Wenzhe Li* Tsinghua University

Antonio Vergari University of California, Los Angeles *Zhe Zeng*^{*} University of California, Los Angeles

Guy Van den Broeck University of California, Los Angeles

*Wenzhe Li** Tsinghua University

Antonio Vergari University of California, Los Angeles *Zhe Zeng*^{*} University of California, Los Angeles

Guy Van den Broeck University of California, Los Angeles

Wenzhe Li* Tsinghua University

Antonio Vergari University of California, Los Angeles *Zhe Zeng*^{*} University of California, Los Angeles

Guy Van den Broeck University of California, Los Angeles

*Wenzhe Li** Tsinghua University

Antonio Vergari University of California, Los Angeles *Zhe Zeng*^{*} University of California, Los Angeles

Guy Van den Broeck University of California, Los Angeles



Given two distributions ${\bf p}$ and ${\bf q}$, and a kernel ${\bf k}$, the task is to compute the *expected kernel*

 $\mathbb{E}_{\mathbf{x} \sim \mathbf{p}, \mathbf{x}' \sim \mathbf{q}}[\mathbf{k}(\mathbf{x}, \mathbf{x}')]$



Given two distributions ${\bf p}$ and ${\bf q}$, and a kernel ${\bf k}$, the task is to compute the *expected kernel*

$$\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')]$$

 \Rightarrow In kernel-based frameworks, expected kernels are omnipresent!



Given two distributions ${\bf p}$ and ${\bf q},$ and a kernel k, the task is to compute the <code>expected kernel</code>

 $\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')]$

 \Rightarrow In kernel-based frameworks, expected kernels are omnipresent!

squared Maximum Mean Discrepancy (MMD) $\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{p}}[\mathbf{k}(\mathbf{x},\mathbf{x}')] + \mathbb{E}_{\mathbf{x}\sim\mathbf{q},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')] - 2\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')]$



Given two distributions ${\bf p}$ and ${\bf q},$ and a kernel k, the task is to compute the <code>expected kernel</code>

 $\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')]$

 \Rightarrow In kernel-based frameworks, expected kernels are omnipresent!

Discrete Kernelized Stein Discrepancy (KDSD) $\mathbb{E}_{\mathbf{x},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}_{\mathbf{p}}(\mathbf{x},\mathbf{x}')]$



$$\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')] = \int_{\mathbf{x},\mathbf{x}'} \mathbf{p}(\mathbf{x}) \mathbf{q}(\mathbf{x}') \mathbf{k}(\mathbf{x},\mathbf{x}') \, d\mathbf{x} \, d\mathbf{x}'$$



$$\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')] = \int_{\mathbf{x},\mathbf{x}'} \mathbf{p}(\mathbf{x})\mathbf{q}(\mathbf{x}')\mathbf{k}(\mathbf{x},\mathbf{x}') \, d\mathbf{x} \, d\mathbf{x}'$$

$$\begin{split} \mathbf{p}, \mathbf{q}, \mathbf{k} \text{ fully factorized} \\ \mathbf{p}(\mathbf{x}) &= \prod_i \mathbf{p}(x_i), \mathbf{q}(\mathbf{x}) = \prod_i \mathbf{q}(x_i) \\ \mathbf{k}(\mathbf{x}, \mathbf{x}') &= \prod_i \mathbf{k}(x_i, x'_i) \\ \Rightarrow \text{ expected kernel is tractable} \\ \prod_i (\int_{x_i, x'_i} \mathbf{p}(x_i) \mathbf{q}(x'_i) \mathbf{k}(x_i, x'_i)) \end{split}$$



$$\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')] = \int_{\mathbf{x},\mathbf{x}'} \mathbf{p}(\mathbf{x})\mathbf{q}(\mathbf{x}')\mathbf{k}(\mathbf{x},\mathbf{x}') \, d\mathbf{x} \, d\mathbf{x}'$$

p, q, k fully factorized

PRO. Tractable exact computation **CON.** Model being too restrictive



$$\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')] = \int_{\mathbf{x},\mathbf{x}'} \mathbf{p}(\mathbf{x})\mathbf{q}(\mathbf{x}')\mathbf{k}(\mathbf{x},\mathbf{x}') \, d\mathbf{x} \, d\mathbf{x}'$$

 $\mathbf{p}, \mathbf{q}, \mathbf{k}$ fully factorized

PRO. Tractable exact computation **CON.** Model being too restrictive

Hard to compute in general. *approximate with MC or variational inference* **PRO.** Efficient computation **CON.** *no guarantees* on error bounds



$$\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')] = \int_{\mathbf{x},\mathbf{x}'} \mathbf{p}(\mathbf{x})\mathbf{q}(\mathbf{x}')\mathbf{k}(\mathbf{x},\mathbf{x}') \, d\mathbf{x} \, d\mathbf{x}'$$

 $\mathbf{p}, \mathbf{q}, \mathbf{k}$ fully factorized

PRO. Tractable exact computation **CON.** Model being too restrictive



trade-off? Hard to compute in general. approximate with MC or variational inference **PRO.** Efficient computation

CON. *no guarantees* on error bounds

Expressive distribution models + Exact computation of expected kernels?

Expressive distribution models + Exact computation of expectated kernels = Circuits!



Probabilistic Circuits

deep generative models + deep guarantees



Probabilistic Circuits

deep generative models + deep guarantees

Kernel Circuits

express kernels as circuits



Probabilistic Circuits

deep generative models + deep guarantees



express kernels as circuits

$$\Rightarrow \mathbb{E}_{\mathbf{x} \sim \mathbf{p}, \mathbf{x}' \sim \mathbf{q}}[\mathbf{k}(\mathbf{x}, \mathbf{x}')]$$

Tractable computational graphs

I. A simple tractable distribution is a PC



e.g., a multivariate Gaussian

 X_1

Tractable computational graphs

I. A simple tractable distribution is a PC

II. A convex combination of PCs is a PC

e.g., a mixture model



Tractable computational graphs

I. A simple tractable distribution is a PCII. A convex combination of PCs is a PCIII. A product of PCs is a PC



Tractable computational graphs



Tractable computational graphs



Probabilistic queries = **feedforward** evaluation

$$p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$$



Probabilistic queries = **feedforward** evaluation

$$p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$$



Probabilistic queries = **feedforward** evaluation

$$p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2) = 0.75$$





PCs are computational graphs



PCs are computational graphs encoding *deep mixture models*

 \Rightarrow stacking (categorical) latent variables



PCs are computational graphs encoding *deep mixture models*

 \Rightarrow stacking (categorical) latent variables

PCs compactly represent *polynomials with exponentially many terms*

 \Rightarrow universal approximators



PCs are computational graphs encoding *deep mixture models*

 \Rightarrow stacking (categorical) latent variables PCs compactly represent *polynomials with exponentially many terms* \Rightarrow universal approximators

PCs are expressive *deep generative models*!



 \Rightarrow we can learn PCs with millions of parameters in minutes on the GPU [Peharz et al. 20201

On par with intractable models!

How expressive are PCs?

dataset	best circuit	BN	MADE	VAE	dataset	best circuit	BN	MADE	VAE
nltcs	-5.99	-6.02	-6.04	-5.99	dna	-79.88	-80.65	-82.77	-94.56
msnbc	-6.04	-6.04	-6.06	-6.09	kosarek	-10.52	-10.83	-	-10.64
kdd	-2.12	-2.19	-2.07	-2.12	msweb	-9.62	-9.70	-9.59	-9.73
plants	-11.84	-12.65	-12.32	-12.34	book	-33.82	-36.41	-33.95	-33.19
audio	-39.39	-40.50	-38.95	-38.67	movie	-50.34	-54.37	-48.7	-47.43
jester	-51.29	-51.07	-52.23	-51.54	webkb	-149.20	-157.43	-149.59	-146.9
netflix	-55.71	-57.02	-55.16	-54.73	cr52	-81.87	-87.56	-82.80	-81.33
accidents	-26.89	-26.32	-26.42	-29.11	c20ng	-151.02	-158.95	-153.18	-146.9
retail	-10.72	-10.87	-10.81	-10.83	bbc	-229.21	-257.86	-242.40	-240.94
pumbs*	-22.15	-21.72	-22.3	-25.16	ad	-14.00	-18.35	-13.65	-18.81

Peharz et al., "Random sum-product networks: A simple but effective approach to probabilistic deep learning", 2019

Unifying existing tractable models



[Chow and Liu 1968]



Junction trees
[Bach and Jordan 2001]



HMMs [Rabiner and Juang 1986]

Classical tractable models can be compactly represented as PCs

Dang et al., "Strudel: Learning Structured-Decomposable Probabilistic Circuits", 2020



Chow-Liu trees

[Chow and Liu 1968]



Junction trees

[Bach and Jordan 2001]



HMMs

[Rabiner and Juang 1986]



CNets

[Rahman et al. 2014]



SPNs [Poon et al. 2011] $\begin{array}{c} 1 & 4 & 1 \\ .31 & 67 & .57 & .55 & .75 & .25 \\ \hline & & & & & & \\ A & B & -A & -B & & & A & -B & -A & B \end{array}$

PSDDs

[Kisa et al. 2014]



PDGs [Jaeger 2004]



PCs are expressive deep generative models!

&

Certifying tractability for a class of queries

verifying structural properties of the graph

Which structural constraints ensure tractability?



A PC is *decomposable* if all inputs of product units depend on disjoint sets of variables



decomposable circuit

Darwiche and Marquis, "A knowledge compilation map", 2002


A PC is *decomposable* if all inputs of product units depend on disjoint sets of variables A PC is *smooth* if all inputs of sum units depend of the same variable sets



decomposable circuit



smooth circuit



Choi et al., "Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Modeling", 2020

decomposable + smooth PCs = ...

MAR

sufficient and necessary conditions for computing any marginal

$$p(\mathbf{y}) = \int_{\mathsf{val}(\mathbf{Z})} p(\mathbf{z}, \mathbf{y}) \, d\mathbf{Z}, \quad \forall \mathbf{Y} \subseteq \mathbf{X}, \quad \mathbf{Z} = \mathbf{X} \setminus \mathbf{Y}$$

 $\implies by a single feed forward evaluation$

Choi et al., "Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Modeling", 2020

decomposable + smooth PCs = ...

MAR

sufficient and necessary conditions for computing any marginal $\int p(\mathbf{z},\mathbf{y}) \, d\mathbf{Z}$

CON

sufficient and necessary conditions for any conditional distribution

$$p(\mathbf{y} \mid \mathbf{z}) = \frac{\int_{\mathsf{val}(\mathbf{H})} p(\mathbf{z}, \mathbf{y}, \mathbf{h}) \, d\mathbf{H}}{\int_{\mathsf{val}(\mathbf{H})} \int_{\mathsf{val}(\mathbf{Y})} p(\mathbf{z}, \mathbf{y}, \mathbf{h}) \, d\mathbf{H} \, d\mathbf{Y}}, \quad \forall \mathbf{Z}, \mathbf{Y} \subseteq \mathbf{X}$$

$$\implies by \, \textit{two} \, \textit{feedforward evaluations}$$

Choi et al., "Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Modeling", 2020

decomposable + smooth PCs = ...



Choi et al., "Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Modeling", 2020

Can we represent kernels as circuits to characterize tractability of its queries?



Kernel Circuits (KCs)

Exa. Radial basis function (RBF) kernel $\mathbf{k}(\mathbf{x}, \mathbf{x}') = \exp\left(-\sum_{i=1}^{4} |X_i - X'_i|^2\right)$



Kernel Circuits (KCs)

Exa. Radial basis function (RBF) kernel $\mathbf{k}(\mathbf{x}, \mathbf{x}') = \exp\left(-\sum_{i=1}^{4} |X_i - X'_i|^2\right)$



decomposable if all inputs of product units depend on disjoint sets of variables

Kernel Circuits (KCs)

Exa. Radial basis function (RBF) kernel $\mathbf{k}(\mathbf{x}, \mathbf{x}') = \exp\left(-\sum_{i=1}^{4} |X_i - X'_i|^2\right)$



decomposable if all inputs of product units depend on disjoint sets of variables

smooth if all inputs of sum units depend of the same variable sets



Common kernels can be compactly represented as decomposable + smooth KCs:

RBF, (exponentiated) Hamming, polynomial ...



tractable computation via circuit operations

i) PCs p and q, and KC k are **decomposable** + **smooth**



tractable computation via circuit operations

i) PCs p and q and KC k are decomposable + smooth ii) PCs p and q and KC k are compatible

 \Rightarrow decompose in the same way

Expected Kernel

tractable computation via circuit operations

i) PCs \mathbf{p} and \mathbf{q} , and KC \mathbf{k} are **decomposable** + **smooth**

ii) PCs p and q and KC k are $\mbox{compatible}$



 ${X_1}{X_2}$





Expected Kernel

tractable computation via circuit operations

i) PCs ${f p}$ and ${f q}$, and KC ${f k}$ are <code>decomposable</code> + <code>smooth</code>

ii) PCs p and q and KC k are $\mbox{compatible}$





Expected Kernel

tractable computation via circuit operations

i) PCs \mathbf{p} and \mathbf{q} , and KC \mathbf{k} are **decomposable** + **smooth**

ii) PCs p and q and KC k are $\mbox{compatible}$



 ${X_1, X_2, X_3}{X_4}$





 $\{(X_1, X_1'), (X_2, X_2'), (X_3, X_3')\}\{(X_4, X_4')\}$



tractable computation via circuit operations

i) PCs p and q and KC k are <code>decomposable</code> + <code>smooth</code> ii) PCs p and q and KC k are <code>compatible</code>



tractable computation via circuit operations

i) PCs p and q and KC k are decomposable + smooth ii) PCs p and q and KC k are compatible

Then computing expected kernels can be done *tractably* by a forward pass

 \Rightarrow product of the sizes of each circuit!

[Sum Nodes] $\mathbf{p}(\mathbf{X}) = \sum_{i} w_i \mathbf{p}_i(\mathbf{X}), \mathbf{q}(\mathbf{X}') = \sum_{j} w'_j \mathbf{q}_j(\mathbf{X}'), \text{ and kernel } \mathbf{k}(\mathbf{X}, \mathbf{X}') = \sum_{l} w''_l \mathbf{k}_l(\mathbf{X}, \mathbf{X}')$:

[Sum Nodes] $\mathbf{p}(\mathbf{X}) = \sum_{i} w_i \mathbf{p}_i(\mathbf{X}), \mathbf{q}(\mathbf{X}') = \sum_{j} w'_j \mathbf{q}_j(\mathbf{X}'), \text{ and kernel } \mathbf{k}(\mathbf{X}, \mathbf{X}') = \sum_{l} w''_l \mathbf{k}_l(\mathbf{X}, \mathbf{X}')$:

VO

[Sum Nodes] $\mathbf{p}(\mathbf{X}) = \sum_{i} w_i \mathbf{p}_i(\mathbf{X}), \mathbf{q}(\mathbf{X}') = \sum_{j} w'_j \mathbf{q}_j(\mathbf{X}'), \text{ and kernel } \mathbf{k}(\mathbf{X}, \mathbf{X}') = \sum_{l} w''_l \mathbf{k}_l(\mathbf{X}, \mathbf{X}')$:

 $\mathbb{E}_{\mathbf{p},\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')] = \sum_{i,j,l} w_i w'_j w''_l \mathbb{E}_{\mathbf{p}_i,\mathbf{q}_j}[\mathbf{k}_l(\mathbf{x},\mathbf{x}')]$ $\implies \text{ expectation is "pushed down" to children}$

[**Product Nodes**] $\mathbf{p}_{\times}(\mathbf{X}) = \prod_{i} \mathbf{p}_{i}(\mathbf{X}_{i}), \mathbf{q}_{\times}(\mathbf{X}') = \prod_{i} \mathbf{q}_{j}(\mathbf{X}'_{i}), \text{ and kernel } \mathbf{k}_{\times}(\mathbf{X}, \mathbf{X}') = \prod_{i} \mathbf{k}_{i}(\mathbf{X}_{i}, \mathbf{X}'_{i}):$

[**Product Nodes**] $\mathbf{p}_{\times}(\mathbf{X}) = \prod_{i} \mathbf{p}_{i}(\mathbf{X}_{i}), \mathbf{q}_{\times}(\mathbf{X}') = \prod_{i} \mathbf{q}_{j}(\mathbf{X}'_{i}), \text{ and kernel } \mathbf{k}_{\times}(\mathbf{X}, \mathbf{X}') = \prod_{i} \mathbf{k}_{i}(\mathbf{X}_{i}, \mathbf{X}'_{i}):$

q

$$\begin{split} \sum_{\mathbf{x},\mathbf{x}'} \mathbf{p}_{\times}(\mathbf{x}) \mathbf{q}_{\times}(\mathbf{x}') \mathbf{k}_{\times}(\mathbf{x},\mathbf{x}') \\ &= \sum_{\mathbf{x},\mathbf{x}'} \prod_{i} \mathbf{p}(\mathbf{x}_{i}) \mathbf{q}(\mathbf{x}_{i}) \mathbf{k}_{i}(\mathbf{x}_{i},\mathbf{x}_{i}') \\ &= \prod_{i} (\sum_{\mathbf{x}_{i},\mathbf{x}_{i}'} \mathbf{p}(\mathbf{x}_{i}) \mathbf{q}(\mathbf{x}_{i}) \mathbf{k}_{i}(\mathbf{x}_{i},\mathbf{x}_{i}')) \end{split}$$

[**Product Nodes**] $\mathbf{p}_{\times}(\mathbf{X}) = \prod_{i} \mathbf{p}_{i}(\mathbf{X}_{i}), \mathbf{q}_{\times}(\mathbf{X}') = \prod_{i} \mathbf{q}_{j}(\mathbf{X}'_{i}), \text{ and kernel } \mathbf{k}_{\times}(\mathbf{X}, \mathbf{X}') = \prod_{i} \mathbf{k}_{i}(\mathbf{X}_{i}, \mathbf{X}'_{i})$:

$$\mathbb{E}_{\mathbf{p}_{ imes},\mathbf{q}_{ imes}}[\mathbf{k}_{ imes}(\mathbf{x},\mathbf{x}')] = \prod_{i} \mathbb{E}_{\mathbf{p},\mathbf{q}}[\mathbf{k}(\mathbf{x}_{i},\mathbf{x}'_{i})]$$

expectation decomposes into easier ones

Algorithm 1 $\mathbb{E}_{\mathbf{p}_n,\mathbf{q}_m}[\mathbf{k}_l]$ — Computing the expected kernel **Input:** Two compatible PCs \mathbf{p}_n and \mathbf{q}_m , and a KC \mathbf{k}_l that is kernel-compatible with the PC pair \mathbf{p}_n and \mathbf{q}_m .

 $\begin{array}{ll} \text{1: if } m,n,l \text{ are } \textit{input} \text{ nodes then} \\ \text{2: return } \mathbb{E}_{\mathbf{p}n,\mathbf{q}m}[\mathbf{k}_l] \\ \text{3: else if } m,n,l \text{ are } \textit{sum} \text{ nodes then} \\ \text{4: return } \sum_{i\in in(n),j\in in(m),c\in in(l)} w_i w_j' w_c'' \mathbb{E}_{\mathbf{p}i,\mathbf{q}j}[\mathbf{k}_c] \\ \text{5: else if } m,n,l \text{ are } \textit{product} \text{ nodes then} \\ \text{6: return } \mathbb{E}_{\mathbf{p}n_L,\mathbf{q}m_L}[\mathbf{k}_L] \cdot \mathbb{E}_{\mathbf{p}n_R,\mathbf{q}m_R}[\mathbf{k}_R] \end{array}$

Computation can be done in one forward pass!

 $\begin{array}{l} \textbf{Algorithm 2} \ \mathbb{E}_{\mathbf{p}n,\mathbf{q}m}[\mathbf{k}_l] - \text{Computing the expected kernel} \\ \hline \textbf{Input:} \ \text{Two compatible PCs } \mathbf{p}_n \ \text{and} \ \mathbf{q}_m, \ \text{and} \ \text{a KC } \mathbf{k}_l \ \text{that is} \\ \hline \text{kernel-compatible with the PC pair } \mathbf{p}_n \ \text{and} \ \mathbf{q}_m. \end{array}$

```
 \begin{array}{ll} \text{1: if } m,n,l \text{ are } \textit{input} \text{ nodes then} \\ \text{2: } & \text{return } \mathbb{E}_{\mathbf{p}n,\mathbf{q}m}[\mathbf{k}_l] \\ \text{3: } & \text{else if } m,n,l \text{ are } \textit{sum} \text{ nodes then} \\ \text{4: } & \text{return } \sum_{i \in \text{in}(n), j \in \text{in}(m), c \in \text{in}(l)} w_i w_j' w_c'' \mathbb{E}_{\mathbf{p}_i,\mathbf{q}_j}[\mathbf{k}_c] \\ \text{5: } & \text{else if } m,n,l \text{ are } \textit{product} \text{ nodes then} \\ \text{6: } & \text{return } \mathbb{E}_{\mathbf{p}n_L,\mathbf{q}m_L}[\mathbf{k}_L] \cdot \mathbb{E}_{\mathbf{p}n_R,\mathbf{q}m_R}[\mathbf{k}_R] \end{array}
```

Computation can be done in one forward pass!

 \Rightarrow squared maximum mean discrepancy $MMD[\mathbf{p}, \mathbf{q}]$ [Gretton et al. 2012] + determinism, kernelized discrete Stein discrepancy (KDSD) [Yang et al. 2018]

Empirical KDSD $\mathbb{S}(\{\underbrace{w^{(i)}}_{\text{weights}}, \underbrace{\mathbf{x}^{(i)}}_{\text{samples}}\}_{i=1}^n \parallel \mathbf{p})$

$$\mathbb{S}^2(\{w^{(i)}, \mathbf{x}^{(i)}\}_{i=1}^n \parallel \mathbf{p}) = \boldsymbol{w}^\top \boldsymbol{K_p} \boldsymbol{w}, \text{ with } [\boldsymbol{K_p}]_{ij} = k_p(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$$

Given a distribution \mathbf{p} , and samples $\{\mathbf{x}^{(i)}\}_{i=1}^{n}$, the black-box importance sampling obtains weights by solving optimization problem

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w}} \left\{ \boldsymbol{w}^\top \boldsymbol{K}_{\boldsymbol{p}} \boldsymbol{w} \, \middle| \, \sum_{i=1}^n w_i = 1, \; w_i \ge 0 \right\}$$

Empirical KDSD $\mathbb{S}(\{\underbrace{w^{(i)}}_{\text{weights}}, \underbrace{\mathbf{x}^{(i)}}_{\text{samples}}\}_{i=1}^n \parallel \mathbf{p})$

$$\mathbb{S}^2(\{w^{(i)}, \mathbf{x}^{(i)}\}_{i=1}^n \parallel \mathbf{p}) = \boldsymbol{w}^\top \boldsymbol{K_p} \boldsymbol{w}, \text{ with } [\boldsymbol{K_p}]_{ij} = k_p(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$$

Given a distribution \mathbf{p} , and samples $\{\mathbf{x}^{(i)}\}_{i=1}^{n}$, the black-box importance sampling obtains weights by solving optimization problem

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w}} \left\{ \boldsymbol{w}^\top \boldsymbol{K}_{\boldsymbol{p}} \boldsymbol{w} \, \middle| \, \sum_{i=1}^n w_i = 1, \; w_i \geq 0
ight\}$$

Empirical KDSD $\mathbb{S}(\{\underbrace{w^{(i)}}_{\text{weights}}, \underbrace{\mathbf{x}^{(i)}}_{\text{samples}}\}_{i=1}^n \parallel \mathbf{p})$

$$\mathbb{S}^2(\{w^{(i)}, \mathbf{x}^{(i)}\}_{i=1}^n \parallel \mathbf{p}) = \boldsymbol{w}^\top \boldsymbol{K_p} \boldsymbol{w}, \text{ with } [\boldsymbol{K_p}]_{ij} = k_p(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$$

Given a distribution \mathbf{p} , and samples $\{\mathbf{x}^{(i)}\}_{i=1}^{n}$, the black-box importance sampling obtains weights by solving optimization problem

$$\boldsymbol{w}^* = \operatorname*{argmin}_{\boldsymbol{w}} \left\{ \boldsymbol{w}^\top \boldsymbol{K_p} \boldsymbol{w} \left| \sum_{i=1}^n w_i = 1, \; w_i \geq 0 \right. \right\}$$

Can we use less samples but maintain the same or even better performance?

Empirical KDSD $\mathbb{S}(\{\underbrace{w^{(i)}}_{\text{weights}}, \underbrace{\mathbf{x}^{(i)}}_{\text{samples}}\}_{i=1}^n \parallel \mathbf{p})$

$$\mathbb{S}^2(\{w^{(i)}, \mathbf{x}^{(i)}\}_{i=1}^n \parallel \mathbf{p}) = \boldsymbol{w}^\top \boldsymbol{K_p} \boldsymbol{w}, \text{ with } [\boldsymbol{K_p}]_{ij} = k_p(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$$

Given a distribution \mathbf{p} , and samples $\{\mathbf{x}^{(i)}\}_{i=1}^{n}$, the black-box importance sampling obtains weights by solving optimization problem

$$oldsymbol{w}^* = \operatorname*{argmin}_{oldsymbol{w}} \left\{ oldsymbol{w}^{ op} oldsymbol{K}_{oldsymbol{p}} oldsymbol{w} \left| \sum_{i=1}^n w_i = 1, \ w_i \geq 0
ight\}$$

Can we use less samples but maintain the same or even better performance?

 \Rightarrow Collapsed samples!

Given partial samples {x_s⁽ⁱ⁾}ⁿ_{i=1}, with (X_s, X_c) a partition of X,
 Represent the conditional distributions p(X_c | x_s⁽ⁱ⁾) as PCs p_i by knowledge compilation [Shen et al. 2016]

Compile the kernel function $k(\mathbf{X_c}, \mathbf{X_c}')$ as KC k

Empirical KDSD between collapsed samples and the target distribution ${f p}$

$$\mathbb{S}^2_{\mathbf{s}}({\{\mathbf{x}_{\mathbf{s}}^{(i)}, w_i\}} \parallel p) = \boldsymbol{w}^\top \boldsymbol{K}_{p,\mathbf{s}} \boldsymbol{w}$$

with $[\mathbf{K}_{p,\mathbf{s}}]_{ij} = \mathbb{E}_{\mathbf{x_c} \sim \mathbf{p}_i, \mathbf{x'_c} \sim \mathbf{p}_j} [\mathbf{k}_p(\mathbf{x}, \mathbf{x'})]$

$$oldsymbol{w}^* = \operatorname*{argmin}_{oldsymbol{w}} \left\{ oldsymbol{w}^ op oldsymbol{K}_{p,\mathbf{s}} oldsymbol{w} \ \left| \ \sum_{i=1}^n w_i = 1, \ w_i \ge 0
ight\}
ight.$$

- Given partial samples $\{\mathbf{x_s}^{(i)}\}_{i=1}^n$, with $(\mathbf{X_s}, \mathbf{X_c})$ a partition of \mathbf{X} ,
- Represent the conditional distributions $\mathbf{p}(\mathbf{X}_{c} \mid \mathbf{x}_{s}^{(i)})$ as PCs \mathbf{p}_{i} by knowledge compilation [Shen et al. 2016]
- Compile the kernel function $k(\mathbf{X_c}, \mathbf{X_c}')$ as KC k

Empirical KDSD between collapsed samples and the target distribution ${f p}$

$$\mathbb{S}^2_{\mathbf{s}}(\{\mathbf{x}_{\mathbf{s}}^{(i)}, w_i\} \parallel p) = \boldsymbol{w}^\top \boldsymbol{K}_{p,\mathbf{s}} \boldsymbol{w}_i$$

with $[\mathbf{K}_{p,\mathbf{s}}]_{ij} = \mathbb{E}_{\mathbf{x_c} \sim \mathbf{p}_i, \mathbf{x'_c} \sim \mathbf{p}_j} [\mathbf{k}_p(\mathbf{x}, \mathbf{x'})]$

$$oldsymbol{w}^* = \operatorname*{argmin}_{oldsymbol{w}} \left\{ oldsymbol{w}^ op oldsymbol{K}_{p,\mathbf{s}} oldsymbol{w} \ \left| \ \sum_{i=1}^n w_i = 1, \ w_i \ge 0
ight\}
ight.$$

Given partial samples { x_s⁽ⁱ⁾ }ⁿ_{i=1}, with (X_s, X_c) a partition of X,
 Represent the conditional distributions p(X_c | x_s⁽ⁱ⁾) as PCs p_i by knowledge compilation [Shen et al. 2016]

Compile the kernel function $k(\mathbf{X_c}, \mathbf{X_c}')$ as KC k

Empirical KDSD between collapsed samples and the target distribution p

$$\mathbb{S}^2_{\mathbf{s}}(\{\mathbf{x_s}^{(i)}, w_i\} \parallel p) = \boldsymbol{w}^{\top} \boldsymbol{K}_{p, \mathbf{s}} \boldsymbol{u}$$

with $[\mathbf{K}_{p,\mathbf{s}}]_{ij} = \mathbb{E}_{\mathbf{x_c} \sim \mathbf{p}_i, \mathbf{x'_c} \sim \mathbf{p}_j} [\mathbf{k}_p(\mathbf{x}, \mathbf{x'})]$

$$oldsymbol{w}^* = rgmin_{oldsymbol{w}} \left\{ oldsymbol{w}^ op oldsymbol{K}_{p, \mathbf{s}} oldsymbol{w} \ \left| \ \sum_{i=1}^n w_i = 1, \ w_i \geq 0
ight\}
ight.$$

Given partial samples {x_s⁽ⁱ⁾}ⁿ_{i=1}, with (X_s, X_c) a partition of X,
 Represent the conditional distributions p(X_c | x_s⁽ⁱ⁾) as PCs p_i by *knowledge compilation* [Shen et al. 2016]

Compile the kernel function $k(\mathbf{X_c}, \mathbf{X_c}')$ as KC k

Empirical KDSD between collapsed samples and the target distribution ${f p}$

 $\mathbb{S}^2_{\mathbf{s}}(\{\mathbf{x_s}^{(i)}, w_i\} \parallel p) = \boldsymbol{w}^\top \boldsymbol{K}_{p, \mathbf{s}} \boldsymbol{w}$

with $[m{K}_{p,\mathbf{s}}]_{ij} = \mathbb{E}_{\mathbf{x_c}\sim\mathbf{p}_i,\mathbf{x'_c}\sim\mathbf{p}_j} \left[\mathbf{k}_p(\mathbf{x},\mathbf{x'})
ight]$

$$oldsymbol{w}^* = \operatorname*{argmin}_{oldsymbol{w}} \left\{ oldsymbol{w}^ op oldsymbol{K}_{p,\mathbf{s}} oldsymbol{w} \ \left| \ \sum_{i=1}^n w_i = 1, \ w_i \geq 0
ight\}
ight.$$

Given partial samples $\{\mathbf{x_s}^{(i)}\}_{i=1}^n$, with $(\mathbf{X_s}, \mathbf{X_c})$ a partition of \mathbf{X} ,

Represent the conditional distributions $p(X_c | x_s^{(i)})$ as PCs p_i by knowledge compilation [Shen et al. 2016]

 \mid Compile the kernel function ${f k}({f X_c},{f X_c}')$ as KC f k

Empirical KDSD between collapsed samples and the target distribution ${f p}$

$$\mathbb{S}^2_{\mathbf{s}}(\{\mathbf{x_s}^{(i)}, w_i\} \parallel p) = \boldsymbol{w}^\top \boldsymbol{K}_{p, \mathbf{s}} \boldsymbol{w}_{p, \mathbf{s}}$$

with $[\boldsymbol{K}_{p,\mathbf{s}}]_{ij} = \mathbb{E}_{\mathbf{x_c} \sim \mathbf{p}_i, \mathbf{x'_c} \sim \mathbf{p}_j} \left[\mathbf{k}_p(\mathbf{x}, \mathbf{x'}) \right]$

$$oldsymbol{w}^* = \operatorname*{argmin}_{oldsymbol{w}} \left\{ oldsymbol{w}^{ op} oldsymbol{K}_{p, \mathbf{s}} oldsymbol{w} \ \left| \ \sum_{i=1}^n w_i = 1, \ w_i \geq 0
ight\}
ight.$$

Given partial samples $\{\mathbf{x_s}^{(i)}\}_{i=1}^n$, with $(\mathbf{X_s}, \mathbf{X_c})$ a partition of \mathbf{X} ,

Represent the conditional distributions $p(X_c | x_s^{(i)})$ as PCs p_i by knowledge compilation [Shen et al. 2016]

 \mid Compile the kernel function ${f k}({f X_c},{f X_c}')$ as KC f k

Empirical KDSD between collapsed samples and the target distribution ${f p}$

$$\mathbb{S}^2_{\mathbf{s}}(\{\mathbf{x_s}^{(i)}, w_i\} \parallel p) = \boldsymbol{w}^{ op} \boldsymbol{K}_{p,\mathbf{s}} \boldsymbol{w}_{p,\mathbf{s}}$$

with $[\boldsymbol{K}_{p,\mathbf{s}}]_{ij} = \mathbb{E}_{\mathbf{x_c} \sim \mathbf{p}_i, \mathbf{x'_c} \sim \mathbf{p}_j} [\mathbf{k}_p(\mathbf{x}, \mathbf{x'})]$

$$oldsymbol{w}^* = \operatorname*{argmin}_{oldsymbol{w}} \left\{ oldsymbol{w}^ op oldsymbol{K}_{p, \mathbf{s}} oldsymbol{w} \, igg|_{i=1}^n w_i = 1, \ w_i \geq 0
ight\}$$
Collapsed Black-box Importance Sampling



methods with collapsed samples all outperform their non-collapsed counterparts
 CBBIS performs equally well or better than other baselines

Friedman and Broeck, "Approximate Knowledge Compilation by Online Collapsed Importance Sampling", 2018 Liu and Lee, "Black-box importance sampling", 2016



Collapsed black-box importance sampling

Support vector regression with missing features



Takeaways

#1: you can be both tractable and expressive#2: circuits are a foundation for tractable inference over kernels



What other applications would benefit from the tractable computation of the expected kernels?

More on circuits ...

Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Models
starai.cs.ucla.edu/papers/ProbCirc20.pdf

Probabilistic Circuits: Representations, Inference, Learning and Theory
youtube.com/watch?v=2RAG5-L9R70

Probabilistic Circuits
arranger1044.github.io/probabilistic-circuits/

Foundations of Sum-Product Networks for probabilistic modeling tinyurl.com/w65po5d

Questions?



References I

- Chow, C and C Liu (1968). "Approximating discrete probability distributions with dependence trees". In: IEEE Transactions on Information Theory 14.3, pp. 462–467.
- Babiner, Lawrence and Biinghwang Juang (1986). "An introduction to hidden Markov models". In: ieee assp magazine 3.1, pp. 4–16.
- Bach, Francis R. and Michael I. Jordan (2001). "Thin Junction Trees". In: Advances in Neural Information Processing Systems 14. MIT Press, pp. 569–576.
- Darwiche, Adnan and Pierre Marquis (2002). "A knowledge compilation map". In: Journal of Artificial Intelligence Research 17, pp. 229–264.
- Jaeger, Manfred (2004). "Probabilistic decision graphs—combining verification and AI techniques for probabilistic inference". In: International Journal of Uncertainty, Fuzziness and Knowledge-Based Systems 12.supp01, pp. 19–42.
- Kisa, Doga, Guy Van den Broeck, Arthur Choi, and Adnan Darwiche (July 2014). "Probabilistic sentential decision diagrams". In: Proceedings of the 14th International Conference on Principles of Knowledge Representation and Reasoning (KR). Vienna, Austria. URL: http://starai.cs.ucla.edu/papers/KisaKR14.pdf.
- Liu, Qiang and Jason D Lee (2016). "Black-box importance sampling". In: arXiv preprint arXiv:1610.05247.
- Friedman, Tal and Guy Van den Broeck (Dec. 2018). "Approximate Knowledge Compilation by Online Collapsed Importance Sampling". In: Advances in Neural Information Processing Systems 31 (NeurIPS). URL: http://starai.cs.ucla.edu/papers/FriedmanNeurIPS18.pdf.
- Peharz, Robert, Antonio Vergari, Karl Stelzner, Alejandro Molina, Xiaoting Shao, Martin Trapp, Kristian Kersting, and Zoubin Ghahramani (2019). "Random sum-product networks: A simple but effective approach to probabilistic deep learning". In: UAI.
- 🕀 🛛 Choi, YooJung, Antonio Vergari, and Guy Van den Broeck (2020). "Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Modeling". In:
- 🕀 Dang, Meihua, Antonio Vergari, and Guy Van den Broeck (2020). "Strudel: Learning Structured-Decomposable Probabilistic Circuits". In: PGM abs/2007.09331.

References II

Peharz, Robert, Steven Lang, Antonio Vergari, Karl Stelzner, Alejandro Molina, Martin Trapp, Guy Van den Broeck, Kristian Kersting, and Zoubin Ghahramani (2020). "Einsum Networks: Fast and Scalable Learning of Tractable Probabilistic Circuits". In: International Conference of Machine Learning.