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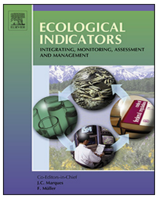

Original Articles

Uncertainty in site classification and its sensitivity to sample size and indicator quality – Bayesian misclassification rate in ecological risk assessment

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ABSTRACT

The aim of this study was to quantify uncertainty when assigning field investigation sites according to their species community composition to either undisturbed or disturbed reference sites by use of ecological indicators. In ecological risk assessment this problem arises when selecting control investigation sites or defining reference species communities. Uncertainty is quantified using a Type II error or misclassification rate. A probabilistic Bayesian model is used to integrate a priori domain knowledge, assess the error rate and come to recommendations about an adequate sample size. Application is demonstrated using data from a case study investigating off-crop arthropod communities in German grassy field margins and consequences for impact assessment of pesticides on terrestrial ecosystems. The model allows calculating statistical power when using such a classification system. By means of stochastic simulations, recommendations about experimental design and indicator size are derived. The study shows that to develop a classification system to typify newly observed sites a well-balanced ratio of undisturbed and disturbed sites as well as a high relevance of reference sites are needed. For the given data set, a much larger number of reference sites as well as increased relevance of selected reference sites would be needed to achieve a good classification result. An optimal number of indicators is calculated allowing for a compromise between sampling error and indicator quality. Uncertainty for correct assignment of an investigation site is compared using indicators for disturbance and reference conditions. Finally, misclassification rate is proposed as a new measure for indicator quality.

1. Introduction

The European Union requires that an ecological risk assessment (ERA) be performed for the authorisation process of plant protection products (PPP) (EC 1107/2009). The aim of ERA is to decide whether there may be a risk of unacceptable adverse effects on the environment, e.g. caused by the chemical substances used in pesticides (www.efsa.europa.eu). Negative effects of pesticides on biodiversity are still a problem in European agricultural landscapes (Geiger et al., 2010). However, to provide important ecosystem functions and services (e.g. pollination, food web support, pest control) it is important that the biodiversity of non-target organisms, like plants and soil arthropods be supported (EFSA PPR Panel, 2014, 2015). This holds for in-field sites, as well as those areas surrounding a field (off-field sites). The latter include field margins and buffer strips that may serve as sources of non-target species, facilitating recovery from impacts in the cropped area (Holland and Luff, 2000). Landscape structures are known to determine properties that to a large extent affect the external recovery of populations (EFSA SC, 2016a,b). The spatial distribution of exposed and non-exposed refuge areas is a particularly important driver for the underlying sink-source dynamics. Thus, to make general protection goals operational, effects of plant protection products on the occupancy of non-target organisms must be quantified at the landscape level.

Potential stressors, such as pesticide exposure, can alter the acceptable range of environmental conditions for populations, communities or ecosystems as normally observed in a reference ecosystem (Normal Operating Range, NOR) (Kersting, 1984; Ravera, 1989). In order to uncover such unacceptable effects of plant protection products, the normal operation range has to be defined using suitable local reference sites (Hughes, 1995; Kilgour et al., 1998; Ottermanns et al., 2010). In

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ecological risk assessment these reference sites have to be found in off-field areas, where the presence of potential stressors can more or less be excluded.

To define reference sites in an ecological risk assessment, the sites have to be assigned to a class of undisturbed or opposed to a class of disturbed sites (statistically referred to as a discriminant analysis). Bioindicators from the observed species compositions can be used to achieve this (Golden and Rattner, 2003). One advantage of using bioindicators is that they tend to integrate effects over time. Indicators can be calculated from species compositions under undisturbed and disturbed conditions using indicator analysis (De Cáceres et al., 2012; Dufrêne and Legendre, 1997). Such an assessment is often focused on detecting a disturbance within the site under investigation. A species that is positively associated with disturbance is called a 'negative indicator' (Carignan and Villard, 2002), and finding such a species can lead to the conclusion that the investigated site is disturbed, and the presence of a potential stressor can be assumed. Not finding the indicator can result in discounting any disturbance or the presence of a potential stressor (statistically referred to as a two-class prediction problem). A species that is positively associated with undisturbed conditions is called a 'positive indicator'. Finding such a species can lead to the conclusion that the investigated site is undisturbed and thus the absence of a potential stressor can be assumed.

When detecting disturbances in such a way, one can make two types of error (Table 1) corresponding to a set of hypotheses. The first hypothesis states that there is no disturbance at the site under investigation. The second hypothesis states that there is a disturbance at the site under investigation. In Type I errors, a disturbance at the site is stated due to finding the indicator for disturbance, despite the absence of a disturbance (α-error, false positive assignment). In Type II errors, a disturbance is neglected due to not finding the indicator for disturbance, despite there being a disturbance (β-error, false negative assignment). A Type II error can be interpreted in different but consistent ways. First, it means that a site is assigned to the undisturbed class although it belongs to the disturbed class. In this case β can be called a misclassification rate. Second, it is the probability of a site belonging to the disturbed class although the indicator for disturbance has not been observed. The same applies to the detections of undisturbed conditions.

It has been pointed out that, in accordance with precautionary principles, β should be minimized in environmental risk assessment and decision-making based on negative indicators. This results in more powerful statistical testing (Power = 1 − β) (Buhl-Mortensen, 1996; Peterman and M'Gonigle, 1992; Sanderson and Petersen, 2002; Santillo et al., 1998; Underwood and Chapman, 2003). In terms of risk protection, for consumers as well as parts of the ecosystem false negative assignments are much more severe and relevant than false positives. The demand for protectiveness is especially important when looking at non-target organisms (Atlas et al., 1978; Montesinos, 2003; Pereira et al., 2009). Due to their important role in ecosystem functioning and services, as well as their sensitivity, arthropods are suitable bioindicators to detect adverse effects. One example is studying the effects of pesticides in impacted German agricultural landscapes (Frampton, 1997; Holland and Luff, 2000; Huusela-Veistola, 1996; Kremen et al., 1993; Rob-Nickoll et al., 2004; Ottermanns, 2008). Given this context and the probabilistic interpretation for β from above, the Type II error can also be referred to as the probability that a pesticide effect exists at a site, but was overlooked using arthropods as bioindicators.

Table 1
The two types of error that can be made when detecting disturbance or undisturbed conditions.

Observation: Disturbance or undisturbed conditions stated?	yes	Type I error α	✓
	no	✓	Type II error β
		no	yes
		Truth: Disturbance or undisturbed conditions present?	

Uncertainty arises at different stages of the risk assessment due to a lack of knowledge and to natural variability (EFSA SC, in press, 2016b). In risk assessment in the field, a crucial source of uncertainty comes from the selection of potentially unaffected references sites. It is especially difficult to find suitable reference systems in heavily modified agricultural landscapes (EFSA SC, 2016b). Nevertheless, to understand the impact of uncertainty on the final assessment outcome, ecological risk assessment must (1) clearly identify the sources of uncertainty, (2) reliably find the range of possible outcomes and (3) exactly quantify the probability of their occurrence (EFSA SC, in press).

The aim of this study was to quantify uncertainty when assigning field investigation sites according to their species community composition by use of ecological indicators to one of two classes, either undisturbed or disturbed sites. In ecological risk assessment this problem arises, for example, when selecting control investigation sites or defining reference species communities. Uncertainty is quantified using the Type II error or misclassification rate. Both classes are characterized by specific indicators, consisting of one or more indicator species i.e., a multiple indicator set. A simple probabilistic Bayesian model was used to integrate a priori domain knowledge, assess the error rate and come to recommendations about an adequate sample size when developing indicators for assessment. Misclassification rate is proposed as a new measure for indicator quality. This is demonstrated using a data set of vegetation and arthropods in grassy field margins from three German macrochores belonging to a class of undisturbed off-field sites not affected by adjacent land use (called references) or a class of off-field sites potentially affected by adjacent land use (spray-drift, called non-target sites). Finally the uncertainty in the correct assignment of an investigation site to the class of undisturbed references was compared using indicators for disturbance (negative indicators) and indicators for reference conditions (positive indicators).

2. Material and methods

2.1. Notation

Throughout this study the following notation is used:

$G = 1$: site belongs to disturbed class = group 1
$G = 0$: site belongs to undisturbed class = group 0
$IG1 = 1$: characteristic indicator (set) for disturbed conditions has been found
$IG1 = 0$: characteristic indicator (set) for disturbed conditions has not been found
$IG0 = 1$: characteristic indicator (set) for undisturbed conditions has been found
$IG0 = 0$: characteristic indicator (set) for undisturbed conditions has not been found
$occ(i,G = k)$: Occurrence of species i over all sites belonging to class k ($k = \{0,1\}$)
$abu(i,G = k)$: Abundance of species i over all sites belonging to class k ($k = \{0,1\}$)
$P(IG1 = 1|G = 1)$: Probability of finding the indicator for disturbed conditions at a site given the site belongs to the disturbed class ($B(G = 1)$) (resp. $IG1 = 0$, $IG0 = 1$, $IG0 = 0$ and $G = 0$), B means the sensitivity from indicator species analysis
$P(G = 1|IG1 = 1)$: Probability of a site belonging to the disturbed class given the indicator for disturbed conditions has been found ($A(G = 1)$), A means the positive predictive value from the indicator species analysis
$P(G = 1|IG1 = 0)$: Probability of a site belonging to the disturbed class given the indicator for disturbed conditions has not been found → false-negative assignment