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Soss: Declarative Probabilistic Programming via Runtime Code Generation

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We present Soss, a declarative probabilistic programming language embedded in the Julia language. Soss represents statistical models in terms of abstract syntax trees, and uses staged compilation for on-demand generation of "inference primitives" (random sampling, log-density, etc) without requiring casual users to worry about such details.

The approach taken by Soss makes it easy to extend to take advantage of other packages in the rapidlygrowing Julia ecosystem. At the time of this writing, Soss users can choose from several inference back-ends and connect easily with larger systems SymPy and Gen.

INTRODUCTION

There are many approaches to building a Probabilistic Programming Language ("PPL"). Soss is distinct from most alternatives in a number of ways:

- Model specification in Soss is *declarative*; statements are represented not by the order entered by the user, but by the partial order given by their variable dependencies.
- Soss models are typically expressed in terms of *inference combinators* (like "For") that combine distributions in some way to arrive at a new distribution.
- Soss models are first-class; models can be passed as arguments to other models, or used in place of distribution functions like Normal within a model.
- Soss models are function-like; abstractly, a model may be considered a function from its arguments to a joint distribution. In particular, specification of "observed variables" is separated from model definition.
- Values and distributions in Soss are represented internally as abstract syntax trees, keeping the internal representation close to that given by the user for maximum flexibility.
- Soss uses staged compilation for inference primitives like rand and logpdf, via novel generalized generated functions from GeneralizedGenerated.jl.
- Soss supports *model transformations*, functions that take a model and return another model.
- Soss supports symbolic simplification, making it easy to inspect or manipulate a symbolic representation of the log-density, or to use it to generate optimized code.
- Soss is extensible; users can define new inference primitives or model transformations externally, and use them as if they had been included in Soss.

Finally, Soss uses Cockney rhyming slang to address the well-known challenge of naming things in computer science ("sauce pan" rhymes with "Stan"). Soss is open-source software.

MODELING IN SOSS

Figure 1 shows a plate diagram and Soss implementation of a simplified two-way ANOVA model. The Soss model m has arguments I and J. Each line of a model is either a sample statement ($v \sim rhs$) or an assign statement (v = rhs). In either case, v must be a valid Julia variable name, and rhs must be a valid Julia expression. For a sample statement, rhs should also be "distribution-like", supporting logpdf and/or rand methods (depending on the inference algorithm to be used).

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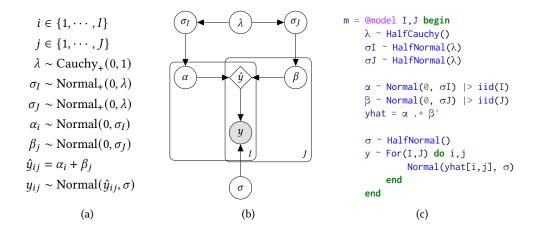


Fig. 1. A generative model (a), plate diagram (b), and Soss model (c) for a two-way analysis of variance model. Note the specification that y will later be observed is not part of the model, but is instead given at inference time.

2.1 Joint Distributions

 A Soss model is *function-like*, taking values for its arguments and returning a *joint distribution*. For example, given m from Figure 1, we can build the joint distribution d=m(I=2, J=3). This supports the usual rand and logpdf functions, as well as some others provided by Soss described in the following sections. For example, ¹

```
julia> d = m(I=2, J=3); rand(d) # or just rand(m(I=2, J=3)) (I = 2, J = 3, yhat = [-0.52 -1.5 0.0037; -0.81 -1.85 -0.28], \sigma = 2.5, \lambda = 1.3, \sigmaJ = 0.72, \sigmaI = 0.41, \beta = [-0.54, -1.5, -0.023], \alpha = [0.026, -0.26], \gamma = [-0.45 -2.0 2.2; -3.4 -3.9 2.3])
```

2.2 Inference Primitives

A given inference algorithm can be expressed in terms of a collection of functions on a model or joint distribution. For example, we often need to evaluate the log-density or its gradient or draw random samples. In Soss, these *inference primitives* generate model-specific code at execution time.

At this writing, the following inference primitive are available:

```
rand draws a random point or sample from a given distribution.
```

particles draws a *systematic sample*, as described in [Douc et al. 2005].

logpdf takes a distribution and a point, and returns the log-density at that point.

xform takes a distribution and some known data, and returns a bijection from \mathbb{R}^n to the space of unknowns. This is useful for algorithms like Hamiltonian Monte Carlo [Neal 2011].

symlogpdf takes a model, and returns a SymPy [Meurer et al. 2017] representation of the log-density, with some additional Julia-based simplifications.

codegen calls symlogpdf, and uses the result to generate a more efficient version of logpdf.

In the above, a *distribution* refers to a joint distribution, while *point* refers to a named tuple in the space space of a distribution.

```
cite MonteCarloMeasurements.jl and TransformVariables.jl
```

¹This and future outputs are lightly edited for space, for example rounding floating point values.

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$$\ell = -3\log(2) - 5\log(\pi) - \sigma^{2}$$

$$-4\log(\lambda) - 2\log(\lambda^{2} + 1) - \frac{\sigma_{I}^{2}}{\lambda^{2}} - \frac{\sigma_{J}^{2}}{\lambda^{2}}$$

$$+ \sum_{i=1}^{I} \left(-\log(\sigma_{I}) - \frac{\log \pi}{2} - \frac{\log 2}{2} - \frac{\alpha_{i}^{2}}{2\sigma_{I}^{2}} \right)$$

$$+ \sum_{j=1}^{J} \left(-\log(\sigma_{J}) - \frac{\log \pi}{2} - \frac{\log 2}{2} - \frac{\beta_{j}^{2}}{2\sigma_{J}^{2}} \right)$$

$$+ \sum_{1 \le i \le I} \left(-\log(\sigma) - \frac{\log \pi}{2} - \frac{\log 2}{2} - \frac{(y_{ij} - \hat{y}_{ij})^{2}}{2\sigma^{2}} \right)$$

$$+ \sum_{1 \le i \le I} \left(-\log(\sigma) - \frac{\log \pi}{2} - \frac{\log 2}{2} - \frac{(y_{ij} - \hat{y}_{ij})^{2}}{2\sigma^{2}} \right)$$

$$= -7.8 - 0.92I - 0.92J - 0.92IJ - \sigma^{2}$$

$$- 4 \log \lambda - 2 \log(\lambda^{2} + 1) - IJ \log \sigma$$

$$- I\log \sigma_{I} - J \log \sigma_{J} - \frac{\sigma_{I}^{2}}{\lambda^{2}} - \frac{\sigma_{J}^{2}}{\lambda^{2}}$$

$$- \frac{1}{2\sigma_{I}^{2}} \sum_{i=1}^{I} \alpha_{i}^{2} - \frac{1}{2\sigma_{J}^{2}} \sum_{j=1}^{J} \beta_{j}^{2}$$

$$- \frac{1}{2\sigma^{2}} \sum_{1 \le i \le I} (y_{ij} - \hat{y}_{ij})^{2}$$

(a) Direct implementation

(b) After symbolic simplification

Fig. 2. Symbolic log-density of *m* before (a) and after (b) simplification steps.

The set of inference primitives is not fixed, but can be extended by users. New primitives can be added in outside packages, and does not require making changes to the Soss codebase.

Figure 2 show the simplification performed automatically by symlogpdf. Note the reduction in the terms included in summations, which account for the bulk of evaluation cost.

2.3 Inference

Together with automatic differentiation, the above inference primitives enable a wide variety of inference algorithms. Rather than building such algorithms specific to Soss, we defer this to external packages. So far, our focus has been Hamiltonian Monte Carlo [Neal 2011], as implemented in DynamicHMC.jl [Papp and Piibeleht 2019] and AdvancedHMC.jl [Ge et al. 2018]; Soss has interfaces to these in the **dynamicHMC** and **advancedHMC** functions, respectively.

2.4 Functions on Models

Soss includes several functions for querying sets of variables associated with a model. As described above, models are function-like, with the inputs given by **arguments**. In the body of a model every statement declares that some variable is either **sampled** or **assigned**. The sampled and assigned variables together comprise the **parameters**, and all of the above are **variables**. Each of these is a Soss function that takes a model and returns a vector of distinct Julia symbols.

Soss ignores the ordering of statements given by the user, instead working in terms of the DAG ordering. You can access this graph with **digraph**, or use **poset** to get the partial order. Finally, **toposort** returns a topologically-ordered vector of the parameters. Each of these three functions takes a model as input.

Soss represents and manipulates variable dependencies using SimpleGraphs, SimplePosets, and SimplePartitions from [Scheinerman 2019].

2.5 Model Transformations

Do implements Pearl's do operator for causal intervention [Pearl 1995].²

²Our Do operator is capitalized because do is a keyword in Julia.

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```
struct Model{A,B,M}
                                                               julia> m.vals
                                                               (yhat = :(\alpha .+ \beta'),)
     args :: Vector{Symbol}
     vals :: NamedTuple
     dists :: NamedTuple
                                                               julia> typeof(m)
     retn :: Union{Nothing, Symbol, Expr}
                                                              Model{NamedTuple{(:I, :J),T} where T<:Tuple,</pre>
end
                                                                    TypeEncoding(begin
                                                                         \sigma \sim HalfNormal()
julia> m.dists
                                                                         \lambda \sim HalfCauchy()
( \lambda = :(HalfCauchy())
                                                                         \sigma J \sim HalfNormal(\lambda)
                                                                         \sigma I \sim HalfNormal(\lambda)
, \sigma I = :(HalfNormal(\lambda))
\sigma J = :(HalfNormal(\lambda))
                                                                         \beta \sim Normal(0, \sigma J) \mid > iid(J)
, \alpha = :(Normal(\emptyset, \sigma I) \mid > iid(I))
                                                                         \alpha \sim Normal(0, \sigma I) \mid > iid(I)
                                                                         yhat = \alpha .+ \beta'
, \beta = :(Normal(\emptyset, \sigma J) \mid > iid(J))
\sigma = :(HalfNormal())
                                                                         y \sim For(I, J) do i, j
, y = :(For(I, J) do i, j)
                                                                                   Normal(yhat[i, j], \sigma)
          Normal(yhat[i, j], σ)
                                                                    end),TypeEncoding(Main)}
          end))
```

Fig. 3. The definition of the Model type, and some details of the m model from Figure 1.

predictive is like Do, but only returns the strongly-connected components containing the specified variables. This is useful for sampling from the posterior predictive distribution.markovBlanket takes a model and a variable, and returns a model representing the Markov blanket at the given variable.

3 IMPLEMENTATION

Soss's inference primitives generate code on demand using the GeneralizedGenerated.jl library, which introduces a <code>@gg</code> macro that works as an extension of Julia's built-in <code>@generated</code> macro for <code>generated functions</code> [Bezanson et al. 2012]. Similarly to <code>@generated</code>, code generated using a <code>@gg</code> function cannot depend on the values of its arguments, but only on their types.

This *staged compilation* introduces some additional overhead on the first call on a given argument type, due to generation and compilation of specialized code. Subsequent calls on this same type have no such overhead, and generally benefit from specialization. To acheive a net gain from this requires making enough function calls to offset the cost of code generation. This makes the approach a natural fit for the PPL domain, where long-running tight loops are very common.

However, the requirement that the generated code only depends on the types presents a challenge, since we clearly need it to depend on the model itself. To address this, GeneralizedGenerated includes facilities for lifting Julia values to the type level.

The type of a Soss model is thus Model {A,B,M}, where

- A gives the type of the *arguments* (A=NamedTuple{T} for some tuple of symbols T),
- B is a type-level representation of the body, and
- M is a type-level representation of the module in which the model was defined.

In this, the "body" is the begin...end following the (possibly empty) arguments of a model. Knowing the module is important in case values from that module are referenced in the model.

The flexibility of code generation in Soss makes it difficult to measure performance. When a performance bottleneck is found, developers or users can ask Soss to generate something different. This design places no a priori constraints on performance.

4 RELATED WORK

The idea of code generation and symbolic simplification in an embedded PPL goes back to *Passage* [Scherrer et al. 2012].

Hakaru [Narayanan et al. 2016] takes a more ambitious symbolic approach in a stand-alone PPL, allowing a wider variety of program transformations.

Soss began with a goal of representing models with continuous, fixed-dimensionality parameter spaces, inspired by *Stan* [Carpenter et al. 2017].

Gen [Cusumano-Towner et al. 2019] was developed independently from Soss, but takes a similar approach (and distinct from most PPLs) in its representation of a model as a function from its arguments to a "trace" (to use Gen's terminology). In both Soss and Gen's static DSL, this trace is a mapping from variable names to values. The similarity of these systems makes interoperability relatively straightforward, as demonstrated in SossGen (https://github.com/cscherrer/SossGen.jl).

ACKNOWLEDGMENTS

Turing [Ge et al. 2018]

We would like to acknowledge...

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```
246
                                                               (model)
                                                                                                                          ⊨ @model ⟨args⟩ begin ⟨statements⟩ end
247
                                                                                                                          \models \lambda \mid \langle Symbol \rangle \mid \langle Symbol \rangle, \langle args \rangle
                                                                          ⟨args⟩
                                                                                                                           |= \langle statement \rangle | \langle statement \rangle |
249
                                    (statements)
250
                                           (statement)
                                                                                                                          ⊨ ⟨assign⟩ | ⟨sample⟩
251
                                                                                                                           \models \langle \text{Symbol} \rangle = \langle \text{Expr} \rangle
                                                               (assign)
                                                                                                                           ⊨ ⟨Symbol⟩ ~ ⟨Measure⟩
                                                          (sample)
253
                                                                                                                          ⊨ return ⟨Expr⟩
                                                                          ⟨retn⟩
255
                                                       (Symbol)
                                                                                                                          ⊨ Julia Symbol
                                                                                                                          ⊨ Julia Expr
                                                                       ⟨Expr⟩
257
                                                                                                                          ⊨ Probability measure (see text)
                                                 (Measure)
```

Fig. 4. Backus-Naur Form representation for a user-specified model.

```
julia> Soss.sourceRand()(m)
                                                                   julia> Soss.sourceLogpdf()(m)
quote
                                                                   quote
     \sigma = rand(HalfNormal())
                                                                        _{ e 0.0
     \lambda = rand(HalfCauchy())
                                                                        _{\ell} += logpdf(HalfNormal(), \sigma)
     \sigma J = rand(HalfNormal(\lambda))
                                                                        _{\ell} += logpdf(HalfCauchy(), \lambda)
     \sigma I = rand(HalfNormal(\lambda))
                                                                        _{\ell} += logpdf(HalfNormal(\lambda), \sigmaJ)
     \beta = rand(iid(J, Normal(0, \sigma J)))
                                                                        _{\ell} += logpdf(HalfNormal(\lambda), \sigmaI)
     \alpha = rand(iid(I, Normal(0, \sigma I)))
                                                                        _{\ell} += logpdf(Normal(0, \sigmaJ) |> iid(J), \beta)
     yhat = \alpha .+ \beta'
                                                                        _{\ell} += logpdf(Normal(0, \sigmaI) |> iid(I), \alpha)
     y = rand(For(I, J) do i, j
                                                                        yhat = \alpha . + \beta'
                      Normal(yhat[i, j], σ)
                                                                        _{\ell} += logpdf(For(I, J) do i, j
                                                                                         Normal(yhat[i, j], σ)
     (I=I, J=J, yhat=yhat, \lambda = \lambda, \sigmaI=\sigmaI,
                                                                                    end, y)
     \sigma J = \sigma J, \alpha = \alpha, \beta = \beta, \sigma = \sigma, \gamma = \gamma
                                                                        return \ell
                                                                   end
end
                            (a) rand
                                                                                              (b) logpdf
```

Fig. 5. Generated code when calling rand(m) and logpdf(m,x).

A MODEL SYNTAX

B SYMBOLIC SIMPLIFICATION

C EXTENDED EXAMPLE

```
Break this up! This is just a staging area
```

```
julia> using Revise, Soss, Random
286
287
        julia> Random.seed!(1);
288
         julia> m = @model I,J begin
289
                        λ ~ HalfCauchy()
290
                        \sigma I \sim HalfNormal(\lambda)
291
                        \sigma J \sim HalfNormal(\lambda)
292
                        \alpha \sim Normal(0, \sigma I) \mid > iid(I)
                       \beta \sim Normal(0, \sigma J) \mid > iid(J)
293
```

```
295
                     yhat = \alpha .+ \beta'
                     \sigma \sim HalfNormal()
296
                     y ~ For(I,J) do i,j
297
                              Normal(yhat[i,j], σ)
298
299
                end;
300
        julia> truth = rand(m(I=2, J=3)); pairs(truth);
301
302
        julia> post = dynamicHMC(m(I=2,J=3), (y=truth.y,));
303
304
        julia> postpred = predict(m(I=2, J=3), post) |> particles;
        julia> postpred.yhat
306
        2×3 Array{Particles{Float64,1000},2}:
        0.241 ± 0.26 0.527 ± 0.3 -0.556 ± 0.38
308
        0.22 \pm 0.26 0.506 \pm 0.32 -0.577 \pm 0.37
310
        julia> postpred.y
        2×3 Array{Particles{Float64,1000},2}:
311
        0.224 ± 0.58 0.529 ± 0.58 -0.58 ± 0.64
312
        0.223 \pm 0.56 0.483 \pm 0.58 -0.58 \pm 0.61
313
314
        julia> m.args
315
        2-element Array{Symbol,1}:
        : I
316
        : J
317
318
        julia> pairs(m.vals)
319
        pairs(::NamedTuple) with 1 entry:
320
          :yhat \Rightarrow :(\alpha .+ \beta')
321
        julia> pairs(m.dists)
322
        pairs(::NamedTuple) with 7 entries:
323
          \lambda \Rightarrow :(HalfCauchy())
324
          : \sigma I \implies : (HalfNormal(\lambda))
325
          : \sigma J \Rightarrow : (HalfNormal(\lambda))
          :\alpha \Rightarrow :(Normal(0, \sigma I) \mid > iid(I))
326
          :\beta \Rightarrow :(Normal(\emptyset, \sigma J) \mid > iid(J))
327
          :\sigma \Rightarrow :(HalfNormal())
328
          :y => :(For(I, J) do i, j. . .
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```

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