Tractable Computation of Expected Kernels by Circuits

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April 29th, 2021 - ***Yahoo Research Seminar***

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Motivation

A Fundamental Task

Given two distributions $\mathbf{p}$ and $\mathbf{q}$, and a kernel $\mathbf{k}$, 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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$\Rightarrow$ *In kernel-based frameworks, expected kernels are omnipresent!*

squared Maximum Mean Discrepancy (MMD)

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

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

$\mathbf{p}(\mathbf{x}) = \prod_i \mathbf{p}(x_i)$, $\mathbf{q}(\mathbf{x}) = \prod_i \mathbf{q}(x_i)$

$\mathbf{k}(\mathbf{x},\mathbf{x}') = \prod_i \mathbf{k}(x_i, x_i')$

$\Rightarrow$ expected kernel is **tractable**

$\prod_i (\int_{x_i, x_i'} \mathbf{p}(x_i)\mathbf{q}(x_i')\mathbf{k}(x_i, x_i'))$

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$\prod_i (\int_{x_i,x_i'} \mathbf{p}(x_i)\mathbf{q}(x_i')\mathbf{k}(x_i,x_i'))$

A computation is **tractable** if it can be done exactly in polynomial time

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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PRO. Tractable exact computation

CON. Model being too restrictive

Challenge

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Hard to compute in general.

$\Longrightarrow$ *approximate with MC or variational inference*

PRO. Efficient computation

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Challenge

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PRO. Tractable exact computation

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trade-off?

Hard to compute in general.

$\Longrightarrow$ *approximate with MC or variational inference*

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Expressive distribution models

+

Exact computation of expected kernels?

Expressive distribution models

+

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

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

Probabilistic Circuits (PCs)

Tractable computational graphs

I. *A simple tractable distribution is a PC*

$\Rightarrow$ *e.g., a multivariate Gaussian*

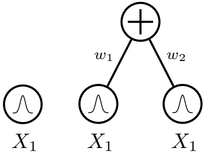
Probabilistic Circuits (PCs)

Tractable computational graphs

I. *A simple tractable distribution is a PC*

II. *A convex combination of PCs is a PC*

$\Rightarrow$ *e.g., a mixture model*



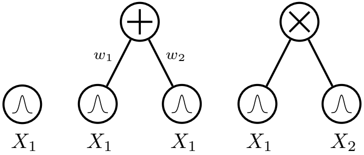
Probabilistic Circuits (PCs)

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*



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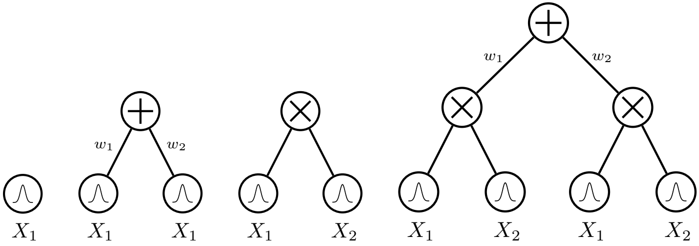

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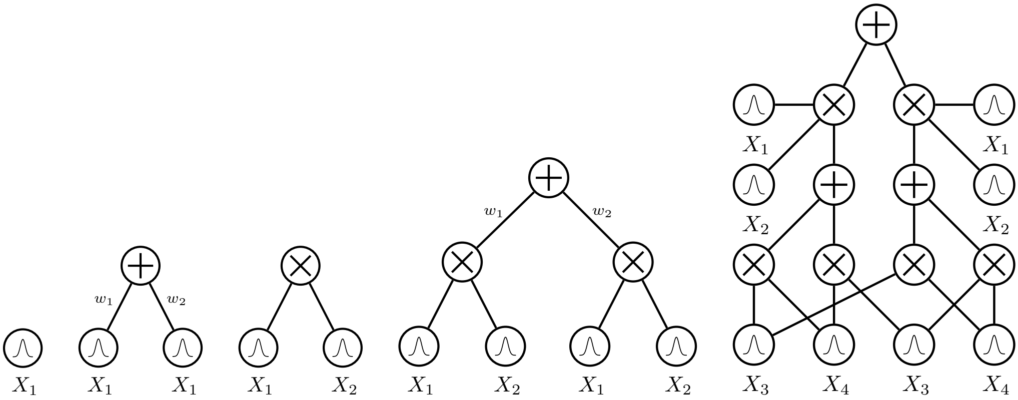
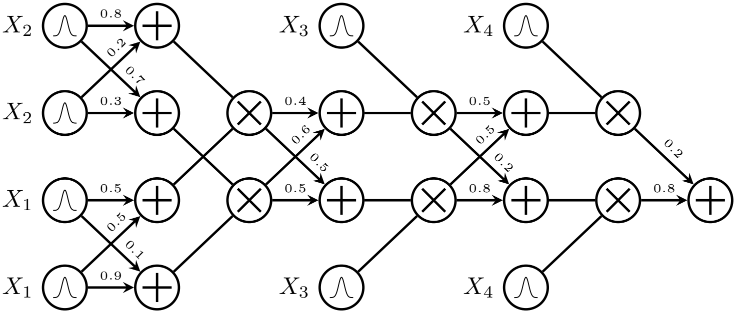


Probabilistic queries = feedforward evaluation

$$p(X_1 = \mathbf{-1.85}, X_2 = \mathbf{0.5}, X_3 = \mathbf{-1.3}, X_4 = \mathbf{0.2})$$



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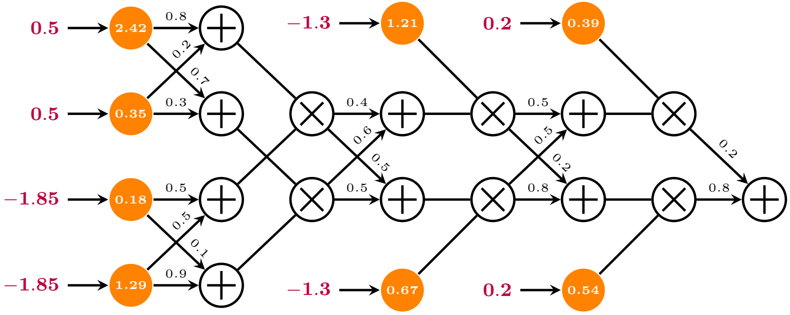
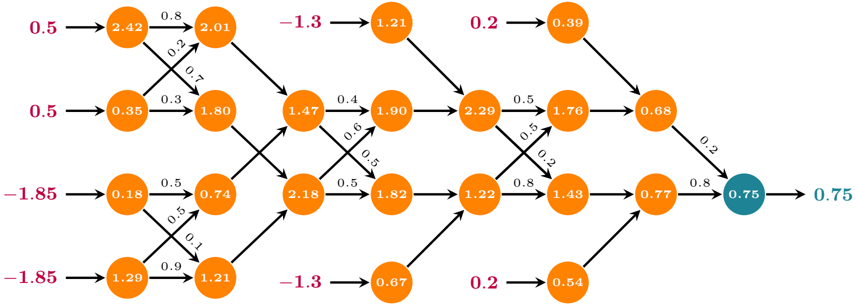


Probabilistic queries = feedforward evaluation

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



PCs = *deep learning*

PCs are computational graphs

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PCs are computational graphs encoding ***deep mixture models***

$\Longrightarrow$ *stacking (categorical) latent variables*

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PCs compactly represent ***polynomials with exponentially many terms***

$\Longrightarrow$ *universal approximators*

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PCs are computational graphs encoding ***deep mixture models***

$\Longrightarrow$ *stacking (categorical) latent variables*

PCs compactly represent ***polynomials with exponentially many terms***

$\Longrightarrow$ *universal approximators*

PCs are expressive *deep generative models*!

$\Longrightarrow$ *we can learn PCs with millions of parameters in minutes on the GPU [Peharz et al. 2020]*

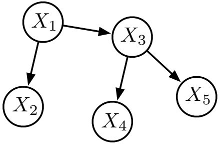
On par with intractable models!

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

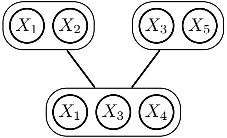
Peharz et al., "Random sum-product networks: A simple but effective approach to probabilistic deep learning", 2019

Unifying existing tractable models



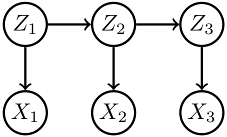
Chow-Liu trees

[Chow and Liu 1968]



Junction trees

[Bach and Jordan 2001]

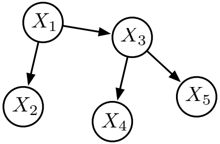


HMMs

[Rabiner and Juang 1986]

Classical tractable models can be compactly represented as PCs

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



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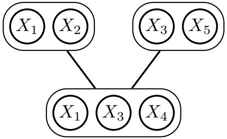

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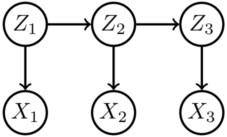

HMMs

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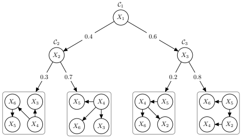
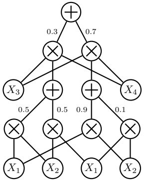


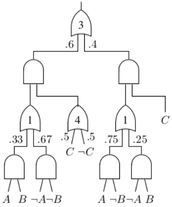
CNets

[Rahman et al. 2014]



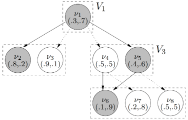
SPNs

[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

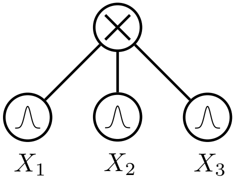
=

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

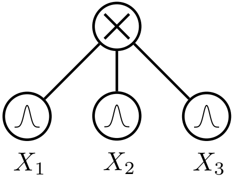


decomposable circuit

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

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



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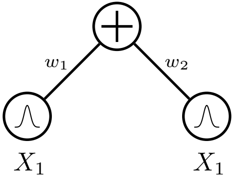


smooth circuit

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

decomposable + *smooth* PCs = ...

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*

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

$\Longrightarrow$ *by a single feedforward 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*

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

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

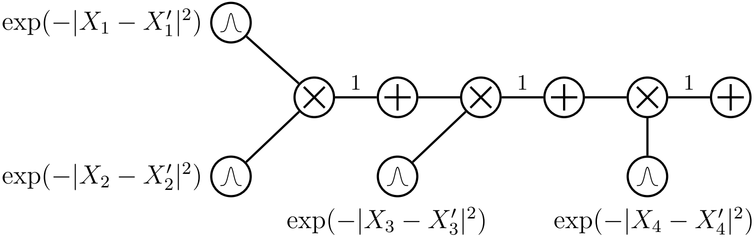
? *What about the* ***expected kernel*** $\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x}, \mathbf{x}')]$*?*

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 $\mathbf{k}(\mathbf{x}, \mathbf{x}') = \exp\left(-\sum_{i=1}^{4} \mid X_i - X_i' \mid^2\right)$



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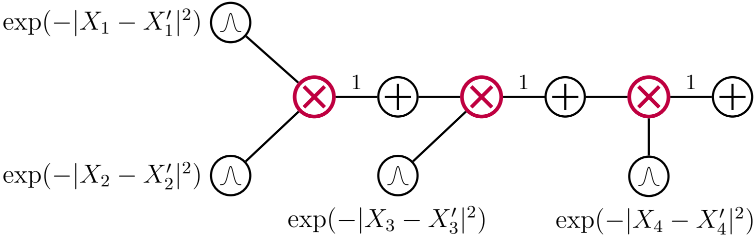

decomposable if all inputs of product units depend on disjoint sets of variables

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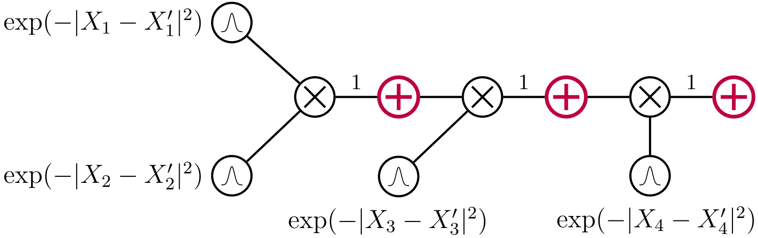

decomposable if all inputs of product units depend on disjoint sets of variables

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

Kernel Circuits (KCs)

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

RBF, (exponentiated) Hamming, polynomial ...

Expected Kernel

tractable computation via circuit operations

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

Expected Kernel

tractable computation via circuit operations

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

ii) PCs $\mathbf{p}$ and $\mathbf{q}$, and KC $\mathbf{k}$ are **compatible**

$\Longrightarrow$ *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**

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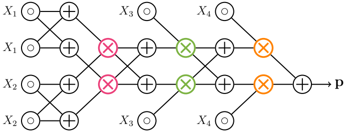
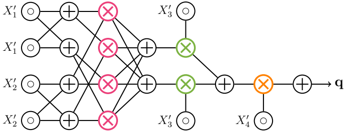
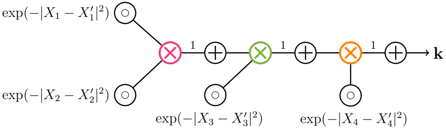


$\{X_1\}\{X_2\}$



$\{X'_1\}\{X'_2\}$



$\{(X_1, X'_1)\}\{(X_2, X'_2)\}$

Expected Kernel

tractable computation via circuit operations

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

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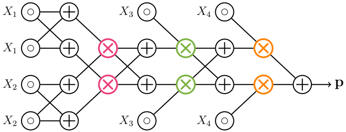
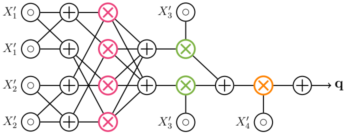
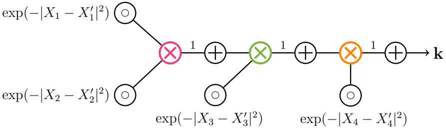


$\{X_1, X_2\}\{X_3\}$



$\{X_1', X_2'\}\{X_3'\}$



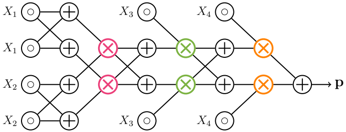
$\{(X_1, X_1'), (X_2, X_2')\}\{(X_3, X_3')\}$

Expected Kernel

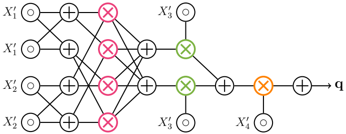
tractable computation via circuit operations

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

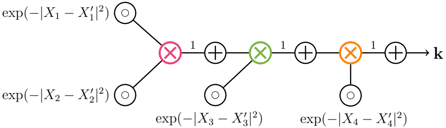
ii) PCs $\mathbf{p}$ and $\mathbf{q}$, and KC $\mathbf{k}$ are **compatible**



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



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



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

Expected Kernel

tractable computation via circuit operations

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

ii) PCs $\mathbf{p}$ and $\mathbf{q}$, and KC $\mathbf{k}$ are **compatible**

Expected Kernel

tractable computation via circuit operations

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

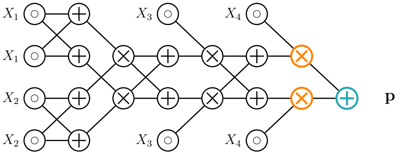
ii) PCs $\mathbf{p}$ and $\mathbf{q}$, and KC $\mathbf{k}$ are **compatible**

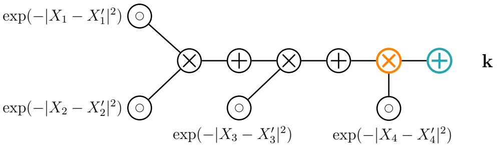
Then computing expected kernels can be done ***tractably*** by a forward pass

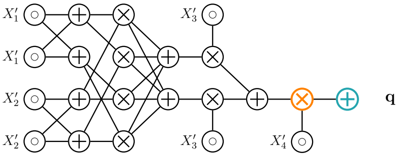
$\Longrightarrow$ *product of the sizes of each circuit!*

smooth + **decomposable** + **compatible** = **tractable E[k]**

[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 $\mathbf{k}(\mathbf{X}, \mathbf{X}') = \sum_l w''_l \mathbf{k}_l(\mathbf{X}, \mathbf{X}')$:







smooth + decomposable + compatible = tractable E[k]

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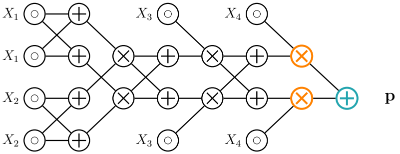

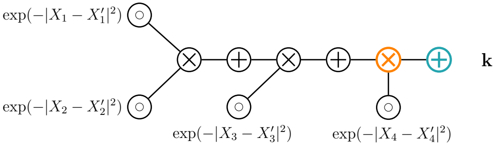

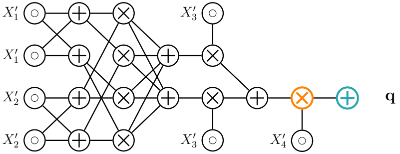

$$\sum_{\mathbf{x},\mathbf{x}'} \mathbf{p}(\mathbf{x})\mathbf{q}(\mathbf{x}')\mathbf{k}(\mathbf{x}, \mathbf{x}')$$

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

smooth + **decomposable** + **compatible** = **tractable E[k]**

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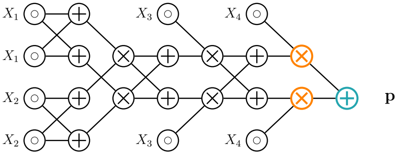
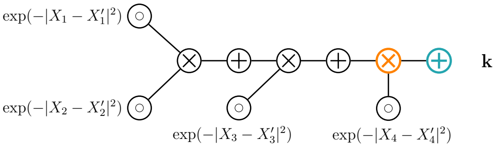
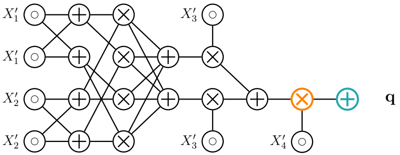




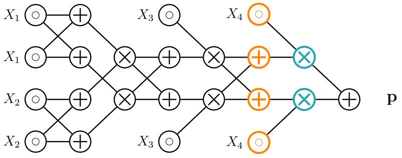


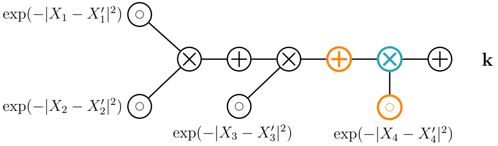
$$\mathbb{E}_{\mathbf{p},\mathbf{q}}[\mathbf{k}(\mathbf{x}, \mathbf{x}')] = \sum_{i,j,l} w_i w'_j w''_l \mathbb{E}_{\mathbf{p}_i,\mathbf{q}_j}[\mathbf{k}_l(\mathbf{x}, \mathbf{x}')]$$

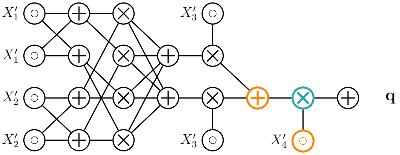
$\Longrightarrow$ *expectation is "pushed down" to children*

smooth + **decomposable** + **compatible** = **tractable E[k]**

[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 $\mathbf{k}_\times(\mathbf{X}, \mathbf{X}') = \prod_i \mathbf{k}_i(\mathbf{X}_i, \mathbf{X}'_i)$:







smooth + **decomposable** + **compatible** = **tractable E[k]**

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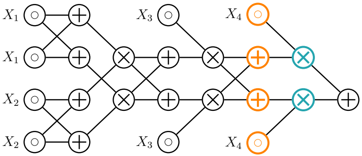
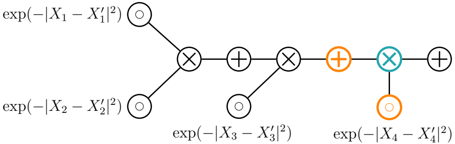
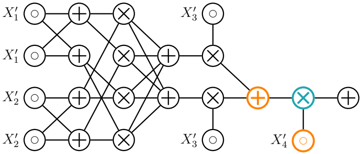


$\mathbf{p}$



$\mathbf{k}$



$\mathbf{q}$

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

smooth + *decomposable* + *compatible* = *tractable E[k]*

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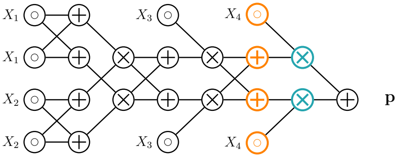

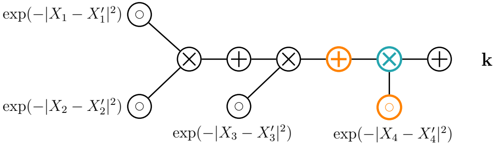

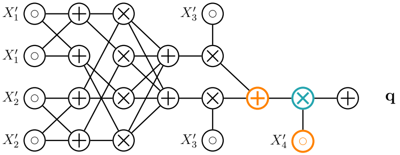

$$\mathbb{E}_{\mathbf{p}_\times, \mathbf{q}_\times}[\mathbf{k}_\times(\mathbf{x}, \mathbf{x}')] = \prod_i \mathbb{E}_{\mathbf{p},\mathbf{q}}[\mathbf{k}(\mathbf{x}_i, \mathbf{x}'_i)]$$

$\Longrightarrow$ *expectation decomposes into easier ones*

smooth + **decomposable** + **compatible** = **tractable E[k]**

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**
2: **return** $\mathbb{E}_{\mathbf{p}_n,\mathbf{q}_m}[\mathbf{k}_l]$
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!

smooth + decomposable + compatible = tractable E[k]

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: **if** m, n, l are ***input*** nodes **then**
2: **return** $\mathbb{E}_{\mathbf{p}_n,\mathbf{q}_m}[\mathbf{k}_l]$
3: **else if** m, n, l are ***sum*** nodes **then**
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Computation can be done in one forward pass!

$\Longrightarrow$ *squared maximum mean discrepancy* $MMD[\mathbf{p}, \mathbf{q}]$ *[Gretton et al. 2012]*

$\Longrightarrow$ + *determinism, kernelized discrete Stein discrepancy (KDSD) [Yang et al. 2018]*

Applications

- ***Support vector regression with missing features***

Support vector regression with missing features

- Given training data,
- we can learn a *support vector regression (SVR) model* $f(\mathbf{x}) = \sum_{i=1}^{m} w_i \mathbf{k}(\mathbf{x}_i, \mathbf{x}) + b$;
- also we can learn a *generative model* for features in PC $\mathbf{p}(\mathbf{X})$.

Support vector regression with missing features

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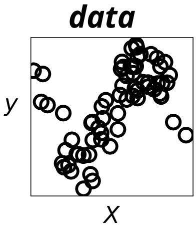

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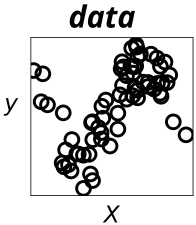

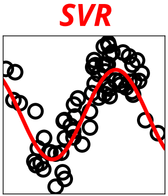

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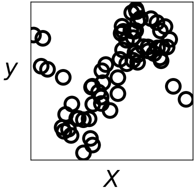
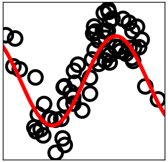
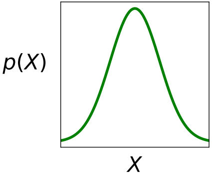
data



SVR



PC



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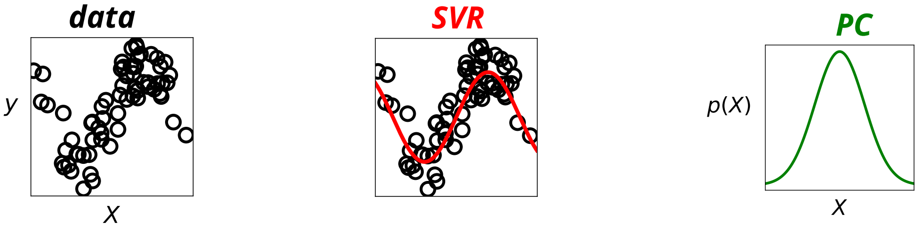

At deployment time, what happen if we observe partial features and some are missing?

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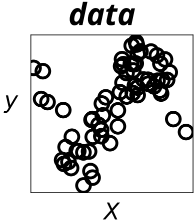

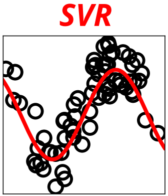

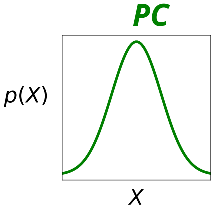

At deployment time, what happen if we observe partial features and some are missing?

$\Longrightarrow$ ***Expected prediction!***

Support vector regression with missing features

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At deployment time, in the case when only features $\mathbf{X}_o = \mathbf{x}_o$ are *observed* and features $\mathbf{X}_m$ are *missing*, with $\mathbf{X} = (\mathbf{X}_o, \mathbf{X}_m)$, the expected prediction is

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$$\mathbb{E}_{\mathbf{x}_m \sim \mathbf{p}(\mathbf{X}_m | \mathbf{x}_o)} [f(\mathbf{x}_o, \mathbf{x}_m)]$$

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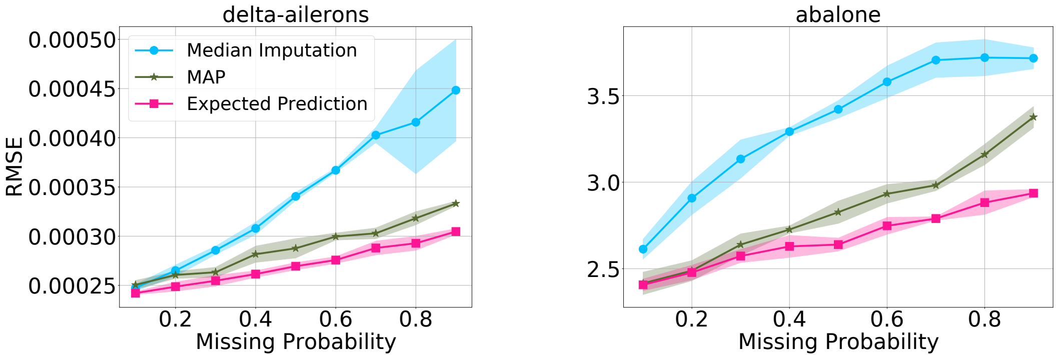
$$\mathbb{E}_{\mathbf{x}_m \sim \mathbf{p}(\mathbf{X}_m|\mathbf{x}_o)}[f(\mathbf{x}_o, \mathbf{x}_m)] = \sum_{i=1}^{m} w_i \mathbb{E}_{\mathbf{x}_m \sim \mathbf{p}(\mathbf{X}_m|\mathbf{x}_o)}[\mathbf{k}(\mathbf{x}_i, (\mathbf{x}_o, \mathbf{x}_m))] + b$$

Support vector regression with missing features



$\Longrightarrow$ *Expected prediction improves over the baselines*

Applications

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

Recap **Black-box Importance Sampling** [Liu et al. 2016]

- 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

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

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

Recap Black-box Importance Sampling [Liu et al. 2016]

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

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

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

$\Longrightarrow$ ***Collapsed samples!***

Collapsed Black-box Importance Sampling

- 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 $\mathbf{p}$

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

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

- Finally, obtain the importance weights $\boldsymbol{w}$ by solving

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

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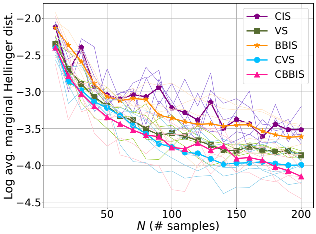
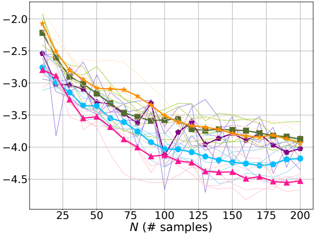
Collapsed Black-box Importance Sampling





$\Longrightarrow$ *methods with collapsed samples all outperform their non-collapsed counterparts*

$\Longrightarrow$ *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

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

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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