Modeling Soil Test Phosphorus Changes under Fertilized and Unfertilized Managements Using Artificial Neural Networks

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ABSTRACT

The build-up and maintenance criteria have been introduced for P fertilizer management in the Pampas of Argentina. However, methods for predicting soil test P changes under contrasting fertilizer rates are not available. We performed a meta-analysis using results from 18 local field experiments performed under the most common crop rotations, in which soil test P changes with and without P fertilization and soil P balance were assessed. We assembled 329 soil test P variation data sets corresponding to a period 12 yr and 129 P balance records. The P balance was not a good predictor of annual soil test P changes $(R^2 = 0.33)$. In 38% of the cases, the P balance and soil test P changes showed opposite trends. Polynomial regression and artificial neural networks were tested for soil test P modeling. The neural networks performed better than the regressions $(R^2 = 0.91 \text{ vs. } 0.83; P < 0.01)$. The network that yielded the best results used the initial soil test P level, the P fertilization rate and time as inputs. According to the model, unfertilized crops growing in soils with low initial P levels (soil test $P = 10 \text{ mg kg}^{-1}$ or lower) were subjected to only small decreases in soil test P levels, whereas greater decreases occurred in soils with initial high P levels. For fertilized crops, the model showed that P-rich soils were less enriched in P than P-poor soils. A simple meta-model was developed for the prediction of soil test P changes under contrasting fertilizer managements.

Core Ideas

- An artificial neural network was developed to describe soil P dynamics.
- The model accurately predicts soil test P increases and decreases.
- A meta-model was derived to apply the build-up and maintenance philosophy.

▼ HE DEVELOPMENT of methods to predict changes in soil P in cropped soils under contrasting management scenarios is of environmental and agronomic importance. Significant amounts of P may be lost annually from agroecosystems by runoff and lixiviation (Haygarth and Jarvis, 1999), resulting in negative environmental impacts (Foy, 2005). These losses are associated with changes in P concentration in the soil solution (Sharpley, 1995), which in turn is correlated with soil test P levels (Dodd et al., 2012). As soil test P levels decrease, losses also decrease (Dodd et al., 2012). Consequently, knowledge of how much the soil test P level decreases in unfertilized soils with initial high fertility or the impact that high P fertilization rates may have on soil test P levels would provide information on the risk of P losses under specific soil management scenarios. The build-up and maintenance philosophy of fertilizer recommendations is based on a single, large P application that increases the soil test P level to the critical crop level and on the maintenance of this level on the subsequent years through smaller P additions (Black, 1993). Building up the soil test P level in one growing season may lead to better economic returns than a gradual increase in soil test P resulting from small annual applications (Bundy et al., 2005). The negative return of the first year will be counteracted by the gains obtained during the following years because crops will be grown under non-limiting P conditions. To adequately implement this methodology, suitable tools for soil test P change predictions under different fertilizer rates and maintenance requirements must be developed.

The simplest way to estimate the association between changes in soil test P levels and fertilizer use is to regress soil test P levels or changes in these levels as dependent variables against soil P balance (P input as fertilizer – P output in harvested products) or the P output/P input ratio as the predictor variables. In some soils, good fits have been attained using linear models (Aulakh et al., 2007; Tang et al., 2008; Withers et al., 2005); in other cases, curvilinear relationships were more appropriate (Johnston et al., 2014; Wyngaard et al., 2012). However, in some experiments, a poor association was observed between the soil test P level and the P balance. For example, soil test P decreased in the presence of a positive P balance, which was attributed to fixation of labile P into a more stable form (Johnston et al., 2014). In other cases, soil test P did not decrease despite a negative P balance (Johnston et al., 2014; Leikam, 1992). These results were attributed to the

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release of stable P forms into the pool captured in the soil P test (Johnston et al., 2014). Phosphorus losses from the sampled layer or absorption of P from deep soil layers not sampled for soil test P determination could also be responsible for the lack of association between P balance and soil test P changes (Blake et al., 2000). Some experimental networks also showed that P balance was a good predictor of soil test P changes when soils were gaining P but was not adequate for soils in which soil test P declined (Li et al., 2012; Ma et al., 2009). Maintenance requirements are usually not equal to P export in harvested products, are greater than P export in soils that fix P (Black, 1993; Withers et al., 2005), and can be nearly zero in soils that release P (Johnston et al., 2014; Leikam, 1992). Determination of the maintenance requirements must therefore be performed by empirically regressing soil test P against different P fertilization rates (Fixen and Ludwick, 1983).

The Argentine Pampas is one of the most important grain production regions in the world because of its extensive area and yield potential (Satorre and Slafer, 1999). High soil test P (Bray-1) levels are measured in uncropped soils, in which a regional average of approximately 60 mg kg⁻¹ is estimated for the upper 0- to 25-cm layer (Alvarez et al., 2013b). Cropping leads to a sharp decline in soil test P levels, with losses of up to 70 to 80% of the initial values (Alvarez et al., 2015). The build-up and maintenance philosophy was adopted by some farmers, but as the fertilizer/grain price ratio is high, the buildup is usually performed over several growing seasons (Alvarez et al., 2013a). Many short duration (45-90 d) laboratory tests were developed locally to estimate the fertilizer P rate required to increase soil test P levels (Quintero et al., 1999; Rubio et al., 2008; Suñer and Galantini, 2013). When a surplus of P is applied to a soil, either because the P rate is greater than plant absorption or because the experiment is performed without plants, the ratio P surplus/soil test P change indicates the amount of P fertilizer needed to increase soil test P by one unit (Bundy et al., 2005; Leikam, 1992) and can be referred to as the soil test buffering capacity. Extrapolating laboratory results to field conditions with a soil depth of 20 cm, and assuming a local modal value for bulk density, the soil test buffering capacity of Pampean soils that will increase soil test P by 1 mg kg⁻¹ ranges from 3 to 10 kg P ha⁻¹, with an average value of approximately 5 to 6 kg P ha⁻¹. This procedure assumes that the fixation-release transformations that occur in different soil P pools are similar in pot experiments and under field conditions and that losses through runoff or lixiviation are zero. However, stabilization of the soil test P level is not attained during short incubation periods and 1 yr after P addition, the soil test P level may be much lower in many of these soils than 45 to 90 d after P addition (Cabello et al., 2008; Rubio et al., 2016). Experiments performed under field conditions to estimate the soil test buffering capacity in some Pampean soils (Ciampitti et al., 2011; Ferraris et al., 2012; Fernandez Lopez and Ferraris, 2006) show that to increase soil test P by 1 mg kg⁻¹, an average P addition of approximately 10 kg P ha⁻¹ (observed range of 6-14 kg P ha⁻¹) is required. This value is double the laboratory estimates and is similar to values observed in other agricultural regions of the world (Leikam, 1992). Consequently, methods for estimating P build-up requirements under field rather than laboratory conditions are needed. Additionally, there are

no available tools for estimating the decline rate of soil test P level under contrasting fertilizer management scenarios. Our objective was to develop simple methods to predict soil test P changes under contrasting fertilization scenarios that could be used by agronomists when applying the build-up and maintenance philosophy to P fertilization. For this purpose we reviewed results from local experiments in which soil test P evolution was documented over a period of years under contrasting fertilization regimes. In many of these experiments, P balance data were also available or could be calculated to relate P balance to soil test P changes. A meta-analysis was performed using complex techniques, and the results were converted into simple meta-models.

MATERIALS AND METHODS Study Area

The Argentine Pampa is a vast plain that covers an area of approximately 60 Mha located between 28° S and 40° S and 57° W and 68° W. The natural vegetation of this biome is grassland (Hall et al., 1992). The climate is humid and warmtemperate with mean annual rainfall ranging from 500 mm in the West to 1200 mm in the East and mean temperature ranging from 14°C in the South to 23°C in the North. The relief is flat or slightly rolling and the predominant soils are Mollisols (mainly Argiudolls, Hapludolls, and Haplustolls in cropped areas), formed on loess-like materials (Alvarez and Lavado, 1998). Soil texture varies from sandy in the West (up to 900 g kg⁻¹ of sand) to clay in the East (<100 g kg⁻¹ of sand) (Alvarez and Lavado, 1998); the organic C content is low to medium (common range from 5–30 mg kg⁻¹), and the pH of agricultural soils is approximately 6 (Berhongaray et al., 2013). Around half of the area is under agriculture, with soybean [Glycine max (L.) Merr.], wheat (Triticum aestivum L.), and corn (*Zea mays* L.) being the main crops (Min Agri, 2016).

Data Search

To gather all relevant information related to soil test P changes as a function of cropping and fertilization in the Pampas, a literature search of peer-reviewed journals was performed based on the results obtained by using Scopus (https://www.scopus.com/home.uri) and Scholar (https:// scholar.google.com/). The key word combinations used were: Argentina, Pampean Region, soil P test, P fertilization, P balance, P surplus, soil P buffer capacity, and soil test P change. A volume by volume online search of Informaciones Agronómicas, the International Plant Nutrition Institute (IPNI) official publication for the Southern Cone, was also performed. In addition, we searched for papers published in the proceedings of the last 20 yr of the National Congresses of Soils, Wheat, and Corn and in symposiums organized by IPNI in Argentina (25 proceedings) from our archives. Special care was taken so as to not repeat information as in many cases; data were first published in a proceeding or in the IPNI journal, followed by later publication in a peer-reviewed journal with local or international circulation. In these cases, data from the peer-reviewed journal were used. Data from a total of 18 field experiments were compiled (Table 1, Fig. 1); these met the following selection criteria: (i) experiments were performed by official institutions, (ii) management practices were similar

Table I. Some characteristics of the experiments analyzed. Temperature and rainfall data are averages of 30 yr at each experimental site.

Authors	MAT	MAR	Soil	Depth	Clay		님	Duration	Rotation	Soil test P	Avg. P rate	Avg. vield	Avg. harvested P	Avg. P balance
	ပ	mm.		- 5				vears		mg kg ⁻¹	kg P ha ⁻¹ vr ⁻¹	t DM ha ⁻¹ vr ⁻¹		
Barbagelata (2012)	6	1130	₹	0-70	270			4		19–48	0-200		0	
Barbagelata (2012)	6	1130	AC	0-70	400			2		4-15	0-200			
Barraco et al. (2014)	9	830	픋	0-20		27	6.2	12	C-So-Su-W/	15–29	7–23	5.5–5.9	17–18	-9-5
Berardo and Grattone (1998, 2000)	4	950	≰	0-18		62	5.7	9	; >	8–39	0-176	3.2-4.2		
Berardo and Marino (2000a)	4	950	≰	0-15		4	6.2	4	Pasture	5–32	0-100	5.5–8.6		
Berardo and Marino (2000b)	4	950	₹	0-15		4	6.2	4	Alfalfa	5–23	0-100	8.3-13.0		
Ciampitti et al. (2011); García et al. (2010)	17	1050	Ŧ	0-20	8	21	5.9	6	C-W/So	9–15	0–37	8.0–9.0	27–31	-27-4
Ciampitti et al. (2011); García et al. (2010)	17	1050	≰	0-20	8	23	0.9	6	C-W/So	9-26	0–37	8.3–8.9	28–33	-28-3
Ciampitti et al. (2011); García et al. (2010)	8	016	Ŧ	0-20	155	54	9.9	6	C-So-W/So	12–29	0-46	5.8–6.1	26–28	-27-8
Ciampitti et al. (2011); García et al. (2010)	8	016	≰	0-20	205	23	5.6	6	C-So-W/So	40–72	0-46	6.3–6.2	27–28	-28-6
Divito et al. (2010)	4	950	TA-PP	0-20	210	32	5.5	9	C-So-W/So	11–37	0–23	5.1–5.7	14-17	-17-3
Echeverría et al. (2004)	8	016		0-20				-	W/So	15–50	0-150		27–33	-27-117
Echeverría et al. (2004)	8	016		0-20				_	W/So	14-45	0-150		27–32	-27-118
Echeverría et al. (2004)	8	910		0-20				-	W/So	11–36	0-150		31–33	-31-117
Echeverría et al. (2004)	4	940		0-20				_	W/So	8–21	0-150		18–27	-18-123
Ferraris et al. (2015)	9	1030		0-20				∞	C-So-W/ So-B/So	4–26	0–52			-14-28
Vidaurreta et al. (2012)	4	950	TA-PP	0-20		26	2.8	0	W/So-C-So	11-40	0-30			6-71-
Vivas et al. (2007)	8	1030	≰	0-20		76	0.9	٣	W/So-C-So	8 <u>-</u> 18	0–27			-22-3
Wyngaard et al. (2011, 2012)	4	950	TA-PP	0-20		26	5.8	œ	W/So-C-So	11–37	0-30		19–22	6-61-

† MAT = mean annual temperature, MAR = mean annual rainfall, AA = Acuic Argindoll, AC = Argilic Cromudert, TH = Typic Hapludoll, TA = Typic Argindoll, PP = Petrocalcic Paleudoll, OM = organic matter, P = phosphorus, C = corn, So = soybean, Su = sunflower, W/So = wheat/soybean double crop in a year, B/So = barley/soybean double crop in a year.

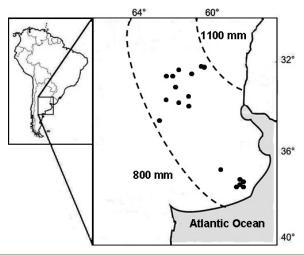


Fig. 1. Map of the Pampean Region indicating location of experimental sites. Some points were slightly moved to avoid overlapping. Dotted lines show isohyets.

to those used by farmers, (iii) P fertilization rates and time of application were clearly specified, (iv) soil test P levels were determined in the upper soil layer, usually 0 to 20 cm, using the Bray 1 method throughout the duration of the experiment, and (v) soils did not receive P fertilizer at least 1 yr before the first soil test P determination. All experiments were located in the humid Pampa, mostly on Mollisols in areas with higher than 800 mm annual rainfall. They generally included an unfertilized control treatment and one or more P fertilization rates. Their duration varied from 1 to 12 yr and in some cases, yield data and P concentration in harvested grains were available, which allowed the calculation of soil P balance (fertilizer P rate- harvested P). Data were obtained from tables or graphs using a program for data acquisition (Getdata Graph Digitizer 2.24). This compilation resulted in 329 data sets on soil test P dynamics, of which 160 consisted of unfertilized control data, and 169 consisted of fertilized treatment data. In addition, 129 P balances records could be calculated.

Modeling Techniques

The evolution of soil test P over time as a function of the P fertilization rate was modeled using two techniques: the common second-order polynomial regression, which included linear, quadratic, and interaction effects (Colwell, 1994) and a feed-forward artificial neural network approach (Jørgensen and Bendoricchio, 2001). The latter methodology has been widely adopted in biological research because it is simpler than process-based models and has high predictive power (Özesmi et al., 2006). Neural networks are adaptive analytical methods that function similarly to human brain neurons, capable of learning on the basis of information that has been presented to them (Jørgensen and Bendoricchio, 2001). Neural networks do not require data normality and produce good fits to nonlinear relationships and complex interactions (Batchelor et al., 1997). The most common network structure consists of three neuron layers: an input layer where each neuron corresponds to an independent (or input) variable, a hidden layer with the number of neurons determined during network development, and an output layer with one neuron equivalent to the dependent variable (or output). Information flows from the input layer,

through the hidden layer, to the output layer. The adjustment of the weights associated to the transfer functions between neurons is called the learning process and consists of comparing network outputs with observed data by using an iterative procedure (Jørgensen and Bendoricchio, 2001). The back propagation algorithm is usually applied (Kaul et al., 2005). This algorithm fits the weights from the output layer to the input layer during the learning process.

Methods for fitting regressions and neural networks have previously been described in detail (Alvarez, 2009). Briefly, data were randomly partitioned as follows: 75% for training (fitting) the models and 25% for cross-validation. Network fitting was performed using 50% of the data while 25% of the data were used for early stopping of weight fitting to avoid overlearning (overfitting) (Park and Vlek, 2002). Linear transfer functions were used between the input layer and the hidden layers and between the output layer and network output, with a sigmoid function connecting the hidden layer to the output layer. The back-propagation algorithm was applied for weight fitting (Rogers and Dowla, 1994). The variables tested as inputs were the mean annual temperature and rainfall of the experimental sites, time since initiation of the experiment, number of crops within a year and soil C (when available), initial soil test P level, annual fertilizer P rate, and cumulative P fertilization rate. A stepwise methodology was applied for model input selection (Gevrey et al., 2003). The learning rate, epoch size, and number of neurons in the hidden layer were fitted as described in Alvarez (2009). The simplest network architecture was applied to use the lowest possible number of inputs and neurons in the hidden layer without losing predictive power as defined by R^2 . Only inputs with a sensitivity ratio larger than one were included in the networks (Miao et al., 2006), and the number of neurons was decreased one at a time from an initial number determined following Somaratne et al. (2005) untill the R^2 value decreased. Statistica (www.statsoft.com) software was used for this purpose.

A polynomial regression was fitted and tested using the same training and validation data sets used for the neural network development. Variables tested as predictors were the same as those tested when fitting the neural networks. A forward stepwise procedure was applied for predictor selection; and the predictors were included in the models only if their effect was significant (P < 0.05). The variance inflator factor was used to prevent autocorrelation (Neter et al., 1990).

Model performance was tested using IRENE, contrasting ordinates and slopes of observed vs. estimated values against 0 and 1, respectively (Fila et al., 2003). The generalization ability of the models was determined by comparing the R^2 value of the training and validation data sets with the Z transformation of Fisher's test (Kleinbaum and Kupper, 1979). When no significant differences were detected between both determination coefficients, it was concluded that the models could be used for generalization for different data sets than those used for their fitting. The root mean square error (RMSE) (Kobayashi and Salam, 2000) was also calculated to evaluate model performance.

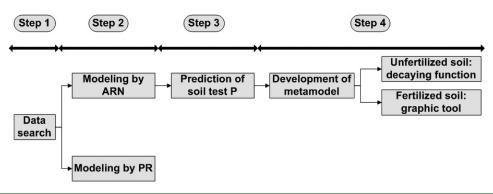


Fig. 2. Flow diagram of the steps followed for development of a meta-model for soil test P changes prediction. ARN = artificial neural network, PR = polynomial regression.

Modeling Soil Test Phosphorus Changes and Meta-Model Generation

Once the best model for soil test P change prediction was selected, variations of the soil P level under contrasting scenarios of initial soil test P level and P fertilization rate were modeled over time using different combinations of these variables and copying observed combinations of the original data set. The output of the selected modeling method was used for meta-model development (Fig. 2). Under unfertilized conditions, the modeled output of the soil test P decay trend in response to cropping and P export was fitted using simple regression functions (linear, quadratic, logarithmic, potential, etc.). Additionally, three kinetic functions, previously used for describing soil test P dynamics, were also fitted (Table 2).

First, the capacity of all tested functions to fit the modeled soil test P decay was assessed using the R^2 value as a decision criterion. After selecting the best function, the parameters of the function were regressed against P_i , and predictive equations were fitted. Then, the overall performance of the function for estimating P_t was assessed using P_i as an independent variable for the estimation of P_t for all soils and sampling times of the original data set. Subsequently, observed (measured in the experiments) vs. estimated (using the selected function) P_t values were compared using regression methods (testing the R^2 value, ordinate and slope). All functions used for soil test P decay fitting were also tested for describing P build-up under different P fertilization rates. The functions were fitted

using Tablecurve software (Systat Software, Inc.). A graphic tool (monogram) was also developed by fitting functions to the outputs of the selected modeling method for build-up P requirements as a function of the soil test P level and P fertilization rate.

RESULTS

Variability of the Data Set

Soil test P levels decreased with time in unfertilized cropped soils (Fig. 3A). The depletion of soil test P was much higher in soils with high initial fertility than in low P soils. Soils with low initial soil test P levels (approximately 10 mg P kg⁻¹ soil) exhibited only a small reduction in soil test P. In these soils, after 2 to 4 yr of cropping without fertilization, the soil test P stabilized with values ranging from 5 to 7 kg P kg⁻¹. When fertilizers were applied, the soil test P levels generally increased. At some sites, fertilized plots had a fivefold higher soil test P level than in their corresponding unfertilized control treatments (Fig. 3B), but in other cases, P fertilization had no impact on soil test P levels. Consequently, fertilization generated a broad range of changes in soil test P levels. The possible relationship between soil test P, soil test P depletion, and yield could not be explored with our data set because cultivated crops, soil, climate, and management conditions varied between the experiments located at different sites and the number of data obtained for possible comparison were very small.

Table 2. Simple kinetic models tested for fitting to soil test P decay.

Model	Equation	Definitions	References
Exponential decay-one pool	$P_t = P_i e^{-kt}$ $k = 0.693/t_{1/2}$	P_t = soil test phosphorus (mg kg ⁻¹) at time t (years) P_i = initial soil test phosphorus k = decaying constant (soil test P fraction depleted by year) $t_{1/2}$ = half-life (time in which soil test P decreases by 50%	Dodd et al., 2012; Eghball et al., 2003; Johnston et al., 2014; McCollum, 1991; Withers et al., 2005
Exponential decay-two pools	$P_t = P_l e^{-klt} + P_r$ $P_i = P_l + P_r$	 P_t = soil test phosphorus (mg kg⁻¹) at time t (years) P_l = labil phosphorus pool P_t = stable phosphorus pool P_i = initial soil test phosphorus kl = decaying constant of the labil phosphorus pool 	Modified from the model used by Ma et al., 2009
Geometric decay	$F = (1+a \times t)^{-b}$ $P_{t} = P_{i} \times F$	F = fraction of initial soil test phosphrous (P_i) remaining at time t (years) a and b = parameters P_t = soil test phosphorus (mg kg ⁻¹) at time t (years)	Barrow, 1980

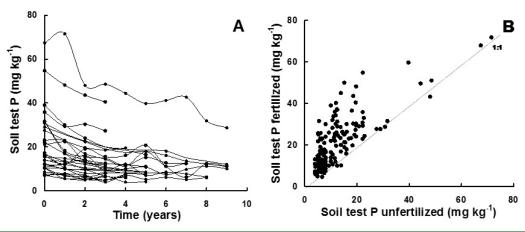


Fig. 3. (A) Change over time of soil test P in the unfertilized treatments of the experiments. Lines connect data from the same experiment. (B) Relationship between soil test P of fertilized and unfertilized treatments of each experiment.

Phosphorus Balance

Phosphorus balance was a poor predictor of soil test P changes (Fig. 4). The correlation between these variables was low and in many soils, showed opposite trends. At some sites, the soil test P levels decreased despite having a positive P balance. This occurred in soils with very high soil test P levels (more than 40 mg P kg⁻¹ soil). Conversely, in other cases, there was no soil test P depletion in spite of a negative P balance. This usually occurred in soils with low soil test P levels (<10 mg P kg⁻¹ soil or lower). In these cases, another method than the balance approach would be needed for soil test P change estimation.

Modeling Method Performance

Changes in soil test P were accurately modeled using polynomial regression and artificial neural networks, among which the latter performed better (P < 0.01). The predictors included in both techniques were the initial soil test P level, time, and cumulative P addition rate. The best network fitted had seven neurons in the hidden layer. The R^2 values of the training and validation data sets did not differ (P < 0.05) for both methodologies, indicating that the models had good generalization ability. The ordinates and slopes of the linear function between

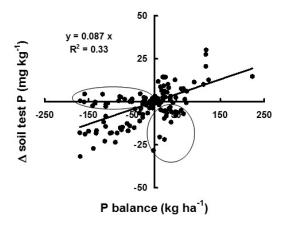


Fig. 4. Changes (Δ) of soil test P as a function of cumulative P balance for each experiment. Ellipses contain the data points for cases in which soil test P decreased despite having positive or null P balances and cases where in spite of negative P balance, the soil test P did not change or even increased.

observed vs. estimated values did not differ from 0 and 1, respectively (Fig. 5). The RMSE values of both methods were acceptable, accounting for an average bias of approximately 4 to 5 mg kg⁻¹ in the soil test P estimates. Despite this, the polynomial regression method predicted some inconsistent results. In P-poor soils (<10 mg P kg⁻¹ soil), a small depletion in soil test P was predicted by the regression when the soils were cropped without fertilization, very similar to the network estimates. However, after 7 to 8 yr of cropping, the regression model also predicted a build-up of soil test P, not accounted for in the observed data. Consequently, the artificial neural network model was selected for soil test P prediction under contrasting management scenarios.

Modeling Soil Test Phosphorus Changes

The best fitted network was used for soil test P modeling as a function of time under contrasting scenarios of soil fertility and fertilizer management (Fig. 6). The model showed that without fertilizer application, soil test P depletion was higher in high P soils. For example, at an initial soil test P level of 50 mg kg⁻¹, 9 yr of cropping without fertilizer application decreased the soil test P level by 27 mg kg⁻¹ ($\Delta P = -54\%$). By contrast, at an initial soil test P level of 10 mg kg⁻¹ the decrease was nearly 3 mg kg⁻¹ $(\Delta P = -30\%)$. Under fertilized management the decreases in soil test P levels were smaller, or a build-up of soil test P occurred. For example, at an initial soil test P value of 50 mg kg⁻¹, the application of 10 kg P ha⁻¹ yr⁻¹ over nine cropping years decreased the soil test P level by 21 mg kg⁻¹ ($\Delta P = -42\%$); resulting in a final value that was 6 mg kg⁻¹ higher than that estimated under non-fertilized conditions. This decrease was the consequence of greater P harvest related to P application. By contrast, the same P fertilization rate increased the soil test P level by nearly 2 mg kg⁻¹ in a soil whose initial soil test P value was 10 mg kg⁻¹ (ΔP = +20%). In the latter case, P build-up may be expected with low P fertilization rates. As expected, higher P fertilization rates resulted in greater soil test P increases.

Meta-Model Development

A meta-model was developed, based on the artificial neural network estimates, to predict soil test P changes under contrasting fertilizer management scenarios. The meta-model was the combination of a kinetic equation and a graphic tool.

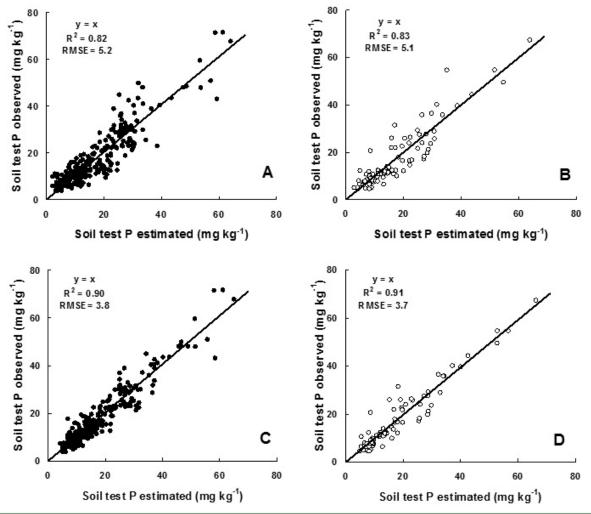


Fig. 5. Relationship between soil test P observed and estimated by the tested modeling methods. (A) Fit by polynomial regression to the training data, (B) fit by polynomial regression to the validation data set, (C) fit by neural network to the training data set, (D) fit by neural network to the validation data set. Subfigures A and B. The regression model fitted was: $P_t = -0.88 + 0.96 \times P_i + 0.087 \times P_c \times$

Under unfertilized scenarios, among the different equations tested for soil test P fitting to the outputs of the artificial network model, the most simple equations yielded poor results, whereas the kinetic models fitted soil test P decay with contrasting performances. The one-pool negative exponential model provided a good fit when the initial soil test P level was >20 mg kg⁻¹ (R^2 > 0.83), but in lower P soils this function underestimated soil test P after a certain number of years, and the fits were poor ($R^2 = 0.1-0.4$). The model could not simulate the steady-state soil test P level in these soils. This problem could be overcome using the two-pool exponential function, which fitted soil test P decay fairly well at both low and high initial soil test P values ($R^2 > 0.97$). Similarly, the geometric model showed very good performance with respect to fitting soil test P decay in unfertilized soils, independent of the initial P level ($R^2 > 0.98$). Because of simplicity, we chose the later model for the meta-model, as it requires two parameters in comparison to the three required by the two-pool exponential function.

The parameters of the geometric model were highly correlated with the initial soil test P level ($R^2 > 0.99$) and could be predicted using this variable (Fig. 7A and 7B). Consequently, the soil test P level at time t in soils that did not receive

fertilization could be estimated by knowing only the initial soil test P value and the time since its measurement. The prediction ability of the decay model was tested against the observed data of soil test P dynamics in unfertilized soils (Fig. 7D). It performed as well as the neural network model, and both the data used for training the network and those used for independent validation were estimated with the same degree of accuracy (\mathbb{R}^2). The ordinate and slope of the linear regression between observed field data and those estimated by the geometric function did not differ from 0 and 1, respectively.

Under the fertilized scenarios, simple regression models or kinetic functions could not be fitted to the network soil test P outputs in many cases. Consequently, as part of the meta-model, a graphic tool was developed for estimating P fertilizer requirements for the maintenance of soil test P (Fig. 8A) or its changes as a function of the P fertilization rate and cropping duration (Fig. 8B). As a simple rule, the P fertilization rates needed for soil test P maintenance were similar to the target soil test P levels. For example, to sustain a soil test P value of 15 mg kg⁻¹, the P fertilization rate must be approximately 15 kg P ha⁻¹ yr⁻¹. The build-up requirements of P depend on the soil test P value and the P fertilization rate. In P-poor soils, soil test P build-up was

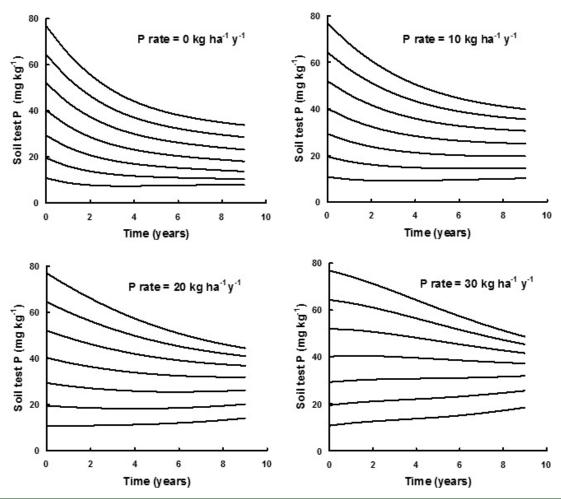


Fig. 6. Predicted dynamics of soil test P modeled using an artificial neural network model as a function of different initial soil test P levels and contrasting application of fertilizer P rates. Phosphorus rates are absolute rates without taken into account harvested P.

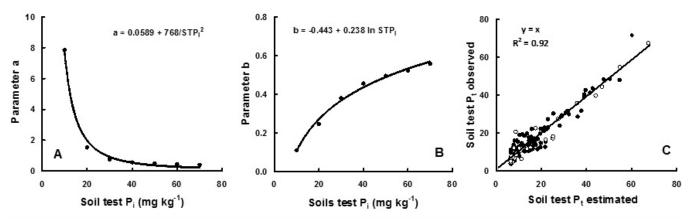


Fig. 7. (A and B) Relationships between the parameters a and b of the geometric decaying model respectively with initial soil test P. (C) Regression of observed soil test P values of unfertilized treatments measured in the experiments along time against those estimated by the metamodel at time t. After determining that the geometric function fitted neural network modeled data the determination of its performance was assessed in a three step procedure: (I) a and b were estimated using equations in panels A and B; (2) soil test P at time t was estimated by the decaying model; (3) observed soil test P data in the field at time t were regressed against estimated values (full drops: training data set used for neural network fit; empty drops: validation data set used for neural network fit).

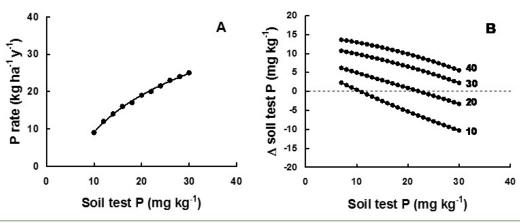


Fig. 8. (A) Required annual P rate for maintenance of the soil test P level (Bray-I). (B) Change (Δ) of soil test P as a function of different annual P rates applied during I0 yr of fertilization. Numbers close to the end of the lines indicate P rates (kg P ha^{-I} yr^{-I}). Points are estimations of the neural network model and lines represent functions fitted to those data points. In both cases P rates were calculated as absolute rates independently of P removed in grains. The meta-model must not be applied to rotations in which annual P off-take in grains is much different than values reported on Table I.

attained under low P fertilization rates, but high rates were needed for P-rich soils. For example, at a P fertilization rate of 20 kg P ha $^{-1}$ yr $^{-1}$, it was possible to build-up soil test P in a soil with an initial level of 10 mg kg $^{-1}$ but not in a soil with an initial soil test P level of 25 mg kg $^{-1}$. Similarly, high P fertilization rates were more efficient for increasing soil test P levels compared with low rates. For example, if 20 kg P ha $^{-1}$ year $^{-1}$ were applied to a soil with a soil test P level of 15 mg kg $^{-1}$, soil test P would increase by 2.9 mg kg $^{-1}$ in 10 yr (the application of approximately 69 kg P increased soil test P by 1 mg kg $^{-1}$), but if the P fertilization rate was 40 kg P ha $^{-1}$ yr $^{-1}$ the soil test P level would increase by 11.6 mg kg $^{-1}$ (the application of approximately 34 kg P increased soil test P in by 1 mg kg $^{-1}$).

DISCUSSION

Dataset Domain

Soil test P data for model fitting were obtained mainly from the 0- to 20-cm soil layer, but in three experiments, the sampling depth was lower (0-15 or 0-18 cm). These experiments were conducted on soils under moldboard plow tillage, in which the average differences in the soil test P level between the 0 to 20 cm and the 0- to 15-cm/0- to 18-cm layers were usually 6% or less (Alvarez and Steinbach, 2012). As this difference would have only a minimal impact on our estimates, these data were incorporated in the analysis. As the available data corresponded to Mollisols with a loam to fine texture in nearly all cases, and no data were available for sandy soils, the developed meta-model cannot be used for the latter soil type. Additionally, the fitted models must not be extrapolated to soils of different mineralogy than the loessic ones to which they were fitted. Soil organic matter did not appear to impact the soil test buffering capacity. When available, this property could not be included in the prediction models despite its considerable variation in the studied soils. Conversely, soil pH usually has a strong impact on the buffering capacity of the soil (Barrow, 2016). The soil pH in our dataset exhibited a small variation, which is common in the Pampas, and therefore the fitted models must not be used for acidified soils.

The ranges of the soil test P level and the P fertilization rates applied were very broad, ensuring ample domain for the graphic tool. This tool can also be used for different rotations

and P balance scenarios but care must be taken if average yields and harvested P values are markedly different from those in our data set, which varied between 20 and 30 kg P ha⁻¹ yr⁻¹. If future yield gains lead to large increases in harvested P, the model must be recalibrated.

Soil Test Phosphorus Dynamics

In these Pampean soils, we observed faster depletion of soil test P in high P soils than in low P soils, and there was a tendency for a steady-state level to be attained even under a negative P balance in very low P soils. Similar results have previously been reported for other areas (Johnston et al., 2014; Ma et al., 2009; Withers et al., 2005). Two conceptual models have been proposed to explain soil P dynamics: the adsorption-diffusion model (Barrow, 2015) and the pool model (Johnston et al., 2014). In the adsorption-diffusion model, it is hypothesized that P added to a soil passes to the soil solution and is then adsorbed on heterogeneous surfaces of soil particles. Subsequently, a solid-state diffusion process takes place into adsorbing particles. This process is sometimes called fixation. Adsorbed P can be desorbed and liberated to the soil solution in a short to medium time period; fixed P cannot. In the pool model, it is hypothesized that soil P is partitioned into four pools: P in the soil solution, surface-absorbed P, strongly absorbed P and precipitated P or P included in minerals. The different pools are connected by fluxes of P between them of different magnitude. The first two pools are highly accessible to plants and captured in common soil test P determinations, whereas the last two pools are not easy accessible to plant. Both models can help to explain the prediction of the artificial neural network. When soil test P declines rapidly in soils with high initial soil test P levels, a flux of P occurs from the soil solution and from P adsorbed onto particles surfaces that do not strongly retain P to more stable forms. This flux declines as soil test P decreases. Phosphorus release from stable forms to the adsorbed P and the soil solution results in steady-state levels of soil test P measured in unfertilized soils under cropping and P off take in harvested products. As a consequence, soil test P in unfertilized soils will decrease to the minimum level that soils can sustain for a certain period of time. This trend can be observed in the Pampean data and was simulated by the network model.

Soil Test Buffering Capacity and Phosphorus Surplus

The inverse of the slope of the regression between soil test P change and cumulative P balance (Fig. 4) is the soil test buffering capacity. An average soil test buffering capacity of 11.5 was estimated using the linear regression model, that is, 11.5 kg ha⁻¹ of P fertilizer would be needed over crop P off take to increase the soil test P level by 1 mg kg⁻¹. Furthermore, the soil test P level would decrease by 1 mg kg⁻¹ when the P balance was –11.5 kg P ha⁻¹. However, the fit of the regression line was poor, and the model cannot be used to apply the build-up and maintenance philosophy to different soils. Soil-specific models appear to be necessary due to the considerable heterogeneity of Pampean soils (Berhongaray et al., 2013). For example, the soil test buffering capacity was strongly influenced by the initial soil test P level in Pampean Argiudolls (Ciampitti et al., 2011). The developed neural model and the meta-model derived from this neural model allowed the estimation of the soil test buffering capacity under a wide range of conditions, which replaced the need for additional extensive experimentation, except for coarse-textured soils.

Modeling Method Selection

The fitted polynomial regression model was more userfriendly; however the neural network was preferred, not only because of its better fit but because of inconsistencies in some estimates of the polynomial model. The second-order exponential model accurately described the decrease in the soil test P level in soils with medium to high P content, but it could not fit the soil test P dynamics in low P soils. The quadratic function and interaction terms on which it was based could not simulate cases where soil test P declined slightly over a few years and then reached a steady-state value. A quadratic multiple regression model is usually not suitable for estimates near data range limits (Onken et al., 1985), as in our case. In addition, the model did not simulate linear P build-up trends. On the other hand, artificial neural networks are especially useful for depicting complex interactions and alterations in curvatures in natural processes (Bishop, 2006) and, as occurs with process-based models, these may be translated into meta-models for providing more user-friendly tools (Haefner, 2005).

Phosphorus Decay Trend in Unfertilized Soils

A decrease in the soil test P levels in unfertilized Pampean soils could be modeled using the one-pool exponential function only when the initial soil test P level was higher than 20 mg P kg⁻¹. In low P soils, in which the decline trend approached linearity, the model did not fit. Above this value, the decay rate was approximately 10% yr⁻¹, and the halflife was 7.5 yr. Studies from other regions showed that the soil test P decline can be accurately described by the negative exponential model (Dodd et al., 2012; Johnston et al., 2014; Withers et al., 2005) despite that in some soils, values from the first or second year of the time series were discarded (Dodd and Mallarino, 2005) or another pool of rapid decline was incorporated into the exponential function (Ma et al., 2009) to improve the fits. The average half-life of soil test P usually ranges from 6 to 9 yr (Eghball et al., 2003; Johnston et al., 2014; Withers et al., 2005), and Johnston et al. (2014)

proposed the use of a simple rule (only one decay constant) for P decline modeling despite the soil initial soil test P level. This cannot be applied to Pampean soils. The two-pools exponential model overcame this problem but it requires the estimation of three parameters (three functions) for its application in the meta-model. Therefore, the geometric progression function appeared to be the best alternative for users.

Build-Up and Maintenance Requirements

Maintenance requirements can be easily estimated using our meta-model on the basis of only the soil test P level. The greater the soil test P value, the greater the P fertilization rate that should be used. Theoretically, the P maintenance rate must counterbalance P export by crops, fixation, and losses (Black, 1993). In soils where fixation is high, the maintenance rate is much greater than harvested P (Fixen and Ludwick, 1983; Withers et al., 2005). As the soil test P level declines, fixation decreases and the maintenance rate is reduced (Leikam, 1992; McCallister et al., 1987), as predicted by the neural network. The network estimated that for soils with low soil test P levels of 10 mg P kg⁻¹, the maintenance rate would approach 10 kg P ha⁻¹ yr⁻¹. Soils with lower soil test P levels would need very low or even no P applications to sustain their P levels, as has been reported for other regions (Leikam, 1992; McCallister et al., 1987), because of P release from low accessibility P pools. In the Pampas, crop critical levels of soil test P commonly varied from 15 to 30 mg kg⁻¹. Consequently, despite soil test P level can be easily maintained in soils with low soil test P, yield response would be expected in these soils with P fertilization and the target soil test P must be the experimental adjusted soil test P threshold beyond which crop response to P is improbable.

The neural model estimated that P build-up can be attained with low P fertilization rates applied to soil with low soil test P levels, but high rates are needed for P-rich soils (Fig. 8B). This type of response of soil test P to fertilizers is common in many soils (Dodd and Mallarino, 2005; McCollum, 1991; Randall et al., 1997) and can be attributed to greater fixation in high P soils (Johnston et al., 2014). The greater efficiency of higher fertilizer P rates in increasing soil test P in comparison to low rates estimated by the model can also be ascribed to an inverse relationship between the P fertilization rate and the fraction fixed (Dobermann et al., 2002; Pote et al., 2003). However, opposite results have been reported (Blake et al., 2003), which have been attributed to an increase in P losses.

The prediction of soil test P changes for different soils based on P balance may be a successful technique when (i) processes such as fixation, runoff, lixiviation, and absorption from deep soil layers are similar between soils and can be summarized into a single slope of the soil test P change–P balance relationship and (ii) the initial soil test P values of the soils are not very different (Ma et al., 2009). This is not the case in Pampean soils. Zhang et al. (1995, 2004) developed a model for predicting soil test P changes using P fertilization rates; the model performed well for the soil for which it was fitted, but it could not be extrapolated to other soils. The artificial neural model developed for the Pampean soils can predict soil test P changes over time using the P fertilization rate and the soil test P levels in different soils. This model does not require yield data or

estimates of P concentration in harvested products, but it must not be applied to rotations that have average harvested P values that are very different from those used for fitting the model. Our estimations are independent of yield data and P surplus only for rotations in which P removed in grains is similar to the values presented in Table 1.

CONCLUSIONS

Our results showed that artificial neural networks are suitable tools for predicting soil test P changes under a wide range of soil and fertilization scenarios. Despite their complexity, neural networks were chosen instead of the balance method or polynomial regression approaches to predict soil test P changes in Pampean soils. The networks are especially appropriate for scientific purposes but when the build-up and maintenance philosophy must be applied by agronomists, simpler methods are needed. A meta-model was developed for predicting soil test P changes with or without P fertilizer application. The soil test P decay rate in unfertilized soils was modeled using a geometric function for which the parameters were estimated using the initial soil test P level. Simple regression models were fitted to achieve this goal. Under fertilized conditions, simple calculation procedures could not be developed, and a graphic tool was proposed for estimating P fertilization requirements for the build-up or maintenance of soil test P.

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