Exact Inference for Discrete Probabilistic Programs via Generating Functions

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An Inference Problem

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Probabilistic program

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$$\begin{split} &X \sim \mathsf{Poisson}(10) \\ &Y \sim \mathsf{Binomial}(X, 0.2) \\ &\mathsf{observe}\, Y = 1 \end{split}$$

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PSI

SOLVER ^X Outputs a symbolic expression involving infinite sums.

PSI [Gehr et al. 2016]

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Not computable exactly using probability mass functions!

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Klinkenberg et al. 2020

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Nested inference: normalize {P}

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 \rightsquigarrow can express real-world models, e.g. population dynamics & change point models

Klinkenberg

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$$= \sum_{n=0}^{\infty} p_n x^n \quad \text{(only discrete } X\text{)}$$
$$\text{where } p_n = \mathbb{P}[X = n]$$

This infinite sum can often be expressed in closed form!

$$\begin{array}{cc} \mathcal{D} & \mathsf{pgf}_{\mathcal{D}}(x) \\ \\ \mathsf{Binomial}(n,p) & (px+1-p)^n \\ \mathsf{Poisson}(\lambda) & e^{\lambda(x-1)} \end{array}$$

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Transformer semantics:



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To evaluate *G*, no computer algebra is needed, just **automatic differentiation**.

Semantics of Conditioning

$$[observe X = c](G)(x) = \frac{G^{(c)}(0)}{c!} \cdot x^{c}$$

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Observations are expensive!

observe X = 100 requires evaluating the 100th derivative!

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- Then the expected value is: $\mathbb{E}[X] = G'(1)$.
- Then the variance and higher moments can be expressed with higher derivatives $G^{(n)}(1)$.

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Extracting information:

$$\mathbb{P}[X=10] = \left. \frac{1}{10!} \frac{\partial^{10}}{\partial x^{10}} xy e^{8x-8} \right|_{x=0,y=1} = \frac{1048576}{2835} e^{-8}$$

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$$\blacktriangleright \mathbb{E}[X] = \frac{\partial}{\partial x} xy e^{8x-8} \big|_{x=1,y=1} = 9$$

Demo (population model)

```
p(68) = 0.028328180265953493
normalize {
                                                        p(69) = 0.023065973853818575
 population := 0;
                                                       p(70) = 0.01838674214279982
 arrivals ~ Poisson(58.15):
                                                        p(71) = 0.01435492147905039
 survivors ~ Binomial(population, 0.2636);
                                                        p(72) = 0.01098084809984991
 population := arrivals + survivors;
                                                        p(73) = 0.008233399343568646
  observed ~ Binomial(population, 0.2):
                                                        p(74) = 0.006053318560300744
 observe observed = 0:
                                                       p(75) = 0.004365517352330878
                                                       p(76) = 0.0030892768898579935
 arrivals ~ Poisson(105.2);
                                                       p(77) = 0.0021458658791949775
 survivors ~ Binomial(population, 0.2636);
                                                       p(78) = 0.0014635700766538772
                                                       p(79) = 0.0009804499356385623
  population := arrivals + survivors:
                                                       p(80) = 0.0006453115328326522
 observed ~ Binomial(population, 0.2);
                                                       p(81) = 0.00041741910372653385
  observe observed = 12:
                                                       p(82) = 0.0002654341174435854
                                                       p(83) = 0.00016597450666935572
 arrivals ~ Poisson(75.2):
                                                       p(84) = 0.00010208012245584834
 survivors ~ Binomial(population, 0.2636);
                                                       p(85) = 0.00006176856103264198
  population := arrivals + survivors;
                                                       p(86) = 0.0000367813977215097
  observed ~ Binomial(population, 0.2);
                                                       p(87) = 0.000021558974254102993
 observe observed = 24:
                                                       p(88) = 0.000012441382544265904
                                                       p(89) = 7.070472990081274e-6
                                                       p(90) = 3.95788624737007e-6
  arrivals ~ Poisson(21.4);
                                                       p(n) <= 4.693893727897103e-6 for all n >= 91
 survivors ~ Binomial(population, 0.2636);
 population := arrivals + survivors;
                                                       Total measure: Z = 1.0000000000000002
 observed ~ Binomial(population, 0.2);
                                                       Expected value: E = 60,28009872152928
 observe observed = 21:
                                                       Variance: V = 38,29566931328145
return population
                                                        Time elapsed: 1.3375798s
```

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- Manual implementation of autodiff is faster
- Computing directly with Taylor expansions is even better

Limitations

Language features:

- only affine functions
- only comparisons X = c (e.g. no X = Y)
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Performance:

- GFs can grow exponentially with constants in the program
- worst-case exponential time



Generating functions **represent distributions** with infinite support **compactly**.

They are a **powerful tool** for **exact inference** in probabilistic programming.