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Deep Learning

[11: Generative Models (Part 1)]

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(last compiled at 16:01:00 on 2018/11/04)

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Generative Models

Approximate Inference

Summary

References

- *Deep Learning* by Goodfellow, Bengio and Courville [▶ Link](#)
 - ▶ Chapter 19: Approximate Inference
 - ▶ Chapter 20: Deep Generative Models
- *Pattern Recognition and Machine Learning* by Bishop
 - ▶ Chapter 10: Approximate Inference
- online resources:
 - ▶ *Stanford CS231n: CNN for Visual Recognition* [▶ Link](#)
 - ▶ *CVPR 2018 GAN Tutorial* [▶ Link](#)
 - ▶ *NIPS 2016 Variational Inference Tutorial* [▶ Link](#)
 - ▶ *NIPS 2016 GAN Tutorial* [▶ Link](#)

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Generative Models

Introduction

Autoregressive Models

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Summary

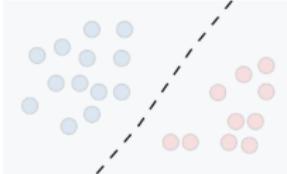
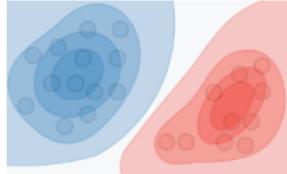
Supervised vs unsupervised learning

	supervised	unsupervised
data	(x, y) x : data, y : label	x just data, no _____
goal	learn a <i>function</i> to map $x \mapsto y$	learn inherent <i>structure</i> of the data
examples	classification regression object detection semantic segmentation	clustering dimensionality reduction representation learning density estimation

(source: cs231n)

Discriminative vs generative models

- assume supervised learning
 - goal: learn a *function* f to map $x \mapsto y$

	discriminative	generative
goal	directly estimate $p(y x)$	estimate $p(x y)$; then deduce ¹ $p(y x)$
should evaluate	$f(x) = \operatorname{argmax}_y p(y x)$	$f(x) = \operatorname{argmax}_y p(x y)p(y)$
what's learned	decision boundary	probability _____ of data
examples		
	SVM, neural nets	Gaussian mixture, Bayes nets

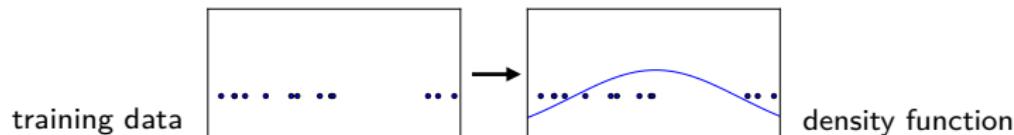
(source: [Ng and Jordan, 2002], stackoverflow)

¹ e.g. using Bayes rule: $p(y | x) = \frac{p(x | y)p(y)}{p(x)}$

Generative modeling in unsupervised learning

- **density estimation**

- ▶ goal: learn $p(x)$

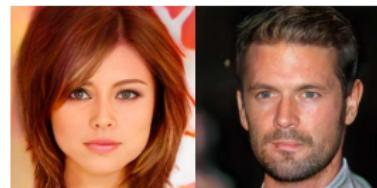


- generation

- ▶ given training data, generate new samples from the same distribution



training data $\sim p_{\text{data}}(x)$

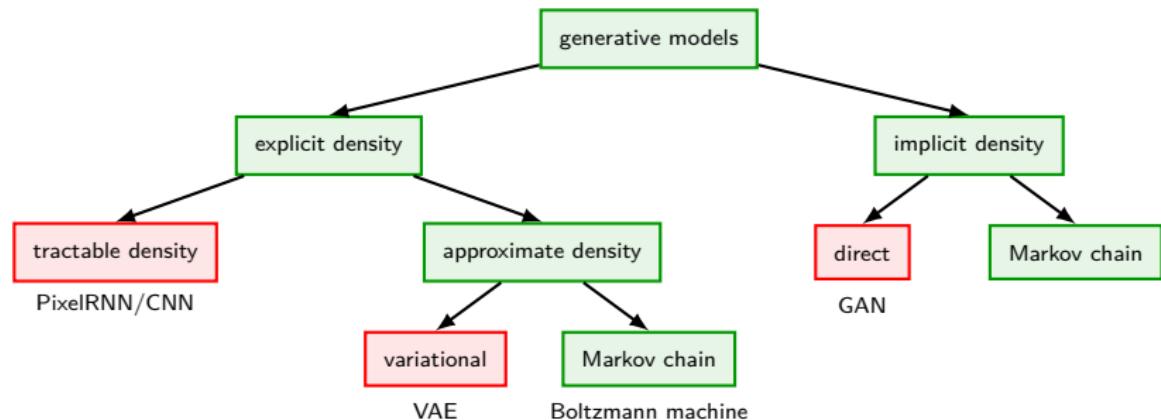


generated samples $\sim p_{\text{model}}(x)$

- ▶ want to learn $p_{\text{model}}(x)$ similar to $p_{\text{data}}(x)$

(source: Goodfellow (2018), Karras (2017))

Taxonomy of generative models



(source: Goodfellow, 2017)

1. explicit density estimation

- ▶ explicitly define and solve for $p_{\text{model}}(\mathbf{x})$

2. implicit density estimation

- ▶ learn a model that can sample from $p_{\text{model}}(\mathbf{x})$ w/o explicitly defining it

Trends in generative models

- conventional GM approaches have one of three drawbacks [Doersch, 2016]:
 1. require strong assumptions about structure in data
 2. make approximations \Rightarrow suboptimal results
 3. rely on computationally expensive inference procedures (*e.g.* MCMC)
- recent advances
 - ▶ train **neural nets** as powerful function approximators through backprop
 \Rightarrow gives framework for **backprop-based function approximators** to build GMs

e.g. variational autoencoder: one of the most popular such frameworks

- ▶ assumptions of this model: weak
- ▶ training: fast via _____
- ▶ make an approximation but error is small given high-capacity models

- generative models based on neural nets

1. autoregressive models (or fully visible belief nets)

- ▶ model $p(\mathbf{x})$ as $\prod_{i=1}^n p(x_i | x_1, \dots, x_{i-1})$

e.g. PixelRNN, PixelCNN, WaveNet

2. Helmholtz machines

- ▶ model $p(\mathbf{x})$ as $\int p(\mathbf{z})p(\mathbf{x} | \mathbf{z})d\mathbf{z}$

- ▶ two components: _____ net (encoder) + generative net (decoder)

- ▶ use variational inference to maximize ELBO

e.g. variational autoencoder (VAE)

3. generative adversarial network (GAN)

- ▶ no explicit density modeling

- ▶ two components: generator + discriminator

- ▶ train models by solving minimax problem

Why study generative models?

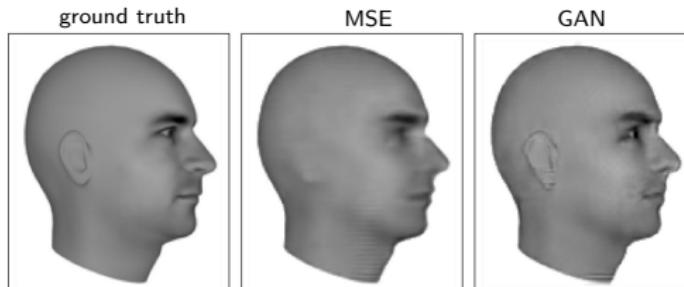
- excellent test of our ability
 - ▶ to represent/manipulate **high-dim/complicated probability distributions**
- can be incorporated into **reinforcement learning** (RL)
 - ▶ simulate possible futures for planning
- can be trained with missing data
 - ▶ can provide predictions on inputs that are missing data
 - ⇒ facilitate -supervised learning



(source: Chen+, 2018)

- enable machine learning to work with multi-modal outputs

e.g. a single input → many different correction answers



← video frame prediction

- ▶ MSE: averaging
- ⇒ blurry
- ▶ GAN: sharp

(source: Lotter+, 2015)

- enable inference of _____ representations

⇒ can be useful as general features

e.g. identity-preserving latent representations →

(source: Antipov+, 2017)

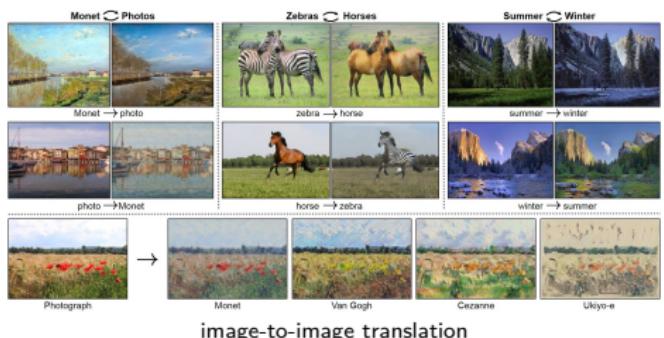


age conditional GAN

- many tasks require **realistic** generation of samples
 - e.g. single image super-resolution, art creation, image-to-image translation



first AI art sold at Christie (\$432,000)



3.5 years of progress on faces

(source: Christie's, Zhu+ (2017), Brundage+ (2018))

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Fully visible belief network (FVBN)

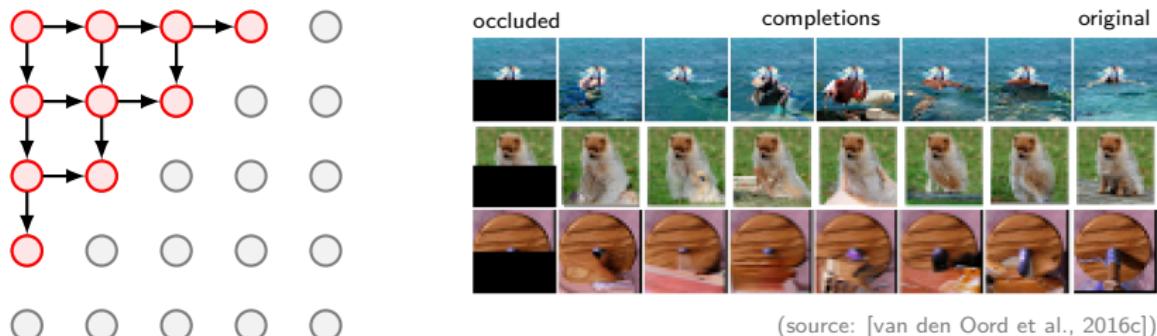
- explicit density model
- how it works:
 1. decompose likelihood of each input x into a product of 1D distributions

$$\underbrace{p(\mathbf{x})}_{\text{likelihood of input } \mathbf{x}} = \prod_{i=1}^n \underbrace{p(x_i | x_1, \dots, x_{i-1})}_{\text{probability of } i\text{-th feature given all previous features}}$$

2. maximize likelihood of training data
- complex distribution over feature values
 - ▶ we express it using a **neural net**
 - main issue:
 - ▶ need to define _____ of “previous features”

PixelRNN

- context: image (ICML 2016 best paper²)
- idea: the same as _____ modeling applied to image
 - ▶ generate image pixels starting from corner
 - ▶ model dependency on previous pixels using 2D LSTM
- limitation
 - ▶ sequential generation \Rightarrow slow



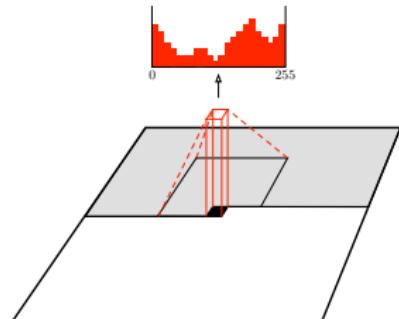
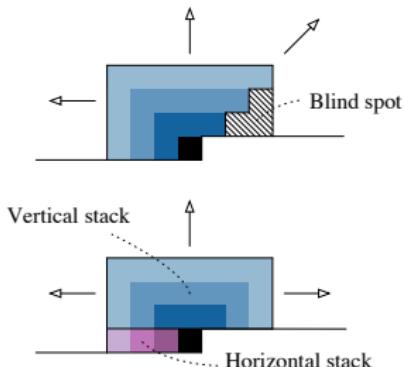
(source: [van den Oord et al., 2016c])

²this paper also proposed a simple PixelCNN, which was revised later in their NIPS paper (next page)

PixelCNN

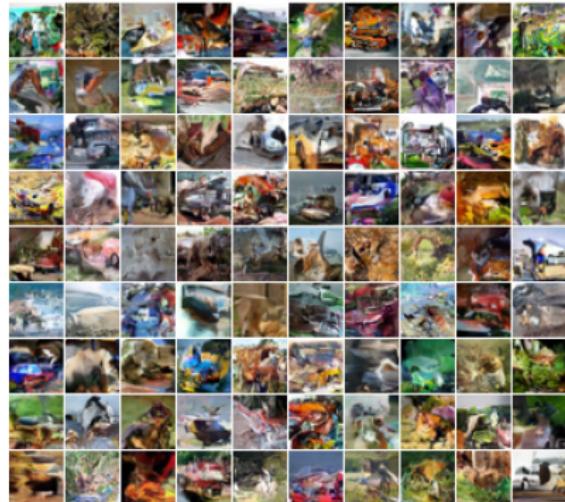
- still generate image pixels starting from corner
- what's new
 - ▶ use CNN (not LSTM) to model dependency on previous pixels
 - ▶ two **conv stacks** to remove _____ spots
- training
 - ▶ maximize likelihood of training images
 - ▶ loss: softmax loss at each pixel
 - ▶ faster³ than PixelRNN
- image generation
 - ▶ must still proceed sequentially
 - ⇒ still slow

(source: [van den Oord et al., 2016b])

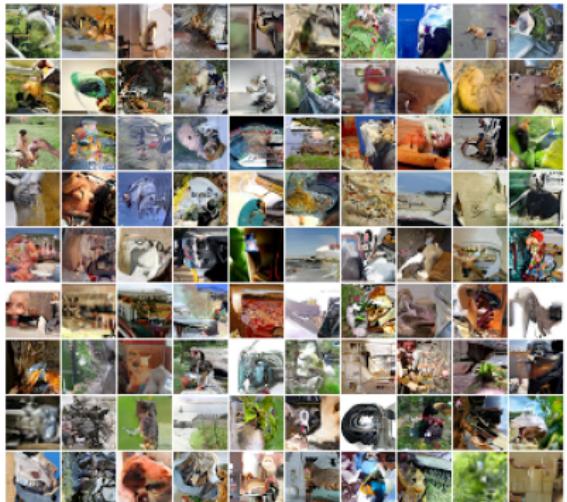


³we can parallelize convolutions since context region values are known from training images

Examples of generated samples



32×32 CIFAR-10

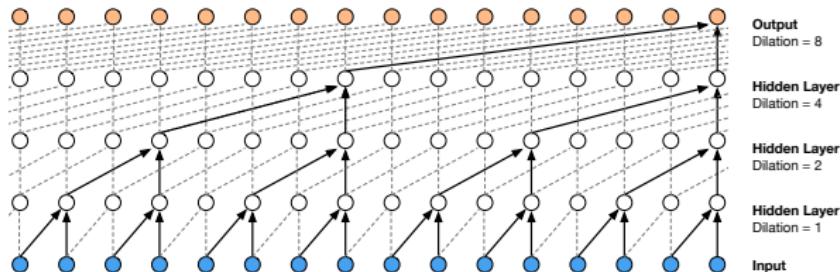


32×32 ImageNet

(source: [van den Oord et al., 2016c])

WaveNet

- can generate raw audios (trained on raw audio waveforms)
 - ▶ similar to PixelCNN in structure, but much more successful
 - ▶ amazing quality but **slow generation** (2 min to synthesize 1 sec audio)
- architecture
 - ▶ use **dilated convolution** to vastly _____ receptive field



(source: [van den Oord et al., 2016a])

- ▶ stack many layers like the above together
- ▶ use classification (not regression) to generate next sample point
- ▶ convert continuous audio → 256-level quantized classes

Remarks

- autoregressive models: pros and cons
 - ▶ can explicitly compute $p(x)$
 - ▶ good samples
 - ▶ sequential generation: _____
- to improve performance
 - ▶ gated convolution layers
 - ▶ short-cut connections
 - ▶ discretized logistic loss
 - ▶ multi-scale
 - ▶ parallelization
 - ▶ and many more!
- more information: [▶ Link](#)

(source: cs231n, [Salimans et al., 2017])



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Probabilistic machine learning

- a probabilistic model
 - ▶ a joint distribution of hidden variables \mathbf{z} and observed variables \mathbf{x}

$$p(\mathbf{z}, \mathbf{x})$$

- ▶ describes how (a portion of) the world works
- inference about the unknowns:
 - ▶ through **posterior** _____
i.e. conditional distribution of the hidden variables given the observations

$$p(\mathbf{z} | \mathbf{x}) = \frac{p(\mathbf{z}, \mathbf{x})}{p(\mathbf{x})} \leftarrow \begin{array}{l} \text{model} \\ \text{data} \end{array}$$

- ▶ the posterior links data and model \Rightarrow used in all downstream analyses
- posterior inference:
 - ▶ therefore a central task in probabilistic models

Posterior inference

- refers to
 - (1) computing posterior distribution $p(z | x)$ or
 - (2) taking expectations computed wrt this distribution

e.g. expectation-maximization (EM) algorithm

- ▶ evaluates expectation of **complete-data log likelihood**
wrt **posterior distribution of latent variables**:

$$\mathcal{Q}(\theta, \theta^{\text{old}}) \triangleq \sum_z p(z | x, \theta^{\text{old}}) \log p(x, z | \theta)$$

- for many models of practical interest
 - ▶ it is intractable to do (1)/(2) \Rightarrow called “challenge of inference”
- challenge of inference
 - ▶ makes it difficult to ____ probabilistic models

Challenge of inference

- general reasons
 - ▶ dimensionality of latent space: too high to work with directly
 - ▶ posterior: highly complex \Rightarrow expectations are not analytically tractable
- reasons in deep learning
 - ▶ interactions between _____ variables (*e.g.* connections between layers)
 - ▶ most neural nets with multiple layers of hidden variables
 - ▷ have intractable posterior distributions
- a solution: approximate posterior inference

Bayesian view

- we setup the general problem
 - ▶ consider a joint density of latent variables \mathbf{z} and observations \mathbf{x}
$$p(\mathbf{z}, \mathbf{x}) = p(\mathbf{z})p(\mathbf{x} | \mathbf{z})$$
- latent variables help govern distribution of data in Bayesian models
- a Bayesian model
 - ▶ draws _____ variables from a prior $p(\mathbf{z})$, and then
 - ▶ relates them to observations through likelihood $p(\mathbf{x} | \mathbf{z})$
- inference in a Bayesian model
 - ▶ conditions on data and computes posterior $p(\mathbf{z} | \mathbf{x})$

↑
this often requires approximate inference

Approximate posterior inference

1. stochastic (e.g. Markov chain Monte Carlo: MCMC)

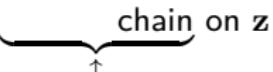
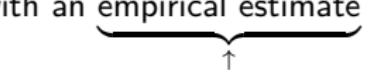
- ▶ given infinite computational resource, can generate exact results
- ▶ approximation arises from using a finite amount of processor time
- ⌚ sampling methods can be computationally demanding
- ⇒ their use is often limited to small-scale problems
- ⌚ difficult to know whether _____ samples are being generated

2. deterministic (e.g. variational inference: VI)

- ▶ some of which scale well to large applications
 - ▶ based on analytical approximations to posterior $p(z | x)$
- e.g. assume it factorizes or has a _____ form (like Gaussian)
- ⇒ never generate exact results

Markov chain Monte Carlo (MCMC)

- dominant paradigm for decades

1. construct an ergodic⁴ 
chain on z
its stationary distribution = posterior $p(z|x)$
2. sample from the chain to collect samples from the stationary distribution
3. approximate the posterior with an empirical estimate

constructed from (a subset of) the collected samples

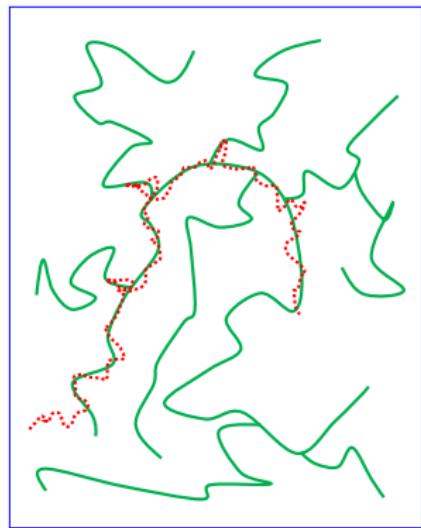
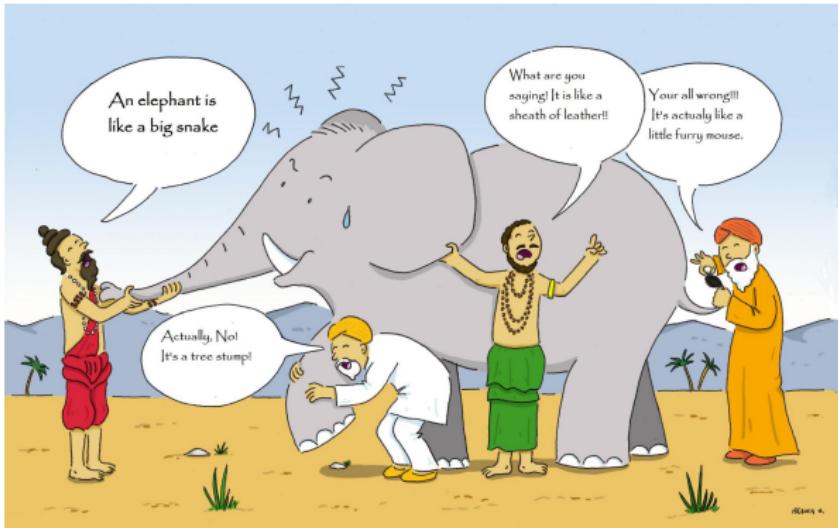
- widely studied, extended, and applied

e.g. Metropolis-Hastings algorithm, Gibbs sampling

- too slow for large data sets/complex models

► a good alternative in these settings: variational inference

⁴an ergodic system is a dynamical system with the following property: no matter where you start, you run the system and keep running it, then any other points in the space you will eventually reach



- goal: sample from a small subset of high-dim region where sampling is ____
 - ▶ often p has some (connected) structure
 - ▶ start somewhere, and start moving around (**red dots**)
 - ▶ try to move toward a region of high probability, and then get there
 - ▶ try to stay in the **regions of high probability (green regions)**, doing random walks
 - ✳ MCMC: do this by forming a Markov chain

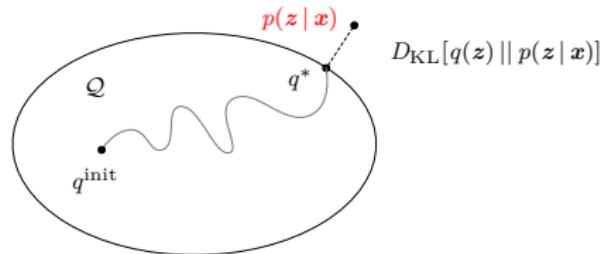
Variational inference (VI)

- main idea: turn inference into optimization (rather than sampling)

1. posit \mathcal{Q} , a *family* of approximate _____ over \mathbf{z}
 - ▶ each $q(\mathbf{z}) \in \mathcal{Q}$: a candidate approximation to the exact posterior
2. find the member of \mathcal{Q} that minimizes D_{KL} to the exact posterior

$$q^*(\mathbf{z}) = \operatorname{argmin}_{q(\mathbf{z}) \in \mathcal{Q}} D_{\text{KL}}[q(\mathbf{z}) \parallel p(\mathbf{z} \mid \mathbf{x})]$$

3. approximate the posterior with q^*
 - ▶ use $q^*(\mathbf{z})$ in place of $p(\mathbf{z} \mid \mathbf{x})$ in downstream modeling



(source: [Blei et al., 2017])

Comparison

- different approaches to solving the same problem

	Markov chain Monte Carlo	variational inference
what it does	samples a Markov chain	solves an _____ problem
approximates posterior with	samples from the chain	optimization results
a tool for	simulating (sampling) from densities	approximating densities

when to use MCMC and when to use VI?

- **MCMC**

- ▶ more computationally intensive than VI, but
- ▶ guarantees producing (asymptotically) _____ samples from target density
 - ⇒ suited to smaller data sets/scenarios
 - ▷ where we happily pay a heavier cost for more **precise** samples

- **VI**

- ▶ has no such guarantees (only finds a density close to the target)
- ▶ but faster than MCMC (also can use stochastic/distributed optimization)
 - ⇒ suited to large data sets/scenarios
 - ▷ where we want to **quickly** explore many models

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The phrase “variational” [Wainwright et al., 2008]

- an umbrella term that refers to mathematical tools for
 - ▶ optimization-based formulations of problems
 - ▶ associated techniques for their solution
- origin: *calculus of variations* (optimization over a space of functions)
- general idea:
 - ▶ express a quantity of interest as the solution of an optimization problem
- the optimization problem can then be “_____”
 - ▶ either by approximating
 - ▷ the function to be optimized or
 - ▷ the set over which the optimization takes place
 - ▶ such relaxations allow us to
 - ▷ approximate the original quantity of interest

Variational inference (variational Bayes)

- inference = solving the following optimization:

$$q^*(\mathbf{z}) = \operatorname{argmin}_{q(\mathbf{z}) \in \mathcal{Q}} D_{\text{KL}}[q(\mathbf{z}) \parallel p(\mathbf{z} \mid \mathbf{x})] \quad (1)$$

- ▶ complexity of \mathcal{Q} determines complexity of this optimization
- choosing \mathcal{Q} needs a good balance
 1. restrict \mathcal{Q} sufficiently [for efficiency]
⇒ it comprises only _____ distributions
 2. allow \mathcal{Q} to be sufficiently rich/flexible [for accuracy]
⇒ it can provide a good approximation to the true posterior

Optimization challenge

- the objective (1): not computable

$$q^*(\mathbf{z}) = \operatorname{argmin}_{q(\mathbf{z}) \in \mathcal{Q}} D_{\text{KL}}[q(\mathbf{z}) \parallel p(\mathbf{z} \mid \mathbf{x})] \quad (1)$$

- reason:

$$\begin{aligned} D_{\text{KL}}[q(\mathbf{z}) \parallel p(\mathbf{z} \mid \mathbf{x})] &= \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})}[\log q(\mathbf{z})] - \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})}[\log p(\mathbf{z} \mid \mathbf{x})] \\ &= \mathbb{E}_{\mathbf{z}}[\log q(\mathbf{z})] - \mathbb{E}_{\mathbf{z}}[\log p(\mathbf{z}, \mathbf{x})] + \underbrace{\log p(\mathbf{x})}_{\text{intractable}} \end{aligned} \quad (2)$$

- solution:

► optimize an alternative objective called evidence lower bound ()
also known as negative variational free energy

Evidence lower bound (ELBO)

- rearranging (2) gives

$$\underbrace{\log p(\mathbf{x}) - D_{\text{KL}}[q(\mathbf{z}) \parallel p(\mathbf{z} \mid \mathbf{x})]}_{\substack{\text{a constant} \\ \text{wrt } q(\mathbf{z})}} = \underbrace{\mathbb{E}_{\mathbf{z}}[\log p(\mathbf{z}, \mathbf{x})] - \mathbb{E}_{\mathbf{z}}[\log q(\mathbf{z})]}_{\triangleq \mathcal{L}(q) \quad \text{"ELBO"}} \quad (3)$$

► ELBO = minimizing the D_{KL}

- examining ELBO gives intuitions about optimal variational density

$$\begin{aligned}\mathcal{L}(q) &= \mathbb{E}_{\mathbf{z}}[\log p(\mathbf{z}, \mathbf{x})] - \mathbb{E}_{\mathbf{z}}[\log q(\mathbf{z})] \\ &= \mathbb{E}_{\mathbf{z}}[\log p(\mathbf{z})] + \mathbb{E}_{\mathbf{z}}[\log p(\mathbf{x} \mid \mathbf{z})] - \mathbb{E}_{\mathbf{z}}[\log q(\mathbf{z})] \\ &= \underbrace{\mathbb{E}_{\mathbf{z}}[\log p(\mathbf{x} \mid \mathbf{z})]}_{\substack{\text{expected log likelihood} \\ \text{of the data}}} - \underbrace{D_{\text{KL}}[q(\mathbf{z}) \parallel p(\mathbf{z})]}_{\substack{D_{\text{KL}} \text{ between} \\ \text{prior } p(\mathbf{z}) \text{ and } q(\mathbf{z})}}\end{aligned}$$

$$\text{ELBO ("variational objective")}: \mathcal{L}(q) = \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})}[\log p(\mathbf{x} | \mathbf{z})] - D_{\text{KL}}[q(\mathbf{z}) || p(\mathbf{z})]$$

which values of \mathbf{z} will this objective encourage $q(\mathbf{z})$ to place its mass on?

- first term: $\mathbb{E}_{\mathbf{z}}[\log p(\mathbf{x} | \mathbf{z})]$
 - i.e. an expected likelihood
 - ▶ encourages densities that explain _____ data⁵
- second term: $-D_{\text{KL}}[q(\mathbf{z}) || p(\mathbf{z})]$
 - i.e. negative divergence between variational density and prior
 - ⇒ encourages densities close to prior
- thus the variational objective mirrors
 - ▶ usual balance between likelihood and prior

⁵i.e. densities that place their mass on configurations of the latent variables that explain the observed data

Why called ELBO?

- ELBO $\mathcal{L}(q)$ lower-bounds the (log) evidence $p(\mathbf{x})$

i.e. for any $q(z)$

$$\log p(\mathbf{x}) \geq \mathcal{L}(q)$$

- proof:

- ▶ notice that (3) gives

$$\log p(\mathbf{x}) = \mathcal{L}(q) + \underbrace{D_{\text{KL}}[q(\mathbf{z}) || p(\mathbf{z} | \mathbf{x})]}_{\geq 0}$$

- ▶ can also be derived through Jensen's inequality

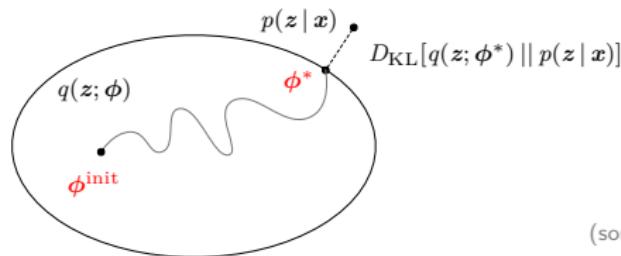
Common restrictions on \mathcal{Q}

1. parameterization

- ▶ use a parametric distribution governed by parameters ϕ

$$q(z; \phi) = q_\phi(z)$$

- ▶ ϕ : variational parameters



(source: [Blei et al., 2017])

- ▶ ELBO \mathcal{L} now becomes a function of ϕ : $\mathcal{L}(q, \phi)$
- ▶ _____ = finding ϕ^*
- ▶ spoiler: VAE uses a neural net to model $q_\phi(z)$ and sgd to train it

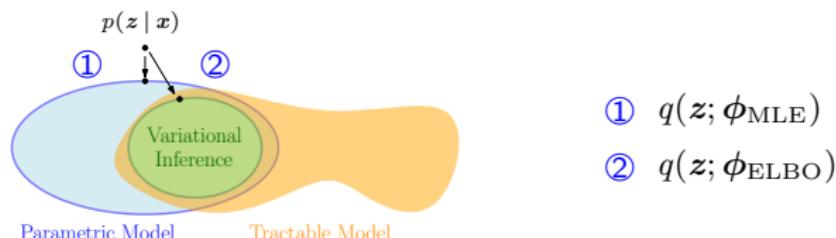
2. factorization

- ▶ assume q factorizes (called “mean-field approach”)

$$q(\mathbf{z}) = \prod_{j=1}^m q_j(z_j)$$

- ▶ each latent variable z_j :
 - ▷ governed by its own variational factor, the density $q_j(z_j)$
 - ▷ can take on any form appropriate to the corresponding random var
- e.g. a continuous variable: a _____ factor
a categorical variable: a categorical factor

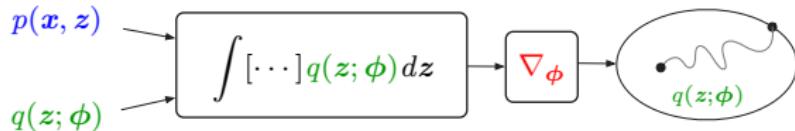
core idea behind VI: maximize \mathcal{L} over a **restricted** family of distributions q



(source: [Chen et al., 2018])

Variational inference recipe

1. start with a **model**: $p(\mathbf{x}, \mathbf{z})$
2. choose a **variational approximation**: $q(\mathbf{z}; \boldsymbol{\phi}) = q_{\boldsymbol{\phi}}(\mathbf{z})$
3. write down **ELBO**: $\mathcal{L}(\boldsymbol{\phi}) = \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}; \boldsymbol{\phi})} [\log p(\mathbf{x}, \mathbf{z}) - q(\mathbf{z}; \boldsymbol{\phi})]$
4. compute the expectation/integral: **e.g.** $\mathcal{L}(\boldsymbol{\phi}) = \mathbf{x}\boldsymbol{\phi}^2 + \log \boldsymbol{\phi}$
5. take derivatives: **e.g.** $\nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi}) = 2\mathbf{x}\boldsymbol{\phi} + \frac{1}{\boldsymbol{\phi}}$
6. optimize: $\boldsymbol{\phi}_{t+1} = \boldsymbol{\phi}_t + \underline{\hspace{10mm}}$



(source: [Blei et al., 2017])

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Summary

- generative models: density estimation and sample generation
 - ▶ explicit density: PixelRNN/CNN, variational autoencoder (VAE)
 - ▶ implicit density: generative adversarial network (GAN)
- generative models are versatile and useful for many tasks
 - ▶ representation/manipulation of high-dim distributions
 - ▶ reinforcement learning, semi-supervised learning
 - ▶ multi-modal outputs, inference of latent representations
- approximate inference schemes fall into two classes: stochastic or deterministic
 - ▶ their strengths and weaknesses are complementary to each other
- variational inference: inference → optimization
 - ▶ goal: approximate posterior $p(z|x) \approx q(z) \in \mathcal{Q}$ [z: latent, x: observed]
 - ▶ \mathcal{Q} : a family of restricted (parameterized/factorized) distributions over z
 - ▶ $q^*(z) = \operatorname{argmin}_{q(z) \in \mathcal{Q}} D_{\text{KL}}[q(z) || p(z|x)]$
 - ▶ VAE: we parameterize q using a neural net and optimize by backprop

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