Probabilistic Programming

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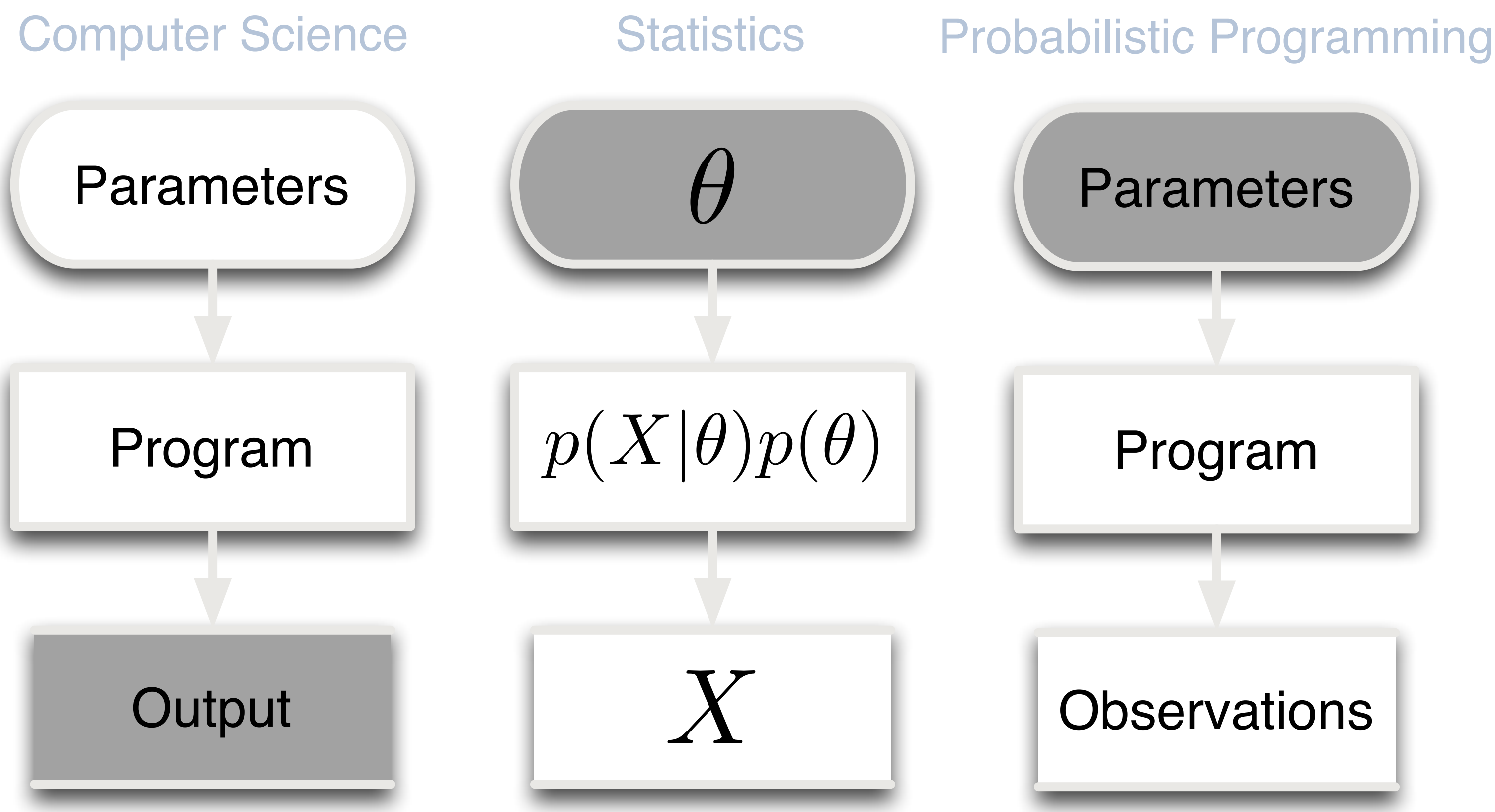
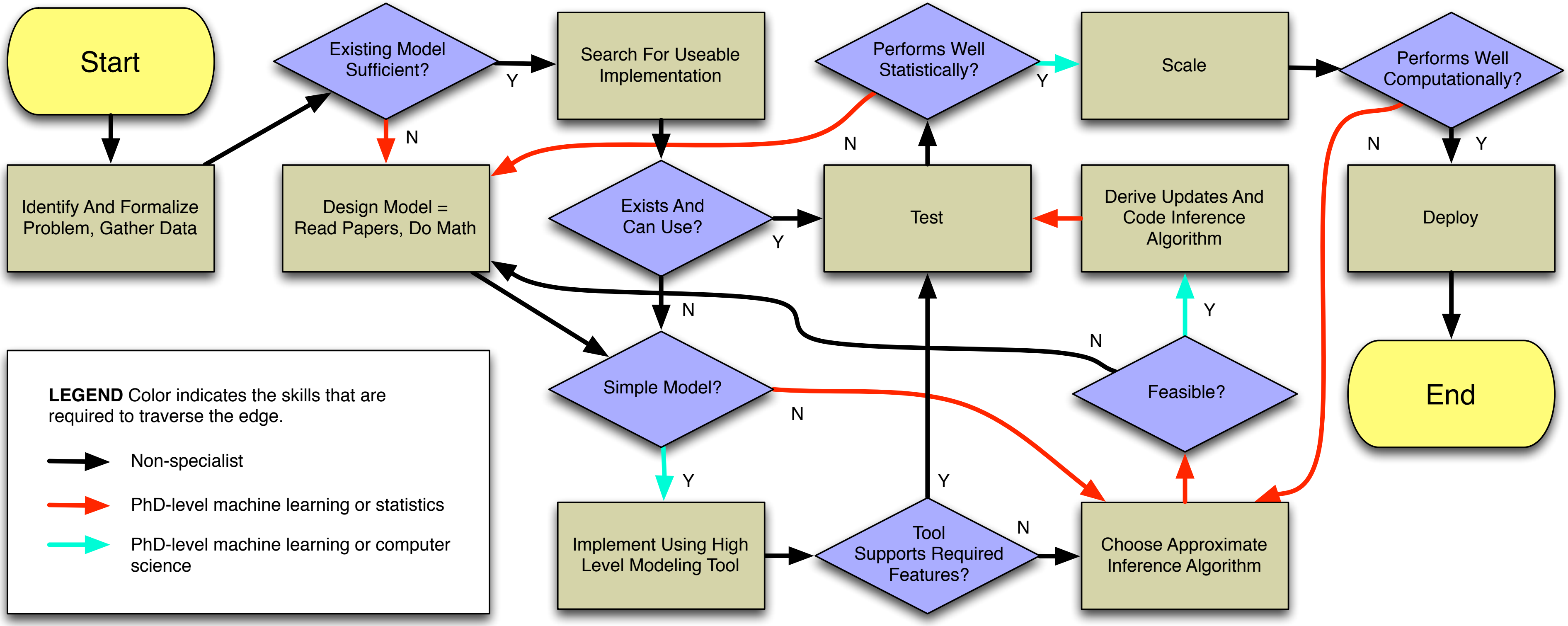
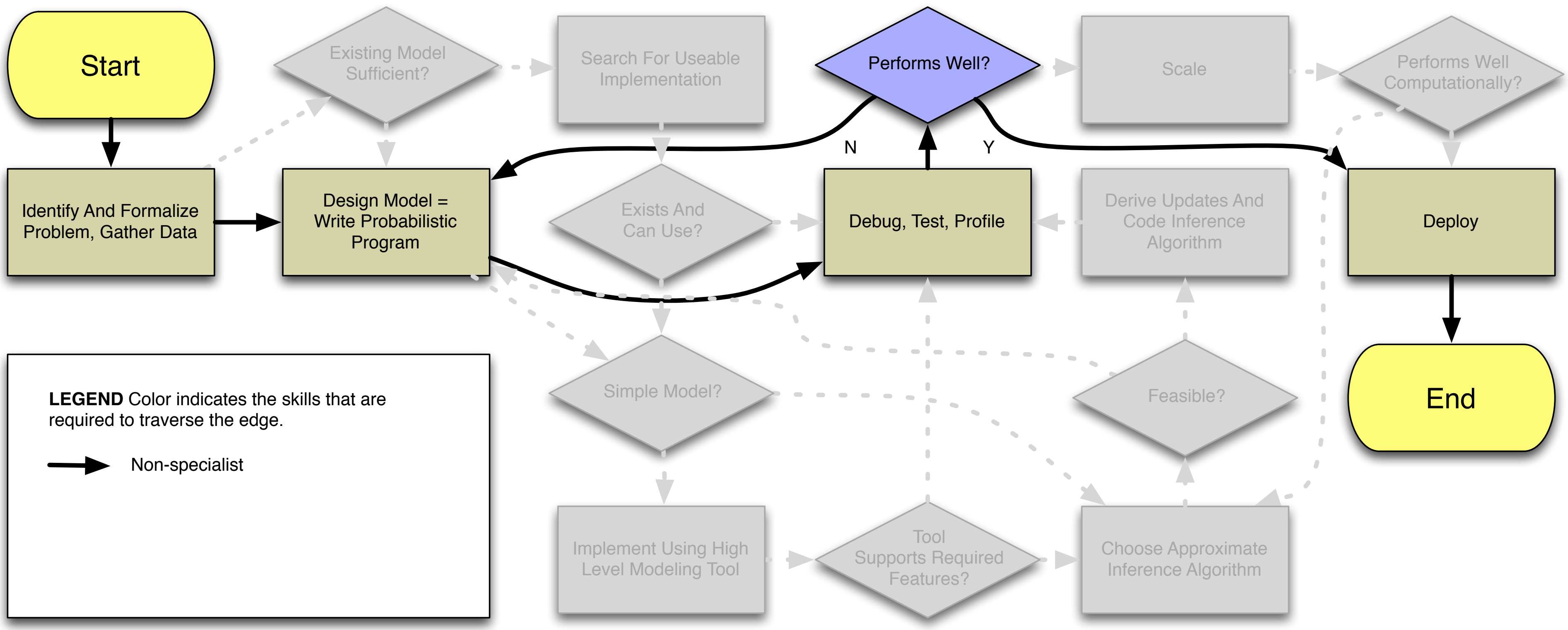
What Is It?


Computer Science
Parameters
Program
Output
Statistics
θ
$p(X|\theta)p(\theta)$
X
Probabilistic Programming
Parameters
Program
Observations

The Way Machine Learning Is

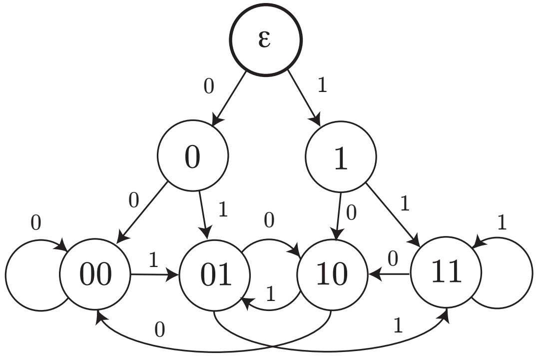


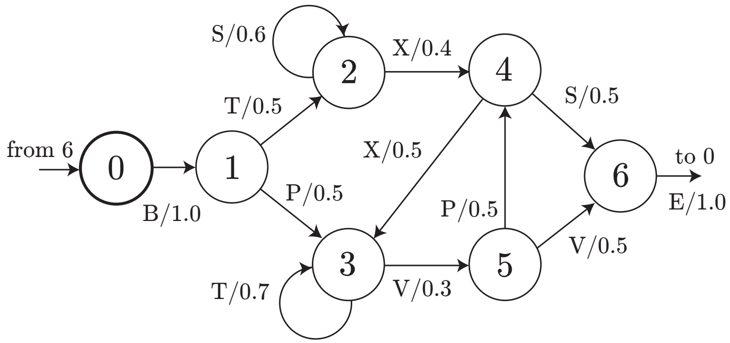
The Way Machine Learning Will Be



Larger Goal: Expressive Compact Models (AI)

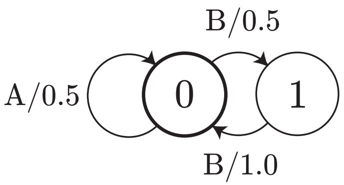
Probabilistic Deterministic Finite Automata



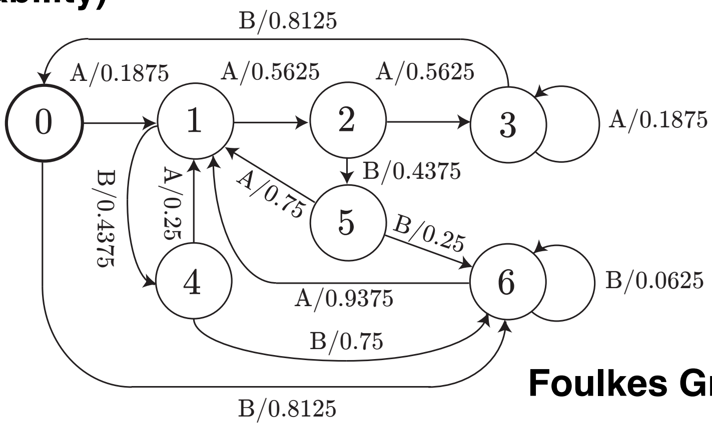


Reber Grammar

Trigram as DFA (without probability)



Even Process



Foulkes Grammar

(Streaming) Sequence Memoizer

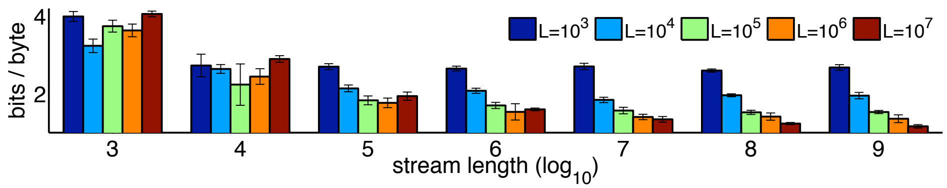
Model

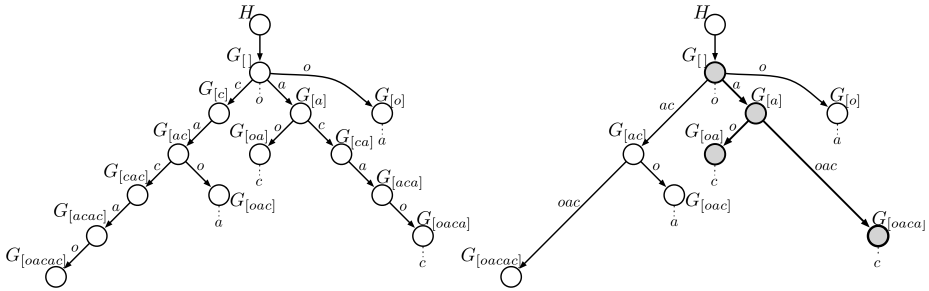
- World state = (infinite) history of emissions
- Per-state emissions *learned*
  - Requires careful smoothing
- Deterministic transitions *fixed*

Problem

- ~2500 lines of Java code
- New student re-implementation
  - 6-12 months
- High-arity state space brings out statistical inefficiencies

- Wikipedia next-byte predictive performance in range of Shannon's human-estimate of the entropy of written English





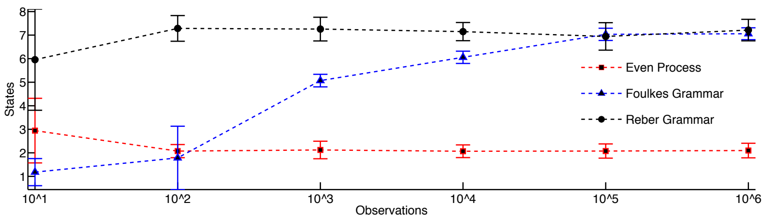
Wood, Archambeau, Gasthaus, James, and Teh A Stochastic Memoizer for Sequence Data, ICML 2009
Bartlett and Wood Deplump for Streaming Data, DCC 2011

Probabilistic Deterministic Infinite Automata

Model

- World state ≈ sufficient statistic of emissions
- Per-state emissions *learned*
- Per-state deterministic transition functions *learned*

- Unsupervised PDFA structure learning biases towards compact (few states) world models that are fast approximate predictors



Problem

- ~4000 lines of Java code
- New student re-implementation
  - 6-12 months

A Prior over PDFA with a bounded number of states

$$\delta$$

$$\begin{array}{c} \\ q_0 \\ q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \\ \vdots \end{array} \begin{array}{c} \begin{array}{ccc} \sigma_0 & \sigma_1 & \sigma_2 \end{array} \\ \left[\begin{array}{ccc} q_3 & q_1 & q_{12} \\ \bullet & q_3 & \bullet \\ q_6 & q_4 & \bullet \\ q_3 & \bullet & q_5 \\ q_3 & q_{42} & q_5 \\ \bullet & q_1 & q_2 \\ \vdots & \vdots & \vdots \end{array}\right] \end{array}$$

$$\pi$$

$$\begin{array}{c} \\ q_0 \\ q_1 \\ \vdots \end{array} \begin{array}{c} \begin{array}{ccc} \sigma_0 & \sigma_1 & \sigma_2 \end{array} \\ \left[\begin{array}{c} \text{(iid probability vector)} \\ \text{(iid probability vector)} \\ \vdots \quad \vdots \quad \vdots \end{array}\right] \end{array}$$

$$\frac{q_0\ q_1\ q_3\ q_3\ q_3\ q_5\ q_2\ q_4\ q_5\ q_2 \ldots}{1\ \ 1\ \ 0\ \ 0\ \ 2\ \ 2\ \ 1\ \ 2\ \ 1\ \ 0 \ldots}$$

$\mu \sim \mathrm{Dir}(\alpha_0/|Q|)$

$\phi_j \sim \mathrm{Dir}(\alpha\mu) \qquad j = 0, \ldots, |\Sigma| - 1$

$\delta(q_i, \sigma_j) = \delta_{ij} \sim \phi_j \qquad i = 0, \ldots, |Q| - 1$

$\pi_{q_i} \sim \mathrm{Dir}(\beta/|\Sigma|) \qquad i = 0, \ldots, |Q| - 1$

$\xi_0 = q_0,\ \xi_t = \delta(\xi_{t-1}, x_{t-1})$

$x_t \sim \pi_{\xi_t}$

Notation:

Q - finite set of states

Σ - finite alphabet

$\delta : Q \times \Sigma \longrightarrow Q$ - transition function

$\pi : Q \times \Sigma \longrightarrow [0, 1]$ - emission distribution

$q_0 \in Q$ - initial state

$x_t \in \Sigma$ - data at time t

$\xi_t \in Q$ - state at time t

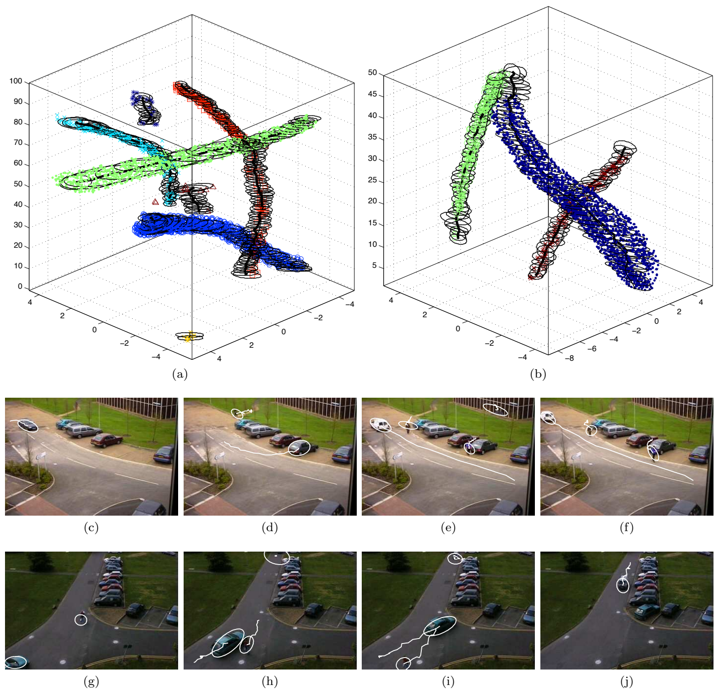
α, α_0, β - hyperparameters

Pfau, Bartlett, and Wood Probabilistic Deterministic Infinite Automata, NIPS, 2011
Doshi-Velez, Pfau, Wood, and Roy Bayesian Nonparametric Methods for Partially-Observable Reinforcement Learning, TPAMI, 2013

Mixture of Objects Markov Model

Model

- World state ≈ infinite mixture of objects
- Per-state, per-object emissions *learned*
- Per-state, per-object *complex* transition functions *learned*



Problem

- ~5000 lines of Matlab code
- Implementation
  - ~ 1 year
- Generative model
  - ~1 *page* latex math
- Inference algorithm
  - ~3 *pages* latex math

Neiswanger, Wood, and Xing The Dependent Dirichlet Process Mixture of Objects for Detection-free Tracking and Object Modeling, AISTATS, 2014

Motivation, Proposal, Honesty

- Existing tools for modeling are cumbersome
  - Akin to writing code in assembly language
  - Model specification and forward sampling “easy”
  - Inference hard

- Probabilistic programming systems
  - Efficient model development and testing
  - Decoupling of modeling and inference
  - More compact notation
  - Bigger more expressive models
  - Automated inference

- Problem
  - Existing probabilistic programming systems not quite there yet

Probabilistic Programming

- Inverse Computing
- Automated Inference For Generative Modeling
- Stochastic Black-box Simulator Inversion

- "Probabilistic programs are usual functional or imperative programs with two added constructs: (1) the ability to draw values at random from distributions, and (2) the ability to condition values of variables in a program via observations. Models from diverse application areas such as computer vision, coding theory, cryptographic protocols, biology and reliability analysis can be written as probabilistic programs."

Gordon et al, "Probabilistic Programming", ICSE 2014

Teaching and Research Language

Anglican

A “Church” of England “Venture”

http://www.robots.ox.ac.uk/~fwood/anglican/

Please report bugs to

https://bitbucket.org/fwood/anglican/issues

van de Meent

Perov

Wood, van de Meent, Mansinghka “A New Approach to Probabilistic Programming Inference” AISTATS 2014

Modeling Language Syntax

Outer Directives

```
[assume symbol expr]
[observe expr value]
[predict expr]
```

Inner Expressions - Scheme/Lisp/Clojure

- Functional except stochastic procedures
- Pure (no side-effects) except mem
- Higher order

Ugh, Why Lisp?

- Redefinition prohibited ("pure functional")

```
[assume (a (normal 5 10))]
[assume (b (normal a 2 ))]
[assume (a (normal b 7 ))]
=> Error
```

- Imperative languages (i.e. Probabilistic-C) allow (!?!!)

```
int a = normal(5,10);
int b = normal(a,2 );
int a = normal(b,7 );
```

Anglican Stochastic Procedures

(flip p) sample a single binomial trial. Returns true with probability p and false with probability 1-p.

(gamma a b) samples from a Gamma distribution with shape a and rate b. Returns a double on the domain (0, Inf).

(invgamma a b) samples from an inverse Gamma distribution with shape a and rate b. Returns a double on the domain (0, Inf).

(normal m s) samples from a univariate normal distribution with mean m and stdev s. Returns a double on the domain (-Inf, Inf)

Higher Order

```
(lambda (& symbols) body) => compound procedure
(lambda symbol body) => compound procedure

Constructs a compound procedure.

Example

    ((lambda (n m)
             (* (+ n 1) m))
        1 2)

    => 4
```

Memoization

```
(mem proc)

    Constructs a memoized procedure instance from an
    expression proc that must evaluate to a procedure. If a
    memoized procedure call is made with a previously used
    set of arguments, a cached value is returned instead of
    re-doing computation. This is typically used both to get
    dynamic programming for free and to incrementally
    construct complex datastructures.
```

Example

```
[assume H (mem (lambda (k) (list (normal 3 4) (gamma 1 1))))]
[assume theta_1 (H 1)]
[assume theta_2 (H 2)]
[assume theta_3 (H 1)]
[predict (= theta_1 theta_3 )] => always true
```

http://www.robots.ox.ac.uk/~fwood/anglican/language/

Complex Control Flow

```
(if bool-expr cons-expr alt-expr)

Example

    (if (= 1 (poisson 2))
            "the predicate is true"
            (normal 18 (/ 45 3.98)))

    => "the predicate is true" w.p. 0.2707
```

Birthday Coincidence

Approximately, what's the probability that in a room filled with 23 people at least one pair of people have the same birthday?

Solution

```
[assume birthday (mem (lambda (i) (uniform-discrete 1 366)))]
[assume N 23]
[assume pair-equal
  (lambda (i j)
    (if (> i N)
      false
      (if (> j N)
        (pair-equal (+ i 1) (+ i 2))
        (if (= (birthday i) (birthday j))
          true
          (pair-equal i (+ j 1))))))]
[predict (pair-equal 1 2)]
```

Invoking Anglican

```
anglican  -s *yoursourcefile*
```

- or –

```
cat *yoursourcefile* | anglican
```

Some command line switches

```
Switches                                                Default   Desc
--------                                                -------   ----
-h, --no-help, --help                                   false     Show help
-s, --source-file                                       *in*      Anglican source file to interpret
-p, --predict-file                                      *out*     File into which to print predicts
-n, --num-samples                                       Infinity  Number of samples
```

Anglican Semantics Lite

- Applying a (random) procedure generates a sample.

- Running an Anglican program yields a stream of predict expression samples generated from a sequence of program execution paths sampled via a Markov chain Monte Carlo exploration of the space of execution paths.

Inference

$$\mu \sim N(1, 5)$$
$$y_i|\mu \sim N(\mu, 2)$$

$$y_1 = 9$$
$$y_2 = 8$$

$$\mu|y_{1:2} \sim N(7.25, 0.8333)$$

Solution

```
[assume sigma (sqrt 2)]
[assume mu (normal 1 (sqrt 5))]
[observe (normal mu sigma) 9]
[observe (normal mu sigma) 8]
[predict mu]
```

Addition

What numbers added together equal seven?

Solution

```
[assume a (- (poisson 100) 100)]
[assume b (- (poisson 100) 100)]
[observe (normal (+ a b) .00001) 7]
[predict (list a b)]
```

Anglican Semantics

- Running an Anglican program yields a stream of predict expression samples generated from a dependent sequence of program execution paths sampled via a Markov chain Monte Carlo exploration of the posterior of execution paths conditioned on observed data.

- Test function averages converge in the usual sense.

Leaving The Beaten Path

$$\mu \sim \text{Poisson}(1)$$

$$y_i|\mu \sim N(\mu, 2)$$

$$y_1 = 9$$

$$y_2 = 8$$

$$\mu|y_{1:2} \sim ?$$

Solution

```
[assume sigma (sqrt 2)]
[assume mu (poisson 1)]
[observe (normal mu sigma) 9]
[observe (normal mu sigma) 8]
[predict mu]
```

Multivariate Logistic Regression

$$\sigma^2 \sim \mathrm{Gamma}(1, 1)$$

$$\beta_j \sim \mathrm{Normal}(0, \sigma^2)$$

$$p(z_i = 1) = \frac{1}{1 + e^{-\beta^T x}}$$

Solution

```
[assume dot-product (lambda (u v)
  (if (= (count u) 0)
     0
     (+ (* (first u) (first v))
        (dot-product (rest u) (rest v)))))]
[assume sigma (sqrt (gamma 1 1))]
[assume beta (list (normal 0 sigma) (normal 0 sigma) (normal 0 sigma) (normal 0 sigma)
(normal 0 sigma))]
[assume z (lambda (x)
  (/ 1 (+ 1 (exp (* -1 (dot-product beta x))))))]
[observe-csv
   "http://www.robots.ox.ac.uk/~fwood/anglican/examples/logistic_regression/iris.csv"
   (flip (z (list 1 $1 $2 $3 $4))) (= $5 "Iris-setosa")]
[predict beta]
; should be Iris-setosa,    i.e. 1 (from training data)
[predict (z (list 1 5.1 3.5 1.4 0.2 ))]
; should be Iris-virginica, i.e. 0 (from training data)
[predict (z (list 1 7.7 2.6 6.9 2.3 ))]
```

Hidden Markov Model

```
[assume initial-state-dist (list (/ 1 3) (/ 1 3) (/ 1 3))]
[assume get-state-transition-dist
    (lambda (s) (cond ((= s 0) (list .1  .5  .4))
                      ((= s 1) (list .2  .2  .6))
                      ((= s 2) (list .15 .15 .7))))]
[assume transition (lambda (prev-state)
     (discrete (get-state-transition-dist prev-state)))]
[assume get-state (mem (lambda (index)
     (if (<= index 0) (discrete initial-state-dist)
                      (transition (get-state (- index 1)))))))]
[assume get-state-observation-mean
     (lambda (s) (cond ((= s 0) -1)
                       ((= s 1)  1)
                       ((= s 2)  0)))]
[observe (normal (get-state-obs-mean (get-state 1 )) 1) .9]
[observe (normal (get-state-obs-mean (get-state 2 )) 1) .8]
…
[observe (normal (get-state-obs-mean (get-state 16)) 1) -1]
[predict (get-state 0)]
[predict (get-state 1)]
…
[predict (get-state 16)]
```

Bayesian Nonparametrics

- One way : lazy stick sampling

```
; sample-stick-index is a procedure that samples an index from
; a potentially infinite dimensional discrete distribution
; lazily constructed using a stick breaking rule

[assume sample-stick-index (lambda (breaking-rule index)
      (if (flip (breaking-rule index))
           index
          (sample-stick-index breaking-rule (+ index 1))))]
```

Sethuraman Stick Breaking

```
; sethuraman-stick-picking-procedure returns a procedure
; that picks a stick each time its called from the set of sticks
; lazily constructed via a closed-over one-parameter stick
; breaking rule

[assume make-sethuraman-stick-picking-procedure
   (lambda (concentration)
       (begin (define V
                 (mem (lambda (x) (beta 1.0 concentration))))
       (lambda () (sample-stick-index V 1))))]
```

DPMem

```
; DPmem is a procedure that takes two arguments -- the concentration
; to a Dirichlet process and a base sampling procedure
; DPmem returns a procedure

[assume DPmem (lambda (concentration base)
   (begin
      (define get-value-from-cache-or-sample
         (mem (lambda (args stick-index)
             (apply base args))))
       (define get-stick-picking-procedure-from-cache
         (mem (lambda (args)
             (make-sethuraman-stick-picking-procedure concentration))))
   (lambda varargs
       ; when the returned function is called , the first thing
       ; it does is get the cached stick breaking
       ; procedure for the passed in arguments
       ; and _calls_ it to get an index
       (begin
          (define index ((get-stick-picking-procedure-from-cache varargs)))
          ; if , for the given set of arguments and
          ; just sampled index a return value has already
          ; been computed , get it from the cache
          ; and return it , otherwise sample a new value
       (get-value-from-cache-or-sample varargs index))))))]
```

Dirichlet Process Mixture

```
[assume H (lambda ()
     (begin
       (define v (/ 1.0 (gamma 1 10)))
       (list (normal 0 (sqrt (* 10 v))) (sqrt v))))]
[assume gaussian-mixture-model-parameters (DPmem 1.72 H)]
[observe-csv "http:// ... "
     (apply normal (gaussian-mixture-model-parameters)) $2]
[predict (apply normal (gaussian-mixture-model-parameters))]
```

Example:

```
curl -s http://www.robots.ox.ac.uk/~fwood/anglican/examples/
dp_mixture_model/dp-church.anglican | anglican | grep 'normal' |
awk -F',' '{print $2}' | feedgnuplot --stream --histogram 0 --with
boxes  --xlabel 'x' --ylabel Frequency --binwidth 1
```

Expressivity

- Easily implement modern machine learning methods
  - 10’s of lines of code
- Higher-order functionality

Symbolic Function Induction

What's the next value? And the function?

Input	Output
1	5
2	3
3	1
4	?

Solution

```
[assume get-int-constant
  (lambda () (uniform-discrete 0 10))]

[assume safe-div
  (lambda (x y) (if (= y 0) 0 (/ x y)))]

[assume pcfg
  (lambda ()
    (define expression-type (discrete (list 0.40 0.30 0.30)))
      (cond
        ((= expression-type 0) (get-int-constant))
        ((= expression-type 1) 'x)
        (else
          (list
            (nth (list (quote +) (quote -) (quote *) (quote safe-div))
                 (discrete (list 0.25 0.25 0.25 0.25)))
              (pcfg) (pcfg)))))]

[assume induced-procedure-code (list 'lambda (list 'x) (pcfg))]
[assume induced-procedure (eval induced-procedure-code)]

[assume noise 0.00001]
[observe (normal (induced-procedure 1) noise) 5]
[observe (normal (induced-procedure 2) noise) 3]
[observe (normal (induced-procedure 3) noise) 1]

[predict induced-procedure-code]
[predict (induced-procedure 4)]
```

Goals and Aims

(i) Accelerate iteration over models

- Inference is automatic
- Writing generative code is easier than deriving model inverses
- Lower technical barrier of entry to development of new models

(ii) Accelerate iteration over inference procedures

- Computer language is an abstraction barrier
  - Inference procedures can be tested against a library of models
  - Inference procedures become “compiler optimizations”

(iii) Enable development of more expressive models

- Probabilistic programs can express a superset of graphical models
- Modern machine learning models are tens of lines of code

How Does it Work?

Probabilistic Programming Concepts

- First half
  - Procedures “sample”
  - Programs are generative models

- This half
  - “Sampling” execution traces = inference

  - Different traces arise from stochastic procedure outputs
    - Elementary

```
flip, normal, discrete, poisson, gamma, …
```

    - Compound

```
(lambda (a b) (if (flip a)
                  (+ (poisson b) 7)
                  (normal a b)))
```

  - Various sampling algorithms apply
    - Rejection sampling
    - Metropolis Hastings
    - Sequential Monte Carlo
    - Particle Markov Chain Monte Carlo

Outline

- Trace Probability
- Probabilistic Program Interpretation
- Monte Carlo-based probabilistic inference
  - Rejection Sampling
  - MCMC
  - SMC
  - PMCMC

Probabilistic Inference

Inference, prediction, and inspection can all be expressed as expectations

$$\mathbb{E}[f] \equiv \int f(\mathbf{x})p(\mathbf{x})d\mathbf{x}$$

Where $\mathbf{x}$ is *all* latent variables, f is a test function, and p is the distribution against which we're integrating.

Monte Carlo Integration

Recipe

1. Sample $\mathbf{x}^{(\ell)} \sim p(\mathbf{x})$ for $\ell = 1 \dots L$
2. Estimate $\mathbb{E}[f] \approx \hat{f} = \frac{1}{L} \sum_{\ell=1}^{L} f(\mathbf{x}^{(\ell)})$

How To Sample Execution Traces

- What is an execution trace?
- What is its probability?

Execution Trace Probability

Observed value

Parameter of observation distribution

Posterior Distribution of Trace Given Observations

$$p(\mathbf{x}_{1:N}|\mathbf{y}_{1:N}) \propto \tilde{p}(\mathbf{y}_{1:N}, \mathbf{x}_{1:N}) \equiv \prod_{n=1}^{N} g(y_n|\theta_{t_n}, \mathbf{x}_{1:n}) f(\mathbf{x}_n|\mathbf{x}_{1:n-1})$$

Joint Distribution of Trace And Observations

Type of observation distribution

Interpreter memory state

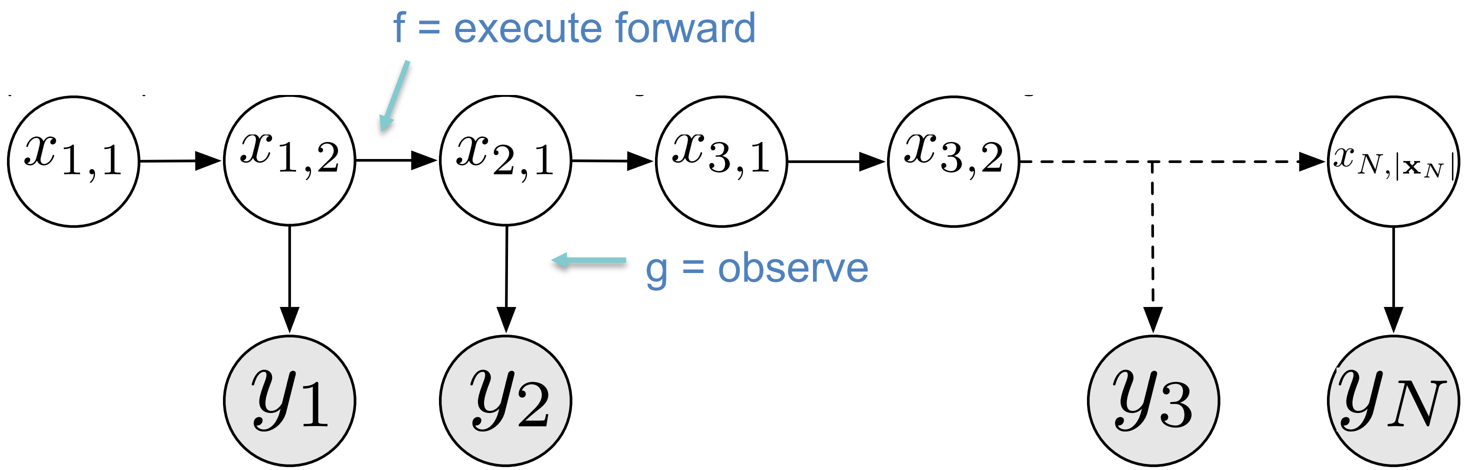
Parameter of stochastic procedure

$$f(\mathbf{x}_n|\mathbf{x}_{1:n-1}) = \prod_{k=1}^{|\mathbf{x}_n|} f(x_{n,k}|\theta_{t_{n,k}}, x_{n,1:(k-1)}, \mathbf{x}_{1:(n-1)})$$

Type of stochastic procedure

Suggests Relationship To State Space Modeling

- Program generates all random variables



- State is interpreter memory state
- Transition is stochastic procedure application
- Only observes need be indexed

Program Interpretation

eval

```
(define (eval exp env)
 (cond
   ((self-evaluating? exp) exp)
   ((variable? exp) (lookup-variable-value exp env))
   ((quoted? exp) (text-of-quotation exp))
   ((assignment? exp) (eval-assignment exp env))
   ((definition? exp) (eval-definition exp env))
   ((if? exp) (eval-if exp env))
   ((lambda? exp)
     (make-procedure (lambda-parameters exp)
                     (lambda-body exp) env))
   ((begin? exp)
     (eval-sequence (begin-actions exp) env))
   ((cond? exp) (eval (cond->if exp) env))
   ((application? exp)
     (apply (eval (operator exp) env)
            (list-of-values (operands exp) env)))
   (else
     (error
      "Unknown expression type -- EVAL" exp))))
```

apply

```
(define (apply procedure arguments)
 (cond
  ((primitive-procedure? procedure)
    (apply-primitive-procedure procedure arguments))
  ((compound-procedure? procedure)
   (eval-sequence
     (procedure-body procedure)
     (extend-environment
       (procedure-parameters procedure)
       arguments
       (procedure-environment procedure)
     )
    )
   )
 (else
  (error
    "Unknown procedure type – APPLY" procedure))))
```

Copied from **Abelson, Sussman and Sussman** “Structure and Interpretation of Computer Programs”

What is $\mathbf{x}_1$?

$$
\begin{aligned}
x_{1,1} &\sim \text{Beta}(7,4) \\
x_{1,2}|x_{1,1}=0.4 &\sim \text{Poisson}(8) \\
x_{1,3}|x_{1,2}=6, x_{1,1}=0.4 &\sim \text{Binomial}(0.4) \\
x_{1,4}|x_{1,3}=\text{true}, x_{1,2}=6, x_{1,1}=0.4 &\sim \text{Poisson}(7) \\
y_1=18|x_{1,4}=7, x_{1,3}=\text{true}, x_{1,2}=6, x_{1,1}=0.4 &\sim \text{Normal}(14,1) \\
x_{2,1}|\ldots &\sim \text{Gamma}(0.4,7) \\
y_2=6|x_{2,1}=6.92,\ldots &\sim \text{Normal}(0,6.92)
\end{aligned}
$$

```
[assume poi-1 (beta 7 4)]
[assume poi-2 (+ 1 (poisson 8))]
[assume generative-model-part-1 (lambda (a b)
                                  (if (flip a)
                                      (+ (poisson b) 7)
                                      (normal a b)))]
[assume generative-model-part-2 (lambda () (gamma poi-1 poi-2))]
[observe (normal (generative-model-part-1 poi-1 poi-2) 1) 18]
[observe (normal 0 (generative-model-part-2)) 6]
[predict (list poi-1 poi-2)]
```

What is $\mathbf{x}_{1:2}$?

[redacted]

$$
\begin{aligned}
x_{2,1} | \ldots &\sim \text{Gamma}(0.4, 7) \\
y_2 = 6 | x_{2,1} = 6.92, \ldots &\sim \text{Normal}(0, 6.92)
\end{aligned}
$$

```
[assume poi-1 (beta 7 4)]
[assume poi-2 (+ 1 (poisson 8))]
[assume generative-model-part-1 (lambda (a b)
                                  (if (flip a)
                                      (+ (poisson b) 7)
                                      (normal a b)))]
[assume generative-model-part-2 (lambda () (gamma poi-1 poi-2))]
[observe (normal (generative-model-part-1 poi-1 poi-2) 1) 18]
[observe (normal 0 (generative-model-part-2)) 6]
[predict (list poi-1 poi-2)]
```

Observe Statements

$$f(y_n|\theta_{t_n}, \mathbf{x}_{1:n})$$

```
[observe (normal (generative-model-part-1 poi-1 poi-2) 1) 18]
```

Original Church : Rejection Sampling

- Run program forward and condition on all observations exactly matching the observed output

```
(define (rejection-query thunk condition)
  (let ((val (thunk)))
    (if (condition val)
        val
        (rejection-query thunk condition))))
```

Goodman, Mansinghka, Roy, Bonawitz, and. Tenenbaum Church: A language for generative models, UAI, 2008

Review: Rejection Sampling

Assume

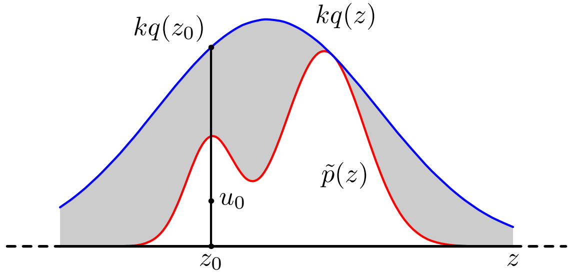
- Want sample from $p(\mathbf{x})$
- $p(\mathbf{x})$ is easy to evaluate, but only up to an unknown normalising constant, i.e.

$$p(\mathbf{x}) = \frac{1}{Z_p}\tilde{p}(\mathbf{x})$$

- A *proposal distribution* $q(\mathbf{x})$ s.t. $kq(\mathbf{x}) \geq \tilde{p}(\mathbf{x})$ for all $\mathbf{x}$ can be designed

Note $\mathbf{x}$ is, in general, a vector of random variables.

Rejection Sampling



Sampling $\mathbf{x}^{(\tau)} \sim q$ and $u^{(\tau)} \sim \mathrm{Uniform}(0, kq(\mathbf{x}^{(\tau)}))$ yields a pair of values uniformly distributed in the gray region.

If $u_0 \leq \tilde{p}(\mathbf{x})$ then $\mathbf{x}^{(\tau)}$ is accepted, otherwise it is rejected and the process repeats until a sample is accepted.

Accepted pairs are uniformly distributed in the white area; dropping $u^{(\tau)}$ yields a sample distributed according to $\tilde{p}(\mathbf{x})$, and equivalently, $p(\mathbf{x})$.

Rejection Sampling

Assume we have a model $p(\mathbf{x})$, some variables of which are known, some of which are not. Also let $\mathbf{x}_{\mathrm{obs}}$ be the "observed" variables and $\mathbf{x}_{\mathrm{lat}}$ be latent variables such that $\mathbf{x}_{\mathrm{obs}} \cup \mathbf{x}_{\mathrm{lat}} = \mathbf{x}$.

We would like samples from $p(\mathbf{x}_{\mathrm{lat}}|\mathbf{x}_{\mathrm{obs}}) = \frac{p(\mathbf{x})}{p(\mathbf{x}_{\mathrm{obs}})}$

Equivalently we can write the conditional distribution of interest as an unnormalised distribution $\tilde{p}(\mathbf{x}_{\mathrm{lat}}|\mathbf{x}_{\mathrm{obs}}) = p(\mathbf{x})\mathbb{I}[\mathbf{x}_{\mathrm{obs}} = \mathbf{v}]$ using an indicator function that imposes the constraint that the observed variables are constrained to take values $\mathbf{v}$.

Rejection sampling with $q(\mathbf{x}) = p(\mathbf{x})$ (i.e. proposing via ancestral sampling of the joint) can be used to generate samples distributed according to $\tilde{p}(\mathbf{x}_{\mathrm{lat}}|\mathbf{x}_{\mathrm{obs}})$. Note that $q(\mathbf{x}) \geq \tilde{p}(\mathbf{x}_{\mathrm{lat}}|\mathbf{x}_{\mathrm{obs}})\ \forall \mathbf{x}$ by construction.

Rejection Sampling

Conditioning via Rejection and Ancestral Sampling

1. Sample $\mathbf{x}^{(\tau)} \sim q(\mathbf{x})$ (i.e. generate via ancestral sampling)
2. Sample $u^{(\tau)} \sim \mathrm{U}(0, q(\mathbf{x}))$
3. Accept $\mathbf{x}^{(\tau)}$ only if $u^{(\tau)} \leq p(\mathbf{x})\mathbb{I}[\mathbf{x}_{\mathrm{obs}} = \mathbf{v}]$
4. Repeat

A sample will only ever be accepted when $\mathbf{x}_{\mathrm{obs}} = \mathbf{v}$ and then it will always be because $q(\mathbf{x}) = p(\mathbf{x})$

Unless the prior and posterior are extremely well matched this will be an extremely inefficient sampler.

Original Church : Rejection Sampling

- Run program forward and condition on all observations exactly matching the observed output

```
(define (rejection-query thunk condition)
  (let ((val (thunk)))
    (if (condition val)
        val
        (rejection-query thunk condition))))
```

Goodman, Mansinghka, Roy, Bonawitz, and. Tenenbaum Church: A language for generative models, UAI, 2008

New Church : Single-Site Independent MH

Sample posterior distribution of execution traces using joint with observed values plugged in

$$p(\mathbf{x}|\mathbf{y}) \propto \tilde{p}(\mathbf{y} = \text{observes}, \mathbf{x})$$

Metropolis-Hastings acceptance rule

$$\min\left(1, \frac{p(\mathbf{y}|\mathbf{x}')p(\mathbf{x}')q(\mathbf{x}|\mathbf{x}')}{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})q(\mathbf{x}'|\mathbf{x})}\right)$$

Need

- Proposal

Have

- Likelihoods (via observe statement restrictions)
- Prior (sequence of ERP returns; scored in interpreter)

Wingate, Stuhlmüller et al Lightweight Implementations of Probabilistic Programming Languages Via Transformational Compilation, 2011
Wood, van de Meent, and Mansinghka "A New Approach to Probabilistic Programming Inference" AISTATS 2014
Mansinghka, Selsam, and Perov "Venture: an interactive, Turing-complete probabilistic programming platform" arXiv 2014

Review : Metropolis Hastings

Algorithm

Initialize $\tau \leftarrow 1, \mathbf{x}^{(\tau)} \leftarrow ?$

Repeat Forever Yielding $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots\}$

1. Propose $\mathbf{x}^* \sim q(\mathbf{x}^*|\mathbf{x}^{(\tau)})$
2. Accept $\mathbf{x}^*$ w.p. $A(\mathbf{x}^*, \mathbf{x}^{(\tau)}) = \min\left(1, \frac{p(\mathbf{x}^*)q(\mathbf{x}^{(\tau)}|\mathbf{x}^*)}{p(\mathbf{x}^{(\tau)})q(\mathbf{x}^*|\mathbf{x}^{(\tau)})}\right)$
3. If $\mathbf{x}^*$ accepted set $\mathbf{x}^{(\tau+1)} \leftarrow \mathbf{x}^*$ else $\mathbf{x}^{(\tau+1)} \leftarrow \mathbf{x}^{(\tau)}$
4. Increment τ

Common choices of proposal include $q(\mathbf{x}^*|\mathbf{x}^{(\tau)}) = \mathcal{N}(\mathbf{x}^{(\tau)}|\sigma^2\mathbf{I})$ (random-walk Metropolis) and/or $q(\mathbf{x}^*|\mathbf{x}^{(\tau)}) = q(\mathbf{x}^*)$ (independent MH). Rules of thumb suggest aiming for acceptance rates of between 25% and 50% by tuning the proposal distribution.

Random Database (RDB) MH Proposal

Single stochastic procedure (SP) output

Probability of new part of proposed execution trace

$$q(\mathbf{x}'|\mathbf{x}) = \frac{\kappa(x'_{m,j}|x_{m,j})}{|\mathbf{x}|} \frac{p(\mathbf{x}'\backslash\mathbf{x} \mid \mathbf{x}' \cap \mathbf{x})}{p(x'_{m,j}|\mathbf{x}' \cap \mathbf{x})}$$

Number of SP's in original trace

Probability of new SP return value (sample) given trace prefix

RDB Implementation

Single site update = sample from the prior = run program forward

$$\kappa(x'_{m,j}|x_{m,j}) = p(x'_{m,j}|\mathbf{x}' \cap \mathbf{x})$$

MH acceptance ratio simplifies

Number of SP applications in original trace

Probability of regenerating current trace continuation given proposal trace beginning

$$\frac{p(\mathbf{y}|\mathbf{x}')\, p(\mathbf{x}')\, |\mathbf{x}|\, p(\mathbf{x} \backslash \mathbf{x}' \mid \mathbf{x} \cap \mathbf{x}')}{p(\mathbf{y}|\mathbf{x})\, p(\mathbf{x})\, |\mathbf{x}'|\, p(\mathbf{x}' \backslash \mathbf{x} \mid \mathbf{x}' \cap \mathbf{x})}$$

Number of SP applications in new trace

Probability of generating proposal trace continuation given current trace beginning

RDB Implementation Sketch

$$
\begin{aligned}
x_{1,1} &\sim \mathrm{Beta}(7,4) \\
x_{1,2}|x_{1,1} = 0.4 &\sim \mathrm{Poisson}(8) \\
\boxed{x_{1,3}|x_{1,2} = 6, x_{1,1} = 0.4 \sim \mathrm{Binomial}(0.4)} & \\
x_{1,4}|x_{1,3} = \textcolor{red}{\text{false}}, x_{1,2} = 6, x_{1,1} = 0.4 &\cancel{\sim \mathrm{Poisson}(7)} \\
\cancel{y_1 = 18|x_{1,4} = 7, x_{1,3} = \text{true}, x_{1,2} = 6, x_{1,1} = 0.4} &\cancel{\sim \mathrm{Normal}(14,1)} \\
\cancel{x_{2,1}|\ldots} &\cancel{\sim \mathrm{Gamma}(0.4,7)} \\
\cancel{y_2 = 6|x_{2,1} = 6.92,\ldots} &\cancel{\sim \mathrm{Normal}(0,6.92)}
\end{aligned}
$$

```
[assume poi-1 (beta 7 4)]
[assume poi-2 (+ 1 (poisson 8))]
[assume generative-model-part-1 (lambda (a b)
                                    (if (flip a)
                                        (+ (poisson b) 7)
                                        (normal a b)))]
[assume generative-model-part-2 (lambda () (gamma poi-1 poi-2))]
[observe (normal (generative-model-part-1 poi-1 poi-2) 1) 18]
[observe (normal 0 (generative-model-part-2)) 6]
[predict (list poi-1 poi-2)]
```

SMC for Prob. Prog. Inference

State-space-model-like decomposition

$$p(\mathbf{x}_{1:n}|y_{1:n}) = g(y_n|\mathbf{x}_{1:n})f(\mathbf{x}_n|\mathbf{x}_{1:n-1})p(\mathbf{x}_{1:n-1}|y_{1:n-1})$$

Suggests Sequential Importance Resampling (SIR)

$$\frac{p(\mathbf{x}_{1:n}|y_{1:n})}{q(\mathbf{x}_{1:n}|y_{1:n})} = \frac{g(y_n|\mathbf{x}_{1:n})f(\mathbf{x}_n|\mathbf{x}_{1:n-1})p(\mathbf{x}_{1:n-1}|y_{1:n-1})}{f(\mathbf{x}_n|\mathbf{x}_{1:n-1})p(\mathbf{x}_{1:n-1}|y_{1:n-1})} = g(y_n|\mathbf{x}_{1:n})$$

Proposal

Run program forward
until next observe directive

Weight of particle
Is observation likelihood

Fischer, Kiselyov, and Shan "Purely functional lazy non-deterministic programming" ACM Sigplan 2009
Wood, van de Meent, and Mansinghka "A New Approach to Probabilistic Programming Inference" AISTATS 2014
Paige and Wood "A Compilation Target for Probabilistic Programming Languages" ICML 2014

Review : Sequential Importance Resampling

SIR Targets

$$p(\mathbf{x}_{1:N}|\mathbf{y}_{1:N}) \propto \tilde{p}(\mathbf{y}_{1:N}, \mathbf{x}_{1:N}) \quad \equiv \quad \prod_{n=1}^{N} g(y_n|\mathbf{x}_{1:n}) f(\mathbf{x}_n|\mathbf{x}_{1:n-1})$$

With a weighted set of particles

$$p(\mathbf{x}_{1:N}|y_{1:N}) \approx \sum_{\ell=1}^{L} w_N^\ell \delta_{\mathbf{x}_{1:N}^\ell}(\mathbf{x}_{1:N})$$

Noting the identity

$$p(\mathbf{x}_{1:n}|y_{1:n}) = g(y_n|\mathbf{x}_{1:n}) f(\mathbf{x}_n|\mathbf{x}_{1:n-1}) p(\mathbf{x}_{1:n-1}|y_{1:n-1})$$

We can use importance sampling to generate samples from

$$p(\mathbf{x}_{1:n}|y_{1:n})$$

Given our sample-based approximation to

$$p(\mathbf{x}_{1:n-1}|y_{1:n-1})$$

Review : Importance Sampling

$$
\begin{aligned}
E_{p(\mathbf{x}|\mathbf{y})}[h(\mathbf{x})] &= \int h(\mathbf{x}) p(\mathbf{x}|\mathbf{y}) d\mathbf{x} \\
&= \int h(\mathbf{x}) \frac{p(\mathbf{x}|\mathbf{y})}{q(\mathbf{x}|\mathbf{y})} q(\mathbf{x}|\mathbf{y}) d\mathbf{x} \\
&\approx \frac{1}{L} \sum_{\ell=1}^{L} h(\mathbf{x}^{\ell}) \frac{p(\mathbf{x}^{\ell}|\mathbf{y})}{q(\mathbf{x}^{\ell}|\mathbf{y})} && x^{\ell} \sim q(\mathbf{x}|\mathbf{y}) \\
&= \frac{1}{L} \sum_{\ell=1}^{L} h(\mathbf{x}^{\ell}) w_n^{\ell} && x^{\ell} \sim q(\mathbf{x}|\mathbf{y}), w_n^{\ell} = \frac{p(\mathbf{x}^{\ell}|\mathbf{y})}{q(\mathbf{x}^{\ell}|\mathbf{y})}
\end{aligned}
$$

Review: Sequential Importance Resampling

$$p(\mathbf{x}_{1:n-1}|\mathbf{y}_{1:n-1}) \approx \sum_{\ell=1}^{L} w_{n-1}^{\ell} \delta_{\mathbf{x}_{1:n-1}^{\ell}}(\mathbf{x}_{1:n-1})$$

$$p(\mathbf{x}_{1:n}|y_{1:n}) = g(y_n|\mathbf{x}_{1:n}) f(\mathbf{x}_n|\mathbf{x}_{1:n-1}) p(\mathbf{x}_{1:n-1}|y_{1:n-1})$$

$$q(\mathbf{x}_{1:n}|y_{1:n}) = f(\mathbf{x}_n|\mathbf{x}_{1:n-1}) p(\mathbf{x}_{1:n-1}|y_{1:n-1})$$

$$p(\mathbf{x}_{1:n}|y_{1:n}) \approx \sum_{\ell=1}^{L} g(y_n|\mathbf{x}_{1:n}^{\ell}) \delta_{\mathbf{x}_{1:n}^{\ell}}(\mathbf{x}_{1:n}), \qquad \mathbf{x}_{1:n}^{\ell} = \mathbf{x}_n^{\ell} \mathbf{x}_{1:n-1}^{a_{n-1}^{\ell}} \sim f$$

SMC Methods Discussed Require Only

Initialization

$p(\mathbf{x}_1)$ can be sampled

Forward Simulation

$f(\mathbf{x}_n|\mathbf{x}_{1:n-1})$ can be sampled (blackbox)

Observation Likelihood Weight Computation

$g(y_n|\mathbf{x}_{1:n})$ can be point-wise evaluated up to constant multiple

Sequential Monte Carlo for Prob. Prog.

Algorithm 1 Parallel SMC program execution

Assume: N observations, L particles
  launch L copies of the program (parallel)
  for $n = 1 \ldots N$ **do**
    wait until all L reach `observe` y_n (barrier)
    update unnormalized weights $\tilde{w}_n^{1:L}$ (serial)
    if $ESS < \tau$ **then**
      sample number of offspring $O_n^{1:L}$ (serial)
      set weight $\tilde{w}_n^{1:L} = 1$ (serial)
      for $\ell = 1 \ldots L$ **do**
        fork or exit (parallel)
      end for
    else
      set all number of offspring $O_n^\ell = 1$ (serial)
    end if
    continue program execution (parallel)
  end for
  wait until L program traces terminate (barrier)
  `predict` from L samples from $\hat{p}(\mathbf{x}_{1:N}^{1:L}|y_{1:N})$ (serial)

Probabilistic-C

```c
#include "probabilistic.h"
#define K 3
#define N 11

/* Markov transition matrix */
static double T[K][K] = { { 0.1,  0.5,  0.4 },
                          { 0.2,  0.2,  0.6 },
                          { 0.15, 0.15, 0.7 } };

/* Observed data */
static double data[N] = { NAN, .9, .8,  .7,   0, -.025,
                               -5, -2, -.1,   0,  0.13 };

/* Prior distribution on initial state */
static double initial_state[K] = { 1.0/3, 1.0/3, 1.0/3 };

/* Per-state mean of Gaussian emission distribution */
static double state_mean[K] = { -1, 1, 0 };

/* Generative program for a HMM */
int main(int argc, char **argv) {

    int states[N];
    for (int n=0; n<N; n++) {
        states[n] = (n==0) ? discrete_rng(initial_state, K)
                           : discrete_rng(T[states[n-1]], K);
        if (n > 0) {
            observe(normal_lnp(data[n], state_mean[states[n]], 1));
        }
        predict("state[%d],%d\n", n, states[n]);
    }

    return 0;
}
```

Paige and Wood “A Compilation Target for Probabilistic Programming Languages” ICML 2014

Inverse Stochastic Simulation

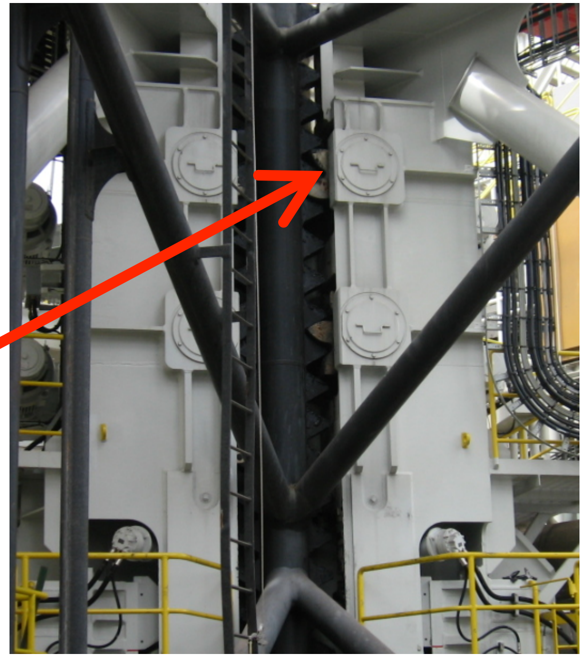
- Deterministic simulator exists as code
- Parameter uncertainties exist
  - Varying parameters to simulator = stochastic simulator

- What to do with observations?
  - Update estimates of parameters
  - Posterior predictions

Example : Jack-Up Units

60m

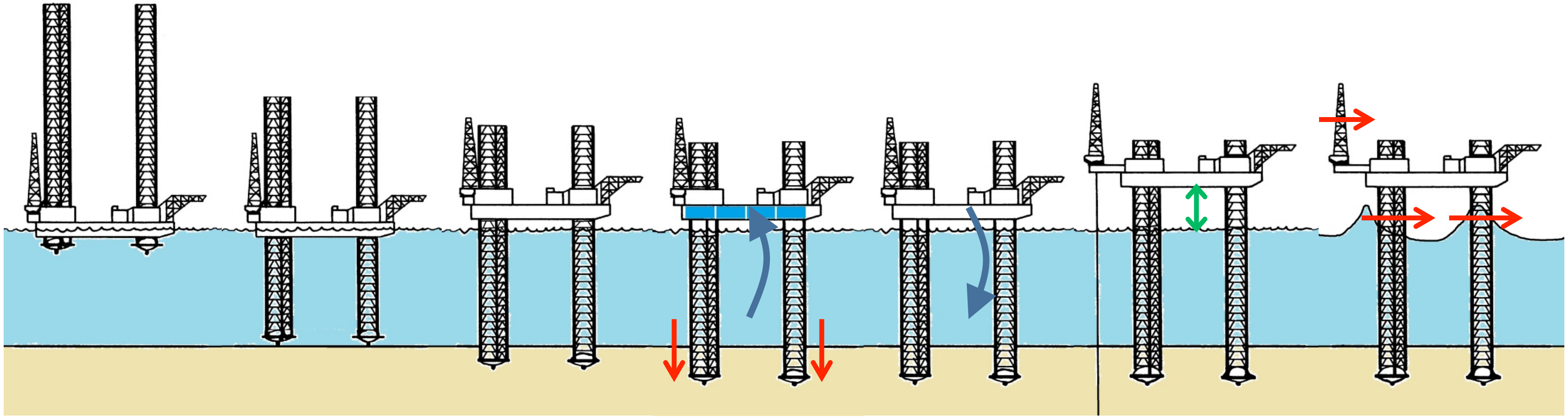
Maersk



Keppel FELS

Keppel FELS

Jack-up operations

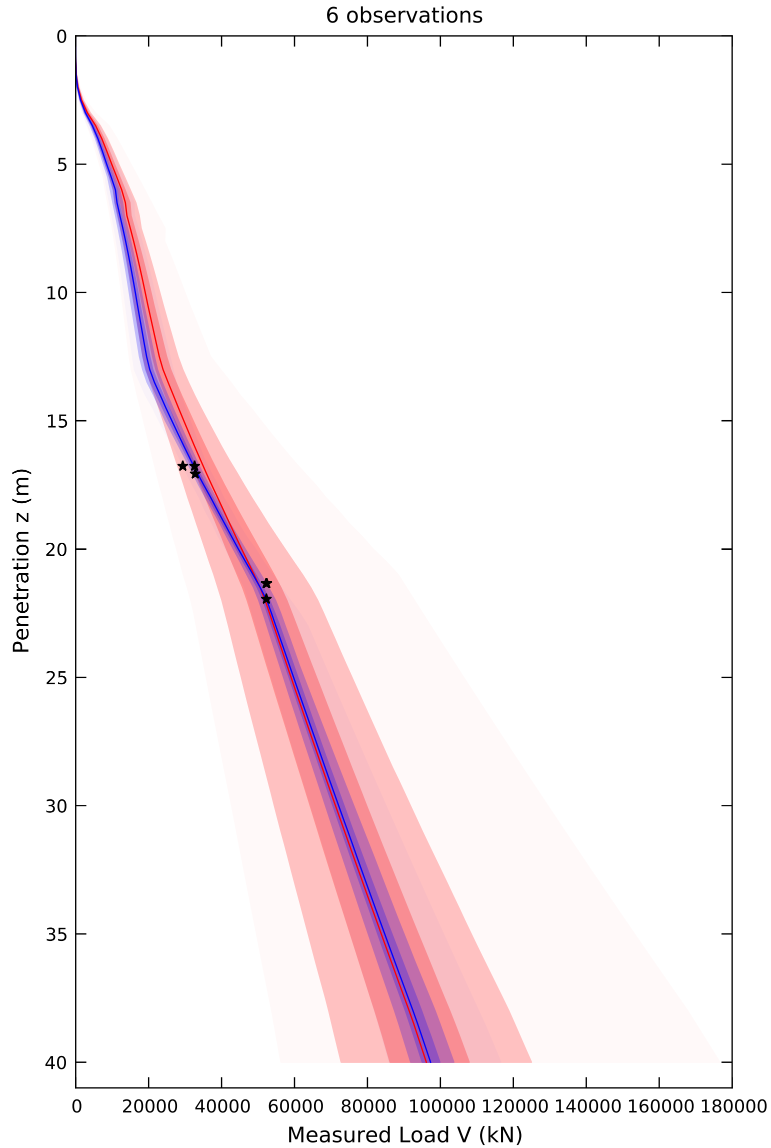


sketches after Poulos (1988)
Slide from Houlsby

Spudcan Simulator + Probabilistic-C -> Inference

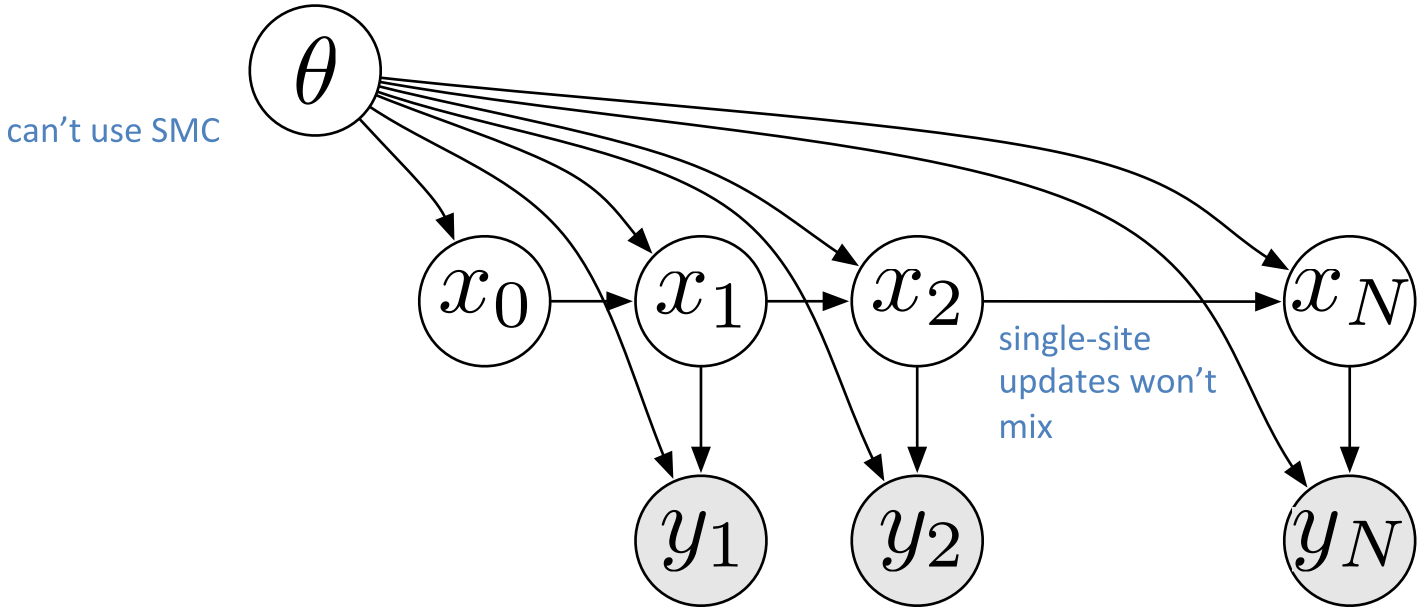
- Deterministic simulator
  - ~750 lines of C code
  - 10-100's of parameters
  - Black-box
  - Not differentiable
- Stochastic simulator
  - +150 lines of C code
  - Priors on parameters
- Automatic inference
  - +15 lines of Probabilistic-C

- ~1000 samples / second



Review : Inference In State Space Models

Consider inference in a state space model that depends on fixed parameters

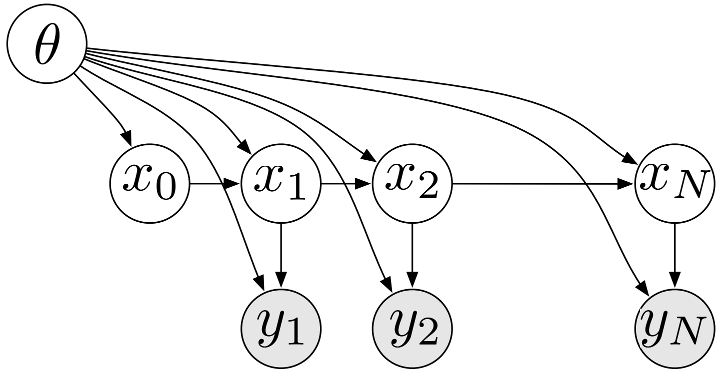


“Ideal” Inference

Ideal MH

$$\min\left(1, \frac{p(y_{1:N}|\theta')p(\theta')q(\theta|\theta')}{p(y_{1:N}|\theta)p(\theta)q(\theta'|\theta)}\right)$$

intractable.

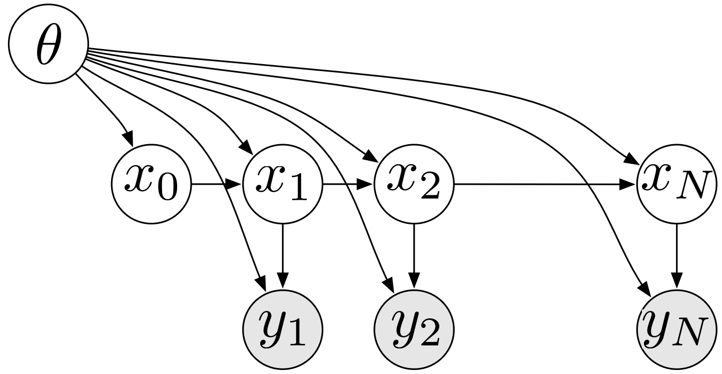


SMC provides *unbiased* estimate

$$\hat{Z} \equiv p(y_{1:N}|\theta) \approx \prod_{n=1}^{N}\left[\frac{1}{N}\sum_{\ell=1}^{L} w_n^\ell\right]$$

Particle Marginal Metropolis Hastings

MH with unbiased likelihood estimates



$$\min\left(1, \frac{\hat{Z}' p(\theta')q(\theta|\theta')}{\hat{Z} p(\theta)q(\theta'|\theta)}\right)$$

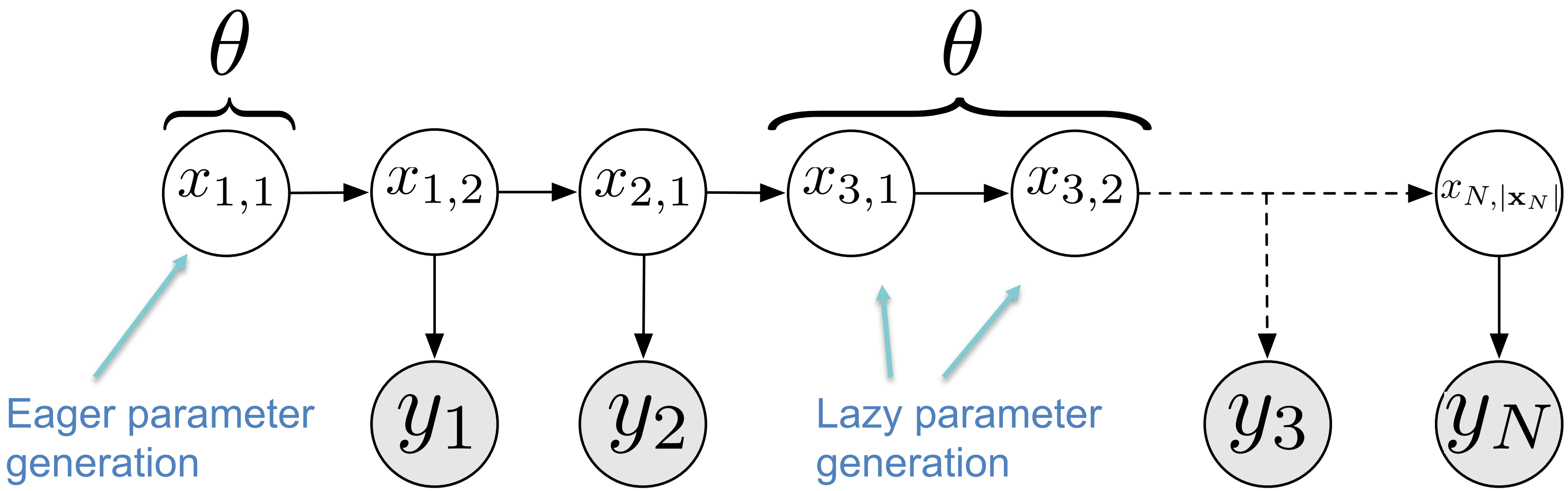
computed via SMC proposal

$$\hat{Z} \equiv p(y_{1:N}|\theta) \approx \prod_{n=1}^{N}\left[\frac{1}{N}\sum_{\ell=1}^{L} w_n^\ell\right]$$

targets correct distribution!

Conditional SMC for Prob. Prog. Inference

- No fixed parameter
- Program generates all random variables



- State is interpreter memory state
- Transition is stochastic procedure application
- Only observes need be indexed

PIMH For Probabilistic Programming

- Run SMC Once
- Compute marginal likelihood estimate

$$\hat{Z} \equiv p(y_{1:N}) \approx \prod_{n=1}^{N} \left[\frac{1}{N} \sum_{\ell=1}^{L} w_n^\ell \right]$$

No theta!

- Do forever
  - Re-run SMC
  - Compute new marginal likelihood estimate

$$\hat{Z}'$$

  - Accept particle set with probability

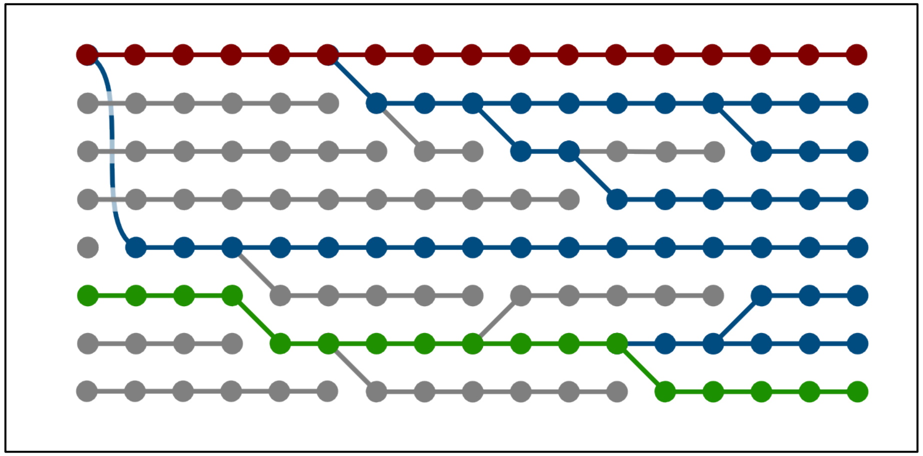
$$\min(1, \hat{Z}'/\hat{Z})$$

  - Emit predictions from all particles in next set (new and/or old)

Particle Gibbs for Prob. Prog.

- MH w/ accept prob. = 1
- SMC "inner-loop" proposal
- "Retained particle"
- *Non-local*
  - Single "sweep" can propose changes to many variable values at once

[Holenstein 2009; Andrieu, Doucet, Holenstein 2010; etc]

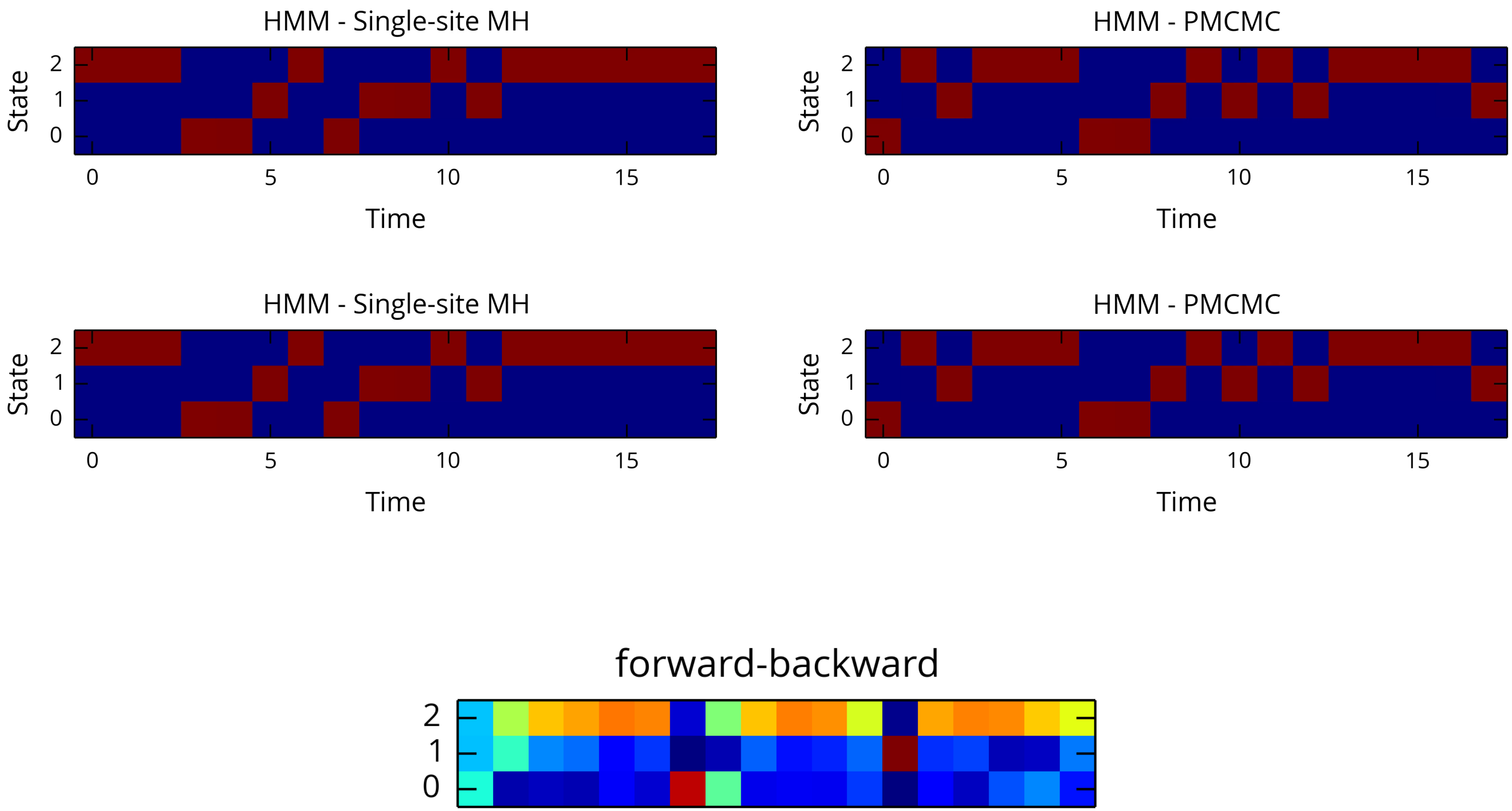


Algorithm 1 Particle Gibbs Prob. Prog. Inference

$L \leftarrow$ number of particles
$S \leftarrow$ number of sweeps
$\{\tilde{w}_N^{(\ell)}, \mathbf{x}_{1:N}^{(\ell)}\} \leftarrow$ Run SMC
for $s < S$ **do**
  $\{\cdot, \mathbf{x}^*_{1:N}\} \leftarrow \mathtt{r}(1, \{1/L, \mathbf{x}_{1:N}^{(\ell)}\})$
  $\{\cdot, \mathbf{x}_0^{(\ell)} = \emptyset\} \leftarrow$ initialize $L-1$ interpreters
  for $d \in$ ordered lines of program **do**
    for $\ell < L-1$ **do**
      $\bar{\mathbf{x}}_{1:(n-1)}^{(\ell)} \leftarrow \mathtt{fork}(\mathbf{x}_{1:(n-1)}^{(\ell)})$
    end for
    if $\mathtt{directive}(\mathrm{d}) == \mathtt{assume}$ **then**
      for $\ell < L-1$ **do**
        $\bar{\mathbf{x}}_{1:n}^{(\ell)} \leftarrow \mathtt{interpret}(d, \bar{\mathbf{x}}_{1:(n-1)}^{(\ell)})$
      end for
      $\{\mathbf{x}_{1:n}^{(\ell)}\} \leftarrow \{\bar{\mathbf{x}}_{1:n}^{(\ell)}\} \cup \mathbf{x}^*_{1:n}$
    else if $\mathtt{directive}(\mathrm{d}) == \mathtt{predict}$ **then**
      for $\ell < L-1$ **do**
        $\mathtt{interpret}(d, \bar{\mathbf{x}}_{1:(n-1)}^{(\ell)})$
      end for
      $\mathtt{interpret}(d, \mathbf{x}^*_{1:(n-1)})$
    else if $\mathtt{directive}(\mathrm{d}) == \mathtt{observe}$ **then**
      for $\ell < L-1$ **do**
        $\{\bar{w}_n^{(\ell)}, \bar{\mathbf{x}}_{1:n}^{(\ell)}\} \leftarrow \mathtt{interpret}(d, \bar{\mathbf{x}}_{1:(n-1)}^{(\ell)})$
      end for
      $\mathcal{T} \leftarrow \mathtt{r}(L-1, \{\bar{w}_n^{(\ell)}, \bar{\mathbf{x}}_{1:n}^{(\ell)}\} \cup \{\tilde{w}^*_{1:n}, \mathbf{x}^*_{1:n}\})$
      $\{\tilde{w}_n^{(\ell)}, \mathbf{x}_{1:n}^{(\ell)}\} \leftarrow \mathcal{T} \cup \{\tilde{w}^*_n, \mathbf{x}^*_{1:n}\}$
    end if
  end for
end for

Wood, van de Meent, Mansinghka "A New Approach to Probabilistic Programming Inference" AISTATS 2014
Paige and Wood "A Compilation Target for Probabilistic Programming Languages" ICML 2014

PMCMC Prob. Prog. Example



Goals and Aims

(i) Accelerate iteration over models

- Inference is automatic
- Writing generative code is easier than deriving model inverses
- Lower technical barrier of entry to development of new models

(ii) Accelerate iteration over inference procedures

- Computer language is an abstraction barrier
  - Inference procedures can be tested against a library of models
  - Inference procedures become “compiler optimizations”

(iii) Enable development of more expressive models

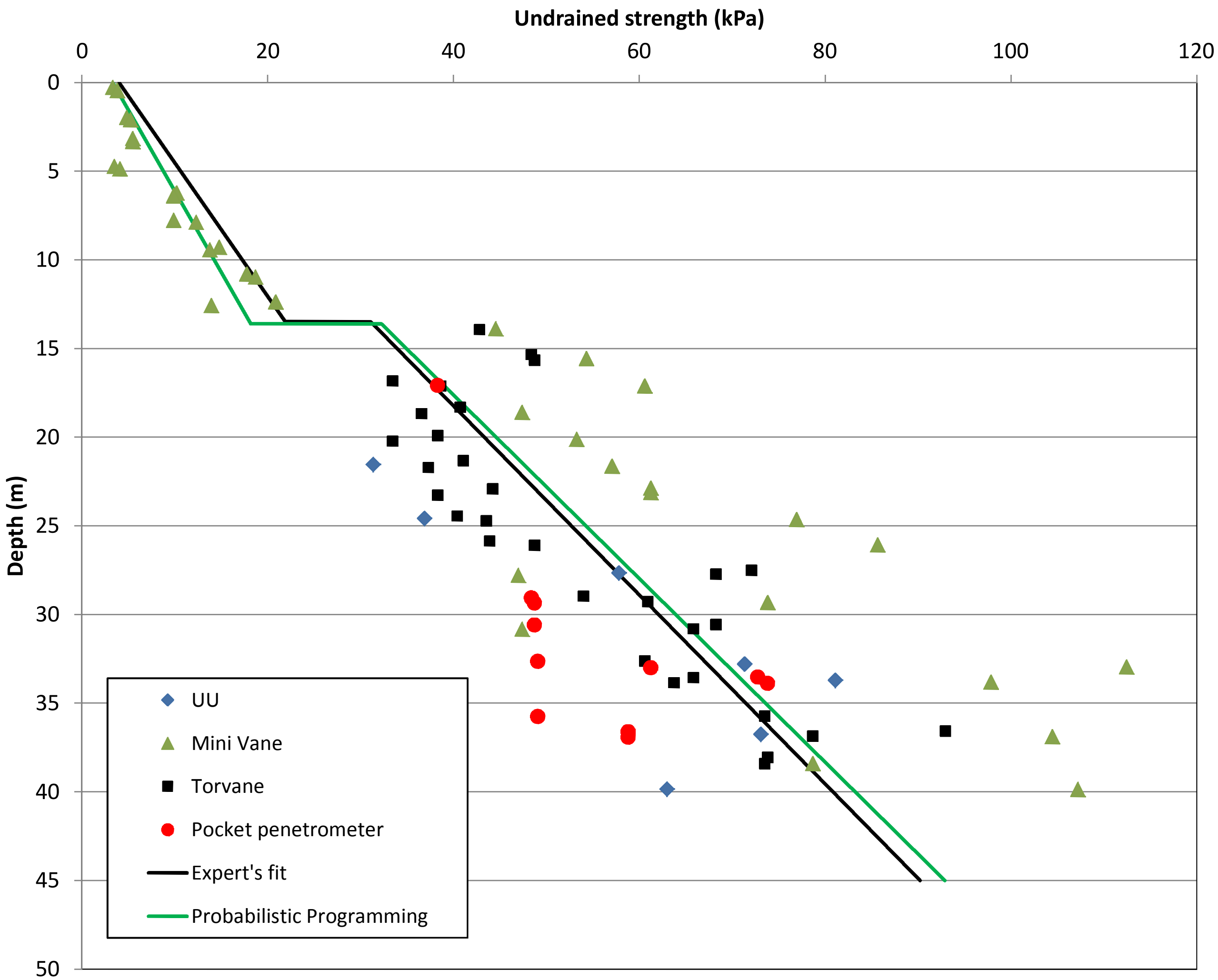
- Probabilistic programs can express a superset of graphical models
- Modern machine learning models are tens of lines of code

Wrap-Up

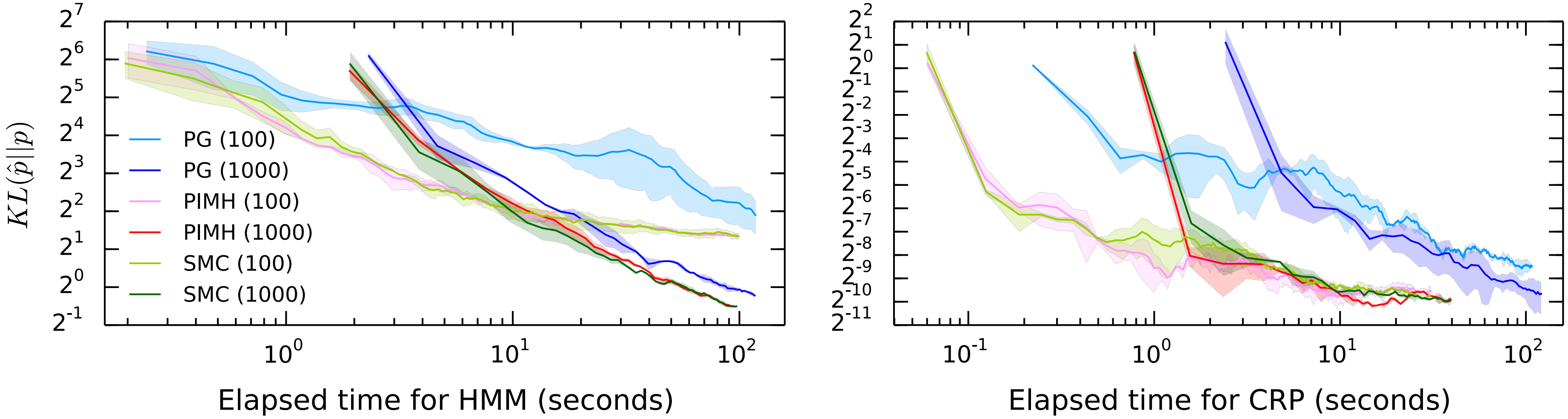
- Research
  - New paths to efficient, scalable probabilistic programming inference
  - True hope for general purpose automatic inference
  - New models (soon)

- Resources
  - http://www.robots.ox.ac.uk/~fwood/anglican/
  - http://www.robots.ox.ac.uk/~brooks/probabilistic-c/
  - http://probabilistic-programming.org/wiki/Home
  - http://forestdb.org/

Parameter Posterior vs. Expert



Compiled PMCMC Algorithm Performance



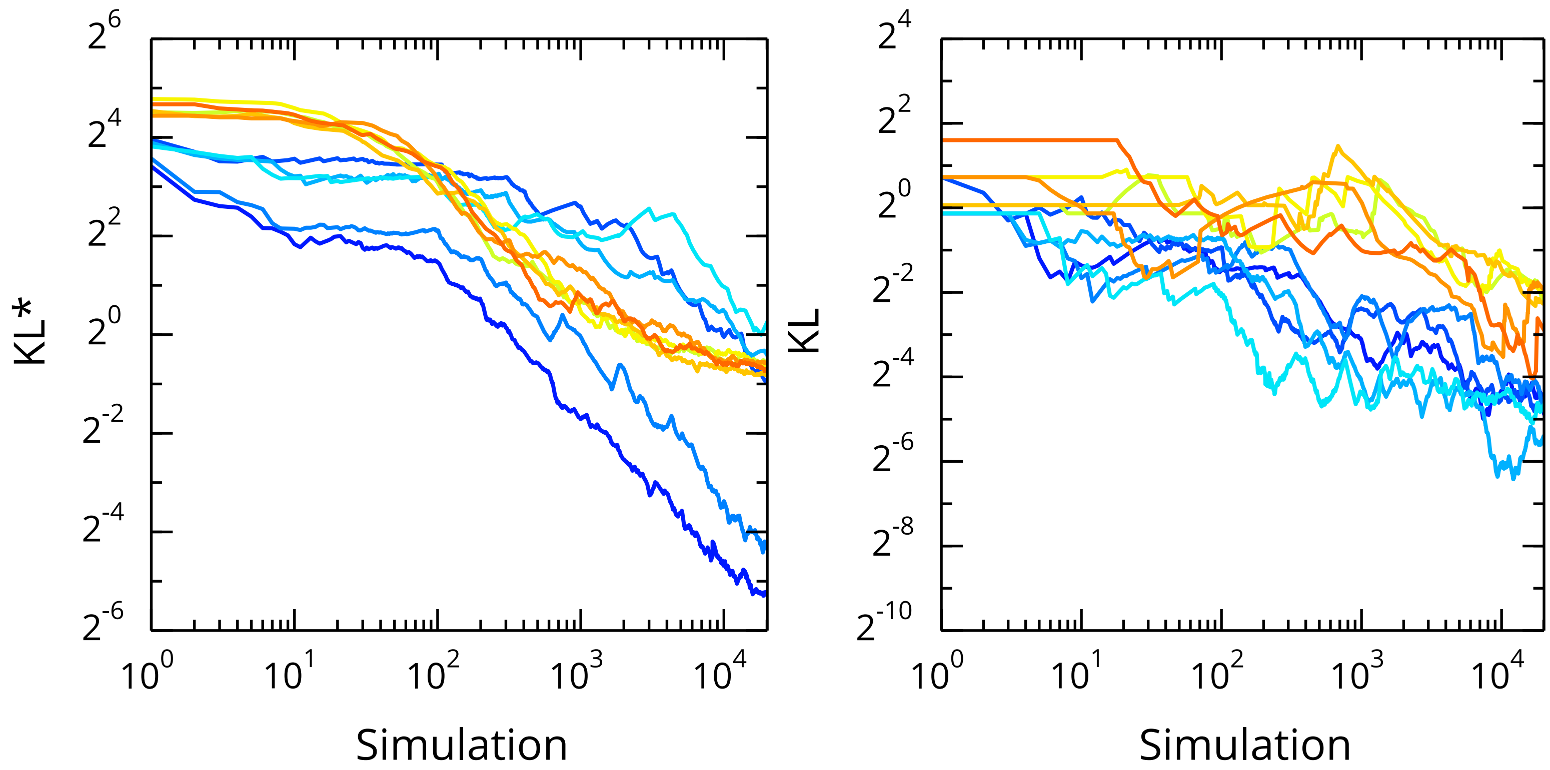
What if `dirac` Observes?

`dirac` observes are constraints

$$
\begin{aligned}
p(\mathbf{x}_{1:N}|\mathbf{y}_{1:N}) \propto \tilde{p}(\mathbf{y}_{1:N}, \mathbf{x}_{1:N}) &= \prod_{n=1}^{N} \mathbb{I}[y_n = a_n(\mathbf{x}_{1:n})] f(\mathbf{x}_n|\mathbf{x}_{1:n-1}) \\
&= p(\mathbf{x}_{1:N}) \mathbb{I}[\mathbf{y}_{1:N} = \mathbf{a}_{1:N}(\mathbf{x}_{1:N})]
\end{aligned}
$$

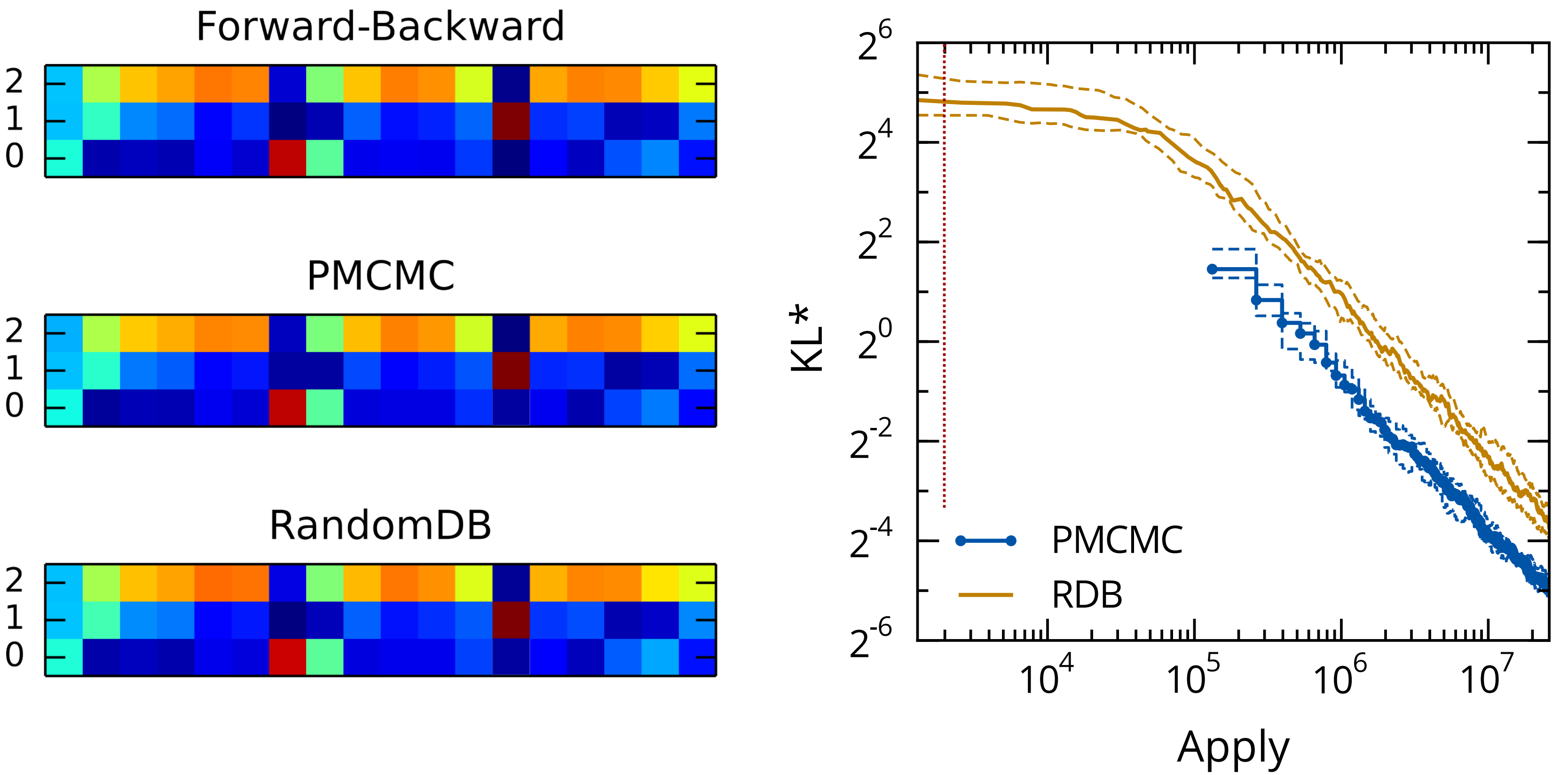
=> SMC / PMCMC reduce to rejection / repeated rejection sampling if all observes are constraints

Opportunity : Optimizing Inference by Program Line Reordering



(a) HMM (b) DP Mixture

Anglican : Particle MCMC Inference



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