Automatic Learning of Summary Statistics for Approximate Bayesian Computation Using Deep Learning

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What we will talk about today

- Introduction to ABC;
- How to leverage deep learning methods to learn the summary statistics for ABC;
  - Present the main results from the paper: *Partially Exchangeable Networks and Architectures for Learning Summary Statistics in Approximate Bayesian Computation* (accepted for ICML 2019);
- We will have a practical focus and run ABC for a simple model (the Beta-Binomial model).

Approximate Bayesian Computation: Simulation based inference

- ABC in a nut-shell: Simulations-based inference method where we generate parameter proposals $\theta^\star$ and accept $\theta^\star$ if the generated data $y^\star \sim p(y|\theta^\star)$ is *similar* to our observed data y^{obs};
- ABC only requires that we can simulate data from a computer simulator of our model $p(y|\theta)$.
- Thus ABC is very generic, and can be applied for models where the likelihood function is intractable.

- *Curse-of-dimensionality*: Instead of comparing the data sets we compare a set of summary statistics $s = S(y)$. The main focus of our work is how to *automatically* learn the summary statistics. (For example for dynamic models, summaries can be autocorrelations, cross-covariances, stationary mean. For i.i.d. data could be quantiles, mean and standard deviation etc.;)

Approximate Bayesian Computation: Rejection sampling method

- Generate $\tilde{N}$ independent proposals $\theta^i \sim p(\theta)$, and corresponding data sets $y^\star \sim p(y|\theta^i)$ from the computer simulator $p(y|\theta)$;

- Compute the summary statistics $s^i = S(y^i)$ for each $i = 1, \ldots, \tilde{N}$;

- Compute the distances $\Delta(s^i, s^{\text{obs}})$ for each $i = 1, \ldots, \tilde{N}$.

- Retain proposals θ^i corresponding to those $\Delta(s^i, s^{\text{obs}})$ such that $\Delta(s^i, s^{\text{obs}}) \leq \epsilon$, for some $\epsilon \geq 0$;

- We sample from $p^\epsilon_{\text{ABC}}(\theta^\star|s^{\text{obs}})$.

ABC rejection sampling for the Beta-Binomial model

Model

$$\begin{aligned} y &\sim \text{Binomial}(m, p), \\ p &\sim \text{Beta}(\alpha, \beta) \end{aligned}$$

In [36]:

```
# Define the model and the prior distribution.

Random.seed!(12) # fix random numbers

# model parameters
m = 4; n = 5; p_true = 0.7

 # define the data generating function
data_generator(p) = rand(Binomial(m,p),n)

# generate data
y_obs = data_generator(p_true)

# prior
α = 2; β = 2
prior = Beta(α,β);
```

ABC rejection sampling for the Beta-Binomial model

In [38]:

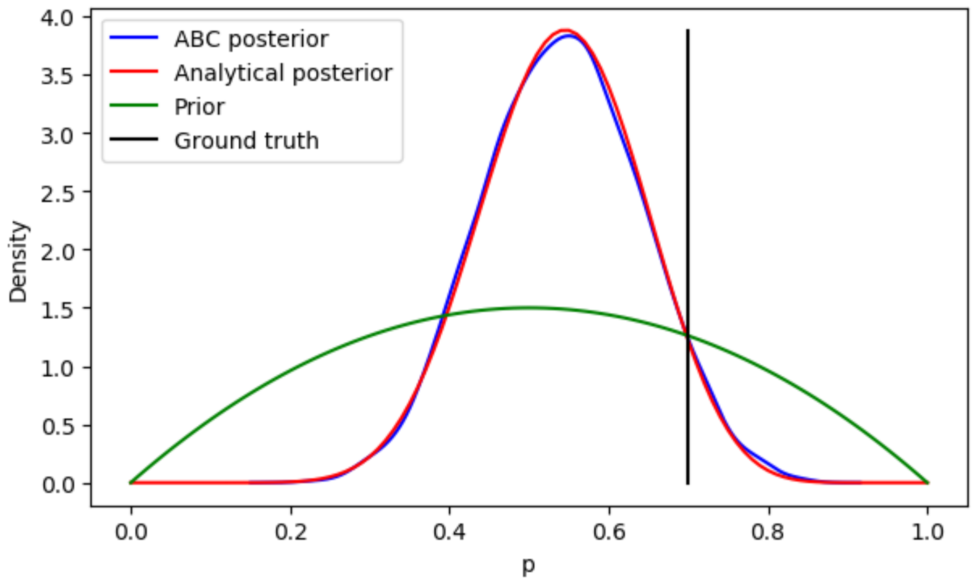
```
# ABC rejection sampling algorithm
function abc_rs(;N_proposals::Int, ϵ::Real)

    abc_posterior_samples = zeros(N_proposals)
    nbr_accepted_proposals = 0

    for i in 1:N_proposals

        p_star = rand(prior) # sample parameter proposal from prio
r
        y_star = data_generator(p_star) # generate data from the d
ata model
        Δ = sum(abs.(sort(y_star)-sort(y_obs))) # compute ABC dist
ance

        if Δ <= ϵ # accept proposal
            nbr_accepted_proposals += 1
            abc_posterior_samples[nbr_accepted_proposals] = p_star
        end
    end

    return abc_posterior_samples[1:nbr_accepted_proposals]
end;
```

ABC rejection sampling for the Beta-Binomial model

In [56]:
```
# Run ABC rejection sampling
abc_posterior_samples = abc_rs(N_proposals = 10^6, ϵ  = 0);
@printf "Acceptance rate: %.2f %%" length(abc_posterior_samples)/1
0^6*100
```

```
Acceptance rate: 0.35 %
```

In [57]:
```
# plot posterior inference results
plot_abc_inference_results(abc_posterior_samples);
```



ABC rejection sampling for the Beta-Binomial model (with summary statistics)

In [43]:
```
# define the summary statistics
S(y) = sum(y); # canonical statistic, i.e. the statistic is suffic
ient!
```

In [46]:

```
# ABC rejection sampling algorithm
function abc_rs_summary_stats(;N_proposals::Int, ϵ::Real, S::Funct
ion)

    abc_posterior_samples = zeros(N_proposals)
    nbr_accepted_proposals = 0

    for i in 1:N_proposals

        p_star = rand(prior) # sample parameter proposal from prio
r
        y_star = data_generator(p_star) # generate data from the d
ata model
        Δ =  abs(S(y_star)-S(y_obs)) # compute ABC distance

        if Δ <= ϵ # accapte proposal
            nbr_accepted_proposals += 1
            abc_posterior_samples[nbr_accepted_proposals] = p_star
        end
    end

    return abc_posterior_samples[1:nbr_accepted_proposals]
end;
```

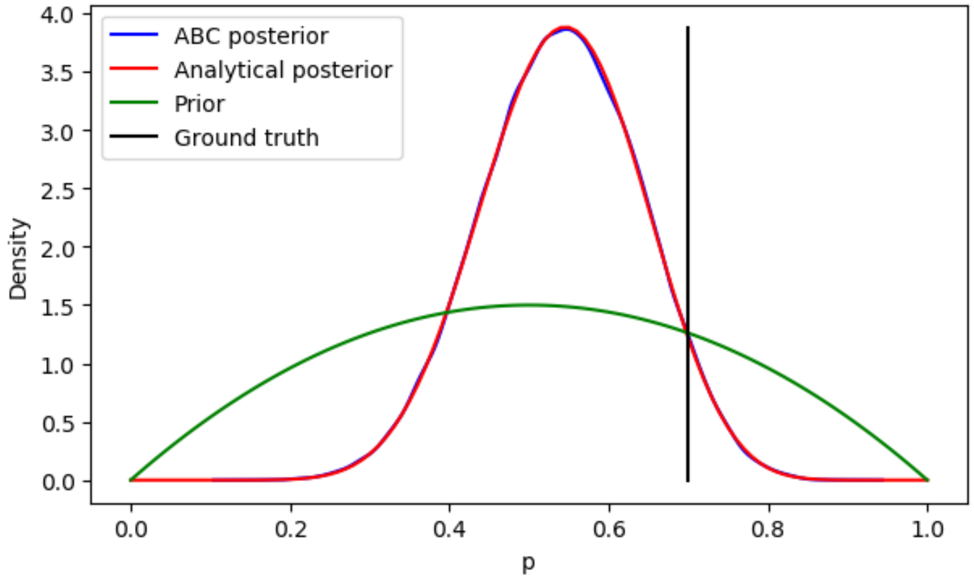
ABC rejection sampling for the Beta-Binomial model (with summary statistics)

In [62]:

```
# Run ABC rejection sampling
abc_posterior_samples = abc_rs_summary_stats(N_proposals = 10^6, ϵ
= 0.1, S=S);
@printf "Acceptance rate: %.2f %%" length(abc_posterior_samples)/1
0^6*100
```

```
Accaptance rate: 6.77 %
```

In [63]:
```
# plot posterior inference results
plot_abc_inference_results(abc_posterior_samples);
```



How to select/learn summary statistics

- The summary statistics *should* be low-dimensional and informative for the parameters (in the ideal case sufficient).
- The problem of selecting informative summary statistics is the main challenge when applying ABC in practice;
- Usually, summary statistics are ad-hoc and "handpicked" out of subject-domain expertise. For example for dynamic models, summaries can be autocorrelations, cross-covariances, stationary mean. For i.i.d. data could be quantiles, mean and standard deviation etc.;
- Several methods to learn/select summary statistics have been developed (see (Prangle, 2015) for a review on these methods);

Learning summary statistics using linear regression

- An important paper is Fearnhead & Prangle, 2012 where they use linear regression to learn summary statistics, they also show that the posterior mean is the *best* (in terms of loss for the posterior mean) summary statistic;

- The semi-automatic ABC (the method from Fearnhead, 2012):
  - We can sample a set of parameter-data pairs $(\theta^i, y^i)_{1 \leq i \leq N}$, by sampling θ^i from the prior, and then simulate corresponding data set y^i from the simulator $p(y|\theta)$;
  - Learn the posterior mean from the N simulations, using a linear regression model:
$$\theta_j^i = E(\theta_j | y^i) + \xi_j^i = b_{0_j} + b_j h(y^i) + \xi_j^i.$$
  - After fitting the linear regression model $S_j(y^\star) = \tilde{b}_{0_j} + \tilde{b}_j h(y^\star)$ is the j:th summary statistics for the proposed data set $y^\star$.

Semi-automatic ABC for the Beta-Binomial model: Step 1: Generate data

In [65]:
```
# generate parameter-data pairs
N = 1000
parameters = rand(prior, N)
data = zeros(N,5)
for i in 1:N; data[i,:] = data_generator(parameters[i]); end
```

Semi-automatic ABC for the Beta-Binomial model: Step 2: Fit linear regression model

In [66]:
```
# Fit linear regression model
β = (data'*data)\data'*parameters # ls estimation
```

Out[66]:
```
5-element Array{Float64,1}:
 0.04676202786457585
 0.04294071054160597
 0.04782352905708373
 0.05299754219974466
 0.05234867025531753
```

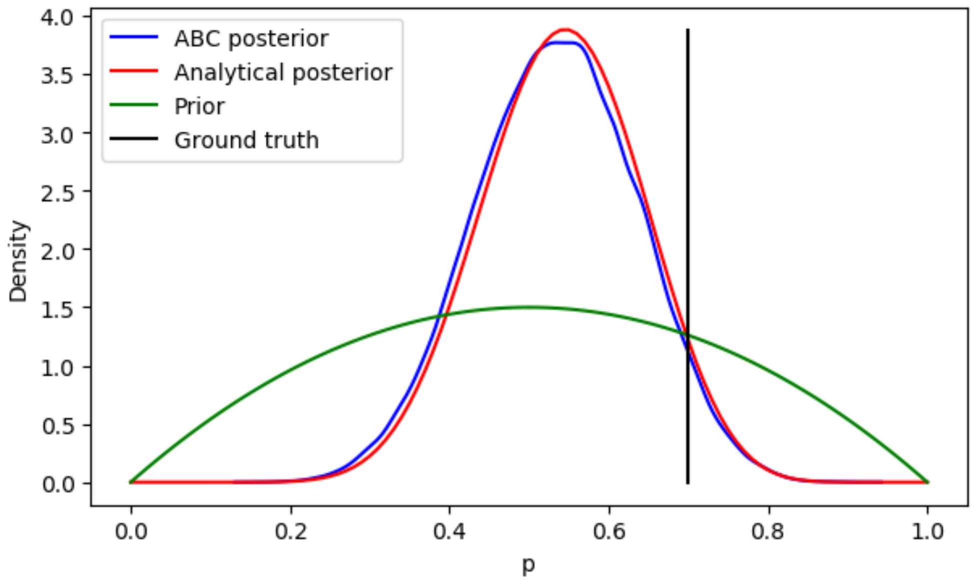
In [33]:
```
# Define the new function to compute the summary statsitic
S_semi_auto(y) = y'*β;
```

Semi-automatic ABC for the Beta-Binomial model: Step 2: Run ABC algorithm

In [67]:
```
# Run ABC rejection sampling
abc_posterior_samples = abc_rs_summary_stats(N_proposals = 10^6, ϵ
= 0.025, S=S_semi_auto);
@printf "Acceptance rate: %.2f %%" length(abc_posterior_samples)/1
0^6*100
```

```
Acceptance rate: 7.15 %
```

In [68]:
```
# plot posterior inference results
plot_abc_inference_results(abc_posterior_samples);
```



Replacing linear regression with multilayer perceptron (MLP) network

- In Jiang et al., 2017 they replace the linear regression model with a MLP network, thus they have following regression model:
$$\theta^i = E(\theta|y^i) + \xi^i = f_\beta(y^i) + \xi^i.$$
Where f_β is the MLP parameterized by the weights β.

Source: (Jiang et al., 2017).

The partially exchangeable network (PEN)

- Markovian data is *partially exchangable* (which is a property that charaterizes Markovian data the same way as $exchangeability$ characterizes i.i.d data);

- Now, PEN is desigen such that it is invariant to the partial exchangeabiliy property of Markovian data;

- We can write the PEN regression model as:
$$\theta^i = E(\theta|y^i) + \xi^i = \rho_{\beta_\rho}\left(y^i_{1:d}, \sum_{l=1}^{M-d} \phi_{\beta_\phi}(y^i_{l:l+d})\right) + \xi^i.$$

- The advantage of PEN is that the archtecture leverge the partial exchangeabiliy property of Markovian data, and thus PEN does not have to *learn* this property.

Results for the AR2 model

Model:
$$y_l = \theta_1 y_{l-1} + \theta_2 y_{l-2} + z_l, \qquad z_l \sim N(0,1).$$

Conclusions

- A practical introduction to ABC for a simple model (the Beta-Binomial model)

- We have studied how deep learning methods can be used to learn summary statistics for ABC, and presented the entire workflow for a simple example;

- PEN is particular useful to use for timeseries data since the network leverage the Markovina structure of the data.

- In Wiqvist et al. 2019 we show how it is possible to obtain good results for several models, including non-Markovian data (for many more details and examples see (Wiqvist et al. 2019)).

The end

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Slides: https://github.com/SamuelWiqvist/bayesatlund2019presentation (https://github.com/SamuelWiqvist/bayesatlund2019presentation)

Github: SamuelWiqvist

Twitter: samuel_wiqvist

References

Fearnhead, P. and Prangle, D. *Constructing summary statistics for approximate bayesian computation: semi-automatic approximate Bayesian computation*. Journal of the Royal Statistical Society: Series B, 74(3):419–474, 2012.

Jiang, B., Wu, T.-y., Zheng, C., and Wong, W. H. *Learning summary statistic for approximate Bayesian computation via deep neural network*. Statistica Sinica, pp. 1595–1618, 2017.

Prangle, D. *Summary statistics in approximate Bayesian computation*. arXiv:1512.05633, 2015.

Wiqvist, S., Mattei P-A., Picchini U., and Frellsen J. *Partially Exchangeable Networks and Architectures for Learning Summary Statistics in Approximate Bayesian Computation*, arXiv:1901.10230, 2019.

Extra slide: Approximate Bayesian Computation: Approximate posterior

- The joint distribution of accapted parameter-data paris $(\theta^\star, s^\star)$ is
$$p(\theta^\star, s^\star) = p(s^\star|\theta^\star)p(\theta^\star)I(\Delta(s^\star, s^{\text{obs}}) \leq \epsilon),$$
where $s^{\text{obs}} = S(y^{\text{obs}})$, I indicator kernel, Δ distance function, and ϵ the threshold.

- Now assume that $S(s^\star) = S(s^{\text{obs}}) \text{ iff } y^\star = y^{\text{obs}}$ and let $\epsilon = 0$. Now marginlizing $s^\star$ yields the true posterior:
$$p(\theta^\star) = \int p(s^\star|\theta^\star)p(\theta^\star)I(\Delta(s^\star, s^{\text{obs}}) \leq \epsilon)ds^\star = p(y|\theta^\star)p($$

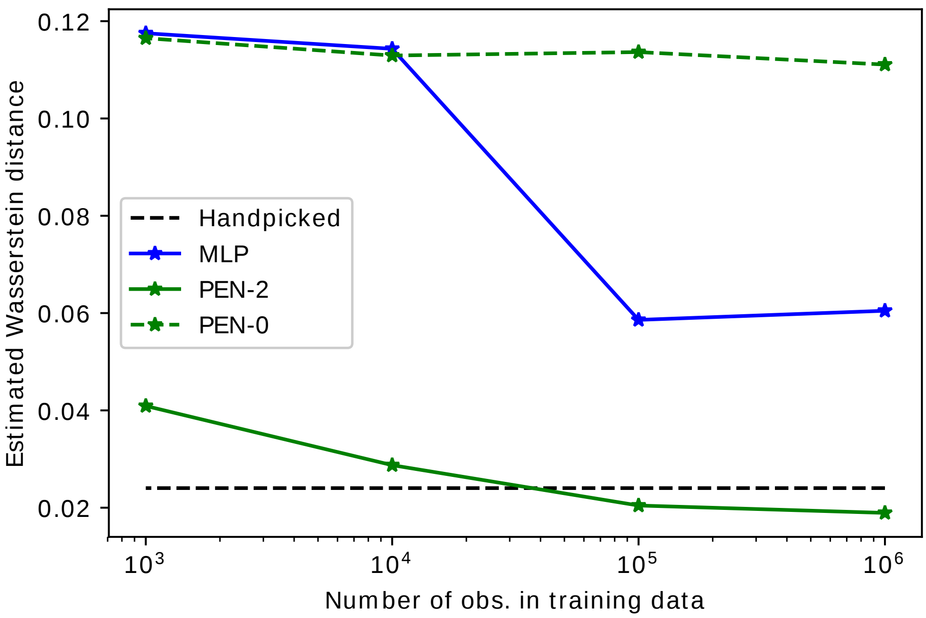
- However, in (almost) all situations we sample from an approximate posterior:

$$p^{\epsilon}_{\text{ABC}}(\theta^\star|s^{\text{obs}}) \propto \int p(s^\star|\theta^\star)p(\theta^\star)I(\Delta(s^\star, s^{\text{obs}}) \leq \epsilon)ds^\star.$$

Extra slide: Results for the AR2 model with observation noise

Model:

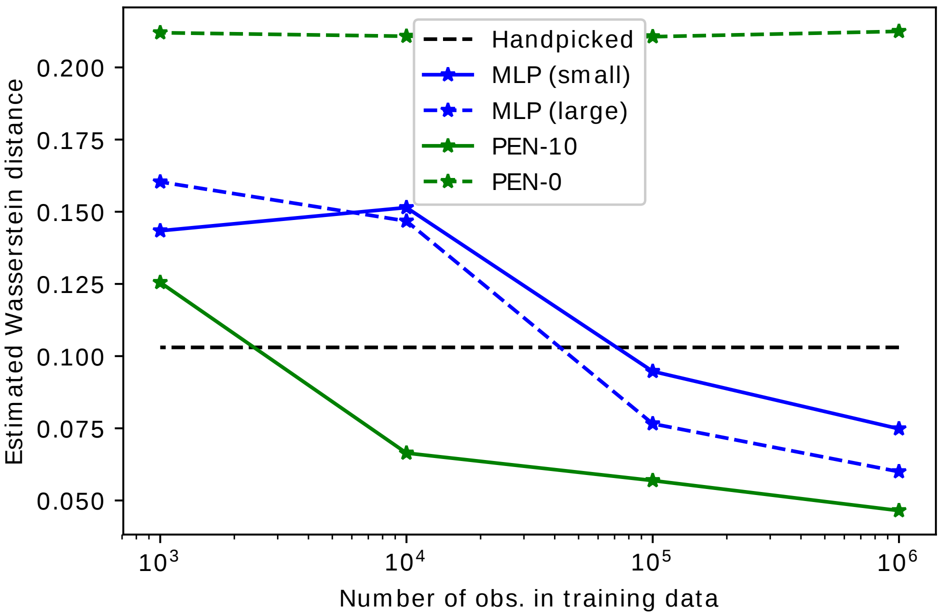
$$y_l = \theta_1 y_{l-1} + \theta_2 y_{l-2} + z_l, \qquad z_l \sim N(0, 1).$$



Extra slide: Results for the MA2 model with observation noise

Model:

$$y_i = x_i + e_i, \qquad e_i \sim N(0, \sigma_\epsilon),$$
$$x_i = z_i + \theta_1 z_{i-1} + \theta_2 z_{i-2}, \qquad z_i \sim N(0, 1).$$


Handpicked
MLP (small)
MLP (large)
PEN-10
PEN-0
0.200
0.175
0.150
0.125
0.100
0.075
0.050
Estimated Wasserstein distance
10^3
10^4
10^5
10^6
Number of obs. in training data