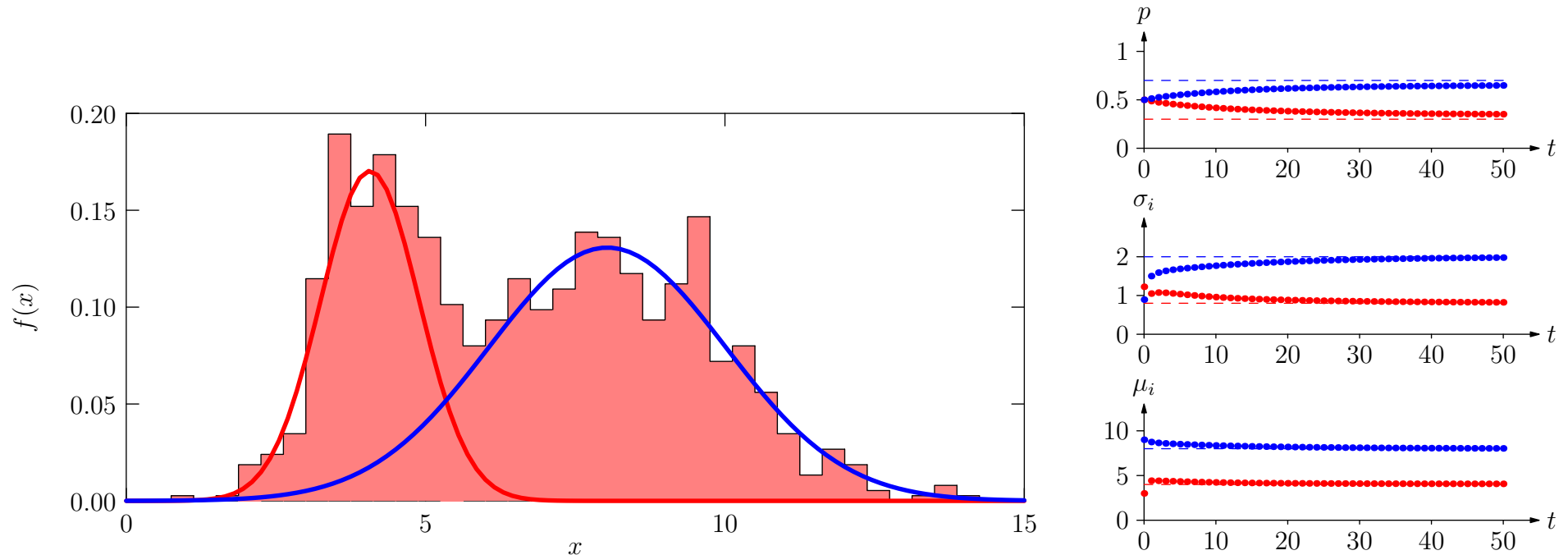


Advanced Machine Learning

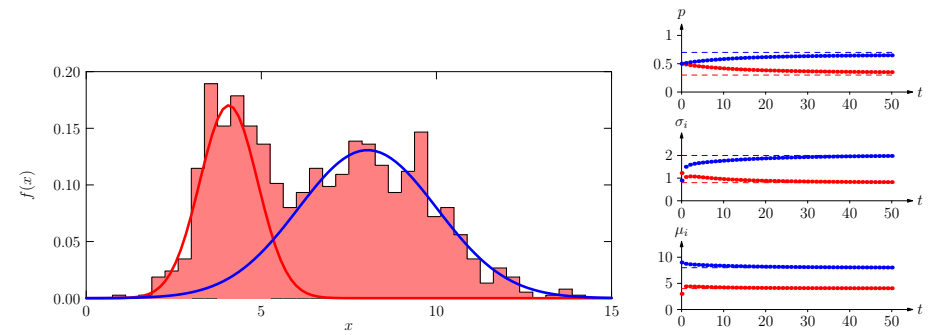
Probabilistic Inference



*Hierarchical Models, Mixture of Gaussians, Expectation
Maximisation*

Outline

1. **Building Probabilistic Models**
2. Mixture of Gaussians
3. Expectation Maximisation



Building Probabilistic Models

- To describe a system with uncertainty we use random variables, X, Y, Z , etc.■
- We use the convention of writing random variables in capitals (this is sometimes confusing as when you observe a random variables it is no longer random)■
- The variables are described by probability mass function $\mathbb{P}(X, Y, Z)$ or if our variables are continuous, but probability densities $f_{X, Y, Z}(x, y, z)$ ■
- A major rule of probability is

$$\sum_X \mathbb{P}(X, Y, Z) = \mathbb{P}(Y, Z) \blacksquare$$

Conditional Probabilities

- When developing models it is often useful to consider conditional probabilities e.g. $\mathbb{P}(X, Y|Z)$ or $f_{X|Y, Z}(x|y, z)$ ■
- A second major rule in probabilistic modelling is

$$\mathbb{P}(X, Y) = \mathbb{P}(X|Y) \mathbb{P}(Y) = \mathbb{P}(Y|X) \mathbb{P}(X) \blacksquare$$

- This is a mathematical identity that does not imply causality (it defines conditional probability)■
- It is the origins of Bayes' rule: $\mathbb{P}(X|Y) = \frac{\mathbb{P}(Y|X) \mathbb{P}(X)}{\mathbb{P}(Y)}$ ■

Discriminative Models

- We often think of our observations as given and the predictions as random variables■
- For example we might be given some features x and we wish to predict a class $C \in \mathcal{C}$ ■
- Our objective is then to find the probability $\mathbb{P}(C|x)$ ■
- This is known as a **discriminative model**■
- E.g. in *foundations of machine learning* you learnt how to find the Bayes' optimal discrimination surface■

Generative Models

- Sometimes it is easy to think about the joint process of generating the features and outputs together■
- This leads to a joint distribution $\mathbb{P}(\mathbf{X}, Y)$ where \mathbf{X} are your features and Y is your output you are trying to predict■
- This is known as a **generative model**■
- Generative models are often more natural to think about■
- We can use them to do discrimination using

$$\mathbb{P}(Y|\mathbf{X}) = \frac{\mathbb{P}(\mathbf{X}, Y)}{\mathbb{P}(\mathbf{X})} = \frac{\mathbb{P}(\mathbf{X}, Y)}{\sum_Y \mathbb{P}(\mathbf{X}, Y)} \quad \blacksquare$$

Latent Variables

- Sometimes we have models that involve random variables that we don't observe and we don't care about
- These are called **latent variables**
- If we have a latent variable Z and observed variable X and we are predicting a variable Y then we would **marginalise** over the latent variable

$$\mathbb{P}(X, Y) = \sum_Z \mathbb{P}(X, Y, Z)$$

Modelling Virus

- Suppose we want to estimate the number of hospitalisation from Corona virus in the next month■
- Our observable is the number of reported cases■
- In our model we might want to estimate the number of actual cases■
- This would be a latent variable (it is not an observable or our final target, but it is very useful intermediate in our model)■
- This will be a random variable (we are uncertain, but we can build a probabilistic model giving a distribution of number of actual cases)■

Hierarchical Models

- Of course, if I was really modelling the spread of a disease I would care about the probability, $f(C|A,V)$, of catching the disease, C , given the persons age A and the variant of the disease V ■
- I would want to know the distribution of ages $f(A)$ and try to infer the probability of different variants $\mathbb{P}(V)$ ■
- I would care about the probability, $f(R|A,V)$, of cases being reported given age and variant■
- And the probability, $f(H|A,V)$, of hospitalisation given A and V ■
- This would involve an elaborate (hierarchical) model with a large number of latent variables■

Probabilistic Inference

- We can use Bayes' rules to learn a set of parameter Θ that occur in our likelihood function

$$\mathbb{P}(\Theta|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|\Theta) \mathbb{P}(\Theta)}{\mathbb{P}(\mathcal{D})}$$

- This provides us a full probabilistic description of the parameters
- It doesn't overfit (we are not choosing the best)
- Bayesian inference provides a description of its own uncertainty
- We need to specify a likelihood and prior, but this is usually not difficult

Problem with Bayes

- Bayes is problematic because it is often hard■
- The posterior is often not expressible as a nice probability function■
- We need to compute the *evidence* or *margin likelihood* we use

$$\mathbb{P}(\mathcal{D}) = \sum_{\Theta} \mathbb{P}(\mathcal{D}|\Theta) \mathbb{P}(\Theta) \blacksquare$$

- But sometimes the number of values that Θ can take are so large that we cannot easily compute this■
- Nevertheless we can usually do this using Monte Carlo techniques■

Maximum A Posteriori (MAP) Solution

- One work around is to compute the mode of the posterior

$$\Theta_{\text{MAP}} = \underset{\Theta}{\operatorname{argmax}} f(\mathcal{D}|\Theta) f(\Theta) = \underset{\Theta}{\operatorname{argmax}} \log(f(\mathcal{D}|\Theta)) + \log(f(\Theta))$$

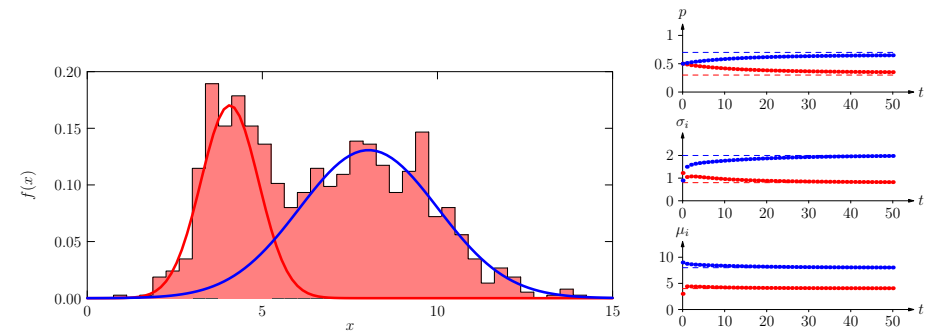
- We don't need to calculate $f(\mathcal{D})$ or explicitly calculate the posterior distribution
- But it is not Bayesian (despite what you are sometime told)—its not properly probabilistic
- You can overfit and you don't get an estimate of the error in your inference

Maximum Likelihood

- When we assume a uniform prior then the MAP solution is just maximising the likelihood■
- Weirdly this hack was accepted as part of mainstream statistics even when Bayesian statistics was considered unscientific■
- Maximum likelihood is often sufficient for *government work*, but it isn't the best you can do■
- In high-dimensional problems using a non-uniform prior can make a big difference■
- And, of course, doing a full probabilistic calculation has real advantages■

Outline

1. Building Probabilistic Models
2. **Mixture of Gaussians**
3. Expectation Maximisation



Mixture of Gaussians

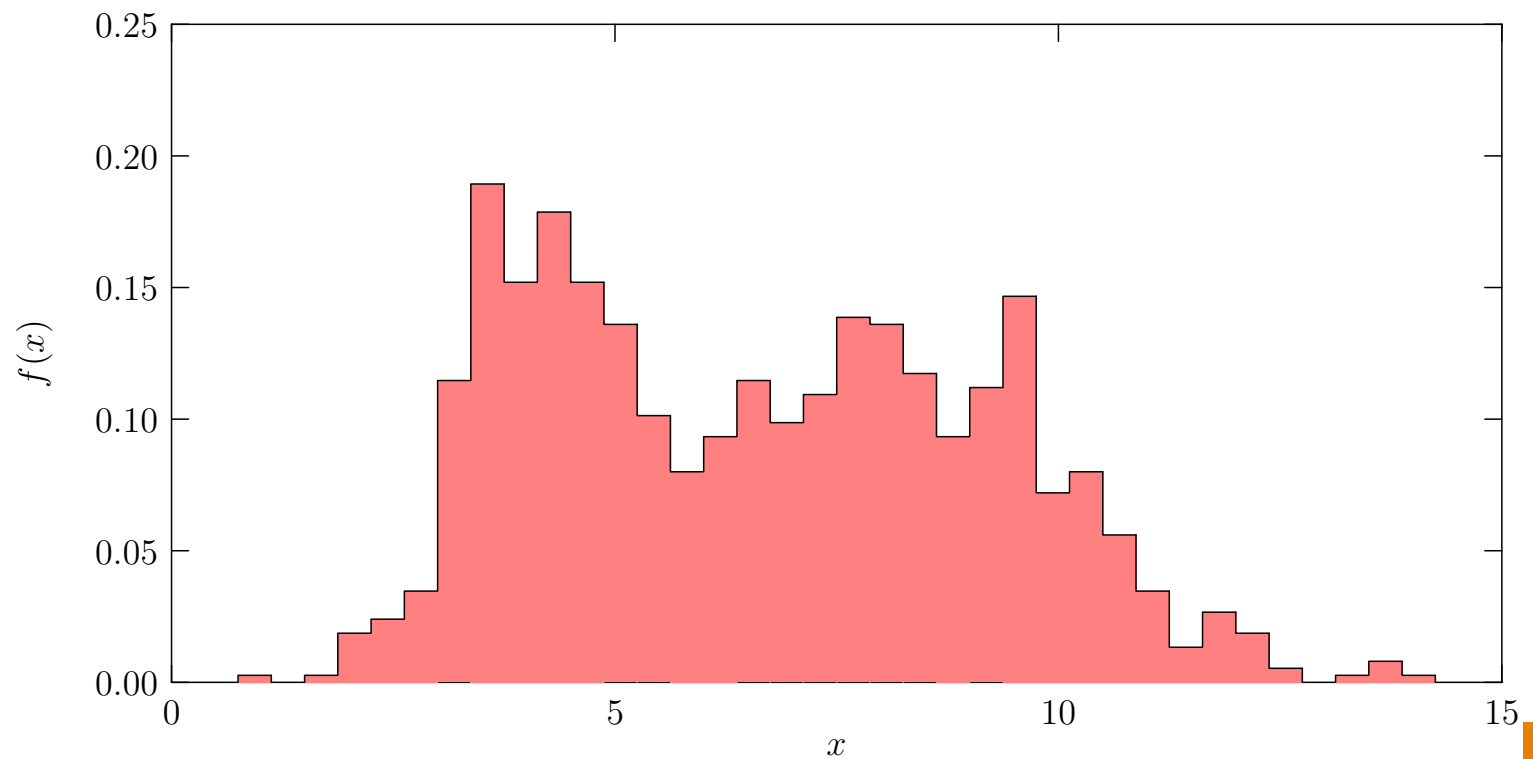
- Suppose we were observing the decays from two types of short-lived particle, A or B ■
- We observe the half life, X_i , but not the particle type■
- We assume X_i is normally distributed with unknown means and variances: $\Theta = \{\mu_A, \sigma_A^2, \mu_B, \sigma_B^2\}$ ■
- Let $Z_i \in \{0,1\}$ be an indicator that particle i is of type A ■
- The probability of X_i is given by

$$f(X_i|Z_i, \Theta) = Z_i \mathcal{N}(X_i|\mu_A, \sigma_A^2) + (1 - Z_i) \mathcal{N}(X_i|\mu_B, \sigma_B^2) \blacksquare$$

Data

- Note that

$$\begin{aligned} f(X_i|\Theta) &= \sum_{Z_i \in \{0,1\}} f(X_i, Z_i|\Theta) \quad \color{brown}{=} \sum_{Z_i \in \{0,1\}} f(X_i|Z_i, \Theta) \mathbb{P}(Z_i) \quad \color{brown}{=} \\ &= \mathbb{E}_{Z_i}[f(X_i|Z_i, \Theta)] \quad \color{brown}{=} p\mathcal{N}(X_i|\mu_A, \sigma_A^2) + (1-p)\mathcal{N}(X_i|\mu_B, \sigma_B^2) \quad \color{brown}{=} \end{aligned}$$



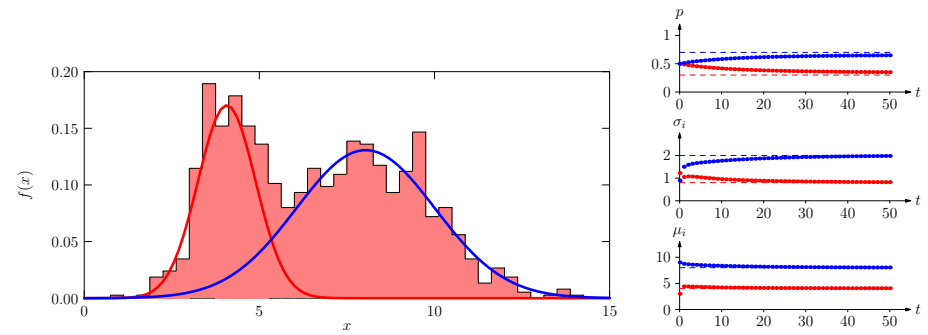
Maximum Likelihood

- To solve the model as a Bayesian we would have to assign priors to our parameters $\Theta = (\mu_A, \sigma_A, \mu_B, \sigma_B, p)$ ■
- This is doable, but complicated (we would also end up with a distribution for our parameters)■
- Often we only want a reasonable estimate for some of our parameters (e.g. the half-lives μ_A and μ_B)■
- A reasonable approach is to seek those parameters that maximise the likelihood of our observed data

$$f(\mathcal{D}|\Theta) = \prod_{X \in \mathcal{D}} f(X|\Theta) \blacksquare$$

Outline

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Maximum Likelihood with Latent Variables

- The maximum likelihood is a non-linear function of the parameters so cannot be immediately maximised■
- If we knew which type of particle a data-point belongs to (Z_i) then it would be straightforward to maximise the likelihood■
- As we don't we need to estimate $\mathbb{P}(Z_i = 1)$, but this depends on $\mu_A, \sigma_A^2, \mu_B, \sigma_B^2$ and p ■
- We could use a standard optimiser, but this is slightly inelegant■

EM Algorithm

- Instead we can use an **expectation-maximisation algorithm** usually known as an **EM algorithm**■
- We proceed iteratively by maximising the expected log-likelihood with respect to the current set of parameters

$$\Theta^{(t+1)} = \operatorname{argmax}_{\Theta} \sum_{\mathbf{Z}} \mathbb{P}(\mathbf{Z} | \mathcal{D}, \Theta^{(t)}) \log(f(\mathcal{D} | \mathbf{Z}, \Theta)) \blacksquare$$

- It isn't obvious why this works■

Why EM Algorithm Works

- The argument around why this works is quite involved
- Note that at each step we maximise

$$Q(\Theta|\Theta^{(t)}) = \sum_{\mathbf{Z} \in \{0,1\}^m} \mathbb{P}(\mathbf{Z}|\mathcal{D}, \Theta^{(t)}) \log(f(\mathcal{D}|\mathbf{Z}, \Theta))$$

- We can show that the maximum, $\Theta^{(t+1)}$, is such that

$$\log(f(\mathcal{D}|\Theta^{(t+1)})) - \log(f(\mathcal{D}|\Theta^{(t)})) \geq Q(\Theta^{(t+1)}|\Theta^{(t)}) - Q(\Theta^{(t)}|\Theta^{(t)}) \geq 0$$

- The details are given in the supplemental notes

Conditional Latent Variables

- We need to compute the distribution of latent variables conditioned on the data and current estimated parameters ■
- For our problem

$$\mathbb{P}\left(\mathbf{Z}|\mathcal{D},\Theta^{(t)}\right) = \prod_{i=1}^m \mathbb{P}\left(Z_i|X_i,\Theta^{(t)}\right) \blacksquare$$

where

$$\mathbb{P}\left(Z_i = 1|X_i,\Theta^{(t)}\right) = \frac{p^{(t)} \mathcal{N}\left(X_i|\mu_A^{(t)},\sigma_A^{2(t)}\right)}{p^{(t)} \mathcal{N}\left(X_i|\mu_A^{(t)},\sigma_A^{2(t)}\right) + (1 - p^{(t)}) \mathcal{N}\left(X_i|\mu_B^{(t)},\sigma_B^{2(t)}\right)}$$

$$\mathbb{P}\left(Z_i = 0|X_i,\Theta^{(t)}\right) = 1 - \mathbb{P}\left(Z_i = 1|X_i,\Theta^{(t)}\right) \blacksquare$$

EM for Mixture of Gaussians

- Maximise with respect to parameters θ

$$\begin{aligned} Q(\theta|\theta^{(t)}) &= \sum_{\mathbf{Z}} \mathbb{P}(\mathbf{Z}|\mathcal{D}, \Theta^{(t)}) \log(f(\mathcal{D}|\mathbf{Z}, \Theta)) \quad \blacksquare = \sum_{i=1}^m \sum_{Z_i} \mathbb{P}(Z_i|\mathcal{D}, \Theta^{(t)}) \log(f(X_i|Z_i, \Theta)) \quad \blacksquare \\ &= \sum_{i=1}^m \sum_{Z_i \in \{0,1\}} \mathbb{P}(Z_i|X_i, \theta_i^{(t)}) (Z_i \log(p) + (1 - Z_i) \log(1 - p) \\ &\quad - \frac{(X_i - \mu_{Z_i})^2}{2\sigma_{Z_i}^2} - \log(\sqrt{2\pi}\sigma_{Z_i})) \quad \blacksquare \end{aligned}$$

- Compute update equations

$$\frac{\partial Q(\theta|\theta^{(t)})}{\partial \mu_k} = 0, \quad \frac{\partial Q(\theta|\theta^{(t)})}{\partial \sigma_k} = 0, \quad \frac{\partial Q(\theta|\theta^{(t)})}{\partial p} = 0 \quad \blacksquare$$

Update Equations

- Means

$$\mu_{Z_i}^{(t+1)} = \frac{\sum_{i=1}^n \mathbb{P}(Z_i | X_i, \boldsymbol{\theta}^{(t)}) X_i}{\sum_{i=1}^n \mathbb{P}(Z_i | X_i, \boldsymbol{\theta}^{(t)})},$$

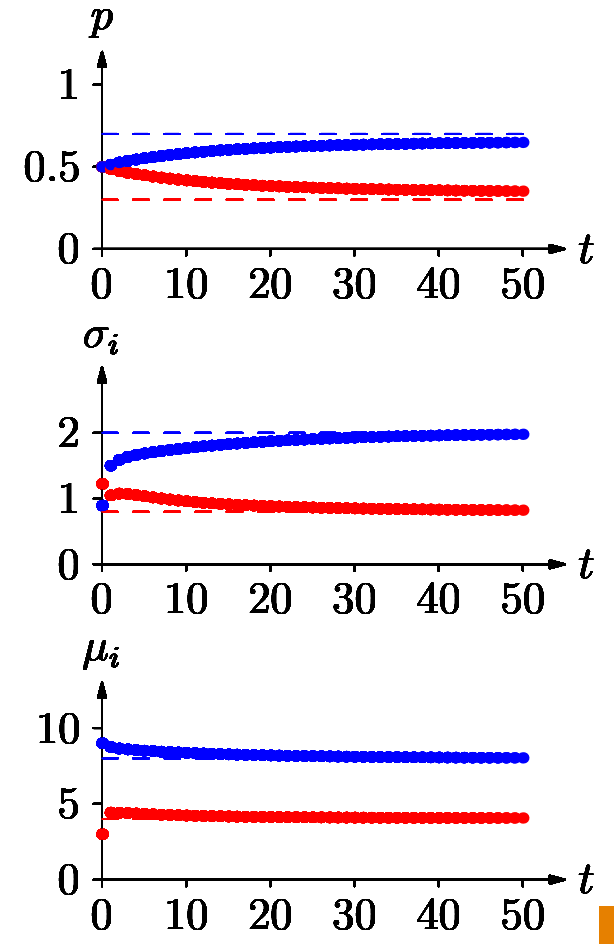
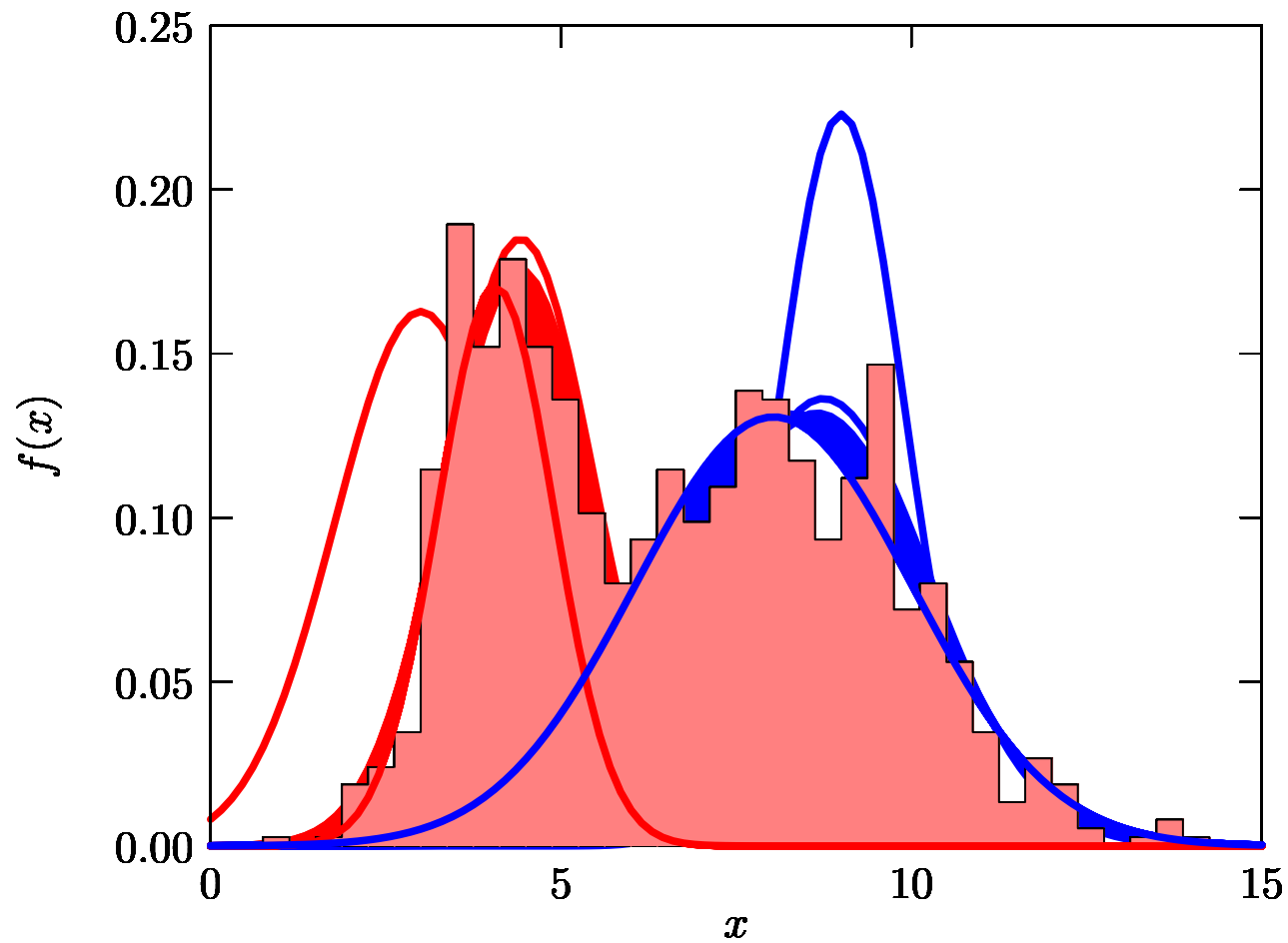
- Variances

$$(\sigma_{Z_i}^{(t+1)})^2 = \frac{\sum_{i=1}^n \mathbb{P}(Z_i | X_i, \boldsymbol{\theta}^{(t)}) (X_i - \mu_{Z_i}^{(t+1)})^2}{\sum_{i=1}^n \mathbb{P}(Z_i | X_i, \boldsymbol{\theta}^{(t)})}$$

- Probability of being type 1

$$p^{(t+1)} = \frac{1}{n} \sum_{i=1}^n \mathbb{P}(Z_i = 1 | X_i, \boldsymbol{\theta}_i^{(t)})$$

Example



Summary

- Building probabilistic models is an intricate process■
- Identifying random variables that describe the system is the first step■
- Often we need to introduce variables that we don't observe and need to be marginalised out■
- The EM algorithm provide one approach to maximising likelihoods or MAP solutions when we have latent variables■
- It often gives nice update equations, but convergence can be slow■