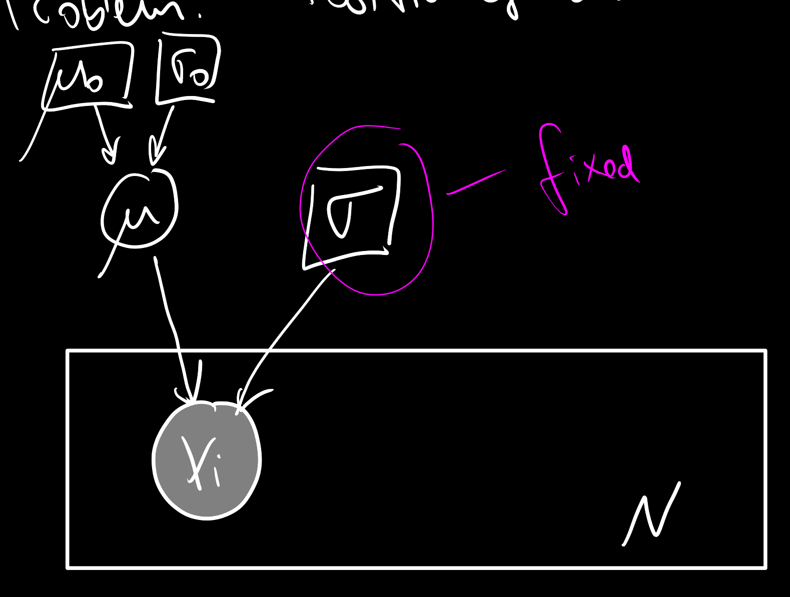
Variational Inference by Automatic Differentiation

$$q(z)^* = \underset{q(z)}{\arg\max} \left(\underbrace{\mathbb{E}_{z \sim q(z)}\left[\log \frac{p(z, x=D)}{q(z)}\right]}_{\text{Evidence Lower Bound (ELBO)}} \right)$$

now propose a parametric distribution $q(z)$ and optimize its parameters

→ by AutoDiff in TensorFlow Probability

Problem: Posterior of a Normal with unknown mean



$$\mu \sim \mathcal{N}(\mu; \mu_0, \sigma_0)$$

$$X_i \sim \mathcal{N}(X_i \mid \mu, \sigma)$$

we have some data $D = \underbrace{\{1.3, 1.5, 1.1, -0.1, \dots\}}_{N \text{ data points}}$

$z = \mu$

$p(\mu \mid \underline{X} = D)$

seek: posterior $p(\mu \mid D)$

we know: $p(\mu \mid D) = \mathcal{N}(\mu; \mu_N, \sigma_N)$

$$\boxed{\mu_N = \frac{\sigma^2 \mu_0 + \sigma_0^2 \sum_{i=0}^{N-1} x^{[i]}}{\sigma^2 + N\sigma_0^2}}$$

$$\boxed{\sigma_N = \frac{\sigma_0 \sigma}{\sqrt{\sigma^2 + N\sigma_0^2}}}$$

Assume we don't know the true posterior

propose surrogate $q(\mu) = \mathcal{N}(\mu; \mu_S, \sigma_S)$

learnable parameters

Maximize ELBO $\quad q(\mu)^* = \underset{q(\mu) \in Q}{\arg\max} (\text{ELBO})$

$$\mu_S^*, \sigma_S^* = \underset{\substack{\mu_S \\ \sigma_S > 0}}{\arg\max} (\text{ELBO})$$

log joint prob: can be evaluated by the DGM

$p(\mu, \underline{X} = D) = p(\mu)\, p(\underline{X} = D \mid \mu)$

$$\mu_S^*, \sigma_S^* = \underset{\substack{\mu_S \\ \sigma_S > 0}}{\overset{\text{argmin}}{\cancel{\arg\max}}} \underbrace{\left(\mathbb{E}_{\mu \sim q(\mu)}\left[\log \frac{p(\mu, \underline{X} = D)}{q(\mu)}\right]\right)}_{\text{negative ELBO} \;\hat{=}\; \text{loss}}$$

$$-\mathcal{L}(\mu_S, \sigma_S)$$

Build a gradient tape / computational while evaluating ELBO

→ then gradients

$$\left.\begin{aligned} \frac{\partial -\mathcal{L}(\mu_S, \sigma_S)}{\partial \mu_S} &= \dots \\ \frac{\partial -\mathcal{L}(\mu_S, \sigma_S)}{\partial \sigma_S} &= \dots \end{aligned}\right\} \text{by reverse-mode auto-diff ("back-propagation")}$$

↳ use gradient-based optimizer, like ADAM

iterative solution $\mu_S^{[j]}, \sigma_S^{[j]}$

$$\mu_S^{[j]} \xrightarrow{j \to \infty} \mu_S^* \qquad \sigma_S^{[j]} \xrightarrow{j \to \infty} \sigma_S^* \qquad \left(\begin{aligned} &\text{we expect} \\ &= \mu_N \\ &= \sigma_N \end{aligned}\right)$$

Approximate Expectation (here: ELBO) by sampling

$$-\mathcal{L}(\mu_S, \sigma_S) \approx -\frac{1}{L} \sum_{l=0}^{L-1} \log \frac{p(\mu = \mu^{[l]}, \underline{X} = D)}{q(\mu = \mu^{[l]})}$$

$$\mu^{[l]} \sim q(\mu)$$

① Sample L samples from $q(\mu)$

② Evaluate approximate ELBO

μ_S & σ_S appear in:

↳ creation of the samples

↳ evaluation of the log-prob