Amortized Learning. Term Paper. Notes

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Contents

1 Goals

Common branch problems that we're trying to solve

1. Evaluate $p(\theta \mid x)$
2. Sample $p(\theta \mid x)$
3. $\mathbb{E}[\theta \mid x], \mathbb{D}[\theta \mid x]$, quantiles
4. $\theta_{MLE} = argmax_{\theta \sim p(\theta)} p(x \mid \theta)$
5. $\theta_{MAP} = argmax_{\theta \sim p(\theta)} p(\theta \mid x)$

2 Projects

1. FMPE, NPSI implementation
2. Summary network experiments (Mamba, CNN, RNN, RevRNN)
3. ABC methods
4. Develop benchmark

3 Papers Summaries

Here I summarize some main thoughts from papers and add questions that arised after reading joint with answers for some. Papers are organized in the order I read them, so there might be dumb questions that have answer in later articles.

3.1 BayesFlow: Learning Complex Stochastic Models With Invertable Neural Networks [Rad+20]

Problem: We have the standart Bayesian setup: model with parameters θ and data x. We want to estimate the posterior $p(\theta \mid x)$. From Bayes theorem we have

$$p(\theta \mid x) \propto p(x \mid \theta) p(\theta)$$

The problem is that in some cases (namely, likelihood-free cases) right-hand side is intractible because we cannot evaluate the $p(x \mid \theta)$, but we can sample from it, i.e.

$$x_i \sim p(x \mid \theta) \iff x_i = g(\theta, \xi_i), \xi_i \sim p(\xi)$$

Solution: Introducing normalizing flow that converts prior into Gaussian

$$\theta \sim p(\theta \mid x) \iff \theta = f_{\varphi}^{-1}(z; x), z \sim N(z \mid 0, \mathbb{I})$$

and considering right loss function we can now learn a summary and inference NN and it will work much more faster for all θ's and x's

Q&A

1. How does the noise ξ selection affects the result? **Preanswer**: it depends also on simulation we use, and, of course, it does matter what noise we'll choose, because it changes the $p(x)$ and so $p(x \mid \theta)$
2. Why do we use Gaussian in normalizing flow?
3. Why don't we minimize the reverse KL divergence? **Answer**: it is also an option, which is considered in [Mur12], Chapter 21 and according to [ZSH24]: «*minimizing the reverse KL divergence leads to approximate distributions that are under-dispersed and that tend to concentrate mass on a single mode of the target distribution, whereas minimizing the forward KL divergence leads to ones that are over-dispersed and that cover all modes of the target distribution*». Both approaches are ubiquitious, but forward KL is easier to implement and it is likelihood-free in contrast to reverse KL.

3.2 Neural Methods for Amortized Inference [ZSH24]

They introduce Bayes risk as the common case of loss function in [Rad+20], where it was the KL divergence. blah-blah Minimizing KL divergence vs reverse KL divergence:

different setups and different method

Summary networks

stopped reading here

Q&A

1. *Average optimality* and what is it, and why do we use it?

3.3 Flow Matching Guide and Code [Lip+24]

Q&A

1. Prove that conditional optimal transport is really linear, i.e.

$$p_t(x) = \int p_{t|1}(x \mid x_1) q(x_1) dx_1$$

   where $p_{t|1}(x \mid x_1) = \mathcal{N}(x \mid tx_1, (1-t)^2 I)$ and

$$X_t \sim p_t \iff X_t = tX_1 + (1-t)X_0$$

2. Verify that u_t and p_t satisfy the Continiuty Equation:

$$\frac{\mathrm{d}}{\mathrm{d}t} p_t(x) + \operatorname{div}(p_t u_t)(x) = 0$$

   Proof. We have $p_t(x) = p_0(\psi_t^{-1}(x))|J(\psi_t^{-1}(x))|$ so

$$\frac{\mathrm{d}}{\mathrm{d}t} p_t(x) = \frac{\mathrm{d}}{\mathrm{d}t} p_0(\psi_t^{-1}(x))|J(\psi_t^{-1}(x))|$$

   □

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□

3.4 Approximate Bayesian Computation in Population Genetic, [BZB02]

Q&A

1. Prove the formula for local-linear regression
2. Provide formulas for multidim local-linear regression + code examples
   (a) Make class LLRegression with methods
   (b) Train and test it in various situations (different δ's, try other kernels instead of K_Δ)
   (c) Compare to analytic solutions and MCMC

4 Questions

1. Continious Flows (FMPE, NPSI) recent papers implementation
2. Sequential Methods (SNPE-A,B,C)

References

[BZB02] Mark A Beaumont, Wenyang Zhang, and David J Balding. "Approximate Bayesian Computation in Population Genetics". In: *Genetics* 162.4 (Dec. 2002), pp. 2025–2035. ISSN: 1943-2631. DOI: 10.1093/genetics/162.4.2025. eprint: https://academic.oup.com/genetics/article-pdf/162/4/2025/42049447/genetics2025.pdf. URL: https://doi.org/10.1093/genetics/162.4.2025.

[Mur12] Kevin P. Murphy. "Machine learning - a probabilistic perspective". In: *Adaptive computation and machine learning series*. 2012. URL: https://api.semanticscholar.org/CorpusID:17793133.

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