Hierarchical Bayesian modeling under covariate shift in supernova cosmology

> Presenter: Max Autenrieth Supervisor: David A. van Dyk Co-Supervisor: Roberto Trotta, David Stenning

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Overview



Image Credit: http://hyperphysics.phy-astr.gsu.edu/hbase/astro/snovcn.html

- Supernova type Ia (SNIa) have common "flashpoint" (standard candles)
- SNIa allow cosmological parameter estimation (e.g. dark energy density).

Statistical Challenges:

- (i) Reliable classification of SNIa given a non-representative training set.
- (ii) Secondary analysis needs to account for contamination arising through (i).

Covariate shift in supernova cosmology

• Confirming Ia is easy with spectra



• Much harder with just photometry





- Probabilistic classification of photometric light curve data
- Confirmed (training) set non-representative

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Definitions and Notation:

- Feature space $\mathcal{X} \subset \mathbb{R}^n$, and label space \mathcal{Y} .
- Different domains: *p*(*x*, *y*) differs in source and target.
- Labeled source (training) data $D_S = \{(x_S^{(i)}, y_S^{(i)})\}_{i=1}^{n_s}$.
- Unlabeled target data $D_T = \{x_T^{(i)}\}_{i=1}^{n_t}$.

Definition 1.1 (Moreno-Torres et al. (2012))

Covariate shift is defined as $p_S(y|x) = p_T(y|x)$ but $p_S(x) \neq p_T(x)$.

Objective: Accurately predicting target labels y_T , by minimizing target risk

$$\mathcal{R}_{\mathcal{T}}(f) \coloneqq \mathbb{E}_{(x,y) \sim \rho_{\mathcal{T}}(x,y)} [\ell(f(x),y)]. \quad (1)$$



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Methodology – Stratified Learning (StratLearn):

• We define the propensity score (PS) as:

$$e(x_i) := P(s_i = 1 | x_S, x_T), \text{ with } 0 < e(x_i) < 1.$$
 (2)

• PS well-established in causal inference (Rosenbaum and Rubin 1983).

Proposition 1 (Learning conditional on the propensity score)

Under covariate shift conditions, conditional on the propensity score:

$$p_T(x, y|e(x)) = p_S(x, y|e(x)),$$
 (3)

eliminating covariate shift. Thus, for any loss function $\ell = \ell(f(x), y)$,

$$E_{(x,y)\sim p_{T}(x,y|e(x))}[\ell(f(x),y)] = E_{(x,y)\sim p_{S}(x,y|e(x))}[\ell(f(x),y)].$$
(4)

StratLearn for SN Ia classification

- Stratify source and target data on propensity score.
- Classify separately within strata, via Random Forest.



StratLearn balances covariates (and outcome) within strata.

Performance close to unbiased "Gold Standard" (AUC: 0.965).

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Bayesian Modelling for Supernova Type Ia Cosmology

- Scientifically justified model for SNIa available.
- Account for measurement errors via Bayesian hierarchical model.



Supernova Cosmology with Contaminated Data

Secondary analysis: needs to account for classification uncertainties!



Intrinsic Magnitude

- Fully Bayes: with target distribution $p(\theta|y, g(D))p(y|f(D), g(D))$
- Requires model specification for contaminants (unknown).
- Parts of data used twice for type probabilities.
- We avoid this using Pragmatic Bayes!

- **Pragmatic** target distribution: $p(\theta|y = SNIa, g(D))p(y = SNIa|f(D))$
- Assumption: Contaminants non-informative for parameters of interest *θ*.

SN Cosmology with Contamination: A pragmatic Bayesian Approach



Iteratively:

- (i) Resample y, with p(y = SNIa|f(D))
- (ii) Fit SNIa model to obtain posterior sample (e.g. via Multinest).

(Results for 500 simulated SNe (SNcosmo) with 5% contamination.)

Ongoing and Future Work

Cosmological parameter estimation (secondary analysis):

- Comparison to fully Bayes (with/without model misspecification).
- Incorporation of (photometric) redshift uncertainties.
- Consideration of selection effects (photometry not representative).

StratLearn:

- Scientific applications (e.g. redshift calibration for weak lensing).
- Balance diagnostics via predicted marginal outcome distributions.

References I

- Autenrieth, M., Van Dyk, D. A., Trotta, R., and Stenning, D. C. (2021). Stratified learning: a general-purpose statistical method for improved learning under covariate shift. *arXiv preprint arXiv:2106.11211*.
- Bickel, S., Brückner, M., and Scheffer, T. (2009). Discriminative learning under covariate shift. *Journal of Machine Learning Research*, 10(Sep):2137–2155.
- Kunz, M., Bassett, B. A., and Hlozek, R. A. (2007). Bayesian estimation applied to multiple species. *Physical Review D*, 75(10):103508.
- Moreno-Torres, J. G., Raeder, T., Alaiz-RodríGuez, R., Chawla, N. V., and Herrera, F. (2012). A unifying view on dataset shift in classification. *Pattern Recognition*, 45(1):521–530.
- Revsbech, E. A., Trotta, R., and van Dyk, D. A. (2018). Staccato: a novel solution to supernova photometric classification with biased training sets. *Monthly Notices of the Royal Astronomical Society*, 473(3):3969–3986.

- Rosenbaum, P. R. and Rubin, D. B. (1983). The central role of the propensity score in observational studies for causal effects. *Biometrika*, 70(1):41–55.
- Shariff, H., Jiao, X., Trotta, R., and van Dyk, D. A. (2016). Bahamas: new analysis of type ia supernovae reveals inconsistencies with standard cosmology. *The Astrophysical Journal*, 827(1):1.
- Shimodaira, H. (2000). Improving predictive inference under covariate shift by weighting the log-likelihood function. *Journal of statistical planning and inference*, 90(2):227–244.
- Zadrozny, B. (2004). Learning and evaluating classifiers under sample selection bias. In *Proceedings of the twenty-first international conference on Machine learning*, page 114. ACM.

Thank you very much for your time!

Future work - Balance diagnostics via predicted outcome

Remark 1 (Outcome balance:)

In covariate shift framework

- Potential outcomes are identical (Y₀ ≡ Y₁), no "treatment effect"
- Only source data is observed $(Y_1 \equiv Y)$
- Given e(x), with 0 < e(x) < 1, and covariate shift conditions, source data assignment is 'strongly ignorable'
- Then, conditional on PS, source and target outcome are the same in expectation [invoking Rosenbaum and Rubin (1983), Theorem 4].
- Target labels y_T in practice not observed, only source labels y_S
- Target and source label predictions (\hat{y}_T and \hat{y}_S) given.
- Can we use predicted outcomes to test for remaining confounding?

Future work - Balance diagnostics via predicted outcome

Table: **StratLearn** strata composition (including all 102 covariates in PS).

Table: Composition with two covariates (redshift and brightness) in PS.

		Number	Number	Prop.			Number	Number	Prop.
Stratum	Set	of SNe	of SNIa	of SNIa	Stratum	Set	of SNe	of SNIa	of SNIa
1	Source	958	518	0.54	1	Source	947	652	0.69
	Target	3306	1790	0.54		Target	2519	1242	0.49
2	Source	120	28	0.23	2	Source	245	181	0.74
	Target	4144	927	0.22		Target	3221	1147	0.36
3	Source	13	4	0.31	3	Source	17	12	0.71
	Target	4250	540	0.13		Target	3449	754	0.22
4	Source	7	4	0.57	4	Source	6	6	1
	Target	4257	610	0.14		Target	3460	342	0.10
5	Source	4	4	1	5	Source	2	0	0
	Target	4259	662	0.16		Target	3464	107	0.03

- Outcome proportions balanced within stratum 1 and 2.
- Imbalance due to remaining confounding.

Previous methods – Importance weighting:

Under covariate shift conditions:

Proposition 2 (Shimodaira (2000), Bickel et al. (2009))

If the support of $p_T(x)$ is contained in $p_S(x)$, then

$$\mathbb{E}_{(x,y)\sim\mathcal{D}_{T}}\left[\ell(f(x),y)\right] = \mathbb{E}_{(x,y)\sim\mathcal{D}_{S}}\left[\frac{p_{T}(x)}{p_{S}(x)}\ell(f(x),y)\right].$$
(5)

Proposition 3 (Bias Correction (Zadrozny 2004))

Let (x, y, s) be examples drawn from a distribution \mathcal{D} , with feature-label-selection space $X \times \mathcal{Y} \times S$. Then,

$$\mathbb{E}_{(x,y)\sim\mathcal{D}}\left[\ell(f(x),y)\right] = \mathbb{E}_{(x,y)\sim\hat{\mathcal{D}}}\left[\ell(f(x),y)|s=1\right],\tag{6}$$

with
$$\hat{\mathcal{D}}(x, y, s) \coloneqq \frac{P(s=1)}{P(s=1|x)} \mathcal{D}(x, y, s).$$
 (7)

Photo-z – Target results:

The target risk $\hat{R}_T(\hat{f})$ is computed as

$$\hat{R}_{T}(\hat{t}) = \frac{1}{n_{T}} \sum_{k=1}^{n_{T}} \int \hat{t}^{2}(z | x_{T}^{(k)}) dz - 2 \frac{1}{n_{T}} \sum_{k=1}^{n_{T}} \hat{t}(z_{T}^{(k)} | x_{T}^{(k)}),$$
(8)

where z_T is the true target redshift, used for evaluation purposes only.



Figure: Target risk (\hat{R}_T) of photometric redshift estimation.