Tractable Computation of Expected Kernels by Circuits

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A Fundamental Task

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

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

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In kernel-based frameworks, expected kernels are omnipresent!

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⇒ In kernel-based frameworks, expected kernels are omnipresent!

squared Maximum Mean Discrepancy (MMD)

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

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⇒ In kernel-based frameworks, expected kernels are omnipresent!

Discrete Kernelized Stein Discrepancy (KDSD)

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

Challenge

Reliability vs. Flexibility

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

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



Reliability vs. Flexibility

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

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

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



Reliability vs. Flexibility

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 ${f p},{f q},{f k}$ 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

Challenge

Reliability vs. Flexibility

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

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

4

Exact computation of expectated kernels

Circuits!

Circuits

Probabilistic Circuits

deep generative models + deep guarantees

Circuits

Probabilistic Circuits

deep generative models + deep guarantees

Kernel Circuits

express kernels as circuits

Circuits

Probabilistic Circuits

deep generative models + deep guarantees

Kernel Circuits

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

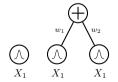
⇒ e.g., a multivariate Gaussian



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

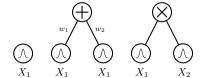


Tractable computational graphs

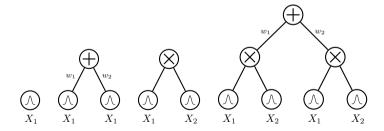
I. A simple tractable distribution is a PC

II. A convex combination of PCs is a PC

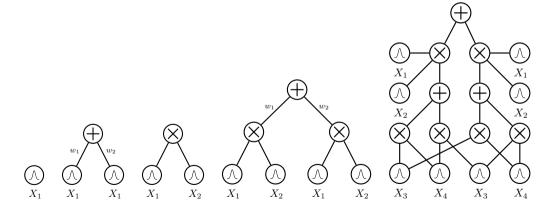
III. A product of PCs is a PC



Tractable computational graphs

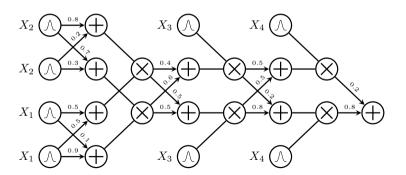


Tractable computational graphs



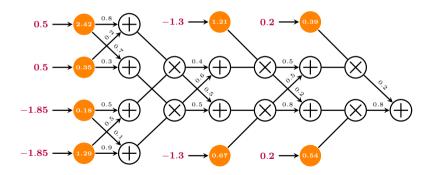
Probabilistic queries = **feedforward** evaluation

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



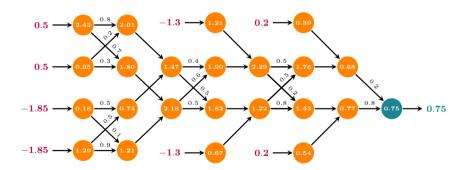
Probabilistic queries = **feedforward** evaluation

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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*

⇒ stacking (categorical) latent variables

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PCs compactly represent *polynomials with exponentially many terms*

⇒ universal approximators

PCs are computational graphs encoding *deep mixture models*

⇒ stacking (categorical) latent variables

PCs compactly represent polynomials with exponentially many terms

⇒ universal approximators

PCs are expressive *deep generative models*!



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

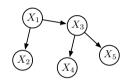
On par with intractable models!

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

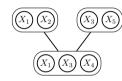
Peharz et al., "Random sum-product networks: A simple but effective approach to probabilistic deep learning", 2019

Unifying existing tractable models



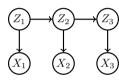
Chow-Liu trees

[Chow and Liu 1968]



Junction trees

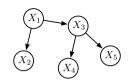
[Bach and Jordan 2001]



HMMs

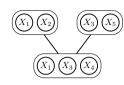
[Rabiner and Juang 1986]

Classical tractable models can be compactly represented as PCs



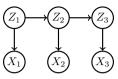
Chow-Liu trees

[Chow and Liu 1968]



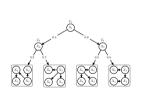
Junction trees

[Bach and Jordan 2001]



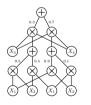
HMMs

[Rabiner and Juang 1986]



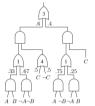
CNets

[Rahman et al. 2014]



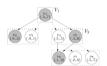
SPNs

[Poon et al. 2011]



PSDDs

[Kisa et al. 2014]



PDGs

[Jaeger 2004]

PCs = deep learning + deep guarantees

PCs are expressive deep generative models!

&

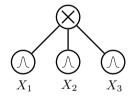
Certifying tractability for a class of queries

verifying structural properties of the graph

Which structural constraints ensure tractability?

decomposable + smooth PCs

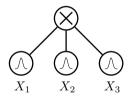
A PC is *decomposable* if all inputs of product units depend on disjoint sets of variables



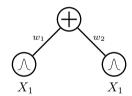
decomposable circuit

decomposable + smooth PCs

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

decomposable + smooth PCs = ...

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

MAR

sufficient and necessary conditions for computing any marginal

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

⇒ by a single feedforward evaluation

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

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

$$\implies \text{by two feedforward evaluations}$$

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 $\frac{\int p(\mathbf{z}, \mathbf{y}, \mathbf{h}) d\mathbf{H}}{\int \int p(\mathbf{z}, \mathbf{y}, \mathbf{h}) d\mathbf{H} d\mathbf{Y}}$

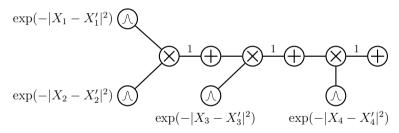
? What a

What about the **expected kernel** $\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')]$?

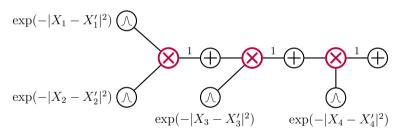
Can we represent kernels as circuits to characterize tractability of its queries?



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

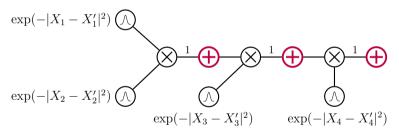


Exa. Radial basis function (RBF) kernel $\mathbf{k}(\mathbf{x}, \mathbf{x}') = \exp\left(-\sum_{i=1}^{4} |X_i - X_i'|^2\right)$



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

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



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

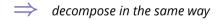
decomposable + **smooth** KCs:

RBF, (exponentiated) Hamming, polynomial ...

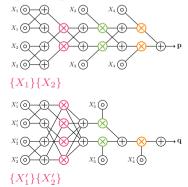
tractable computation via circuit operations

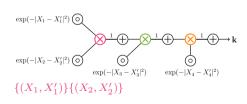
i) PCs ${f p}$ and ${f q}$, and KC ${f k}$ are decomposable + smooth

- i) PCs ${\bf p}$ and ${\bf q}$, and KC ${\bf k}$ are decomposable + smooth
- ii) PCs ${f p}$ and ${f q}$, and KC ${f k}$ are compatible

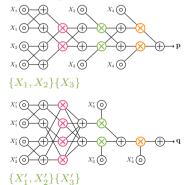


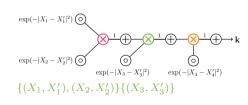
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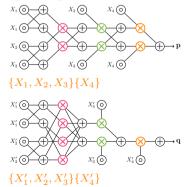


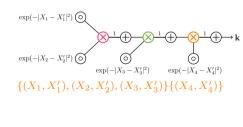
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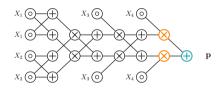
tractable computation via circuit operations

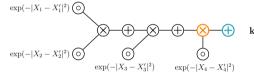
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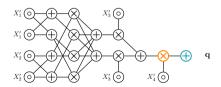
Then computing expected kernels can be done *tractably* by a forward pass

product of the sizes of each circuit!

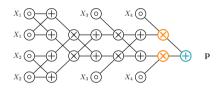
[Sum Nodes] $\mathbf{p}(\mathbf{X}) = \sum_{i} w_{i} \mathbf{p}_{i}(\mathbf{X}), \mathbf{q}(\mathbf{X}') = \sum_{j} w'_{j} \mathbf{q}_{j}(\mathbf{X}'),$ and kernel $\mathbf{k}(\mathbf{X}, \mathbf{X}') = \sum_{l} w''_{l} \mathbf{k}_{l}(\mathbf{X}, \mathbf{X}')$:

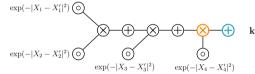


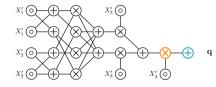




[Sum Nodes] $\mathbf{p}(\mathbf{X}) = \sum_{i} w_{i} \mathbf{p}_{i}(\mathbf{X}), \mathbf{q}(\mathbf{X}') = \sum_{j} w'_{j} \mathbf{q}_{j}(\mathbf{X}'), \text{ and kernel } \mathbf{k}(\mathbf{X}, \mathbf{X}') = \sum_{l} w''_{l} \mathbf{k}_{l}(\mathbf{X}, \mathbf{X}')$:



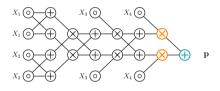


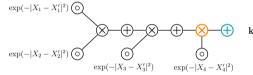


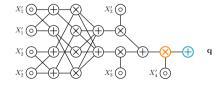
$$\sum_{\mathbf{x},\mathbf{x}'} \mathbf{p}(\mathbf{x}) \mathbf{q}(\mathbf{x}') \mathbf{k}(\mathbf{x},\mathbf{x}')$$

$$= \sum_{i,j,l} w_i w'_j w''_l \mathbf{p}_i(\mathbf{x}) \mathbf{q}_j(\mathbf{x}) \mathbf{k}_l(\mathbf{x},\mathbf{x}')$$

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



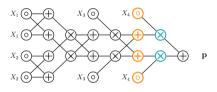


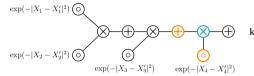


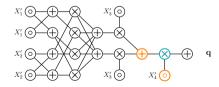
$$\mathbb{E}_{\mathbf{p},\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')] = \sum_{i,j,l} w_i w_j' w_l'' \mathbb{E}_{\mathbf{p}_i,\mathbf{q}_j}[\mathbf{k}_l(\mathbf{x},\mathbf{x}')]$$

expectation is "pushed down" to children

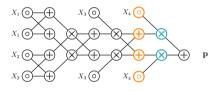
[Product Nodes] $\mathbf{p}_{\times}(\mathbf{X}) = \prod_{i} \mathbf{p}_{i}(\mathbf{X}_{i}), \mathbf{q}_{\times}(\mathbf{X}') = \prod_{i} \mathbf{q}_{j}(\mathbf{X}'_{i}),$ and kernel $\mathbf{k}_{\times}(\mathbf{X}, \mathbf{X}') = \prod_{i} \mathbf{k}_{i}(\mathbf{X}_{i}, \mathbf{X}'_{i})$:

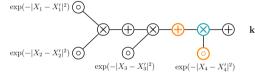


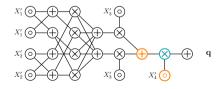




[**Product Nodes**] $\mathbf{p}_{\times}(\mathbf{X}) = \prod_{i} \mathbf{p}_{i}(\mathbf{X}_{i}), \mathbf{q}_{\times}(\mathbf{X}') = \prod_{i} \mathbf{q}_{j}(\mathbf{X}'_{i}), \text{ and kernel } \mathbf{k}_{\times}(\mathbf{X}, \mathbf{X}') = \prod_{i} \mathbf{k}_{i}(\mathbf{X}_{i}, \mathbf{X}'_{i})$:

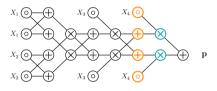


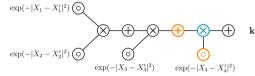


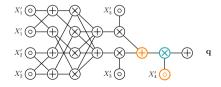


$$\begin{aligned} & \sum_{\mathbf{x},\mathbf{x}'} \mathbf{p}_{\times}(\mathbf{x}) \mathbf{q}_{\times}(\mathbf{x}') \mathbf{k}_{\times}(\mathbf{x},\mathbf{x}') \\ \mathbf{q} & = \sum_{\mathbf{x},\mathbf{x}'} \prod_{i} \mathbf{p}(\mathbf{x}_{i}) \mathbf{q}(\mathbf{x}_{i}) \mathbf{k}_{i}(\mathbf{x}_{i},\mathbf{x}'_{i})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

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







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

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 .

- 1: **if** m, n, l are **input** nodes **then**
- $\mathbb{E}_{\mathbf{p}_n,\mathbf{q}_m}[\mathbf{k}_l]$
- 3: **else if** m, n, l are **sum** nodes **then**
- 4: return $\sum_{i \in \mathsf{in}(n), j \in \mathsf{in}(m), c \in \mathsf{in}(l)} w_i w_j' w_c'' \mathbb{E}_{\mathbf{p}_i, \mathbf{q}_j}[\mathbf{k}_c]$
- 5: **else if** m, n, l are **product** nodes **then**
- 6: return $\mathbb{E}_{\mathbf{p}_{n_{\mathsf{L}}},\mathbf{q}_{m_{\mathsf{L}}}}[\mathbf{k}_{\mathsf{L}}]\cdot\mathbb{E}_{\mathbf{p}_{n_{\mathsf{R}}},\mathbf{q}_{m_{\mathsf{R}}}}[\mathbf{k}_{\mathsf{R}}]$

Computation can be done in one forward pass!

Algorithm 2 $\mathbb{E}_{\mathbf{p}_n,\mathbf{q}_m}[\mathbf{k}_l]$ — 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 .

- 1: $\mathbf{if}\ m,n,l$ are \mathbf{input} nodes \mathbf{then}
- $\mathbb{E}_{\mathbf{p}_n,\mathbf{q}_m}[\mathbf{k}_l]$
- 3: **else if** m, n, l are **sum** nodes **then**
- 4: return $\sum_{i \in \text{in}(n), j \in \text{in}(m), c \in \text{in}(l)} w_i w_j' w_c'' \mathbb{E}_{\mathbf{p}_i, \mathbf{q}_j}[\mathbf{k}_c]$
- 5: **else if** m, n, l are **product** nodes **then**
- 6: **return** $\mathbb{E}_{\mathbf{p}_{n_{\mathsf{L}}},\mathbf{q}_{m_{\mathsf{L}}}}[\mathbf{k}_{\mathsf{L}}] \cdot \mathbb{E}_{\mathbf{p}_{n_{\mathsf{R}}},\mathbf{q}_{m_{\mathsf{R}}}}[\mathbf{k}_{\mathsf{R}}]$

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]

Applications

Collapsed black-box importance sampling

lacksquare Empirical KDSD $\mathbb{S}(\{\underline{w}^{(i)},\ \mathbf{x}^{(i)}\}_{i=1}^n\parallel\mathbf{p})$

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

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

| Empirical KDSD $\mathbb{S}(\set{w^{(i)},\ \mathbf{x}^{(i)}}_{i=1}^n \parallel \mathbf{p})$

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

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

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

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

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

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

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



- 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 $\mathbf{k}(\mathbf{X_c},\mathbf{X_c}')$ as KC \mathbf{k}
- Empirical KDSD between collapsed samples and the target distribution p

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

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

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

- lacksquare 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 $\mathbf{k}(\mathbf{X_c},\mathbf{X_c}')$ as KC \mathbf{k}
- Empirical KDSD between collapsed samples and the target distribution p

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

with
$$[K_{p,\mathbf{s}}]_{ij} = \mathbb{E}_{\mathbf{x}_{\mathbf{c}} \sim \mathbf{p}_i, \mathbf{x}_o' \sim \mathbf{p}_i} [\mathbf{k}_p(\mathbf{x}, \mathbf{x}')]$$

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- lacksquare Empirical KDSD between collapsed samples and the target distribution ${f r}$

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

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} \, \middle| \, \sum_{i=1}^n w_i = 1, \, w_i \geq 0
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- lacksquare 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]
- lacksquare 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 **p**

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

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

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- 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]
- \blacksquare Compile the kernel function $k(X_c, X_c{'})$ as KC k
- lacksquare Empirical KDSD between collapsed samples and the target distribution ${f p}$

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

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

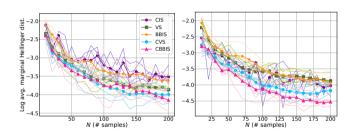
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methods with collapsed samples all outperform their non-collapsed counterparts CBBIS performs equally well or better than other baselines

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

Applications

- Collapsed black-box importance sampling
- Support vector regression with missing features

Conclusion

Takeaways

#1: you can be both tractable and expressive

#2: circuits are a foundation for tractable inference over kernels

What else?

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?



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