Deep Probabilistic Models – Unobserved Data

Deep Learning 2 – 2023

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- with a tractable and differentiable likelihood function, gradient-based search for NN parameters gives us a general purpose mechanism to approach supervised learning

Finally, once the probabilistic model is fully specified (which includes parameter estimation), together with a decision rule, it can power applications (tasks).

Goals for this session

1. Prescribe joint distribution involving discrete and unobserved random variables
2. Estimate parameter via gradient-based MLE
3. Recognise the role of a model's posterior distribution in parameter estimation

Outline

Modelling observed random variables

Our goal is to learn a distribution over a set of **observed** random variables.

Observed random variables are the result of random experiments that have already happened: e.g., sentences in a collection of news articles, number of stars in a product review.

Modelling unobserved random variables

Unobserved random variables are variables that are

- observable in principle, but not available for observation (e.g., the topic of a piece of text, a semantic graph)
- unobservable (e.g., a 100-dimensional sentence embedding)

they help us prescribe and even estimate our models.

Our goal is to learn a distribution over *observed and unobserved rvs*

- make explicit assumptions about statistical dependence
- discover hidden structure
- mimic intuitions/knowledge about the data generating process
- deal with missing data
- estimate uncertainty about predictions

Deterministic predictors may also be available.

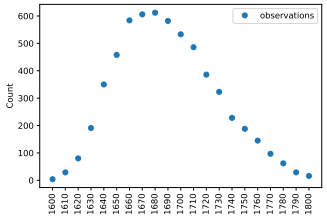
Unobserved random variables are also called latent variables.

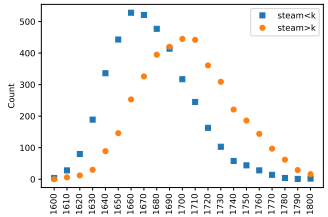
For those interested in Bayesian statistics, note that the presence of unobserved random variables does not imply Bayesian modelling. Bayesian principles are a collection of ideas organised in what is called the Bayesian Theory (or Bayesian Decision Theory) for rational decision making under uncertainty (Bernardo and Smith, 2009). These ideas may cross paths with many aspects of our ML solutions.

Outline

Latent Structure and Over-Dispersion

We found some old manuscripts in an excavation site, historians began labelling them for publication date.





Marginally (left), it looked like our observations could have been drawn from a Poisson distribution.

Left: publication date of documents in the labelled collection.

Our historians claim that above some threshold k a document was likely written after 1699 (when Thomas Savery demonstrated his first steam engine to the British Royal society).

Right: data as a function of the frequency of the word *steam*.

Plotting two streams of data under such criterion reveals what could have been 2 different Poisson distributions.

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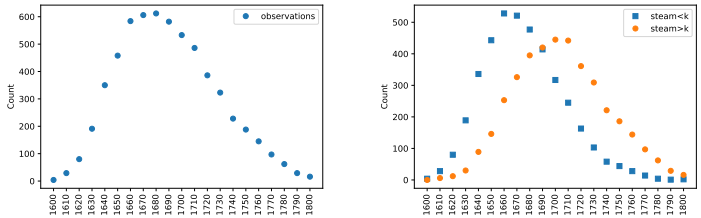

But they might also have been the result of mixing (right) into one population draws from two different Poisson distributions.

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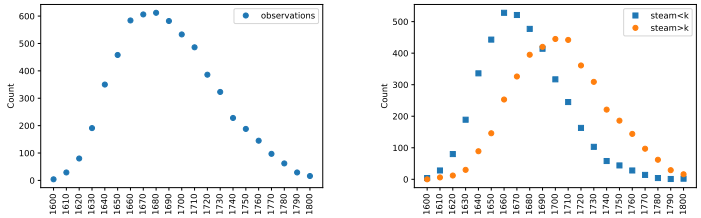

The way a model *views* the data tells us something about latent factors that account for (cause or correlate with) observed variance.

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Plotting two streams of data under such criterion reveals what could have been 2 different Poisson distributions.

"Oh, latent variables are like hidden units, right?"

Latent structure here has to do with a partitioning of the probability space in terms of intermediate outcomes that depend on one another.

Hidden layers in an NN output deterministic transformations of their observed inputs. They are not statements about statistical dependence.

Example:

$$Y|h \sim \text{Poisson}\left(\underbrace{\exp\left(\sum_{i=1}^{D} w_i h_i\right)}_{\text{shallow NN}}\right)$$

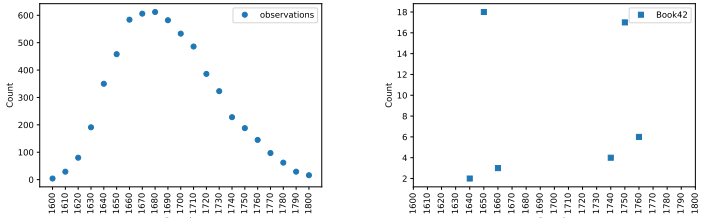
any one draw comes from the exact same Poisson.

To reveal latent structure that is likely supported by observations, we need to postulate a joint distribution where observations and latent variables interact.

'Interacting' is a matter of **statistical dependence**.

Latent Structure and Multimodality

For a few manuscripts, we obtained labels from multiple experts.



Left: observations for Y across the collection. Right: observations for Y given doc is book-42.

a unimodal conditional $Y|\mathrm{doc}$ seems inappropriate.

When we plot observations for Y (e.g., left) we see the data *marginally*.

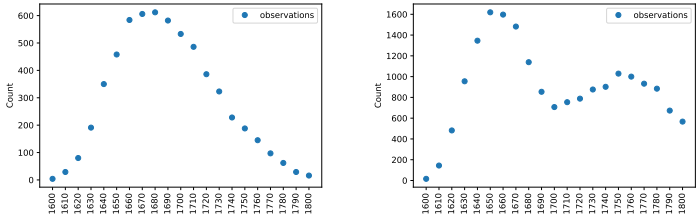
If we intend to model the data conditionally, that plot won't help us pick a family. That is because our choice should be informed by plots of the kind $Y|\mathrm{doc}$. If we group our data into bins, where bin membership depends on matching a specific value of doc, more often than not our bins will each contain a single data point. Should we conclude that *conditionally* our data can be seen as deterministic? By no means!

Be aware of sneaky modelling assumptions. The combination of *'1 bin per unique document'* and *'one plot per bin'* is a modelling choice (for visualisation purposes, but still). One that suffers from data sparsity so tremendously that it makes a random variable look deterministic. Concluding that we can model the data deterministically is in fact an instance of overfitting (by humans).

Note that sometimes we can *construct* more meaningful $Y|\mathrm{doc}$ plots that reveal the stochastic nature of the data. For example, if we have direct access to the mechanism by which observations are generated, we can fix doc and draw Y multiple times (rightmost plot on the slide).

"But NNs can, in principle, learn anything, right?"

Not quite. We identify a *probability measure* by parameterising a joint pdf (or pmf). Thus our models are limited by the expressiveness of the families we choose.



Left: data look unimodal and could have been drawn from a Poisson.
Right: data look bimodal and a single Poisson seems less likely.

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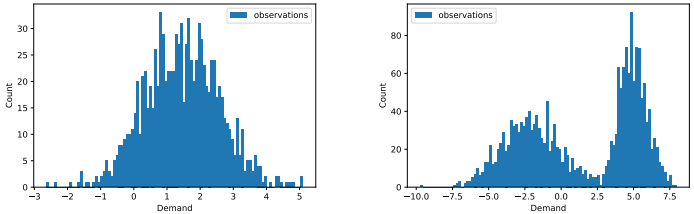


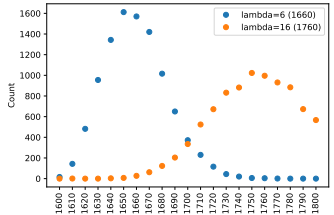
Left: data look unimodal and could have been drawn from a Gaussian.
Right: data look bimodal and a single Gaussian seems less likely.

Can we combine simple distributions?

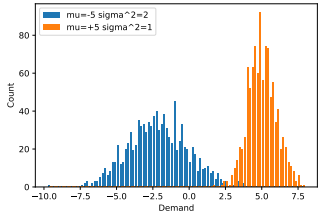
We can however *mix* K members of each family to get a good fit:

For example, with $K = 2$

$$Z|b \sim \text{Bernoulli}(b)$$
$$Y|\lambda, b \sim \text{Poisson}(\lambda_z)$$



$$Z|b \sim \text{Bernoulli}(b)$$
$$Y|\mu, \sigma, b \sim \mathcal{N}(\mu_z, \sigma_z^2)$$



This is known as a **mixture model**. The specific ones on the slide combines two conditional distributions, namely, $Y|Z = 0$ and $Y|Z = 1$. The model mixes its conditional *components* stochastically, a process controlled by a distribution over components, whose probabilities $p(z|\theta)$ are known as *mixing weights*. That is, with probability $p(z|\theta)$ the component $Y|Z = z$ generates a draw in $\mathcal{Y}$. In this example, $p(Z = 1|\theta) = b$ and $p(Z = 0|\theta) = 1 - b$.

For $K > 2$ components, $Z \sim \text{Cat}(\pi_1, \ldots, \pi_K)$, thus $p(z|\pi) = \pi_z$.

Mixture model

A **mixture model** assigns probability density

$$p_{ZY}(z, y|\theta) = p_Z(z|\theta)_{Y|Z} p(y|z, \theta)$$

to joint outcomes in $\mathcal{Z} \times \mathcal{Y}$. That is, it prescribes a *joint distribution* over observed and unobserved random variables.

A mixture model encodes the assumption that data points are each drawn from one of a finite number of independent distributions.

The latent variable Z captures this *unobserved component assignment*. It is governed by a distribution we call the *prior*. Oftentimes this is as simple as a uniform distribution over the sample space $\mathcal{Z}$.

Given an observation y drawn from the mixture, we can *infer* a distribution over component assignments by basic probability calculus, this very famous result is known as Bayes rule:

$$p(z|y, \theta) = \frac{p(z, y|\theta)}{p(y|\theta)} = \frac{p(y|z, \theta)p(z|\theta)}{\sum_{z' \in \mathcal{Z}} p(y|z', \theta)p(z'|\theta)}$$

Note that this *posterior pdf* $p(z|y, \theta)$ involves the *marginal pdf* $p(y|\theta)$, which we discuss next.

Prescribing Flexible Distributions

The **marginal** distribution of the mixture model is potentially multimodal and exhibits richer covariance structure. It assigns probability density

$$p(y|\theta) = \sum_{z=1}^{K} p(z|\theta)p(y|z,\theta)$$

to an outcome $y \in \mathcal{Y}$ by *marginalisation* of assignments $z \in \mathcal{Z}$ of the latent random variable.

Marginal inference for the MM scales linearly in the number of *components*. This is a key type of computation, for example, indispensable for parameter estimation / learning via maximum likelihood.

Say we have a dataset $\mathcal{D}$ of N i.i.d. observations for Y. MLE depends on the log-likelihood function, which in turn depends on assessments of the *marginal probability* of each observation:

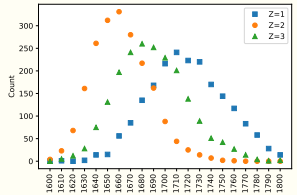
$$\begin{aligned}
\mathcal{L}_{\mathcal{D}}(\theta) &= \sum_{n=1}^{N} \log p(y^{(n)}|\theta) \\
&= \sum_{n=1}^{N} \log \sum_{z^{(n)}=1}^{K} p(y^{(n)}, z^{(n)}|\theta) \\
&= \sum_{n=1}^{N} \log \sum_{z^{(n)}=1}^{K} p(y^{(n)}|z^{(n)}, \theta)p(z^{(n)}|\theta)
\end{aligned}$$

Posterior component assignment

Given an observation y we can infer a distribution over component assignments via Bayes rule

$$p(z|y,\theta) = \frac{p(z,y|\theta)}{p(y|\theta)} = \frac{p(y|z,\theta)p(z|\theta)}{\sum_{z' \in \mathcal{Z}} p(y|z',\theta)p(z'|\theta)}$$

MMs are one of the first options when it comes to organising massive collections of unlabelled data into smaller groups (clustering).



Here is a mixture model (3 Poisson components) of our historical data.

Components in a mixture model are not *labelled* with self-evident information such as *'pre-steam-engine'* and *'post-steam-engine'*, but sometimes by inspecting likely component assignments we can recognise some salient features data bring data points together under a certain component. We can also use it to target annotation efforts, for example, to avoid under-representing certain decades (in our running example).

Labelling components with self-evident information can be done by experts with assistance of posterior queries or even semi-automatically by extending mixture models in interesting ways. See LDA (Blei et al., 2003), for example.

Predictors are welcome

It is also possible to use mixture models in conditional models:

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

and we may use x in different ways, e.g.

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

Whether to use predictors to parameterise mixing weights, the conditional model, or both will depend on the application.

'Parameterising mixing weights' means specifying a distribution over K mixture components, e.g.

$$Z|x \sim \text{Cat}(g(x; \theta))$$

An alternative to giving control of mixing weights to a neural network, or fixing the weights to something superficially intuitive (like a uniform distribution), is to prescribe a *prior* distribution over the mixing coefficients. This would get you very close to Bayesian realms. Do you know any distribution which has the space of K-dimensional probability vectors as support?

Semi-supervised learning

Suppose some documents are annotated and others are not (as in the example), and say we model generatively.

For labelled documents, we observe (x, y) whose joint probability is

$$p_{XY}(x, y|\theta) = p_Y(y|\theta)_{X|Y} p(x|y, \theta)$$

and the marginal probability of an unlabelled document x is

$$p_X(x|\theta) = \sum_{y \in \mathcal{Y}} p_Y(y|\theta) p_{X|Y}(x|y, \theta)$$

For a countably finite set $\mathcal{Y}$, this is a **mixture model**!

This is a very special mixture model for its components are *labelled* with self-evident information (e.g., decades).

A generative model of this kind can be thought of as a classifier (the *task* point of view), we need only apply Bayes rule to obtain a conditional $p(y|x_*, \theta)$ that can power a decision rule for a novel document x_*.

But, above all, a generative model of this kind is a model of all of our observations (the *random experiment* point of view). Our observations are indeed a collection of documents, where some documents (very few) are labelled for decade. When we model conditionally we call the labelled instances *training data* and ignore all unlabelled instances (the vast majority of our observations).

Besides powering a classification rule, the generative formulation could be used to shed light onto vocabulary shifts over the decades. One way to specify the component $p(x|y, \theta)$ is to assume it generates a document by drawing words independently given a decade-specific parameter θ_y. That is, $X_i|Y = y \sim \text{Cat}(\theta_y)$ for $i = 1, \ldots, |x|$.

Competition or cooperation?

In a mixture model the components *compete* to generate a data point. This means they cannot *cooperate* to account for some observed variance.

Sometimes, however, we want to stipulate the presence of a number of latent factors that together contribute to our observations distributing the way they do. Think of it in terms of clustering: sometimes we need overlapping clusters, or rather, *attributes*.

For example, our documents are scientific documents, and the period in consideration covers the European Scientific Revolution, as it came to be named. A number of inventions and new ideas marked this period. Documents were likely influenced by subsets of those ideas, rather than any singe idea in particular.

Like in mixture models we can recognise two roles for the class of models we are about to develop.

They can serve task-driven goals and power models that can predict attributes of an input (e.g., attributes of product, aspects of review, morphological features of a word).

They can serve knowledge-seeking goals and power inferences about latent structure that account (cause or correlate with) observed variance (e.g., in what latent aspects/dimensions are data points related).

Latent factor document model

Let us consider a latent factor model for document modelling:

- a document $x = (x_1, \ldots, x_I)$ consists of I i.i.d. categorical draws from that model
- the categorical distribution in turn depends on binary latent factors $z = (z_1, \ldots, z_D)$ which are also i.i.d.

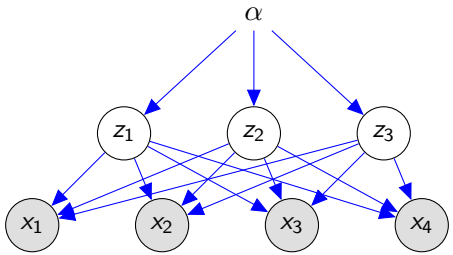
$$\begin{aligned} Z_j &\sim \text{Bernoulli}(\alpha) && (1 \leq d \leq D) \\ X_i|z &\sim \text{Categorical}\left(f(z;\theta)\right) && (1 \leq i \leq I) \end{aligned}$$

Here $f(\cdot;\theta)$ is an NN and θ its parameters.

To keep the model simple we will assume $X_i \perp X_j|Z$ for $i \neq j$. We could, however, relax this conditional independence if we wanted. For example, we could model $X_i|z, x_{<i} \sim \text{Cat}(f(z, x_{<i};\theta))$.

Graphical model

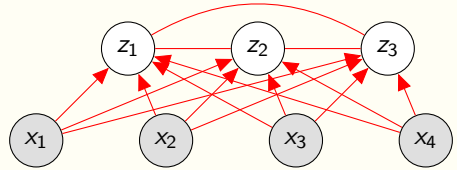
Joint distribution: independent latent variables



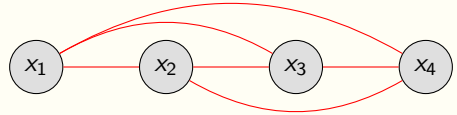
I omit θ from the graphical model, but every $X_i|z$ depends on it.

Suppose, for example, $D = 3$ and $I = 4$.

Posterior



Marginal



I'm omitting θ and α from the graphical models.

Intractable Marginals

In the latent factor model, marginalisation takes time $\mathcal{O}(2^D)$

$$
\begin{aligned}
p(x|\alpha,\theta) &= \sum_{z\in\{0,1\}^D} p(z|\alpha)p(x|z,\theta) \\
&= \sum_{z\in\{0,1\}^D} \prod_{d=1}^{D} \text{Bern}(z_d|\alpha) \prod_{i=1}^{I} \text{Cat}(x_i|f(z;\theta))
\end{aligned}
$$

As a consequence, we cannot assess $\log p(x|\alpha,\theta)$ nor its gradient.

Thinking ahead: if we cannot assess $\log p(x|\alpha,\theta)$ for an observation x, nor its gradient, how are we going to estimate parameters for this model?

Combinatorial Latent Structure

The posterior of the latent factor model reveals attributes that are relevant to an observation.

Sampling from it can help discover discrete factors of variation (e.g. morphological attributes of a word).

Unfortunately, the posterior in this case is a Gibbs distribution whose parameter is intractable to compute

- its natural parameter has length 2^D
- its log-normaliser requires a summation over $z \in \{0, 1\}^D$

Applications

Alignment Learn to match two data structures (e.g., word alignment, phrase alignment, visual question answering).

Data: $\langle x_1, \ldots, x_I \rangle$ and $\langle y_1, \ldots, y_J \rangle$

Generate each part of y using a subset of the parts of x.

- this can be a mixture model
- or a latent factor model
- and there can be constraints on the parts (e.g., disjoint)

(Rios et al., 2018; Deng et al., 2018; Kawakami et al., 2019)

Applications

Latent attribution What parts of the input (or of a computation graph) affect predictions.

Data: $\langle x_1, \ldots, x_I \rangle$ and y

$$Z_i \sim \text{Bern}(\alpha)$$
$$Y|x, z \sim \text{Cat}(f(x \odot z; \theta))$$

x could also be every hidden state internal to a given NN, and y could be that NN's output $y = g(x; \phi)$

(Lei et al., 2016; Bastings et al., 2019; Cao et al., 2020)

Applications

Compositionality Learn a computation graph.

Sample a structure z from a prior or conditional distribution $Z|x$ and let this structure determine a composition function to parameterise a distribution $Y|x, z$. This can be used for semi-supervised learning of syntactic/semantic representations, for learning to solve arithmetic expressions, interpretable text classifiers, etc.

(Yogatama et al., 2017; Corro and Titov, 2018; Niculae et al., 2018; Havrylov et al., 2019)

Applications

Controllable generation Learn to affect a conditional generator by controlling a latent prompt.

For example, translation models parameterise a conditional distribution $Y|x, \theta$ over translations of a given input x.

The source may contain a certain word (e.g., doctor), and the target language gender-marks nouns. The source sentence *does not* contain enough information to resolve the ambiguity, wouldn't it be nice to have a mechanism, other than requiring the user to produce a less ambiguous x, to control inflections?

(Hu et al., 2017; Zhou and Neubig, 2017; Ataman et al., 2020)

Applications

(Hu et al., 2017; Zhou and Neubig, 2017; Ataman et al., 2020)

Summary

Mixture model ('learning clusters')

Latent factor model ('learning attributes or overlapping clusters')

Applications:

- unsupervised learning (e.g., word alignments, LDA, IBP)
- semi-supervised learning (e.g., generative classifiers, disentanglement learning)
- transparency (e.g., latent rationales)

Examples:

- word alignments (Brown et al., 1993; Vogel et al., 1996; Rios et al., 2018)
- LDA (Blei et al., 2003)
- IBP (Ghahramani and Griffiths, 2006)
- semi-supervised deep generative models (Kingma et al., 2014; **?**)
- latent rationales (Lei et al., 2016; Bastings et al., 2019)

Outline

Latent Variable Models

When talking about some generic model I will follow this convention

- X is an rv taking on values in $\mathcal{X}$
- $x \in \mathcal{X}$ is an observation
- Z is a *discrete* rv taking on values in $\mathcal{Z}$
- $z \in \mathcal{Z}$ is a latent assignment
- the joint pdf factorises as $p(x, z|\theta) = p(z|\theta)p(x|z, \theta)$
- $p(z|\theta)$ is called the *prior*
- $p(x|z, \theta)$ is called the *observational model*
- $p(x|\theta)$ is the *marginal* (or *evidence*)
- and $p(z|x, \theta) = \frac{p(x,z|\theta)}{p(x|\theta)}$ is the posterior
- anything in the model can be parameterised by NNs

Throughout, we shall assume we have N i.i.d. observations. With deterministic parameters θ, we can make all our arguments in terms of a single observation x. Recall, the likelihood-function $\mathcal{L}_{\mathcal{D}}(\theta)$ is just $\sum_{x\sim\mathcal{D}} \log p(x|\theta)$.

By the way, can you draw a plate diagram for our generic latent variable model?

Many models admit exact marginals

Examples (and the algorithms for marginalisation)

- Mixture models (enumeration)
- HMMs (forward algorithm)
- CFGs (inside algorithm)
- Spanning-tree random fields (matrix-tree theorem)

Tractable marginalisation depends on the conditional independence assumptions of a model (e.g., in an HMM a hidden state is independent of all but its preceding state), not on how that model's probability distributions are parameterised (e.g., a transition distribution in the HMM may be stored in a table, predicted by a log-linear model or by an NN).

Marginalisation algorithms are generally harder to parallelise on GPUs.

Recall that to use NNs in probabilistic models we converged to two constraints on the log-likelihood function:

- differentiability with respect to parameters
- and tractability

If $p(z|\theta)$ and $p(x|z,\theta)$ are differentiable functions of their parameters, there is no impediment to gradient-based parameter estimation. Can you show that to yourself? Hint: expand $\nabla_\theta \log p(x|\theta)$.

Tractability depends on whether $p(x|\theta) = \sum_{z \in \mathcal{Z}} p(x, z|\theta)$, or its logarithm, can be evaluated in feasible time. Though it may seem so, this is not always a matter of cardinality of $\mathcal{Z}$.

For example, there is a Catalan number of trees in a CFG, yet because of the strong independence assumptions in the model, the marginal $p(x|\theta)$ is computable in cubic-time (w.r.t. sequence length) via the inside algorithm. Similarly, there is an exponential number of state sequences in an HMM, but its marginal is computable in linear-time (w.r.t. sequence length) via the forward algorithm.

Neural {MM, HMM, CFG, CRF, ... }

An NN-parameterisation of a classic discrete LVM, for which exact marginals are tractable, still needs to preserve all of that model's statistical assumptions about unobserved random variables.

We won't necessarily achieve a more complex distribution.

Though we may condition on complex data more effectively.

A neural HMM could look like:

$$p(x|\theta) = \sum_{z \in \{1,\dots,K\}^{|x|}} \prod_{i=1}^{|x|} \underbrace{p(z_i|z_{i-1}, x_{<i}, \theta)}_{\mathrm{Cat}(z_i|g(x_{<i}, z_{i-1}; \theta))} \underbrace{p(x_i|z_i, x_{<i})}_{\mathrm{Cat}(x_i|f(x_{<i}, z_i; \theta))}$$

the entire history of already generated words is available for conditioning

NNs allow us to condition on complex observations, like a long history of words $x_{<i}$ in unsupervised part-of-speech tagging.

We cannot, as easily, exploit that power to relax statistical conditional independence assumptions, for those assumptions are crucial in order to maintain *exact and tractable* access to marginal probabilities.

Think of it this way, what makes the HMM the HMM is the first-order (or n-order) Markov assumption $Z_i \perp Z_j | Z_{i-1}$ for j other than i and $i-1$. Relaxing that turns the HMM into something else, for which exact inference is likely impossible. See Wang et al. (2018) for a neural HMM.

Gradient-based MLE

What happens when we autodiff the quantity $\log p(x|\theta)$, which we computed exactly and tractably?

Let's inspect this gradient ourselves $\nabla_\theta \log p(x|\theta)$

Gradient of log-marginal

- It all starts with the derivative of log, followed by chain rule again.

Gradient-based MLE

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$$= \frac{1}{p(x|\theta)} \nabla_\theta p(x|\theta) =$$

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- Sums are fine, but let's use the log identity $f' = f(\log f)'$

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&= \sum_{z \in \mathcal{Z}} \frac{p(z, x|\theta)}{p(x|\theta)} \nabla_\theta \log p(z, x|\theta) = \sum_{z \in \mathcal{Z}} p(z|x, \theta) \nabla_\theta \log p(z, x|\theta)
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- The marginal is constant for $z \in \mathcal{Z}$, so distribute it over the sum.
- This gives us a recognisable object! Joint probability, divided by evidence, that's the posterior! And we have a weighted average, coefficients given by a pmf, and we sum over the entire support $\mathcal{Z}$.

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&= \mathbb{E}_{p(z|x,\theta)} \left[\nabla_\theta \log p(z, x|\theta) \right]
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- This gives us a recognisable object! Joint probability, divided by evidence, that's the posterior! And we have a weighted average, coefficients given by a pmf, and we sum over the entire support $\mathcal{Z}$.
- We have an expectation! The gradient of the log-marginal of x is the expected gradient of the log joint probability of x and z, where x is observed and z is a draw from the posterior distribution $Z|x, \theta$. Dependency on Z makes the gradient of log-joint $G(Z) = \nabla_\theta \log P(Z, X = x)$ a random variable.

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Autodiff performs **exact posterior inference** for us!

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- The gradient of the log-marginal $\nabla_\theta \log p(x|\theta)$ is deterministic, it is the expected value $\mathbb{E}_{Z|X=x,\theta}[G(Z)]$. You evaluate the marginal, autodiff evaluates the expectation.

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- The gradient of the log-marginal $\nabla_\theta \log p(x|\theta)$ is deterministic, it is the expected value $\mathbb{E}_{Z|X=x,\theta}[G(Z)]$. You evaluate the marginal, autodiff evaluates the expectation.

Summary

Many discrete LVMs admit tractable marginalisation

Assessing the gradient of the log-marginal probability of an observation corresponds to assessing an expectation under the posterior distribution over latent variables. Think of it this way:

- we need posterior inference to compute the gradient
- and we need the gradient for parameter estimation
- with exact marginals, autodiff assesses the gradient thus abstracting posterior inference away

What happens when we cannot solve $\sum_{z \in \mathcal{Z}} p(x, z|\theta)$?

Many interesting models are such that the exact marginal is intractable. We've seen, for example, the case where $p(x, z|\theta)$ is a latent factor model.

Autodiff cannot differentiate a quantity that cannot be assessed. So if we cannot compute the exact log-marginal probability of an observation, we won't get automatic posterior inference for free. We will have to resort to rather explicit approaches to approximate inference.

Final Remarks

- Probabilistic models are extremely flexible tools.
- They are interesting precisely because we can make choices about unobserved aspects of the data.
- Discrete latent variables are oftentimes key to revealing interpretable structure, or to imposing some interpretable structure on a joint distribution.
- Learning discrete LVMs is challenging due posterior inference.
- When posterior inference is tractable, MLE training via stochastic gradient optimisation is available out of the box.

What next?

To model with *any* type of unobserved data we need the power of approximate inference tools, see our Amortised Variational Inference module.

Curious about concrete instances of probabilistic models that are state-of-the-art? Check our Advanced Generative Models module.

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