Accelerating Metropolis-Hastings with Lightweight Inference Compilation

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Facebook Probability, Facebook AI Infrastructure, UC Berkeley

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Background

Two competing philosophies

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Probabilistic ML

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Deep Learning

Irrelevant [LeCun et al., 2015, Goodfellow et al., 2016]

Probabilistic programming languages (PPLs)

> *Just as programming beyond the simplest algorithms requires tools for abstraction and composition, complex probabilistic modeling requires new progress in model representation—probabilistic programming languages.*

[Goodman, 2013]

Abstractions over deterministic computations

Low Level Assembly

```
mov   dx, msg
; ah=9 - "print string" sub-function
mov   ah, 9
int   0x21

"terminate␣program" sub-function
mov   ah, 0x4c
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msg
db  'Hello,␣World!', 0x0d, 0x0a, '$'
```

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```

High Level Python

```
print("Hello,␣World!")
```

Abstractions over probabilistic computations

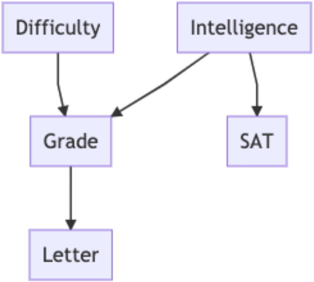

Figure 1:
[Koller and Friedman, 2009]

Abstractions over probabilistic computations

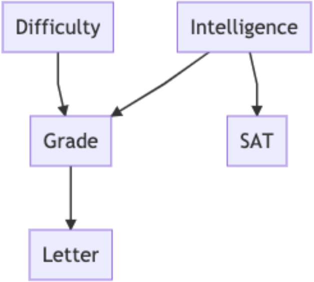

Figure 1:
[Koller and Friedman, 2009]

```
d ~ Bernoulli
i ~ Normal
g ~ g(d, i)
s ~ s(i)
l ~ Multinomial(g)
```

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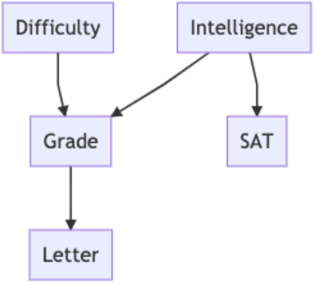


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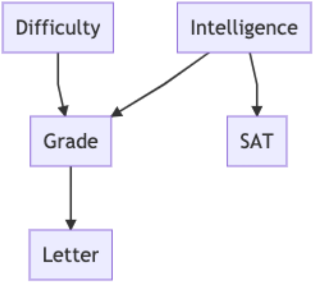
Generative model:

$$P(D, I, G, S, L) = P(D)P(I)P(G \mid D, I)P(S \mid I)P(G \mid L)$$

Abstractions over probabilistic computations

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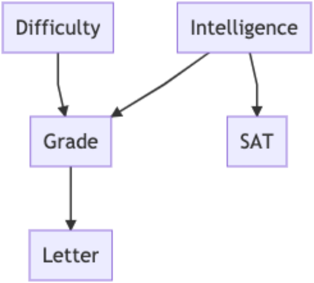
Question : Given a student's recommendation *letter* and *SAT* score, what should I expect their *intelligence* to be?

Abstractions over probabilistic computations

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Question : Given a student's recommendation *letter* and *SAT* score, what should I expect their *intelligence* to be?

PPL Query : `infer(i, {l=Good, s=800})`

Bayesian Inference Basics

Latent Variables X

Observed Variables Y

Prior $P(X)$

Likelihood $P(Y \mid X)$

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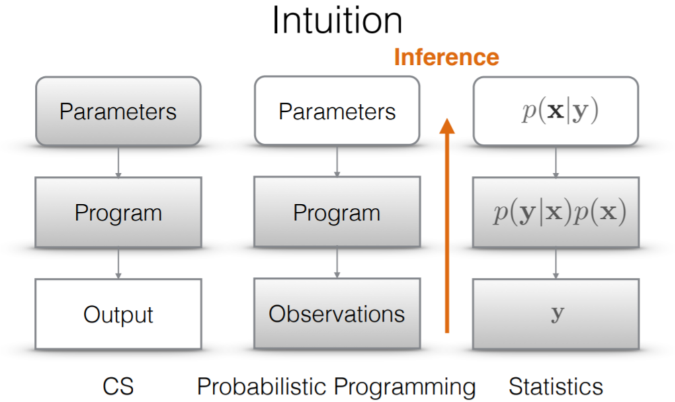

Figure 2: [van de Meent et al., 2018]

Bayesian Inference Basics

Goal: Approximate the posterior $P(X \mid Y)$

X	Y
intelligence	letter and grade
scene description	image
simulation	simulator output
program source code	program return value
policy prior and world simulator	rewards
cognitive decision making process	observed behavior

Table 1: [van de Meent et al., 2018]

Why only approximate?

$$P(X \mid Y) = \frac{P(Y \mid X)P(X)}{P(Y)} = \frac{P(Y \mid X)P(X)}{\underbrace{\int_X P(Y \mid X)P(X)dX}_{=:Z(Y)}}$$

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Denominator $Z(Y)$ (i.e. partition function, marginal likelihood $P(Y)$) high-dimensional integral, known only for a small family of *conjugate* prior/likelihood pairs

How to approximate?

Variational Inference

Monte Carlo

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Variational Inference

Let q_ϕ be a tractable parametric family (e.g. Gaussian mean-field $q_\phi(X) = \prod_{i=1}^{d} N(X_i \mid \phi_{1,i}, \phi_{2,i})$)

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$$\mathbb{E}[g(X)|Y]$$

$$= \int g(X) \cdot P(X \mid Y) dX$$

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Inference compilation in declarative PPLs

Imperative vs Declarative PPLs

Imperative: Evaluation-based, samples (linear) execution traces (Pyro, Church, WebPPL)

Imperative vs Declarative PPLs

Imperative: Evaluation-based, samples (linear) execution traces (Pyro, Church, WebPPL)

```
(begin
    (define geometric
        (lambda (p)
        (if (flip p)
        1
        (+ 1 (geometric p)))))
    (geometric .7))
```

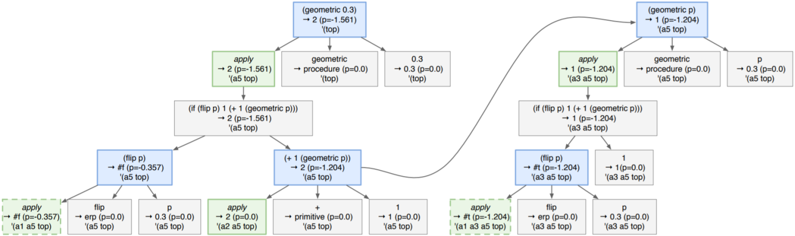

Figure 2: [Wingate et al., 2011]

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$$\mathbb{E}_{P(X|Y)}[g(X)] = \mathbb{E}_{P(X|Y)}\left[\frac{q(X)}{q(X)}g(X)\right] = \frac{\mathbb{E}_q\left[\frac{P(X,Y)}{q(X)}g(X)\right]}{P(Y)}$$

$$\approx \frac{1}{N}\sum_i^N \frac{\frac{P(X_i,Y)}{q(X_i)}}{P(Y)}g(X_i) \approx \sum_i^N \frac{\frac{P(X_i,Y)}{q(X_i)}}{\sum_i^N \frac{P(X_i,Y)}{q(X_i)}}g(X_i)$$

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Convergence rate $\mathrm{Var}_q\left[\frac{P(X,Y)}{q(X)}g(X)\right]^{-1/2}$ [Yuan and Druzdzel, 2007]

SIS of execution traces

1. Execute the probabilistic program forwards
2. At each stochastic variable (i.e. `sample` statement), sample from proposer $q(\cdot)$ and assign value
3. At each observed random variable (i.e. `observe` statement), multiply likelihood into trace's importance weight

SIS of execution traces

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Problem: Myopic choices from sampling q early in the trace may result in low importance weights later. Would like q to account for observations Y.

Constructing a proposal distribution

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Likelihood-Weighting [Norvig and Intelligence, 2002]:
$q(X) = P(X)$

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Key Idea: Exploit access to $P(X, Y)$ to build a proposer q "close" to $P(X \mid Y)$?

Trace-based inference compilation (IC)

- Construct DNN with parameters ϕ mapping observations Y (amortized inference, [Goodman, 2013]) and execution prefix to proposal distribution $q_\phi(\cdot \mid Y)$
- Train q_ϕ against forward samples from the probabilistic program $p(x, y)$ (inference compilation)

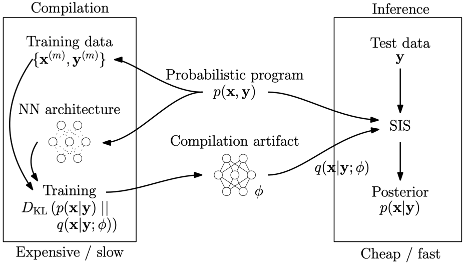
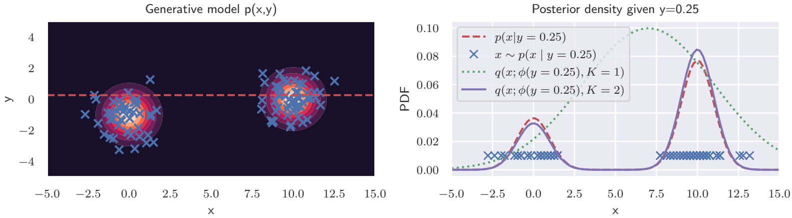


Figure 3: [Le et al., 2017]

Intuition for inference compilation



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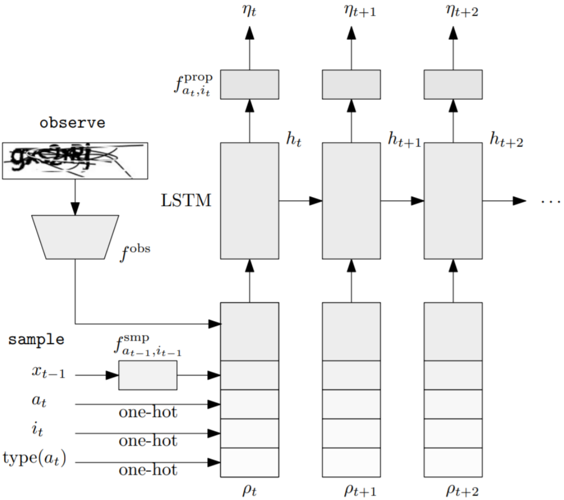

Figure 4: [Le et al., 2017]

Sensitivity to nuisance random variables

```
def magnitude(obs, M):
    x = sample(Normal (0, 10))
    [sample(Normal (0 ,10)) for _ in range(M)] # extend trace with nuisance
    y = sample(Normal (0 ,10))
    observe(obs**2, Likelihood=Normal(x**2 + y**2, 0.1)0
    return x, y
```

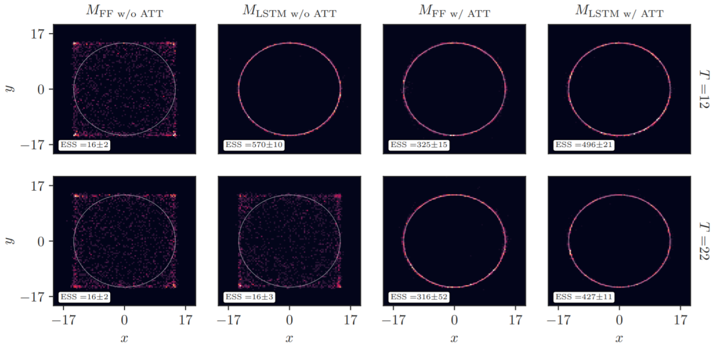

Figure 5: [Harvey et al., 2019]

Imperative vs Declarative PPLs

Declarative: Graph-based, samples instantiated graphical models (i.e. worlds) (BUGS, BLOG, Stan, beanmachine)

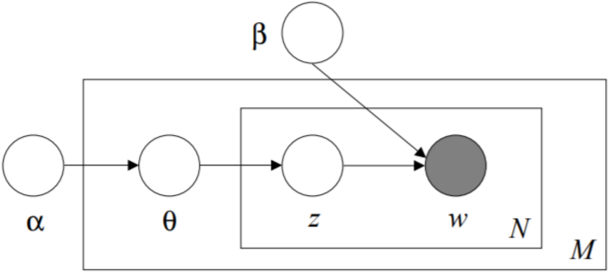

Figure 6: [Blei et al., 2003]

Key Idea: Markov blanket MB(X_i) available in declarative PPL

MCMC sampling of graphical models

Metropolis-within-Gibbs / Lightweight MH ([Wingate et al., 2011]):

- Fix observed nodes Y to their values.
- Repeat:
  - Pick single random unobserved node X_i
  - Sample proposal $q(X_i)$ to propose new value
  - Accept with probability α and revert otherwise

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Theorem ([Hastings, 1970])
With appropriately chosen α, the above algorithm yields a Markov Chain with the posterior as the invariant distribution.

MH proposal distributions

Different $q(\cdot) \implies$ different MCMC algorithms

- Random walk MH: $q(\cdot)$ isotropic Gaussian

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Theorem ([Pearl, 1987])
Gibbs distributions $P(X_i \mid X_i^c) = P(X_i \mid MB(X_i))$ are optimal proposers $q(\cdot)$

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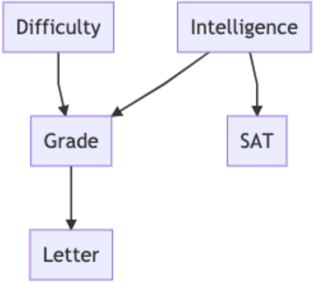
Theorem ([Pearl, 1987])
Gibbs distributions $P(X_i \mid X_i^c) = P(X_i \mid MB(X_i))$ are optimal proposers $q(\cdot)$

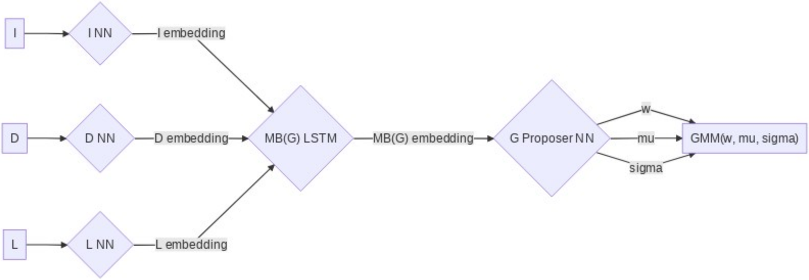
$\therefore$ $\mathrm{MB}(X_i)$ is the minimal sufficient inputs for generating proposal distribution

LIC artifacts for example student network

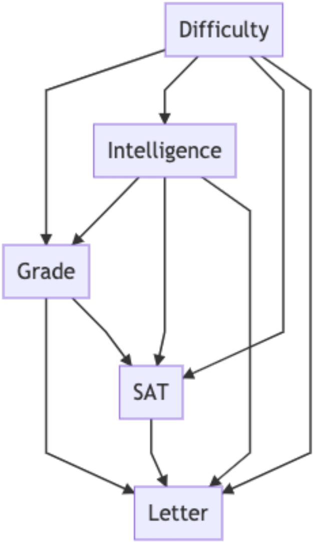


$$q(d|g,i)$$
$$q(i|g,d,s)$$
$$q(g|i,d,l)$$
$$q(s|i)$$
$$q(l|g)$$

Example LIC proposer for grade



Compare against SIS IC's (non-minimal) proposer



$q(d|\text{observations})$

$q(i|d, \text{observations})$

$q(g|i, d, \text{observations})$

$q(s|g, i, d, \text{observations})$

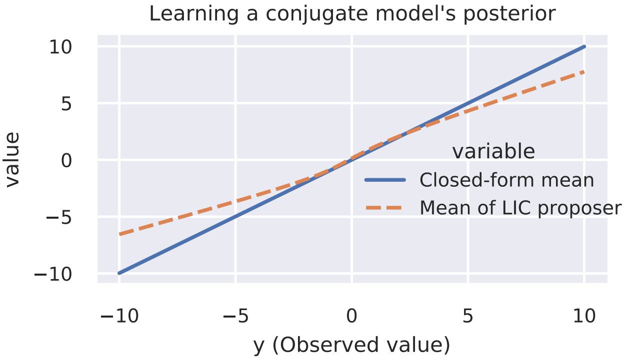
$q(l|s, g, i, d, \text{observations})$

Results

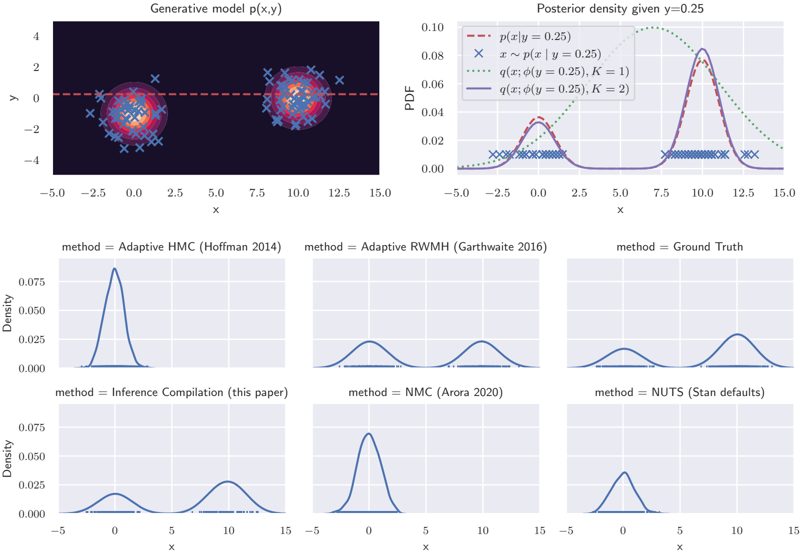
Recovering conjugate expressions in normal-normal

$$x \sim N(0, 2),\ y \mid x \sim N(x, 0.1)$$

Know: $y \mid x \sim N(0.999x, 0.0001)$



GMM Mode Escape



Robustness to nuisance random variables

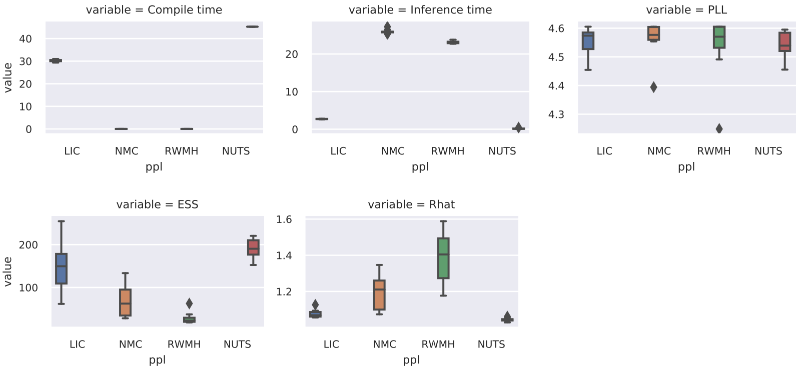
```
def magnitude(obs):
  x = sample(Normal(0, 10))
  for _ in range(100):
    nuisance = sample(Normal(0, 10))
  y = sample(Normal(0, 10))
  observe(
    obs**2,
    likelihood=Normal(x**2 + y**2, 0.1))
  return x
```

```
class NuisanceModel:
  @random_variable
  def x(self):
      return dist.Normal(0, 10)
  @random_variable
  def nuisance(self, i):
      return dist.Normal(0, 10)
  @random_variable
  def y(self):
      return dist.Normal(0, 10)
  @random_variable
  def noisy_sq_length(self):
      return dist.Normal(
          self.x()**2 + self.y()**2,
          0.1)
```

	# params	compile time	ESS
LIC (this paper)	3,358	44 sec.	49.75
[Le et al., 2017]	21,952	472 sec.	10.99

Bayesian Logistic Regression

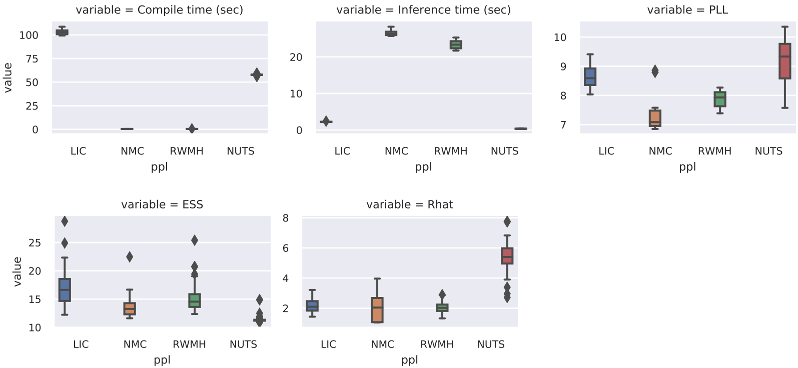
$$\beta \sim \mathcal{N}_{d+1}(0_{d+1}, \mathrm{diag}(10, 2.51_d)),$$
$$y_i \mid \boldsymbol{x}_i \overset{\text{iid}}{\sim} \mathrm{Bernoulli}(\sigma(\beta^\top \boldsymbol{x}_i)) \text{ where } \sigma(t) = (1 + e^{-t})^{-1}$$



n-Schools

$$
\begin{aligned}
\beta_0 &\sim \mathrm{StudentT}(3, 0, 10) \\
\tau_i &\sim \mathrm{HalfCauchy}(\sigma_i) \qquad \text{for } i \in [\text{district}, \text{state}, \text{type}] \\
\beta_{i,j} &\sim \mathcal{N}(0, \tau_i) \qquad \text{for } i \in [\text{district}, \text{state}, \text{type}], j \in [n_i] \\
y_k &\sim \mathcal{N}(\beta_0 + \sum_i \beta_{i,j_k}, \sigma_k)
\end{aligned}
$$

n-Schools


variable = Compile time (sec)
variable = Inference time (sec)
variable = PLL
variable = ESS
variable = Rhat
value
ppl
LIC
NMC
RWMH
NUTS
100
75
50
25
0
20
10
9
8
7
15
6
4
2

Future directions

Adaptive LIC

Problem: forward samples during compilation may not sufficiently represent observations (obs) encountered at inference

RWMH adapts step size [Garthwaite et al., 2016], HMC adapts mass matrix [Hoffman and Gelman, 2014], can LIC adapt NN weights?

Solution: perform MCMC with IC artifact to draw posterior samples $(\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)} = \text{obs}) \sim P(\boldsymbol{x} \mid \boldsymbol{y} = \text{obs})$, hill-climb inclusive KL between *conditional* (rather than joint) posterior

$$\arg\min_{\phi} D_{KL}(p(\boldsymbol{x}|\boldsymbol{y} = \text{obs}) || q(\boldsymbol{x}|\boldsymbol{y} = \text{obs}; \phi))$$

$$\approx \arg\min_{\phi} \sum_{m=1}^{N} \log Q(\boldsymbol{x}^{(m)} \mid \boldsymbol{y} = \text{obs}, \phi)$$

IAF density estimators

Problem: GMM in LIC may not be as expressive as more recently developed density estimators [Kingma et al., 2016]

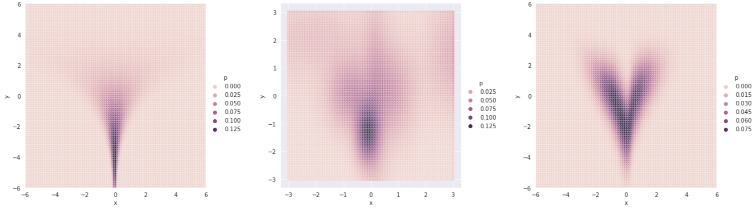
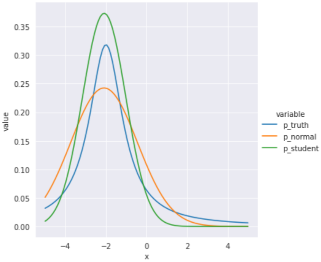


Figure 7: Neal's funnel (left) and a 7-component isotropic GMM (middle) and 7-layer IAF (right) density approximation

Heavy-tailed density estimators

Problem: GMMs and standard IAFs (Lipschitz functions of Gaussians) remain sub-Gaussian, *n*-schools is heavy tailed

Idea: IAFs with heavy-tailed base distribution



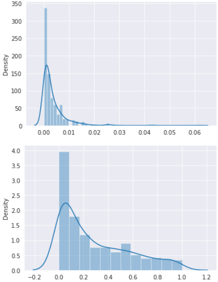


Figure 8: IAF density estimation of a Cauchy$(-2, 1)$ (left) and their K-S statistics when using a Normal (right top) and StudentT (right bottom) base distribution

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