MEASURING ECOLOGICAL NICHE OVERLAP FROM OCCURRENCE AND SPATIAL ENVIRONMENTAL DATA

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ABSTRACT

1. Aim – Concerns over how global change will influence species distributions, in conjunction with increased emphasis on understanding niche dynamics in evolutionary and community contexts, highlight the growing need for robust methods to quantify niche differences between or within taxa. We propose a statistical framework to describe and compare environmental niches from occurrence and spatial environmental data.
2. Location – Europe, North America, South America
3. Methods – The framework applies kernel smoothers to densities of species occurrence in gridded environmental space to calculate metrics of niche overlap and test hypotheses regarding niche conservatism. We use this framework and simulated species with predefined distributions and amounts of niche overlap to evaluate several ordination and species distribution modeling techniques for quantifying niche overlap. We illustrate the approach with data on two well-studied invasive species.
4. Results – We show that niche overlap can be accurately detected with the framework when variables driving the distributions are known. The method is robust to known and previously undocumented biases related to the dependence of species occurrences on the frequency of environmental conditions that occur across geographic space. The use of a kernel smoother makes the process of moving from geographical space to multivariate environmental space independent of both sampling effort and arbitrary choice of resolution in environmental space. However, the use of ordination and species distribution model techniques for selecting, combining and weighting variables on which niche overlap is calculated provide contrasting results.
5. Main conclusions – The framework meets the increasing need for robust methods to quantify niche differences. It is appropriate to study niche differences between species, subspecies or intraspecific lineages that differ in their geographical distributions. Alternatively, it can be used to measure the degree to which the environmental niche of a species or intraspecific lineage has changed over time.

KEYWORDS

Niche conservatism, niche equivalency, niche similarity, ordination, species distribution model, ecological niche model, kernel density, virtual species, *Centaurea stoebe*, *Solenopsis invicta*.

BIOSKETCH

This work originates from a Workshop on "Progress in predictive species distribution modeling", held in 2008 in Riederalp, Switzerland. OB, MCF, PBP and AG conceived the ideas; OB wrote the scripts and performed the simulations and analyses; OB, MCF, PBP led the writing; OB and MCF provided data for the two invasive species used for illustrating the approach; BP tested the script on further species data not presented here; NGY provided statistical support; AG, CHG, BP, LP, NGY, WT, MJF, CR, and NEZ suggested important corrections to the manuscript.

INTRODUCTION

"It is, of course, axiomatic that no two species regularly established in a single fauna have precisely the same niche relationships" Grinnell (1917)

An ongoing challenge for ecologists is quantifying species distributions and determining which factors influence species range limits (Guisan & Thuiller, 2005; Colwell & Rangel, 2009). Factors that can constrain species distributions include abiotic gradients, such as climate, sunlight, topography and soils, and biotic interactions, such as the identity and abundance of facilitators (e.g. pollinators, seed dispersers), predators, parasites and competitors (Gaston, 2003). The study of how species vary in their requirements for and tolerance of these factors has advanced, in part due to the continued conceptual development and quantification of the ecological niche of species (Chase & Leibold, 2003; Soberón, 2007). The complementary concepts of the environmental niche (sensu Grinnell, 1917) and the trophic niche (sensu Elton, 1927) serve as a basis for assessing ecological and biogeographical similarities and differences among species. Toward this end, a variety of measures have been used to quantify niche characteristics. Historically, such assessments have focused primarily on differences in local trophic and reproductive habits (reviewed in Chase & Leibold, 2003) and have asked: How much does resource use by species A overlap with that of species B? Recent concern over the effects of global change on species distributions has emphasized the need to quantify differences among species in their environmental requirements in a geographical context and at an extent comparable to that of species ranges. Consistent with aspects of the Grinnellian niche, such assessments pursue questions regarding similarities and differences in the environmental conditions associated with species geographical distributions and how they change over time (Devictor *et al.*, 2010). Despite improvements in our ability to model species distributions (Guisan & Thuiller, 2005), development of techniques to quantify overlap of different environmental niches has received relatively little attention (but see Warren *et al.*, 2008).

A variety of approaches and metrics have been used to measure niche overlap (e.g., Horn, 1966; MacArthur & Levins, 1967; Schoener, 1970; Colwell & Futuyma, 1971; May & Arthur, 1972; Pianka, 1980). Generally, these methods date to the period in which competition was widely believed to be the primary mechanism structuring ecological communities and measures of niche overlap were developed to quantify differences due to competition (Chase & Leibold, 2003). More recently, research has elucidated how changing environmental conditions could affect future distributions of native species (e.g. Etterson & Shaw, 2001; Jump & Penuelas, 2005) and invasive exotic species (e.g. Broennimann *et al.*, 2007; Fitzpatrick *et al.*, 2007; Steiner *et al.*, 2008; Medley, 2010). Further, changes in climatic tolerances and requirements of species accompany the diversification of lineages in a variety of taxa (e.g., Silvertown *et al.*, 2001; Losos *et al.*, 2003; Graham *et al.*, 2004b; Yesson & Culham, 2006; Fitzpatrick *et al.*, 2007; Evans *et al.*, 2009). A common theme among these studies is the quantification of environmental niches, how they change over time and differ among species. Yet the inadequacy of methods for comparing species environmental niches has fueled debate over the validity of conclusions derived from comparative studies of niche dynamics (Fitzpatrick *et al.*, 2008; Peterson & Nakazawa, 2008).

Assessing differences in the environmental niches of species requires identification and consideration of the factors that influence species distributions. In practice, distributions of species are often characterized using occurrence records (Graham *et al.*, 2004a). Differences in niches that are quantified using observed occurrences of species reflect an unknown conjunction of the environmental niches of the species, the biotic interactions they experience, and the habitats available to species and colonized by them (Soberón, 2007; Colwell & Rangel, 2009).

Although it has often been assumed that these effects are negligible at broad spatial scales, recent studies indicate that biotic interactions may play an important role in defining the lower thermal boundaries of species' distributions (e.g. Gotelli *et al.*, 2010; Sunday *et al.*, 2011). This subset of the environmental niche that is actually occupied by the species corresponds to the realized niche (Hutchinson, 1957). The environmental conditions comprising the realized niche are described using a set of geographically referenced environmental variables. These variables come from widely used, on-line collections such as WorldClim (Hijmans *et al.*, 2005), a wealth of other variables of some physiological and demographic importance (e.g. Zimmermann *et al.*, 2009), and physical habitat variation as represented by country and regional land cover as well as land use classifications (e.g. Lutolf *et al.*, 2009). Hereafter, the use of geographically referenced variables is often implicit when we refer to niche comparison, but the approaches and metrics we present can be applied to any quantitative niche dimension.

Methods for quantifying the environmental niche and estimating niche differences typically rely on either ordination techniques (e.g. Thuiller *et al.*; 2005a; Hof *et al.*, 2010) or species distribution models (SDMs; Guisan & Thuiller, 2005) Ordination techniques allow for direct comparisons of species-environment relationships in environmental space, and employ various maximization criteria to construct synthetic axes from associated environmental variables (Jongman *et al.*, 1995). In contrast, assessment of niche differences with SDMs involves calibration (for each species) of statistical or machine-learning functions that relate environmental variables to georeferenced data on species occurrence (Guisan & Thuiller, 2005). SDMs can select and emphasize, via weighting, certain variables associated with processes that determine the distribution of the species (through their environmental niches) while down-weighting or excluding variables that do not help to discriminate between species presence and absence (Wintle *et al.*, 2003; Guisan & Thuiller, 2005). Niche overlap is then estimated through the projection of those functions across a landscape (i.e. the overlap is calculated in geographic space). Recently, Warren *et al*. (2008) developed such an SDM-based method that uses cell-by-cell comparisons of geographic predictions of occurrences and randomization tests to quantify niche differences and assess their statistical significance. However, niche overlap analyses using geographic projections of niches derived from SDMs could prove problematic because the measured niche overlap is likely to vary depending on the extent and distribution of environmental gradients in the study area and potentially because of unquantified statistical artifacts related to model fitting.

Here, we present a new statistical framework to describe and compare niches in a gridded environmental space (i.e. where each cell corresponds to a unique set of environmental conditions). Within this framework, we quantify niche overlap using several ordination and SDM techniques and evaluate their performances. The framework overcomes some of the shortcomings of current approaches to quantifying niche differences. It (i) accounts for biases introduced by spatial resolution (grid size), (ii) makes optimal use of both geographic and environmental spaces, and (iii) corrects observed occurrence densities for each region in light of the availability of environmental space. Case studies from nature are unlikely to provide an unbiased assessment of methods used to quantify niche overlap because of sampling errors and unknown biases. To overcome these issues, we test the methods using simulated species distributions for which niche overlap and the constraining environmental gradients are known without error. Finally, we illustrate our approach using two invasive species that have native and invaded ranges on different continents and which have been subjects of recent studies of niche dynamics (Broennimann *et al.*, 2007; Fitzpatrick *et al.*, 2007).

METHODS

A FRAMEWORK TO COMPARE ENVIRONMENTAL NICHES

We present a framework to quantify niche overlap between two species (e.g. sister taxa, subspecies, etc.) or two distinct sets of populations of a same species (e.g. native and invasive populations of an invasive species, geographically disjunct populations of the same species, etc.). The framework also applies to comparisons among the same species but at different times (e.g. before and after climate change). More broadly, the framework can be applied to compare any taxonomical, geographical or temporal groups of occurrences (hereafter called “entities”). The framework involves three steps: (1) calculation of the density of occurrences and of environmental factors along the environmental axes of a multivariate analysis, (2) measurement of niche overlap along the gradients of this multivariate analysis and (3) statistical tests of niche equivalency and similarity (*cf.* Warren *et al.*, 2008). All the analyses are done in R (R Development Core Team 2010) and scripts are available online as Supplementary Material.

1) Calibration of the niche and occurrence density

The environmental space is defined by the axes of the chosen analysis and is bounded by the minimum and maximum environmental values found across the entire study region. In this application, we consider the first two axes for ordinations such as PCA and one axis for SDMs (i.e. the output of an SDM is comprised of a single vector of predicted probabilities of occurrence derived from complex combinations of functions of original environmental variables; the overlap of the two species is analyzed along this gradient of predictions). We recognize that in principle niche overlap analyses can consider greater dimensionality than we do here. However, in practice increased dimensionality brings greater challenges in terms of interpretation, visualization, and additional technical aspects. Nonetheless, a greater number of dimensions should be considered in further development of the present approach. The environmental space is divided into a grid of $r \times r$ cells (or a vector of r values when the analysis considers only one axis). For our analyses we set the resolution r to 100. Each cell corresponds to a unique vector of environmental conditions v_{ij} present at one or more sites in geographical space, where "i" and "j" refer to the cell corresponding respectively to i^{th} and j^{th} bin of the environmental variables. The bins are defined by the chosen resolution r, and the minimum and maximum values present in the study area along these variables.

Since the number of occurrences is dependent on sampling strategy, sampled occurrences may not represent the entire distribution of the species or other taxon nor the entire range of suitable environmental conditions, resulting in underestimated densities in some cells and potentially large bias in measured niche overlap (Supplementary Material, Fig. S1a). Interestingly, this problem is similar to the delimitation of the utilization distribution of species in geographical space. Traditionally, methods such as minimum convex polygons have been used to delimitate utilization distributions (e.g. Blair, 1940). But, newer developments have shown that kernel methods provide more informative estimations (Worton, 1989) and such methods have seen recent application in modeling species distributions (Ferrier *et al.*, 2007; Hengl *et al.*, 2009). We thus apply a kernel density function to determine the "smoothed" density of occurrences in each cell in the environmental space for each dataset. We use the standard smoothing parameters used in most density estimation studies (Gaussian kernel with a standard bandwidth, which corresponds to 0.9 times the minimum of the standard deviation and the interquartile range of the data divided by 1.34 times the sample size to the negative one-fifth power; Silverman, 1986). The smoothed density of occurrence o_{ij} for each cell is thus calculated as

$$o_{ij} = \frac{\delta(n_{ij})}{\max(n_{ij})}, \qquad (1)$$

where $\delta(n_{ij})$ is the kernel density estimation of the number of occurrences of the entity at sites with environment v_{ij}, $\max(n_{ij})$ is the maximum number of occurrences in any one cell, and o_{ij} is a relative abundance index that ranges from 0, for environmental conditions in which the entity has not been observed, to 1 for environmental conditions in which the entity was most commonly observed. In a similar manner, the smoothed density of available environments e_{ij} is calculated as

$$e_{ij} = \frac{\delta(N_{ij})}{\max(N_{ij})}, \qquad (2)$$

where $\delta(N_{ij})$ is the number of sites with environment v_{ij} and $\max(N_{ij})$ is the number of cells with the most common environment in the study area. Finally, we calculate z_{ij} , the occupancy of the environment v_{ij} by the entity, as

$$z_{ij} = \frac{\frac{o_{ij}}{e_{ij}}}{\max\left(\frac{o}{e}\right)} \text{ if } e_{ij} \neq 0, \qquad z_{ij} = 0 \text{ if } e_{ij} = 0, \qquad (3)$$

where z_{ij} ranges between 0 and 1 and ensures a direct and unbiased comparison of occurrence densities between different entities occurring in ranges where environments are not equally available.

2) Measurement of niche overlap

The comparison of z_{ij} between two entities can be used to calculate niche overlap using the D metric (Schoener 1970; reviewed in Warren *et al.*, 2008) as

$$\mathrm{D} = 1 - \frac{1}{2}\left(\sum_{ij} \left| z_{1ij} - z_{2ij} \right|\right),$$

where z_{1ij} is entity 1 occupancy, z_{2ij} is entity 2 occupancy. This metric varies between 0 (no overlap) and 1 (complete overlap). Note that regions of the environmental space that do not exist in geography have z_{ij} set to 0. These regions thus do not contribute to the measure of the D metric and niche overlap is measured among real habitats only (see discussion in Warren *et al.*, 2008, Appendix S2). Note also that the use of a kernel density function when calculating the density is critical for an unbiased estimate of D. When no kernel density function is applied, the calculated overlap depends on the resolution *r* chosen for the gridded environmental space (Supplementary Material, Fig. S1a). Using smoothed densities from a kernel density function ensures that the measured overlap is independent of the resolution of the grid (Supplementary Material, Fig. S1b).

3) Statistical tests of niche equivalency and similarity

We build from the methodology described in Warren *et al.* (2008) to perform niche equivalency and similarity tests. The niche equivalency test determines whether niches of two entities in two geographical ranges are equivalent (i.e. whether the niche overlap is constant when randomly reallocating the occurrences of both entities among the two ranges). All occurrences are pooled and randomly split into two datasets, maintaining the number of occurrences as in the original datasets, and the niche overlap statistic D is calculated. This process is repeated 100 times (to ensure that the null hypothesis can be rejected with high confidence) and a histogram of simulated values is constructed. If the observed value of D falls within the density of 95% of the simulated values, the null hypothesis of niche equivalency cannot be rejected.

The niche similarity test differs from the equivalency test because the former examines whether the overlap between observed niches in two ranges is different from the overlap between the observed niche in one range and niches selected at random from the other range. In other words, the niche similarity test addresses whether the environmental niche occupied in one range is more similar to the one occupied in the other range than would be expected by chance? For this test, we randomly shift the entire observed density of occurrences in one range (the center of the simulated density of occurrence is randomly picked among available environments) and calculate the overlap of the simulated niche with the observed niche in the other range. The test of niche similarity is also based on 100 repetitions. If the observed overlap is greater than 95% of the simulated values, the entity occupies environments in both of its ranges that are more similar to each other than expected by chance. Note that in some instances, it may be difficult to define the extent of the study areas to be compared. When species occur on different continents, the choice cab be straightforward and should consider the complete gradient of environmental space that the study species could reasonably encounter, including consideration of dispersal ability and major biogeographical barriers or transitions. When species occur in the same region or on an island, the environment can be the same for all species and therefore correcting for differences in the densities of environment is not necessary.

TESTING THE FRAMEWORK WITH VIRTUAL ENTITIES

A robust test of the framework described above requires entities that have distributions determined by known environmental parameters and that exhibit known levels of niche overlap. To achieve this, we simulated pairs of virtual entities with varying amounts of niche overlap (see Supplementary Material, Appendix S1), in a study region comprised of all temperate climates in Europe (EU) and North America (NA) and defined by 8 bioclimatic variables at 10' resolution that were derived from raw climatic data from the CRU CL 2.0 dataset (New *et al.*, 2002). These variables included: ratio of actual and potential evapotranspiration (aetpet), number of growing degree days above 5°C (gdd), annual precipitation (p), potential evapotranspiration (pet), number of months with drought (ppi), seasonality in precipitation (stdp), annual mean temperature (t), annual maximum temperature (tmax), and annual minimum temperature (tmin). Procedures to calculate aetpet, pet and gdd from the raw CRU CL 2.0 data are detailed in Thuiller *et al.* (2005b).

We first apply the framework to 100 pairs of virtual entities that differ in niche position and that exhibit decreasing amounts of niche overlap, from perfect overlap (D=1, all areas in common under the normal density curves) to no overlap (D=0, no area in common under the normal density curves). We compare these simulated levels of niche overlap to that measured along the p and t gradients (instead of the two first axes of a multivariate analysis). Since the normal density curves defining the niches of the virtual entities (Supplementary Material, Appendix S1) are built along these two gradients, we postulate that the overlap detected by the application of the framework should be the same as the simulated level of niche overlap across the full range of possible overlap (0:1).

Next, we apply the framework to matched pairs of virtual entities but compare the simulated level of niche overlap to the niche overlap detected along axes calibrated using several ordination (Table 1) and SDM techniques (Table 2). For methods with maximization criteria that do not depend on an *a priori* grouping (here EU vs. NA, Table 1), we run two sets of simulations, using information from either EU alone or both EU and NA to calibrate the method (‘Areas of Calibration’, Tables 1, 2). To compare the outcomes of the methods quantitatively, for each analysis we first calculate the average absolute difference between the simulated and measured overlap (Δ_{abs}). This difference indicates the magnitude of the errors (deviation from the simulated=measured diagonal). To test for biases in the method (i.e. whether or not scores are centered on the diagonal), we then perform a Wilcoxon signed-rank test on these differences. A method that reliably measures simulated levels of niche overlap should both show small errors (small Δ_{abs}) and low bias (non-significant Wilcoxon test).

CASE STUDIES OF REAL SPECIES

We also test the framework using two invasive species that have native and invaded ranges on different continents and which have been subjects of recent analyses of niche dynamics. The first case study concerns spotted knapweed (*Centaurea stoebe,* Asteraceae), native to Europe, and highly invasive in North America (see Broennimann *et al.*, 2007; Broennimann & Guisan, 2008 for details). The second case study addresses the fire ant (*Solenopsis invicta*), native to South America and invasive in the USA (see Fitzpatrick *et al.*, 2007; Fitzpatrick *et al.*, 2008 for details).

RESULTS

EVALUATION OF THE FRAMEWORK

Before applying ordination and SDM methods to our datasets, we examine whether we could accurately measure simulated levels of niche overlap along known gradients. We use 100 pairs of virtual entities with known levels of niche overlap along p and t climate gradients. The overlap we detect between each pair of virtual entities is almost identical to the simulated overlap (i.e. the shared volume between the two simulated bivariate normal curves; filled circles, Fig. 2). This is the case for all levels of overlap except for highly overlapping distributions (>0.8) where the actual overlap is slightly underestimated, and where the effects of sampling are likely to be most evident. Because detected overlap cannot be larger than 100 percent, any error in the measurement of highly overlapping distribution necessarily must result in underestimation. This underestimation is, however, very small (Δ_{abs}:μ = 0.024) and does not alter interpretation. Note that when overlap is measured using virtual entities that follow a univariate normal distribution along a precipitation gradient, no underestimation was observed (Supplementary material, Fig. S2). When we leave differences in environmental availability uncorrected, niche overlap is consistently underestimated (open circles, Fig. 2), except for niches with low overlap (<0.3). This bias is on average five times larger than that of the corrected measure.

NICHE OVERLAP DETECTED BY ORDINATION AND SDM METHODS

Simulated entities

Ordination and SDM techniques vary in their ability to measure simulated niche overlap (Figs. 3-5). Among methods with maximization criteria that do not depend on *a priori* grouping (Fig. 3), PCA-env calibrated on both EU and NA ranges most accurately measures simulated niche overlap (Δ_{abs}:μ = 0.054, *W*: ns; Fig. 3b). Note, however, that highly overlapping distributions are somewhat underestimated but significance of the Wilcoxon test is unaffected. The only other predominantly unbiased method in this category is ENFA, also calibrated on environmental data from both ranges. However, errors generated by ENFA are comparatively high (Δ_{abs}:μ = 0.156, *W*: ns; Fig. 3d). Scores of PCA-occ and MDS are significantly biased, with measured overlap consistently lower than simulated (Fig. 3a, b), especially in ordination of data combined from both EU and NA ranges.

Among methods with maximization criteria based on *a priori* grouping (Fig. 4), WITHIN-env provides the lowest errors of measured overlap. However, WITHIN-env significantly underestimates the simulated overlap (Δ_{abs}:μ = 0.084, *W*:*** Fig. 4b), though the amount of underestimation is small. By contrast, WITHIN-occ overestimates simulated overlap (Δ_{abs}:μ =

0.195, *W*:***; Fig. 4a). Predictably, techniques that maximize discrimination between groups (BETWEEN-occ and LDA; Fig. 4c, d) fail to measure simulated levels of niche overlap adequately. Both methods provide similar results in which overlap is underestimated across all simulated levels.

Compared to ordinations, SDM methods show different patterns when measuring overlap (Fig. 5). When calibrated on both ranges, all SDM methods report high levels of overlap (0.6-1), regardless of simulated overlap. SDMs apparently calibrate bimodal curves that tightly fit the two distributions as a whole. However, when calibrated on the EU range only, all SDM methods report increasing levels of overlap along the gradient of simulated overlap. MaxEnt achieves the best results (Δ_{abs}:μ = 0.111, *W*:ns; Fig. 5b), followed by GBM (Δ_{abs}:μ = 0.134, *W*:*; Fig. 5c). MaxEnt is the only SDM method providing non-significant bias. GLM exhibits a similar amount of error as GBM, but with lower reported overlap (Δ_{abs}:μ = 0.147, *W*:***; Fig. 5a). RF provides very poor results in term of both error and bias (Δ_{abs}:μ = 0.393, *W*:***; Fig. 5d).

Case studies

Analyses of spotted knapweed and fire ant occurrences using PCA-env, the most accurate method in terms of niche overlap detection, show that for both species the niche in the native and invaded ranges overlap little (0.25 and 0.28 respectively, Figs. 6, 7). For spotted knapweed, the invaded niche exhibits both shift and expansion (Fig. 6a-b) relative to its native range. Interestingly, two regions of dense occurrence in NA indicate two known areas of invasion in Western and Eastern NA. In contrast, the fire ant exhibits a shift from high density in warm and wet environments in South America towards occupying cooler and drier environments in NA (Fig. 7a-b). For both species, niche equivalency is rejected, indicating that the two species have undergone significant alteration of their environmental niche during the invasion process (Figs. 6d, 7d). However, for both species, niche overlap falls within the 95% confidence limits of the null distributions, leading to non-rejection of the hypothesis of retained niche similarity (Figs. 6e and 7e).

DISCUSSION

The framework we have presented helps meet the increasing need for robust methods to quantify niche differences between or within taxa (Wiens & Graham, 2005; Pearman *et al.*, 2008a). By using simulated entities with known amounts of niche overlap, our results show that niche overlap can be accurately detected within this framework (Fig. 2). Our method is appropriate to study between-species differences of niches (e.g. Thuiller *et al.*, 2005a; Hof *et al.*, 2010), as well as to compare subspecies or distinct populations of the same species that differ in their geographical distributions and which are therefore likely to experience different climatic conditions (e.g. Broennimann *et al.*, 2007; Fitzpatrick *et al.*, 2007; Steiner *et al.*, 2008; Medley, 2010). Alternatively, when a record of the distribution of the taxa (and corresponding environment) through time exists, our approach can be used to answer the question of whether and to what degree environmental niches have changed through time (e.g. Pearman *et al.*, 2008b; Varela *et al.*, 2010).

This framework presents two main advantages over methods developed previously. First, it disentangles the dependence of species occurrences from the frequency of different climatic conditions that occur across a region. This is accomplished by dividing the number of times a species occurs in a given environment by the frequency of locations in the region that have those environmental conditions, thereby correcting for differences in the relative availability of environments. Without this correction, the measured amount of niche overlap between two entities is systematically underestimated (Fig. 2). For example, in the approach of Warren *et al.* (2008), an SDM-based method using comparisons of geographic predictions of occurrences, projections depend on a given study area. Measured differences between niches could represent differences in the environmental characteristics of the study area rather than real differences between species. Second, application of a kernel smoother to standardized species' densities makes moving from geographical space, where the species occur, to the multivariate environmental space, where analyses are performed, independent of both sampling effort and of the resolution in environmental space (Supplementary Material, Fig. S1). This is a critical consideration, because it is unlikely that species occurrences and environmental datasets from different geographic regions or times always present the same spatial resolution. Without accounting for these differences, measured niche overlap will partially be a function of data resolution.

Although niche overlap can be detected accurately when variables driving the distribution are known (e.g. with niches defined along precipitation and temperature, Fig. 2), the use of ordination and SDM techniques for selecting, combining and weighting variables on which the overlap is calculated provide contrasting results. The causes of the differences in the performance among techniques remain unclear, but several factors might be responsible. Among the important factors are (i) how the environment varies in relation to species occurrences versus the study region (or time period) as a whole, (ii) how techniques select variables based on this variation, and (iii) the level of collinearity that exists between variables within each area/time and whether it remains constant among areas/times. Hereafter we discuss the performance of the techniques we tested in the light of these factors.

ORDINATIONS VERSUS SDMS

Ordinations and SDMs use contrasting approaches to reduce the dimension of an environmental dataset. While ordinations find orthogonal and linear combinations of original predictors that maximize a particular ratio of environmental variance in the dataset, SDMs fit non-linear response curves, attributing different weights to variables according to their capacity to discriminate presences from absences (or pseudo-absences). When using both study regions for the calibration, SDMs consistently overestimate the simulated level of niche overlap (Fig. 5, black circles). Likely, SDMs fit bimodal response curves that tightly match the data and artificially predict occurrences in both ranges (i.e. SDMs model the range of each entity as a single complex, albeit overfitted, niche). As a result, prediction values for occurrences are high for both ranges. Since the overlap is measured on the gradient of predicted values, measured overlap is inevitably high. In contrast, ordinations calibrated on both areas provide a simpler environmental space (i.e. linear combination of original predictors), in which niche differences are conserved. As a result, ordinations usually show a monotonic relationship between detected and simulated overlap (Figs. 3 and 4, black circles).

When calibrating SDMs using only one study area and subsequently projecting the model to another area, estimated overlap increases with simulated overlap (Fig. 5, crosses). However, the pattern of detected overlap using SDMs is irregular (i.e., Δ_{abs}:μ is high), again likely because of overfitting. Bias in detected overlap may also arise from differing spatial structure of environments between study areas. Unlike ordinations, which remove collinearity between variables by finding orthogonal axes, the variable selection procedure of SDMs is sensitive to collinearity. A variable that is not important for the biology of the species, but correlated to one that is, might be given a high weight in the model (e.g. as in the case of microclimatic decoupling of macroclimatic conditions; Scherrer & Korner, 2010). Projection of the model to another area (or continent in the present case) could then be inconsistent with the actual requirements of the species and lead to spurious patterns of detected overlap. In contrast, ordination techniques calibrated on only one study area show a more stable pattern of detected overlap (i.e. monotonic increase, low Δ_{abs}:μ). In general, no SDM method exceeded the performance of the best ordination method.

Based on our results, ordinations seem to be more appropriate than SDMs for investigating niche overlap. However, unlike ordination techniques, SDMs are able to select and rank variables according to their importance in delimiting the niche. SDMs thus could be used to identify variables that are closely related to the processes driving the distribution of the species, while excluding variables that do not discriminate presence and absence. It remains to be tested whether the use of simpler SDM models with more proximal variables (i.e. thus reducing the potential influence of model overfitting and variable collinearity, Guisan & Thuiller, 2005) would improve accuracy of estimated niche overlap. The best practice is to use variables thought to be crucial (i.e. eco-physiologically meaningful) for the biology of the species (Guisan & Thuiller, 2005). Often, uncertainties surrounding the biology of focal species leave us to select variables relevant to the eco-physiology of the higher taxonomic group to which it belongs (e.g. all vascular plants).

DIFFERENCES IN OVERLAP DETECTION AMONG ORDINATIONS

Of the ordination techniques we considered, PCA-env most accurately quantified the simulated level of niche overlap and did so without substantial bias. Unlike PCA-occ, PCA-env summarizes the entire range of climatic variability found in the study area and it is in this multivariate space that occurrences of the species are then projected. Thus, PCA-env is less prone to artificial maximization of ecologically irrelevant differences between distributions of the species.

However, the possibility remains that superior performance of PCA-env might be partly attributable to the fact that our study areas (i.e. Europe and North America) have relatively similar precipitation and temperature gradients that explain most of the environmental variation. The highest performance of PCA-env is likely in situations where species respond to gradients that also account for most of the environmental variation throughout the study region as a whole (i.e. the maximization of the variation of the environment in the study area also maximizes the variation in the niche of the species). Moreover, if this environmental setting prevails in both study areas, issues regarding changes in the correlation structure of variables may be minimal.

PCA-occ, in contrast, uses environmental values at species occurrences only and selects variables that vary most among occurrences. The resulting principal components are calibrated to discriminate even the slightest differences in the correlation of variables at each occurrence. A variable that differs little among locations where the species occurs, but exhibits substantial variation across the study region, likely represents meaningful ecological constraint. Therefore, depending on the environment of the study region (which PCA-occ does not consider), these variables may have undetected ecological relevance (Calenge *et al.*, 2008). If the noise (e.g., climatic variation between regions) is large relative to the signal to measure (i.e. differences in niches between species), the degree of niche overlap could be underestimated (Fig. 3a).

LDA and BETWEEN-occ analyses calibrated using occurrences alone tend to underestimate the simulated level of niche overlap. Both of these methods attempt to discriminate *a priori* chosen groups along environmental gradients. Therefore, these methods will give a higher weight to variables that discriminate the two niches in terms of average positions. For example, in the case of a perfect overlap between the niches on temperature (t) and precipitation (p) variables, these methods will ignore environmental variables most correlated with t and p, and will instead select variables that discriminate the niches, no matter their ecological relevance. Therefore, these methods will tend to erroneously suggest that niches differ more than they actually do. If such group discriminant analyses show high overlap, there is no difference in the average position of the niches along any variable. However, if they show low overlap, one should be aware of the ecological relevance of the components along which the niche average positions differ.

WITHIN-env was the second most reliable method for quantifying niche overlap. This method aims at first remove differences between the two environments and subsequently focuses on differences between the niches in a common multivariate environmental space. All information that is not shared by the two environments is not retained. This approach is more conservative and therefore may be more robust in analyses where two areas (or times) widely differ regarding some variables. A niche shift detected after removing the effect of the different environments is unlikely a statistical artifact and therefore probably represents a true difference or change in the ecology of the species. That said, the superior performance of WITHIN-env in our study is likely related to the manner in which distributions were simulated (equal variance, but different means) and this approach may not perform well if the excluded variables (i.e. the gradients showing largest differences between the two areas) are relevant with respect to niche quantification and, thus, niche overlap between the two distributions. In such cases, only limited conclusions regarding niche differences are possible, although the retained variables may actually be important determinants of the species' niche. In contrast, the WITHIN-occ method (i.e. calibrated on occurrences only) significantly overestimated the simulated degree of overlap. This was expected since the method removes most of the environmental differences found between the two sets of occurrences before comparing the niches. For this reason, we anticipated even greater overestimation of niche overlap.

In the case of ENFA, information is also lost because the two selected axes do not maximize the explained variation. Instead, ENFA constructs the niche using a model with *a priori* ecological hypotheses that are based on the concepts of marginality and specificity (Hirzel *et al.*, 2002). Therefore, ENFA tends to suggest niches are more similar than they actually are.

Despite differences between ordination methods, all were consistent in one aspect. When calibrated on both the EU and NA ranges, the measured niche overlap (filled circles, Fig. 3) was generally lower than the simulated level and also lower than the measured values when calibrated on EU alone (crosses, Fig. 3). When only one range is used in the calibration process, less climatic variation is depicted in the environmental space, thus increasing the overlap between distributions.

REANALYSIS OF CASE STUDIES

In the cases of spotted knapweed, *Centaurea stoebe* (Broennimann *et al.*, 2007) and the fire ant, *Solenopsis invicta* (Fitzpatrick, 2007; Fitzpatrick *et al.*, 2008) niche overlap was originally assessed through the use of a BETWEEN-occ analysis and the calculation of the between-class ratio of inertia that does not correct for environmental availability (spotted knapweed: 0.32; fire ant: 0.40). Although our framework produced different values of niche overlap with PCA-env (spotted knapweed and fire ant 0.25 and 0.28, respectively; Figs. 6 and 7), the conclusions in the original papers do not change. Namely, this reanalysis confirms earlier findings that both spotted knapweed and the fire ant experienced measurable changes in environmental niche occupancy as they invaded North America. The application of our framework to these species results in rejection of the niche equivalency hypothesis. Despite claims to the contrary (e.g. Peterson & Nakazawa, 2008), our analyses confirm that any attempt to predict the niche characteristics from one range to another is inadequate for these species. The results also show that, as would be expected, the invasive niches tend to be more similar to the native niche than random and, thus, niche similarity could not be rejected. In the perspective of niche conservatism, we thus conclude that, as invasive species, spotted knapweed and the fire ant did not significantly retain their environmental niche characteristics from their native ranges.

PERSPECTIVES

We developed and tested our framework using only one set of study areas comprised of all environments present in EU and NA. Virtual entities were created with varying niche positions along environmental gradients but constant niche breadths. We used this setting, which obviously is a subset of situations encountered in nature, because of computational limitations and to simplify the interpretation of the results. Though we believe that this setting provides robust insights to develop best practices for quantification of niche overlap, other situations should be investigated. To explore differences between ordination and SDM techniques more fully, one would need to simulate species distributions with low to high variance of the environment in the study region as a factor that is crossed with low/high variance of the environmental conditions at species occurrences. We cannot exclude that some modeling technique (i.e. such as MaxEnt, the only SDM method which provided irregular, but non-significantly biased results) could be more robust when differences between environments are important.

The framework we illustrate here measures niche overlap using the metric D (Schoener, 1970). Different metrics exist to measure niche overlap (e.g. MacArthur & Levins, 1967; Colwell &

Futuyma, 1971; Warren *et al.*, 2008) and since we provide a description of the niche in a gridded environmental space, these additional measures or metrics could be easily implemented. However we feel that the metric D is the easiest to interpret. This measure indicates an overall match between two niches over the whole climatic space and determines whether we can infer the niche characteristics of one species (subspecies, population) from the other. We argue that SDMs can be reasonably projected outside the calibration area only if the niche overlap is high ($D \approx 1$) and if the test of niche equivalency could not be rejected.

The metric D (as most overlap metrics) does not indicate directionality or type of niche difference and alone cannot tell us whether the niche has expanded, shrunk, or remained unchanged. In a similar vein, because D is symmetrical, the amount of overlap is the same for both entities being compared, even though it is unlikely that the niches of two entities are of the same size. Moreover, D provides no quantitative indication concerning the position and the breadth of the niches (but does provide a visual indication). These additional measures of the directionality of niche change could be easily implemented in our framework in the future.

CONCLUSIONS

How the environmental niches of taxa change across space and time is fundamental to our understanding of many issues in ecology and evolution. We anticipate that such knowledge will have practical importance as ecologists are increasingly asked to forecast biological invasions, changes in species distributions under climatic change, or extinction risks. To date, our ability to rigorously investigate intra- or inter-specific niche overlap has been plagued by methodological limitations coupled with a lack of clarity in the hypotheses being tested. The result has been ambiguity in interpretation and inability to decipher biological signals from statistical artifacts. The framework we present allows niche quantification through ordination and SDM techniques while taking into account the availability of environments in the study area. As in Warren *et al.* (2008), our framework allows statistical tests of niche hypotheses (i.e. niche similarity and equivalency), but under our framework these tests are performed directly in environmental space, thereby allowing correction of bias associated with geographical dimension. Our comparative analysis of virtual entities with known amounts of niche overlap shows that such ordination techniques quantify niche overlap more accurately than SDMs. However, we show that the choice of technique, depending on the structure of the data and the hypotheses to test, remains critical for an accurate assessment of niche overlap. Focusing on rates of change of species niches and a search for consistent patterns of niche lability and/or stability across many taxa will most readily compliment the synthesis of ecological and evolutionary analyses already firmly underway.

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FIGURES AND TABLES

Table 1 – Ordination techniques for quantifying niche overlap. In addition to a general description of the technique, an explanation of its application to the comparison of simulated niches between the European (EU) and North American (NA) continents is provided. Depending on the type of analysis and whether *a priori* groups are used or not, the different areas of calibration we tested are specified.

Name	**Description**	**Areas of Calibration**
PCA-occ	Principal component analysis (Pearson, 1901) transforms a number of correlated variables into a small number of uncorrelated linear combinations of the original variables (principal components). These components are the best predictors – in terms of R^2 – of the original variables. In other terms, the first principal component accounts for as much of the variability in the data as possible, and each following component accounts for as much of the remaining variability as possible. For the study of niche overlap, the data used to calibrate the PCA is the climate values associated with the occurrences of the species. Additional occurrence data can be projected in the same environmental space. When calibrating the PCA with EU and NA occurrences, differences in position along the principal components discriminate environmental differences between the two distributions. When calibrating with EU occurrences only, differences in position along the principal components maximize the discrimination of differences among the EU distribution.	1. Occ. in EU 2. Occ. in EU+NA
PCA-env	Same as PCA-occ but calibrated on the entire environmental space of the two study areas, including species occurrences. When calibrating PCA-env on EU and NA ranges, differences in position along the principal components discriminate differences between the EU and NA environmental spaces whereas a calibration on the EU full environmental space maximizes the discrimination among this range only.	1. EU range 2. EU&NA ranges
BETWEEN-occ & WITHIN-occ	Between-group and Within-group Analyses (Doledec & Chessel, 1987) are two ordination techniques that rely on a primary analysis (here PCA, but could be CA or MCA) but use *a priori* groups to optimize the combination of variable in the principal components. Here the *a priori* groups correspond to EU and NA. BETWEEN-occ and WITHIN-occ are calibrated with EU&NA occurrences, and respectively maximizes or minimizes the discrimination of niche differences between EU and NA occurrences.	1. Occ. in EU+NA
WITHIN-env	Same as WITHIN but calibrated on the entire environmental spaces of the two continents. WITHIN-env minimizes the discrimination of environmental differences between EU and	1. EU&NA

	NA ranges.	ranges
LDA	Linear Discriminant Analysis (LDA; Fisher, 1936) finds linear combinations of variables which discriminate the differences between two or more groups. The objective is thus similar to BETWEEN but uses a different algorithm. Distances between occurrences are calculated with Mahalanobis distance.	1. Occ. in EU+NA
MDS	Multidimensional Scaling (MDS; Gower, 1966) is a non-parametric generalization of PCA that allows various choices of measures of associations (not limited to correlation and covariance as in PCA). Here we use the distance in the Euclidean space. The degree of correspondence between the distances among points implied by MDS plot and the input distance structure is measured (inversely) by a *stress* function. Scores are juggled to reduce the stress until stress is stabilized.	1. Occ. In EU 2. Occ. in EU+NA
ENFA	Ecological Niche Factor Analysis (ENFA; Hirzel *et al.*, 2002). ENFA is an ordination technique that compares environmental variation in the species distribution to the entire area. This method differs from other ordination techniques in that the principal components have a direct ecological interpretation. The first component corresponds to a marginality factor: the axis on which the species niche differs at most from the available conditions in the entire area. The next components correspond to specialization factors: axes that maximize the ratio of the variance of the global distribution to that of the species distribution.	1. Occ. in EU + EU range 2. Occ. in EU&NA + EU&NA ranges

Table 2 – SDM techniques for quantifying niche overlap. GLM, GBM and RF were fitted with species presence-absence as the response variable and environmental variables as predictors (i.e. explanatory variables) using the BIOMOD package in R (Thuiller *et al.*, 2009, R-Forge.R-project.org) and default settings. MaxEnt was fitted using the *dismo* package in R with default settings. For all techniques, we use pseudo-absences that were generated randomly throughout the area of calibration. Two sets of models were created using two areas of calibration: one using presence-absence data in EU only and a second using presence-absence data in both EU and NA. The resulting predictions of occurrence of the species (ranging between 0 and 1) are used as environmental axes in the niche overlap framework.

Name	**Description**
GLM	Generalized linear models (GLM; McCullagh & Nelder, 1989) constitute a flexible family of regression models, which allow several distributions for the response variable and non-constant variance functions to be modeled. Here we use binomial (presence-absence) response variables with a logistic link function (logistic regression) and allow linear and quadratic relationship between the response and explanatory variables. A stepwise procedure in both directions was used for predictor selection, based on the Akaike information criterion (AIC; Akaike, 1974).
MaxEnt	MaxEnt (Phillips *et al.*, 2006) is a machine learning algorithm that estimate the probability of occurrence of a species in contrast to the background environmental conditions. MaxEnt estimates species' distributions by finding the distribution of maximum entropy (i.e. that is most spread out, or closest to uniform) subject to the constraint that the expected value for each environmental variable under this estimated distribution matches its empirical average. MaxEnt begins with a uniform distribution then uses an iterative approach to increase the probability value over locations with conditions similar to samples. The probability increases iteration by iteration, until the change from one iteration to the next falls below the convergence threshold. MaxEnt uses L-1 regularization as an alternative to stepwise model selection to find parsimonious models.
GBM	The gradient boosting machines (GBM; Friedman, 2001) is an iterative computer learning algorithm. In GBMs, model fitting occurs not in parameter space but instead in function space. The GBM iteratively fits shallow regression trees, updating a base function with additional regression tree models. A randomly chosen part of the training data is used for function fitting, leaving the other part for estimating the optimal number of trees to use during prediction with the model (out-of-bag estimate).
RF	Random Forests (RF; Breiman, 2001). Random Forests grows many classification trees. To classify the species observations (i.e. presences and absences) from the environmental variables, RFs puts the variables down each of the trees in the forest. Each tree gives a classification, and the tree "votes" for that class. The forest chooses the classification having the most votes (over all the trees in the forest). Random forests is designed to avoid overfitting.

Figure 1 - Example of virtual species following a bivariate normal density along precipitation and temperature gradients with 50% overlap between the European and North American niche in environmental space. Red to blue color scale shows the projection of the normal densities in the geographic space from low to high probabilities. Black dots show random occurrences.

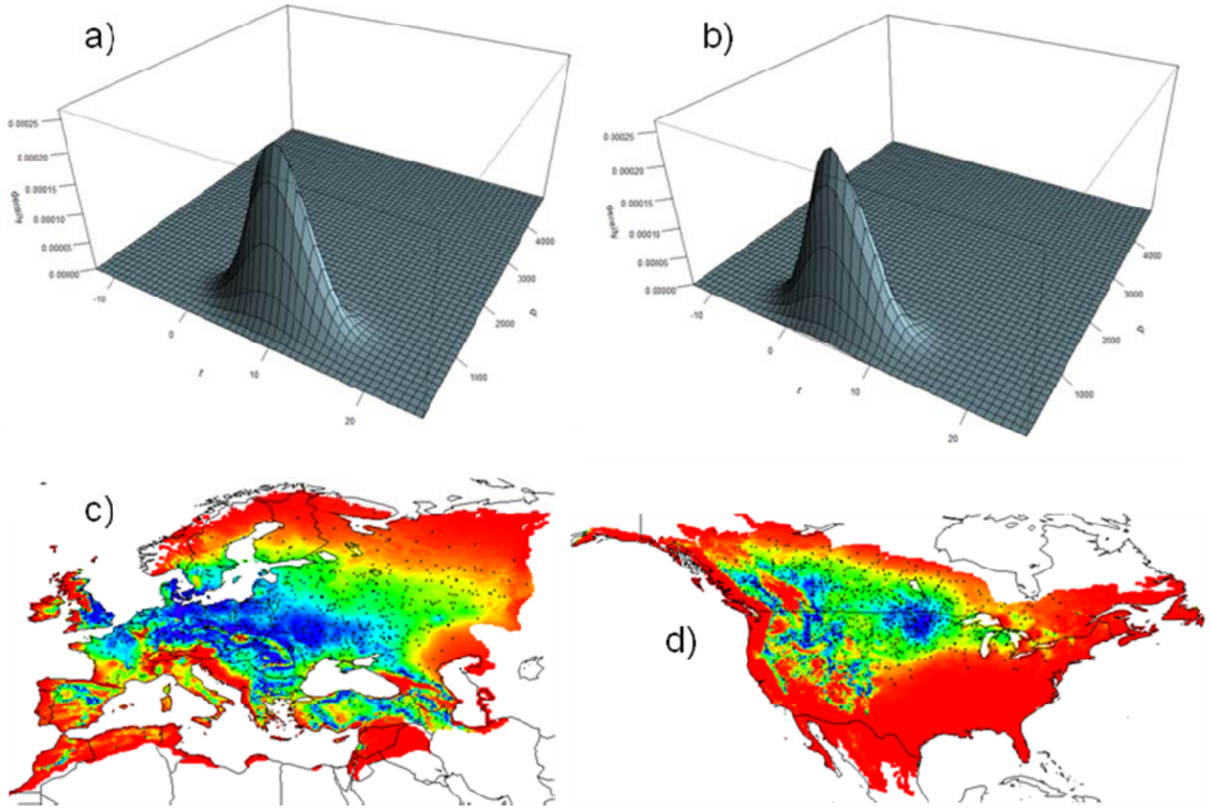

Figure 2 - Agreement between simulated and detected niche overlap. Each dot corresponds to a pair of simulated entities. Simulated overlap corresponds to the volume in common between the two bivariate normal distributions with different means on p and t gradients (see Fig. 1). Filled circles represent the detected overlap with correction for climate availability (density of occurrences divided by the density of climate across the entire climate space). Open circles show the detected overlap when no correction for climate availability is applied. The average absolute difference between the simulated and measured overlap (abs(Δ): μ) is indicated for both corrected and uncorrected measures.

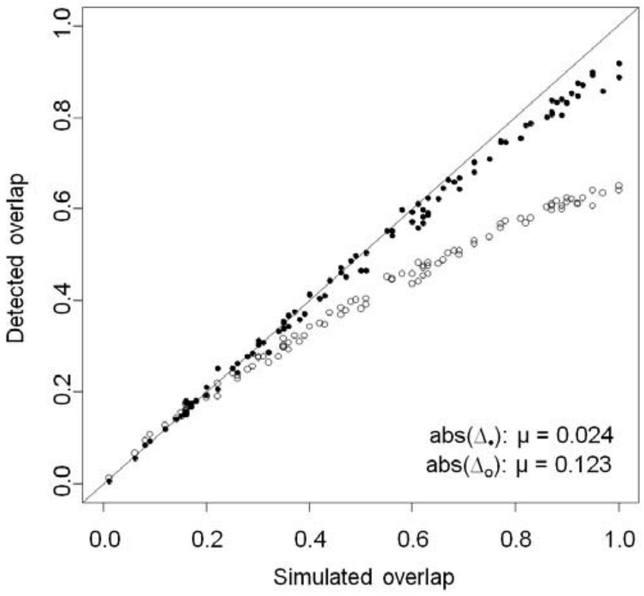

Figure 3 - Sensitivity analysis of simulated versus detected niche overlap for ordinations not using a grouping factor. The axes of the analyses on which the overlap is measured correspond to a) PCA-occ, b) PCA-env, c) MDS and d) ENFA. Crosses refer to models calibrated on the EU range only. Black dots indicate models calibrated on both EU and NA ranges. Results for ENFA calibrated on the EU range only could not be provided because of computational limitations. Abs(Δ): μ indicate the average absolute difference between simulated and detected overlaps. The significance of the Wilcoxon signed-rank test, *W*, is shown (ns: non-significant, *: 0.05<*p*-value<0.01, **: 0.01<*p*-value<0.001, ***: *p*-value<0.001)

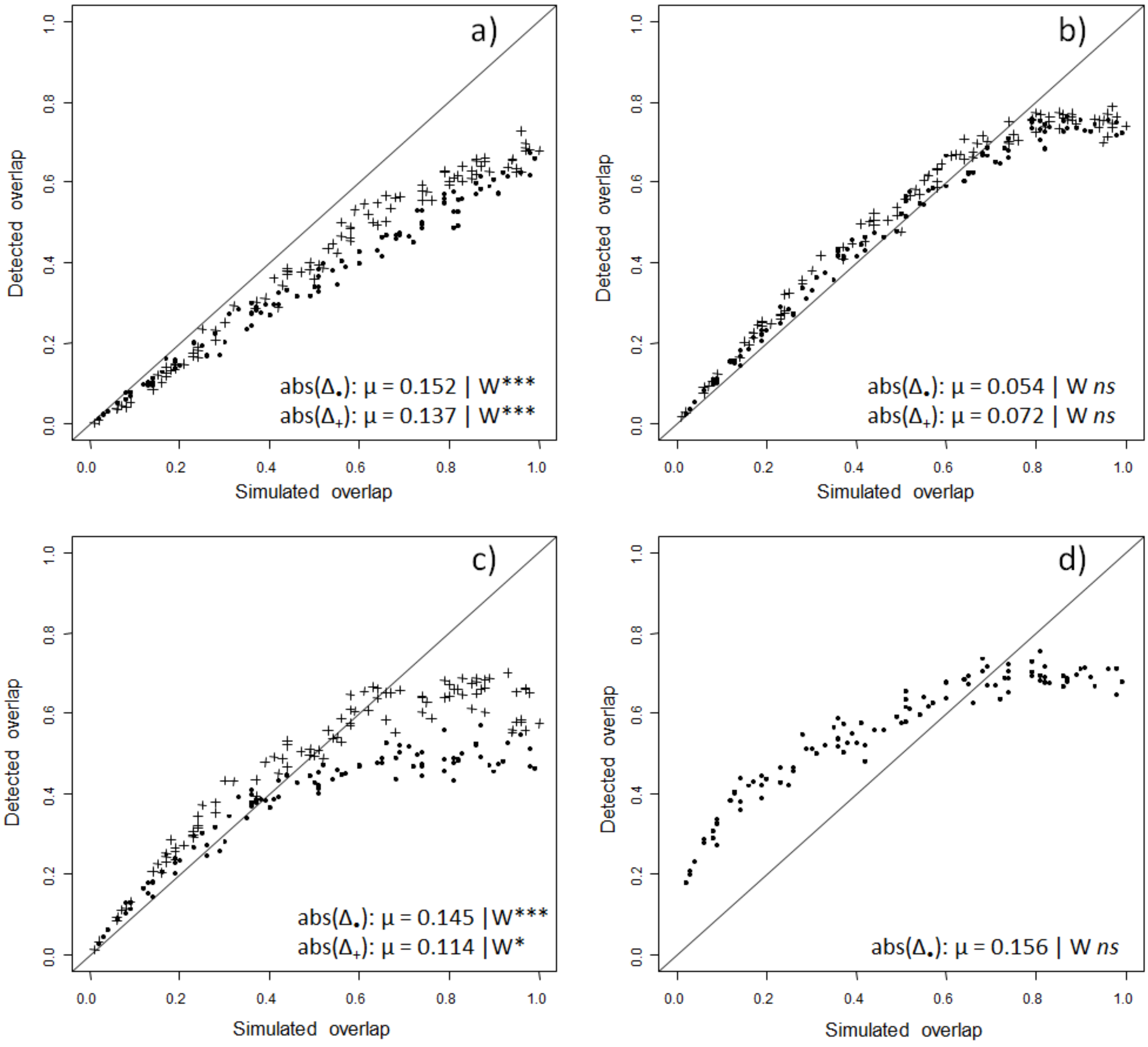

Figure 4 - Sensitivity analysis of simulated versus detected niche overlap for ordinations using a priori grouping factor. The axes of the analyses on which the overlap is measured correspond to a) WITHIN-occ, b) WITHIN-env, c) BETWEEN-occ and d) LDA. Black dots indicate models calibrated on both EU and NA ranges. Abs(Δ): μ indicates the average absolute difference between simulated and detected overlaps. The significance of the Wilcoxon signed-rank test, *W*, is shown (ns: non-significant, *: 0.05<p-value<0.01, **: 0.01<p-value<0.001, ***: p-value<0.001)

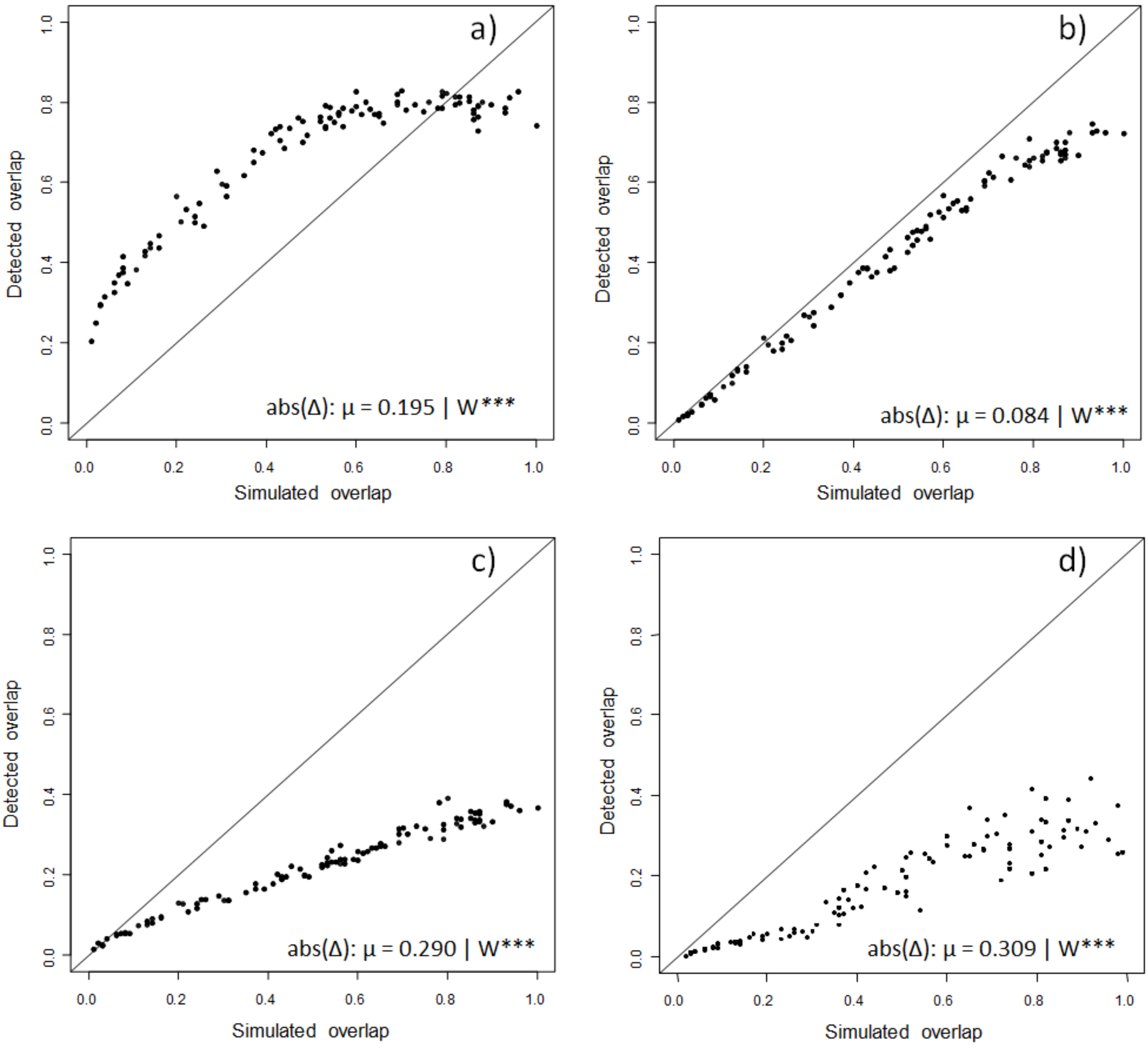

Figure 5 - Sensitivity analysis of simulated versus detected niche overlap for different SDM algorithms. The axes of the analyses on which the overlap is measured correspond to a) GLM, b) MaxEnt, c) GBM and d) RF. Crosses refer to models calibrated on the EU range only. Black dots indicate models calibrated on both EU and NA ranges. Abs(Δ): μ indicates the average absolute difference between simulated and detected overlaps. The significance of the Wilcoxon signed-rank test, *W*, is shown (ns: non-significant, *: 0.05<*p*-value<0.01, **: 0.01<*p*-value<0.001, ***: *p*-value<0.001).

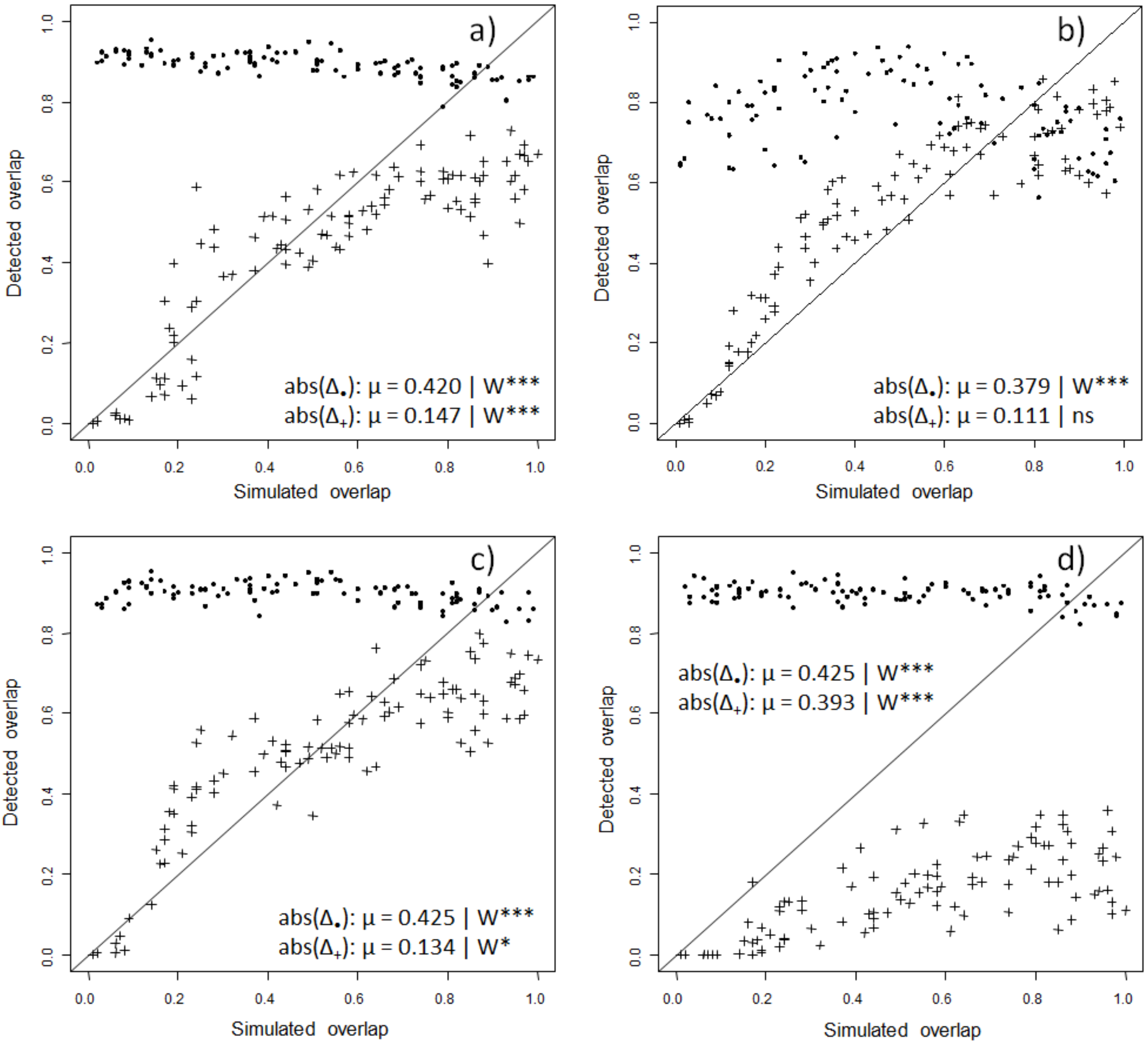

Figure 6. Niche of spotted knapweed in climatic space - example of a Principal Component Analysis (PCA-env). a) and b) represent the niche of the species along the two first axes of the PCA in the European native (EU) and North American invaded range (NA) respectively. Grey shading shows the density of the occurrences of the species by cell. The solid and dashed contour lines illustrate respectively 100% and 50% of the available (background) environment. The arrows represent how the center of the niche has changed between EU and NA. c) shows the contribution of the climatic variables on the two axes of the PCA and the percentage of inertia explained by the two axes. Histograms (d-f) show the observed niche overlap D between the two ranges (bar with a diamond) and simulated niche overlaps (gray bars) on which tests of niche equivalency (d)**,** niche similarity of NA to EU (e)**,** and niche similarity of EU to NA (f) are calculated from 100 iterations. The significance of the tests are shown (ns: non-significant, *: 0.05<*p*-value<0.01, **: 0.01<*p*-value<0.001, ***: *p*-value<0.001)**.**

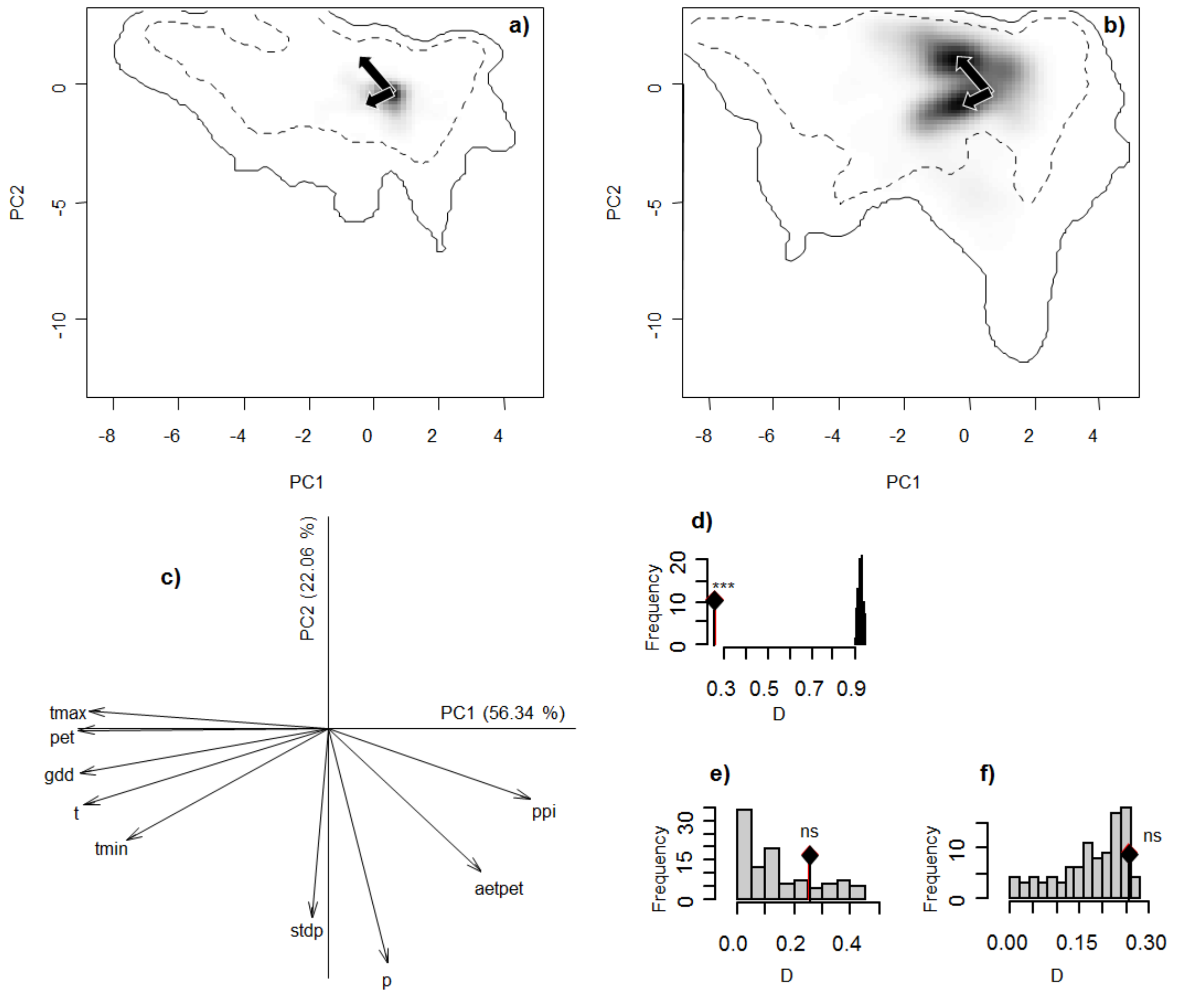

Figure 7. Niche of the imported fire ant in climatic space - example of a Principal Component Analysis (PCA-env). a) and b) represent the niche of the species along the two first axes of the PCA in the European native (EU) and North American invaded range (NA) respectively. Grey shading shows the density of the occurrences of the species by cell. The solid and dashed contour lines illustrate respectively 100% and 50% of the available (background) environment. The arrows represent how the center of the niche has changed between EU and NA. c) shows the contribution of the climatic variables on the two axes of the PCA and the percentage of inertia explained by the two axes. Histograms (d-f) show the observed niche overlap D between the two ranges (bars with a diamond) and simulated niche overlaps (gray bars) on which tests of niche equivalency (d)**,** niche similarity of NA to EU (e)**,** and niche similarity of EU to NA (f) are calculated from 100 iterations. The significance of the tests are shown (ns: non-significant, *: $0.05<p$-value<0.01, **: $0.01<p$-value<0.001, ***: p-value<0.001)**.**