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INTERVAL ESTIMATION OF ECONOMICALLY OPTIMAL NITROGEN DOSE

Paweł Kobus

*Department of Agricultural Economics and International Economic Relations,
Warsaw University of Life Sciences*

ABSTRACT

The aim of this paper is to propose a procedure for interval estimate of nitrogen dose x_r , which allows to achieve a chosen value of wheat production function derivative r . It is shown that the point estimator of x_r follows asymptotically normal distribution. That fact is used for construction of an asymptotic confidence interval for x_r . It is also shown that substituting r with proportion of input and product unit prices allows to use the proposed formula for interval estimation of economically optimal nitrogen dose. An example of such application based on winter wheat fertilizing experiment is given.

Key words: economical optimization, nonlinear regression, interval estimation.

INTRODUCTION

The choice of fertilizer doses is one of the most basic choices which must be made by a farmer. It influences yield achieved and, consequently, income from plant production.

In this paper the choice of optimal nitrogen dose for winter wheat will be considered. The relationship of wheat yield and nitrogen dose is an instance of production function $f(x)$, where x is a value of the nitrogen dose. Consequently, calculation of optimal dose must be preceded by the choice of an applicable production function. Some of the most popular functions for modelling relationship between yield and nitrogen dose are the quadratic function and the segmented linear function. Nevertheless, they have some flaws. In the case of the quadratic function it is symmetry: in reality, the decrease of yield after reaching maximum, even when physically observed, is slower than the increase before it. For the segmented linear function, it is the sharp change of yield reaction to slightly different doses. In this paper the exponential function proposed earlier by the author [Kobus 2000] will be used as production function.

In an economically optimal point, the proportion (*price of expenditure unit / price of product unit*) equals the value of production function's derivative [Panek 1993]. In our case, the product unit is one ton of winter wheat and the expenditure unit is one kilogram of nitrogen.

Let's assume that the mentioned proportion is r .

Hence the problem of estimating economically optimal nitrogen dose is reduced to the estimation of x for a given value of derivative r .

The main aim of this paper is to assess the possibility of interval estimation of economically optimal nitrogen dose in the case of nonlinear regression function.

Production function

The yield of any plant is a random variable highly dependent on weather and soil conditions, hence the production function can be understood as a relation of the conditional expected value of yield and fertilizer doses rather than relation between yield and fertilizer doses.

Let's consider the following nonlinear regression function:

$$f(x) = \theta_0 - \theta_1 \exp(-\theta_2 x), \quad (1)$$

where $\theta_0, \theta_1, \theta_2$ are positive real number parameters. The derivative of regression function (1) is $f'(x) = \theta_1 \theta_2 \exp(-\theta_2 x)$. Let r be a given value. The problem is to estimate x_r such that $f'(x_r) = r$. Solving that equation gives the following function of parameters θ_1 and θ_2 :

$$x_r = \frac{\log(\theta_2) + \log(\theta_1) - \log(r)}{\theta_2} \quad (2)$$

The natural estimator of x_r may be obtained by substituting parameters θ_1 and θ_2 in equation (2) with their least squares estimates

$$x_r = \frac{\log(\hat{\theta}_2) + \log(\hat{\theta}_1) - \log(r)}{\hat{\theta}_2} \quad (3)$$

Since it was not possible to give explicit formula for θ_1 and θ_2 estimators under the assumption of independent additive normal error, i.e.

$$y_i = \theta_0 - \theta_1 \exp(-\theta_2 x_i) + \varepsilon_i, \quad i = 1, \dots, n, \quad (4)$$

the exact theoretical distribution of x_r estimator remains unknown. In the next section asymptotic approach to distribution of the vector θ and x_r estimates will be explained.

Asymptotic distribution of the vector θ and x_r estimators

In case of normally distributed error, the least squares estimator (LSE) vector θ is equivalent to maximal likelihood estimator (MLE) which has several useful properties: strong consistency, asymptotic normality and asymptotic efficiency [Rao 1982], [Serfling 1991]. In this section asymptotic distribution of vector θ will be identified using existing results for MLE.

Maximal likelihood function for considered model is:

$$L(y, \theta) = \left(\frac{1}{\sigma \sqrt{2\pi}} \right)^n \exp \left[\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - (\theta_0 - \theta_1 e^{-\theta_2 x_i}))^2 \right]. \quad (5)$$

According to properties of MLE, the estimator of vector θ follows an asymptotic normal distribution with an expected value equal to the vector θ and covariance matrix equal to inverse of a Fisher information matrix:

$$\mathbf{I}_\theta = -\mathbf{E}_\theta \left[\frac{\partial^2 \log L(\mathbf{y}, \boldsymbol{\theta})}{\partial \theta_p \partial \theta_m} \right]_{3 \times 3} \quad (6)$$

It is easy to see that due to the form of model (4) \mathbf{I}_{θ} may be written down in a form more friendly to use:

$$\mathbf{I}_\theta = -\mathbf{E}_\theta \left[\frac{\partial^2 \log L(\mathbf{y}, \boldsymbol{\theta})}{\partial \theta_p \partial \theta_m} \right]_{3 \times 3} = \frac{1}{\sigma^2} \left[\sum_{i=1}^n \left(\frac{\partial f(x_i)}{\partial \theta_p} \cdot \frac{\partial f(x_i)}{\partial \theta_m} \right) \right]_{3 \times 3} \quad (7)$$

Where the partial derivative of $f(x_i)$ with respect to θ_0 equals 1, with respect to θ_1 it is $-\exp(-\theta_2 x_i)$, and with respect to θ_2 it is $\theta_1 x_i \exp(-\theta_2 x_i)$.

If we denote by V matrix of derivatives with elements v_{ip} equal to the partial derivative from $f(x_i)$ with respect to θ_p , then

$$\mathbf{I}_\theta = \frac{1}{\sigma^2} \mathbf{V}^T \mathbf{V} \quad (8)$$

Where

$$V^T V = \begin{bmatrix} n & -\sum e^{-\theta_2 x_i} & \theta_1 \sum x_i e^{-\theta_2 x_i} \\ -\sum e^{-\theta_2 x_i} & \sum e^{-2\theta_2 x_i} & -\theta_1 \sum x_i e^{-2\theta_2 x_i} \\ \theta_1 \sum x_i e^{-\theta_2 x_i} & -\theta_1 \sum x_i e^{-2\theta_2 x_i} & \theta_1^2 \sum x_i^2 e^{-2\theta_2 x_i} \end{bmatrix}. \quad (9)$$

Summing up the above facts the covariance matrix of the vector theta estimator may be expressed as $\sigma^2(\mathbf{V}^T \mathbf{V})^{-1}$, and consequently the estimator of x_r is a function of asymptotically normal vector of theta parameters estimators.

According to the theorem given by Serfling [Serfling 1991], a vector function \mathbf{g} of the asymptotically normally distributed vector variable $\mathbf{Z}_n \sim \text{AN}(\mathbf{mu}, \mathbf{b}_n^2 * \mathbf{Sigma})$ is also asymptotically normally distributed i.e. $\mathbf{g}(\mathbf{Z}_n) \sim \text{AN}(\mathbf{g}(\mathbf{mu}), \mathbf{b}_n^2 * \mathbf{D} \mathbf{Sigma} \mathbf{D}^T)$, assuming that every component of the vector function is a real function and the differential \mathbf{D} of function \mathbf{g} in the point $\mathbf{z} = \mathbf{E}(\mathbf{Z})$ is non-zero.

Applying the above-mentioned theorem to the estimator of x_r gives its asymptotic distribution:

$$x_r \sim \text{AN}\left(x_r, \sigma^2 \mathbf{D}(\mathbf{V}^T \mathbf{V})^{-1} \mathbf{D}^T\right) \quad (10)$$

where the derivative vector

$$D = \left[\begin{array}{c} \frac{\partial x_r}{\partial \theta_p} \Big|_{\hat{\theta}=0} \end{array} \right]_{1 \times 3} = \left[\begin{array}{cc} 0 & \frac{\log\left(\frac{r}{\theta_1 \theta_2}\right) + 1}{\theta_2^2} \end{array} \right]. \quad (11)$$

Confidence interval

The problem of interval estimate of x_r is reduced now to well-known estimation of expected value of normal distribution though both parameters of normal distribution expected value and standard deviation, depend on parameters of regression function: θ_1 and θ_2 and on given value of derivative r . In that case the construction of confidence interval can be based on central function:

$$\frac{x_r - x_0}{S_{x_r}}, \quad (12)$$

with assumption that it follows *t-student* distribution with ν degrees of freedom [Rao 1982]. Such assumption can be justified if estimator of x_r and its variation estimate are independent variables with following distributions:

$$x_r \sim N(x_r, \sigma_{x_r}^2), \quad (\nu S_{x_r}^2 / \sigma_{x_r}^2) \sim \chi_\nu^2. \quad (13)$$

The first postulate of x_r estimator normality was validated in the previous chapter. The second postulate has been also checked for various number of Y 's observations n . For each number there was fitted, with satisfactory result, *Gamma* distribution for variable $(S_{x_r}^2 / \sigma_{x_r}^2)$ with shape and scale parameters close to $(n-3)/2$ regardless of the values of parameters: θ_1 and θ_2 of regression function (1).

For example for $n=6$ was fitted $\text{Gamma}(1.56758; 1.49895)$ and for $n=96$ $\text{Gamma}(48.6025, 46.3893)$. Multiplying $(S_{x_r}^2 / \sigma_{x_r}^2)$ by $(n-3)$ resulted in $\text{Gamma}(1.56758, 0.49965)$ and $\text{Gamma}(48.6025, 0.498809677)$ respectively. Hence

$$\frac{(n-3)S_{x_r}^2}{\sigma_{x_r}^2} \sim \chi_{(n-3)}^2, \quad (14)$$

and

$$\frac{x_r - x_r}{S_{x_r}} \sim t_{(n-3)}. \quad (15)$$

Use of central function (15) resulted in following formula for two-sided confidence intervals:

$$P\left\{x_r \in \left(x_r - S_{x_r} t_{(\alpha, n-3)}, x_r + S_{x_r} t_{(\alpha, n-3)}\right)\right\} = 1 - \alpha, \quad (16)$$

and in following formula:

$$P\left\{x_r \in \left(x_r - S_{x_r} t_{(2\alpha, n-3)}, \infty\right)\right\} = 1 - \alpha, \quad (17)$$

for left-sided, where $t(\alpha, n-3)$ is a critical value from Student's t distribution with $(n-3)$ degrees of freedom.

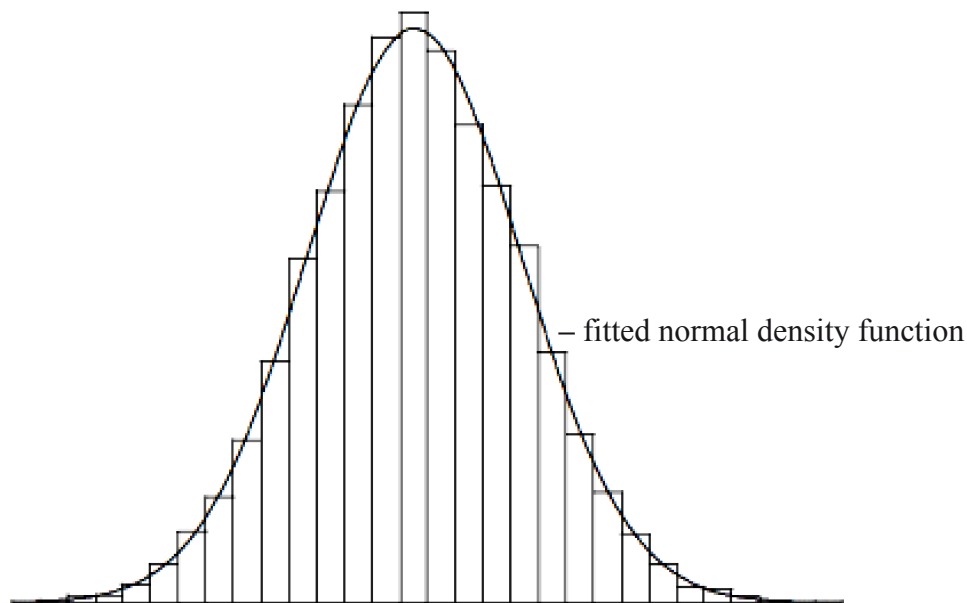
SIMULATIONS

The confidence intervals derived in the previous chapter are asymptotic. The remaining question is whether any number of observations short of infinity is sufficient for the asymptotic properties of x_r estimator distribution to show. In this chapter the results of simulations concerning that question will be shown.

The paper was inspired by a real experiment [Fotyma et al. 1992] where for each value of independent variable x (0, 50, 100, 150, 200, 250) there were 16 observations of dependent variable Y . Calculated values of θ_1 and θ_2 estimators were respectively 1.997 and 0.0278. Hence for the simulations purpose following values of parameter θ_2 were chosen: (0.020, 0.025, 0.030, 0.035, 0.040) and for parameter θ_1 : (1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0). For each combination of parameters values 96 observations of variable Y were generated (16 for each level of the variable x), with error term following normal distribution $N(0, 0.01)$. For every set of generated values of variable Y parameters θ_1 and θ_2 were estimated, and using formula (2) value of x_r estimator was calculated. That procedure was repeated 10000 times.

Picture 1 is typical for all investigated values of parameters: θ_1 , θ_2 and considered values r of derivative.

Empirical distribution of x_r estimator is approximately normal.



Picture 1. Empirical distribution of x_r estimator for $\theta_2=0.035$, $\theta_1=4$ and $r=0.005$.
Source: own calculations.

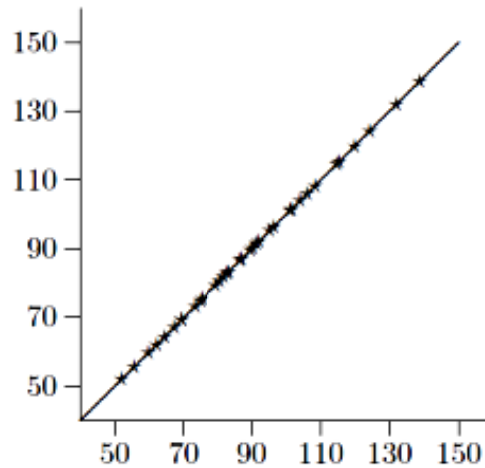
Parameters of x_r estimator distribution for all combinations of parameters: θ_1 , θ_2 and $r=0.005$ are presented in tables 1 and 2.

Table 1. Mean values of x_r estimator

theta ₁	theta ₂				
	0.020	0.025	0.030	0.035	0.040
1.0	69.293	64.348	59.678	55.518	51.856
1.5	89.615	80.606	73.234	67.156	62.068
2.0	104.003	92.119	82.833	75.390	69.285
2.5	115.158	101.045	90.274	81.772	74.875
3.0	124.271	108.336	96.352	86.984	79.439
3.5	131.976	114.501	101.490	91.390	83.296
4.0	138.650	119.841	105.941	95.206	86.637

Source: own calculations.

In all cases the difference between mean x_r estimator and the real value of x_r was very small, ranging from -4.3% up to 1.3% of standard deviation σ_{x_r} on average -0.2%. Hence the bias of x_r estimator can be treated as irrelevant for practical application, see picture 2.



Picture 2. Average values of x_r estimator versus true values of x_r .
Source: own calculations.

Dependence of σ_{x_r} value and parameters θ_1 and θ_2 is more complicated than respective relation for expected value. As one may see in table 2 σ_{x_r} decreases with the increase of parameter θ_1 . The increase of parameter θ_2 results at first in reduction of σ_{x_r} and from some point in the enlarging of σ_{x_r} again. The position of the turning point depends on the value of parameter θ_1 .

Table 2. Standard deviations of x_r estimator

theta ₁	theta ₂				
	0.020	0.025	0.030	0.035	0.040
1.0	2.340	2.445	2.610	2.831	3.122
1.5	2.481	2.428	2.471	2.582	2.757
2.0	2.391	2.263	2.251	2.314	2.437
2.5	2.249	2.089	2.051	2.087	2.180
3.0	2.106	1.931	1.879	1.900	1.975
3.5	1.974	1.794	1.735	1.746	1.807
4.0	1.855	1.675	1.612	1.616	1.669

Source: own calculations.

Also in the case of the standard deviation σ_{x_r} the difference between empirical and theoretical values was very small, ranging this time from -0.3% up to 2.5% of the standard deviation theoretical value, on average it was 0.3%.

What remains to be verified is empirical confidence level of asymptotic interval for x_r .

In table 3 there are presented percentages of covering x_r by two-sided confidence intervals for considered combinations of parameters of θ_1 and θ_2 .

Table 3. Observed level of confidence for theoretical value 95%

θ_1	θ_2				
	0.020	0.025	0.030	0.035	0.040
1.0	79.7%	88.6%	91.5%	92.8%	94.2%
1.5	90.3%	92.3%	93.2%	93.8%	94.3%
2.0	92.2%	93.4%	93.7%	94.1%	94.4%
2.5	93.0%	93.8%	94.0%	94.2%	94.5%
3.0	93.4%	94.1%	94.2%	94.3%	94.6%
3.5	93.7%	94.2%	94.3%	94.4%	94.6%
4.0	93.8%	94.3%	94.4%	94.5%	94.6%

Source: own calculations.

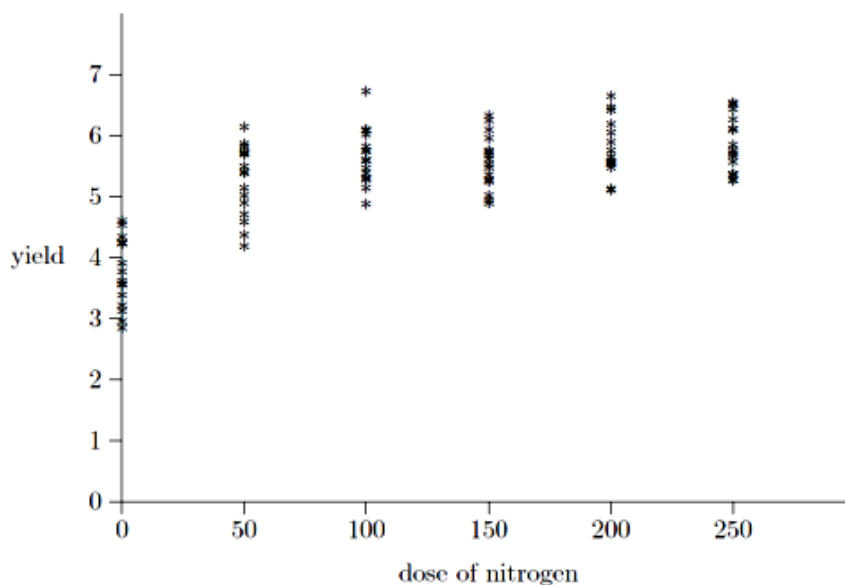
The observed confidence level is on average lower by 1.8% than theoretical one. It may be noted that divergence is getting bigger when values of the parameters θ_1 and θ_2 are small, and on the other hand when θ_1 and θ_2 increase the divergence almost disappear.

Example of application

In picture 3 there are presented results of fertilizing experiment for winter wheat. Fitting of regression function (1) resulted in values of estimators of: $\theta_2=0.0278$, $\theta_1=1.997$ and $\theta_0=5.53$, while their covariance matrix

$$\hat{\sigma}^2(V^T V)^{-1} = 0.3175 \begin{bmatrix} 96.000 & -21.302 & 702.461 \\ -21.302 & 17.058 & -112.657 \\ 702.461 & -112.657 & 12736.512 \end{bmatrix}^{-1}.$$

One of the questions stated by researchers was: "what dose of nitrogen is economically optimal"? or rather to be more precise: "what is the minimal dose of nitrogen which gives reasonable chance of achieving maximal profit"?



Picture 3. Yields of winter wheat for different levels of fertilizing.
Source: own calculations.

Let's assume that proportion (*price of expenditure unit / price of product unit*) is the same as an average in third quarter of the last year [Ceny w ... 2010] i.e. 0.00462.

Hence the problem of estimating economically optimal nitrogen dose is reduced to estimation x_r for given value of derivative $r=0.00462$.

The point estimator of x_r calculated by formula (2) equals 89.43. To calculate standard deviation of that estimator one must first calculate the vector of derivatives \mathbf{D} , in our case

$$\hat{D} = [0 \quad 18.017 \quad -1923.150]$$

Now the estimator of x_r standard deviation can be calculated with application of the following formula:

$$S_{x_r} = \sqrt{\hat{\sigma}^2 \mathbf{D}(\mathbf{V}^T \mathbf{V})^{-1} \mathbf{D}^T}, \quad (18)$$

which results in $S_{x_r}=13.29$.

Having determined the values of x_r estimator and its standard deviation it is possible to obtain two-sided or one-sided confidence intervals for x_r using formula (16) or (17) respectively.

Now it is time to recall the question of researchers: "what is the minimal dose of nitrogen which gives reasonable chance of achieving maximal profit"? Let's denote "minimal dose" by x_m and "reasonable chance" by (1-alpha). Now x_m is such value that: $P(x_r \geq x_m) = \alpha$ and $P(x_r \leq x_m) = 1 - \alpha$. It could be argued that if one wants to be confident on (1-alpha) level that dose x_m is minimal but sufficient for achieving the highest profit, he should set x_m to such value that probability that x_r exceeds x_m is alpha.

In table 4 are presented values of x_m .

Table 4. Approximate x_m

1-alpha	x_m
0.05	67.35
0.1	72.28
0.2	78.19
0.3	82.44
0.4	86.05
0.5	89.43
0.6	92.81
0.7	96.42
0.8	100.67
0.9	106.58

Source: own calculations.

Therefore, if we assume that "reasonable chance" *1-alpha* was set to 0.90 we should use about 106.5kg of nitrogen per hectare.

FINAL CONCLUSION

Distribution of x_r estimator can be modelled with satisfactory quality by normal distribution with an estimator of expected value given by formula (3) and an estimator of standard deviation given by formula (18).

Proposed interval estimation procedure of x_r allows taking into account preferred level of probability of using economically optimal nitrogen dose.

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Department of Agricultural Economics and International Economic Relations
Warsaw University of Life Sciences
ul. Nowoursynowska 166, PL-02-787 Warszawa
e-mail: pawel_kobus@sggw.pl

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