

STATISTICAL SCIENCE

Volume 38, Number 3

August 2023

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Statistical Science [ISSN 0883-4237 (print); ISSN 2168-8745 (online)], Volume 38, Number 3, August 2023. Published quarterly by the Institute of Mathematical Statistics, 9760 Smith Road, Waite Hill, Ohio 44094, USA. Periodicals postage paid at Cleveland, Ohio and at additional mailing offices.

POSTMASTER: Send address changes to *Statistical Science*, Institute of Mathematical Statistics, Dues and Subscriptions Office, PO Box 729, Middletown, Maryland 21769, USA.

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The Role of Exchangeability in Causal Inference

Olli Saarela, David A. Stephens and Erica E. M. Moodie

Abstract. Though the notion of exchangeability has been discussed in the causal inference literature under various guises, it has rarely taken its original meaning as a symmetry property of probability distributions. As this property is a standard component of Bayesian inference, we argue that in Bayesian causal inference it is natural to link the causal model, including the notion of confounding and definition of causal contrasts of interest, to the concept of exchangeability. Here, we propose a probabilistic between-group exchangeability property as an identifying condition for causal effects, relate it to alternative conditions for unconfounded inferences (commonly stated using potential outcomes) and define causal contrasts in the presence of exchangeability in terms of posterior predictive expectations for further exchangeable units. While our main focus is on a point treatment setting, we also investigate how this reasoning carries over to longitudinal settings.

Key words and phrases: Bayesian inference, causal inference, confounding, exchangeability, posterior predictive inference.

REFERENCES

- ARJAS, E. (2012). Causal inference from observational data: A Bayesian predictive approach. In *Causality: Statistical Perspectives and Applications* (C. Berzuini, A. P. Dawid and L. Bernardinelli, eds.) 71–84. Wiley, NY.
- ARJAS, E. and PARNER, J. (2004). Causal reasoning from longitudinal data. *Scand. J. Stat.* **31** 171–187. MR2066247 <https://doi.org/10.1111/j.1467-9469.2004.02-134.x>
- BAKER, S. G. (2013). Causal inference, probability theory, and graphical insights. *Stat. Med.* **32** 4319–4330. MR3118357 <https://doi.org/10.1002/sim.5828>
- BERNARDO, J.-M. and SMITH, A. F. M. (1994). *Bayesian Theory*. Wiley Series in Probability and Mathematical Statistics: Probability and Mathematical Statistics. Wiley, Chichester. MR1274699 <https://doi.org/10.1002/9780470316870>
- BIJLSMA, M. J., TARKIAINEN, L., MYRSKYLÄ, M. and MARTIKAINEN, P. (2017). Unemployment and subsequent depression: A mediation analysis using the parametric G-formula. *Soc. Sci. Med.* **194** 142–150.
- BÜHLMANN, P. (2020). Invariance, causality and robustness: 2018 Neyman Lecture. *Statist. Sci.* **35** 404–426. MR4148216 <https://doi.org/10.1214/19-STS721>
- CHAKRABORTY, B. and MURPHY, S. A. (2014). Dynamic treatment regimes. *Annu. Rev. Stat. Appl.* **1** 447–464.
- CHIB, S. (2007). Analysis of treatment response data without the joint distribution of potential outcomes. *J. Econometrics* **140** 401–412. MR2408912 <https://doi.org/10.1016/j.jeconom.2006.07.009>
- COLE, S. R. and FRANGAKIS, C. E. (2009). The consistency statement in causal inference: A definition or an assumption? *Epidemiology* **20** 3–5.
- COMMENGES, D. (2019). Causality without potential outcomes and the dynamic approach. Preprint. Available at [arXiv:1905.01195](https://arxiv.org/abs/1905.01195).
- COMMENGES, D. and GÉGOUT-PETIT, A. (2015). The stochastic system approach for estimating dynamic treatments effect. *Lifetime Data Anal.* **21** 561–578. MR3397506 <https://doi.org/10.1007/s10985-015-9322-3>
- DAWID, A. P. (2000). Causal inference without counterfactuals. *J. Amer. Statist. Assoc.* **95** 407–448. MR1803167 <https://doi.org/10.2307/2669377>
- DAWID, P. (2021). Decision-theoretic foundations for statistical causality. *J. Causal Inference* **9** 39–77. MR4289525 <https://doi.org/10.1515/jci-2020-0008>
- DAWID, A. P. and DIDELEZ, V. (2010). Identifying the consequences of dynamic treatment strategies: A decision-theoretic overview. *Stat. Surv.* **4** 184–231. MR2740837 <https://doi.org/10.1214/10-SS081>
- DAWID, A. P., MUSIO, M. and FIENBERG, S. E. (2016). From statistical evidence to evidence of causality. *Bayesian Anal.* **11** 725–752. MR3498044 <https://doi.org/10.1214/15-BA968>
- DE FINETTI, B. (1929). Funzione caratteristica di un fenomeno aleatorio. In *Atti del Congresso Internazionale dei Matematici: Bologna del 3 al 10 de Settembre di 1928* 179–190.
- DE FINETTI, B. (1938). Sur la condition d'équivalence partielle. *Actual. Sci. Ind.* **739**. Translated In: *Studies in Inductive and Prob-*

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- bility. II. Jeffrey, R. (ed.) University of California Press: Berkeley 1980.
- DIACONIS, P. (1988). Recent progress on de Finetti's notions of exchangeability. In *Bayesian Statistics*, 3 (Valencia, 1987). *Oxford Sci. Publ.* 111–125. Oxford Univ. Press, New York. [MR1008047](#)
- FERREIRA, J. A. (2015). Some models and methods for the analysis of observational data. *Stat. Surv.* **9** 106–208. [MR3396384](#) <https://doi.org/10.1214/15-SS110>
- FERREIRA, J. A. (2019). Causality from the point of view of statistics. Preprint. Available at [arXiv:1908.07301](https://arxiv.org/abs/1908.07301).
- GELMAN, A., CARLIN, J. B., STERN, H. S. and RUBIN, D. B. (2004). *Bayesian Data Analysis*, 2nd ed. *Texts in Statistical Science Series*. CRC Press/CRC, Boca Raton, FL. [MR2027492](#)
- GREENLAND, S. (2003). Quantifying biases in causal models: Classical confounding vs collider-stratification bias. *Epidemiology* **14** 300–306.
- GREENLAND, S. (2012). Causal inference as a prediction problem: Assumptions, identification and evidence synthesis. In *Causality: Statistical Perspectives and Applications* (C. Berzuini, A. P. Dawid and L. Bernardinelli, eds.) 43–58. Wiley, NY.
- GREENLAND, S. and ROBINS, J. M. (1986). Identifiability, exchangeability, and epidemiological confounding. *Int. J. Epidemiol.* **15** 413–419. <https://doi.org/10.1093/ije/15.3.413>
- GREENLAND, S. and ROBINS, J. M. (2009). Identifiability, exchangeability, and epidemiological confounding revisited. *Epidemiol. Perspect. Innov.* **6**. <https://doi.org/10.1186/1742-5573-6-4>.
- GREENLAND, S., ROBINS, J. M. and PEARL, J. (1999). Confounding and collapsibility in causal inference. *Statist. Sci.* **14** 29–46.
- HERNÁN, M. A., BRUMBACK, B. and ROBINS, J. M. (2001). Marginal structural models to estimate the joint causal effect of nonrandomized treatments. *J. Amer. Statist. Assoc.* **96** 440–448. [MR1939347](#) <https://doi.org/10.1198/016214501753168154>
- HERNÁN, M. A. and ROBINS, J. M. (2006). Estimating causal effects from epidemiological data. *J. Epidemiol. Community Health* **60** 578–586.
- HEWITT, E. and SAVAGE, L. J. (1955). Symmetric measures on Cartesian products. *Trans. Amer. Math. Soc.* **80** 470–501. [MR0076206](#) <https://doi.org/10.2307/1992999>
- HOLLAND, P. W. (1986). Statistics and causal inference. *J. Amer. Statist. Assoc.* **81** 945–970. [MR0867618](#)
- JAIN, P., DANAEI, G., ROBINS, J. M., MANSON, J. E. and HERNÁN, M. A. (2016). Smoking cessation and long-term weight gain in the Framingham Heart Study: An application of the parametric g-formula for a continuous outcome. *Eur. J. Epidemiol.* **31** 1223–1229. <https://doi.org/10.1007/s10654-016-0200-4>
- KEIDING, N. and CLAYTON, D. (2014). Standardization and control for confounding in observational studies: A historical perspective. *Statist. Sci.* **29** 529–558. [MR3300358](#) <https://doi.org/10.1214/13-STS453>
- KEIL, A. P., EDWARDS, J. K., RICHARDSON, D. R., NAIMI, A. I. and COLE, S. R. (2014). The parametric g-formula for time-to-event data: Towards intuition with a worked example. *Epidemiology* **25** 889.
- LAURITZEN, S. L., ANDERSEN, A. H., EDWARDS, D., JÖRESKOG, K. G. and JOHANSEN, S. (1989). Mixed graphical association models [with discussion and rejoinder]. *Scand. J. Stat.* **16** 273–306.
- LINDLEY, D. V. (2002). Seeing and doing: The concept of causation. *Int. Stat. Rev.* **70** 191–214.
- LINDLEY, D. V. and NOVICK, M. R. (1981). The role of exchangeability in inference. *Ann. Statist.* **9** 45–58. [MR0600531](#)
- NEOPHYTOU, A. M., COSTELLO, S., PICCIOTTO, S., BROWN, D. M., ATTFIELD, M. D., BLAIR, A., LUBIN, J. H., STEWART, P. A., VERMEULEN, R. et al. (2019). Diesel exhaust, respirable dust, and ischemic heart disease: An application of the parametric g-formula. *Epidemiology* **30** 177–185.
- PEARL, J. (2009). *Causality: Models, Reasoning, and Inference*, 2nd ed. Cambridge Univ. Press, Cambridge. [MR2548166](#) <https://doi.org/10.1017/CBO9780511803161>
- PEARL, J. (2010). On the consistency rule in causal inference: Axiom, definition, assumption, or theorem? *Epidemiology* **21** 872–875. <https://doi.org/10.1097/EDE.0b013e3181f5d3fd>
- ROBINS, J. M. and GREENLAND, S. (1992). Identifiability and exchangeability for direct and indirect effects. *Epidemiology* **3** 143–155. <https://doi.org/10.1097/00001648-199203000-00013>
- ROBINS, J. M., HERNÁN, M. A. and BRUMBACK, B. (2000). Marginal structural models and causal inference in epidemiology. *Epidemiology* **11** 550–560.
- ROBINS, J. M. and WASSERMAN, L. (1997). Estimation of effects of sequential treatments by reparameterizing directed acyclic graphs. In *Proceedings of the Thirteenth Conference on Uncertainty in Artificial Intelligence, Providence Rhode Island, August 1–3, 1997* (D. Geiger and P. Shenoy, eds.) 409–420. Morgan Kaufmann, San Francisco, CA.
- ROSENBAUM, P. R. and RUBIN, D. B. (1983). The central role of the propensity score in observational studies for causal effects. *Biometrika* **70** 41–55. [MR0742974](#) <https://doi.org/10.1093/biomet/70.1.41>
- RØYSLAND, K. (2011). A martingale approach to continuous-time marginal structural models. *Bernoulli* **17** 895–915. [MR2817610](#) <https://doi.org/10.3150/10-BEJ303>
- RUBIN, D. B. (1978). Bayesian inference for causal effects: The role of randomization. *Ann. Statist.* **6** 34–58. [MR0472152](#)
- SAARELA, O., BELZILE, L. R. and STEPHENS, D. A. (2016). A Bayesian view of doubly robust causal inference. *Biometrika* **103** 667–681. [MR3551791](#) <https://doi.org/10.1093/biomet/asw025>
- SAARELA, O., STEPHENS, D. A. and MOODIE, E. E. (2023). Supplement to “The Role of Exchangeability in Causal Inference.” <https://doi.org/10.1214/22-STS879SUPP>
- SAARELA, O., STEPHENS, D. A., MOODIE, E. E. M. and KLEIN, M. B. (2015). On Bayesian estimation of marginal structural models. *Biometrics* **71** 279–288. [MR3366229](#) <https://doi.org/10.1111/biom.12269>
- SHAHN, Z., LI, Y., SUN, Z., MOHAN, A., SAMPAIO, C. and HU, J. (2019). G-computation and hierarchical models for estimating multiple causal effects from observational disease registries with irregular visits. *AMIA Joint Summits on Translational Science Proceedings* **2019** 789–798.
- TAUBMAN, S. L., ROBINS, J. M., MITTLEMAN, M. A. and HERNÁN, M. A. (2009). Intervening on risk factors for coronary heart disease: An application of the parametric g-formula. *Int. J. Epidemiol.* **38** 1599–1611. <https://doi.org/10.1093/ije/dyp192>
- VANDERWEELE, T. J. (2009a). Concerning the consistency assumption in causal inference. *Epidemiology* **20** 880–883. <https://doi.org/10.1097/EDE.0b013e3181bd5638>
- VANDERWEELE, T. J. (2009b). Marginal structural models for the estimation of direct and indirect effects. *Epidemiology* **20** 18–26. <https://doi.org/10.1097/EDE.0b013e31818f69ce>
- VANSTEELENDT, S., BEKAERT, M. and CLAESKENS, G. (2012). On model selection and model misspecification in causal inference. *Stat. Methods Med. Res.* **21** 7–30. [MR2867536](#) <https://doi.org/10.1177/0962280210387717>
- VAN DER VAART, A. W. (1998). *Asymptotic Statistics. Cambridge Series in Statistical and Probabilistic Mathematics* **3**. Cambridge Univ. Press, Cambridge. [MR1652247](#) <https://doi.org/10.1017/CBO9780511802256>
- VON PLATO, J. (1989). De Finetti's earliest works on the foundations of probability. *Erkenntnis* **31** 263–282.

WESTREICH, D., COLE, S. R., YOUNG, J. G., PALELLA, F., TIEN, P. C., KINGSLEY, L., GANGE, S. J. and HERNÁN, M. A. (2012). The parametric g-formula to estimate the effect of highly

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31 2000–2009. MR2956032 <https://doi.org/10.1002/sim.5316>

Aitchison's Compositional Data Analysis 40 Years on: A Reappraisal

Michael Greenacre , Eric Grunsky , John Bacon-Shone , Ionas Erb  and Thomas Quinn 

Abstract. The development of John Aitchison's approach to compositional data analysis is followed since his paper read to the Royal Statistical Society in 1982. Aitchison's logratio approach, which was proposed to solve the problematic aspects of working with data with a fixed-sum constraint, is summarized and reappraised. It is maintained that the properties on which this approach was originally built, the main one being subcompositional coherence, are not required to be satisfied exactly—quasi-coherence is sufficient, that is near enough to being coherent for all practical purposes. This opens up the field to using simpler data transformations, such as power transformations, that permit zero values in the data. The additional property of exact isometry, which was subsequently introduced and not in Aitchison's original conception, imposed the use of isometric logratio transformations, but these are complicated and problematic to interpret, involving ratios of geometric means. If this property is regarded as important in certain analytical contexts, for example, unsupervised learning, it can be relaxed by showing that regular pairwise logratios, as well as the alternative quasi-coherent transformations, can also be quasi-isometric, meaning they are close enough to exact isometry for all practical purposes. It is concluded that the isometric and related logratio transformations such as pivot logratios are not a prerequisite for good practice, although many authors insist on their obligatory use. This conclusion is fully supported here by case studies in geochemistry and in genomics, where the good performance is demonstrated of pairwise logratios, as originally proposed by Aitchison, or Box–Cox power transforms of the original compositions where no zero replacements are necessary.

Key words and phrases: Box–Cox transformation, compositional modeling, correspondence analysis, isometry, logratio transformations, log-contrast, principal component analysis, Procrustes analysis, subcompositional coherence.

REFERENCES

- [1] AITCHISON, J. (1982). The statistical analysis of compositional data. *J. Roy. Statist. Soc. Ser. B* **44** 139–177. [MR0676206](#)
- [2] AITCHISON, J. (1986). *The Statistical Analysis of Compositional Data. Monographs on Statistics and Applied Probability*. CRC Press, London. [MR0865647](#) <https://doi.org/10.1007/978-94-009-4109-0>
- [3] AITCHISON, J. (1997). The one-hour course in compositional data analysis, or compositional data analysis is simple. In *Proceedings of IAMG'97* (V. Pawlowsky-Glahn, ed.) 3–35. CIMNE, Barcelona.
- [4] AITCHISON, J. (2008). The single principle of compositional data analysis, continuing fallacies, confusions and misunderstandings and some suggested remedies. In *Proceedings of CodaWork'08, Keynote Address* 3–35 URL: <https://core.ac.uk/download/pdf/132548276.pdf>.
- [5] AITCHISON, J. and BACON-SHONE, J. (1984). Log contrast models for experiments with mixtures. *Biometrika* **71** 323–330.
- [6] AITCHISON, J. and GREENACRE, M. (2002). Biplots of com-

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- positional data. *J. R. Stat. Soc., Ser. C* **51** 375–392. MR1977249 <https://doi.org/10.1111/1467-9876.00275>
- [7] AMARI, S. (2016). *Information Geometry and Its Applications. Applied Mathematical Sciences* **194**. Springer, Tokyo. MR3495836 <https://doi.org/10.1007/978-4-431-55978-8>
- [8] BENÉCRI, J.-P. (1980). *L'analyse des Données. II: L'analyse des correspondances*, 3rd ed. Dunod, Paris. MR0593139
- [9] BOOESHAGHI, A. S., HALLGRÍMSDÓTTIR, I. B., GÁLVEZ-MERCHÁN, Á. and PACTER, L. (2022). Depth normalization for single-cell genomics count data. bioRxiv, Cold Spring Harbor Laboratory.
- [10] BÓNA, M. (2006). *A Walk Through Combinatorics: An Introduction to Enumeration and Graph Theory*, 2nd ed. World Scientific, Hackensack, NJ. MR2361255 <https://doi.org/10.1142/6177>
- [11] BUCCIANI, A. (2015). The FOREGS repository: Modelling variability in stream water on a continental scale revising classical diagrams from CoDA (compositional data analysis) perspective. *J. Geochem. Explor.* **154** 94–104.
- [12] BUETTNER, M., OSTNER, J., MUELLER, C. L., THEIS, F. J. and SCHUBERT, B. (2021). scCODA is a Bayesian model for compositional single-cell data analysis. *Nat. Commun.* **12** 1–10.
- [13] BUTLER, A. and GLASBEY, C. (2008). A latent Gaussian model for compositional data with zeros. *J. R. Stat. Soc., Ser. C* **57** 505–520. MR2528668 <https://doi.org/10.1111/j.1467-9876.2008.00627.x>
- [14] COENDERS, G. and GREENACRE, M. (2022). Three approaches to supervised learning for compositional data with pairwise log-ratios. <https://doi.org/10.1080/02664763.2022.2108007>
- [15] COENDERS, G. and PAWLOWSKY-GLAHLN, V. (2020). On interpretations of tests and effect sizes in regression models with a compositional predictor. *SORT* **44** 201–220. MR4121257 <https://doi.org/10.2436/20.8080.02.100>
- [16] COMBETTES, P. L. and MÜLLER, C. L. (2021). Regression models for compositional data: General log-contrast formulations, proximal optimization, and microbiome data applications. *Stat. Biosci.* **13** 217–242. <https://doi.org/10.1007/s12561-020-09283-2>
- [17] CORTÉS, J. A. (2009). On the Harker variation diagrams; a comment on “The statistical analysis of compositional data. Where are we and where should we be heading?” by Aitchison and Egozcue (2005). *Math. Geosci.* **41** 817–828. <https://doi.org/10.1007/s11004-009-9222-8>
- [18] DAVID, M., DAGBERT, M. and BEAUCHEMIN, Y. (1977). Statistical analysis in geology: Correspondence analysis method. *Colo. Sch. Mines Q.* **72** 11–57.
- [19] EGOZCUE, J. J. and PAWLOWSKY-GLAHLN, V. (2005). Groups of parts and their balances in compositional data analysis. *Math. Geol.* **37** 795–828. MR2183639 <https://doi.org/10.1007/s11004-005-7381-9>
- [20] EGOZCUE, J. J. and PAWLOWSKY-GLAHLN, V. (2019). Compositional data: The sample space and its structure. *TEST* **28** 599–638. MR3992128 <https://doi.org/10.1007/s11749-019-00670-6>
- [21] GREENACRE, M. (2019). Discussion of “Compositional data: the sample space and its structure”, by Egozcue and Pawlowsky-Glahn. *TEST* **2019** 20–24.
- [22] ERB, I. and AY, N. (2021). The information-geometric perspective of compositional data analysis. In *Advances in Compositional Data Analysis* (P. Filzmoser, K. Hron, J. A. Martín-Fernández and J. Palarea-Albaladejo, eds.) 21–43. Springer, New York.
- [23] ERB, I. and NOTREDAME, C. (2016). How should we measure proportionality on relative gene expression data? *Theory Biosci.* **135** 21–36.
- [24] ERB, I., QUINN, T. P., LOVELL, D. and NOTREDAME, C. (2017). Differential proportionality — a normalization-free approach to differential gene expression. In *Proceedings of CoDaWork 2017, the 7th Compositional Data Analysis Workshop*. Available under bioRxiv, pp. 134536. <https://doi.org/10.1101/134536>
- [25] FILZMOSER, P., HRON, K. and TEMPL, M. (2018). *Applied Compositional Data Analysis. Springer Series in Statistics*. Springer, Cham. MR3839314 <https://doi.org/10.1007/978-3-319-96422-5>
- [26] FIŠEROVÁ, E. and HRON, K. (2011). On the interpretation of orthonormal coordinates for compositional data. *Math. Geosci.* **43** 455.
- [27] GABRIEL, K. R. (1972). Analysis of meteorological data by means of canonical decomposition and biplots. *J. Appl. Meteorol. Climatol.* **11** 1071–1077.
- [28] GORDON-RODRIGUEZ, E., QUINN, T. P. and CUNNINGHAM, J. P. (2021). Learning sparse log-ratios for high-throughput sequencing data. *Bioinformatics*. btab645. <https://doi.org/10.1093/bioinformatics/btab645>
- [29] GOWER, J. C. and DIJKSTERHUIS, G. B. (2004). *Procrustes Problems. Oxford Statistical Science Series* **30**. Oxford Univ. Press, Oxford. MR2051013 <https://doi.org/10.1093/acprof:oso/9780198510581.001.0001>
- [30] GRAEVE, M. and GREENACRE, M. (2020). The selection and analysis of fatty acid ratios: A new approach for the univariate and multivariate analysis of fatty acid trophic markers in marine organisms. *Limnol. Oceanogr., Methods* **18** 196–210.
- [31] GRALINSKA, E., KOHL, C., FADAKAR, B. S. and VINGRON, M. (2022). Visualizing cluster-specific genes from single-cell transcriptomics data using association plots. *J. Mol. Biol.* **434** 167525. <https://doi.org/10.1016/j.jmb.2022.167525>
- [32] GREENACRE, M. (2003). Singular value decomposition of matched matrices. *J. Appl. Stat.* **30** 1101–1113. MR2037841 <https://doi.org/10.1080/0266476032000107132>
- [33] GREENACRE, M. (2009). Power transformations in correspondence analysis. *Comput. Statist. Data Anal.* **53** 3107–3116. MR2667615 <https://doi.org/10.1016/j.csda.2008.09.001>
- [34] GREENACRE, M. (2010). Log-ratio analysis is a limiting case of correspondence analysis. *Math. Geosci.* **42** 129–34.
- [35] GREENACRE, M. (2011). Measuring subcompositional incoherence. *Math. Geosci.* **43** 681–93.
- [36] GREENACRE, M. (2013). Contribution biplots. *J. Comput. Graph. Statist.* **22** 107–122. MR3044325 <https://doi.org/10.1080/10618600.2012.702494>
- [37] GREENACRE, M. (2016). Data reporting and visualization in ecology. *Polar Biol.* **39** 2189–2205.
- [38] GREENACRE, M. (2016). *Correspondence Analysis in Practice*, 3rd ed. CRC Press, Boca Raton, FL.
- [39] GREENACRE, M. (2017). ‘Size’ and ‘shape’ in the measurement of multivariate proximity. *Methods Ecol. Evol.* **8** 1415–1424. <https://doi.org/10.1111/2041-210X.12776>
- [40] GREENACRE, M. (2018). *Compositional Data Analysis in Practice*. Chapman & Hall / CRC Press, Boca Raton, Florida.
- [41] GREENACRE, M. (2019). Variable selection in compositional data analysis using pairwise logratios. *Math. Geosci.* **51** 649–682. MR3981436 <https://doi.org/10.1007/s11004-018-9754-x>
- [42] GREENACRE, M. (2020). Amalgamations are valid in compositional data analysis, can be used in agglomerative clustering, and their logratios have an inverse transformation. *Appl. Comput. Geosci.* **5** 100017.
- [43] GREENACRE, M. (2021). Compositional data analysis. *Annu. Rev. Stat. Appl.* **8** 271–299. MR4243548 <https://doi.org/10.1146/annurev-statistics-042720-124436>

- [44] GREENACRE, M. (2022). Compositional data analysis – linear algebra, visualization and interpretation. In *Innovations in Multivariate Statistical Modelling: Navigating Theoretical and Multidisciplinary Domains* (A. Bekker and J. Ferreira, eds.) Springer, New York. <https://arxiv.org/abs/2110.12439>.
- [45] GREENACRE, M., GRUNSKY, E. and BACON-SHONE, J. (2020). A comparison of amalgamation and isometric logratios in compositional data analysis. *Comput. Geosci.* **148** 104621.
- [46] GREENACRE, M., GRUNSKY, E., BACON-SHONE, J., ERB, I. and QUINN, T. (2023). Supplement to “Aitchison’s Compositional Data Analysis 40 Years on: A Reappraisal.” <https://doi.org/10.1214/22-STSS880SUPPA>, <https://doi.org/10.1214/22-STSS880SUPPB>, <https://doi.org/10.1214/22-STSS880SUPPC>, <https://doi.org/10.1214/22-STSS880SUPPD>, <https://doi.org/10.1214/22-STSS880SUPPE>
- [47] GREENACRE, M. and LEWI, P. (2009). Distributional equivalence and subcompositional coherence in the analysis of compositional data, contingency tables and ratio-scale measurements. *J. Classification* **26** 29–54. MR2507824 <https://doi.org/10.1007/s00357-009-9027-y>
- [48] GREENACRE, M., MÁRTINEZ-ÁLVARO, M. and BLASCO, A. (2021). Compositional data analysis of microbiome and anyomics datasets: A validation of the additive logratio transformation. *Front. Microbiol.* **12** 2625. <https://doi.org/10.3389/fmicb.2021.727398>
- [49] GRUNSKY, E. C. (1985). Recognition of alteration in volcanic rocks using statistical analysis of lithochemical data. *J. Geochem. Explor.* **25** 157–183.
- [50] HAFEMEISTER, C. and SATIJA, R. (2019). Normalization and variance stabilization of single-cell RNA-seq data using regularized negative binomial regression. *Genome biology* **20** 1–15.
- [51] HAUG, T., FALK-PETERSEN, S., GREENACRE, M. et al. (2017). Trophic level and fatty acids in harp seals compared with common minke whales in the Barents Sea. *Marine Biol. Res.* **13** 919–932. <https://doi.org/10.1080/17451000.2017.1313988>
- [52] HELLINGER, E. (1909). Neue Begründung der Theorie quadratischer Formen von unendlichvielen Veränderlichen. *J. Reine Angew. Math.* **136** 210–271. MR1580780 <https://doi.org/10.1515/crll.1909.136.210>
- [53] HRON, K., COENDERS, G., FILZMOSER, P., PALAREA-ALBALADEJO, J., FAMÉRA, M. and GRYGAR, T. M. (2021). Analysing pairwise logratios revisited. *Math. Geosci.* **54** <https://www.x-mol.com/paperRedirect/1381133593200320512>.
- [54] HRON, K., FILZMOSER, P., DE CARITAT, P., FIŠEROVÁ, E. and GARDLO, A. (2017). Weighted pivot coordinates for compositional data and their application to geochemical mapping. *Math. Geosci.* **49** 797–814. MR3672426 <https://doi.org/10.1007/s11004-017-9684-z>
- [55] HSU, L. L. and CULHANE, A. C. (2023). Correspondence analysis for dimension reduction, batch integration, and visualization of single-cell RNA-seq data. *Sci. Rep.* **13** 1197.
- [56] HUBERT, L. and ARABIE, P. (1985). Comparing partitions. *J. Classification* **2** 193–218.
- [57] JACKSON, D. A. (1997). Compositional data in community ecology: The paradigm or peril of proportions? *Ecology* **78** 929–940.
- [58] KRAFT, A., GRAEVE, M., JANSSEN, D. et al. (2017). Arctic pelagic amphipods: Lipid dynamics and life strategy. *J. Plankton Res.* **37** 790–807.
- [59] KRZANOWSKI, W. (1987). Selection of variables to preserve multivariate data structure, using principal components. *J. R. Stat. Soc. Ser. C. Appl. Stat.* **36** 22–33.
- [60] KYNČLOVÁ, P., HRON, K. and FILZMOSER, P. (2017). Correlation between compositional parts based on symmetric balances. *Math. Geosci.* **49** 777–796. MR3672425 <https://doi.org/10.1007/s11004-016-9669-3>
- [61] LEWI, P. J. (1976). Spectral mapping, a technique for classifying biological activity profiles of chemical compounds. *Arz. Forsch.* **26** 1295–300.
- [62] LEWI, P. J. (1986). Analysis of biological activity profiles by Spectramap. *Eur. J. Med. Chem.* **21** 155–62.
- [63] LEWI, P. J. (2005). Spectral mapping, a personal and historical account of an adventure in multivariate data analysis. *Chemom. Intell. Lab. Syst.* **77** 215–23.
- [64] LOVELL, D., PAWLOWSKY-GLAHN, V., EGOZCUE, J. J., MARGUERAT, S. and BÄHLER, J. (2015). Proportionality: A valid alternative to correlation for relative data. *PLoS Comput. Biol.* **11** e1004075.
- [65] LUECKEN, M. D. and THEIS, F. J. (2019). Current best practices in single-cell RNA-seq analysis: a tutorial. *Mol. Syst. Biol.* **15** e8746.
- [66] MARTÍN-FERNÁNDEZ, J. A., PAWLOWSKY-GLAHN, V., EGOZCUE, J. J. and TOLOSONA-DELGADO, R. (2018). Advances in principal balances for compositional data. *Math. Geosci.* **50** 273–298. MR3779069 <https://doi.org/10.1007/s11004-017-9712-z>
- [67] MARTÍNEZ-ÁLVARO, M., AUFFRET, M. D., DUTHIE, C. A., DEWHURST, R., CLEVELAND, M., WATSON, M. and ROEHE, R. (2021). Bovine host genome acts on specific metabolism, communication and genetic processes of rumen microbes host-genomically linked to methane emissions. Submitted for Publication <https://www.researchsquare.com/article/rs-290150/v1>.
- [68] MARTÍNEZ-ÁLVARO, M., ZUBIRI-GAITÁN, A., HERNÁNDEZ, P., GREENACRE, M., FERRER, A. and BLASCO, A. (2021). Comprehensive comparison of the cecum microbiome functional core in genetically obese and lean hosts under similar environmental conditions. Accepted by *Commun. Biol.*
- [69] MCKINLEY, J. M., GRUNSKY, E. and MUELLER, U. (2018). Environmental monitoring and peat assessment using multivariate analysis of regional-scale geochemical data. *Math. Geosci.* **50** 235–246. MR3772992 <https://doi.org/10.1007/s11004-017-9686-x>
- [70] MEIER, S., FALK-PETERSEN, S., GADE-SØRENSEN, L. A. et al. (2016). Fatty acids in common minke whale (*Balaenoptera acutorostrata*) blubber reflect the feeding area and food selection, but also high endogenous metabolism. *Marine Biol.*
- [71] MURTAGH, F. (1984). Counting dendrograms: A survey. *Discrete Appl. Math.* **7** 191–199. MR0727923 [https://doi.org/10.1016/0166-218X\(84\)90066-0](https://doi.org/10.1016/0166-218X(84)90066-0)
- [72] PALAREA-ALBALADEJO, J. and MARTÍN-FERNÁNDEZ, J. (2015). zCompositions – R package for multivariate imputation of left-censored data under a compositional approach. *Chemom. Intell. Lab. Syst.* **143** 85–96.
- [73] PAWLOWSKY-GLAHN, V. and BUCCIANTI, A., eds. (2011) *Compositional Data Analysis: Theory and Applications* Wiley, Chichester. MR2920574 <https://doi.org/10.1002/9781119976462>
- [74] PAWLOWSKY-GLAHN, V., EGOZCUE, J. J. and TOLOSONA-DELGADO, R. (2015). *Modeling and Analysis of Compositional Data. Statistics in Practice.* Wiley, Chichester. MR3328965
- [75] QUINN, T. P. and ERB, I. (2020). Amalgams: Data-driven amalgamation for the dimensionality reduction of compositional data. *NAR Genomics Bioinform.* **2**. lqaa076. <https://doi.org/10.1093/nargab/lqaa076>
- [76] QUINN, T. P., ERB, I., RICHARDSON, M. F. and CROWLEY, T. M. (2018). Understanding sequencing data as compositions: An outlook and review. *Bioinformatics* **34** 2870–2878. <https://doi.org/10.1093/bioinformatics/bty175>

- [77] QUINN, T. P., RICHARDSON, M. F., LOVELL, D. and CROWLEY, T. M. (2017). Propr: An R-package for identifying proportionally abundant features using compositional data analysis. *Sci. Rep.* **7** 16252–16259.
- [78] RAND, W. M. (1971). Objective criteria for the evaluation of clustering methods. *J. Amer. Statist. Assoc.* **66** 846–850.
- [79] REN, B., BACALLADO, S., FAVARO, S., HOLMES, S. and TRIPPA, L. (2017). Bayesian nonparametric ordination for the analysis of microbial communities. *J. Amer. Statist. Assoc.* **112** 1430–1442. MR3750866 <https://doi.org/10.1080/01621459.2017.1288631>
- [80] REY, F., GREENACRE, M., SILVA NETO, G. M., BUENO-PARDO, J., DOMINGUES, M. R. and CALADO, R. (2022). Fatty acid ratio analysis identifies changes in competent meroplanktonic larvae sampled over different supply events. *Mar. Environ. Res.* **173** 105517.
- [81] SCEALY, J. L. and WELSH, A. H. (2011). Regression for compositional data by using distributions defined on the hypersphere. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **73** 351–375. MR2815780 <https://doi.org/10.1111/j.1467-9868.2010.00766.x>
- [82] SCEALY, J. L. and WELSH, A. H. (2014). Colours and cocktails: Compositional data analysis 2013 Lancaster lecture. *Aust. N. Z. J. Stat.* **56** 145–169. MR3226434 <https://doi.org/10.1111/anzs.12073>
- [83] SMITHSON, M. and BROOMELL, S. B. (2022). Compositional data analysis tutorial. *Psychol. Methods* **27**. <https://doi.org/10.1037/met0000464>
- [84] SMYTH, D. (2007). Methods used in the Tellus Geochemical Mapping of Northern Ireland. British Geological Survey, Open Report, OR/07/022.
- [85] STANLEY, C. R. (2019). Molar element ratio analysis of litho-geochemical data: A toolbox for use in mineral exploration and mining. *Geochem., Explor. Environ. Anal.* **20** 233–256.
- [86] STEPHENS, M. A. (1982). Use of the von Mises distribution to analyse continuous proportions. *Biometrika* **69** 197–203. MR0655685 <https://doi.org/10.1093/biomet/69.1.197>
- [87] TE BEEST, D. E., NIJHUIS, E. H., MÖHLMANN, T. W. R. and TER BRAAK, C. J. F. (2021). Log-ratio analysis of microbiome data with many zeroes is library size dependent. *Mol. Ecol. Resour.* **21** 1866–1874. <https://doi.org/10.1111/1755-0998.13391>
- [88] R CORE TEAM (2021). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria.
- [89] TOWNES, F. W., HICKS, S. C., ARYEE, M. J. and IRIZARRY, R. A. (2019). Feature selection and dimension reduction for single-cell RNA-Seq based on a multinomial model. *Genome Biol.* **20** 295. <https://doi.org/10.1186/s13059-019-1861-6>
- [90] VAN DEN BOOGAART, K. G. and TOLOSANA-DELGADO, R. (2013). *Analyzing Compositional Data with R. Use R!* Springer, Heidelberg. MR3099409 <https://doi.org/10.1007/978-3-642-36809-7>
- [91] VAN DEN WOLLENBERG, A. L. (1977). Redundancy analysis, an alternative for canonical analysis. *Psychometrika* **42** 207–219.
- [92] WOOD, J. and GREENACRE, M. (2021). Making the most of expert knowledge to analyse archaeological data: A case study on Parthian and Sasanian glazed pottery. *Archaeol. Anthropol. Sci.* **13** 110.
- [93] YOO, J., SUN, Z., GREENACRE, M., MAD, Q., CHUNG, D. and KIM, Y. M. (2022). A guideline for the statistical analysis of compositional data in immunology. *Commun. Stat. Appl. Methods* **29** 453–469.

Statistical Embedding: Beyond Principal Components

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Abstract. There has been an intense recent activity in embedding of very high-dimensional and nonlinear data structures, much of it in the data science and machine learning literature. We survey this activity in four parts. In the first part, we cover nonlinear methods such as principal curves, multidimensional scaling, local linear methods, ISOMAP, graph-based methods and diffusion mapping, kernel based methods and random projections. The second part is concerned with topological embedding methods, in particular mapping topological properties into persistence diagrams and the Mapper algorithm. Another type of data sets with a tremendous growth is very high-dimensional network data. The task considered in part three is how to embed such data in a vector space of moderate dimension to make the data amenable to traditional techniques such as cluster and classification techniques. Arguably, this is the part where the contrast between algorithmic machine learning methods and statistical modeling, represented by the so-called stochastic block model, is at its greatest. In the paper, we discuss the pros and cons for the two approaches. The final part of the survey deals with embedding in \mathbb{R}^2 , that is, visualization. Three methods are presented: t -SNE, UMAP and LargeVis based on methods in parts one, two and three, respectively. The methods are illustrated and compared on two simulated data sets; one consisting of a triplet of noisy Ranunculoid curves, and one consisting of networks of increasing complexity generated with stochastic block models and with two types of nodes.

Key words and phrases: Statistical embedding, principal component, nonlinear principal component, multidimensional scaling, local linear method, ISOMAP, graph spectral theory, diffusion mapping, reproducing kernel Hilbert space, random projection, topological data analysis and embedding, persistent homology, persistence diagram, the Mapper, network embedding, spectral embedding, stochastic block modeling, Skip-Gram, neighborhood sampling strategies, visualization, t -SNE, LargeVis, UMAP.

REFERENCES

- AIZERMAN, M. A., BRAVERMAN, E. M. and ROZONOER, L. I. (1956). Theoretical foundations of the potential function method in pattern recognition learning. *Autom. Remote Control* **25** 821–137.
- ARMILLOTTA, M., FOKIANOS, K. and KRIKIDIS, I. (2022). Generalized linear models network autoregression. In *Network Science* 112–125. International Conference on Network Science.
- BAGLAMA, J. and REICHEL, L. (2005). Augmented implicitly restarted Lanczos bidiagonalization methods. *SIAM J. Sci. Comput.* **27** 19–42. MR2201173 <https://doi.org/10.1137/04060593X>
- BELKIN, M. and NIYOGI, P. (2002). Laplacian eigenmaps and spectral techniques for embedding and clustering. In *Advances in Information Processing Systems* (T. K. Leen, T. G. Dietterich and V. Treps, eds.). MIT Press, Cambridge, MA.
- BELKIN, M. and NIYOGI, P. (2003). Laplacian eigenmaps for dimensionality reduction and data representation. *Neural Comput.* **15** 1373–1396.
- BIAN, R., KOH, Y. S., DOBBIE, G. and DIVOLI, A. (2019). Network embedding and change modeling in dynamic heterogeneous networks. In *Proceedings of the 42nd International ACM SIGIR Conference on Research and Development in Information Retrieval* 861–864.
- BICKEL, P. and CHEN, A. (2009). A nonparametric view of network models and Newman–Girvan and other modularities. *Proc. Natl. Acad. Sci.* **106** 21068–21073.

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- BICKEL, P. J. and SARKAR, P. (2016). Hypothesis testing for automated community detection in networks. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **78** 253–273. MR3453655 <https://doi.org/10.1111/rssb.12117>
- BICKEL, P., CHOI, D., CHANG, X. and ZHANG, H. (2013). Asymptotic normality of maximum likelihood and its variational approximation for stochastic blockmodels. *Ann. Statist.* **41** 1922–1943. MR3127853 <https://doi.org/10.1214/13-AOS1124>
- BLONDEL, V. D., GUILLAUME, J.-L., LAMBIOTTE, R. and LEFEBVRE, E. (2008). Fast unfolding of communities in large networks. *J. Stat. Mech. Theory Exp.* **2008** P10008.
- BOSER, B. E., GUYON, I. M. and VAPNIK, V. N. (1992). A training algorithm for optimal margin classifiers. In *Fifth Annual Workshop on COLT*, ACM, Pittsburgh, PA.
- BUKKURI, A., ANDOR, N. and DARCY, I. K. (2021). Applications of topological data analysis on oncology. *Front. Artif. Intell. Mach. Learn. Artif. Intell.* **4** 1–14.
- CANNINGS, T. I. and SAMWORTH, R. J. (2017). Random-projection ensemble classification. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **79** 959–1035. MR3689307 <https://doi.org/10.1111/rssb.12228>
- CARLSSON, G. (2009). Topology and data. *Bull. Amer. Math. Soc. (N.S.)* **46** 255–308. MR2476414 <https://doi.org/10.1090/S0273-0979-09-01249-X>
- CARRIÈRE, M., MICHEL, B. and OUDOT, S. (2018). Statistical analysis and parameter selection for Mapper. *J. Mach. Learn. Res.* **19** Paper No. 12, 39 pp. MR3862419
- CARRIÈRE, M. and RABADÁN, R. (2020). Topological data analysis of single-cell Hi-C contact maps. In *Topological Data Analysis—The Abel Symposium 2018. Abel Symp.* **15** 147–162. Springer, Cham. MR4338672 https://doi.org/10.1007/978-3-030-43408-3_6
- CHAZAL, F. and MICHEL, B. (2017). An introduction to topological data analysis: Fundamental and practical aspects for data scientists. Preprint. Available at [arXiv:1710.04019v1](https://arxiv.org/abs/1710.04019v1).
- CHAZAL, F. and MICHEL, B. (2021). An introduction to topological data analysis: Fundamental and practical aspects for data scientists. *Front. Artif. Intell. Mach. Learn. Artif. Intell.* **4** 1–28.
- CHEN, Y.-C., GENOVESE, C. R. and WASSERMAN, L. (2015). Asymptotic theory for density ridges. *Ann. Statist.* **43** 1896–1928. MR3375871 <https://doi.org/10.1214/15-AOS1329>
- CHEN, Y. C., HO, S., FREEMAN, P. E., GENOVESE, C. R. and WASSERMAN, L. (2015a). Cosmic web reconstruction through density ridges: Methods and algorithm. *Mon. Not. R. Astron. Soc.* **454** 1140–1156.
- CHEN, Y. C., HO, S., TENNETI, A., MANDELBAUM, R., CROFT, R., DIMATTEO, T., FREEMAN, P. E., GENOVESE, C. R. and WASSERMAN, L. (2015b). Investigating galaxy-filament alignments in hydrodynamic simulations using density ridges. *Mon. Not. R. Astron. Soc.* **454** 3341–3350.
- CLAESKENS, G., CROUX, C. and VAN KERCKHOVEN, J. (2008). An information criterion for variable selection in support vector machines. *J. Mach. Learn. Res.* **9** 541–558. MR2417246 <https://doi.org/10.2139/ssrn.1094652>
- COIFMAN, R. R. and LAFON, S. (2006). Diffusion maps. *Appl. Comput. Harmon. Anal.* **21** 5–30. MR2238665 <https://doi.org/10.1016/j.acha.2006.04.006>
- CORMEN, T. H., LEISERSON, C. E., RIVEST, R. L. and STEIN, C. (2022). *Introduction to Algorithms*, 3rd ed. MIT Press, Cambridge, MA. MR2572804
- CRANE, H. and DEMPSEY, W. (2015). A framework for statistical network modeling. Preprint. Available at [arXiv:1509.08185](https://arxiv.org/abs/1509.08185).
- CRAWFORD, L., MONOD, A., CHEN, A. X., MUKHERJEE, S. and RABADÁN, R. (2020). Predicting clinical outcomes in glioblastoma: An application of topological and functional data analysis. *J. Amer. Statist. Assoc.* **115** 1139–1150. MR4143455 <https://doi.org/10.1080/01621459.2019.1671198>
- CUI, P., WANG, X., PEI, J. and ZHU, W. (2019). A survey on network embedding. *IEEE Trans. Knowl. Data Eng.* **31** 833–852.
- DE SILVA, V. and TENENBAUM, J. (2002). Global versus local methods in nonlinear dimensionality reduction. *Adv. Neural Inf. Process. Syst.* **15**.
- DECELLE, A., KRZAKALA, F., MOORE, C. and ZDEBOROVÁ, L. (2011). Asymptotic analysis of the stochastic block model for modular networks and its algorithmic applications. *Phys. Rev. E* **84** 066106.
- DEVROYE, L. and WISE, G. L. (1980). Detection of abnormal behavior via nonparametric estimation of the support. *SIAM J. Appl. Math.* **38** 480–488. MR0579432 <https://doi.org/10.1137/0138038>
- DONG, Y., CHAWLA, N. V. and SWAMI, A. (2017). Metapath2vec: Scalable representation learning for heterogeneous networks. Kid 17, 2017, Halifax, NS, Canada.
- DONG, W., MOSES, C. and LI, K. (2018). Efficient k -nearest neighbour graph construction for generic similarity measures. In *Proceedings of the 20th International Conference of the World Wide Web* 577–586, New York.
- DU, L., WANG, Y., SONG, G., LU, Z. and WANG, J. (2018). Dynamic network embedding: An extended approach for Skip-Gram based network embedding. In *Proceedings of the 27th International Joint Conference on Artificial Intelligence, IJAI-18*.
- DUCHAMP, T. and STUETZLE, W. (1996). Extremal properties of principal curves in the plane. *Ann. Statist.* **24** 1511–1520. MR1416645 <https://doi.org/10.1214/aos/1032298280>
- EDELSBRUNNER, H., LETCHER, D. and ZOMORODIAN, A. (2002). Topological persistence and simplification. *Discrete Comput. Geom.* **28** 511–533. MR1949898 <https://doi.org/10.1007/s00454-002-2885-2>
- GENOVESE, C. R., PERONE-PACIFICO, M., VERDINELLI, I. and WASSERMAN, L. (2012). Manifold estimation and singular deconvolution under Hausdorff loss. *Ann. Statist.* **40** 941–963. MR2985939 <https://doi.org/10.1214/12-AOS994>
- GENOVESE, C. R., PERONE-PACIFICO, M., VERDINELLI, I. and WASSERMAN, L. (2014). Nonparametric ridge estimation. *Ann. Statist.* **42** 1511–1545. MR3262459 <https://doi.org/10.1214/14-AOS1218>
- GHOJOGH, B., GHODSI, A., KARRAY, F. and CROWLEY, M. (2021). Johnson–Lindenstrauss lemma, linear and nonlinear random projections, random Fourier features and random kitchen sinks: Tutorial and survey. Preprint. Available at [arXiv:2108.04172v1](https://arxiv.org/abs/2108.04172v1).
- GHRIST, R. (2018). Homological algebra and data. In *The Mathematics of Data. IAS/Park City Math. Ser.* **25** 273–325. Amer. Math. Soc., Providence, RI. MR3839171
- GIRVAN, M. and NEWMAN, M. E. J. (2002). Community structure in social and biological networks. *Proc. Natl. Acad. Sci. USA* **99** 7821–7826. MR1908073 <https://doi.org/10.1073/pnas.122653799>
- GREENE, D. and CUNNINGHAM, P. (2011). Tracking the evolution of communities in dynamic social networks. Report Idiro Technologies, Dublin, Ireland.
- GRETTON, A. (2019). Introduction to RKHS, and some simple kernel algorithms. Lecture notes.
- GROVER, A. and LESKOVEC, J. (2016). node2vec: Scalable feature learning for networks. In *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining* 855–864.
- HAGHVERDI, L., BUETTNER, F. and THEIS, F. J. (2015). Diffusion maps for high-dimensional single-cell analysis of differentiation data. *Bioinformatics* **31** 2989–2998. <https://doi.org/10.1093/bioinformatics/btv325>
- HASTIE, T. (1984). Principal curves and surfaces. Laboratory for Computational Statistics Technical Report 11, Stanford Univ., Dept. Statistics. MR2634007

- HASTIE, T. and STUETZLE, W. (1989). Principal curves. *J. Amer. Statist. Assoc.* **84** 502–516. [MR1010339](#)
- HASTIE, T., TIBSHIRANI, R. and FRIEDMAN, J. (2019). *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*, 2nd ed. *Springer Series in Statistics*. Springer, New York. [MR2722294](#) <https://doi.org/10.1007/978-0-387-84858-7>
- HINTON, G. E. and ROWEIS, S. T. (2002). Stochastic neighbour embedding. *Adv. Neural Inf. Process. Syst.* **15** 833–840.
- HINTON, G. E. and SALAKHUTDINOV, R. R. (2006). Reducing the dimensionality of data with neural networks. *Science* **313** 504–507. [MR2242509](#) <https://doi.org/10.1126/science.1127647>
- HOFF, P. D., RAFTERY, A. E. and HANDCOCK, M. S. (2002). Latent space approaches to social network analysis. *J. Amer. Statist. Assoc.* **97** 1090–1098. [MR1951262](#) <https://doi.org/10.1198/016214502388618906>
- HOLLAND, P. W., LASKEY, K. B. and LEINHARDT, S. (1983). Stochastic blockmodels: First steps. *Soc. Netw.* **5** 109–137. [MR0718088](#) [https://doi.org/10.1016/0378-8733\(83\)90021-7](https://doi.org/10.1016/0378-8733(83)90021-7)
- HOTELLING, H. (1933). Analysis of a complex of statistical variables into principal components. *J. Educ. Psychol.* **24** 417–441.
- HOTELLING, H. (1936). Relations between two sets of variates. *Biometrika* **28** 321–377.
- HYVÄRINEN, A. and OJA, E. (2000). Independent component analysis: Algorithms and applications. *Neural Netw.* **13** 411–430.
- JOHNSON, W. B. and LINDENSTRAUSS, J. (1984). Extensions of Lipschitz mappings into a Hilbert space. In *Conference in Modern Analysis and Probability (New Haven, Conn., 1982)*. *Contemp. Math.* **26** 189–206. Amer. Math. Soc., Providence, RI. [MR0737400](#) <https://doi.org/10.1090/conm/026/737400>
- JOLLIFFE, I. T. (2002). *Principal Component Analysis*, 2nd ed. *Springer Series in Statistics*. Springer, New York. [MR2036084](#)
- JOSSE, J. and HUSSON, F. (2012). Selecting the number of components in principal component analysis using cross-validation approximations. *Comput. Statist. Data Anal.* **56** 1869–1879. [MR2892383](#) <https://doi.org/10.1016/j.csda.2011.11.012>
- KARRER, B. and NEWMAN, M. E. J. (2011). Stochastic blockmodels and community structure in networks. *Phys. Rev. E* (3) **83** 016107, 10 pp. [MR2788206](#) <https://doi.org/10.1103/PhysRevE.83.016107>
- KAZEMI, S. M., GOEL, R., JAIN, K., KOPYZEV, I., SETHI, A., FORSYTH, P. and POUPART, P. (2020). Representation learning for dynamic graphs: A survey. *J. Mach. Learn. Res.* **21** Paper No. 70, 73 pp. [MR4095349](#)
- KIM, J., RINALDO, A. and WASSERMAN, L. (2019). Minimax rates for estimating the dimension of a manifold. *J. Comput. Geom.* **10** 42–95. [MR3918925](#) <https://doi.org/10.20382/jocg.v10i1a3>
- KOBOUROV, S. (2012). Spring embedders and forced directed graph drawing algorithms. Preprint. Available at [arXiv:1201.3011](https://arxiv.org/abs/1201.3011).
- KOHONEN, T. (1982). Self-organized formation of topologically correct feature map. *Biol. Cybernet.* **43** 59–69.
- KONISHI, S. and KITAGAWA, G. (2008). *Information Criteria and Statistical Modeling*. *Springer Series in Statistics*. Springer, New York. [MR2367855](#) <https://doi.org/10.1007/978-0-387-71887-3>
- KOSSINET, G. and WATTS, D. J. (2006). Empirical analysis of an evolving social network. *Science* **311** 88–90. [MR2192483](#) <https://doi.org/10.1126/science.1116869>
- LEE, C. and WILKINSON, D. J. (2019). A review of stochastic block models and extensions for graph clustering. *Appl. Netw. Sci.* **4** 122.
- LEI, J. and RINALDO, A. (2015). Consistency of spectral clustering in stochastic block models. *Ann. Statist.* **43** 215–237. [MR3285605](#) <https://doi.org/10.1214/14-AOS1274>
- LEVINA, E. and BICKEL, P. (2004). Maximum likelihood estimation of intrinsic dimension. In *Advances in Neural Information Processing Systems* (L. Saul, Y. Weiss and L. Bottou, eds.) **17**. MIT Press, Cambridge, MA.
- LI, P., HASTIE, T. J. and CHURCH, K. W. (2007). Nonlinear estimators and tail bounds for dimension reduction in l_1 using Cauchy random projections. *J. Mach. Learn. Res.* **8** 2497–2532. [MR2353840](#) https://doi.org/10.1007/978-3-540-72927-3_37
- LIM, B. and ZOHREN, S. (2021). Time-series forecasting with deep learning: A survey. *Philos. Trans. R. Soc. Lond. A* **379** Paper No. 20200209, 14 pp. [MR4236146](#) <https://doi.org/10.1098/rsta.2020.0209>
- LITTLE, A. V., MAGGIONI, M. and ROSASCO, L. (2011). Multiscale geometric methods for estimating intrinsic dimension. In *Proc. SampTA* 4:2.
- LUDKIN, M., ECKLEY, I. and NEAL, P. (2018). Dynamic stochastic block models: Parameter estimation and detection of changes in community structure. *Stat. Comput.* **28** 1201–1213. [MR3850391](#) <https://doi.org/10.1007/s11222-017-9788-9>
- LUNDE, B. Å. S., KLEPPE, T. S. and SKAUG, H. J. (2020). An information criterion for automatic gradient tree boosting. Preprint. Available at [arXiv:2008.05926](https://arxiv.org/abs/2008.05926).
- MARKOV, A. (1958). The insolubility of the problem of homeomorphy. *Dokl. Akad. Nauk SSSR* **121** 218–220. [MR0097793](#)
- MCINNIS, L., HEALY, J. and MELVILLE, J. (2018). UMAP: Uniform manifold approximation for dimension reduction. Preprint. Available at [arXiv:1802.03426v2](https://arxiv.org/abs/1802.03426v2).
- MIKOLOV, T., SUTSKEVER, I., CHEN, K., CORRADO, G. and DEAN, J. (2013). Distributed representation of words and phrases and their composability. In *Advances in Neural Information Processing Systems 26: Proceedings Annual 27th Conference on Neural Information Processing Systems, Lake Tahoe, Nevada, USA*.
- NEWMAN, M. E. J. (2006). Modularity and community structure in networks. *Proc. Natl. Acad. Sci.* **103** 8577–8582.
- NEWMAN, M. (2020). *Networks*, 2nd ed. Oxford Univ. Press, Oxford. [MR3838417](#) <https://doi.org/10.1093/oso/9780198805090.001.0001>
- NEWMAN, M. E. J. and GIRVAN, M. (2004). Finding and evaluating community networks. *Phys. Rev. E* **69** 026113.
- NEWMAN, M. E. J. and REINERT, G. (2016). Estimating the number of communities in a network. *Phys. Rev. Lett.* **137** 078301.
- NIYOGI, P., SMALE, S. and WEINBERGER, S. (2008). Finding the homology of submanifolds with high confidence from random samples. *Discrete Comput. Geom.* **39** 419–441. [MR2383768](#) <https://doi.org/10.1007/s00454-008-9053-2>
- OTNEIM, H., JULLUM, M. and TJØSTHEIM, D. (2020). Pairwise local Fisher and naive Bayes: Improving two standard discriminants. *J. Econometrics* **216** 284–304. [MR4077395](#) <https://doi.org/10.1016/j.jeconom.2020.01.019>
- OZERTEM, U. and ERDOGMUS, D. (2011). Locally defined principal curves and surfaces. *J. Mach. Learn. Res.* **12** 1249–1286. [MR2804600](#)
- PEARSON, K. (1901). On lines and planes of closest fit to systems of points in space. *Philos. Mag.* **2** 559–572.
- PEIXITO, T. P. (2021). Descriptive vs. inferential community detection: Pitfalls, myths and half-truths. Preprint. Available at [arXiv:2112.00183v1](https://arxiv.org/abs/2112.00183v1).
- PEIXOTO, T. P. (2019). Bayesian stochastic blockmodeling. In *Advances in Network Clustering and Blockmodeling* 289–332.
- PEROZZI, B., AL-RFOU, R. and SKIENA, S. (2014). Deepwalk: Online learning of social representations. In *Proceedings of the 20th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining* 701–710.
- QIAO, W. and POLONIK, W. (2021). Algorithms for ridge estimation with convergence guarantees. Preprint. Available at [arXiv:2014.12314v1](https://arxiv.org/abs/2014.12314v1).
- QIU, J., DONG, Y., MA, H., LI, J., WANG, K. and TANG, J. (2018). Network embedding as matrix factorization: Unifying DeepWalk, LINE, PTE, and node2vec. In *Proceedings WSDM*. ACM, New York.

- QIU, J., DONG, Y., MA, H., LI, J., WANG, K. and TANG, J. (2019). NetSMF: Large-scale network embedding as sparse matrix factorization. In *Proceedings of the 2019 World Wide Web Conference*, May 13–17, San Francisco, CA, USA.
- RAVISSHANKER, N. and CHEN, R. (2019). Topological data analysis (TDA) for time series. Preprint. Available at [arXiv:1909.10604v1](https://arxiv.org/abs/1909.10604v1).
- ROHE, K., CHATTERJEE, S. and YU, B. (2011). Spectral clustering and the high-dimensional stochastic blockmodel. *Ann. Statist.* **39** 1878–1915. [MR2893856 https://doi.org/10.1214/11-AOS887](https://doi.org/10.1214/11-AOS887)
- ROHE, K., QIN, T. and YU, B. (2016). Co-clustering directed graphs to discover asymmetries and directional communities. *Proc. Natl. Acad. Sci. USA* **113** 12679–12684. [MR3576189 https://doi.org/10.1073/pnas.1525793113](https://doi.org/10.1073/pnas.1525793113)
- ROWEIS, S. T. and SAUL, L. K. (2000). Nonlinear dimensionality reduction by locally linear embedding. *Science* **290** 2323–2326. <https://doi.org/10.1126/science.290.5500.2323>
- SALINAS, D., FLUNKERT, V., GASTHAUS, J. and JANUSCHOWSKI, T. (2020). DeepAR: Probabilistic forecasting with autoregressive recurrent networks. *Int. J. Forecast.* **36** 1181–1191.
- SAMMON, J. W. (1969). A nonlinear mapping for data structure analysis. *IEEE Trans. Comput.* **18** 403–409.
- SCHÖLKOPF, B., SMOLA, A. and MÜLLER, K.-L. (2005). Kernel principal components. *Lecture Notes in Comput. Sci.* **1327** 583–588.
- SHAHRIARI, B., SWERSKY, K., WANG, Z., ADAMS, R. P. and DE FREITAS, N. (2015). Taking the human out of the loop: A review of Bayesian optimization. *Proc. IEEE* **104** 148–175.
- SINGH, G., MEMOLI, F. and CARLSSON, G. (2007). Topological methods for the analysis of high dimensional data sets and 3D object recognition. In *Eurographics Symposium on Point Based Graphics* (M. Botsch and R. Pajarola, eds.). The Eurographics Association.
- SUN, Y., NORICK, B., HAN, J., YAN, X., YU, P. and YU, X. (2012). Integrating meta-path selection with user-guided object clustering in heterogeneous information networks. In *KDD '12: Proceedings of the 18th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining* 1348–1356.
- TANG, J., QU, M. and MEI, Q. (2015). PTE: Predictive text embedding through large-scale heterogeneous text networks. Preprint. Available at [arXiv:1508.00200v1](https://arxiv.org/abs/1508.00200v1).
- TANG, J., QU, M., WANG, M., ZHANG, M., YAN, J. and MEI, Q. (2015). LINE: Large-scale information network embedding. In *Proceedings of the 24th International Conference on World Wide Web* 1067–1077.
- TANG, J., LIU, J., ZHANG, M. and MEI, Q. (2016). Visualizing large-scale and high-dimensional data. In *Proceedings of the 25th International Conference on World Wide Web* 287–297.
- TENENBAUM, J. B., DE SILVA, V. and LANGFORD, J. C. (2000). A global geometric framework for nonlinear dimensionality reduction. *Science* **290** 2319–2323. <https://doi.org/10.1126/science.290.5500.2319>
- TJØSTHEIM, D., JULLUM, M. and LØLAND, A. (2023). Some recent trends in embedding of time series and dynamic networks. *J. Time Ser. Anal.* To appear. <https://doi.org/10.1111/jtsa.12677>
- TJØSTHEIM, D., JULLUM, M. and LØLAND, A. (2023). Supplement to “Statistical embedding: Beyond principal components”. <https://doi.org/10.1214/22-STSS881SUPP>
- TJØSTHEIM, D., OTNEIM, H. and STØVE, B. (2022a). Statistical dependence: Beyond Pearson’s ρ . *Statist. Sci.* **37** 90–109. [MR4371097 https://doi.org/10.1214/21-sts823](https://doi.org/10.1214/21-sts823)
- TJØSTHEIM, D., OTNEIM, H. and STØVE, B. (2022b). *Statistical Modeling Using Local Gaussian Approximation*. Elsevier/Academic Press, London. [MR4382419 https://doi.org/10.1016/B978-0-12-822891-6](https://doi.org/10.1016/B978-0-12-822891-6)
- TORGERSON, W. S. (1952). Multidimensional scaling: I. Theory and method. *Psychometrika* **17** 401–419. [MR0054219 https://doi.org/10.1007/BF02288916](https://doi.org/10.1007/BF02288916)
- TUTTE, W. T. (1963). How to draw a graph. *Proc. Lond. Math. Soc.* (3) **13** 743–767. [MR0158387 https://doi.org/10.1112/plms/s3-13.1.743](https://doi.org/10.1112/plms/s3-13.1.743)
- VAN DER MAATEN, L. (2014). Accelerating t-SNE using tree-based algorithms. *J. Mach. Learn. Res.* **15** 3221–3245. [MR3277169 https://doi.org/10.26434/chemrxiv-2014-08-00000](https://doi.org/10.26434/chemrxiv-2014-08-00000)
- VAN DER MAATEN, L. and HINTON, G. (2008). Visualizing data using t-SNE. *J. Mach. Learn. Res.* **9** 2579–2605.
- VAN DER MAATEN, L., POSTMA, E. and VAN DER HERIK, J. (2009). Dimensionality reduction: A comparative review. Tilburg Centre for Creative Computing, TiCC TR 2009.005.
- VON LUXBURG, U. (2007). A tutorial on spectral clustering. *Stat. Comput.* **17** 395–416. [MR2409803 https://doi.org/10.1007/s11222-007-9033-z](https://doi.org/10.1007/s11222-007-9033-z)
- WANG, Y. X. R. and BICKEL, P. J. (2017). Likelihood-based model selection for stochastic block models. *Ann. Statist.* **45** 500–528. [MR3650391 https://doi.org/10.1214/16-AOS1457](https://doi.org/10.1214/16-AOS1457)
- WASSERMAN, L. (2018). Topological data analysis. *Annu. Rev. Stat. Appl.* **5** 501–535. [MR3774757 https://doi.org/10.1146/annurev-statistics-031017-100045](https://doi.org/10.1146/annurev-statistics-031017-100045)
- WEI, Y.-C. and CHENG, C.-K. (1989). Towards efficient hierarchical designs by ratio cut partitioning. In *1989 IEEE International Conference on Computer-Aided Design. Digest of Technical Papers* 298–301. IEEE.
- XIE, H., LI, J. and XUE, H. (2018). A survey of dimensionality reduction techniques based on random projection. Preprint. Available at [arXiv:1706.04371v4](https://arxiv.org/abs/1706.04371v4).
- YOUNG, G. and HOUSEHOLDER, A. S. (1938). Discussion of a set of points in terms of their mutual distances. *Psychometrika* **3** 19–22.
- YOUNG, T., HAZARIKA, D., PORIA, S. and CAMBRIA, E. (2018). Recent trends in deep learning based natural language processing. *IEEE Comput. Intell. Mag.* **13** 55–75.
- ZHANG, J. and CHEN, Y. (2020). Modularity based community detection in heterogeneous networks. *Statist. Sinica* **30** 601–629. [MR4213981 https://doi.org/10.1007/s00445-020-00411-4](https://doi.org/10.1007/s00445-020-00411-4)
- ZHENG, Q. (2016). Spectral techniques for heterogeneous social networks. Ph.D. thesis, Queen’s Univ., Ontario, Canada.
- ZHOU, C., LIU, Y., LIU, X. and GAO, J. (2017). Scalable graph embedding for asymmetric proximity. In *Proceedings of the 31st AAAI Conference on Artificial Intelligence*.
- ZHU, X. and PAN, R. (2020). Grouped network vector autoregression. *Statist. Sinica* **30** 1437–1462. [MR4257540 https://doi.org/10.5705/ss.202017.0533](https://doi.org/10.5705/ss.202017.0533)
- ZHU, X., PAN, R., LI, G., LIU, Y. and WANG, H. (2017). Network vector autoregression. *Ann. Statist.* **45** 1096–1123. [MR3662449 https://doi.org/10.1214/16-AOS1476](https://doi.org/10.1214/16-AOS1476)
- ZOMORODIAN, A. and CARLSSON, G. (2005). Computing persistent homology. *Discrete Comput. Geom.* **33** 249–274. [MR2121296 https://doi.org/10.1007/s00454-004-1146-y](https://doi.org/10.1007/s00454-004-1146-y)

Can We Reliably Detect Biases that Matter in Observational Studies?

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Abstract. In an observational study of the effects caused by a treatment, biases from unmeasured covariates remain a concern even after successful adjustments for measured covariates. This concern is partly addressed by demonstrating that the qualitative conclusions of the primary analysis would not be altered by small or moderate biases—that these conclusions are insensitive to small or moderate bias. Additionally, the concern is partly addressed by collecting additional information, such as outcomes known to be unaffected by the treatment, and using this information as a test of various biases. Is there a gap between these two activities? Perhaps the study is insensitive to small biases, and we can detect large biases, but the study is sensitive to moderate biases that cannot be detected—that is an informal description of a gap. The concept of “no gap” is defined formally in Definition 3.1, and the probability of “no gap” is determined under various sampling situations. When there is no gap, ask: Are causal conclusions measurably strengthened? If so, by how much? The answer depends upon the covering design sensitivity, $\widehat{\Gamma}$, defined to be the smallest bias that can explain both the ostensible effect of the treatment on the primary outcome and the evidence of bias provided by the unaffected outcome. The covering design sensitivity is calculated in various contexts. A small observational study of the effects of light alcohol consumption on HDL cholesterol is used to illustrate ideas and methods.

Key words and phrases: Causal inference, detecting bias, observational study, sensitivity analysis.

REFERENCES

- [1] AGENCY, U. E. P. (2021). How people are exposed to mercury. Available at www.epa.gov/mercury.
- [2] ALBERS, W., BICKEL, P. J. and VAN ZWET, W. R. (1976). Asymptotic expansions for the power of distribution free tests in the one-sample problem. *Ann. Statist.* **4** 108–156. [MR0391373](#)
- [3] BERGER, R. L. and BOOS, D. D. (1994). P values maximized over a confidence set for the nuisance parameter. *J. Amer. Statist. Assoc.* **89** 1012–1016. [MR1294746](#)
- [4] BERK, R. H. and JONES, D. H. (1978). Relatively optimal combinations of test statistics. *Scand. J. Stat.* **5** 158–162. [MR0509452](#)
- [5] BIRCH, M. W. (1964). The detection of partial association. I. The 2×2 case. *J. Roy. Statist. Soc. Ser. B* **26** 313–324. [MR0176562](#)
- [6] BONVINI, M. and KENNEDY, E. H. (2022). Sensitivity analysis via the proportion of unmeasured confounding. *J. Amer. Statist. Assoc.* **117** 1540–1550. [MR4480730](#) <https://doi.org/10.1080/01621459.2020.1864382>
- [7] BROWN, B. M. (1981). Symmetric quantile averages and related estimators. *Biometrika* **68** 235–242. [MR0614960](#) <https://doi.org/10.1093/biomet/68.1.235>
- [8] CAMPBELL, D. T. (1969). Prospective: Artifact and control. In *Artifacts in Behavioral Research* (R. Rosenthal and R. Rosnow, eds.) Academic Press, New York.
- [9] FISHER, R. A. (1935). *The Design of Experiments*. Oliver & Boyd, Edinburgh.
- [10] FOGARTY, C. B. and SMALL, D. S. (2016). Sensitivity analysis for multiple comparisons in matched observational studies through quadratically constrained linear programming. *J. Amer. Statist. Assoc.* **111** 1820–1830. [MR3601738](#) <https://doi.org/10.1080/01621459.2015.1120675>
- [11] GASTWIRTH, J. L. (1966). On robust procedures. *J. Amer. Statist. Assoc.* **61** 929–948. [MR0205397](#)
- [12] GASTWIRTH, J. L., KRIEGER, A. M. and ROSENBAUM, P. R. (2000). Asymptotic separability in sensitivity analysis. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **62** 545–555. [MR1772414](#) <https://doi.org/10.1111/1467-9868.00249>
- [13] GOODMAN, S. N., SCHNEEWEISS, S. and BAIOCCHI, M. (2017). Using design thinking to differentiate useful from misleading evidence in observational research. *J. Amer. Med. Assoc.* **317** 705–707.
- [14] GROENEVELD, R. A. (1972). Asymptotically optimal group rank tests for location. *J. Amer. Statist. Assoc.* **67** 847–849.

- MR0395030
- [15] HASEGAWA, R. B., WEBSTER, D. W. and SMALL, D. S. (2019). Evaluating Missouri's handgun purchaser law: A bracketing method for addressing concerns about history interacting with group. *Epidemiology* **30** 371–379.
- [16] HOGAN, W. W. (1973). Point-to-set maps in mathematical programming. *SIAM Rev.* **15** 591–603. MR0345641 <https://doi.org/10.1137/1015073>
- [17] KARMAKAR, B., FRENCH, B. and SMALL, D. S. (2019). Integrating the evidence from evidence factors in observational studies. *Biometrika* **106** 353–367. MR3949308 <https://doi.org/10.1093/biomet/asz003>
- [18] KIM, H. J., JUNG, S., ELIASSEN, A. H., CHEN, W. Y., WILLET, W. C. and CHO, E. (2017). Alcohol consumption and breast cancer risk in younger women according to family history of breast cancer and folate intake. *Amer. J. Epidemiol.* **186** 524–531.
- [19] KUROKI, M. and PEARL, J. (2014). Measurement bias and effect restoration in causal inference. *Biometrika* **101** 423–437. MR3215357 <https://doi.org/10.1093/biomet/ast066>
- [20] LEHMANN, E. L. (1975). *Nonparametrics*. Holden-Day, Oakland, CA.
- [21] LEHMANN, E. L. and ROMANO, J. P. (2006). *Testing Statistical Hypotheses*. Springer, Berlin.
- [22] LOCONTE, N. K., BREWSTER, A. M., KAUR, J. S., MERRILL, J. K. and ALBERG, A. J. (2018). Alcohol and cancer: A statement of the American society of clinical oncology. *J. Clin. Oncol.* **36** 83–93.
- [23] LU, B., CAI, D. and TONG, X. (2018). Testing causal effects in observational survival data using propensity score matching design. *Stat. Med.* **37** 1846–1858. MR3799844 <https://doi.org/10.1002/sim.7599>
- [24] MARITZ, J. S. (1979). A note on exact robust confidence intervals for location. *Biometrika* **66** 163–166. MR0529161 <https://doi.org/10.1093/biomet/66.1.163>
- [25] MARKOWSKI, E. P. and HETTMANSPERGER, T. P. (1982). Inference based on simple rank step score statistics for the location model. *J. Amer. Statist. Assoc.* **77** 901–907. MR0686416
- [26] MCKILLIP, J. (1992). Research without control groups: A control construct design. In *Methodological Issues in Applied Social Psychology* 159–175. Springer, Berlin.
- [27] MUNAFÒ, M. R., HIGGINS, J. P. T. and SMITH, G. D. (2021). Triangulating evidence through the inclusion of genetically informed designs. *Cold Spring Harbor Perspect. Med.* **11** a040659.
- [28] NEYMAN, J. (1990). On the application of probability theory to agricultural experiments. Essay on principles. Section 9. *Statist. Sci.* **5** 465–472. MR1092986 <https://doi.org/10.1214/ss/1177012031>
- [29] NOETHER, G. E. (1973). Some simple distribution-free confidence intervals for the center of a symmetric distribution. *J. Amer. Statist. Assoc.* **68** 716–719.
- [30] PEDERSEN, G. A., MORTENSEN, G. K. and LARSEN, E. H. (1994). Beverages as a source of toxic trace element intake. *Food Add. Contam.* **11** 351–363.
- [31] PIMENTEL, S. D., SMALL, D. S. and ROSENBAUM, P. R. (2016). Constructed second control groups and attenuation of unmeasured biases. *J. Amer. Statist. Assoc.* **111** 1157–1167. MR3561939 <https://doi.org/10.1080/01621459.2015.1076342>
- [32] QUADE, D. (1979). Using weighted rankings in the analysis of complete blocks with additive block effects. *J. Amer. Statist. Assoc.* **74** 680–683. MR0548265
- [33] REYNOLDS, K. D. and WEST, S. G. (1987). A multiplisat strategy for strengthening nonequivalent control group designs. *Eval. Rev.* **11** 691–714.
- [34] ROSENBAUM, P. R. (1987). The role of a second control group in an observational study. *Statist. Sci.* **2** 292–306.
- [35] ROSENBAUM, P. R. (1989). The role of known effects in observational studies. *Biometrics* **45** 557–569. MR1010518 <https://doi.org/10.2307/2531497>
- [36] ROSENBAUM, P. R. (1989). On permutation tests for hidden biases in observational studies: An application of Holley's inequality to the Savage lattice. *Ann. Statist.* **17** 643–653. MR0994256 <https://doi.org/10.1214/aos/1176347131>
- [37] ROSENBAUM, P. R. (2002). *Observational Studies*, 2nd ed. *Springer Series in Statistics*. Springer, New York. MR1899138 <https://doi.org/10.1007/978-1-4757-3692-2>
- [38] ROSENBAUM, P. R. (2007). Sensitivity analysis for m -estimates, tests, and confidence intervals in matched observational studies. *Biometrics* **63** 456–464. MR2370804 <https://doi.org/10.1111/j.1541-0420.2006.00717.x>
- [39] ROSENBAUM, P. R. (2010). Design sensitivity and efficiency in observational studies. *J. Amer. Statist. Assoc.* **105** 692–702. MR2724853 <https://doi.org/10.1198/jasa.2010.tm09570>
- [40] ROSENBAUM, P. R. (2012). An exact adaptive test with superior design sensitivity in an observational study of treatments for ovarian cancer. *Ann. Appl. Stat.* **6** 83–105. MR2951530 <https://doi.org/10.1214/11-AOAS508>
- [41] ROSENBAUM, P. R. (2012). Testing one hypothesis twice in observational studies. *Biometrika* **99** 763–774. MR2999159 <https://doi.org/10.1093/biomet/ass032>
- [42] ROSENBAUM, P. R. (2014). Weighted M -statistics with superior design sensitivity in matched observational studies with multiple controls. *J. Amer. Statist. Assoc.* **109** 1145–1158. MR3265687 <https://doi.org/10.1080/01621459.2013.879261>
- [43] ROSENBAUM, P. R. (2015). Bahadur efficiency of sensitivity analyses in observational studies. *J. Amer. Statist. Assoc.* **110** 205–217. MR3338497 <https://doi.org/10.1080/01621459.2014.960968>
- [44] ROSENBAUM, P. R. (2017). *Observation and Experiment*. Harvard Univ. Press, Cambridge, MA. MR3702029
- [45] ROSENBAUM, P. R. (2018). Sensitivity analysis for stratified comparisons in an observational study of the effect of smoking on homocysteine levels. *Ann. Appl. Stat.* **12** 2312–2334. MR3875702 <https://doi.org/10.1214/18-AOAS1153>
- [46] ROSENBAUM, P. R. (2020). Modern algorithms for matching in observational studies. *Annu. Rev. Stat. Appl.* **7** 143–176. MR4104189 <https://doi.org/10.1146/annurev-statistics-031219-041058>
- [47] ROSENBAUM, P. R. (2020). *Design of Observational Studies*. Springer, Berlin.
- [48] ROSENBAUM, P. R. (2021). *Replication and Evidence Factors in Observational Studies*. CRC Press/CRC, Boca Raton, FL.
- [49] ROSENBAUM, P. R. (2023). Sensitivity analyses informed by tests for bias in observational studies. *Biometrics* **79**. <https://doi.org/10.1111/biom.13558>
- [50] ROSENBAUM, P. R. and SILBER, J. H. (2009). Amplification of sensitivity analysis in matched observational studies. *J. Amer. Statist. Assoc.* **104** 1398–1405. MR2750570 <https://doi.org/10.1198/jasa.2009.tm08470>
- [51] RUBIN, D. B. (1974). Estimating causal effects of treatments in randomized and nonrandomized studies. *J. Educ. Psychol.* **66** 688–701.
- [52] SCHUEMIE, M., HRIPCSAK, G., RYAN, P., MADIGAN, D. and SUCHARD, M. (2018). Empirical confidence interval calibration for population-level effect estimation studies in observational healthcare data. *Proc. Natl. Acad. Sci. USA* **115** 2571–2577.
- [53] SCHWARTZ, S., LI, F. and REITER, J. P. (2012). Sensitivity analysis for unmeasured confounding in principal stratification settings with binary variables. *Stat. Med.* **31** 949–962. MR2913871 <https://doi.org/10.1002/sim.4472>

- [54] SHI, X., MIAO, W. and TCHETGEN TCHETGEN, E. (2020). A selective review of negative control methods in epidemiology. *Curr. Epidemiol. Rep.* **7** 190–202.
- [55] SUH, I., SHATEN, B. J., CUTLER, J. A. and KULLER, L. H. (1992). Alcohol use and mortality from coronary heart disease: The role of high-density lipoprotein cholesterol. The multiple risk factor intervention trial research group. *Ann. Intern. Med.* **116** 881–887. <https://doi.org/10.7326/0003-4819-116-11-881>
- [56] SUNDARAM, R. K. (1996). *A First Course in Optimization Theory*. Cambridge Univ. Press, Cambridge. MR1402910 <https://doi.org/10.1017/CBO9780511804526>
- [57] TARDIF, S. (1987). Efficiency and optimality results for tests based on weighted rankings. *J. Amer. Statist. Assoc.* **82** 637–644. MR0898370
- [58] TCHETGEN TCHETGEN, E. J. (2014). The control outcome calibration approach for causal inference with unobserved confounding. *Amer. J. Epidemiol.* **179** 633–640.
- [59] TCHETGEN TCHETGEN, E. J., YING, A., CUI, Y., SHI, X. and MIAO, W. (2020). An introduction to proximal causal learning. ArXiv Preprint. Available at [arXiv:2009.10982](https://arxiv.org/abs/2009.10982).
- [60] YU, B. and GASTWIRTH, J. L. (2005). Sensitivity analysis for trend tests: Application to the risk of radiation exposure. *Biostatistics* **6** 201–209.
- [61] ZHAO, Q. (2019). On sensitivity value of pair-matched observational studies. *J. Amer. Statist. Assoc.* **114** 713–722. MR3963174 <https://doi.org/10.1080/01621459.2018.1429277>

Experimental Design in Marketplaces

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Abstract. Classical Randomized Controlled Trials (RCTs), or A/B tests, are designed to draw causal inferences about a population of units, for example, individuals, plots of land or visits to a website. A key assumption underlying a standard RCT is the absence of interactions between units, or the *stable unit treatment value assumption* (*Ann. Statist.* **6** (1978) 34–58). Modern experimentation, however, is often conducted in settings characterized by complex interactions between units. Such interactions can invalidate the standard estimators and make classical experimental designs ineffective. Although the presence of interference forces us to make untestable assumptions on the nature of the interactions even under randomization, sophisticated experimental designs can ameliorate the dependence on such assumptions. In this manuscript, we review the recent and rapidly growing literature on novel experimental designs for these settings. One key feature common to many of these designs is the presence of multiple layers of randomization within the same experiment. We discuss a novel experimental design, called *Multiple Randomization Designs* or MRDs, that provides a general framework for such experiments. Through these complex designs, we can study questions about causal effects in the presence of interference that cannot be answered by classical RCTs.

Key words and phrases: Experimental design, causal inference, online experimentation, multiple randomization designs, two-sided marketplaces.

REFERENCES

- ARONOW, P. M. (2012). A general method for detecting interference between units in randomized experiments. *Sociol. Methods Res.* **41** 3–16. MR3190698 <https://doi.org/10.1177/0049124112437535>
- ARONOW, P. M. and SAMII, C. (2017). Estimating average causal effects under general interference, with application to a social network experiment. *Ann. Appl. Stat.* **11** 1912–1947. MR3743283 <https://doi.org/10.1214/16-AOAS1005>
- ATHEY, S., ECKLES, D. and IMBENS, G. W. (2018). Exact p -values for network interference. *J. Amer. Statist. Assoc.* **113** 230–240. MR3803460 <https://doi.org/10.1080/01621459.2016.1241178>
- ATHEY, S. and IMBENS, G. W. (2022). Design-based analysis in difference-in-differences settings with staggered adoption. *J. Econometrics* **226** 62–79. MR4348786 <https://doi.org/10.1016/j.jeconom.2020.10.012>
- BACKSTROM, L. and KLEINBERG, J. (2011). Network bucket testing. In *Proceedings of the 20th International Conference on World Wide Web* 615–624.
- BAJARI, P., BURDICK, B., IMBENS, G. W., MASOERO, L., MCQUEEN, J., RICHARDSON, T. and ROSEN, I. M. (2021). Multiple randomization designs. arXiv preprint. Available at [arXiv:2112.13495](https://arxiv.org/abs/2112.13495).
- BASSE, G. W., FELLER, A. and TOULIS, P. (2019). Randomization tests of causal effects under interference. *Biometrika* **106** 487–494. MR3949317 <https://doi.org/10.1093/biomet/asy072>
- BOJINOV, I., SIMCHI-LEVI, D. and ZHAO, J. (2020). Design and analysis of switchback experiments. Available at SSRN 3684168.
- BOND, R. M., FARISS, C. J., JONES, J. J., KRAMER, A. D., MARLOW, C., SETTLE, J. E. and FOWLER, J. H. (2012). A 61-million-person experiment in social influence and political mobilization. *Nature* **489** 295–298.
- BRANDT, A. (1938). Tests of significance in reversal or switchback trials. *Iowa Agric. Home Econ. Exp. Stat. Res. Bull.* **21** 1.
- BROWN, B. W. JR. (1980). The crossover experiment for clinical trials. *Biometrics* 69–79.
- COCHRAN, W. (1939). Long-term agricultural experiments. *Suppl. J. R. Stat. Soc.* **6** 104–148.

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- COCHRAN, W. G. (1977). *Sampling Techniques*, 3rd ed. *Wiley Series in Probability and Mathematical Statistics*. Wiley, New York. MR0474575
- COCHRAN, W. G. and COX, G. M. (1948). *Experimental Designs*. Wiley, New York, NY.
- COOK, T. D. and DEMETS, D. L. (2007). *Introduction to Statistical Methods for Clinical Trials*. CRC Press/CRC, Boca Raton, FL.
- CRÉPON, B., DUFLO, E., GURGAND, M., RATHÉLOT, R. and ZAMORA, P. (2013). Do labor market policies have displacement effects? Evidence from a clustered randomized experiment. *Q. J. Econ.* **128** 531–580.
- FISHER, R. A. (1937). *The Design of Experiments*. Oliver & Boyd, Edinburgh.
- GART, J. J. (1963). A median test with sequential application. *Biometrika* **50** 55–62. MR0156424 <https://doi.org/10.1093/biomet/50.1-2.55>
- GASTWIRTH, J. L. (1968). The first-median test: A two-sided version of the control median test. *J. Amer. Statist. Assoc.* **63** 692–706. MR0240933
- GUPTA, S., KOHAVI, R., TANG, D., XU, Y., ANDERSEN, R., BAKSHY, E., CARDIN, N., CHANDRAN, S., CHEN, N. et al. (2019). Top challenges from the first practical online controlled experiments summit. *ACM SIGKDD Explor. Newsl.* **21** 20–35.
- HALLORAN, M. E., and STRUCHINER, C. J. (1991). Study Designs for Dependent Happenings. *Epidemiology*. **2** 331–338.
- HECKMAN, J. J., LOCHNER, L. and TABER, C. (1998). General-equilibrium treatment effects: A study of tuition policy. *Amer. Econ. Rev.* **88** 381–386.
- HEMMING, K., HAINES, T. P., CHILTON, P. J., GIRLING, A. J. and LILFORD, R. J. (2015). The stepped wedge cluster randomised trial: Rationale, design, analysis, and reporting. *BMJ* **350**.
- HOLLAND, P. W. (1986). Statistics and causal inference. *J. Amer. Statist. Assoc.* **81** 945–970. MR0867618
- HOLTZ, D., LOBEL, R., LISKOVICH, I. and ARAL, S. (2020). Reducing interference bias in online marketplace pricing experiments. arXiv preprint. Available at arXiv:2004.12489.
- HORVITZ, D. G. and THOMPSON, D. J. (1952). A generalization of sampling without replacement from a finite universe. *J. Amer. Statist. Assoc.* **47** 663–685. MR0053460
- HUDGENS, M. G. and HALLORAN, M. E. (2008). Toward causal inference with interference. *J. Amer. Statist. Assoc.* **103** 832–842. MR2435472 <https://doi.org/10.1198/016214508000000292>
- IMAI, K., JIANG, Z. and MALANI, A. (2021). Causal inference with interference and noncompliance in two-stage randomized experiments. *J. Amer. Statist. Assoc.* **116** 632–644. MR4270009 <https://doi.org/10.1080/01621459.2020.1775612>
- IMBENS, G. W. and RUBIN, D. B. (2015). *Causal Inference in Statistics, Social, and Biomedical Sciences*. Cambridge Univ. Press, Cambridge.
- JOHARI, R., LI, H. and WEINTRAUB, G. (2020). Experimental design in two-sided platforms: An analysis of bias. arXiv preprint. Available at arXiv:2002.05670.
- JONES, B. and NACHTSHEIM, C. J. (2009). Split-plot designs: What, why, and how. *J. Qual. Technol.* **41** 340–361.
- KOHAVI, R., CROOK, T., LONGBOTHAM, R., FRASCA, B., HENNE, R., FERRES, J. L. and MELAMED, T. (2009). Online experimentation at Microsoft. *Data Mining Case Stud.* 11.
- MANSKI, C. F. (1993). Identification of endogenous social effects: The reflection problem. *Rev. Econ. Stud.* **60** 531–542. MR1236836 <https://doi.org/10.2307/2298123>
- MATHISEN, H. C. (1943). A method of testing the hypothesis that two samples are from the same population. *Ann. Math. Stat.* **14** 188–194. MR0009285 <https://doi.org/10.1214/aoms/1177731460>
- MUNRO, E., WAGER, S. and XU, K. (2021). Treatment effects in market equilibrium. arXiv preprint. Available at arXiv:2109.11647.
- NEYMAN, J. (1923/1990). On the application of probability theory to agricultural experiments. Essay on principles. Section 9. *Statist. Sci.* **5** 465–472.
- UGBURN, E. L. and VANDERWEELE, T. J. (2014). Causal diagrams for interference. *Statist. Sci.* **29** 559–578. MR3300359 <https://doi.org/10.1214/14-STS501>
- PAPADOGEORGOU, G., MEALLI, F. and ZIGLER, C. M. (2019). Causal inference with interfering units for cluster and population level treatment allocation programs. *Biometrics* **75** 778–787. MR4012083 <https://doi.org/10.1111/biom.13049>
- POLLMANN, M. (2020). Causal inference for spatial treatments. arXiv preprint, arXiv:2011.00373.
- POUGET-ABADIE, J., AYDIN, K., SCHUDY, W., BRODERSEN, K. and MIRROKNI, V. (2019). Variance reduction in bipartite experiments through correlation clustering. *Adv. Neural Inf. Process. Syst.* **32**.
- ROSENBAUM, P. R. (2007). Interference between units in randomized experiments. *J. Amer. Statist. Assoc.* **102** 191–200. MR2345537 <https://doi.org/10.1198/016214506000001112>
- RUBIN, D. B. (1978). Bayesian inference for causal effects: The role of randomization. *Ann. Statist.* **6** 34–58. MR0472152.
- UGANDER, J., KARRER, B., BACKSTROM, L. and KLEINBERG, J. (2013). Graph cluster randomization: Network exposure to multiple universes. In *Proceedings of the 19th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, KDD '13* 329–337. Association for Computing Machinery, New York, NY, USA.
- VANDERWEELE, T. J., TCHETGEN, E. J. T. and HALLORAN, M. E. (2014). Interference and sensitivity analysis. *Statist. Sci.* **29** 687–706. MR3300366 <https://doi.org/10.1214/14-STS479>
- WAGER, S. and XU, K. (2021). Experimenting in equilibrium. *Management Sci.* <https://doi.org/10.1287/mnsc.2020.3844>.
- WU, C. J. and HAMADA, M. S. (2011). *Experiments: Planning, Analysis, and Optimization* **552**. Wiley, New York.
- XIONG, R., ATHEY, S., BAYATI, M. and IMBENS, G. W. (2019). Optimal experimental design for staggered rollouts. <http://dx.doi.org/10.2139/ssrn.3483934>.
- YATES, F. (1935). Complex experiments. *Suppl. J. R. Stat. Soc.* **2** 181–247.
- ZIGLER, C. M. and PAPADOGEORGOU, G. (2021). Bipartite causal inference with interference. *Statist. Sci.* **36** 109–123. MR4194206 <https://doi.org/10.1214/19-STS749>

Parameter Restrictions for the Sake of Identification: Is There Utility in Asserting That Perhaps a Restriction Holds?

Paul Gustafson

Abstract. Statistical modeling can involve a tension between assumptions and statistical identification. The law of the observable data may not uniquely determine the value of a target parameter without invoking a key assumption, and, while plausible, this assumption may not be obviously true in the scientific context at hand. Moreover, there are many instances of key assumptions which are untestable, hence we cannot rely on the data to resolve the question of whether the target is legitimately identified. Working in the Bayesian paradigm, we consider the grey zone of situations where a key assumption, in the form of a parameter space restriction, is scientifically reasonable but not incontrovertible for the problem being tackled. Specifically, we investigate statistical properties that ensue if we structure a prior distribution to assert that *maybe* or *perhaps* the assumption holds. Technically this simply devolves to using a mixture prior distribution putting just some prior weight on the assumption, or one of several assumptions, holding. However, while the construct is straightforward, there is very little literature discussing situations where Bayesian model averaging is employed across a mix of fully identified and partially identified models.

Key words and phrases: Bayesian model averaging, Bayes risk, large-sample theory, partial identification.

REFERENCES

- BERGER, J. O. (1985). *Statistical Decision Theory and Bayesian Analysis*, 2nd ed. *Springer Series in Statistics*. Springer, New York. MR0804611 <https://doi.org/10.1007/978-1-4757-4286-2>
- CASELLA, G. and BERGER, R. L. (2002). *Statistical Inference*, 2nd ed. Duxbury, N. Scituate.
- CHEN, C. F. (1985). On asymptotic normality of limiting density functions with Bayesian implications. *J. Roy. Statist. Soc. Ser. B* **47** 540–546. MR0844485
- DANIELS, M. J. and HOGAN, J. W. (2008). *Missing Data in Longitudinal Studies: Strategies for Bayesian Modeling and Sensitivity Analysis*. Chapman & Hall, CRC Press, New York. <https://doi.org/10.1201/9781420011180>
- FOX, M. P., MACLEHOSE, R. F. and LASH, T. L. (2022). *Applying Quantitative Bias Analysis to Epidemiologic Data*, 2nd ed. Springer, Berlin. <https://doi.org/10.1007/978-3-030-82673-4>
- FRANKS, A. M., D’AMOUR, A. and FELLER, A. (2020). Flexible sensitivity analysis for observational studies without observable implications. *J. Amer. Statist. Assoc.* **115** 1730–1746. MR4189753 <https://doi.org/10.1080/01621459.2019.1604369>
- GREENLAND, S. (2003). The impact of prior distributions for uncontrolled confounding and response bias: A case study of the relation of wire codes and magnetic fields to childhood leukemia. *J. Amer. Statist. Assoc.* **98** 47–54. MR1977199 <https://doi.org/10.1198/01621450338861905>
- GREENLAND, S. (2005). Multiple-bias modelling for analysis of observational data. *J. Roy. Statist. Soc. Ser. A* **168** 267–306. MR2119402 <https://doi.org/10.1111/j.1467-985X.2004.00349.x>
- GUSTAFSON, P. (2007). Measurement error modelling with an approximate instrumental variable. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **69** 797–815. MR2368571 <https://doi.org/10.1111/j.1467-9868.2007.00611.x>
- GUSTAFSON, P. (2015). *Bayesian Inference for Partially Identified Models: Exploring the Limits of Limited Data. Monographs on Statistics and Applied Probability* **141**. CRC Press, Boca Raton, FL. MR3642458
- GUSTAFSON, P. (2023). Supplement to “Parameter restrictions for the sake of identification: Is there utility in asserting that perhaps a restriction holds?.” <https://doi.org/10.1214/23-STS885SUPP>
- GUSTAFSON, P. and GREENLAND, S. (2006). The performance of random coefficient regression in accounting for residual confounding. *Biometrics* **62** 760–768. MR2247204 <https://doi.org/10.1111/j.1541-0420.2005.00510.x>
- GUSTAFSON, P. and GREENLAND, S. (2009). Interval estimation for messy observational data. *Statist. Sci.* **24** 328–342. MR2757434 <https://doi.org/10.1214/09-STS305>

- GUSTAFSON, P., LE, N. D. and SASKIN, R. (2001). Case-control analysis with partial knowledge of exposure misclassification probabilities. *Biometrics* **57** 598–609. MR1855698 <https://doi.org/10.1111/j.0006-341X.2001.00598.x>
- HOETING, J. A., MADIGAN, D., RAFTERY, A. E. and VOLINSKY, C. T. (1999). Bayesian model averaging: A tutorial (with comments by M. Clyde, David Draper and E. I. George, and a rejoinder by the authors). *Statist. Sci.* **14** 382–417. MR1765176 <https://doi.org/10.1214/ss/1009212519>
- KASS, R. E. and RAFTERY, A. E. (1995). Bayes factors. *J. Amer. Statist. Assoc.* **90** 773–795. MR3363402 <https://doi.org/10.1080/01621459.1995.10476572>
- KEELE, L. and QUINN, K. M. (2017). Bayesian sensitivity analysis for causal effects from 2×2 tables in the presence of unmeasured confounding with application to presidential campaign visits. *Ann. Appl. Stat.* **11** 1974–1997. MR3743285 <https://doi.org/10.1214/17-AOAS1048>
- LASH, T. L., FOX, M. P., MACLEHOSE, R. F., MALDONADO, G., MCCANDLESS, L. C. and GREENLAND, S. (2014). Good practices for quantitative bias analysis. *Int. J. Epidemiol.* **43** 1969–1985. https://doi.org/10.1007/978-3-030-82673-4_13
- LITTLE, R. J. A. and RUBIN, D. B. (2019). *Statistical Analysis with Missing Data*, Vol. 793, 3rd ed. Wiley, New York.
- MANSKI, C. F. (2003). *Partial Identification of Probability Distributions*. Springer Series in Statistics. Springer, New York. MR2151380
- SCHARFSTEIN, D. O., DANIELS, M. J. and ROBINS, J. M. (2003). Incorporating prior beliefs about selection bias into the analysis of randomized trials with missing outcomes. *Biostatistics* **4** 495–512. <https://doi.org/10.1093/biostatistics/4.4.495>
- VANSTEELENDT, S., GOETGHEBEUR, E., KENWARD, M. G. and MOLENBERGHS, G. (2006). Ignorance and uncertainty regions as inferential tools in a sensitivity analysis. *Statist. Sinica* **16** 953–979. MR2281311
- VERSTRAETEN, T., FARAH, B., DUCHATEAU, L. and MATU, R. (1998). Pooling sera to reduce the cost of HIV surveillance: A feasibility study in a rural Kenyan district. *Trop. Med. Int. Health* **3** 747–750. <https://doi.org/10.1046/j.1365-3156.1998.00293.x>
- WANG, F. and GELFAND, A. E. (2002). A simulation-based approach to Bayesian sample size determination for performance under a given model and for separating models. *Statist. Sci.* **17** 193–208. MR1925941 <https://doi.org/10.1214/ss/1030550861>
- WASSERMAN, L. (2000). Bayesian model selection and model averaging. *J. Math. Psych.* **44** 92–107. MR1770003 <https://doi.org/10.1006/jmps.1999.1278>
- WHITE, H. (1982). Maximum likelihood estimation of misspecified models. *Econometrica* **50** 1–25. MR0640163 <https://doi.org/10.2307/1912526>
- XIA, M. and GUSTAFSON, P. (2016). Bayesian regression models adjusting for unidirectional covariate misclassification. *Canad. J. Statist.* **44** 198–218. MR3507780 <https://doi.org/10.1002/cjs.11284>
- XIA, M. and GUSTAFSON, P. (2018). Bayesian inference for unidirectional misclassification of a binary response trait. *Stat. Med.* **37** 933–947. MR3760458 <https://doi.org/10.1002/sim.7555>

Variational Inference for Cutting Feedback in Misspecified Models

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Abstract. Bayesian analyses combine information represented by different terms in a joint Bayesian model. When one or more of the terms is misspecified, it can be helpful to restrict the use of information from suspect model components to modify posterior inference. This is called “cutting feedback”, and both the specification and computation of the posterior for such “cut models” is challenging. In this paper, we define cut posterior distributions as solutions to constrained optimization problems, and propose variational methods for their computation. These methods are faster than existing Markov chain Monte Carlo (MCMC) approaches by an order of magnitude. It is also shown that variational methods allow for the evaluation of computationally intensive conflict checks that can be used to decide whether or not feedback should be cut. Our methods are illustrated in a number of simulated and real examples, including an application where recent methodological advances that combine variational inference and MCMC within the variational optimization are used.

Key words and phrases: Bayesian model criticism, cutting feedback, model misspecification, modular inference.

REFERENCES

- [1] ALQUIER, P., RIDGWAY, J. and CHOPIN, N. (2016). On the properties of variational approximations of Gibbs posteriors. *J. Mach. Learn. Res.* **17** 239. [MR3595173](#)
- [2] BENNETT, J. and WAKEFIELD, J. (2001). Errors-in-variables in joint population pharmacokinetic/pharmacodynamic modeling. *Biometrics* **57** 803–812. [MR1863449](#) <https://doi.org/10.1111/j.0006-341X.2001.00803.x>
- [3] BISSIRI, P. G., HOLMES, C. C. and WALKER, S. G. (2016). A general framework for updating belief distributions. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **78** 1103–1130. [MR3557191](#) <https://doi.org/10.1111/rssb.12158>
- [4] BLANGIARDO, M., HANSELL, A. and RICHARDSON, S. (2011). A Bayesian model of time activity data to investigate health effect of air pollution in time series studies. *Atmos. Environ.* **45** 379–386.
- [5] BLEI, D. M., KUCUKELBIR, A. and MCAULIFFE, J. D. (2017). Variational inference: A review for statisticians. *J. Amer. Statist. Assoc.* **112** 859–877. [MR3671776](#) <https://doi.org/10.1080/01621459.2017.1285773>
- [6] CARMONA, C. and NICHOLLS, G. (2020). Semi-modular inference: Enhanced learning in multi-modular models by tempering the influence of components. In *Proceedings of the Twenty Third International Conference on Artificial Intelligence and Statistics* (S. Chiappa and R. Calandra, eds.). *Proceedings of Machine Learning Research* **108** 4226–4235.
- [7] CARMONA, C. and NICHOLLS, G. (2022). Scalable Semi-Modular Inference with Variational Meta-Posteriors. Available at [arXiv:2204.00296](#).
- [8] CARPENTER, B., GELMAN, A., HOFFMAN, M. D., LEE, D., GOODRICH, B., BETANCOURT, M., BRUBAKER, M., GUO, J., LI, P. et al. (2017). Stan: A probabilistic programming language. *J. Stat. Softw.* **76** 1–32.
- [9] DEL MORAL, P., DOUCET, A. and JASRA, A. (2006). Sequential Monte Carlo samplers. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **68** 411–436. [MR2278333](#) <https://doi.org/10.1111/j.1467-9868.2006.00553.x>
- [10] EVANS, M. (2015). *Measuring Statistical Evidence Using Relative Belief. Monographs on Statistics and Applied Probability* **144**. CRC Press, Boca Raton, FL. [MR3616661](#)
- [11] FRAZIER, D. T., LOAIZA-MAYA, R., MARTIN, G. M. and KOO, B. (2021). Loss-Based Variational Bayes Prediction. Available at [arXiv:2104.14054](#).
- [12] FRAZIER, D. T. and NOTT, D. J. (2022). Cutting feedback and modularized analyses in generalized Bayesian inference. Available at [arXiv:2202.09968](#).
- [13] GELMAN, A., MENG, X.-L. and STERN, H. (1996). Posterior predictive assessment of model fitness via realized discrepancies. *Statist. Sinica* **6** 733–807. [MR1422404](#)
- [14] HAN, S., LIAO, X., DUNSON, D. and CARIN, L. (2016). Variational Gaussian copula inference. In *Proceedings of the 19th International Conference on Artificial Intelligence and Statistics*

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- (A. Gretton and C. C. Robert, eds.). *Proceedings of Machine Learning Research* **51** 829–838.
- [15] JACOB, P. E., MURRAY, L. M., HOLMES, C. C. and ROBERT, C. P. (2017). Better together? Statistical learning in models made of modules. Available at [arXiv:1708.08719](https://arxiv.org/abs/1708.08719).
- [16] JACOB, P. E., O’LEARY, J. and ATCHADÉ, Y. F. (2020). Unbiased Markov chain Monte Carlo methods with couplings. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **82** 543–600. MR4112777 <https://doi.org/10.1111/rssb.12336>
- [17] KENNEDY, M. C. and O’HAGAN, A. (2001). Bayesian calibration of computer models. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **63** 425–464. MR1858398 <https://doi.org/10.1111/1467-9868.00294>
- [18] KNOBLAUCH, J., JEWSON, J. and DAMOULAS, T. (2022). An optimization-centric view on Bayes’ rule: Reviewing and generalizing variational inference. *J. Mach. Learn. Res.* **23** 132. MR4577084
- [19] KNOWLES, D. A. and MINKA, T. (2011). Non-conjugate variational message passing for multinomial and binary regression. In *Advances in Neural Information Processing Systems 24* (J. Shawe-Taylor, R. S. Zemel, P. L. Bartlett, F. Pereira and K. Q. Weinberger, eds.) 1701–1709. Curran Associates, Red Hook.
- [20] KUCUKELBIR, A., TRAN, D., RANGANATH, R., GELMAN, A. and BLEI, D. M. (2017). Automatic differentiation variational inference. *J. Mach. Learn. Res.* **18** 14. MR3634881
- [21] LIN, W., KHAN, M. E. and SCHMIDT, M. (2019). Fast and simple natural-gradient variational inference with mixture of exponential-family approximations. In *Proceedings of the 36th International Conference on Machine Learning* (K. Chaudhuri and R. Salakhutdinov, eds.). *Proceedings of Machine Learning Research* **97** 3992–4002.
- [22] LITTLE, R. J. A. (1992). Regression with missing X’s: A review. *J. Amer. Statist. Assoc.* **87** 1227–1237.
- [23] LIU, F., BAYARRI, M. J. and BERGER, J. O. (2009). Modularization in Bayesian analysis, with emphasis on analysis of computer models. *Bayesian Anal.* **4** 119–150. MR2486241 <https://doi.org/10.1214/09-BA404>
- [24] LIU, Y. and GOUDIE, R. J. B. (2022). A General Framework for Cutting Feedback within Modularized Bayesian Inference. Available at [arXiv:2211.03274](https://arxiv.org/abs/2211.03274).
- [25] LIU, Y. and GOUDIE, R. J. B. (2022). Stochastic approximation cut algorithm for inference in modularized Bayesian models. *Stat. Comput.* **32** 7. MR4350200 <https://doi.org/10.1007/s11222-021-10070-2>
- [26] LIU, Y. and GOUDIE, R. J. B. (2023). Generalized geographically weighted regression model within a modularized Bayesian framework. *Bayesian Anal.* 1–36. <https://doi.org/10.1214/22-BA1357>
- [27] LOAIZA-MAYA, R., SMITH, M. S., NOTT, D. J. and DANAHER, P. J. (2022). Fast and accurate variational inference for models with many latent variables. *J. Econometrics* **230** 339–362. MR4466728 <https://doi.org/10.1016/j.jeconom.2021.05.002>
- [28] LUNN, D., BEST, N., SPIEGELHALTER, D., GRAHAM, G. and NEUENSCHWANDER, B. (2009). Combining MCMC with ‘sequential’ PKPD modelling. *J. Pharmacokin. Pharmacodyn.* **36** 19–38.
- [29] MAUCORT-BOULCH, D., FRANCESCHI, S. and PLUMMER, M. (2008). International correlation between human papillomavirus prevalence and cervical cancer incidence. *Cancer Epidemiol. Biomark. Prev.* **17** 717–720.
- [30] MCCANDLESS, L. C., DOUGLAS, I. J., EVANS, S. J. and SMEETH, L. (2010). Cutting feedback in Bayesian regression adjustment for the propensity score. *Int. J. Biostat.* **6** 16. MR2602559 <https://doi.org/10.2202/1557-4679.1205>
- [31] MCCANDLESS, L. C., RICHARDSON, S. and BEST, N. (2012). Adjustment for missing confounders using external validation data and propensity scores. *J. Amer. Statist. Assoc.* **107** 40–51. MR2949340 <https://doi.org/10.1080/01621459.2011.643739>
- [32] MINKA, T. (2005). Divergence measures and message passing Technical Report No. MSR-TR-2005-173 Microsoft Research.
- [33] MOSS, D. and ROUSSEAU, J. (2022). Efficient Bayesian estimation and use of cut posterior in semiparametric hidden Markov models. Available at [arXiv:2203.06081](https://arxiv.org/abs/2203.06081).
- [34] MURPHY, K. M. and TOPEL, R. H. (2002). Estimation and inference in two-step econometric models. *J. Bus. Econom. Statist.* **20** 88–97. MR1940632 <https://doi.org/10.1198/073500102753410417>
- [35] NICHOLLS, G. K., LEE, J. E., WU, C.-H. and CARMONA, C. U. (2022). Valid belief updates for prequentially additive loss functions arising in Semi-Modular inference. Available at [arXiv:2201.09706](https://arxiv.org/abs/2201.09706).
- [36] NICHOLSON, G., BLANGIARDO, M., BRIERS, M., DIGGLE, P. J., FJELDE, T. E., GE, H., GOUDIE, R. J. B., JERSAKOVA, R., KING, R. E. et al. (2022). Interoperability of statistical models in pandemic preparedness: Principles and reality. *Statist. Sci.* **37** 183–206.
- [37] NOTT, D. J., WANG, X., EVANS, M. and ENGLERT, B.-G. (2020). Checking for prior-data conflict using prior-to-posterior divergences. *Statist. Sci.* **35** 234–253. MR4106603 <https://doi.org/10.1214/19-STS731>
- [38] OGLE, K., BARBER, J. and SARTOR, K. (2013). Feedback and modularization in a Bayesian meta-analysis of tree traits affecting forest dynamics. *Bayesian Anal.* **8** 133–168. MR3036257 <https://doi.org/10.1214/13-BA806>
- [39] ORMEROD, J. T. and WAND, M. P. (2010). Explaining variational approximations. *Amer. Statist.* **64** 140–153. MR2757005 <https://doi.org/10.1198/tast.2010.09058>
- [40] PAPAMAKARIOS, G., NALISNICK, E., REZENDE, D. J., MOHAMED, S. and LAKSHMINARAYANAN, B. (2021). Normalizing flows for probabilistic modeling and inference. *J. Mach. Learn. Res.* **22** 57. MR4253750
- [41] PETRIN, A. and TRAIN, K. (2010). A control function approach to endogeneity in consumer choice models. *J. Mark. Res.* **47** 3–13.
- [42] PLUMMER, M. (2015). Cuts in Bayesian graphical models. *Stat. Comput.* **25** 37–43. MR3304902 <https://doi.org/10.1007/s11222-014-9503-z>
- [43] POMPE, E. and JACOB, P. E. (2021). Asymptotics of cut distributions and robust modular inference using posterior bootstrap. Available at [arXiv:2110.11149](https://arxiv.org/abs/2110.11149).
- [44] PRESANIS, A. M., OHLSEN, D., SPIEGELHALTER, D. J. and DE ANGELIS, D. (2013). Conflict diagnostics in directed acyclic graphs, with applications in Bayesian evidence synthesis. *Statist. Sci.* **28** 376–397. MR3135538 <https://doi.org/10.1214/13-STS426>
- [45] SALIMANS, T. and KNOWLES, D. A. (2013). Fixed-form variational posterior approximation through stochastic linear regression. *Bayesian Anal.* **8** 837–881. MR3150471 <https://doi.org/10.1214/13-BA858>
- [46] SMITH, M. S., LOAIZA-MAYA, R. and NOTT, D. J. (2020). High-dimensional copula variational approximation through transformation. *J. Comput. Graph. Statist.* **29** 729–743. MR4191239 <https://doi.org/10.1080/10618600.2020.1740097>
- [47] STYRING, A., CHARLES, M., FANTONE, F., HALD, M., MCMAHON, A., MEADOW, R., NICHOLLS, G., PATEL, A., PITRE, M. et al. (2017). Isotope evidence for agricultural extensification reveals how the world’s first cities were fed. *Nature Plants* **3** 17076.

- [48] TITSIAS, M. and LÁZARO-GREDILLA, M. (2014). Doubly stochastic variational Bayes for non-conjugate inference. In *Proceedings of the 31st International Conference on Machine Learning* (E. P. Xing and T. Jebara, eds.). *Proceedings of Machine Learning Research* **32** 1971–1979.
- [49] WAND, M. P. (2017). Fast approximate inference for arbitrarily large semiparametric regression models via message passing. *J. Amer. Statist. Assoc.* **112** 137–156. MR3646558 <https://doi.org/10.1080/01621459.2016.1197833>
- [50] WANG, Y. and BLEI, D. M. (2019). Variational Bayes under model misspecification. In *Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada* (H. M. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. B. Fox and R. Garnett, eds.) 13357–13367.
- [51] WINN, J. and BISHOP, C. M. (2005). Variational message passing. *J. Mach. Learn. Res.* **6** 661–694. MR2249835
- [52] WOODARD, D. B., CRAINICEANU, C. and RUPPERT, D. (2013). Hierarchical adaptive regression kernels for regression with functional predictors. *J. Comput. Graph. Statist.* **22** 777–800. MR3173742 <https://doi.org/10.1080/10618600.2012.694765>
- [53] YAO, Y., VEHTARI, A., SIMPSON, D. and GELMAN, A. (2018). Yes, but did it work?: Evaluating variational inference. In *Proceedings of the 35th International Conference on Machine Learning* (J. Dy and A. Krause, eds.). *Proceedings of Machine Learning Research* **80** 5581–5590.
- [54] YE, L., BESKOS, A., DE IORIO, M. and HAO, J. (2020). Monte Carlo co-ordinate ascent variational inference. *Stat. Comput.* **30** 887–905. MR4108683 <https://doi.org/10.1007/s11222-020-09924-y>
- [55] YU, X., NOTT, D. J., TRAN, M.-N. and KLEIN, N. (2021). Assessment and adjustment of approximate inference algorithms using the law of total variance. *J. Comput. Graph. Statist.* **30** 977–990. MR4356599 <https://doi.org/10.1080/10618600.2021.1880921>
- [56] ZEILER, M. D. (2012). ADADELTA: An Adaptive Learning Rate Method. Available at arXiv:1212.5701.
- [57] ZHANG, L., BEAL, S. L. and SHEINER, L. B. (2003). Simultaneous vs. sequential analysis for population PK/PD data I: Best-case performance. *J. Pharmacokinet. Pharmacodyn.* **30** 387–404. <https://doi.org/10.1023/b:jopa.0000012998.04442.1f>
- [58] ZHANG, L., BEAL, S. L. and SHEINER, L. B. (2003). Simultaneous vs. sequential analysis for population PK/PD data II: Robustness of models. *J. Pharmacokinet. Pharmacodyn.* **30** 305–416.
- [59] ZIGLER, C. M., WATTS, K., YEH, R. W., WANG, Y., COULL, B. A. and DOMINICI, F. (2013). Model feedback in Bayesian propensity score estimation. *Biometrics* **69** 263–273. MR3058073 <https://doi.org/10.1111/j.1541-0420.2012.01830.x>

Note on Legendre's Method of Least Squares

Jukka Nyblom

Abstract. In the first published treatment of the least squares, Legendre applied his new method to the French meridian data measured for the determination of the length of the meter (*Nouvelles méthodes pour la détermination des orbites des comètes* (1805) 76 Firmin Didot). Legendre treated one error term as a constant. It is shown here that it turns out to be equivalent to the generalized least squares solution of his model (*Nouvelles méthodes pour la détermination des orbites des comètes* (1805) 77 Firmin Didot).

Key words and phrases: French meridian data, meridian arc length, generalized least squares, flattening of the Earth, determination of meter.

REFERENCES

- EULER, L. P. (1755). Éléments de la Trigonométrie sphéroïdique tirés de la méthode des plus grandes et plus petits. *Mémoires de Berlin* 1753 **IX** 258–293.
- HALD, A. (1998). *A History of Mathematical Statistics from 1750 to 1930. Wiley Series in Probability and Statistics: Texts and References Section*. Wiley, New York. [MR1619032](#)
- LAPLACE, P. S. (1799). *Traité de Mécanique Céleste* **2**. Duprat, Paris.
- LEGENDRE, A. M. (1805). *Nouvelles méthodes pour la détermination des orbites des comètes*. Firmin Didot, Paris.
- STIGLER, S. M. (1981). Gauss and the invention of least squares. *Ann. Statist.* **9** 465–474. [MR0615423](#)
- STIGLER, S. M. (1986). *The History of Statistics: The Measurement of Uncertainty Before 1900*. The Belknap Press of Harvard Univ. Press, Cambridge, MA. [MR0852410](#)
- TORGE, W. (2001). *Geodesy*. de Gruyter, Berlin.

A Conversation with Mary E. Thompson

Rhonda J. Rosychuk

Abstract. Mary E. Thompson (née Beattie) was born September 9, 1944, in Winnipeg, Manitoba, Canada. She obtained a B.Sc. in Mathematics from the University of Toronto in 1965, and earned M.Sc. (1966) and Ph.D. (1969) degrees in Mathematics from the University of Illinois at Urbana-Champaign. She joined the Department of Statistics at the University of Waterloo as a Lecturer in 1969 and became an Assistant Professor in 1971. In 2004, she was awarded the honour of University Professor and in 2011 became Distinguished Professor Emerita at the University of Waterloo. She has served in many leadership roles including Chair of the Department of Statistics and Actuarial Science, Acting Dean of the Faculty of Mathematics, President of the Statistical Society of Canada (SSC) and Chair of the COPSS Presidents' Award Committee. She chaired the Development Committee for the Canadian Statistical Sciences Institute (CANSSI) and was its founding Scientific Director.

Thompson has received numerous honours and awards including the SSC's Gold Medal, the Elizabeth L. Scott Award, the Waksberg Award of Survey Methodology and the Governor General's Innovation Award. She is an elected member of the International Statistical Institute, an Honorary Member of the SSC and is a Fellow of the American Statistical Association, the Institute of Mathematical Statistics, the Royal Society of Canada and the Fields Institute.

Thompson has made fundamental contributions to several areas in statistics including sampling theory and the analysis of surveys. She is the author of two books in these areas: *Theory of Sample Surveys* (1997) and *Sampling Theory and Practices* (2020 with C. Wu). She has also made key contributions in estimation theory and stochastic processes. As the author of over 150 published, refereed papers, Thompson has influenced the theory and practice of statistics.

The following conversation took place virtually in September 2022 with interviewer Rhonda J. Rosychuk of the University of Alberta.

Key words and phrases: University of Waterloo, Statistical Society of Canada, Canadian Statistical Sciences Institute, sampling theory, survey methodology, estimation theory, stochastic processes.

REFERENCES

- [1] BINDER, D. A. (1983). On the variances of asymptotically normal estimators from complex surveys. *Int. Stat. Rev.* **51** 279–292. [MR0731144](https://doi.org/10.2307/1402588) <https://doi.org/10.2307/1402588>
- [2] BIRNBAUM, A. (1962). On the foundations of statistical inference. *J. Amer. Statist. Assoc.* **57** 269–326. [MR0138176](https://doi.org/10.2307/1402588)
- [3] FISHER, R. A. (1956). *Statistical Methods and Scientific Inference*. Oliver and Boyd, Edinburgh, UK.
- [4] GODAMBE, V. P. (1955). A unified theory of sampling from finite populations. *J. Roy. Statist. Soc. Ser. B* **17** 269–278. [MR0077037](https://doi.org/10.2307/1403139)
- [5] GODAMBE, V. P. (1966). A new approach to sampling from finite populations. I. Sufficiency and linear estimation. *J. Roy. Statist. Soc. Ser. B* **28** 310–319. [MR0216720](https://doi.org/10.2307/1403139)
- [6] GODAMBE, V. P. and THOMPSON, M. E. (1971). Bayes, fiducial and frequency aspects of statistical inference in regression analysis in survey-sampling. *J. Roy. Statist. Soc. Ser. B* **33** 361–390. [MR0362603](https://doi.org/10.2307/1403139)
- [7] GODAMBE, V. P. and THOMPSON, M. E. (1986). Parameters of superpopulation and survey population: Their relationships and estimation. *Int. Stat. Rev.* **54** 127–138. [MR0962931](https://doi.org/10.2307/1403139) <https://doi.org/10.2307/1403139>

- [8] GODAMBE, V. P. and THOMPSON, M. E. (1989). An extension of quasi-likelihood estimation. *J. Statist. Plann. Inference* **22** 137–172. MR1004344 [https://doi.org/10.1016/0378-3758\(89\)90106-7](https://doi.org/10.1016/0378-3758(89)90106-7)
- [9] JIANG, C., WALLACE, M. P. and THOMPSON, M. E. (2022). Dynamic treatment regimes with interference. *Canad. J. Statist.* To appear. <https://doi.org/10.1002/cjs.11702>
- [10] RAMÍREZ-RAMÍREZ, L. L. and THOMPSON, M. E. (2014). Applications of the variance of final outbreak size for disease spreading in networks. *Methodol. Comput. Appl. Probab.* **16** 839–862. MR3270598 <https://doi.org/10.1007/s11009-013-9325-z>
- [11] THOMPSON, M. E. (1984). Model and design correspondence in finite population sampling. *J. Statist. Plann. Inference* **10** 323–334. MR0766648 [https://doi.org/10.1016/0378-3758\(84\)90057-0](https://doi.org/10.1016/0378-3758(84)90057-0)
- [12] THOMPSON, M. E. (1997). *Theory of Sample Surveys. Monographs on Statistics and Applied Probability* **74**. CRC Press, London. MR1462619 [https://doi.org/10.1002/1097-0258\(20000715\)19:13<1825::AID-SIM466>3.0.CO;2-E](https://doi.org/10.1002/1097-0258(20000715)19:13<1825::AID-SIM466>3.0.CO;2-E)
- [13] THOMPSON, M. E. (2001). Likelihood principle and randomization in survey sampling. In *Data Analysis from Statistical Foundations* 9–25. Nova Sci. Publ., Huntington, NY. MR2034504
- [14] THOMPSON, M. E., RAMIREZ RAMIREZ, L. L., LYUBCHICH, V. and GEL, Y. R. (2016). Using the bootstrap for statistical inference on random graphs. *Canad. J. Statist.* **44** 3–24. MR3474218 <https://doi.org/10.1002/cjs.11271>
- [15] THOMPSON, M. E., SEDRANSK, J., FANG, J. and YI, G. Y. (2022). Bayesian inference for a variance component model using pairwise composite likelihood with survey data. *Surv. Methodol.* **48** 73–93.
- [16] THOMPSON, M. E. B. (1969). *Some Aspects of Optimal Stopping Theory*. ProQuest LLC, Ann Arbor, MI. Thesis (Ph.D.)—University of Illinois at Urbana-Champaign. MR2619132
- [17] WU, C. and THOMPSON, M. E. (2020). *Sampling Theory and Practice. ICSA Book Series in Statistics*. Springer, Cham. MR4180686 <https://doi.org/10.1007/978-3-030-44246-0>

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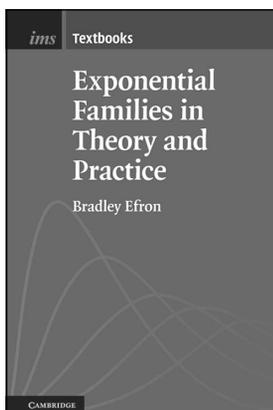
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