Building Probabilistic Models

Mark van der Wilk

Department of Computing Imperial College London

January 16, 2023

Questions

Last time, I gave examples of probabilistic reasoning, e.g. colour perception:

$$P(C|L) = \sum_{i} P(C|L, I = i) P(I = i)$$

$$P(C|L, I = i) = \frac{P(L|C, I = i)P(C)}{P(L|I = i)}$$

- ► But why this structure?
- What assumptions were made?
- How should assumptions be expressed and communicated?
- ► How do we manipulate distributions to the form we want?

How to systematically approach a probabilistic modelling problem?

Mathematical Modelling

Often, we can pose a mathematical model of a phenomenon:

► Reflection (Phong model, different symbol convention)

$$I_{ ext{p}} = k_{ ext{a}} i_{ ext{a}} + \sum_{m \; \in \; ext{lights}} (k_{ ext{d}} (\hat{L}_m \cdot \hat{N}) i_{m, ext{d}} + k_{ ext{s}} (\hat{R}_m \cdot \hat{V})^lpha i_{m, ext{s}})$$

Movement of an object under gravity (Newton's laws)

$$s_t = \frac{1}{2} \frac{F}{m} t^2 + v_0 t \tag{1}$$

So if you are **given** some quantities, you can make a prediction about another.

From Mathematical Models to Probabilistic Models

- ► A mathematical model expresses deterministic relationships.
- ► A probabilistic model expresses relationships with uncertainty.
- ▶ Often, probabilistic models are specified starting with a mathematical model.
- Mathematical relationships can help specify conditional distributions.

Mathematical models are a *special case* of deterministic models. Probability can still express certainty! E.g. from Newton's laws:

$$s_t = \frac{1}{2} \frac{F}{m} t^2 + v_0 t \tag{2}$$

$$p(s_t|v_0, m, F) = \delta(s_t - \frac{1}{2}\frac{F}{m}t^2 + v_0t)$$
(3)

(Remember: $\int_{\mathcal{R}} \delta(\mathbf{x} - \mathbf{y}) d\mathbf{x} = 1$ if $\mathbf{y} \in \mathcal{R}$, 0 otherwise.)

Probabilistic Models: Uncertain Quantities

Given a mathematical model.

$$p(s_t|v_0, m, F) = \delta(s_t - \frac{1}{2}\frac{F}{m}t^2 + v_0t)$$
(4)

A certain relationship like this can be used to work back to uncertain quantities. Imagine we are uncertain about certain quantities:

$$p(v_0, m, F) = \mathcal{N}(v_0; \mu_v, 1.0)\delta(m - 1.0)\mathcal{N}(F; \mu_F, 0.1)$$
 (5)

We can find how our uncertainty over the initial velocity v_0 changes by finding $p(v_0|s_t)$!

Probabilistic Models: Uncertain Relationships

- ► Is the relationship $p(s_t|v_0, m, F) = \delta(s_t \frac{1}{2}\frac{F}{m}t^2 + v_0t)$ realistic?
- If we did an initial value experiment, would we really measure exactly the predicted value?
- Adding uncertainty makes predictions more realistic, by allowing errors.

$$p(s_t|v_0, m, F) = \mathcal{N}\left(s_t; \frac{1}{2}\frac{F}{m}t^2 + v_0t, \sigma^2\right)$$
 (6)

Probability of Everything

How to make these intuitions **systematic**? It's a good idea to start from a representation that:

- 1. clearly expresses the assumptions made in our model,
- 2. allows us to derive any distribution that we are interested in.

The joint distribution over all variables. The **Probability of Everything**.

$$p(x,y,z) \tag{7}$$

Any question we may want to answer corresponds to finding:

$$p(x,z|y) = \frac{p(x,y,z)}{p(y)} \qquad \text{or} \qquad p(x|y) = \int \frac{p(x,y,z)}{p(y)} dz \qquad (8)$$

- ▶ Observe a variable? Conditioning (i.e. divide and renormalise).
- ▶ Not interested in a variable? Marginalise.

Building a Probabilistic Model: Statistical Approach

Understanding how your variables causally interact gives you a factorisation of the joint.

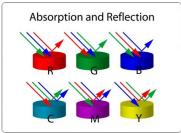
- 1. Identify all the variables that are relevant to your problem.
- 2. Start with a variable that you will observe.
- 3. Determine which variables it depends on, and choose a sensible conditional distribution.
- 4. Repeat previous step for one of the variables that you conditioned on.

Example: Lighting

Step 1: Identify all variables:

- ▶ Object colour *C*.
- ▶ Reflected light *L*.
- ▶ Illumination *I*.

Joint: p(C, L, I).



Step 2: We observe the reflected light *L*. We have a model for the *L* given *I* and *C*: p(L, C, I) = p(L|C, I)p(C, I).

Step 3: Let's pick *C*. Colour does not depend on illumination, so p(C|I) = p(C), showing that *C* and *I* are independent.

While we can use our knowledge for choosing p(L|C, I), we need to choose subjective priors for p(C) and p(I).

Finding the right posterior

- ▶ Now that we have the joint, how do we find p(C|L)?
- Remember: We need to find it in terms of the conditional distributions which we can actually evaluate.
- ► This is why starting with the joint is such a good idea! Given the definitions from the previous slide, we can evaluate it!

$$p(C|L) = \frac{p(C,L)}{p(L)} = \frac{\sum_{I} p(C,L,I)}{\sum_{C,I} p(C,L,I)}$$
(9)

$$=\frac{\sum_{I} p(L|C,I) p(C) p(I)}{\dots} \tag{10}$$

We can take many different routes!

$$p(C|L) = \frac{p(L|C)p(C)}{p(L)} = \frac{\left[\sum_{I}p(L|C,I)p(I)\right]p(C)}{p(L)}$$
(11)

Many roads lead to Rome, but starting from the joint highlights assumptions

Example: Burglars, Earthquakes, and Alarms

"Fred lives in Los Angeles and commutes 60 miles to work. Whilst at work, he receives a phone-call from his neighbour saying that Fred's burglar alarm is ringing. What is the probability that there was a burglar in his house today? While driving home to investigate, Fred hears on the radio that there was a small earthquake that day near his home. 'Oh', he says, feeling relieved, 'it was probably the earthquake that set off the alarm'. What is the probability that there was a burglar in his house?" (MacKay, 2003, §21.1)

Q: How does the joint factorise? What conditionals should we define?

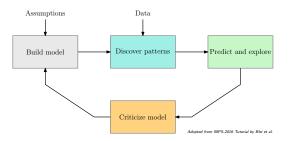
► Variables: **p**honecall, **a**larm, **b**urglar, radio, **e**arthquake p(p,a,b,r,e) = p(p,a,b,r,e) (12)

$$p(p, a, b, r, e) = p(p|a, b, r, e)p(a, b, r, e)$$
 (13)

$$p(p, a, b, r, e) = p(p|a)p(a, b, r, e)$$
 (14)

Probabilistic Pipeline

If your assumptions are good/correct, inference will give accurate results and good predictions.



- ► Good models generate data that is similar to the data we observe.
- ► Predict and explore: Sample from the prior, assess predictions.
- ► Criticize/revise the model.

Building a Probabilistic Model: ML Approach

Q: What happens if we don't have a mathematical/mechanistic model?

- ► For some problems, little is known about the process.
- ► No known latent variables to use for creating a model.
- We mainly want good prediction!

All we really need is $p(\mathcal{D}_{\text{future}}, \mathcal{D}_{\text{observed}})$, so we can find the predictive distribution:

$$p(\mathcal{D}_{\text{future}}|\mathcal{D}_{\text{observed}}) = \frac{p(\mathcal{D}_{\text{future}}, \mathcal{D}_{\text{observed}})}{p(\mathcal{D}_{\text{observed}})}.$$
 (20)

Latent Variables

How do we create a joint with interesting relationships between the observed and future data?

► Invent **latent variables** that are **common** to all data.

$$p(\mathcal{D}_{\text{fut}}, \mathcal{D}_{\text{obs}}, \mathbf{z})$$
 (21)

► For simplicity, often data is iid given latent variables.

$$p(\mathcal{D}_{\text{fut}}, \mathcal{D}_{\text{obs}}, \mathbf{z}) = \prod_{i} p(\mathcal{D}_{i} | \mathbf{z}) p(\mathbf{z})$$
 (22)

- May not have a direct physical basis initially, but can turn out to be interpretable after training.
- ► Induces correlations between data, that can help to predict

$$p(\mathcal{D}_{\text{fut}}, \mathcal{D}_{\text{obs}}) = \int p(\mathcal{D}_{\text{fut}}, \mathcal{D}_{\text{obs}}, \mathbf{z}) d\mathbf{z}$$
 (23)

Example: Linear Basis Function Regression

Linear regression falls under this!

$$p(\mathbf{y}, \mathbf{y}^*) = \int \prod_{i} p(y_i | \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta}$$
 (24)

$$p(y_i|\boldsymbol{\theta}) = \mathcal{N}(y_i; \boldsymbol{\theta}^{\mathsf{T}} \boldsymbol{\phi}(\mathbf{x}), \sigma^2)$$
 (25)

- ► Do we really believe that the data we obtained was generated by sampling some parameters?
- Do we really believe that the relationship is a sum of polynomials?
- No, but it's useful for predicting!

Similar, VAE (which we will also discuss).

How do we know we have a good model?

Model criticism is crucial! Luckily, we have an objective metric on how well it's doing:

Predictive accuracy!

- Hold-out test set.
- Check where it is overconfident and underconfident.
- ▶ Does it predict well when you change the setting?
- ► Bayesian model selection (soon).

The ML philosophy: if you predict well, you understand.

Conclusion

Summary:

- You can do anything with the joint.
- Can create joints from understanding of the world.
- Can create joints by just hypothesising relationships. Just make sure you validate your model...

What you should be able to do:

- ► Create probabilistic model (i.e. joints) by composing conditionals.
- Apply sum and product rules to find desired posteriors.

Reading & exercises:

- Chapter 3 (MacKay, 2003).
- ► Exercise: the burglar alarm (MacKay, 2003, ch.21)
- ► Exercise: bent coin (MacKay, 2003, §3.2)
- ► Exercise: legal evidence (MacKay, 2003, §3.4)

References I

MacKay, D. J. C. (2003). Information Theory, Inference, and Learning Algorithms. Cambridge University Press.