Kinetic diversity indices for the characterization of topsoil formation in natural and augmented ecosystems

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ABSTRACT SUMMARY

We introduce the chemical kinetics for the evaluation of soil ion diversity in order to characterize the relationship between vegetation growth and topsoil formation.
Using two measures that represent invariant features of chemical reaction rate with respect to the total ion concentration and ion balance, we analyzed soil mineral databases from geographically continuous Brazilian savanna and highly biodiverse farming plots and surrounding natural environment in Japan. Combined with the model of self-organized vegetation growth, the developed measures showed distinctiveness and complementarity to interpret the topsoil formation processes through a wide range of spatio-temporal ecological transition. Such a framework of analysis is applicable to wider ecological interactions that can be formalized as a concentration-dependent reaction network.
Keywords: *Soil ion diversity, chemical kinetics, Brazilian Savanna, Synecoculture, augmented ecosystems, ecological optimum, topsoil formation, diversity measure.*

INTRODUCTION, SCOPE AND MAIN OBJECTIVES

We applied two measures of diversity based on the chemical kinetics, to evaluate the topsoil formation with respect to the spatial transition and temporal succession of ecosystems with natural and artificially augmented vegetation. The main objective is to qualitatively characterize the development process of aboveground and underground ecosystems for 1) the total amount, and 2) balance of soil ions, both contribute to maximize chemical reaction rate in soil solution. These measures were defined as invariant quantities that do not depend on the difference of soil moisture, which assures the consistency of the results against local climates' temporal variation such as drought and instantaneous rain.

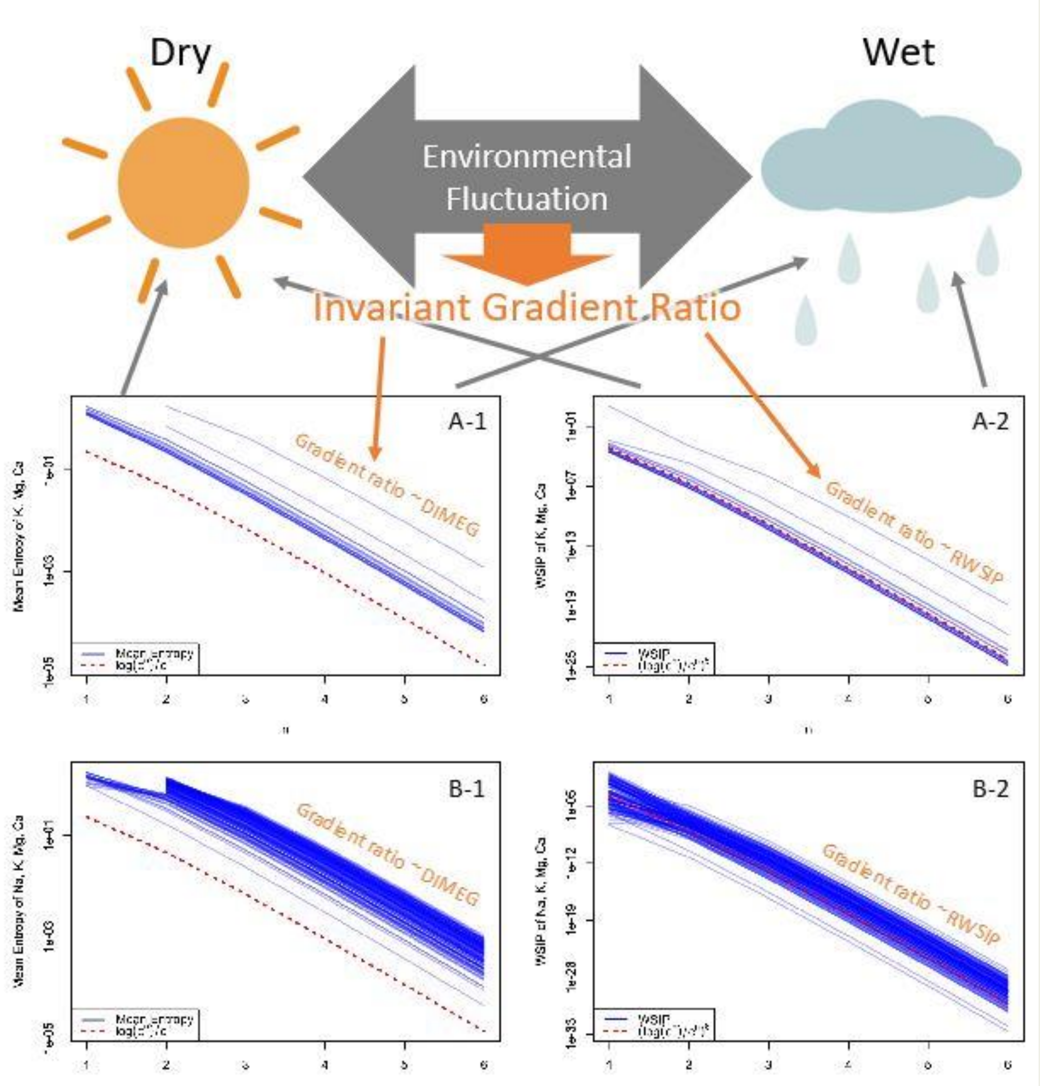

Fig. 1: **Asymptotic behavior of A: Mean Entropy and B: Weighted Self-Information Product (WSIP) in blue lines, applied to soil mineral databases of A-1 and B-1: Brazilian savanna a, and A-2 and B-2: Synecoculture fields and surrounding natural ecosystems b. With respect to the dilution parameters c=10 and n≥1, the gradient ratios between the blue lines and red dotted standard functions converge to constant values, which provide DIMEG and RWSIP scores for each sample. Actual soil solution remains within 4<n<4.7.**

Measure	Sample group 1	Magnitude relation	Sample group 2	p-value
DIMEG	Syneco 0-10cm	>	Syneco 30-40cm	0.0052
DIMEG	Syneco 0-10cm	<	Natural 0-10cm	0.031
DIMEG	Natural 0-10cm	>	Natural 30-40cm	0.00011
DIMEG	Syneco 30-40cm	>	Natural 30-40cm	0.029
DIMEG	Syneco All	<	Natural All	0.29
log(RWSIP)	Syneco 0-10cm	>	Syneco 30-40cm	0.038
log(RWSIP)	Syneco 0-10cm	>	Natural 0-10cm	0.0021
log(RWSIP)	Natural 0-10cm	>	Natural 30-40cm	0.96
log(RWSIP)	Syneco 30-40cm	>	Natural 30-40cm	0.20
log(RWSIP)	Syneco All	>	Natural All	0.0021

Tab 1: **Results of t-test for the difference of mean values between two sample groups from Synecoculture fields ("Syneco") and secondary forests ("Natural") in the same area in Japan. The notation "0-10cm" and "30-40cm" are the sampling depths. "Syneco All" gathers all samples of "Syneco 0-10cm" and "Syneco 30-40cm", and "Natural All" that of "Natural 0-10cm" and "Natural 30-40cm". With respect to the magnitude relationship of mean values, significant differences are highlighted with red (significance level 1%) and blue (5%). To satisfy the normality of distribution, RWSIP was tested in logarithmic scale. Asymptotic behavior of A: Mean Entropy and B: Weighted Self-Information Product (WSIP) in blue lines, applied to soil mineral databases of A-1 and B-1: Brazilian savanna a, and A-2 and B-2: Synecoculture fields and surrounding natural ecosystems b. With respect to the dilution parameters c=10 and n≥1, the gradient ratios between the blue lines and red dotted standard functions converge to constant values, which provide DIMEG and RWSIP scores for each sample. Actual soil solution remains within 4<n<4.7.**

Methodology

Databases: Soil mineral databases of A: four different depths and four transitional vegetation difference from the Cerrado (Brazilian savanna) [a], and B: with two different depths, 34 and 104 samples respectively from natural and augmented ecosystems with edible plant species in Synecoculture project [b].

Measures: 1) **Dilution-Invariant Mean Entropy Gradient (DIMEG)** and 2) **Regularized Weighted Self-Information Product (RWSIP)** defined based on the invariant property of the entropy of chemical reaction [b].

Summary of derivation of the measures: Consider the chemical reaction rate $v = k\prod_{i=1}^{m}[X_i]^{r_i}$ with m reactants, each with concentration $[X_i]$, coefficients r_i, and rate constant k. We convert the unit $[X_i]$ to a probability form, such that ${[X_i]}/{c^n}$, with constant $c > 0$ and scale $n \geq 0$ being the dilution factor. Adding the concentration of inactive elements $q = 1 - \sum_{i=1}^{m}\frac{[X_i]}{c^n} > 0$, the set of $\{[X_i], q\}$ forms a probability distribution, on which we define the Mean Entropy $S = -\sum_{i=1}^{m} r_i \frac{[X_i]}{c^n}\log\frac{[X_i]}{c^n} - q\log q$ as a diversity measure. Since soil solution is largely influenced by external factors in actual open-field situations (e.g., precipitation), we are interested in the measure of chemical reaction that is not affected by a simple dilution. Using the asymptotic analysis, we derive the constant gradient of the mean entropy with respect to the change in dilution parameters represented in the form of standard function ${\log c^n}/{c^n}$:

$$\lim_{n\to\infty}\left(S/\frac{\log c^n}{c^n}\right) = \lim_{n\to\infty}\sum_{i=1}^{m}\left(-r_i\frac{[X_i]}{c^n}(\log[X_i] - n\log c) - q\log q\right)\left(\frac{c^n}{n\log c}\right) = \sum_{i=1}^{m} r_i[X_i],$$

from which we define DIMEG as the dilution-invariant measure of reaction rate,

$$DIMEG := \sum_{i=1}^{m} r_i[X_i].$$

For a given c and n, larger DIMEG value generally represents greater reaction rate. See Fig.1A-1 and B-1 for more intuitive meanings.

Since DIMEG is based on the sum, it can take the same value for different balances of reactants. To distinguish the different reaction rates under the same DIMEG, we develop a complementary measure based on the product of term-wise entropy regularized by DIMEG:

$$\lim_{n\to\infty}\left(\frac{\prod_{i=1}^{m}\left(-\frac{[X_i]}{c^n}\log\frac{[X_i]}{c^n} \Big/ \frac{\log c^n}{c^n}\right)^{r_i}}{\left(S \Big/ \frac{\log c^n}{c^n}\right)^{\sum_{i=1}^{m} r_i}}\right) = \frac{\prod_{i=1}^{m}[X_i]^{r_i}}{DIMEG^{\sum_{i=1}^{m} r_i}},$$

the limit value of which we define as RWSIP,

$$RWSIP := \frac{\prod_{i=1}^{m}[X_i]^{r_i}}{DIMEG^{\sum_{i=1}^{m} r_i}}.$$

It corresponds to the gradient of the weighted self-information product $WSIP := \prod_{i=1}^{m}\left(-\frac{[X_i]}{c^n}\log\frac{[X_i]}{c^n}\right)^{r_i}$ with respect to the dilution parameters $\left({\log c^n}/{c^n}\right)^{\sum_{i=1}^{m} r_i}$. Note that the numerator of RWSIP coincides with the solubility product constant. See Fig.1A-2 and B-2 for the exact relationship between WSIP and RWSIP.

The database analyses in Fig.1 and 2 took after the general chemical equation of soil ion equilibrium:

$$Cl^- + NO_3^- + 2SO_4^{2-} + HCO_3^- + H_2PO_4^- = 2Ca^{2+} + 2Mg^{2+} + K^+ + Na^+$$

The conversion of unit from measured concentration to the probability form of these ions can be calculated from the molecular weight, and in case of choosing $c = 10$, it is situated at the range of $4 < n < 4.7$, which satisfies the convergence of the gradients of Mean Information and WSIP to DIMEG and RWSIP, respectively, in the actual databases as shown in Fig.1.

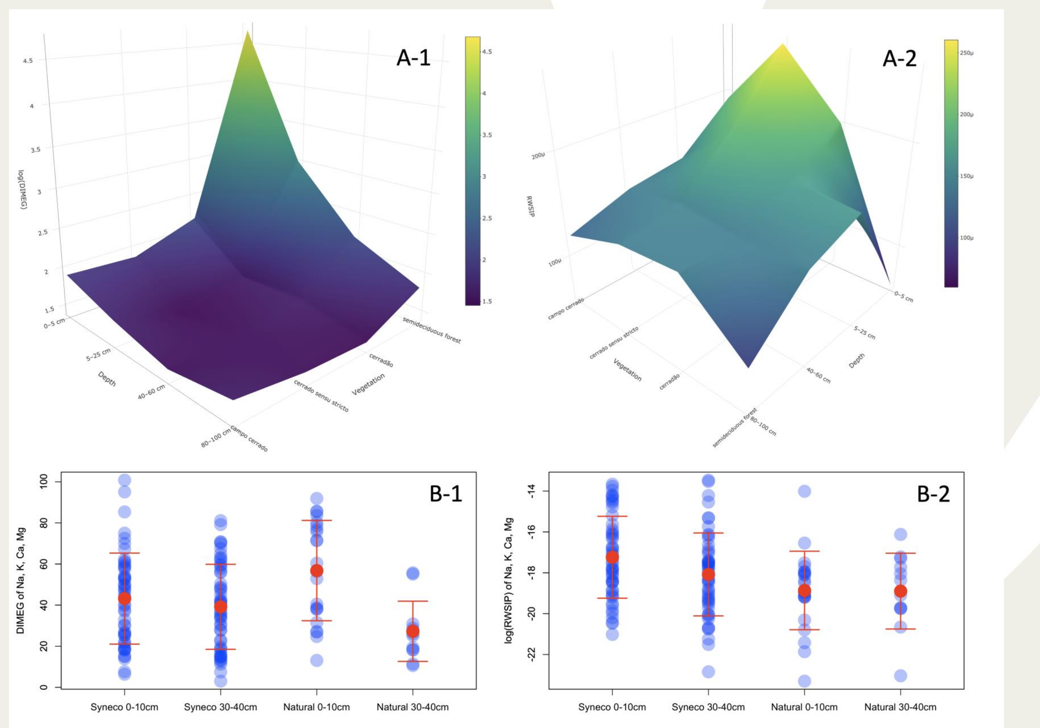

Fig. 2: **A: DIMEG and B: RWSIP scores of A-1 and B-1: Brazilian savanna a (mesh surface), and A-2 and B-2: Synecoculture fields and surrounding natural ecosystems b (blue circles with mean value ± standard deviation in red circles and lines).**

Fig.2 summarize the results of DIMEG and RWSIP scores. In the soil mineral database of Brazilian savanna, the DIMEG scores that represent the total concentration of measured minerals K, Mg, Ca show gradual increase along the vegetation transition from lower savannic formation to semideciduous forest, and the concentration becomes higher towards the soil surface. The RWSIP scores, on the contrary, take the maximum values at higher savannic formation such as cerrado sensu stricto and cerradão (i.e. ecotonic formation between grassland and forest), and remains lower at both ends of campo cerrado and semideciduous forest. The increase of RWSIP towards the soil surface is generally observed, except the low score at the soil surface of semideciduous forest (i.e. established ecosystem with high and dense vegetation). Results from Synecoculture fields and surrounding ecosystems also showed higher concentration of soil minerals Na, K, Mg, Ca at the surface (0-10cm) level, with statistically significant increases of mean DIMEG scores compared to the 30-40cm depth layer (p < 1%). While the surface soil of natural ecosystems showed higher DIMEG values than Synecoculture fields (p < 5%), at the deeper level (30-40cm) the Synecoculture samples contained more concentration of total minerals (p < 5%). There was no significant difference between the overall samples of Synecoculture vs. natural environment. The RWSIP values between Synecoculture vs. surrounding ecosystems showed higher mean value for Synecoculture fields (p < 1%), with significant difference at the surface 0-10cm layer (p < 1%). Only in Synecoculture fields the increase of RWSIP scores towards the surface was significant (p < 5%). The p-values are summarized in Tab.1.

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DISCUSSION

The complementarity between DIMEG and RWSIP shed new insights on the interpretation of savannic formation: while total ion concentration showed monotonal increase towards highly developed vegetation, the soil ion balance became most diverse at the transitional ecotonic formation between grassland and forest. Since natural plant communities that comprise multiple species follow the self-organization process known as ecological optimum c, the qualitative dynamics of DIMEG and RWSIP can be mapped into the different phases of the sigmoidal growth curve (Fig.3): The DIMEG can be interpreted as a proxy of the growth curve of underground ion diversity, while RWSIP corresponds to the growth rate (i.e. differential of the growth curve) because maximizing the diversity in a given concentration leads to the maximization of chemical reaction rate. This model coherently explains the relative magnitude relationship between DIMEG and RWSIP with respect to the spatial transition of vegetation in Brazilian savanna (light blue in Fig.3). Higher mineral concentration at the surface level is another evidence of ecological optimum, where vegetative organic matters mainly stack and decompose at the surface level, which forms nutrient cycle and exerts soil functions supported by chemical buffering capacity (e.g. adsorptive filtration of water through electro-chemical property of soil particles). In coherence with the theory of augmented ecosystems, the qualitative differences between Synecoculture (1-3 years of implementation with an enhanced level of biodiversity) and natural soils (lower species diversity but longer period of topsoil formation) was consistent with such a self-organization view: In both cases soil surface maintained higher concentration of ions, and despite the shorter period of vegetation succession, Synecoculture fields accumulated the same level of soil minerals as in natural ecosystems with longer succession. Major difference was observed at the balance of these ions, which corresponds to the different phases of the growth curve between the ecotonic transition of Synecoculture (i.e. the orange-shaded range in Fig.3, with higher RWSIP values represented as a magenta line) and more established and saturated stage of natural ecosystems (i.e. the green-shaded range in Fig.3, with lower RWSIP values represented as a cyan line).

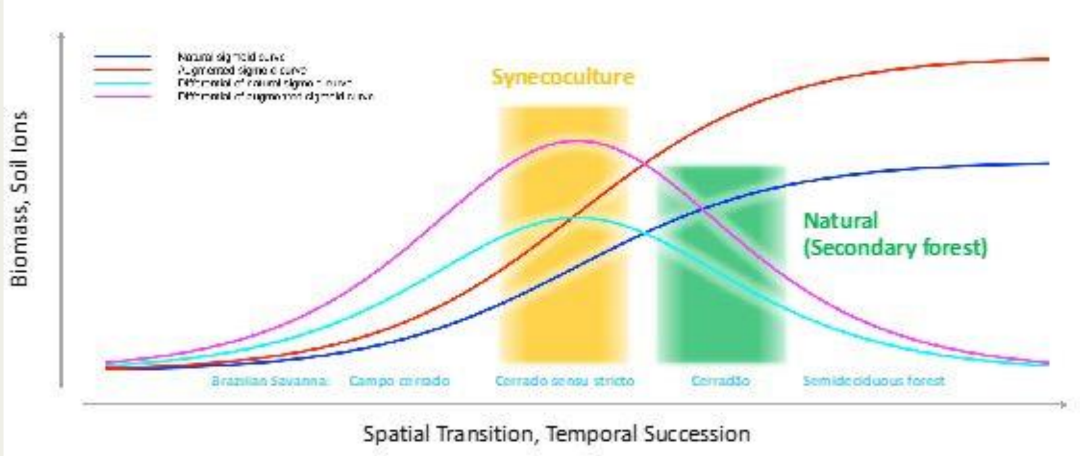

Fig.3 **Qualitative model of vegetation development and soil formation based on the self-organization process of ecological optimum. The cases of Brazilian savanna and Synecoculture experiments are integrated with respect to the relative differences between DIMEG (total ion concentration) and RWSIP (ion balance) scores, which correspond to the sigmoidal growth curves (blue and red lines) and its gradient curves (cyan and magenta lines) , respectively, of the biodiversity measures such as aboveground biomass and underground ion diversity. The blue curve and its cyan gradient represent the spatial transition and temporal succession of natural ecosystems, while the red curve and its magenta gradient those of augmented ecosystems such as Synecoculture fields. The correspondence with analyzed databases is shown as: light blue words indicating the savannic transition in Brazil; orange shade for the succession stage of Synecoculture fields; and green shade for its surrounding ecosystems' sample**

CONCLUSIONS

Two novel diversity indices (DIMEG and RWSIP) incorporating the mechanism of chemical reaction in soil have been constructed, and validated its effectiveness in characterizing natural and augmented ecosystems that contain variability in vegetation transition and succession stages. The developed indices are robust against the open-field fluctuation such as soil water content and provide consistent measures that can be applied to the reinterpretation of existent soil ion databases under variable measurement conditions, and combine with related information on biodiversity. Since the soil chemical property is the essential environment for soil biodiversity, the developed indices may provide important information for the estimation of soil microbial communities using massive data and artificial intelligence d. The complementarity between arithmetic and geometric means is one of the essential strategies for the characterization of complex systems, and further variants of the proposed diversity measures could be considered to unveil hierarchical structure in higher-dimensional databases d. These indices being formally defined on chemical equation, there should be direct applications to dynamical equilibria of general ecological interaction networks beyond soil ion reactions, such as the food chain of soil microorganisms.

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