

# Amortized Learning. Term Paper. Notes

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# 1 Goals

Common branch problems that we're trying to solve

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

# 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  $\theta$  and data  $x$ . We want to estimate the posterior  $p(\theta | x)$ . From Bayes theorem we have

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

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

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

**Solution:** Introducing normalizing flow that converts prior into Gaussian

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

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

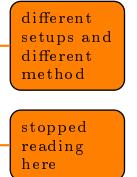
## Q&A

1. How does the noise  $\xi$  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  $p(x | \theta)$
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 ubiquitous, 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:

Summary networks



## 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.

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

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

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

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

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

□

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□

### 3.4 Approximate Bayesian Computation in Population Genetic, [BZB02]

#### Q&A

- Prove the formula for local-linear regression
- Provide formulas for multidim local-linear regression + code examples
  - Make class LLRegression with methods
  - Train and test it in various situations (different  $\delta$ 's, try other kernels instead of  $K_\Delta$ )
  - Compare to analytic solutions and MCMC

## 4 Questions

- Continous Flows (FMPE, NPSI) recent papers implementation
- 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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- [ZSH24] Andrew Zammit-Mangion, Matthew Sainsbury-Dale, and Raphaël Huser. *Neural Methods for Amortized Inference*. 2024. arXiv: 2404.12484 [stat.ML]. URL: <https://arxiv.org/abs/2404.12484>.