Introduction

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VI Tutorial @ University of Alicante
https://vitutorial.github.io/tour/ua2020

This tutorial is about

probabilistic models *parameterised* by **neural networks**

- in this class we will look into what this means, why this is interesting, and when this is challenging

1. Probabilistic Models
2. Supervised Models Powered by NNs
3. Latent Variable Models Powered by NNs

What is a probabilistic model?

A probabilistic model predicts possible outcomes of an experiment.

Most modern machine learning models are probabilistic.

Two Machine Learning Paradigms

Supervised problems: learn a distribution over observed data

- sentences in natural language, images, videos, . . .

Unsupervised problems: learn a distribution over observed and unobserved data

- sentences in natural language + parse trees, images + bounding boxes, . . .

What are the benefits of probabilistic models?

Probabilistic models allows to incorporate assumptions through

- the choice of distribution
- the way that distributions uses side information
- stipulate unobserved data and their properties

They return a distribution over outcomes

Other benefits

- They can generate data
- They allow to model unobserved data
- They can be more compact
- They can provide explanation and can suggest improvements
- They can inform decision makers

Deep Generative Models

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Short answer: *backpropagation breaks!*

Why are we here today?

Because we want to combine the advantages of probabilistic models and neural networks to potentially

- overcome lack of supervision
- learn from partial supervision
- learn from less data
- shape the way models reason about data

and much more!

What are you getting out of this today?

As we progress we will

- develop a shared vocabulary to talk about probabilistic models powered by NNs
- derive crucial results step by step
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Goal

- you should be able to navigate through fresh literature
- and start combining probabilistic models and NNs

Supervised problems

We have data $x^{(1)}, \dots, x^{(N)}$ e.g. sentences, images
generated by some **unknown** procedure which we assume can be captured by a probabilistic model

- with **known** probability (mass/density) function e.g.

$$X \sim \mathrm{Cat}(\theta_1, \dots, \theta_K) \quad \text{or} \quad X \sim \mathcal{N}(\theta_\mu, \theta_\sigma^2)$$

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and estimate parameters θ that assign maximum likelihood $p(x^{(1)}, \ldots, x^{(N)}|\theta)$ to observations

Supervised NN models

Let y be all side information available
e.g. deterministic *inputs/features/predictors*

Have neural networks predict parameters of our probabilistic model

$$X|y \sim \mathrm{Cat}(\pi_\theta(y)) \quad \text{or} \quad X|y \sim \mathcal{N}(\mu_\theta(y), \sigma_\theta(y)^2)$$

and proceed to estimate parameters θ of the NNs

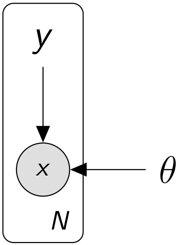
Graphical model

Random variables

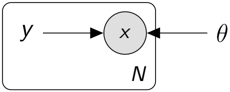
- observed data
  $x^{(1)}, \ldots, x^{(N)}$

Deterministic variables

- inputs or predictors
  $y^{(1)}, \ldots, y^{(N)}$
- model parameters θ



Multiple problems, same language



(Conditional) Density estimation

	Side information (y)	Observation (x)
Parsing	a sentence	its syntactic/semantic parse tree/graph
Translation	a sentence	its translation
Captioning	an image	caption in English
Entailment	a text and hypothesis	entailment relation

Task-driven feature extraction

Often our side information is itself some high dimensional object

- y is a sentence and x a tree
- y is the source sentence and x is the target
- y is an image and x is a caption

and part of the job of the NNs that parametrise our models is to also deterministically encode that input in a low-dimensional space

NN as efficient parametrisation

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Prediction is done by a decision rule outside the statistical model

- e.g. argmax, beam search

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MLE via gradient-based optimisation

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and we can update θ in the direction

$$\gamma \nabla_\theta \mathcal{L}(\theta|x^{(1:N)})$$

to attain a local maximum of the likelihood function

Big Data

For large N, computing the gradient is inconvenient

$$\nabla_\theta \mathcal{L}(\theta | x^{(1:N)}) = \underbrace{\sum_{s=1}^{N} \nabla_\theta \log p(x^{(s)} | \theta)}_{\text{too many terms}}$$

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$$= \mathbb{E}_{S \sim \mathcal{U}({}^{1}/_{N})} \left[N \nabla_\theta \log p(x^{(S)} | \theta) \right]$$

S selects data points uniformly at random

Stochastic optimisation

For large N, we can use a gradient estimate

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and take a step in the direction

$$\gamma\frac{N}{M}\underbrace{\nabla_\theta \mathcal{L}(\theta|x^{(s_1:s_M)})}_{\text{stochastic gradient}}$$

where $x^{(s_1:s_M)}$ is a random mini-batch of size M

DL in NLP recipe

Maximum likelihood estimation

- tells you which loss to optimise (i.e. negative log-likelihood)

Automatic differentiation (*backprop*)

- "give me a tractable forward pass and I will give you gradients"

Stochastic optimisation powered by backprop

- general purpose gradient-based optimisers

Constraints

Differentiability

- intermediate representations must be continuous
- activations must be differentiable

Tractability

- the likelihood function must be evaluated exactly, thus it's required to be tractable

When do we have intractable likelihood?

Latent variable models contain unobserved random variables

$$p(x, z|\theta)$$

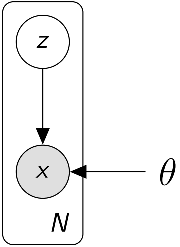
thus assessing the marginal likelihood requires marginalisation of latent variables

$$p(x|\theta) = \int p(x, z|\theta)\,\mathrm{d}z$$

Latent variable model

Latent random variables

- unobserved
- or unobservable



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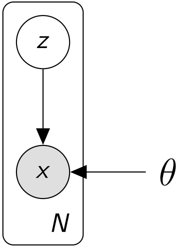

A joint distribution over data and unknowns

$$p(x, z|\theta) = p(z)p(x|z, \theta)$$

Examples of latent variable models

Discrete latent variable, continuous observation

$$\underbrace{p(x|\theta) = \sum_{c=1}^{K} \mathrm{Cat}(c|\pi_1, \ldots, \pi_K) \underbrace{\mathcal{N}(x|\mu_\theta(c), \sigma_\theta(c)^2)}_{\text{forward pass}}}_{\textbf{too many forward passes}}$$

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Continuous latent variable, discrete observation

$$p(x|\theta) = \underbrace{\int \mathcal{N}(z|0, I) \underbrace{\mathrm{Cat}(x|\pi_\theta(z))}_{\text{forward pass}} \mathrm{d}z}_{\textbf{infinitely many forward passes}}$$

Intractable gradient

$$\nabla_\theta \log p(x|\theta)$$

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\end{aligned}
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Approximations

Can we approximate the gradient?

- some approximations introduce bias
- others break differentiability
- some approximations suffer from both problems

We prefer unbiased approximations. A large bulk of DGM research goes to efficient unbiased gradient estimation.

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  e.g. parse trees, dependency graphs, alignments
- uncertainty quantification
  e.g. Bayesian NNs

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a mixture model whose mixture components are labelled by words

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