Probabilistic Programming and AI: Lecture 2

Introduction to Probabilistic Programming Languages

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- · Latent variables ⊖
- Observed variables X
- · Observes are believed to be generated from latents
- Prior distribution $P(\Theta)$ captures our belief/information about the latent variables before observing data
- Likelihood $P(X|\Theta)$ encodes how we believe the observes are generated from latents
- · Posterior distribution is obtained with Bayes Theorem

$$P(\Theta|X) = \frac{P(X|\Theta) \times P(\Theta)}{P(X)}$$

 Posterior is the updated belief, our information about the latents after having observed data

Prior $P(\Theta)$

- design decision: can be constructed from expert knowledge / previous experiments
- · computable

Likelihood $P(X|\Theta)$

- encodes generative process from latents Θ to observes X
- · computable

Joint Probability $P(X, \Theta)$

- product of prior and likelihood $P(X, \Theta) = P(X|\Theta) \times P(\Theta)$
- · computable

Marginal / Evidence P(X)

- can be interpreted as the probability of generating the observed data from a prior
- · can only be **approximated** in most models

Posterior $P(\Theta|X)$

- is the updated belief, the information about the latents after having observed data
- · what we want to know
- · can only be **approximated** in most models

Coin model

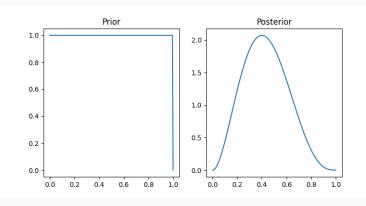
```
x_i \sim \text{Bernoulli}(p)
                                                          observed
\Theta = p, X = (x_1, \dots, x_n), P(X, \Theta) = P(p)P(x_1|p) \cdots P(x_n|p)
\underline{\log P(X,\Theta)} = \underline{\log P(p)} + \underline{\sum_{i=1}^{n} \log P(x_i|p)}
  "log-prob" log-prior log-likelihood
def prior(p):
     return dist.Uniform(0,1, validate_args=False).log_prob(p).exp()
def likelihood(xs,p):
    lp = torch.tensor(0.)
for x in xs:
         lp += dist.Bernoulli(p, validate_args=False).log_prob(x)
    return lp.exp()
def joint(xs, p):
     return prior(p) * likelihood(xs, p)
xs = torch.tensor([0.,1.,1.,0.,0.])
```

latent

 $p \sim \text{Uniform}(0,1)$

Example

ps = torch.linspace(0,1,200)
posterior_unnormalised = torch.hstack([joint(xs, p) for p in ps])
marginal = torch.trapz(posterior_unnormalised, ps)
posterior = posterior_unnormalised / marginal



Example

Compared to Frequentist Statistics

l = torch.hstack([likelihood(xs, p) for p in ps])

Maximum-Likelihood-Estimator:

ps = torch.linspace(0,1,10000)

ps[l.argmax()] Returns: 0.3999

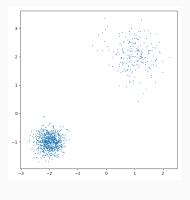
```
Hypothesis testing \mathcal{H}_0: p=0.5:  m=xs.mean() \text{ # test statistic: mean } \\ means=dist.Bernoulli(0.5).sample((len(xs), 10000)).mean(dim=0) \\ a=min(1-m,m) \\ b=max(1-m,m) \\ \text{# probability that sample is more extreme than observations } \\ ((means < a) | (b < means)).float().mean() \\ \text{Returns: } \\ tensor(0.3662) \text{ # p-value -> cannot reject null}
```

Generative Modelling

Generative Modelling

In generative modelling, we encode the way how we believe the observed data was generated in a probabilistic model.

Cluster Model



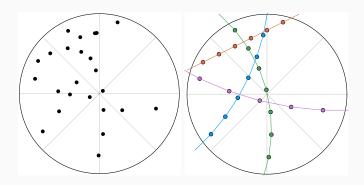
- · How many clusters? Easy: 2
- Model probability of being in cluster 1:
 p ~ Uniform(0,1)
- Cluster centers, k=0,1: $\mu_{\rm X}^k \sim {\rm Uniform(-3,3)}, \; \mu_{\rm V}^k \sim {\rm Uniform(-3,3)}$
- Cluster spread, k = 0, 1: $\sigma^k \sim \text{InverseGamma}(1,1)$
- Cluster membership, i = 1, ..., N: $z_i \sim \text{Bernoulli}(p)$
- Observed data, i = 1, ..., N: $x_i \sim \text{Normal}(\mu^{z_i}, \sigma^{z_i})$

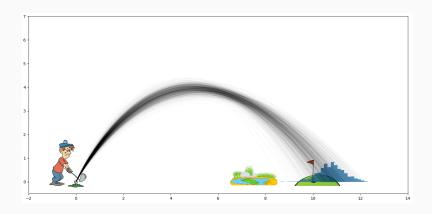
$$P(X,\Theta) = P(p)P(\mu_X^1)P(\mu_Y^1)P(\mu_X^2)P(\mu_Y^2)P(\sigma^1)P(\sigma^2)\prod_{i=1}^N P(z_i|p)P(x_i|\mu,\sigma,z_i)$$

- · How many clusters? Easy: 2
- Model probability of being in cluster 1:
 p ~ Uniform(0,1)
- · Cluster centers, k=0,1: $\mu_{\rm X}^k \sim {\rm Uniform(-3,3)}, \ \mu_{\rm Y}^k \sim {\rm Uniform(-3,3)}$
- Cluster spread, k = 0, 1: $\sigma^k \sim \text{InverseGamma}(1.1)$
- Cluster membership, i = 1, . . . , N:
 z_i ~ Bernoulli(p)
- Observed data, i = 1, ..., N: $x_i \sim \text{Normal}(\mu^{z_i}, \sigma^{z_i})$

```
@model function cluster(x::Vector{Vector{Float64}})
    K = 2 # 2 clusters
    p ~ Uniform(0..1) # probability of being in cluster 1
    mu x = zeros(K)
    mu v = zeros(K)
    sigmas = zeros(K)
    for k in 1:K
        # Cluster centers
        mu x[k] ~ Uniform(-3.3)
        mu v[k] ~ Uniform(-3.3)
        # Cluster spread
        sigmas[k] ~ InverseGamma(1,1)
    end
    z = zeros(Int, length(x))
    for i in 1:length(x)
        z[i] ~ Bernoulli(p) # Cluster membership
        mu = z[i] == 1 ? [mu_x[1], mu_y[1]] : [mu_x[2], mu_y[2]]
        sigma = z[i] == 1 ? sigmas[1] : sigmas[2]
        x[i] ~ MvNormal(mu, sigma) # Observed data
```

Radar Observations





Probabilistic programming is a programming paradigm in which probabilistic models are specified and posterior inference for these models is performed automatically.

In the most general sense:

A **probabilistic program** is a non-deterministic program for which each execution can be weighted with a real number (e.g a probability).

```
def linear regression(x, y):
    lp = torch.tensor(0.0)
    slope = dist.Normal(0.,3.).sample()
    lp += dist.Normal(0.,3.).log_prob(slope)
    intercept = dist.Normal(0..3.).sample()
    lp += dist.Normal(0.,3.).log_prob(intercept)
   sigma = dist. HalfCauchy (1). sample ()
    lp += dist.HalfCauchy(1).log_prob(sigma)
   for i in range(len(x)):
        lp += dist.Normal(slope * x[i] + intercept, sigma).log_prob(y[i])
    return (slope, intercept, sigma), lp
```

$$P(X, \Theta) = P(\text{slope})P(\text{intercept})P(\text{sigma}) \prod_{i=1}^{N} P(x_i|\text{slope}, \text{intercept}, \text{sigma})$$

A probabilistic programming language (PPL) abstracts away the complexities of computing the program weight.

A PPL allows us to conveniently specify a probabilistic model as a program (by using special syntax or primitives).

Internally, the programs are represented in a way to facilitate automated posterior inference.

```
# Turing
@model function linreg(x, y)
    slope ~ Normal(0,3)
   intercept ~ Normal(0.3)
    sigma ~ InverseGamma(1,1)
   for i in eachindex(v)
        v[i] ~ Normal(slope * x[i] + intercept, sigma)
    end
end
# Pvro
def linreg(x, v):
    slope = pyro.sample("slope", dist.Normal(0,3))
    intercept = pyro.sample("intercept", dist.Normal(0,3))
    sigma = pyro.sample("sigma", dist.HalfCauchy(1))
    for i in range(len(x)):
        pyro.sample(
            f"y[{i}]",
            dist.Normal(slope * x[i] + intercept, sigma),
            obs=v[i])
```

Representation-Based

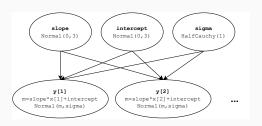
- Translate the program to internal representation
- · Usually the underlying representation is some sort of graph
- · Optimised inference

Evaluation-Based

- Usually embedded in existing languages
- · Have special programming constructs to specify models
- · Run the entire program in different contexts for inference
- · General Purpose

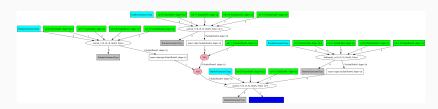
Representation-Based: Graphical Models

Example: PyMC



Representation-Based: Graphical Models

Underlying Computation Graph in PyMC



Representation-Based: Graphical Models

Strengths

- Can exploit structure of model
- Optimised inference

Constraints

- Only works for models with finite number of random variables
- Are not "embedded" in host language

Representation-Based: Unconstrained Function

Example: Stan

```
data {
  int<lower=0> N;
  vector[N] x;
  vector[N] y;
}
parameters {
  real slope;
  real intercept;
  real<lower=0> sigma;
}
model {
  slope - normal(0,3)
  intercept - normal(0,3)
  sigma - inv_gamma(2,1)
  y - normal(slope+intercept*x,sigma);
}
```

```
double model(vector<double> theta,
  int N, vector<double> x, vector<double> y) {
  double target = 0.0;
  slope = theta[0];
  intercept = theta[1];
  sigma = exp(theta[2]); // transformed

  target += normal_lpdf(slope, 0, 3);
  target += normal_lpdf(intercept, 0, 3);
  target += inv_gamma_lpdf(sigma, 2, 1);

for (int i = 0; i++, i < N) {
    target += normal_lpdf(y[i],slope*x[i]+intercept,sigma)
  }
  return target;
}</pre>
```

$model \colon \mathbb{R}^3 \to \mathbb{R}$

a.s. differentiable if all variables are continuous and terminates

Representation-Based: Unconstrained Function

Strengths

- Specialised (gradient-based) inference
- Fast inference

Constraints

- · Black box function
- Only supports finite number of random variables

Representation-Based: Symbolic

Example: Psi

```
\begin{array}{lll} \text{def main()} \{ & \text{flips} := [0,1,1,0,0]; \\ \text{n} := & \text{flips.length;} \\ \text{p} := & \text{uniform(0,1);} \end{array} & p(u) & = & \frac{\int_0^1 p^{2+u} (1-p)^{4-u} dp}{\int_0^1 p^3 (1-p)^3 dp + \int_0^1 p^2 (1-p)^4 dp} \\ & \text{for i in } [0..n) \{ & & & \\ \text{x} := & \text{bernoulli(p);} & & & \\ & & \text{observe(x==flips[i]);} \\ \} & & & & = & \frac{3}{7} \delta_1(u) + \frac{4}{7} \delta_0(u) \end{array}
```

Representation-Based: Symbolic

Strengths

Exact inference

Constraints

Most models are not solvable symbolically

Example: Pyro

```
linreg(x)
returns:
(tensor(0.4707), tensor(3.9712))
with pyro.poutine.trace() as trace:
    linreg(x)
trace.get_trace().nodes["sigma"]
returns:
{ 'type : 'sample',
    'name': 'sigma',
    'fn': HalfCauchy(),
    'is_observed': False,
    'value': tensor(4.4170),
    ...}
```

Example: Pyro

```
with pyro.poutine.trace() as trace:
    with pyro.condition(
        data={f*y{{i}*: y[i] for i in range(5)}}):
    linreg(x)

trace.get_trace().nodes[*y[0]*]
returns:
{'type': 'sample',
    'name': 'y[0]',
    'fn': Normal(loc: -7.59, scale: 2.31),
    'is_observed': True,
    'value': tensor(-1.2000),
    ...}

trace.get_trace().log_prob_sum()
returns:
tensor(-27.8861)
```

Example: Gen

```
@gen function linreg(x, y)
    slope ~ normal(0,3)
end

function var"##linreg#369"(var"##state#294", x::Any, y::Any)
    slope = Gen.traceat(var"##state#294", normal, (0, 3), :slope)
end
```

end

```
@model function linreg(x, y) # Turing
     slope ~ Normal(0.3)
end
function linreg(__model__::Model, __varinfo__::AbstractVarInfo, __context__::AbstractContext . x. y: )
   var"##dist#362" = Normal(0.3)
   var"##vn#359" = (DynamicPPL.resolve_varnames)((AbstractPPL.VarName){:slope}(), var"##dist#362")
   var"##isassumption#360" = begin
           if (DynamicPPL.contextual isassumption)( context . var"##vn#359")
           end
       end
       var"##retval#364" = if (DynamicPPL.contextual_isfixed)(_context__, var"##vn#359")
               slope = (DynamicPPL.getfixed nested)( context . var"##vn#359")
            elseif var"##isassumption#360"
               begin
                   (var"##value#363", __varinfo__) = (DynamicPPL.tilde_assume!!)( __context__, (DynamicPPL.unwr.
                   slope = var"##value#363"
                   var"##value#363"
               end
               if !((DynamicPPL.inargnames)(var"##vn#359". model ))
                   slope = (DynamicPPL.getconditioned_nested)(__context__, var"##vn#359")
               end
               (var"##value#361", __varinfo__) = (DynamicPPL.tilde_observe!!)(__context__, (DynamicPPL.check_ti
               var"##value#361"
           end
       return (var"##retval#364", varinfo )
   end
```

Strengths

- Can represent any probabilistic model
- Can be embedded in host languages

Constraints

General-purpose inference is difficult

Implementing a minimal PPL

Implementing a minimal PPL

Goals:

- · Evaluation-based
- Contextualised execution (Lecture 2)
- · General-purpose inference:
 - Likelihood weighting (Lecture 2 + Assignment 2)
 - Metropolis Hastings (Lecture 3 + Assignment 3)
- · Gradient-based inference:
 - Hamiltonian Monte Carlo (Lecture 3 + Assignment 4)
 - Variational Inference (Lecture 4 + Assignment 4)

PPL Core: Distribution Back-end

torch.distributions

PPL Core: Sample Context

```
_SAMPLE_CONTEXT = None
class SampleContext(ABC):
    def __enter__(self):
        global _SAMPLE_CONTEXT
        SAMPLE CONTEXT = self
    def __exit__(self, *args):
        global SAMPLE CONTEXT
        SAMPLE CONTEXT = None
    @abstractmethod
    def sample(self,
               address: str.
               distribution: dist. Distribution,
               observed: Optional[torch.Tensor] = None) -> torch.Tensor:
        raise NotImplementedError
```

PPL Core: Sample Context

```
1  ctx = MySampleContext()
2  with ctx:
3  do_something()

1  ctx = MySampleContext()
2  ctx.__enter__()
3  do_something()
4  ctx.__exit__()
```

PPL Core: Sample Statement

Example Program

```
def noisy_geometric(p):
    x = 0
   while True:
        b = sample(f"b_{x}", dist.Bernoulli(p))
        if b:
            break
       x += 1
    y = sample("y", dist.Normal(x,1), observed=torch.tensor(3))
   return x
torch.manual_seed(0)
[noisy_geometric(0.25) for _ in range(10)]
returns:
[2, 0, 8, 0, 4, 8, 0, 3, 1, 0]
```

Example Context

```
class LogProb(SampleContext):
   def __init__(self):
        self.log_prob = torch.tensor(0.)
   def sample(self,
               address: str.
               distribution: dist. Distribution.
               observed: Optional[torch.Tensor] = None) -> torch.Tensor:
        if observed is not None:
            value = observed
        else:
            value = distribution.sample()
        self.log_prob += distribution.log_prob(value)
        return value
```

Example Context (cont.)

```
torch.manual_seed(0)
ctx = LogProb()
with ctx:
    x = noisy_geometric(0.25)
x, ctx.log_prob
returns:
(2, tensor(-1.9617))
p = torch.tensor(0.25)
2*torch.log(1-p) + torch.log(p) + dist.Normal(2,1).log_prob(torch.tensor(3))
\# == tensor(-1.9617)
```

Example Context

```
class Trace(SampleContext):
   def __init__(self):
        self.trace = {}
   def sample(self,
               address: str.
               distribution: dist. Distribution,
               observed: Optional[torch.Tensor] = None) -> torch.Tensor:
        if observed is not None:
            value = observed
        else.
            value = distribution.sample()
        self.trace[address] = {
            'value': value.
            'distribution': distribution.
            'is observed': observed is not None,
            'log_prob': distribution.log_prob(value)
        return value
```

Example Context (cont.)

```
torch.manual seed(0)
ctx = Trace()
with ctx.
    x = noisy geometric(0.25)
ctx.trace
returns:
{'b_0': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25, logits: -1.0986123085021973),
  'is_observed': False,
  'log_prob': tensor(-0.2877)},
 'b_1': {'value': tensor(0.),
  'distribution': Bernoulli(probs: 0.25, logits: -1.0986123085021973),
  'is observed': False.
  'log prob': tensor(-0.2877)}.
 'b_2': {'value': tensor(1.),
  'distribution': Bernoulli(probs: 0.25, logits: -1.0986123085021973),
  'is_observed': False,
  'log_prob': tensor(-1.3863)},
 'y': {'value': tensor(3),
  'distribution': Normal(loc: 2.0, scale: 1.0),
  'is observed': True,
  'log prob': tensor(-1.4189)}}
```

Rejection Sampling

Coin model:

```
p \sim \text{Uniform}(0,1)
x_i \sim \text{Bernoulli}(p)
```

```
def rejection_sampling(xs_observed):
    while True:
        # generate samples from joint
        p = dist.Uniform(0,1).sample()
        xs = dist.Bernoulli(p).sample(xs_observed.shape)
        if (xs == xs_observed).all():
            return p # accept
        # reject
```

Rejected 50.54% of iterations for 1 number of observations. Rejected 83.78% of iterations for 2 number of observations. Rejected 91.76% of iterations for 3 number of observations. Rejected 96.68% of iterations for 4 number of observations. Rejected 98.26% of iterations for 5 number of observations.

Likelihood Weighting (Importance Sampling)

Problem: We want to compute statistic $r(\Theta)$ for the posterior $P(\Theta|X)$, but we cannot sample from it or evaluate the density directly.

Solution: Sample from a reference distribution Q.

$$\mathbb{E}_{\Theta \sim P(.|X)}[r(\Theta)]$$

Posterior mean: $r(\Theta) = \Theta$, probability that $\Theta > 0$: $r(\Theta) = \delta_{\Theta > 0}$.

Importance Sampling

$$\mathbb{E}_{\Theta \sim P(.|X)}[r(\Theta)] = \int r(\theta) p_{\Theta|X}(\theta|X) d\theta$$

$$= \int r(\theta) \frac{p_{\Theta|X}(\theta|X)}{p_{Q}(\theta)} p_{Q}(\theta) d\theta$$

$$= \mathbb{E}_{\Theta \sim Q} \left[r(\Theta) \frac{p_{\Theta|X}(\Theta|X)}{p_{Q}(\Theta)} \right]$$

We can use samples θ_i from Q in Monte Carlo simulation:

$$\mathbb{E}_{X \sim Q} \left[r(\Theta) \frac{p_{\Theta|X}(\Theta|X)}{p_{Q}(\Theta)} \right] \approx \frac{1}{N} \sum_{i=1}^{N} r(\theta_{i}) \frac{p_{\Theta|X}(\theta_{i}|X)}{p_{Q}(\theta_{i})}$$

But we cannot compute $p_{\Theta|X}(\theta_i|X)$!?

But we cannot compute $p_{\Theta|X}(\theta_i|X)$!?

$$\frac{p_{\Theta|X}(\theta_i|X)}{p_Q(\theta_i)} = \frac{p_{\Theta,X}(\theta_i,X)}{p_X(X)p_Q(\theta_i)}$$
$$= \frac{1}{p_X(X)} \underbrace{\frac{p_{\Theta,X}(\theta_i,X)}{p_Q(\theta_i)}}_{W_{i:=}}$$

But we cannot compute $p_X(X)$!?

But we cannot compute $p_X(X)$!?

Set $r(\Theta) = 1$

$$1 = \mathbb{E}_{X \sim P(.|X)} [r(\Theta)] = \mathbb{E}_{\Theta \sim Q} \left[\frac{p_{\Theta|X}(\Theta|X)}{p_{Q}(\Theta)} \right]$$
$$= \frac{1}{p_{X}(X)} \mathbb{E}_{\Theta \sim Q} \left[\frac{p_{\Theta,X}(\Theta,X)}{p_{Q}(\Theta)} \right] \approx \frac{1}{p_{X}(X)} \frac{1}{N} \sum_{i=1}^{N} W_{i}$$

Thus,

$$p_X(X) \approx \frac{1}{N} \sum_{i=1}^{N} W_i$$

Putting it all together: $W_i = \frac{p_{\Theta,X}(\theta_i,X)}{p_{Q}(\theta_i)}$

$$\begin{split} \mathbb{E}_{\Theta \sim P(.|X)}\left[r(\Theta)\right] &= \mathbb{E}_{\Theta \sim Q}\left[r(\Theta)\frac{p_{\Theta|X}(\Theta|X)}{p_{Q}(\Theta)}\right] \\ &\approx \frac{1}{N}\sum_{i=1}^{N}\frac{p_{\Theta,X}(\theta_{i},X)}{p_{X}(X)p_{Q}(\theta_{i})} \cdot r(\theta_{i}) \\ &= \frac{1}{N}\sum_{i=1}^{N}\frac{W_{i}}{p_{X}(X)}r(\theta_{i}) \\ &\approx \frac{1}{N}\sum_{i=1}^{N}\frac{W_{i}}{\sum_{k=1}^{N}W_{k}}r(\theta_{i}), \quad \theta_{i} \sim Q \end{split}$$

Q has to satisfy: $p_Q(\theta) = 0 \implies p_{\Theta,X}(\theta,X) = 0$.

Likelihood Weighting is a special case of importance sampling where the reference distribution is the prior $Q = P_{\Theta}$.

The weights reduce to the likelihood

$$W_i = \frac{p_{\Theta,X}(\theta_i,X)}{p_{Q}(\theta_i)} = \frac{p_{\Theta,X}(\theta_i,X)}{p_{\Theta}(\theta_i)} = p_{X|\Theta}(X|\theta_i)$$

Coin model

```
def prior(p):
    return dist.Uniform(0,1, validate_args=False).log_prob(p).exp()

def likelihood(xs,p):
    lp = torch.tensor(0.)
    for x in xs:
        lp += dist.Bernoulli(p, validate_args=False).log_prob(x)
    return lp.exp()

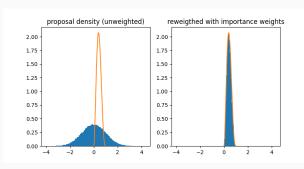
def joint(xs, p):
    return prior(p) * likelihood(xs, p)

xs = torch.tensor([0.,1.,1.,0.,0.])
```

```
proposal = dist.Normal(0,1)
proposal_sample = proposal.sample((N,))

weights = (
    torch.hstack([joint(xs, proposal_sample[i]) for i in range(N)]) /
    proposal.log_prob(proposal_sample).exp()
) # importance sampling

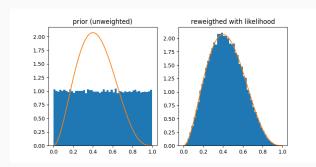
axs[0].hist(proposal_sample, density=True, bins=100)
axs[1].hist(proposal_sample, density=True, bins=100, weights=weights)
```



```
proposal = dist.Uniform(0,1) # prior
proposal_sample = proposal.sample((N,))

weights = torch.hstack([likelihood(xs, proposal_sample[i]) for i in range(N)])
# likelihood weighting

axs[0].hist(proposal_sample, density=True, bins=100)
axs[1].hist(proposal_sample, density=True, bins=100, weights=weights)
```



In our PPL, the coin model can be specified much more compactly.

```
def coin_model(xs):
    p = sample("p", dist.Uniform(0,1))
    for i in range(len(xs)):
        sample(f"x[{i}]", dist.Bernoulli(p), observed=xs[i])
```

In assignment 2, we will write a sample context to make likelihood weighting work automatically with any model.

Resources

Bayesian Inference Framework https://www.youtube.com/watch?v=0w 4QcvBYII Intuition behind Bayesian inference https://www.youtube.com/watch?v=yvWlpwnT1nw Bayesian posterior sampling https://www.youtube.com/watch?v=EHqU9LE9tg8 Generative Models http://probmods.org/chapters/generative-models.html AI That Understands the World, Using Probabilistic Programming https://www.voutube.com/watch?v=8j2S7BRRWus A Personal Viewpoint on Probabilistic Programming https://www.youtube.com/watch?v=TFXcVlKgPlM