How to do it better with neural networks: Amortized SBI

basic observation: given $TS = \{(Y_i \sim p^s(Y),\ X_i = \phi(Y_i, \eta_i))\}_{i=1}^{N}$ $\quad \eta_i \sim p^s(\eta \mid Y_i)$

(easy to create when we know $p^s(Y)$ and $\phi(Y, \eta)$)

we can train conditional normalizing flows for

$$p(X \mid Y) \approx p^s(X \mid Y) \qquad \text{(forward surrogate)}$$

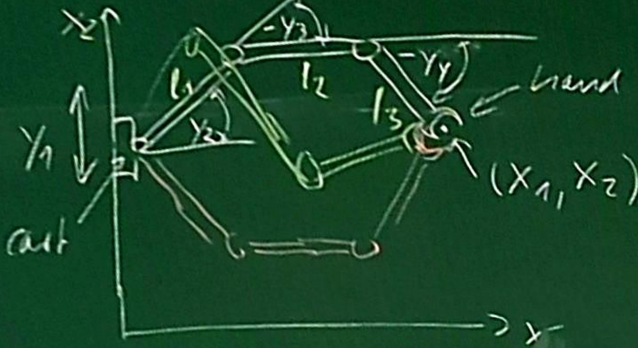
$$p(Y \mid X) \approx p^s(Y \mid X) \qquad \text{(inverse posterior)}$$

[also: estimator for $p(X) \approx p^S(X) = \int p^S(Y)\, p^S(X|Y)\, dy$]

- advantages:
  - likelihood-free: $p^S(X|Y)$ is not needed, $X \sim \phi(Y, \eta)$ suffices
  - scales to high dimensions $\dim(X)$ and $\dim(Y)$
  - can <u>learn</u> summary statistics $h(x)$ such that $p(Y \mid h(x)) \approx p^S(Y|X)$
    - [feature detection network
  - amortized: all simulations in TS contribute to training, no rejections
    - upfront training effort may be high (rule of thumb: roughly as expensive as 5–10 MCMC runs)
    - prediction is very cheap (just network evaluation on GPU)
    - training amortizes if one analyzes <u>many</u> X^{obs} (economics of scale)
  - generalization: networks generalize to unseen (X, Y) pairs
    $\Rightarrow$ even X far from X^{obs} (normally rejected) contribute to accuracy
- disadvantages:
  - so far, no theoretical performance guarantees
  - no cheap way to fine tune networks when $p^S(Y)$ or $\phi(Y, \eta)$ change slightly (open research problem)

• example: inverse kinematics

consider 2D robot arm with 4 DoF $\quad Y = (Y_1, Y_2, Y_3, Y_4)$



(x_1, x_2) desired / observable hand location (2D)

$\Rightarrow$ information loss $Y \rightsquigarrow X$ $\quad (\dim(Y) > \dim(X))$

$\Rightarrow$ no unique solution for $X \rightsquigarrow Y$

define simulation: $\phi_1(Y) = x_1 = 0 + l_1 \cos(Y_2) + l_2 \cos(Y_2 + Y_3) + l_3 \cos(Y_2 + Y_3 + Y_4)$

(deterministic, no noise) $\phi_2(Y) = x_2 = Y_1 + l_1 \sin(Y_2) + l_2 \sin(Y_2 + Y_3) + l_3 \sin(Y_2 + Y_3 + Y_4)$

priors ("preferred joint positions", "convenient situations")

$$p^S(Y) = p_1^S(Y_1) \cdot p_2^S(Y_2) \cdot p_3^S(Y_3)\, p_4^S(Y_4) \quad \text{independent}$$

$$p_1(Y_1) = \mathcal{N}(0, \sigma^2 = 1/16); \quad p_2^S(Y_2) = p_3^S(Y_3) = p_4^S(Y_4) = \mathcal{N}\left(0, \sigma^2 = \frac{1}{4}\right)$$

(in units of rad$^{(2)}$)

task: solve inverse problem:

given desired hand location X^{obs}, compute $p(Y \mid X^{obs}) \approx p^S(Y \mid X^{obs})$

unknown truth

$p^s(Y|X^{obs}) > 0$ for all $Y \in F(X^{obs}) = \{ Y \mid \phi(Y) = X^{obs} \}$

infinite set due to $\dim(Y) > \dim(X)$

$p^s(Y|X^{obs}) \approx 0$ if Y is inconvenient according to prior

$p^s(Y|X^{obs}) \gg 0$ if Y is convenient — " —

joint probability $p^s(X, Y) \propto \delta(X - \phi(Y)) \cdot p^s(Y)$

when Y is guessed (as in MCMC), $\delta(X - \phi(Y)) = 0$ most of the time

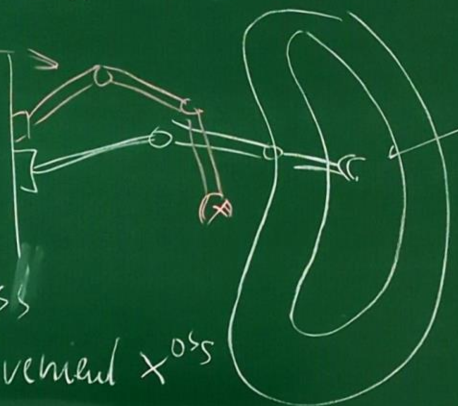
$\Rightarrow$ very high rejection

[even if $\dim(Y) = \dim(X)$ the solution may not be unique,
but $F(X)$ must be a "zero set" $\int_{F(X)} p(Y)\, dY = 0$]

less convenient

$\Rightarrow$ few inconvenient examples in TS

$\Rightarrow$ $p(Y|X^{obs})$ is less accurate for inconvenient X^{obs}



typical set of $p^s(X)$ according to prior
(convenient situations as above: arm is nearly straight)

$$TS = \{ (Y_i \sim p^s(Y), X_i = \phi(Y_i)) \}_{i=1}^{N}$$