Functional tensors for probabilistic programming

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NeurIPS workshop on program transformation 2019-12-14

Outline

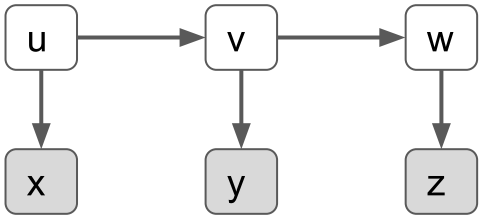
Motivation

What are Funsors?

Language overview

Discrete latent variable models

```
F : Tensor[n,n]
H : Tensor[n,m]
u ~ Categorical(F[0])
v ~ Categorical(F[u])
w ~ Categorical(F[v])
observe x ~ Categorical(H[u])
observe y ~ Categorical(H[v])
observe z ~ Categorical(H[w])
```



Discrete latent variable models

```
F = pyro.param("F", torch.ones(n,n), constraint=simplex)
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u = pyro.sample("u", Categorical(F[0]))
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w = pyro.sample("w", Categorical(F[v]))
pyro.sample("x", Categorical(H[x]), obs=x)
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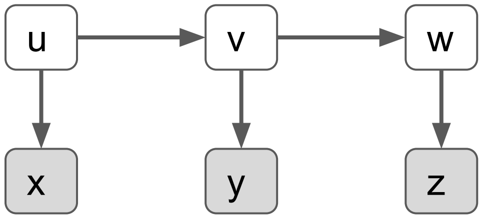
pyro.sample("z", Categorical(H[z]), obs=z)
```



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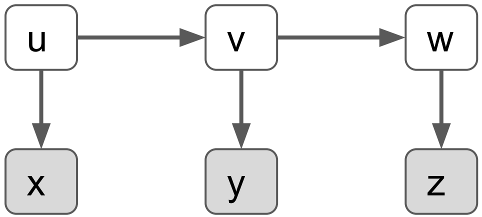

Inference via variable elimination

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Goal: vary F,H to maximize p(x,y,z)

$$p(x, y, z) = \sum_u \sum_v \sum_w p(u, v, w, x, y, z)$$

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```

```
# In PyTorch:
p = einsum("u,vu,vw,u,v,w",
           F[0],F,F,
           H[:,x],H[:,y],H[:,z])
```

```
p.backward()  # backprop to optimize F,H
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~~Discrete~~ Gaussian latent variable models

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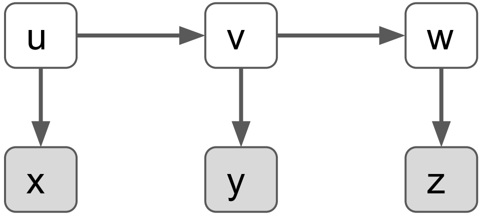

Kalman filters,
Sequential Gaussian Processes,
Linear-Gaussian state space models,
Gaussian conditional random fields,
...

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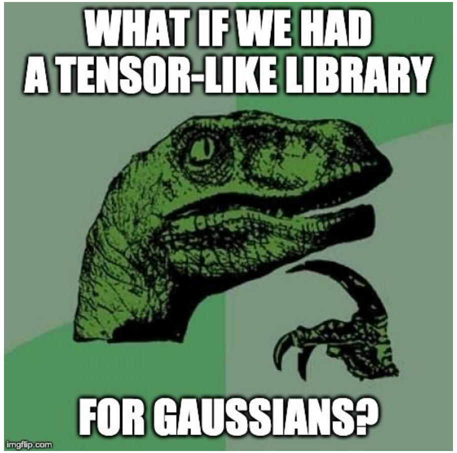

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```
# In a gaussian library:
p = (F(0,"u")*F("v","u")*F("v","w")
     *H("u",x)*H("v",y)*H("w",z)
     ).sum("u").sum("v").sum("z")  # or .integrate() or something?
```

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"Tensors are open terms
whose dimensions are free variables
of type bounded int"

"Funsors are open terms
whose free variables are
of type bounded int or real array"

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Funsor ::= Tensor | Gaussian | ...

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- Gaussians are closed under some operations:
  - Gaussian * Gaussian ⇒ Gaussian
  - Gaussian.sum("a_real_variable") ⇒ Gaussian
  - Gaussian["x" = affine_function("y")] ⇒ Gaussian
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  - Gaussian["x" = affine_function("y")] ⇒ Gaussian
  - (Gaussian * quadratic_function("x")).sum("x") ⇒ Gaussian or Tensor
- Gaussians are not closed under all operations:
  - Gaussian.sum("an_integer_variable") ⇒ ...a mixture of Gaussians…
  - (Gaussian * f("x")).sum("x") ⇒ ...an arbitrary Gaussian expectation...

Funsors are not as simple as Tensors

Approximate computation with Gaussians

```
Gaussian.sum("i") ⇒ ...mixture of Gaussians...
# but approximating...
with interpretation(moment_matching):
    Gaussian.sum("i") ⇒ Gaussian
```

But nonstandard interpretation helps!

Approximate computation with Gaussians

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with interpretation(monte_carlo):
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```

a randomized rewrite rule

But nonstandard interpretation helps!

Monte Carlo approximation via Delta funsors

```
# Three rewrite rules:
with interpretation(monte_carlo):
    (Gaussian * f("x")).sum("x") ⇒ (Delta * f("x")).sum("x")

Delta("x",x,w) * f("x") ⇒ Delta("x",x,w) * f(x)

Delta("x",x,w).sum("x") ⇒ w
```

Monte Carlo approximation via Delta funsors

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```

The point x and weight w are both differentiable:
- x via the reparameterization trick,
- w via REINFORCE, DiCE factor
  (e.g. to track mixture component weight)

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```

The point x and weight w are both differentiable:
- x via the reparameterization trick,
- w via REINFORCE, DiCE factor

Theorem: monte_carlo is correct in expectation at all derivatives.

Inference via delayed sampling

fun $\mathrm{GenerativeModel}(x)$	$p \leftarrow 1$
$\quad z \leftarrow \mathrm{sample}(P_z)$	$p \leftarrow p \times P_z[v = z]$
$\quad y \leftarrow \exp(z)$	
$\quad \mathrm{observe}(P_x[\theta = y],\ x)$	$p \leftarrow p \times P_x[\theta = y, v = x]$
end	maximize: $\sum_z p$

Funsor syntax

```
Funsor ::= Tensor | Gaussian | Delta | Variable
         | Funsor["x"=Funsor]              # substitution
         | f̂(Funsor, …, Funsor)             # application, e.g. +,*
         | ∑ₓ Funsor                        # marginalization
         | ∏ₓ Funsor                        # plate reduction
```

Algorithm 1 TensorVariableElimination

input variabl… F, values $F \subseteq V \times F$,

plate s…

plate s…

output PlatedSumProduct(…

Initialize an empty list of scalars $S \leftarrow []$.

while F is not empty **do**

- Choose a leaf plate set $L \in \{P(f) \mid f \in F\}$ with a maximal number of plates.
- Let $V_L \leftarrow \{v \in V \mid P(v) = L\}$ be the variables in L.
- Let $F_L \leftarrow \{f \in F \mid P(f) = L\}$ be the factors in L.
- Let $E_L \leftarrow E \cap (V_L \times F_L)$ be the edges in L.
- **for** (V_c, F_c) **in** Partition(V_L, F_L, E_L) **do**
  - Let $f \leftarrow$ SumProduct(F_c, V_c).
  - Let $V_f \leftarrow \{v \mid (v, f) \in E \cap ((V \setminus V_c) \times F_c)\}$ be the set of f's remaining variables.
  - Remove component (V_c, F_c) from V, F, E, P.
  - **if** V_f is empty **then**
    - Add Product(f, L, M) to scalars S.
  - **else**
    - Let $L' \leftarrow \bigcup\{P(v) \mid v \in V_f\}$ be the next plate set where f has variables.
    - **if** $L' = L$ **then error**("Intractable!");
    - Let $f' \leftarrow$ Product$(f, L \setminus L', M)$.
    - Add f' to F, E, P appropriately.

return SumProduct$(S, \{\})$

```
def plated_sum_product(sum_op, prod_op, factors, eliminate, plates):
    sum_vars = eliminate - plates
    ...
    scalars = []
    while ordinal_to_factors:
        leaf = max(ordinal_to_factors, key=len)
        leaf_factors = ordinal_to_factors.pop(leaf)
        leaf_vars = ordinal_to_vars[leaf]
        for (group_factors, group_vars) in partition(leaf_factors, leaf_vars):
            f = reduce(prod_op, group_factors).reduce(sum_op, group_vars)
            remaining_sum_vars = sum_vars.intersection(f.inputs)
            if not remaining_sum_vars:
                scalars.append(f.reduce(prod_op, leaf & eliminate))
            else:
                new_plates = frozenset().union(
                    *(var_to_ordinal[v] for v in remaining_sum_vars))
                if new_plates == leaf:
                    raise ValueError("Intractable!")
                f = f.reduce(prod_op, leaf - new_plates)
                ordinal_to_factors[new_plates].append(f)
    return reduce(prod_op, scalars)
```

This would have been heinously complex without Funsors

Questions?

github.com / pyro-ppl / funsor ← code

funsor.pyro.ai ← docs

arxiv.org / abs / 1910.10775 ← longer paper

Extra Material

Variational inference

fun GenerativeModel(x)	$p \leftarrow 1$
$\quad z \leftarrow \text{sample}(P_z)$	$p \leftarrow p \times P_z[v = z]$
$\quad \text{observe}(P_x[\theta = z],\ x)$	$p \leftarrow p \times P_x[v = x, \theta = z]$
end	
fun InferenceModel(x)	$q \leftarrow 1$
$\quad z \leftarrow \text{sample}(Q[\theta = x])$	$q \leftarrow q \times Q[v = z, \theta = x]$
end	maximize: $\sum_z q \log \frac{p}{q}$

Pyro as modeling frontend

A new DSL for inference backend

modeling frontend

```
def model():
    x = pyro.sample("x", Px)
    y = pyro.sample("y", Py(θ=x),
                    obs=data)
```

Pyro

inference backend

```
p = 1
p *= Px(x="x")
p *= Py(θ="x")(y=data)


p = p.sum()  # marginalize out x
loss = -log(p)
loss.backward()
```

PSEUDOCODE

modeling frontend

```
def guide(data):
    x = pyro.sample("x", Qx(data))

def model(data):
    x = pyro.sample("x", Px)
    y = pyro.sample("y", Py(θ=x),
                          obs=data)
```

Pyro

inference backend

```
log_q = 0
log_q += Qx(data)(x="x")

log_p = 0
log_p += Px(x="x")
log_p += Py(θ="x")(y=data)

elbo = log_q.exp() * (log_p - log_q)
elbo = elbo.sum()  # marginalize out x
loss = -elbo
loss.backward()
```

PSEUDOCODE

modeling frontend

semi-symbolic backend

```
y = Tensor(torch.randn(10))
assert isinstance(y + y, Tensor)   # eager

x = Variable("x", reals(10))
assert isinstance(x + x, Binary)   # lazy
assert isinstance(x + y, Binary)   # lazy
```

Funsor

Pyro

```
from pyro.generic import distributions as dist
from pyro.generic import infer, optim, pyro, pyro_backend

def model(data):
    locs = pyro.param("locs", torch.tensor([-1., 0., 1.]))
    with pyro.plate("plate", len(data), dim=-1):
        x = pyro.sample("x", dist.Categorical(torch.ones(3) / 3))
        pyro.sample("obs", dist.Normal(locs[x], 1.), obs=data)

def guide(data):
    with pyro.plate("plate", len(data), dim=-1):
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        pyro.sample("x", dist.Categorical(p))

for backend in ["pyro", "funsor"]:
    with pyro_backend(backend):
        svi = infer.SVI(model,  guide,  optim.Adam({}),  infer.Trace_ELBO())
        svi.step(data=torch.randn(10))
```

Uses funsor under the hood

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Uses funsor under the hood

Funsor

```
def kalman_filter_model(data):
    log_p = 0.
    x_curr = funsor.Tensor(torch.tensor(0.))

    for t, y in enumerate(data):
        x_prev = x_curr
        x_curr = funsor.Variable('x_{}'.format(t), funsor.reals())     # delayed sample
        log_p += dist.Normal(x_prev, trans_noise, value=x_curr)      # transition
        if isinstance(x_prev, funsor.Variable):
            log_p = log_p.reduce(ops.logaddexp, x_prev.name)     # eagerly collapse prev state
        log_p += dist.Normal(x_curr, emit_noise, value=y)           # emission

    return log_p
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        if isinstance(x_prev, funsor.Variable):
            log_p = log_p.reduce(ops.logaddexp, x_prev.name)              # eagerly collapse prev state
        log_p += dist.Normal(x_curr, emit_noise, value=y)                 # emission

    return log_p
```

Funsor

```
def kalman_filter_model(data):
    log_p = 0.
    x_curr = funsor.Tensor(torch.tensor(0.))

    for t, y in enumerate(data):
        x_prev = x_curr
        x_curr = funsor.Variable('x_{}'.format(t), funsor.reals())       # delayed sample
        log_p += dist.Normal(x_prev, trans_noise, value=x_curr)          # transition
        if isinstance(x_prev, funsor.Variable):
            log_p = log_p.reduce(ops.logaddexp, x_prev.name)             # eagerly collapse prev state
        log_p += dist.Normal(x_curr, emit_noise, value=y)                # emission

    return log_p
```

PyTorch

```python
class Encoder(nn.Module):
  def __init__(self):
    super(Encoder, self).__init__()
    self.fc1 = nn.Linear(784, 400)
    self.fc21 = nn.Linear(400, 20)
    self.fc22 = nn.Linear(400, 20)
  def forward(self, image):
    image = image.reshape(
      image.shape[:-2] + (-1,))
    h1 = F.relu(self.fc1(image))
    loc = self.fc21(h1)
    scale = self.fc22(h1).exp()
    return loc, scale

class Decoder(nn.Module):   . . .
```

Funsor

```python
encode = funsor.torch.function(
  reals(28, 28), (reals(20), reals(20)))(Encoder())

decode = funsor.torch.function(
  reals(20), reals(28, 28))(Decoder())

@funsor.interpretation(funsor.monte_carlo)
def vae_loss(data):
  loc, scale = encode(data)
  q = funsor.Independent(
        dist.Normal(loc['i'], scale['i'], value='z'), 'z', 'i')

  probs = decode('z')
  p = dist.Bernoulli(probs['x', 'y'], value=data['x', 'y'])
  p = p.reduce(ops.add, frozenset(['x', 'y']))

  elbo = funsor.Integrate(q, p - q, frozenset(['z']))
  return -elbo.reduce(ops.add, 'batch')
```

Funsor

image : reals(28,28) ⊢ encode : reals(20) × reals(20)

z : reals(20) ⊢ decode : reals(28,28)

```
encode = funsor.torch.function(
    reals(28, 28), (reals(20), reals(20)))(Encoder())

decode = funsor.torch.function(
    reals(20), reals(28, 28))(Decoder())

@funsor.interpretation(funsor.monte_carlo)
def vae_loss(data):
    loc, scale = encode(data)
    q = funsor.Independent(
            dist.Normal(loc['i'], scale['i'], value='z'), 'z', 'i')

    probs = decode('z')
    p = dist.Bernoulli(probs['x', 'y'], value=data['x', 'y'])
    p = p.reduce(ops.add, frozenset(['x', 'y']))

    elbo = funsor.Integrate(q, p - q, frozenset(['z']))
    return -elbo.reduce(ops.add, 'batch')
```