STATISTICAL ECO(-TOXICO)LOGY

IMPROVING THE UTILIZATION OF DATA FOR ECOLOGICAL RISK ASSESSMENT

by

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1 GENERAL DISCUSSION AND OUTLOOK

STATISTICAL ECOTOXICOLOGY

The simulation study performed in chapter **??** clearly showed that common experimental designs exhibit unacceptably low statistical power (Szöcs and Schäfer, 2016; Van Der Hoeven, 1998). This underpins the criticism accumulated over the last 30 years towards the usage of NOEC as endpoint (Fox and Landis, 2016). Nevertheless, the NOEC is still one of the standard endpoint for mesocosm experiments in higher tier risk assessment (EFSA, 2013).

Recently, *a posteriori* calculations of statistical power have been proposed to counteract these limitations and aid the interpretation treatment-related effects in model ecosystems (Brock et al., 2015). The "minimum detectable difference" (MDD) estimates the difference between to means that must exist in order to produce a statistically significant result ($p < 0.05$ (Gelman and Stern, 2006)) and could be used to ínterpret NOEC. However, *a posteriori* calculations have been shown to have logical flaws when used for interpretation of non-significant results (Hoenig and Heisey, 2001; Nakagawa and Foster, 2004). However, conducting and report of *a priori* power calculations, as performed in chapter **??**, might provide researchers important information to optimize their study designs, ensuring that their experimental designs have appropriate power (Johnson et al., 2015).

Moreover, similar simulations can not only be used to analyse data of factorial designs, but also from regression designs. Indeed, simulations could be used to determine optimal designs for dose-response models and EC_x determination, balancing precision and resources. Regression designs are generally more powerful and provide more information than factorial designs (Cottingham et al., 2005). Regression designs in mesocosm experiments, assigning the replicates to more tested concentrations, might also provide more insights. However, currently statistical tools to analyse a community dose-reponse relations, providing a $EC_{x,community}$ are not well explored. Separate dose-response models could be fit to each species (Ritz, 2010), leading to a EC_x for each species in a mesocosm study. Subsequently, this EC_x values could be combined and summarised using Species Sensitivity Distributions (Posthuma et al., 2002), providing a hazardous concentration ($HC_{x,community}$) for x % of species affected (Maltby et al., 2005). Another possibility would be to use a logistic type of ordination (van den Brink et al., 2003). Reduced-Rank vector generalized linear models (RR-VGLM) could be used to fit such type of models (Yee, 2015; Yee and Hastie, 2003) but they have not been applied in ecotoxicology yet.

In a similar vein, community ecology is currently experiencing a shift towards new class of multivariate methods, incorporating statistical models for abundances across many taxa simultaneously (ter Braak and Šmilauer, 2015; Warton et al., 2015a; Warton et al., 2015b; Warton et al., 2012). However, this methods have not been applied frequently and their applicability to ecotoxicological data is currently unclear (Szöcs et al., 2015). All this models have in common, that the choice of statistical model is primarily based ...

LEVERAGING MONITORING DATA FOR ECOLOGICAL RISK ASSESSMENT

CHALLENGES TO UTILIZE 'BIG DATA' IN ECOLOGICAL RISK ASSESSMENT

CONCLUSIONS

REFERENCES

Brock, T. C. M., M. Hammers-Wirtz, U. Hommen, T. G. Preuss, H.-T. Ratte, I. Roessink, T. Strauss, and P. J. Van den Brink (2015). "The minimum detectable difference (MDD) and the interpretation of treatment-related effects of pesticides in experimental ecosystems". *Environmental Science and Pollution Research* 22 (2), 1160–1174.

Cottingham, K. L., J. T. Lennon, and B. L. Brown (2005). "Knowing when to draw the line: designing more informative ecological experiments". *Frontiers in Ecology and the Environment* 3 (3), 145–152.

EFSA (2013). “Guidance on tiered risk assessment for plant protection products for aquatic organisms in edge-of-field surface waters”. *EFSA Journal* 11 (7), 3290.

Fox, D. R. and W. G. Landis (2016). “Comment on ET&C perspectives, November 2015-A holistic view”. *Environmental Toxicology and Chemistry* 35 (6), 1337–1339.

Gelman, A. and H. Stern (2006). “The difference between “significant” and “not significant” is not itself statistically significant”. *The American Statistician* 60 (4), 328–331.

Hoenig, J. M. and D. M. Heisey (2001). “The abuse of power”. *The American Statistician* 55 (1), 19–24.

Johnson, P. C. D., S. J. E. Barry, H. M. Ferguson, and P. Müller (2015). “Power analysis for generalized linear mixed models in ecology and evolution”. *Methods in Ecology and Evolution* 6 (2), 133–142.

Maltby, L., N. Blake, T. C. M. Brock, and P. J. Van Den Brink (2005). “Insecticide species sensitivity distributions: Importance of test species selection and relevance to aquatic ecosystems”. *Environmental Toxicology and Chemistry* 24 (2). pdf RS, 379–388.

Nakagawa, S. and T. M. Foster (2004). “The case against retrospective statistical power analyses with an introduction to power analysis”. *acta ethologica* 7 (2), 103–108.

Posthuma, L., G. W. Suter, and T. P. Traas (2002). *Species sensitivity distributions in ecotoxicology*. Environmental and ecological risk assessment. Boca Raton and Fla: Lewis.

Ritz, C. (2010). “Toward a unified approach to dose-response modeling in ecotoxicology”. *Environmental Toxicology and Chemistry* 29 (1), 220–229.

Szöcs, E., P. J. v. d. Brink, L. Lagadic, T. Caquet, M. Roucaute, A. Auber, Y. Bayona, M. Liess, P. Ebke, A. Ippolito, C. J. F. t. Braak, T. C. M. Brock, and R. B. Schäfer (2015). “Analysing chemical-induced changes in macroinvertebrate communities in aquatic mesocosm experiments: a comparison of methods”. *Ecotoxicology* 24 (4), 760–769.

Szöcs, E. and R. B. Schäfer (2016). "Statistical hypothesis testing—To transform or not to transform?" *Integrated Environmental Assessment and Management* 12 (2), 398–400.

Ter Braak, C. J. and P. Šmilauer (2015). "Topics in constrained and unconstrained ordination". *Plant Ecology* 216 (5), 683–696.

Van den Brink, P. J., N. W. van den Brink, and C. J. F. ter Braak (2003). "Multivariate analysis of ecotoxicological data using ordination: demonstrations of utility on the basis of various examples". *Australasian Journal of Ecotoxicology* 9. RS, 141–156.

Van Der Hoeven, N. (1998). "Power analysis for the NOEC: What is the probability of detecting small toxic effects on three different species using the appropriate standardized test protocols?" *Ecotoxicology* 7 (6), 355–361.

Warton, D. I., F. G. Blanchet, R. B. O'Hara, O. Ovaskainen, S. Taskinen, S. C. Walker, and F. K. C. Hui (2015a). "So Many Variables: Joint Modeling in Community Ecology". *Trends in Ecology & Evolution* 30 (12), 766–779. URL: http://www.sciencedirect.com/science/article/pii/S0169534715002402.

Warton, D. I., S. D. Foster, G. De'ath, J. Stoklosa, and P. K. Dunstan (2015b). "Model-based thinking for community ecology". *Plant Ecology* 216 (5), 669–682.

Warton, D. I., S. T. Wright, and Y. Wang (2012). "Distance-based multivariate analyses confound location and dispersion effects". *Methods in Ecology and Evolution* 3 (1), 89–101.

Yee, T. W. (2015). *Vector Generalized Linear and Additive Models*. Springer Series in Statistics. New York, NY: Springer New York.

Yee, T. W. and T. J. Hastie (2003). "Reduced-rank vector generalized linear models". *Statistical modelling* 3 (1), 15–41.