\} \\ F_{Cg} &= \theta F_{Cvs} \end{aligned} \quad (10)$$

where θ is a constant fraction. The nitrate concentration in the vacuoles, C_{Nv} , can be obtained from the carbon concentration, C_{Cv} , as

$$\begin{aligned} \Gamma_{Cv} + \Gamma_{Nv} &= 1, \\ \Gamma_{Cv} &= \frac{\beta_C C_{Cv}}{\Pi_v}, \\ \Gamma_{CN} &= \frac{\beta_N C_{Nv}}{\Pi_v}, \end{aligned} \quad (11)$$

where β_N and β_C are constants and Π_v is the osmotic pressure in the vacuoles. Nitrogen contents of the vacuole and structure, M_{Nv} and M_{Ns} , are related to the state variables M_{Cv} and M_{Cs} via

$$\begin{aligned} M_{Nv} &= \frac{\lambda \Pi_v}{\beta_N} M_{Cs} - \frac{\beta_C}{\beta_N} M_{Cv} \\ M_{Ns} &= r_{Ns} M_{Cs} \end{aligned} \quad (12)$$

where λ is the permanent water volume associated with one unit of structural carbon; r_{Ns} is the N to C permanent ratio in the structure. A nitrogen balance of the vacuoles has form,

$$\frac{dM_{Nv}}{dt} = F_{Nrv} - r_{Ns} F_{Cvs} \quad (13)$$

where $\frac{dM_{Nv}}{dt}$ is the rate of change of the nitrate- N content of the vacuoles, F_{Nrv} is the uptake of nitrate from the rhizosphere. If growth is limited by nitrate supply, then uptake is equal to supply and F_{Nrv} represents the rate of supply. From (11) and (12) one can easily get

$$\beta_N M_{Nv} + \beta_C M_{Cv} = \Pi_v V_v \quad (14)$$

and

$$\frac{dM_{Nv}}{dt} = \frac{\lambda \Pi_v}{\beta_N} \frac{dM_{Cs}}{dt} - \frac{\beta_C}{\beta_N} \frac{dM_{Cv}}{dt}, \quad (15)$$

where V_v is the volume of the vacuoles per unit ground area. It is now possible to derive an expression for the rate of growth, F_{Cvs} , in terms of the limiting supply rate of nitrate, F_{Nrv} (and other quantities). Using Eqn (15) to substitute

for $\frac{dM_{Nv}}{dt}$ in Eqn (13) and then substituting for time derivatives of M_{Cv} and M_{Cs} from Eqs (7), an expression for F_{Cvs} in terms of the other fluxes is obtained for the N -limiting case:

$$F_{Cvs} = \frac{\beta_N F_{Nrv} + \beta_C (F_{Cav} - F_{Cm})}{\Pi_v \lambda + \beta_C (1 + \theta) + \beta_N r_{Ns}} \quad (16)$$

Using Eqn(16) completes the modification required for the nitrate-limited growth. One way to determine the missing initial condition is to assume that since the plants are initially small and the environment constant, growth is balanced and exponential (EG). The composition of seedlings growing under such conditions is only a function of the environment and hence invariant with time. Therefore the ratio is assumed for the initial data

$$\frac{M_{Cv}}{M_{Cs}} = \frac{dM_{Cv}}{dM_{Cs}}. \quad (17)$$

4. EVALUATION OF THE AVAILABLE EXPERIMENTS

A set of the available experiments for estimation of parameters of the NICOLET model is considered. In these experiments the normal and the extreme climate conditions were expected to be maintained in the greenhouse. The extreme experiments were associated with: low level of the source inputs, namely light and CO_2 , and low sink demand associated with low level of Nitrate supply and low inside air temperature. All the conditions expected to remain permanent (no day-night changes) during the period of one month. Daily measurements of the four outputs were planned. All the experiments were planned in such a way that the Equilibrium Growth (EG) conditions in all cases will be maintained. Following values of climate inputs were taken as the normal (i.e. summer conditions in Israel):

Light, $I = 20 \text{mol}[PAP]m^{-2}d^{-1}$

Nitrate supply, $F_{Nrv} = 0.65 \text{mol}[N]m^{-2}d^{-1}$

Inside air temperature, $T = 24, 47^\circ C$

Inside CO_2 concentration, $CO_2 = 0.0353 \text{mol}[C]m^{-3}$

The inside temperature was chosen to get $h_g = 0.5$ from the EG equation (17). Corresponding values of the Γ_v and values of the inhibition functions for the four extreme experiments are shown below.

Source stress conditions:

Low CO_2 , $C_{Ca} = 0.005 \text{mol}[C]m^{-3}$, $h_g = 0.5$,

$\Gamma_{Cv} = b_g$,

Low light, $I = 8.006 \text{mol}[PAP]m^{-2}d^{-1}$,

$h_g = 0.5$, $\Gamma_{Cv} = b_g$

Sink stress conditions:

Low temperature, $T = 12.62^\circ C$, $h_p = 0.5$,

$\Gamma_{Cv} = b_p$,

Low Nitrate, $F_{Nrv} = 0.0157 \text{mol}[N]m^{-2}d^{-1}$,

$h_p = 0.5$, $\Gamma_{Cv} = b_p$

Four model outputs were planned to be measured

each day during one month period for these experiments. They are:

$FM[gm^{-2}]$ - fresh mass,

$DM[gm^{-2}]$ - dry mass,

$NO3[mg[NO3]kg^{-1}[FM]]$ -Nitrate,

$N_r[g[N]g^{-1}[DM]]$ - reduced Nitrogen.

Altogether 15 model parameters were analyzed for possible selection into the Fisher matrix subset for the estimation. These parameters are related to photosynthesis (ϵ , σ), respiration and growth (θ , k , ν , c), photosynthesis and growth (a), internal relationships (β_N , β_C , λ), inhibition functions (b_p , s_p , b_g , s_g), Nitrogen to Carbon ratio in the structure (r_{Ns}). One could expect that the low source growth experiments will permit to identify some parameters related to the photosynthesis and growth and/or growth inhibition, and the low sink growth experiments will permit to identify some parameters related to the photosynthesis inhibition and/or N to C ratio in structure. The sensitivity analysis was done numerically. Relative sensitivities were calculated (one point per each day) for each of four outputs along the trajectory of each planned experiment with nominal values of parameters. The nominal values of the model parameters are presented in the Appendix 1. The results of the analysis of availability of parameters estimation are presented for these five experiments separately and also for all experiments together (as a combined data set) in the Tables 1 – 4. The selection procedure DPS follows its description in section 2. The thresholds $\alpha_1 = 0.95$, $\alpha_2 = 40$ were used in the DPS procedure. In Tables 1 – 4 for the correspondent treatments the selected parameters are shown with their number in the order by decreasing sorting set of the relative sensitivities and the correspondent condition number (in brackets) for the Fisher sub-matrices where these parameters are selected. In the case when the parameter is the first in the order the condition number is not indicated (because then the dimension of the submatrix matrix is one).

Table 1. Normal conditions

k	ϵ	r_{Ns}
1	2(8.2)	3(10.3)

Table 2. Source limited growth

	ϵ	a	λ	β_N	r_{Ns}
<i>Low Light</i>	1		4(38.2)	3(5.3)	2(1.4)
<i>Low CO₂</i>		1		3(5.7)	2(1.1)

For all experiments considered together as a union

Table 3. Sink limited growth

	a	k	b_p	r_{Ns}
<i>Low T</i>		1	2(1.1)	3(1.6)
<i>Low N</i>	3(12.2)		1	2(3.9)

source of the modelled data the results of the

DPS procedure are presented in Table 4. The eight selected parameters are shown. One can see that

Table 4. All treatments

a	k	b_p	ϵ
1	2(3)	3(4)	4(18)
β_N	λ	σ	c
5(18.9)	6(23.8)	7(35.1)	8(35.2)

in Table 4 almost the union of the parameters selected for the separate treatments is presented. Generally one can see that different parameters are selected for the source limited experiments and for the sink limited experiments. It looks natural that in both source limited experiments with low light and low CO_2 parameter β_N is selected as far as in this case the nitrate concentration prevails in the vacuole. On the other hand it is also expected that parameter b_p from the photosynthesis inhibition function h_p is a significant one when the sink stress occurs as a result of the input reductions in the case of low temperature and also for low nitrate experiments. Parameter r_{Ns} is an important one for the constant N to C ratio in the structure and thus it affects the outputs in both type of experiments. From the first look it is not clear why ϵ is selected in the experiment with low light and σ is not selected in the experiment with low CO_2 . However it can be understood by consideration of the relative sensitivities of the photosynthesis $p\{.\}$ in respect to these parameters. The relative sensitivity of photosynthesis in respect to ϵ is inverse proportional to I and the correspondent relative sensitivity in respect to σ is inverse proportional to C_{Ca} . For the used normal conditions the product ϵI is five fold less then the product σC_{Ca} . The same ratio exists between their relative sensitivities in the experiments with low I and low C_{Ca} respectively. The combination of multiple experiments together provides more variability in conditions and thus permits to select more parameters for the estimation. One can see that the most wide set of parameters (8 parameters) can be extracted from consideration of all treatments together.

5. CONCLUSIONS

An analysis and evaluation of several planned experiments for parameters estimation has been presented. This can be considered as a preliminary and necessary step for optimal design of experiments that overcome difficulty related to the Fisher matrix singularity. A simple preliminary procedure DPS has been used. It gives a suggestion of choosing parameters for estimation as a result of the future experiment. The procedure was demonstrated with set of possible experiments for estimation of parameters of the NICOLET model. It was shown that the type of experiment

(sink or source limited growth) corresponds to the selection of the parameters. A combination of different experiments is more effective rather than consideration of the separate treatments.

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APPENDIX 1. NOMINAL VALUES

Photosynthesis:

$$\epsilon = 0.07 \text{ mol}[C]/\text{mol}[PAP]; \sigma = 1.4 \times 10^{-3} \text{ m/s}$$

Respiration and growth: $\theta = 0.3$; $\nu = 13.6$;

$$k = 0.147(10^{-6} \text{ mol}[C]/(\text{m}^2[\text{ground}]s));$$

$$c = 0.06931/K$$

Photosynthesis and growth:

$$a = 1.7 \text{ m}^2/\text{mol}[C]$$

Internal relationships:

$$\beta_N = 6.0 \text{ kPa}/(\text{mol}[N]/\text{m}^3);$$

$$\beta_C = 0.61 \text{ kPa}/(\text{mol}[C]/\text{m}^3);$$

$$\lambda = 0.833 \times 10^{-3} \text{ m}^3/\text{mol}[C]$$

Inhibition functions:

$$b_p = 0.8; s_p = 10; b_g = 0.2; s_g = 10$$

Nitrogen to Carbon ratio in the structure:

$$r_{Ns} = 0.08 \text{ g}[N]g^{-1}[C]$$

$$\text{Conversion} : \eta = 0.030 \text{ kg}[DM]/\text{mol}[C]$$

Initial condition (fresh mass):

$$W_F^i = 0.0093 \text{ kg}/\text{m}^2$$

Arbitrarily fixed: $T^* = 20^\circ\text{C}$