ANALYSIS OF SIMULATION MODELS BY RESPONSE SURFACE TECHNIQUES

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1.1 Introduction

The Statistical Reporting Service (SRS) of the U.S. Department of Agriculture (USDA) currently uses plant measurements from a probability sample of plots in fields planted to a crop in regression equations, where coefficients are estimated using historic measurements, to forecast yields during the current year. Measurements do not include any meteorological observations or take into account any cultural practice information, except plant density.

These models are adequate in the maturing period (4 to 6 weeks prior to biological maturity) but have not been adequate for yield forecasting in the early and mid-growing period (6 to 12 weeks before harvest) in normal or near-normal years. These models have been less accurate during these periods in abnormal years. UDSA is optimistic that plant process models with feedback capabilities can contribute to better forecasts in the early and mid-growing periods.

As part of USDA yield research, we have attempted to identify the interrelationships (important to yield) which exist between various parameters and functions in plant process models, as a first step toward developing procedures for the evaluation of plant growth simulation models. The need for more (or less) accurate parameter or function determination through experimentation can also be assessed as part of the sensitivity of modeled yield to these factors.

1.2 Plant Process Models

Plant process models have been developed by agronomists, agricultural engineers and other plant scientists to study the response of an average plant, or unit area of plants, to environmental conditions and/or various management practices. These models simulate the growth of plants from sowing to maturity. The models are crop specific and, in some instances, require location and variety calibration. Several stages of plant process models have evolved. After Duncan (1966), among others, successfully modeled photosyntheses, scientists were able to use this process in simulation growth models for corn, cotton, alfalfa, a short grass, barley and wheat. These models use daily inputs of temperature, solar radiation and rainfall to "grow" the specified plant. Current versions of plant process models are beginning to include the more complex relationships of the effects of soil, nitrificiation, insects and disease. The simulation of the individual processes has become more detailed and more complete.

A typical plant process model, sometimes called a soil-plant-atmosphere model, might trace the growth of the plant in a daily cycle and would accept climatic measurements, estimate daily evapotranspiration rates, separate them into evaporation and transpiration rates, extend the roots, monitor soil moisture flow between the plant and the soil, use solar radiation values for photosynthesis, mimic the respiration process, and apportion the dry matter production among the roots, stems, leaves and fruit of the plant. The computed maturity stage of the plant would determine whether to continue the simulation or to print final statistics. The parameters and functions used for the simulation of the growth processes would be estimated from laboratory or field experiements. In most models, the growth process is deterministic with no probability distribution attached to any of the model components.

These models have been used primarily as research tools to examine the changes in yield or in growth behavior under different conditions. Recent models have attempted to simulate the crop yields more accurately. For example, Arkin et al (1980) introduced feedback information into SORGF, a grain sorghum model developed earlier (Arkin et al (1976)). Plant part data, such as number of leaves emerged or number of fully-grown leaves, and plant phenology data, such as Julian dates of floral initiation, anthesis, or physiological maturity, are entered into the program at various growth stages; the model variables are then reset based on this information; and the modeled growth of the plant continues from that point.

1.3 Sensitivity Analysis

The traditional approach to studying the effect of varying relevant parameters in a simulation model is the same as that used in any other interpolation problem: a multidimensional regula falsi technique. The use of fractional factorial designs to limit the number of simulation runs required, is clearly indicated when the number of factors becomes large. Montgomery (1979) presents a detailed discussion of the use of such techniques. In an earlier paper (Montgomery and Evans (1975)) they also suggest the use of response surface designs for the analysis of the sensitivity of responses to changes in input parameters. Steinhorst (1979) utilizes two-level fractional factorial designs as suggested by many authors (e.g., Kleijnen (1979)). Hartley (1979) also proposes to restrict the number of experimental runs required by adopting a form of rotation sampling plan.

1.4 Design Constraints

As is the case with most simulation models, the class of computer programs described in Section 1.1 require extensive computer time. Many of the factors determining the responses of such simulation runs are difficult to quantify. Some simulation models require constants, such as the fraction of wheat florets converted into grains, that must be determined experimentally. A study of the sensitivity of responses to a variation of these constants may be useful in that if the response is not significantly affected, costly experimentation to determine the constant for different varieties of wheat may be unnecessary. It was considerations of this type that prompted us to look for minimal (smallest size) response surface designs. We chose a central composite design with one center-point (since replication in such a deterministic model would yield identical results), and arbitrarily chosen x-values, with the option of choosing a fractional factorial design for the lattice points if the number of factors is five or greater.

Cubic response surface designs were compared to minimal quadratic response surfaces to see whether the quadratic surface is adequate to express the association between input parameters and yield prediction. Work is also in progress to consider the effect of scale transformation of input parameters. The approach is similar to that proposed by Hartley and Rao (1967). In a design matrix for classificatory models, these authors replaced the 0,1 in a given row by θ and $1 - \theta$ for two selected columns, and estimated the value theta by maximum likelihood.

2.1 Model Assumptions

In addition to the usual assumptions that the experiments (simulated growths of a plant) can be performed and the response(s) measured at each of the design points, we have made two special assumptions. First, we have assumed that an available simulation program is the author's best description of the modeled plant processes. The model usually has been validated by the author over several locations and the forecasting (estimation) ability of the model has been evaluated by USDA over time (see Wilson et al (1981)). Thus, the existing values of the factors (the center point values) provide a good indication of the response and the response surface intercept should be close to the center point response. Second, in the calibration of the model parameters (selected as factors), a range of possible values (or a set of bounds) for each factor has been determined by the model author. By setting the factor levels to be +1 and -1 at these bounds, we have defined a design lattice which describes the variation of the "real" response to be expected under variation of parameters.

2.2 Relative Sensitivity

Although the physical units of the factors may be completely different and levels may even be categorical in nature, use of the model author's calibration limits in setting the factor levels standardizes the sensitivity of the response to all of the factors. Since the intercept is the best estimate of the response at the center and "reality" lies inside the unit lattice, the contribution of each factor or factor combination at the boundary (lattice points), i.e., the coefficient of that effect in the standard response equation, can serve as an index of sensitivity. The ratio of this coefficient to the intercept has been defined to be the "relative sensitivity" of the response to variation of a factor or factor combination.

3.1 The Computer Programs

Even for minimal designs, many runs may be necessary. For example, 25 runs of the simulation program are required to estimate the response to variation of four factors in a quadratic response surface design. Thus, it is advisable to study, in each run, as many responses as possible. Care was taken to write analysis programs that could handle multiple responses without unnecessary repetition. Our driver program permits the handling of several responses during one execution of the simulation program. For the analysis of a single response, the procedure RSREG of the Statistical Analysis System (SAS) has been used and is quite efficient. The SAS procedure GLM was used for the estimation of cubic response equations. Special programs are being written to examine the effect of transformation of scales.

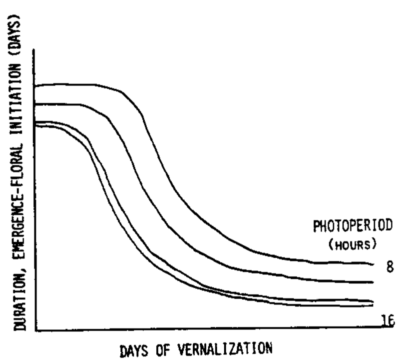
3.2 A Simulation Model

TAMW ("Texas A&M Wheat Simulation Model") (Maas and Arkin 1980a)) was used to demonstrate the response surface techniques. The following factors were used in the analysis:

1. ROSPZ -- spacing between rows(cm)
2. ROWID -- spacing between plants in a row(cm)
3. DENS -- density of plant population (combination of ROSPZ and ROWID) (cm*cm/plant)
4. COMP -- an exponent used in the calculation of a competition factor
5. LAI -- leaf area threshhold
6. CVERN -- an input function which governs the effect of vernalization on the vegetative phase (see Figure 1)
7. BETA -- the limiting value of asymptote for the number of heads(H) possible at head emergence given the number of existing shoots(X) at terminal spikelet in

   $$H = \beta * (1 - EXP(-\alpha * X/\beta))$$
8. CGSET -- the fraction of wheat florets converted to grain.

FIGURE 1: Picture of CVERN



DURATION OF THE PERIOD FROM EMERGENCE TO FLORAL INITIATION AS A FUNCTION OF PHOTOPERIOD AND VERNALIZATION.

Three weather datasets were chosen to provide different kinds of environmental conditions. Maximum and minimum temperatures, precipitation, solar radiation and snow depth were obtained on a daily basis. All data were recorded during the 1978-79 growing season and were used to validate the model. The field sites were located near Temple, Texas (a wet southern latitude growing season); Fort Pierre, South Dakota (a normal northern latitude growing season); and Brewster, Kansas (a severe early-season water stress growing season).

4.1 Comparison of Predicted and Simulated Values

A preliminary study compared prediction errors for points inside the design lattice to extrapolation errors. The effects of interaction and higher order terms were assessed to determine the adequacy of a quadratic response surface. The choice of factors and lattice points produced impossible physical conditions for star points two units from the center point; consequently, the design has $\alpha = 1.5$. Responses were yield (grain weight in grams per plant) and the maximum number of shoots per plant. The weather data were from Temple, Texas.

TABLE 1: Preliminary Study - Design

Factor/Level	-1.5	-1	0	1	1.5
ROSPZ	15	20	30	40	45
ROWID	3	4	6	8	9
COMP	.25	.30	.40	.50	.55
LAI	.7	1.0	1.6	2.2	2.5

The TAMW simulation program was run for 25 points, i.e., the 16 lattice points, the center point, and the eight star points. The maximum errors between the observed yields and those predicted from the response equation for yield occurred at the settings: 30, 9, .40, 1.6 (observed 8.030, predicted 7.816), at 45, 6, .40, 1.6 (observed 8.030, predicted 7.816), and at 40, 8, .30, 1.0 (observed 7.732, predicted 7.932). Of the remaining 22 settings, four had an error between .1 and .2 and 18 had errors less than .1. The following table shows the quality of fit of the quadratic model for extropolated settings:

TABLE 2: Preliminary Study - Extrapolation

ROSPZ	ROWID	COMP	LAI	Yield(PRED)	Yield(OBS)	ERROR
15	3	.25	.7	1.505	2.089	.584
45	9	.55	2.5	9.009	9.064	.055
15	3	.40	.7	1.774	2.270	.496
15	6	.25	1.6	4.301	4.186	-.115
15	6	.40	.7	3.925	3.532	-.393
30	3	.25	1.6	4.301	4.186	-.115
30	3	.40	.7	3.925	3.532	-.393
30	6	.25	.7	6.112	6.162	.050
45	9	.40	1.6	8.729	9.064	.335
45	6	.55	1.6	7.671	8.030	.359
45	6	.40	2.5	8.060	8.030	-.030
30	9	.55	1.6	7.671	8.030	.359
30	9	.40	2.5	8.060	8.030	-.030
30	6	.55	2.5	6.662	6.726	.064
15	3	.25	2.5	1.607	2.324	.717
15	3	.55	.7	1.221	1.732	.511
15	9	.25	.7	5.278	4.855	-.423
45	3	.25	.7	5.278	5.248	-.030

"Observed" in this context refers to the results of TAMW runs at various extrapolation settings, where at least two of the factors were at the level of + or - α. If the user is not satisfied with this degree of approximation, the following options are open: the step-size between intervals could be reduced; α could be chosen closer to the lattice points; factors which have small coefficients for the cross-product terms in the response equation could be left out.

From this study and several other studies which we made, we concluded that the traditional techniques of sensitivity analysis, i.e., variation of each factor at all possible levels, are not needed for the evaluation of these computer simulation programs. The difference between the results of computer simulation studies and the physical growth process would appear to be of a greater order of magnitude than the error of approximation of a quadratic response equation to the computer simulation model (Maas and Arkin (1980)).

4.2 Quadratic vs. Cubic Response Surfaces

The next study concerned the possible advantages of using a cubic response surface design. To reduce the number of computer runs only three factors were used, but at each of the three locations -- Temple, Fort Pierre, and Brewster. The star points were two units from the center point and the levels were based on the precision of measurement indicated by the authors of TAMW.

TABLE 3: Cubic Study

Factor/Level	-2	-1	0	1	2
CVERN	F - 8	F - 4	F	F + 4	F + 8
BETA	620	670	720	770	820
CGSET	.15	.20	.25	.30	.35

All of these factor values are determined experimentally. The function values to define CVERN depend on the current photoperiod, but essentially shift the y-value up and down. When the factor levels were chosen, the model author suggested a vertical shift of four units as one level for the function values. If CVERN does not affect the yield response then less experimentation would be required to determine this function given variety and location changes. Similarly, CGSET is a parameter also established by costly experimental procedures. If it does not affect yield significantly over location and varietal changes, then it could be ignored and costs for experiments to determine varietal and location differences could be reduced.

Using Temple data, the quadratic response surface (with significant coefficients (at .10 level)) is

$$\text{YIELD} = 3.85 - .13*\text{CVERN} + .28*\text{BETA} + .77*\text{CGSET}$$

and has maximum errors of -.175 for point 13 and .171 at point 12, the two star points for BETA (see TABLE 4 for point identification).

TABLE 4: Temple Data and Errors

POINT	CVERN	BETA	CGSET	SIM YIELD	QUAD ERROR	CUBIC ERROR
1	-1	-1	-1	2.875	-0.066	-.012
2	1	-1	-1	2.680	-0.099	-.008
3	-1	1	-1	3.494	0.099	.011
4	1	1	-1	3.246	0.081	.006
5	-1	-1	1	4.313	-0.074	-.036*
6	1	-1	1	4.020	-0.093	-.032*
7	-1	1	1	5.241	0.104*	.033*
8	1	1	1	4.868	0.073	.028
9	0	0	0	3.848	-0.004	-.014
10	-2	0	0	4.051	-0.025	-.013
11	2	0	0	3.597	0.025	-.013
12	0	-2	0	3.435	0.171*	.001
13	0	2	0	4.225	-0.175*	.001
14	0	0	-2	2.308	-0.002	.001
15	0	0	2	5.387	0.001	.001
16	1	0	-1	2.918	0.051	.011
17	0	1	-1	3.201	0.028	.011
18	0	-1	0	3.078	-0.004	-.009
19	-1	0	0	2.980	0.003	.011
20	1	0	0	3.231	-0.056	-.026
21	-1	1	0	3.648	0.085	-.093*
22	0	1	0	4.002	0.031	.009
23	0	-1	1	3.725	0.006	.008
24	-1	0	1	4.189	-0.078	-.035
25	0	0	1	4.039	-0.092	.073*
26	1	0	1	4.802	0.035	.012
27	0	1	1	4.618	-0.002	-.019
28	0	-1	-1	4.470	0.111	.013
29	-1	0	-1	4.847	-0.126*	-.071*
30	0	0	-1	4.377	0.128*	.059
31	-1	-1	0	3.805	0.140*	.058
32	1	-1	0	3.549	0.102*	.049
33	1	1	0	3.894	-0.087	-.025

The cubic response surface (with significant coefficients (at .10 level)) is

YIELD = 3.86 - .15*CVERN + .08*BETA
+ .77*CGSET + .06*BETA*CGSET
+ .03*BETA*BETA*BETA
+ .11*BETA*CVERN*CVERN
+ .13*BETA*CGSET*CGSET

and has a maximum error of .093 at point 21. The errors (.001) at points 12 and 13 are equal and much smaller than the errors from the quadratic analysis.

If the quadratic response surface equation is applied to the points used in the cubic analysis, the maximum errors (.17) are those present from the quadratic analysis although there are four absolute errors between .10 and .14. The cubic fits the quadratic design points better in all but two cases (points 9 and 15), but these errors are less than .02. The cubic surface fits the additional points better except for three cases where both quadratic and cubic errors are less than .02.

When Fort Pierre data was used, the quadratic response surface and error structure were similar. The coefficients changed since yields were less in the northern latitudes.

YIELD = 2.575 - .10 * CVERN + .15 * BETA
+ .52 * CGSET

These coefficients were the only ones significant at the .10 level.

When Brewster data was used as input to TAMW, the severe water stress caused several changes in the quadratic and cubic surfaces; however, the contributions of the factors remained about the same. The behavior of the yield response is essentially linear, with the higher order terms and interaction terms contributing very little to the predicted response, but yet reducing the prediction errors slightly. The quadratic response surface (with significant coefficients (at .10 level)) is

YIELD = 2.99 + .59 * CGSET - .12*CVERN*CVERN

and has maximum errors of -.14 and .13 at points 10 and 11, respectively. These points are the star points for CVERN (see TABLE 5 for errors).

TABLE 5: Brewster Data and Errors

CVERN	BETA	CGSET	SIM YIELD	BREW-STER quad	BREW-STER cubic	TEMPLE quad (ADJ)
-1	-1	-1	2.310	.090	.005	.235
1	-1	-1	2.209	-.051	.005	.296
-1	1	-1	2.392	.080	.006	-.137
1	1	-1	2.289	-.059	.006	-.010
-1	-1	1	3.466	.068	.006	-.057
1	-1	1	3.314	-.072	.005	.067
-1	1	1	3.589	.059	.005	-.682*
1	1	1	3.433	-.081	.005	-.496*
0	0	0	2.982	-.011	-.007	-.004
-2	0	0	2.369	-.144*	-.011*	-.841*
2	0	0	2.669	.132*	-.011*	-.037
0	-2	0	2.852	-.015	-.004	.454*
0	2	0	3.088	.001	-.004	-.446*
0	0	-2	1.789	-.028	-.004	.345
0	0	2	4.175	.014	-.004	-.345
1	0	-1	2.251	-.057	.004	.140
0	1	-1	2.430	-.017	-.006	.009
0	-1	0	2.921	-.013	-.006	.224
-1	0	0	2.942	.072	.003	-.163
1	0	0	2.814	-.068	.004	-.039
-1	1	0	2.991	.069	.005	-.410*
0	1	0	3.038	-.006	-.006	-.227
0	-1	1	3.505	-.004	-.006	.114
-1	0	1	3.531	.063	.005	-.370
0	0	1	3.579	.001	-.006	-.175
1	0	1	3.377	-.077*	.005	-.216
0	1	1	3.645	.006	-.004	-.462*
0	-1	-1	2.336	-.021	-.004	.335
-1	0	-1	2.354	.084*	.005	.047
0	0	-1	2.386	-.020	-.006	.170
-1	-1	0	2.888	.078*	.005	.089
1	-1	0	2.761	-.063	.005	.180
1	1	0	2.861	-.071	.005	-.254

The cubic response surface (with significant coefficients (at .10 level)) is

YIELD = 2.99 - .11*CVERN + .06*BETA
+ .60*CGSET - .11*CVERN*CVERN
- .01*CGSET*CVERN + .01*BETA*CGSET
+ .05*CVERN*CVERN*CVERN
- .02*CGSET*CVERN*CVERN

and has maximum errors of .011 at points 10 and 11, the star points for CVERN. However, these errors are much smaller than the errors from the quadratic surface.

When the behavior of the Brewster simulations was compared with the expected responses obtained by using the Temple quadratic response equation, the predicted responses at Brewster were all less than the simulated yield. When the predictions were adjusted by the difference in center point responses (-.866), the distribution of errors contained both positive and negative values; however, with the exception of an error of .454 at point 12 -- the negative star point for BETA, all of the "large" errors were negative. The largest error (-.841) occurred at the negative star point for CVERN, point 10 -- as it did for both the quadratic and cubic response equations for Brewster.

5.1 Factor Sensitivities

The relative sensitivities of the factors and factor combinations appear in TABLE 6. The center point yield, which represents the model author's best simulation, dominates the response equation. The contributions of the individual terms are small for points within the unit lattice when compared with the intercept of the response equation and hence, the relative sensitivities are also small. The only term which could change the response by more than 7% corresponds to the pure factor CGSET with a relative sensitivity of .20. In fact, the value of the relative sensitivity for CGSET is .20 for all of the models. BETA has a relative sensitivity close to .07 using the quadratic surfaces for the normal growing season (Temple and Fort Pierre), but only .02 for both Temple and Brewster cubic surfaces; BETA is not part of the quadratic response equation for Brewster. The impact of factor combinations is considerably smaller near the center point, as expected since the higher-order and interaction terms are multiplicative. Although these terms are not meaningless (if the effects are significant), the contribution (for these models) to the yield response is negligible and the terms could be discarded.

For this set of factors -- CVERN, BETA, and CGSET -- the relative sensitivities have been consistent from location to location and from quadratic to cubic response equation. CGSET has influenced the yield in all cases and the parameter value should be well-defined if TAMW is to be used for yield forecasts or estimates. Although the cost of experimentation may be expensive, the performance of the model is heavily dependent on CGSET; CGSET must be accurately measured. BETA, on the other hand, plays a lesser role in model performance and may be less accurately determined.

TABLE 6: Relative Sensitivities

FACTOR	TEMPLE QUAD	TEMPLE CUBIC	FT PIERRE QUAD	BREWSTER QUAD	BREWSTER CUBIC
CVERN	.03	.04	.04	-	.04
BETA	.07	.02	.06	-	.02
CGSET	.20	.20	.20	.20	.20
CVERN**2	-	-	-	.04	.04
BETA**2	-	-	-	-	.00
CVERN*CGSET	-	.01	-	-	.00
BETA*CGSET	-	.02	-	-	.00
CVERN**3		-			.02
BETA**3		.01			-
CVERN*CVERN*BETA		.03			-
CVERN*CVERN*CGSET		-			.01
BETA*CGSET*CGSET		.03			-

5.1 Scaling the Factors

In this approach to sensitivity analysis, the author of the simulation program was expected to state, for each factor, where the "center" setting is to be taken, and where the upper and lower boundaries of "reality" would be assumed. These points were translated into the values zero and plus or minus one, respectively. There is, of course, no reason why the center point should be as far from the left boundary as it is from the right. Attempts have been made to improve the fit of a minimal quadratic response surface by choosing irregular spacing of these points. For example, center points for each of the k factors could be chosen so as to minimize a function of the error of fit. If least squares is used for this purpose, "ridges" appear to occur (i.e., the gradient vector at the minimum is not zero). Further work in this area is in progress.

6.1 Conclusions

The use of response surface techniques to evaluate plant process models has provided some important advantages. The central composite design with a single center point enables us to perform sensitivity analyses on multiple variables and parameters at one time; the existence and contributions of higher-order and interaction terms can be assessed and at reduced cost. If the number of factors becomes large (greater than five), then fractional factorial designs can be implemented.

Quadratic designs have produced a prediction equation for the simulation model which have errors generally less than the errors between the model and field data. Cubic designs are much better because of smaller errors, but the additional points (and additional cost) required for this design make this option less attractive. The use of scaling on the factors -- which are in many cases ordinal or nominal -- in a quadratic design may be an important bridge between the need for more points and the need for lower costs.

The relative sensitivities of the various factors and factor combinations have been consistent under different meteorological scenarios for both the quadratic and cubic designs. The impact of the individual factors on the yield response can be measured and the need for more or less accurate determination of the function or parameter can be assessed.

Further work in factor scaling for quadratic designs is in progress and will be reported at a later time.

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