What is Probabilistic Reasoning and why shall you care?

antonio vergari (he/him)

@tetraduzione

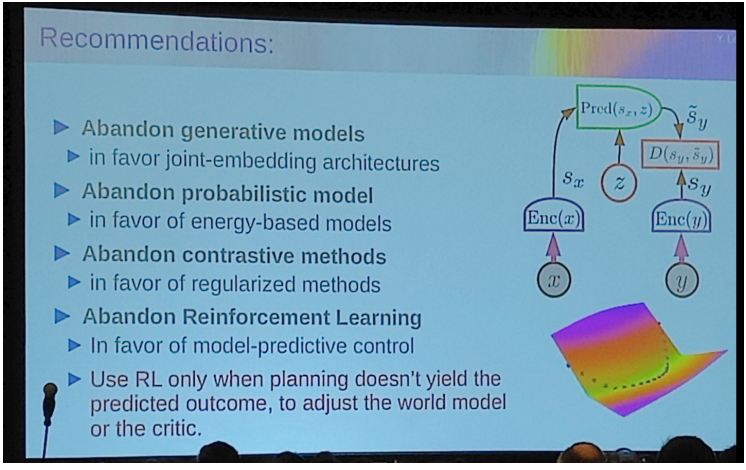
4-5th Mar 2024 - **Advanced Probabilistic Modeling** - *University of Trento*

april

april is probably a recursive identifier of a lab

april

about
probabilities
integrals &
logic

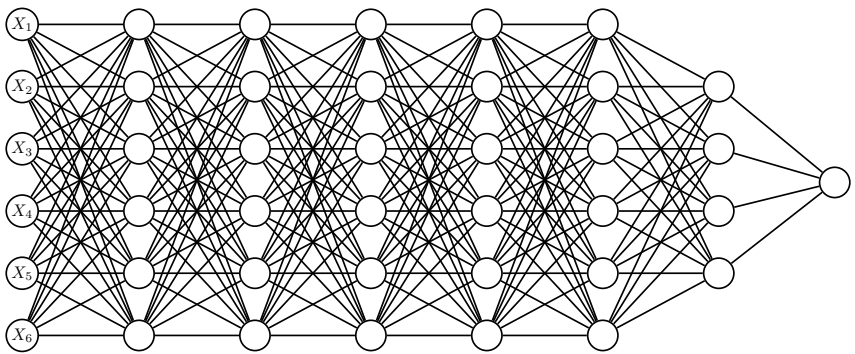


why shall we care about probabilities?

why ***deep generative models***

Computational graphs that encode expressive distributions $p_{\mathbf{m}}(\mathbf{X})$

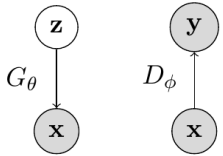
$\Rightarrow$ *by stacking layers of "latent" units*



why ***deep generative models***

Computational graphs that encode expressive distributions $p_{\mathbf{m}}(\mathbf{X})$

$\Rightarrow$ *by stacking layers of "latent" units*



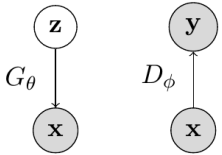
GANs

[Goodfellow et al. 2014]

why ***deep generative models***

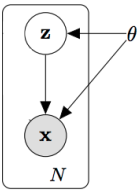
Computational graphs that encode expressive distributions $p_{\mathbf{m}}(\mathbf{X})$

$\Rightarrow$ *by stacking layers of "latent" units*



GANs

[Goodfellow et al. 2014]



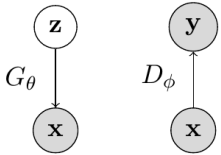
VAEs/Diffusion

[Kingma and Welling 2014]

why *deep generative models*

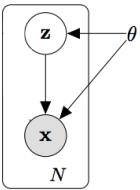
Computational graphs that encode expressive distributions $p_{\mathbf{m}}(\mathbf{X})$

$\Rightarrow$ *by stacking layers of "latent" units*



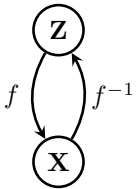
GANs

[Goodfellow et al. 2014]



VAEs/Diffusion

[Kingma and Welling 2014]



Cont/Disc Flows

[Papamakarios et al. 2019]

why ***deep generative models*** ...

[PROS] they encode ***expressive*** distributions with ***millions of parameters***

+

they ***scale learning*** to high-dimensional, large datasets via ***GPU***

...and why they lack ***complex reasoning***

[PROS] they encode ***expressive*** distributions with ***millions of parameters***

+

they ***scale learning*** to high-dimensional, large datasets

[CONS] they are ***limited to simple reasoning*** routine (lack flexibility)

+

their computations come with ***little or no guarantees*** (unreliable)

Deep generative models

+

flexible and reliable advanced probabilistic reasoning?

What is advanced reasoning?

or the inherent trade-off of tractability vs. expressiveness

wait!

the basics first

The "***product***" rule:

$$p(\mathbf{X}, \mathbf{Y}, \mathbf{Z}) = p(\mathbf{X})p(\mathbf{Y}, \mathbf{Z} \mid \mathbf{X}) = p(\mathbf{X})p(\mathbf{Y} \mid \mathbf{X})p(\mathbf{Z} \mid \mathbf{X}, \mathbf{Y})$$

wait!

the basics first

The "***product***" rule:

$$p(\mathbf{X}, \mathbf{Y}, \mathbf{Z}) = p(\mathbf{X})p(\mathbf{Y}, \mathbf{Z} \mid \mathbf{X}) = p(\mathbf{X})p(\mathbf{Y} \mid \mathbf{X})p(\mathbf{Z} \mid \mathbf{X}, \mathbf{Y})$$

The "***sum***" rule:

$$p(\mathbf{X}, \mathbf{Y}) = \quad ???$$

wait!

the basics first

The "***product***" rule:

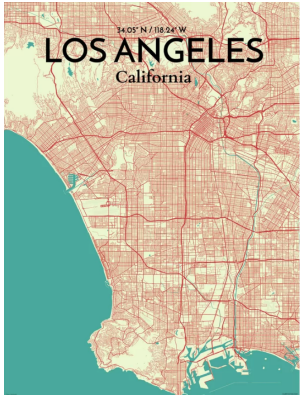
$$p(\mathbf{X}, \mathbf{Y}, \mathbf{Z}) = p(\mathbf{X})p(\mathbf{Y}, \mathbf{Z} \mid \mathbf{X}) = p(\mathbf{X})p(\mathbf{Y} \mid \mathbf{X})p(\mathbf{Z} \mid \mathbf{X}, \mathbf{Y})$$

The "***sum***" rule:

$$p(\mathbf{X}, \mathbf{Y}) = \int_{\mathsf{dom}(\mathbf{z})} p(\mathbf{X}, \mathbf{Y}, \mathbf{z})\, d\mathbf{Z}$$

Why probabilistic inference?

q_1: *What is the probability that today is a Monday and there is a traffic jam on Westwood Blvd.?*

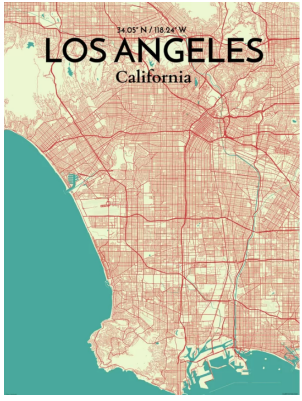


© fineartamerica.com

Why probabilistic inference?

q_1: *What is the probability that today is a Monday and there is a traffic jam on Westwood Blvd.?*

q_2: *Which day is most likely to have a traffic jam on my route to campus?*



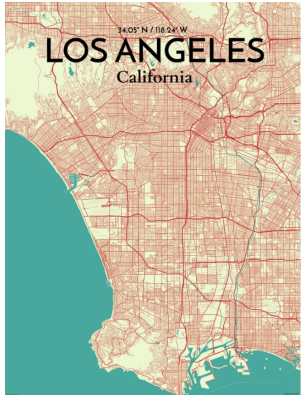
© fineartamerica.com

Why probabilistic inference?

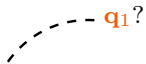
q_1: *What is the probability that today is a Monday and there is a traffic jam on Westwood Blvd.?*

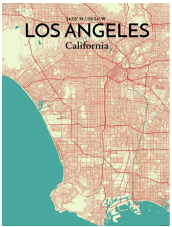
q_2: *Which day is most likely to have a traffic jam on my route to campus?*

How to answer several of these ***probabilistic queries****?*



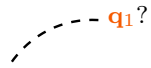
“What is the most likely street to have a traffic jam at 12.00?”

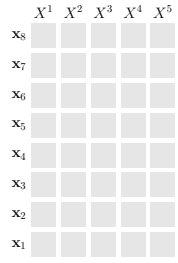




answering queries...

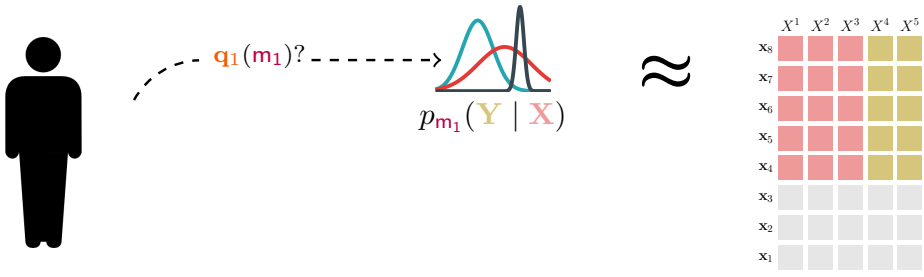
“What is the most likely street to have a traffic jam at 12.00?”





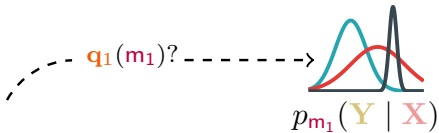
answering queries...

*"What is the most likely **street** to have a traffic jam at **12.00**?"*

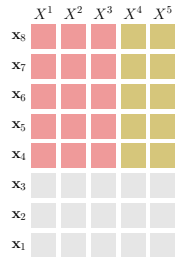


...by fitting predictive models!

*"What is the most likely **street** to have a traffic jam at **12.00**?"*

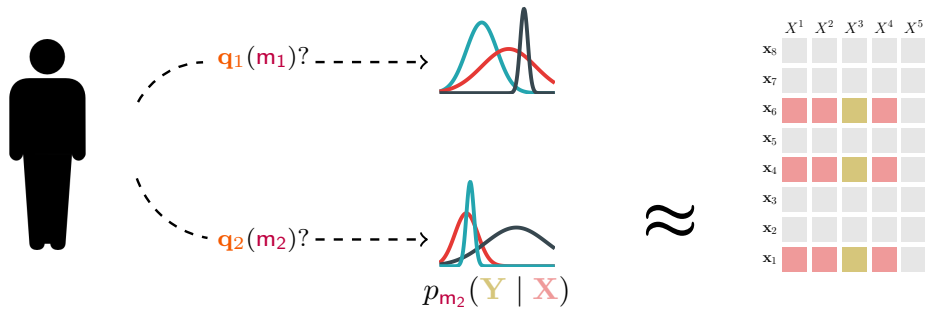


$\approx$



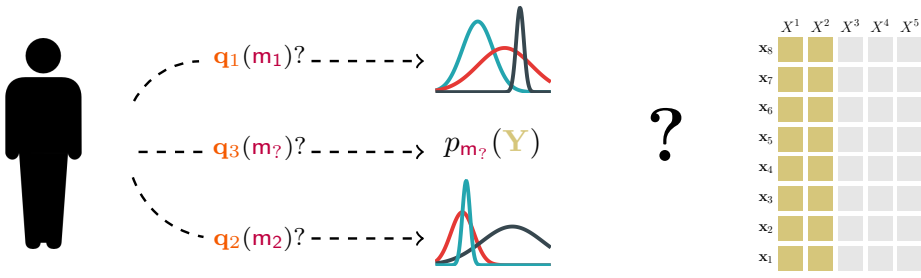
~~***...by fitting predictive models!***~~

*"What is the most likely **time** to see a traffic jam at **Sunset Blvd.**?"*

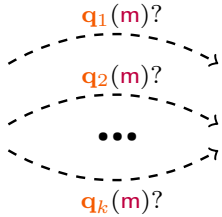


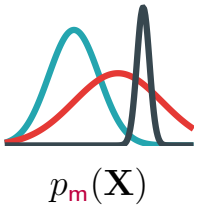
~~...by fitting predictive models!~~

*"What is the probability of a traffic jam on **Westwood Blvd.** on **Monday**?"*



~~...by fitting predictive models!~~

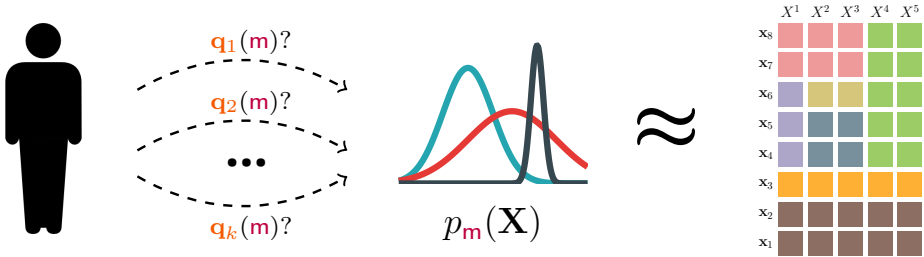




$\approx$

	X^1	X^2	X^3	X^4	X^5
$\mathbf{x}_8$					
$\mathbf{x}_7$					
$\mathbf{x}_6$					
$\mathbf{x}_5$					
$\mathbf{x}_4$					
$\mathbf{x}_3$					
$\mathbf{x}_2$					
$\mathbf{x}_1$					

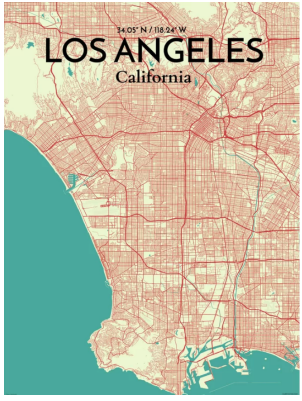
...by fitting generative models!



...e.g. exploratory data analysis

Why probabilistic inference?

q_1: *What is the probability that today is a Monday and there is a traffic jam on Westwood Blvd.?*



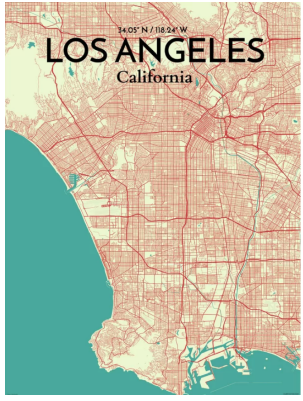
© fineartamerica.com

Why probabilistic inference?

$\mathbf{q}_1$: *What is the probability that today is a Monday and there is a traffic jam on Westwood Blvd.?*

$$\mathbf{X} = \{\mathsf{Day}, \mathsf{Time}, \mathsf{Jam}_{\mathsf{Str1}}, \mathsf{Jam}_{\mathsf{Str2}}, \ldots, \mathsf{Jam}_{\mathsf{StrN}}\}$$

$$\mathbf{q}_1(\mathbf{m}) = p_{\mathbf{m}}(\mathsf{Day} = \mathsf{Mon}, \mathsf{Jam}_{\mathsf{Wwood}} = 1)$$



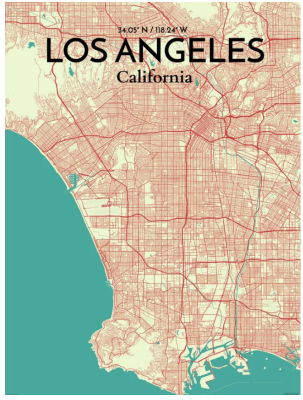
Why probabilistic inference?

$\mathbf{q}_1$: *What is the probability that today is a Monday and there is a traffic jam on Westwood Blvd.?*

$$\mathbf{X} = \{\text{Day}, \text{Time}, \text{Jam}_{\text{Str1}}, \text{Jam}_{\text{Str2}}, \ldots, \text{Jam}_{\text{StrN}}\}$$

$$\mathbf{q}_1(\mathbf{m}) = p_{\mathbf{m}}(\text{Day} = \text{Mon}, \text{Jam}_{\text{Wwood}} = 1)$$

$\Rightarrow$ ***marginals*** *(the sum rule)*

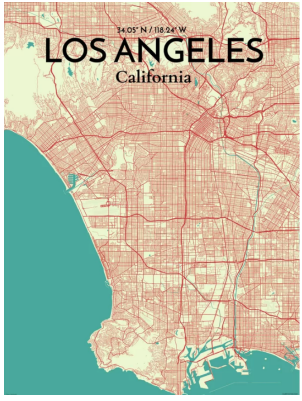


Why probabilistic inference?

$\mathbf{q}_2$: *Which day is most likely to have a traffic jam on my route to campus?*

$$\mathbf{X} = \{\mathsf{Day}, \mathsf{Time}, \mathsf{Jam}_{\mathsf{Str1}}, \mathsf{Jam}_{\mathsf{Str2}}, \ldots, \mathsf{Jam}_{\mathsf{StrN}}\}$$

$$\mathbf{q}_2(\mathbf{m}) = \mathrm{argmax}_{\mathsf{d}}\, p_{\mathbf{m}}(\mathsf{Day} = \mathsf{d} \wedge \bigvee\nolimits_{i \in \mathsf{route}} \mathsf{Jam}_{\mathsf{Str}i})$$



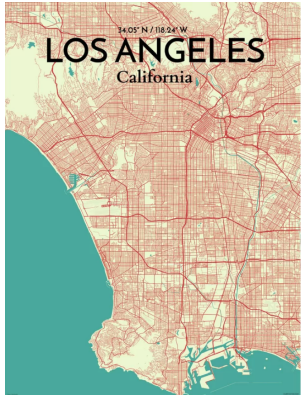
Why probabilistic inference?

$\mathbf{q}_2$: *Which day is most likely to have a traffic jam on my route to campus?*

$\mathbf{X} = \{\mathsf{Day}, \mathsf{Time}, \mathsf{Jam}_{\mathsf{Str1}}, \mathsf{Jam}_{\mathsf{Str2}}, \ldots, \mathsf{Jam}_{\mathsf{StrN}}\}$

$\mathbf{q}_2(\mathbf{m}) = \mathrm{argmax}_{\mathsf{d}}\, p_{\mathbf{m}}(\mathsf{Day} = \mathsf{d} \wedge \bigvee_{i \in \mathsf{route}} \mathsf{Jam}_{\mathsf{Str}i})$

$\Rightarrow$ ***marginals + MAP + logical events***



Tractable Probabilistic Inference

A class of queries $\mathcal{Q}$ *is tractable on a family of probabilistic models* $\mathcal{M}$

iff for any query $\mathbf{q} \in \mathcal{Q}$ *and model* $\mathbf{m} \in \mathcal{M}$

exactly *computing* $\mathbf{q}(\mathbf{m})$ *runs in time* $O(\text{poly}(|\mathbf{m}|))$.

$\Rightarrow$ ***model-centric*** *definition...*

Tractable Probabilistic Inference

A class of queries $\mathcal{Q}$ *is tractable on a family of probabilistic models* $\mathcal{M}$

iff for any query $\mathbf{q} \in \mathcal{Q}$ *and model* $\mathbf{m} \in \mathcal{M}$

exactly *computing* $\mathbf{q}(\mathbf{m})$ *runs in time* $O(\text{poly}(|\mathbf{m}|))$.

$\Rightarrow$ ***model-centric*** *definition...*

$\Rightarrow$ *...and* ***query-centric****: Tractability is not a universal property!*

Tractable Probabilistic Inference

A class of queries $\mathcal{Q}$ *is tractable on a family of probabilistic models* $\mathcal{M}$

iff for any query $\mathbf{q} \in \mathcal{Q}$ *and model* $\mathbf{m} \in \mathcal{M}$

exactly *computing* $\mathbf{q}(\mathbf{m})$ *runs in time* $O(\text{poly}(|\mathbf{m}|))$.

$\Rightarrow$ ***model-centric*** *definition...*

$\Rightarrow$ *...and* ***query-centric****: Tractability is not a universal property!*

$\Rightarrow$ *often* poly *will in fact be* ***linear****!*

Tractable Probabilistic Inference

A class of queries $\mathcal{Q}$ *is tractable on a family of probabilistic models* $\mathcal{M}$

iff for any query $\mathbf{q} \in \mathcal{Q}$ *and model* $\mathbf{m} \in \mathcal{M}$

exactly *computing* $\mathbf{q}(\mathbf{m})$ *runs in time* $O(\text{poly}(|\mathbf{m}|))$.

$\Rightarrow$ ***model-centric*** *definition...*

$\Rightarrow$ *...and* ***query-centric****: Tractability is not a universal property!*

$\Rightarrow$ *often* poly *will in fact be* ***linear****!*

$\Rightarrow$ *Note: if* $|\mathbf{m}| \in O(\text{poly}(|\mathbf{X}|))$*, then query time is* $O(\text{poly}(|\mathbf{X}|))$.

Tractable Probabilistic Inference

A class of queries $\mathcal{Q}$ *is tractable on a family of probabilistic models* $\mathcal{M}$

iff for any query $\mathbf{q} \in \mathcal{Q}$ *and model* $\mathbf{m} \in \mathcal{M}$

exactly *computing* $\mathbf{q}(\mathbf{m})$ *runs in time* $O(\text{poly}(|\mathbf{m}|))$.

$\Rightarrow$ ***model-centric*** *definition...*

$\Rightarrow$ *...and* ***query-centric****: Tractability is not a universal property!*

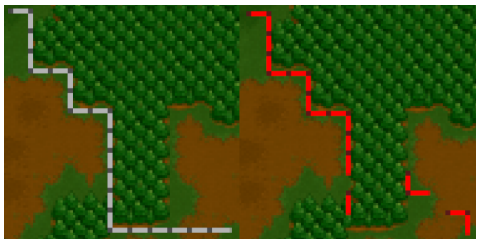
$\Rightarrow$ *often* poly *will in fact be* ***linear****!*

$\Rightarrow$ *Note: if* $|\mathbf{m}| \in O(\text{poly}(|\mathbf{X}|))$*, then query time is* $O(\text{poly}(|\mathbf{X}|))$.

$\Rightarrow$ *Why* ***exactness****? Highest guarantee possible!*

why tractable models?

exactness can be crucial in safety-driven applications



guarantee constraint satisfaction

[Ahmed et al. 2022]

estimation error is bounded (0)

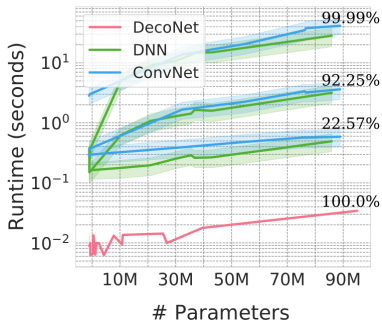
[Choi 2022]

why tractable models?

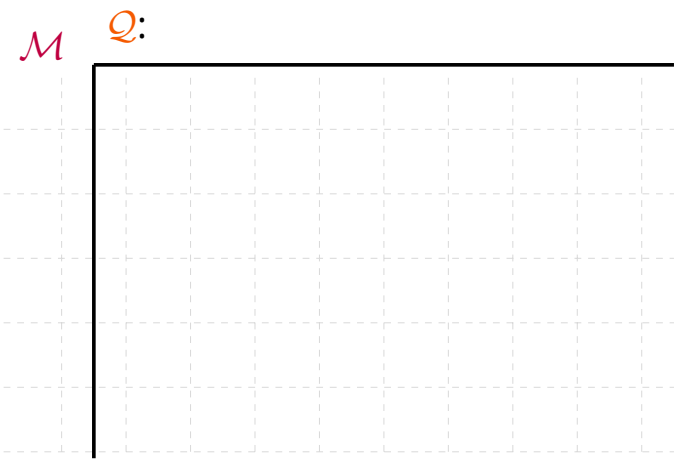
they can be much faster than intractable ones!

Method	MNIST (10,000 test images)		
	Theoretical bpd	Comp. bpd	En- & decoding time
PC (small)	1.26	1.30	**53**
PC (large)	**1.20**	**1.24**	168
IDF	1.90	1.96	880
BitSwap	1.27	1.31	904

[Liu, Mandt, and Broeck 2022]



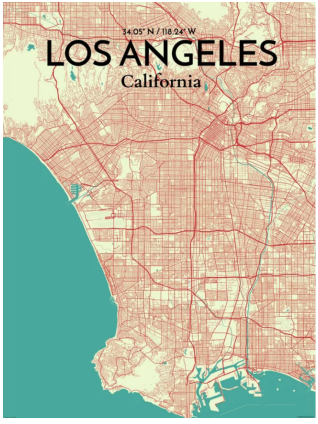
[Subramani et al. 2021]



tractable bands

Complete evidence (EVI)

q_3: *What is the probability that today is a Monday at 12.00 and there is a traffic jam only on Westwood Blvd.?*

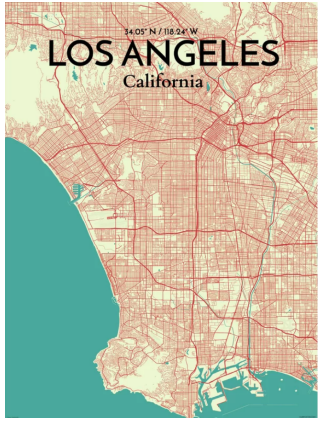


Complete evidence (EVI)

$\mathbf{q}_3$: *What is the probability that today is a Monday at 12.00 and there is a traffic jam only on Westwood Blvd.?*

$$\mathbf{X} = \{\mathsf{Day}, \mathsf{Time}, \mathsf{Jam}_{\mathsf{Wwood}}, \mathsf{Jam}_{\mathsf{Str2}}, \ldots, \mathsf{Jam}_{\mathsf{StrN}}\}$$

$$\mathbf{q}_3(\mathbf{m}) = p_{\mathbf{m}}(\mathbf{X} = \{\mathsf{Mon}, 12.00, 1, 0, \ldots, 0\})$$



Complete evidence (EVI)

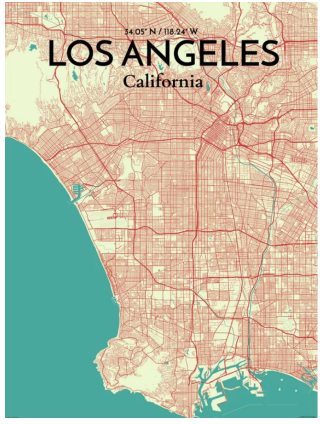
$\mathbf{q}_3$: *What is the probability that today is a Monday at 12.00 and there is a traffic jam only on Westwood Blvd.?*

$$\mathbf{X} = \{\text{Day}, \text{Time}, \text{Jam}_{\text{Wwood}}, \text{Jam}_{\text{Str2}}, \ldots, \text{Jam}_{\text{StrN}}\}$$

$$\mathbf{q}_3(\mathbf{m}) = p_{\mathbf{m}}(\mathbf{X} = \{\text{Mon}, 12.00, 1, 0, \ldots, 0\})$$

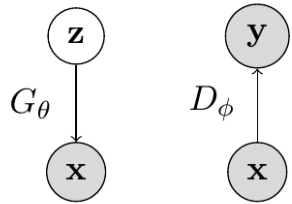
...fundamental in ***maximum likelihood learning***

$$\theta_{\mathbf{m}}^{\text{MLE}} = \text{argmax}_\theta \prod_{\mathbf{x} \in \mathcal{D}} p_{\mathbf{m}}(\mathbf{x}; \theta)$$



Generative Adversarial Networks

$$\min_\theta \max_\phi \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}(\mathbf{x})}\left[\log D_\phi(\mathbf{x})\right] + \mathbb{E}_{\mathbf{z}\sim p(\mathbf{z})}\left[\log(1 - D_\phi(G_\theta(\mathbf{z})))\right]$$



Goodfellow et al., "Generative adversarial nets", , 2014

Generative Adversarial Networks

$$\min_\theta \max_\phi \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}(\mathbf{x})}\left[\log D_\phi(\mathbf{x})\right] + \mathbb{E}_{\mathbf{z}\sim p(\mathbf{z})}\left[\log(1 - D_\phi(G_\theta(\mathbf{z})))\right]$$

no explicit likelihood!

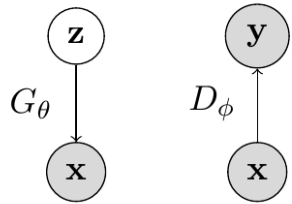
$\Rightarrow$ *adversarial training instead of MLE*

$\Rightarrow$ *no tractable EVI*

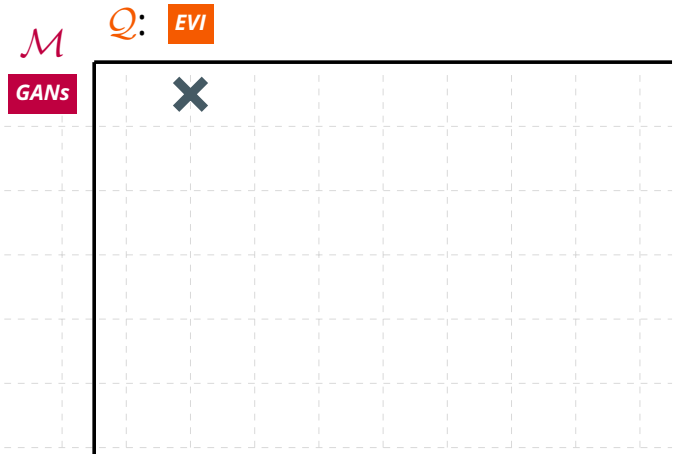
good sample quality

$\Rightarrow$ *but lots of samples needed for MC*

unstable training $\Rightarrow$ *mode collapse*



Goodfellow et al., "Generative adversarial nets", , 2014

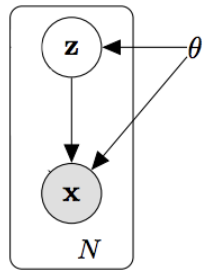


tractable bands

Variational Autoencoders

$$p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{x} \mid \mathbf{z}) p(\mathbf{z}) d\mathbf{z}$$

an explicit likelihood model!



Rezende, Mohamed, and Wierstra, "Stochastic backprop. and approximate inference in deep generative models", arXiv preprint arXiv:1401.4082, 2014
Kingma and Welling, "Auto-Encoding Variational Bayes", , 2014

Variational Autoencoders

$$\log p_\theta(\mathbf{x}) \geq \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}\left[\log p_\theta(\mathbf{x} \mid \mathbf{z})\right] - \mathbb{KL}(q_\phi(\mathbf{z} \mid \mathbf{x})||p(\mathbf{z}))$$

an explicit likelihood model!

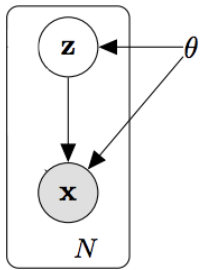
... but computing $\log p_\theta(\mathbf{x})$ is intractable

$\Rightarrow$ *an infinite and uncountable mixture*

$\Rightarrow$ *no tractable EVI*

we need to optimize the ELBO...

$\Rightarrow$ *which is "tricky" [Alemi et al. 2017; Dai and Wipf 2019; Ghosh et al. 2019]*



Energy Based Models

$$p_\theta(\mathbf{x}) = e^{-E(\mathbf{x};\theta)}/Z$$

an explicit likelihood model!

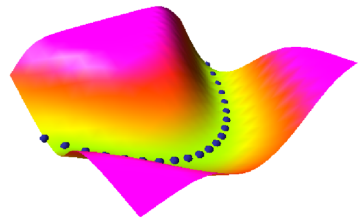
... but computing the partition function $Z = \int e^{-E(\mathbf{x};\theta)}\, d\mathbf{X}$ is intractable

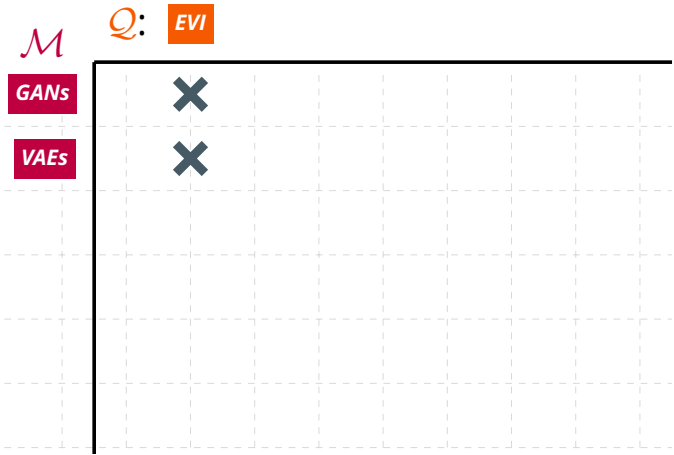
$\Rightarrow$ *no tractable EVI*

alternative ways to train them than MLE...

$\Rightarrow$ *e.g., (denoising) score/ratio matching*

[Song and Kingma 2021]





tractable bands

Normalizing flows

$$p_{\mathbf{X}}(\mathbf{x}) = p_{\mathbf{Z}}(f^{-1}(\mathbf{x})) \left| \det \left(\frac{\delta f^{-1}}{\delta \mathbf{x}} \right) \right|$$

an explicit likelihood!

...plus structured Jacobians

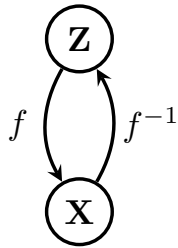
$\Rightarrow$ *tractable EVI queries!*

many neural variants

RealNVP *[Dinh, Sohl-Dickstein, and Bengio 2016],* MAF *[Papamakarios, Pavlakou, and Murray 2017]*

MADE *[Germain et al. 2015],*

PixelRNN *[Oord, Kalchbrenner, and Kavukcuoglu 2016]*



Normalizing flows

$$p_{\mathbf{X}}(\mathbf{x}) = p_{\mathbf{Z}}(f^{-1}(\mathbf{x})) \left| \det \left(\frac{\delta f^{-1}}{\delta \mathbf{x}} \right) \right|$$

an explicit likelihood!

...plus structured Jacobians

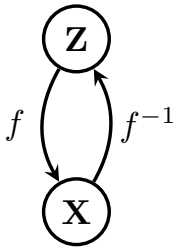
$\Rightarrow$ *tractable EVI queries!*

many neural variants

RealNVP *[Dinh, Sohl-Dickstein, and Bengio 2016],* MAF *[Papamakarios, Pavlakou, and Murray 2017]*

MADE *[Germain et al. 2015],*

PixelRNN *[Oord, Kalchbrenner, and Kavukcuoglu 2016]*



Normalizing flows

$$p_{\mathbf{X}}(\mathbf{x}) = p_{\mathbf{Z}}(f^{-1}(\mathbf{x})) \left| \det \left(\frac{\delta f^{-1}}{\delta \mathbf{x}} \right) \right|$$

an explicit likelihood!

...plus structured Jacobians

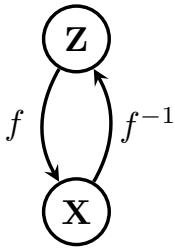
$\Rightarrow$ *tractable EVI queries!*

many neural variants

RealNVP *[Dinh, Sohl-Dickstein, and Bengio 2016],* MAF *[Papamakarios, Pavlakou, and Murray 2017]*

MADE *[Germain et al. 2015],*

PixelRNN *[Oord, Kalchbrenner, and Kavukcuoglu 2016]*



Autoregressive models

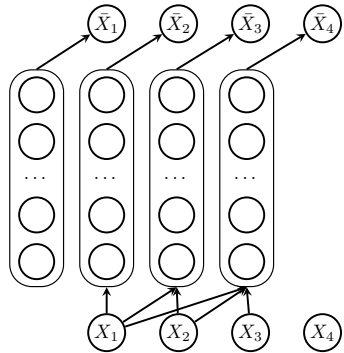
$p_\theta(\mathbf{x}) = \prod_i p_\theta(x_i \mid \mathbf{x}_{<i})$

an explicit likelihood model via the product rule

a special case of normalizing flows!

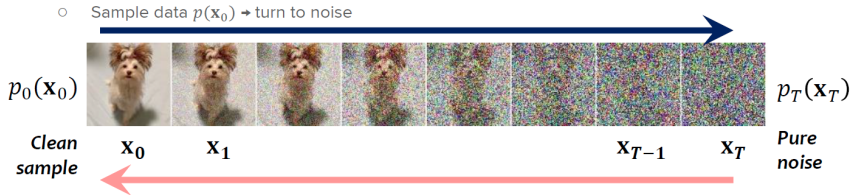
$\Longrightarrow$ *the $\mathbf{Z}$s are the noise used to sample*

[Papamakarios et al. 2021]



Diffusion models

and continuous (time) normalizing flows



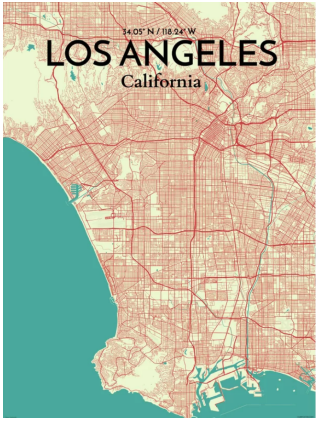
create a continuous-time flow/diffusion process as a P/SDE

$\Rightarrow$ *no close form for the likelihood in general*

$\Rightarrow$ *no tractable EVI*

Marginal queries (MAR)

q_1: *What is the probability that today is a Monday ~~at 12.00~~ and there is a traffic jam ~~only~~ on Westwood Blvd.?*

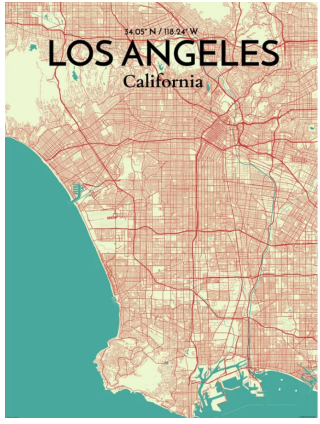


© fineartamerica.com

Marginal queries (MAR)

$\mathbf{q}_1$: *What is the probability that today is a Monday ~~at 12.00~~ and there is a traffic jam ~~only~~ on Westwood Blvd.?*

$$\mathbf{q}_1(\mathbf{m}) = p_{\mathbf{m}}(\mathsf{Day} = \mathsf{Mon}, \mathsf{Jam}_{\mathsf{Wwood}} = 1)$$



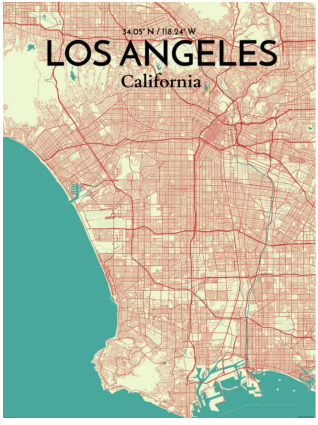
Marginal queries (MAR)

$\mathbf{q}_1$: *What is the probability that today is a Monday ~~at 12.00~~ and there is a traffic jam ~~only~~ on Westwood Blvd.?*

$$\mathbf{q}_1(\mathbf{m}) = p_{\mathbf{m}}(\text{Day} = \text{Mon}, \text{Jam}_{\text{Wwood}} = 1)$$

General: $p_{\mathbf{m}}(\mathbf{e}) = \int p_{\mathbf{m}}(\mathbf{e}, \mathbf{H})\, d\mathbf{H}$

where $\mathbf{E} \subset \mathbf{X}, \quad \mathbf{H} = \mathbf{X} \setminus \mathbf{E}$



© fineartamerica.com

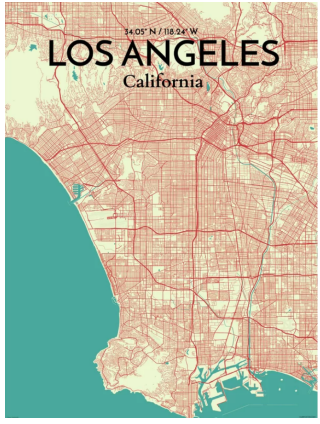
Marginal queries (MAR)

$\mathbf{q}_1$: *What is the probability that today is a Monday ~~at 12.00~~ and there is a traffic jam ~~only~~ on Westwood Blvd.?*

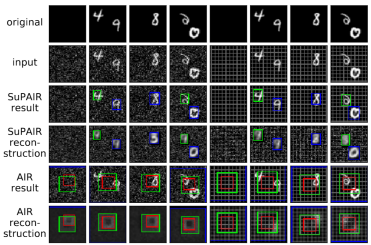
$$\mathbf{q}_1(\mathbf{m}) = p_{\mathbf{m}}(\text{Day} = \text{Mon}, \text{Jam}_{\text{Wwood}} = 1)$$

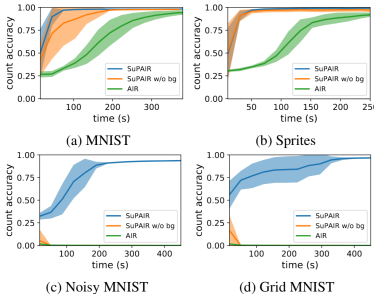
tractable MAR $\Longrightarrow$ tractable ***conditional queries*** (CON):

$$p_{\mathbf{m}}(\mathbf{q} \mid \mathbf{e}) = \frac{p_{\mathbf{m}}(\mathbf{q}, \mathbf{e})}{p_{\mathbf{m}}(\mathbf{e})}$$



Tractable MAR: scene understanding





(a) MNIST (b) Sprites

(c) Noisy MNIST (d) Grid MNIST

~~Fast and exact marginalization over~~ unseen or "do not care" parts in the scene

Stelzner, Peharz, and Kersting, "Faster Attend-Infer-Repeat with Tractable Probabilistic Models", ICML, 2019

Kossen et al., "Structured Object-Aware Physics Prediction for Video Modeling and Planning", arXiv preprint arXiv:1910.02425, 2019

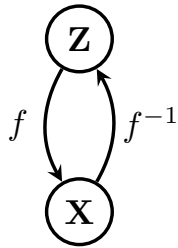
Normalizing flows

$$p_{\mathbf{X}}(\mathbf{x}) = p_{\mathbf{Z}}(f^{-1}(\mathbf{x})) \left| \det \left(\frac{\delta f^{-1}}{\delta \mathbf{x}} \right) \right|$$

an explicit likelihood!

...plus structured Jacobians

$\Rightarrow$ *tractable EVI queries!*



Normalizing flows

$$p_{\mathbf{X}}(\mathbf{x}) = p_{\mathbf{Z}}(f^{-1}(\mathbf{x})) \left| \det \left(\frac{\delta f^{-1}}{\delta \mathbf{x}} \right) \right|$$

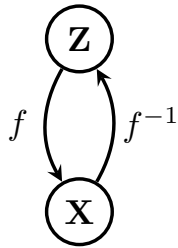
an explicit likelihood!

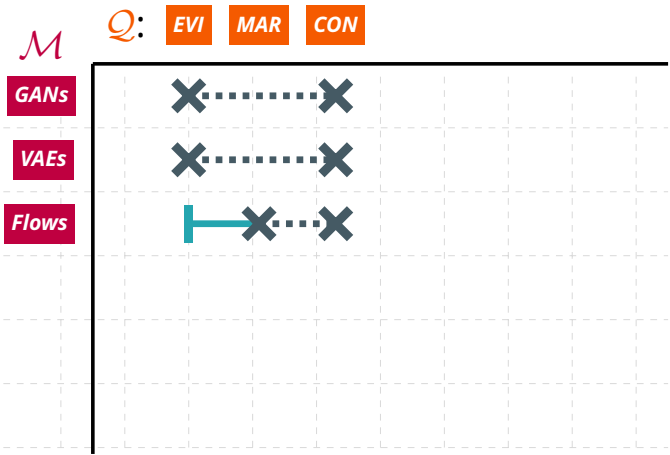
...plus structured Jacobians

$\Rightarrow$ *tractable EVI queries!*

MAR is generally intractable:
we cannot easily integrate over f

$\Rightarrow$ *unless f is "simple", e.g. identity*



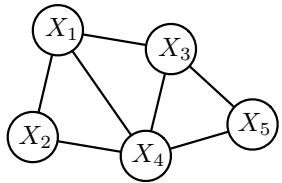


tractable bands

Probabilistic Graphical Models (PGMs)

Declarative semantics: a clean separation of modeling assumptions from inference

Nodes: random variables
Edges: dependencies



+

Inference:

conditioning *[Darwiche 2001; Sang, Beame, and Kautz 2005]*

elimination *[Zhang and Poole 1994; Dechter 1998]*

message passing *[Yedidia, Freeman, and Weiss*

Complexity of MAR on PGMs

Exact complexity: Computing MAR and CON is *#P-hard*

$\Rightarrow$ *[Cooper 1990; Roth 1996]*

Approximation complexity: Computing MAR and CON approximately within a relative error of $2^{n^{1-\epsilon}}$ for any fixed ϵ is *NP-hard*

$\Rightarrow$ *[Dagum and Luby 1993; Roth 1996]*

Why? Treewidth!

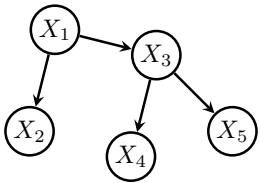
Treewidth:

Informally, how tree-like is the graphical model $\mathbf{m}$?
Formally, the minimum width of any tree-decomposition of $\mathbf{m}$.

Fixed-parameter tractable: MAR and CON on a graphical model $\mathbf{m}$ with treewidth w take time $O(|\mathbf{X}| \cdot 2^w)$, which is linear for fixed width w

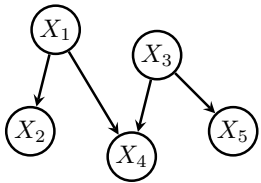
[Dechter 1998; Koller and Friedman 2009]. $\Longrightarrow$ *what about bounding the treewidth by design?*

Low-treewidth PGMs



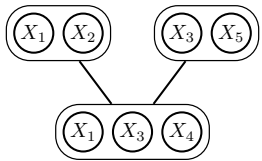
Trees

[Meilă and Jordan 2000]



Polytrees

[Dasgupta 1999]



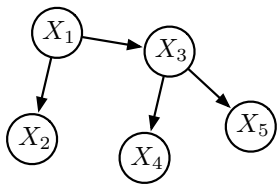
Thin Junction trees

[Bach and Jordan 2001]

If treewidth is bounded (e.g. $\approxeq 20$), exact MAR and CON inference is possible in practice

Tree distributions

A ***tree-structured BN*** *[Meilă and Jordan 2000]* where each $X_i \in \mathbf{X}$ has *at most* one parent Pa_{X_i}.

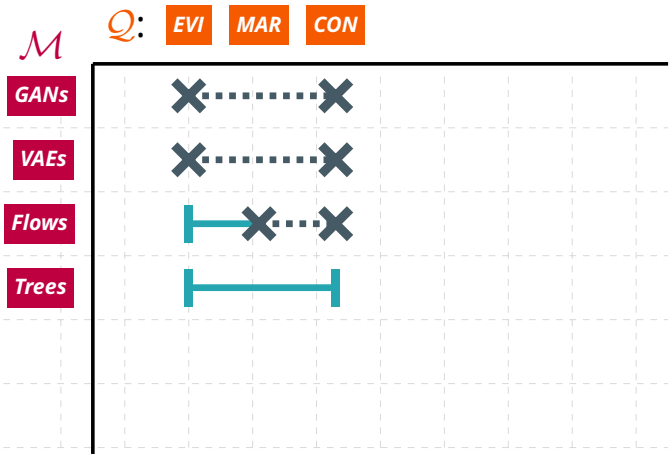


$$p(\mathbf{X}) = \prod_{i=1}^{n} p(x_i|\mathrm{Pa}_{x_i})$$

Exact querying: EVI, MAR, CON tasks *linear* for trees: $O(|\mathbf{X}|)$

Exact learning from d examples takes $O(|\mathbf{X}|^2 \cdot d)$ with the classical Chow-Liu algorithm[1]

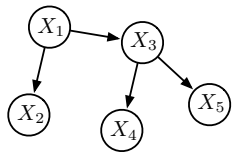
[1] *Chow and Liu, "Approximating discrete probability distributions with dependence trees", 1968*



tractable bands

What do we lose?

Expressiveness: Ability to represent rich and complex classes of distributions

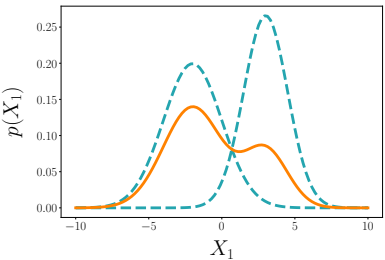


Bounded-treewidth PGMs lose the ability to represent *all possible distributions* ...

Cohen, Sharir, and Shashua, "On the expressive power of deep learning: A tensor analysis", , 2016
Martens and Medabalimi, "On the Expressive Efficiency of Sum Product Networks", CoRR, 2014

Mixtures

Mixtures as a convex combination of k (simpler) probabilistic models

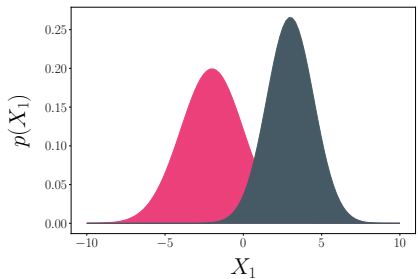


$$p(X) = w_1 \cdot p_1(X) + w_2 \cdot p_2(X)$$

EVI, MAR, CON queries scale linearly in k

Mixtures

Mixtures as a convex combination of k (simpler) probabilistic models



$$p(X) = p(Z = \mathbf{1}) \cdot p_1(X|Z = \mathbf{1}) + p(Z = \mathbf{2}) \cdot p_2(X|Z = \mathbf{2})$$

Mixtures are marginalizing a ***categorical latent variable*** Z with k values

$\Rightarrow$ *increased expressiveness*

Expressiveness and efficiency

Expressiveness: Ability to represent rich and effective classes of functions

$\Rightarrow$ *mixture of Gaussians can approximate any distribution!*

Cohen, Sharir, and Shashua, "On the expressive power of deep learning: A tensor analysis", , 2016
Martens and Medabalimi, "On the Expressive Efficiency of Sum Product Networks", CoRR, 2014

Expressiveness and efficiency

Expressiveness: Ability to represent rich and effective classes of functions

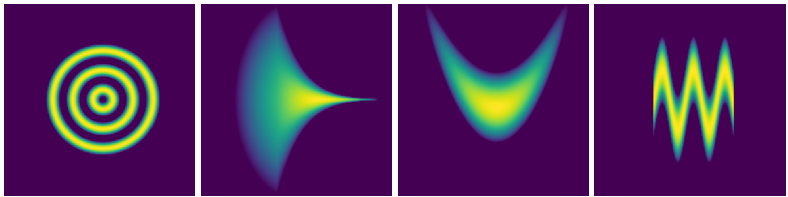
$\Rightarrow$ *mixture of Gaussians can approximate any distribution!*

Expressive efficiency (succinctness) Ability to represent rich and effective classes of functions **compactly**

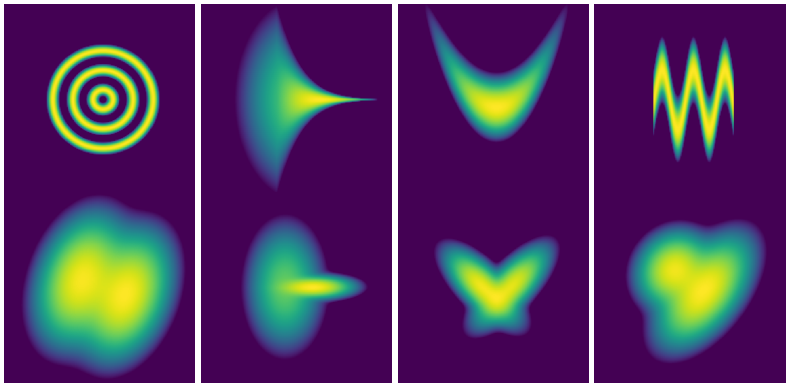
$\Rightarrow$ *but how many components does a Gaussian mixture need?*

Cohen, Sharir, and Shashua, "On the expressive power of deep learning: A tensor analysis", , 2016
Martens and Medabalimi, "On the Expressive Efficiency of Sum Product Networks", CoRR, 2014

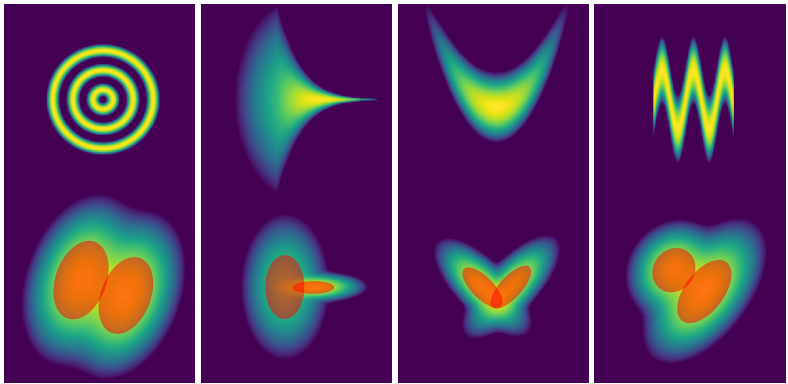
How expressive efficient are mixtures?



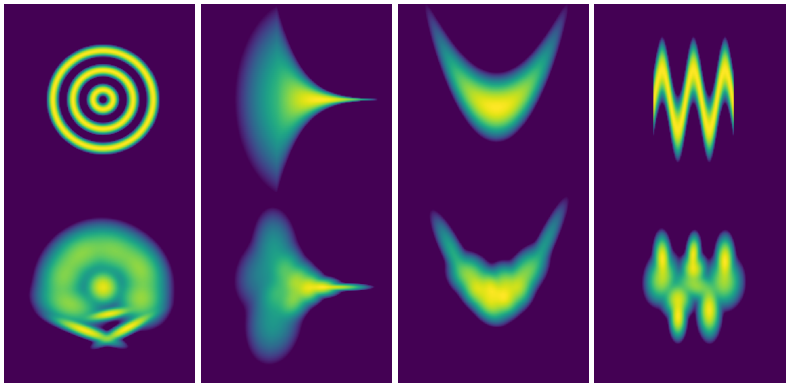
How expressive efficient are mixtures?



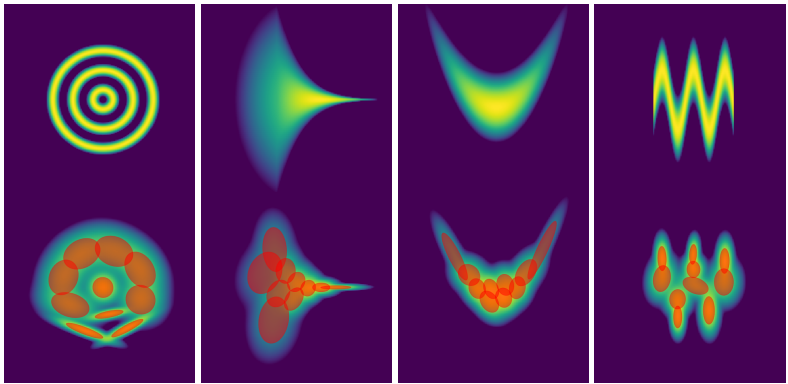
How expressive efficient are mixtures?



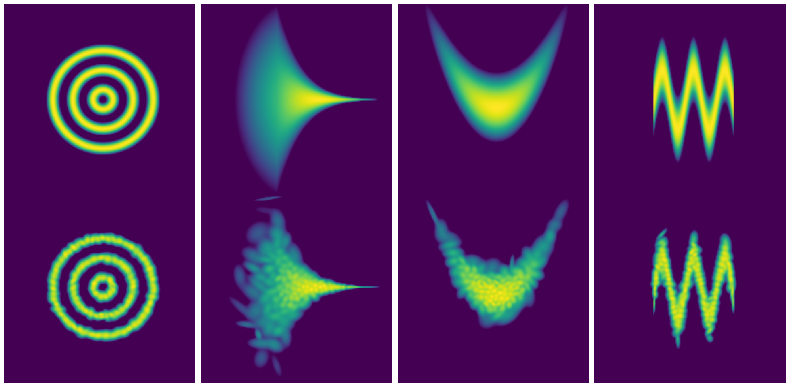
How expressive efficient are mixtures?



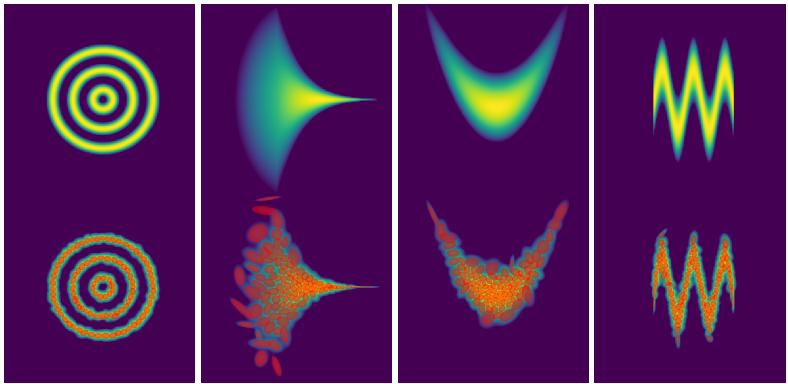
How expressive efficient are mixtures?



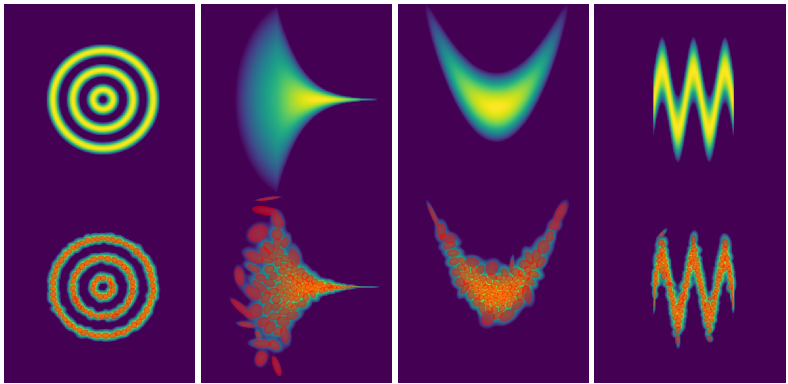
How expressive efficient are mixtures?



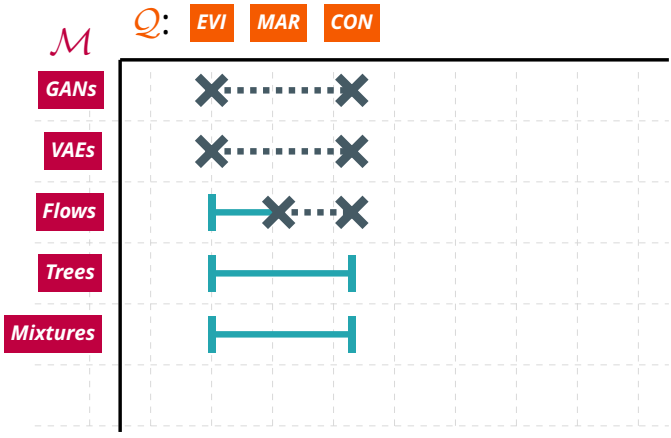
How expressive efficient are mixtures?



How expressive efficient are mixtures?



$\Rightarrow$ *stack mixtures like in deep generative models*

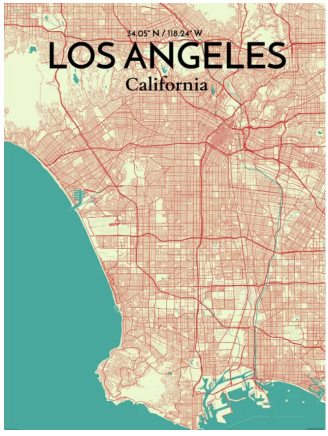


tractable bands

Maximum A Posteriori (MAP)

aka Most Probable Explanation (MPE)

q_5: *Which combination of roads is most likely to be jammed on Monday at 9am?*

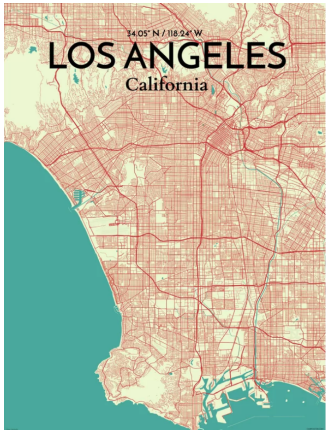


Maximum A Posteriori (MAP)

aka Most Probable Explanation (MPE)

$\mathbf{q}_5$: *Which combination of roads is most likely to be jammed on Monday at 9am?*

$$\mathbf{q}_5(\mathbf{m}) = \operatorname{argmax}_{\mathbf{j}} p_{\mathbf{m}}(\mathbf{j}_1, \mathbf{j}_2, \ldots \mid \mathsf{Day}=\mathsf{M}, \mathsf{Time}=9)$$



Maximum A Posteriori (MAP)

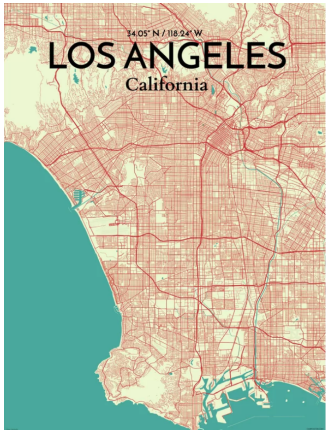
aka Most Probable Explanation (MPE)

$\mathbf{q}_5$: *Which combination of roads is most likely to be jammed on Monday at 9am?*

$\mathbf{q}_5(\mathbf{m}) = \operatorname{argmax}_{\mathbf{j}} p_{\mathbf{m}}(\mathbf{j}_1, \mathbf{j}_2, \ldots \mid \text{Day}=\text{M}, \text{Time}=9)$

General: $\operatorname{argmax}_{\mathbf{q}} p_{\mathbf{m}}(\mathbf{q} \mid \mathbf{e})$

where $\mathbf{Q} \cup \mathbf{E} = \mathbf{X}$



Maximum A Posteriori (MAP)

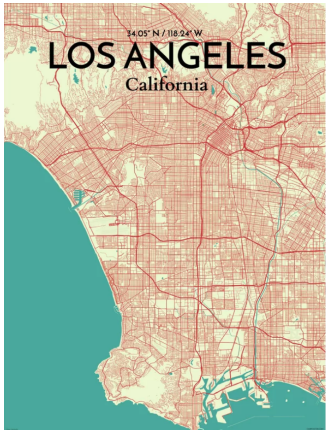
aka Most Probable Explanation (MPE)

$\mathbf{q}_5$: *Which combination of roads is most likely to be jammed on Monday at 9am?*

...***intractable*** for latent variable models!

$$\max_{\mathbf{q}} p_{\mathbf{m}}(\mathbf{q} \mid \mathbf{e}) = \max_{\mathbf{q}} \sum_{\mathbf{z}} p_{\mathbf{m}}(\mathbf{q}, \mathbf{z} \mid \mathbf{e})$$

$$\neq \sum_{\mathbf{z}} \max_{\mathbf{q}} p_{\mathbf{m}}(\mathbf{q}, \mathbf{z} \mid \mathbf{e})$$

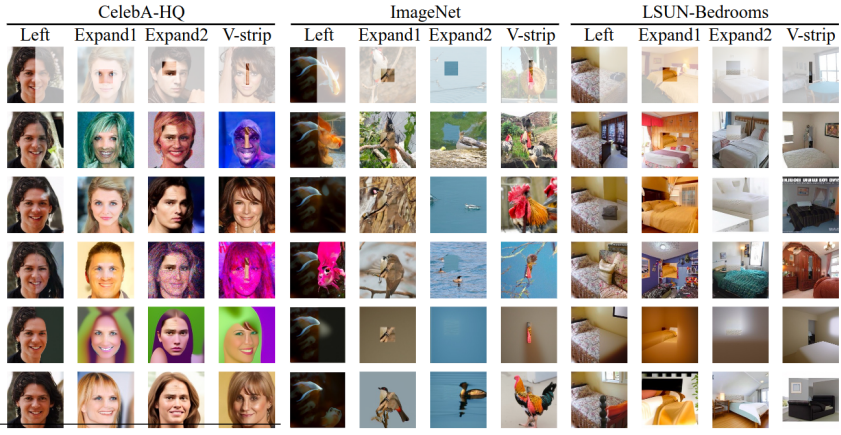


MAP inference : image inpainting

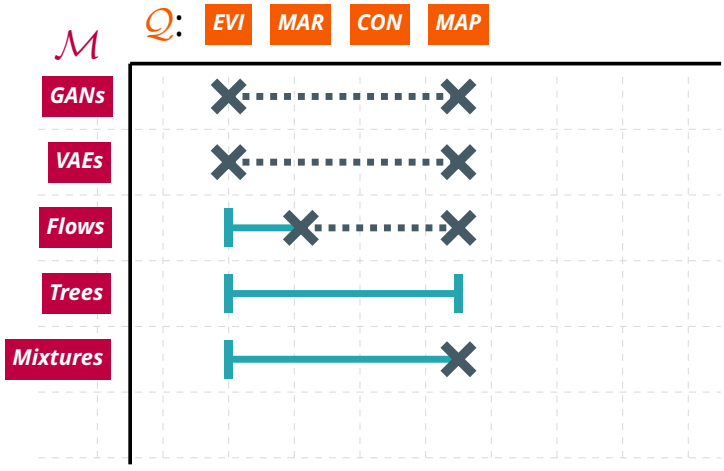
Predicting ***arbitrary patches***
given a ***single*** model
without the need of retraining.

Poon and Domingos, "Sum-Product Networks: a New Deep Architecture", UAI 2011, 2011
Sguerra and Cozman, "Image classification using sum-product networks for autonomous flight of micro aerial vehicles", , 2016

MAP inference : image inpainting



Liu, Niepert, and Broeck, "Image Inpainting via Tractable Steering of Diffusion Models", , 2024

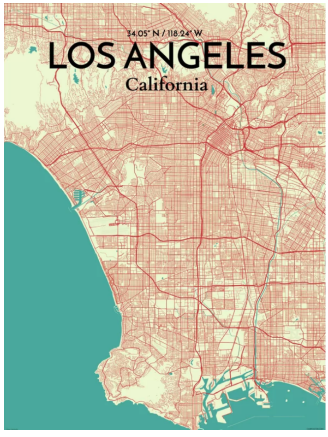


tractable bands

Marginal MAP (MMAP)

aka Bayesian Network MAP

q_6: *Which combination of roads is most likely to be jammed* ~~*on Monday*~~ *at 9am?*

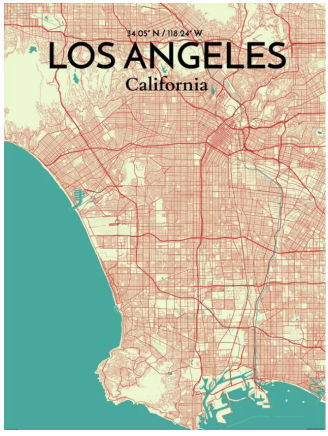


Marginal MAP (MMAP)

aka Bayesian Network MAP

$\mathbf{q}_6$: *Which combination of roads is most likely to be jammed* ~~*on Monday*~~ *at 9am?*

$$\mathbf{q}_6(\mathbf{m}) = \operatorname{argmax}_{\mathbf{j}}\ p_{\mathbf{m}}(\mathbf{j}_1, \mathbf{j}_2, \ldots \mid \mathsf{Time}{=}9)$$



Marginal MAP (MMAP)

aka Bayesian Network MAP

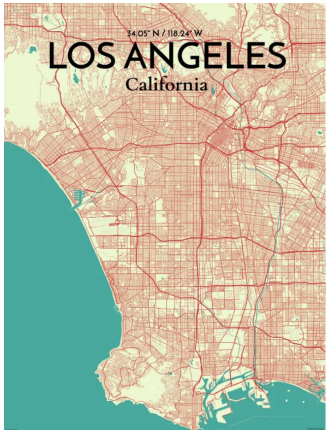
$\mathbf{q}_6$: *Which combination of roads is most likely to be jammed* ~~*on Monday*~~ *at 9am?*

$$\mathbf{q}_6(\mathbf{m}) = \text{argmax}_{\mathbf{j}}\ p_{\mathbf{m}}(\mathbf{j}_1, \mathbf{j}_2, \ldots \mid \text{Time}=9)$$

General: $\text{argmax}_{\mathbf{q}}\ p_{\mathbf{m}}(\mathbf{q} \mid \mathbf{e})$

$$= \text{argmax}_{\mathbf{q}}\ \textstyle\sum_{\mathbf{h}} p_{\mathbf{m}}(\mathbf{q}, \mathbf{h} \mid \mathbf{e})$$

where $\mathbf{Q} \cup \mathbf{H} \cup \mathbf{E} = \mathbf{X}$



Marginal MAP (MMAP)

aka Bayesian Network MAP

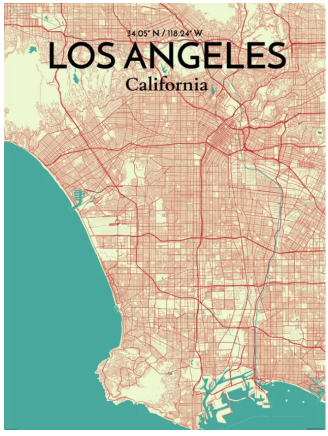
$\mathbf{q}_6$: *Which combination of roads is most likely to be jammed ~~on Monday~~ at 9am?*

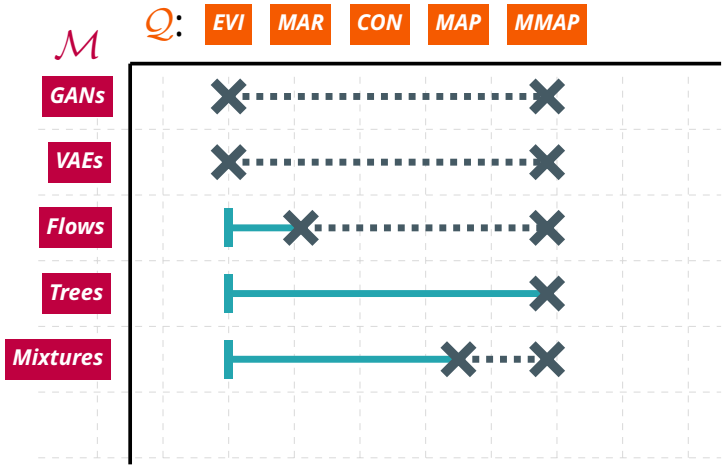
$$\mathbf{q}_6(\mathbf{m}) = \operatorname{argmax}_{\mathbf{j}}\ p_{\mathbf{m}}(\mathbf{j}_1, \mathbf{j}_2, \ldots \mid \mathsf{Time}=9)$$

$\Rightarrow$ *NP^{PP}-complete [Park and Darwiche 2006]*

$\Rightarrow$ *NP-hard for trees [de Campos 2011]*

$\Rightarrow$ *NP-hard even for Naive Bayes [ibid.]*

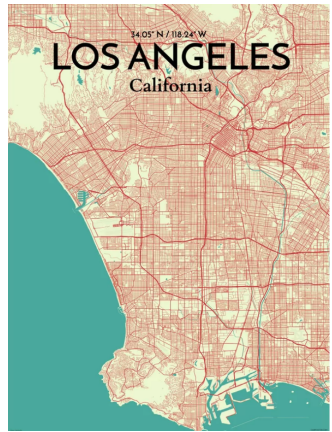




tractable bands

Advanced queries

q_2: *Which day is most likely to have a traffic jam on my route to campus?*



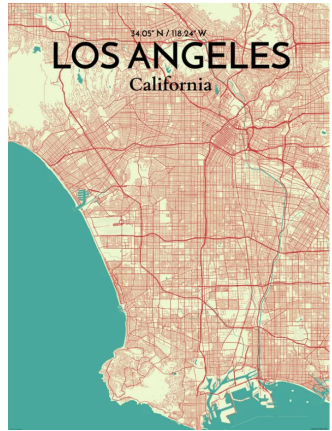
Bekker et al., "Tractable Learning for Complex Probability Queries", , 2015

Advanced queries

$\mathbf{q}_2$: *Which day is most likely to have a traffic jam on my route to campus?*

$$\mathbf{q}_2(\mathbf{m}) = \text{argmax}_{\mathsf{d}}\, p_{\mathbf{m}}(\mathsf{Day} = \mathsf{d} \wedge \bigvee_{i \in \mathsf{route}} \mathsf{Jam}_{\mathsf{Str}\, i})$$

$\Rightarrow$ ***marginals + MAP + logical events***



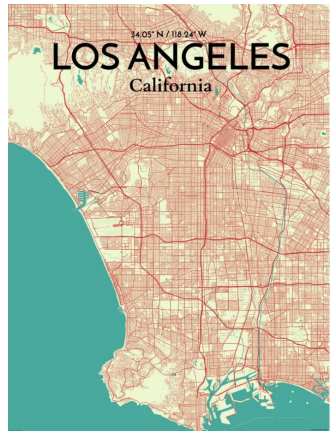
© fineartamerica.com

Bekker et al., "Tractable Learning for Complex Probability Queries", , 2015

Advanced queries

q_2: *Which day is most likely to have a traffic jam on my route to campus?*

q_7: *What is the probability of seeing more traffic jams in Westwood than Hollywood?*



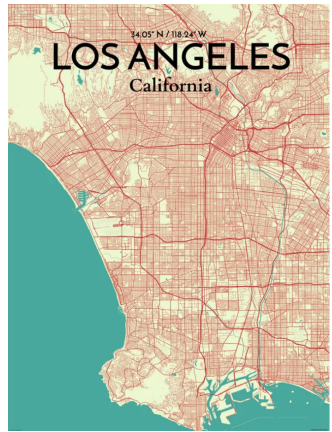
Bekker et al., "Tractable Learning for Complex Probability Queries", , 2015

Advanced queries

q_2: *Which day is most likely to have a traffic jam on my route to campus?*

q_7: *What is the probability of seeing more traffic jams in Westwood than Hollywood?*

$\Rightarrow$ ***counts + group comparison***



Bekker et al., "Tractable Learning for Complex Probability Queries", , 2015

Advanced queries

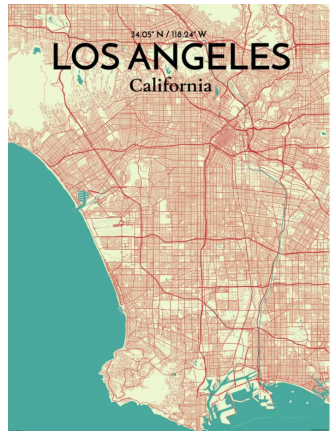
q_2: *Which day is most likely to have a traffic jam on my route to campus?*

q_7: *What is the probability of seeing more traffic jams in Westwood than Hollywood?*

and more:

expected classification agreement
[Oztok, Choi, and Darwiche 2016; Choi, Darwiche, and Broeck 2017; Choi and Broeck 2018]

expected predictions *[Khosravi et al. 2019]*



Bekker et al., "Tractable Learning for Complex Probability Queries", , 2015

more complex reasoning

q_1 *"What is the **expected prediction** for a patient with unavailable records?"*

q_2 *"How **fair** is the prediction is a certain protected attribute changes?"*

q_3 *"Can we certify no **adversarial examples** exist?"*

...asking queries to a ML model

more complex reasoning

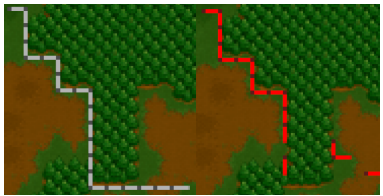
q$_1$ $\mathbb{E}_{\mathbf{x}_m \sim p(\mathbf{x}_m|\mathbf{x}_o)}\left[f(\mathbf{x}_o, \mathbf{x}_m)\right]$
(expected prediction)

q$_2$ $\mathbb{E}_{\mathbf{x}_c \sim p(\mathbf{x}_c|X_s=0)}\left[f_0(\mathbf{x}_c)\right] - \mathbb{E}_{\mathbf{x}_c \sim p(\mathbf{x}_c|X_s=1)}\left[f_1(\mathbf{x}_c)\right]$
(fairness)

q$_3$ $\mathbb{E}_{\mathbf{e} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_D)}\left[f(\mathbf{x} + \mathbf{e})\right]$
(adversarial robust.)

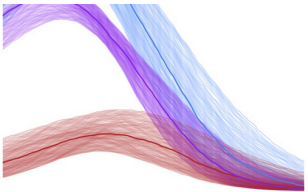
...into math expressions

more complex reasoning



neuro-symbolic AI

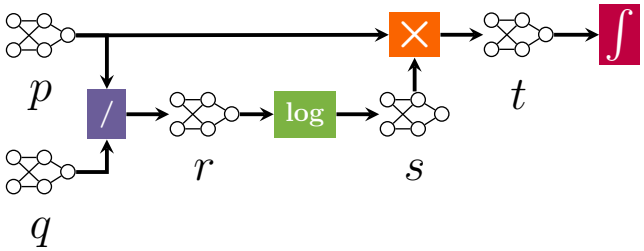
probabilistic programming



computing uncertainties (Bayesian inference

...and more application scenarios

$$\int p(\mathbf{x}) \times \log \left(p(\mathbf{x}) \,/\, q(\mathbf{x}) \right) \, d\mathbf{X}$$



build a LEGO-like query calculus!

Vergari *et al., "A Compositional Atlas of Tractable Circuit Operations: From Simple Transformations to Complex Information-Theoretic Queries", NeurIPS, 2021*

	Query	Tract. Conditions	Hardness
CROSS ENTROPY	$-\int p(\boldsymbol{x}) \log q(\boldsymbol{x}) \, \mathrm{d}\mathbf{X}$	Cmp, q Det	#P-hard w/o Det
SHANNON ENTROPY	$-\sum p(\boldsymbol{x}) \log p(\boldsymbol{x})$	Sm, Dec, Det	coNP-hard w/o Det
RÉNYI ENTROPY	$(1-\alpha)^{-1} \log \int p^{\alpha}(\boldsymbol{x}) \, d\mathbf{X}, \alpha \in \mathbb{N}$	SD	#P-hard w/o SD
	$(1-\alpha)^{-1} \log \int p^{\alpha}(\boldsymbol{x}) \, d\mathbf{X}, \alpha \in \mathbb{R}_{+}$	Sm, Dec, Det	#P-hard w/o Det
MUTUAL INFORMATION	$\int p(\boldsymbol{x}, \boldsymbol{y}) \log(p(\boldsymbol{x}, \boldsymbol{y}) / (p(\boldsymbol{x}) p(\boldsymbol{y})))$	Sm, SD, Det*	coNP-hard w/o SD
KULLBACK-LEIBLER DIV.	$\int p(\boldsymbol{x}) \log(p(\boldsymbol{x}) / q(\boldsymbol{x})) d\mathbf{X}$	Cmp, Det	#P-hard w/o Det
RÉNYI'S ALPHA DIV.	$(1-\alpha)^{-1} \log \int p^{\alpha}(\boldsymbol{x}) q^{1-\alpha}(\boldsymbol{x}) \, d\mathbf{X}, \alpha \in \mathbb{N}$	Cmp, q Det	#P-hard w/o Det
	$(1-\alpha)^{-1} \log \int p^{\alpha}(\boldsymbol{x}) q^{1-\alpha}(\boldsymbol{x}) \, d\mathbf{X}, \alpha \in \mathbb{R}$	Cmp, Det	#P-hard w/o Det
ITAKURA-SAITO DIV.	$\int [p(\boldsymbol{x}) / q(\boldsymbol{x}) - \log(p(\boldsymbol{x}) / q(\boldsymbol{x})) - 1] d\,\mathbf{X}$	Cmp, Det	#P-hard w/o Det
CAUCHY-SCHWARZ DIV.	$-\log \frac{\int p(\boldsymbol{x}) q(\boldsymbol{x}) d\mathbf{X}}{\sqrt{\int p^2(\boldsymbol{x}) d\mathbf{X} \int q^2(\boldsymbol{x}) d\mathbf{X}}}$	Cmp	#P-hard w/o Cmp
SQUARED LOSS	$\int (p(\boldsymbol{x}) - q(\boldsymbol{x}))^2 d\,\mathbf{X}$	Cmp	#P-hard w/o Cmp

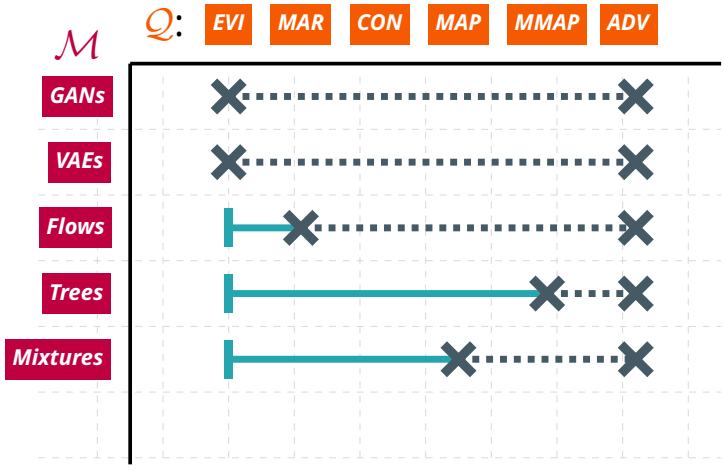
compositionally *derive the tractability of many more queries*

Vergari *et al., "A Compositional Atlas of Tractable Circuit Operations: From Simple Transformations to Complex Information-Theoretic Queries", NeurIPS, 2021*

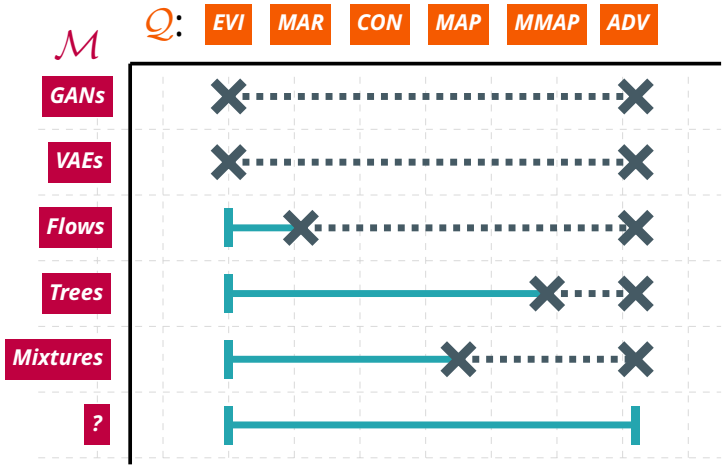
	Query	Tract. Conditions	Hardness
CROSS ENTROPY	$-\int p(\boldsymbol{x}) \log q(\boldsymbol{x}) \, \mathrm{d}\mathbf{X}$	Cmp, q Det	#P-hard w/o Det
SHANNON ENTROPY	$-\sum p(\boldsymbol{x}) \log p(\boldsymbol{x})$	Sm, Dec, Det	coNP-hard w/o Det
RÉNYI ENTROPY	$(1-\alpha)^{-1} \log \int p^{\alpha}(\boldsymbol{x}) \, d\mathbf{X}, \alpha \in \mathbb{N}$	SD	#P-hard w/o SD
	$(1-\alpha)^{-1} \log \int p^{\alpha}(\boldsymbol{x}) \, d\mathbf{X}, \alpha \in \mathbb{R}_{+}$	Sm, Dec, Det	#P-hard w/o Det
MUTUAL INFORMATION	$\int p(\boldsymbol{x}, \boldsymbol{y}) \log(p(\boldsymbol{x}, \boldsymbol{y}) / (p(\boldsymbol{x}) p(\boldsymbol{y})))$	Sm, SD, Det*	coNP-hard w/o SD
KULLBACK-LEIBLER DIV.	$\int p(\boldsymbol{x}) \log(p(\boldsymbol{x}) / q(\boldsymbol{x})) d\mathbf{X}$	Cmp, Det	#P-hard w/o Det
RÉNYI'S ALPHA DIV.	$(1-\alpha)^{-1} \log \int p^{\alpha}(\boldsymbol{x}) q^{1-\alpha}(\boldsymbol{x}) \, d\mathbf{X}, \alpha \in \mathbb{N}$	Cmp, q Det	#P-hard w/o Det
	$(1-\alpha)^{-1} \log \int p^{\alpha}(\boldsymbol{x}) q^{1-\alpha}(\boldsymbol{x}) \, d\mathbf{X}, \alpha \in \mathbb{R}$	Cmp, Det	#P-hard w/o Det
ITAKURA-SAITO DIV.	$\int [p(\boldsymbol{x}) / q(\boldsymbol{x}) - \log(p(\boldsymbol{x}) / q(\boldsymbol{x})) - 1] d\,\mathbf{X}$	Cmp, Det	#P-hard w/o Det
CAUCHY-SCHWARZ DIV.	$-\log \frac{\int p(\boldsymbol{x}) q(\boldsymbol{x}) d\mathbf{X}}{\sqrt{\int p^2(\boldsymbol{x}) d\mathbf{X} \int q^2(\boldsymbol{x}) d\mathbf{X}}}$	Cmp	#P-hard w/o Cmp
SQUARED LOSS	$\int (p(\boldsymbol{x}) - q(\boldsymbol{x}))^2 d\,\mathbf{X}$	Cmp	#P-hard w/o Cmp

*and **prove hardness** when some input properties are not satisfied*

***Vergari** et al., "A Compositional Atlas of Tractable Circuit Operations: From Simple Transformations to Complex Information-Theoretic Queries", NeurIPS, 2021*



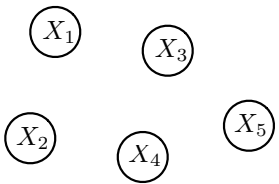
tractable bands



tractable bands

Fully factorized models

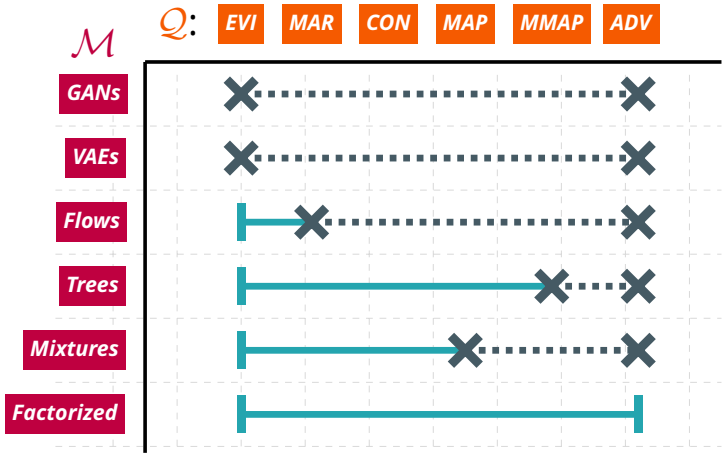
A completely disconnected graph. Example: Product of Bernoullis (PoBs)



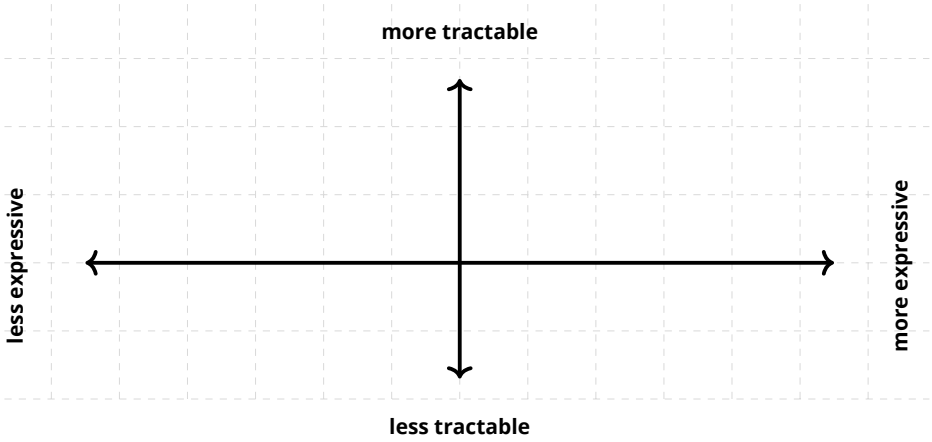
$$p(\mathbf{x}) = \prod_{i=1}^{n} p(x_i)$$

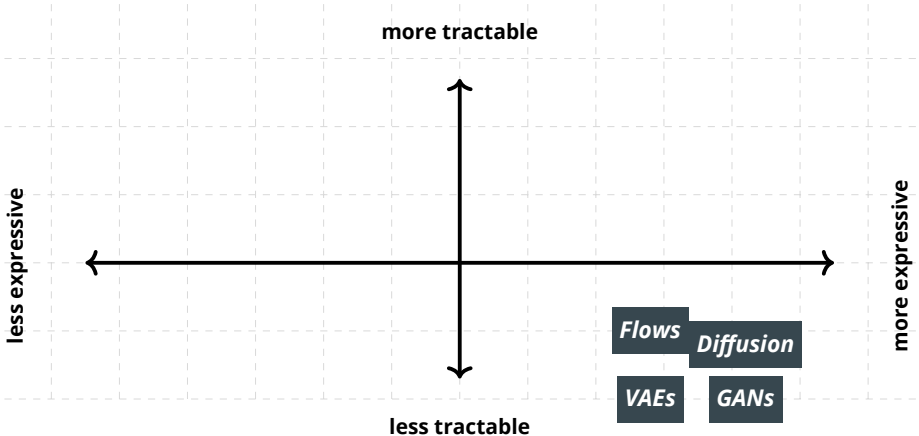
Complete evidence, marginals and MAP, MMAP inference is ***linear***!

$\Longrightarrow$ *but definitely not expressive...*

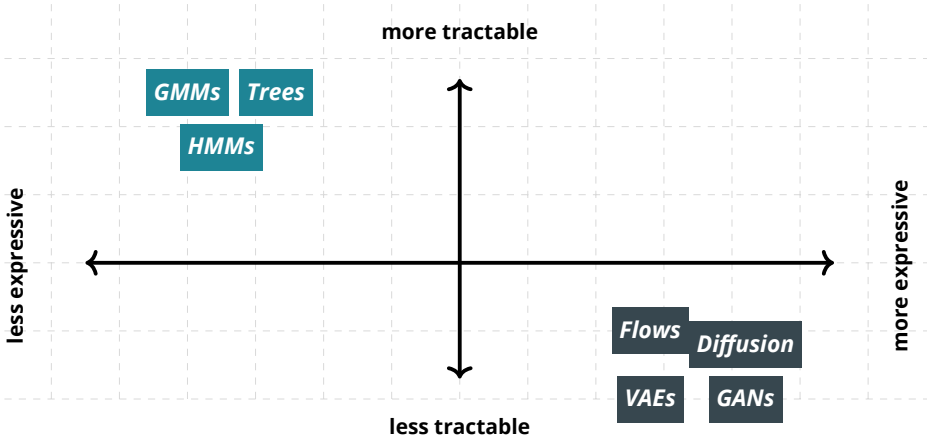


tractable bands

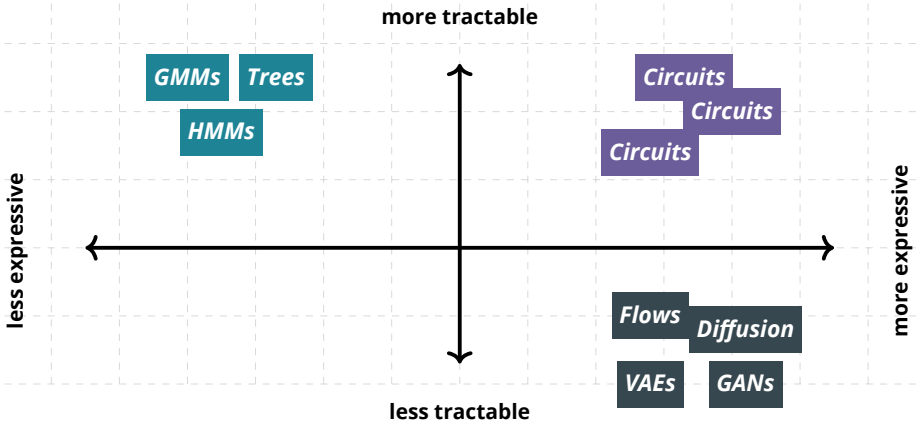

more tractable
less expressive
more expressive
less tractable



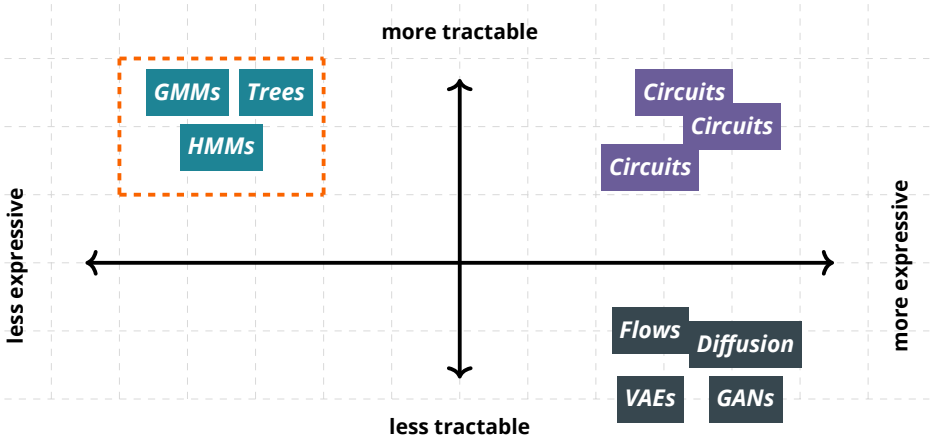
Expressive models are not much tractable...



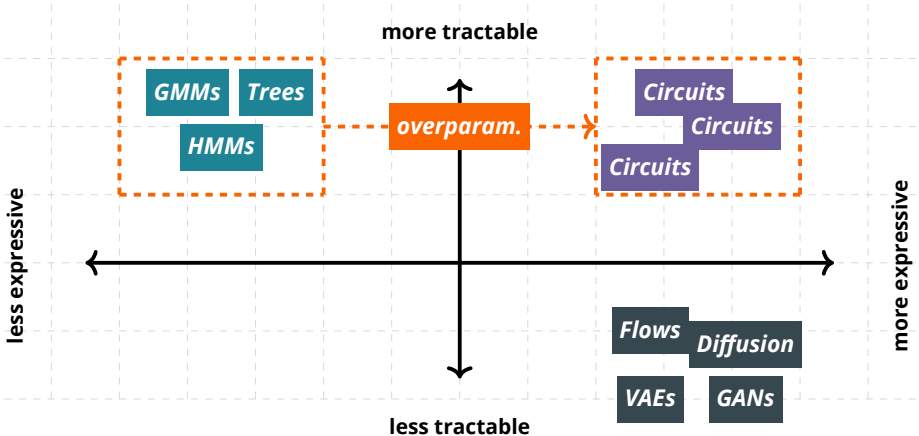
Tractable models are not that expressive...



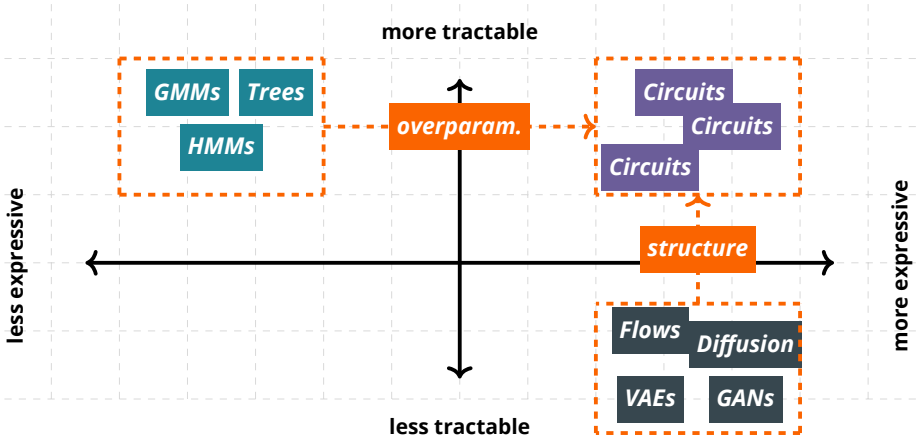
Circuits can be both expressive and tractable!



Start simple...



then make it more expressive!



impose structure!