Welcome and Introduction

Philip Schulz and Wilker Aziz

https:
//github.com/philschulz/VITutorial

About us ...

Wilker Aziz

- Research associate at UvA
- VI, Sampling methods, Machine Translation

Philip Schulz

- Applied Scientist at Amazon
- ▶ VI, Machine Translation, Bayesian Models

Keywords

- supervised vs unsupervised learning
- density estimation
- probabilistic modelling
- deep learning
- maximum likelihood estimation
- gradient-based optimisation
- stochastic gradients
- latent variable models
- posterior inference
- variational inference

Problems

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 . . .

Supervised problems

We have data $x^{(1)}, \dots, x^{(N)}$ e.g.

▶ sentences, images, ...

generated by some unknown procedure

Supervised problems

We have data $x^{(1)}, \ldots, x^{(N)}$ 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.

$$X \sim \mathsf{Cat}(\pi_1, \dots, \pi_K)$$
 or $X \sim \mathcal{N}(\mu, \sigma^2)$

Supervised problems

We have data $x^{(1)}, \ldots, x^{(N)}$ 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.

$$X \sim \mathsf{Cat}(\pi_1, \dots, \pi_K)$$
 or $X \sim \mathcal{N}(\mu, \sigma^2)$

and proceed to estimate parameters that assign maximum likelihood to observations

Multiple problems, same language



(Conditional) Density estimation

Side information (ϕ) Parsing a sentence

Observation (x) its syntactic/semantic

parse tree/graph

Translation a sentence

its translation

Captioning an image

caption in English

Entailment a text and hypothesis

entailment relation

Where does deep learning kick in?

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

Have neural networks predict parameters of our probabilistic model

$$X|\phi \sim \mathsf{Cat}(\pi_{\theta}(\phi))$$
 or $X|\phi \sim \mathcal{N}(\mu_{\theta}(\phi), \sigma_{\theta}(\phi)^2)$

and proceed to estimate parameters θ of the NNs

Task-driven feature extraction

Often our side information ϕ is itself some high dimensional data

- lacktriangledown ϕ is a sentence and x a tree
- lacktriangledown ϕ is the source sentence and x is the target
- $ightharpoonup \phi$ 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

From the statistical point of view NNs do not generate data

- they parametrise distributions that by assumption govern data
- compact and efficient way to map from complex side information to parameter space

NN as efficient parametrisation

From the statistical point of view NNs do not generate data

- they parametrise distributions that by assumption govern data
- compact and efficient way to map from complex side information to parameter space

Prediction is done by a decision rule outside the statistical model

e.g. beam search

Let $p(x|\theta)$ be the probability of an observation x and θ refer to all of its parameters

Let $p(x|\theta)$ be the probability of an observation x and θ refer to all of its parameters

Given a dataset $x^{(1)}, \ldots, x^{(N)}$ of i.i.d. observations,

Let $p(x|\theta)$ be the probability of an observation x and θ refer to all of its parameters

Given a dataset $x^{(1)}, \ldots, x^{(N)}$ of i.i.d. observations, the log-likelihood function gives us a criterion for parameter estimation

$$\mathcal{L}(\theta|x^{(1:N)}) = \log \prod_{s=1}^{N} p(x^{(s)}|\theta)$$

Let $p(x|\theta)$ be the probability of an observation x and θ refer to all of its parameters

Given a dataset $x^{(1)}, \ldots, x^{(N)}$ of i.i.d. observations, the log-likelihood function gives us a criterion for parameter estimation

$$\mathcal{L}(\theta|x^{(1:N)}) = \log \prod_{s=1}^{N} p(x^{(s)}|\theta)$$
$$= \sum_{s=1}^{N} \log p(x^{(s)}|\theta)$$

MLE via gradient-based optimisation

If the log-likelihood is **differentiable** and **tractable** then backpropagation can give us the gradient

$$\mathbf{\nabla}_{\theta} \mathcal{L}(\theta|x^{(1:N)}) = \mathbf{\nabla}_{\theta} \sum_{s=1}^{N} \log p(x^{(s)}|\theta)$$

MLE via gradient-based optimisation

If the log-likelihood is **differentiable** and **tractable** then backpropagation can give us the gradient

$$\boldsymbol{\nabla}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta} | \boldsymbol{x}^{(1:N)}) = \boldsymbol{\nabla}_{\boldsymbol{\theta}} \sum_{s=1}^{N} \log p(\boldsymbol{x}^{(s)} | \boldsymbol{\theta}) = \sum_{s=1}^{N} \boldsymbol{\nabla}_{\boldsymbol{\theta}} \log p(\boldsymbol{x}^{(s)} | \boldsymbol{\theta})$$

MLE via gradient-based optimisation

If the log-likelihood is **differentiable** and **tractable** then backpropagation can give us the gradient

$$\nabla_{\theta} \mathcal{L}(\theta|x^{(1:N)}) = \nabla_{\theta} \sum_{s=1}^{N} \log p(x^{(s)}|\theta) = \sum_{s=1}^{N} \nabla_{\theta} \log p(x^{(s)}|\theta)$$

and we can update θ in the direction

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

to attain a local maximum of the likelihood function

For large N, computing the gradient is inconvenient

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

For large N, computing the gradient is inconvenient

$$\begin{split} \boldsymbol{\nabla}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}|\boldsymbol{x}^{(1:N)}) &= \underbrace{\sum_{s=1}^{N} \boldsymbol{\nabla}_{\boldsymbol{\theta}} \log p(\boldsymbol{x}^{(s)}|\boldsymbol{\theta})}_{\text{too many terms}} \\ &= \underbrace{\sum_{s=1}^{N} \frac{1}{N} N \boldsymbol{\nabla}_{\boldsymbol{\theta}} \log p(\boldsymbol{x}^{(s)}|\boldsymbol{\theta})}_{} \end{split}$$

For large N, computing the gradient is inconvenient

$$\begin{split} \nabla_{\theta} \mathcal{L}(\theta|x^{(1:N)}) &= \underbrace{\sum_{s=1}^{N} \nabla_{\theta} \log p(x^{(s)}|\theta)}_{\text{too many terms}} \\ &= \underbrace{\sum_{s=1}^{N} \frac{1}{N} N \nabla_{\theta} \log p(x^{(s)}|\theta)}_{\text{N}} \\ &= \underbrace{\sum_{s=1}^{N} \mathcal{U}(s|1/N) N \nabla_{\theta} \log p(x^{(s)}|\theta)}_{\text{0}} \end{split}$$

For large N, computing the gradient is inconvenient

$$egin{aligned}
abla_{ heta} \mathcal{L}(heta|x^{(1:N)}) &= \sum_{s=1}^{N}
abla_{ heta} \log p(x^{(s)}| heta) \ &= \sum_{s=1}^{N} rac{1}{N} N
abla_{ heta} \log p(x^{(s)}| heta) \ &= \sum_{s=1}^{N} \mathcal{U}(s|^{1}/N) N
abla_{ heta} \log p(x^{(s)}| heta) \ &= \mathbb{E}_{S \sim \mathcal{U}(1/N)} \left[N
abla_{ heta} \log p(x^{(S)}| heta)
ight] \end{aligned}$$

S selects data points uniformly at random

Stochastic optimisation

For large N, we can use a gradient estimate

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

Stochastic optimisation

For large N, we can use a gradient estimate

$$\begin{split} \boldsymbol{\nabla}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta} | \boldsymbol{x}^{(1:N)}) &= \underbrace{\mathbb{E}_{S \sim \mathcal{U}(^{1/N})} \left[N \boldsymbol{\nabla}_{\boldsymbol{\theta}} \log p(\boldsymbol{x}^{(S)} | \boldsymbol{\theta}) \right]}_{\text{expected gradient :)}} \\ & \overset{\mathsf{MC}}{\approx} \frac{1}{M} \sum_{m=1}^{M} N \boldsymbol{\nabla}_{\boldsymbol{\theta}} \log p(\boldsymbol{x}^{(s_i)} | \boldsymbol{\theta}) \\ S_i &\sim \mathcal{U}(^{1/N}) \end{split}$$

Stochastic optimisation

For large N, we can use a gradient estimate

$$\begin{split} \boldsymbol{\nabla}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta} | \boldsymbol{x}^{(1:N)}) &= \underbrace{\mathbb{E}_{S \sim \mathcal{U}(1/N)} \left[N \boldsymbol{\nabla}_{\boldsymbol{\theta}} \log p(\boldsymbol{x}^{(S)} | \boldsymbol{\theta}) \right]}_{\text{expected gradient :)}} \\ & \overset{\mathsf{MC}}{\approx} \frac{1}{M} \sum_{m=1}^{M} N \boldsymbol{\nabla}_{\boldsymbol{\theta}} \log p(\boldsymbol{x}^{(s_i)} | \boldsymbol{\theta}) \\ S_i \sim \mathcal{U}(1/N) \end{split}$$

and take a step in the direction

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

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

Tractability is central

Likelihood gives us a differentiable objective to optimise for

but we need to stick with tractable likelihood functions

When do we have intractable likelihood?

Unsupervised problems contain unobserved random variables

$$p(x, z | \theta) = \overbrace{p(z)}^{\text{prior}} \underbrace{p(x | z, \theta)}_{\text{observation model}}$$

When do we have intractable likelihood?

Unsupervised problems contain unobserved random variables

$$p(x, z | \theta) = \overbrace{p(z)}^{\text{prior}} \underbrace{p(x | z, \theta)}_{\text{observation model}}$$

thus assessing the marginal likelihood requires marginalisation of latent variables

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

Examples of latent variable models

Discrete latent variable, continuous observation

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

Examples of latent variable models

Discrete latent variable, continuous observation

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

Continuous latent variable, discrete observation

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

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

$$\nabla_{\theta} \log p(x|\theta) = \nabla_{\theta} \log \underbrace{\int p(x,z|\theta) dz}_{\text{marginal}}$$

$$\nabla_{\theta} \log p(x|\theta) = \nabla_{\theta} \log \underbrace{\int p(x,z|\theta) dz}_{\text{marginal}}$$

$$= \underbrace{\frac{1}{\int p(x,z|\theta) dz} \int \nabla_{\theta} p(x,z|\theta) dz}_{\text{chain rule}}$$

$$\nabla_{\theta} \log p(x|\theta) = \nabla_{\theta} \log \underbrace{\int p(x,z|\theta) dz}_{\text{marginal}}$$

$$= \underbrace{\frac{1}{\int p(x,z|\theta) dz} \int \nabla_{\theta} p(x,z|\theta) dz}_{\text{chain rule}}$$

$$= \underbrace{\frac{1}{p(x|\theta)} \int \underbrace{p(x,z|\theta) \nabla_{\theta} \log p(x,z|\theta)}_{\text{log-identity for derivatives}} dz$$

$$\nabla_{\theta} \log p(x|\theta) = \nabla_{\theta} \log \underbrace{\int p(x,z|\theta) dz}_{\text{marginal}}$$

$$= \underbrace{\frac{1}{\int p(x,z|\theta) dz} \int \nabla_{\theta} p(x,z|\theta) dz}_{\text{chain rule}}$$

$$= \underbrace{\frac{1}{p(x|\theta)} \int \underbrace{p(x,z|\theta) \nabla_{\theta} \log p(x,z|\theta)}_{\text{log-identity for derivatives}} dz$$

$$= \int \underbrace{p(z|x,\theta) \nabla_{\theta} \log p(x,z|\theta)}_{\text{d}z} dz$$

$$\nabla_{\theta} \log p(x|\theta) = \nabla_{\theta} \log \underbrace{\int p(x,z|\theta) dz}_{\text{marginal}}$$

$$= \underbrace{\frac{1}{\int p(x,z|\theta) dz} \int \nabla_{\theta} p(x,z|\theta) dz}_{\text{chain rule}}$$

$$= \underbrace{\frac{1}{p(x|\theta)} \int \underbrace{p(x,z|\theta) \nabla_{\theta} \log p(x,z|\theta)}_{\text{log-identity for derivatives}} dz$$

$$= \int \underbrace{p(z|x,\theta) \nabla_{\theta} \log p(x,z|\theta)}_{\text{gradientity for derivatives}} dz$$

$$= \mathbb{E}_{p(z|x,\theta)} [\nabla_{\theta} \log p(x,z|\theta)]$$

Some reasons

organise a massive collection of data e.g. LDA

Some reasons

- organise a massive collection of data e.g. LDA
- learn from unlabelled data
 e.g. semi-supervised learning

Some reasons

- organise a massive collection of data e.g. LDA
- learn from unlabelled data e.g. semi-supervised learning
- induce discrete representations
 e.g. parse trees, dependency graphs,
 permutations, alignments

Some reasons

- organise a massive collection of data e.g. LDA
- learn from unlabelled data e.g. semi-supervised learning
- induce discrete representations
 e.g. parse trees, dependency graphs,
 permutations, alignments
- uncertainty quantification e.g. Bayesian NNs

Probabilistic models parametrised by neural networks

Probabilistic models parametrised by neural networks

 explicit modelling assumptions one of the reasons why there's so much interest

Probabilistic models parametrised by neural networks

- explicit modelling assumptions one of the reasons why there's so much interest
- but requires efficient inference

Probabilistic models parametrised by neural networks

- explicit modelling assumptions one of the reasons why there's so much interest
- but requires efficient inference which is the reason why we are here today