Summary Statistics - CSML Reading Group

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October 30, 2020

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When dealing with high-dimensional data y_{obs}, ABC algorithms use lower-dimensional summary statistics S(y)

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Lower dimensional representation

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- Lower dimensional representation \rightarrow improved acceptance rate

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Optimal S(y) would be "minimal sufficient" statistics

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- Optimal S(y) would be "minimal sufficient" statistics
- Often these are not available \rightarrow resort to summary statistics

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- Idea of sufficiency is to find statistics S(y) of the data that summarise the information about θ

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- Idea of sufficiency is to find statistics S(y) of the data that summarise the information about θ

Definition (Bayes Sufficiency)

For any prior distribution of θ , the posterior density $f(\theta|y, S(y)) = f(\theta|S(y))$

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Theorem (Fisher-Pitman-Koopman-Darmois)

With i.i.d. sampling from a model, exponential families are the only models for which there are sufficient statistics whose dimensions remain bounded as the sample size grows.

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Need methods for selecting appropriate low dimensional insufficient summaries

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Choice of S(y) will impact the **efficiency** and **accuracy** of ABC

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First two methods rely on training data and candidate summary statistics $z = (z_1, z_2, ..., z_k)$ where each z_i is a scalar function of data y

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Subset selection

Projection methods

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- Subset selection
- Projection methods
- Auxiliary likelihood

Last method uses an approximating model to provide a more tractable "auxiliary" likelihood to derive summary statistics from

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All these approaches require subjective input from the user

Example Data Features

Example data features used for Estimation of mutation rate in coalescent simulation (Nunes and Balding, 2010).

Table 1: The pool of summary statistics Ω considered for summarising datasets of DNA sequence haplotypes in the simulation study. For each statistic, we show the number of observed datasets (out of 100) for which it was included in the optimal set in univariate, unadjusted ABC inference by the methods described in the text.

		Selected for θ (%)			Selected for ρ (%)		
Statistic	Description	AS	ME	2-stage	\mathbf{AS}	ME	2-stage
C_1	no. of segregating sites	75	67	100	73	67	97
C_2	Uniform[0,25] random variable	4	3	0	2	5	0
C_3	mean no. of differences over all pairs of haplotypes	27	54	25	52	30	19
C_4	25^{*} (mean r^{2} across pairs separated by $< 10\%$						
	of the simulated genomic region)	56	35	50	35	59	78
C_5	no. of distinct haplotypes	43	19	20	78	73	100
C_6	frequency of the most common haplotype	36	20	1	11	23	2
C_7	no. of singleton haplotypes	16	14	5	16	31	5

Figure: Nunes and Balding, 2010

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Example Data Features

Data features used for Random walk models (Barnes et al. 2012).

- S1 Mean square displacement.
- S2 Mean x and y displacement.
- S3 Mean square x and y displacement.
- S4 Straightness index.
- S5 Eigenvalues of gyration tensor (reference random walks book).

Applying our summary statistic selection framework to data simulated from the three different models over 100

Figure: Barnes et al.

Attempts to find a subset of z that produces a low dimensional approximately sufficient set of statistics S'

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- Requires training data, simplest way is to sample (θ, y) pairs by sampling θ from prior, then generating y

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- Approximate sufficiency, Entropy minimisation, Mutual information maximisation
- Good for producing interpretable summaries subset of interpretable candidates z more interpretable than some projection of z

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- Problems include large computational expense, often ABC must be run on all candidate subsets of z

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Can use more candidate summaries because of this

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- Can use more candidate summaries because of this
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• All methods apply to multi-dimensional θ
Need an approximate and tractable likelihood for the data

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- ► Need an **approximate** and **tractable** likelihood for the data
- Auxiliary likelihood p_A(y|φ), auxiliary parameters φ don't need to correspond to generative parameters θ

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Maximum likelihood estimators, Likelihood distance, Scores

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- Maximum likelihood estimators, Likelihood distance, Scores
- No need for training data
- Subjective choice of this approximating model may be difficult/poorly approximating

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- Want small number of parameters to produce low-dimensional summaries

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Hard to assess whether the auxiliary likelihood is producing informative summaries for the generative model

- General model with tractable likelihood e.g. Gaussian Mixture
- Approximate the generative likelihood with tractable alternative e.g. Composite likelihood
- Want small number of parameters to produce low-dimensional summaries
- Hard to assess whether the auxiliary likelihood is producing informative summaries for the generative model

Example

4.1. The structural model: An Ornstein-Uhlenbeck type stochastic volatility model

Our structural model \mathcal{M}_S is defined in terms of the following two stochastic differential equations:

$$dx^{*}(t) = (\mu + \beta\sigma^{2}(t)) dt + \sigma(t) dW(t)$$
 (4.1)

$$d \sigma^2(t) = -\lambda \sigma^2(t) dt + dZ(\lambda t).$$
 (4.2)

Here we denote with $(z^*(t))_{t\geq 0}$ the log price process of an asset, $(W(t))_{t\geq 0}$ is a standard Brownian motion and $(\sigma^2(t))_{t\geq 0}$ is the underlying latent instantaneous volatility process of OU type, independent of $(W(t))_{t\geq 0}$ with $(Z(td))_{t\geq 0}$ being the background driving Lévy process

Blum et al. (2013) - 'What is very apparent from this study is that there is no single "best" method of dimension reduction for ABC.'

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- With low k = dim(z), subset selection methods are computationally feasible and perform best
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- Chapter could have discussed the selection of data features z could initially better selection of z reduce the need for complex and expensive summary selection?

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Is there any room for improving this initial selection of features?

- Blum et al. (2013) 'What is very apparent from this study is that there is no single "best" method of dimension reduction for ABC.'
- With low k = dim(z), subset selection methods are computationally feasible and perform best
- With high k, projection methods are favoured
- Chapter could have discussed the selection of data features z could initially better selection of z reduce the need for complex and expensive summary selection?
- Is there any room for improving this initial selection of features?
- No analysis of how these methods affect the accuracy of the posterior approximation

K2-ABC: Approximate Bayesian Computation with Kernel Embeddings - Park et al., (2016)

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- Circumvents need for selecting summary statistics - uses MMD to give a dissimilarity measure between y_{obs} and simulated y

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- Still need to pick the characteristic kernel, this is subjective

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 Approximate Bayesian computation via the energy statistic - Nguyen et al., (2020)

Approximate Sufficiency - Joyce and Marjoram, 2008

Approximate Sufficiency - Joyce and Marjoram, 2008 Candidate statistics randomly added, and are only accepted if there is a great enough change in posterior approximation

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- Entropy Minimisation Nunes and Balding, 2010 Complex two-step approach.
 - Minimise estimate of ABC posterior entropy to pick $S_{\rm ME}$, retain $n_{\rm obs}$ 'best' datasets for training
 - Repeatedly run rejection-ABC, minimise the RMSE of parameters compared to best datasets over subsets of z

Mutual Information Maximisation - Barnes et al., 2012

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- Add in z_i that maximises estimated \mathcal{KL} -divergence between ABC posteriors

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Regularisation
Subset Selection Methods

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Regularisation

- Local-linear regression model with response $\theta,$ and covariates z, in the region of $S(y_{\rm obs})$

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Regularisation

- Local-linear regression model with response θ , and covariates z, in the region of $S(y_{obs})$

- Use the AIC/BIC criterion to penalise complexity, and select relevant data features

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- Local-linear regression model with response θ , and covariates z, in the region of $S(y_{\rm obs})$

- Use the AIC/BIC criterion to penalise complexity, and select relevant data features

- Post-processing allows for samples $||S(y_{obs}) - S(y)|| < h$ to be adjusted based on the local-linear regression

Further refinements - regression

Beaumont, Zhang and Balding, 2002, Blum, 2010, Blum and François, 2010



Location model: $y \sim N(\theta, 1), \theta \sim N(0, 1)$

Partial Least Squares - Wegmann et al., 2009

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- *i*th PLS component $u_i = \alpha_i^T z$ maximises $\sum_{j=1}^p \text{Cov}(u_i, \theta_j)^2$, s.t. $\text{Cov}(u_i, u_j) = 0$ for j < i. Also normalisation constraint $\alpha_i^T \alpha_i = 1$

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Linear Regression - Fearnhead and Prangle, 2012

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 - Fit linear model to training data, $heta \sim \mathcal{N}(Az + b, \Sigma)$

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- Motivated by $S(y) = \mathbb{E}[\theta|y]$ being optimal choice of S to minimise quadratic loss of parameter means in the target distribution $\pi(\theta|S(y_{obs}))$ when h = 0

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Boosting - Aeschbacher et al., 2012

- Non-linear regression method, uses training data and outputs predictors $\hat{\theta}(y)$ of $\mathbb{E}(\theta|y)$, which are used as summary statistics

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- Generates an ensemble of weak learners to construct a strong learner