Probabilistic & Unsupervised Learning

Week 2: Latent Variable Models

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Unsupervised Learning

The story so far . . .

- beliefs about data represented by parameterised distribution

\[ P(\mathcal{D} | \theta, m) = \prod_{i=1}^{n} P(x_{i} | \theta, m) \]

- learning involves estimating a value (or distribution) for \( \theta \)

Bayes \[ P(\theta | \mathcal{D}, m) = \frac{P(\mathcal{D} | \theta, m)P(\theta | m)}{P(\mathcal{D} | m)} \]

MAP \[ \theta^{*} = \arg\max_{\theta} P(\theta | \mathcal{D}, m) \]

ML \[ \theta^{*} = \arg\max_{\theta} P(\mathcal{D} | \theta, m) \]

and (possibly) model selection

\[ P(m|\mathcal{D}) \propto \int d\theta \ P(\mathcal{D}|\theta, m)P(\theta|m) \]
Aren’t We Done?

No!

- direct application of Bayes’ rule is intractable for all but the simplest models.
- even maximum-likelihood (or similar) learning may be prohibitive.
- algorithms (and approximations) are dictated by form of distribution.
Correlated Continuous-Valued Data

Assume:

• we have a data set $D = \{x_1, \ldots, x_N\}$
• each data point is a vector of $D$ features:
  $x_i = [x_{i1} \ldots x_{iD}]$
• the data points are i.i.d. (independent and identically distributed).

One of the simplest forms of unsupervised learning: model the **mean** of the data and the **correlations** between the $D$ features in the data.

We can use a multi-variate Gaussian (or Multi-Variate Normal) model:

$$p(\mathbf{x}|\mu, \Sigma) = |2\pi\Sigma|^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \mu)^\top \Sigma^{-1} (\mathbf{x} - \mu) \right\}$$
ML Estimation of a Gaussian

Data set $\mathcal{D} = \{x_1, \ldots, x_N\}$, likelihood: $p(\mathcal{D} | \mu, \Sigma) = \prod_{n=1}^{N} p(x_n | \mu, \Sigma)$

Maximise likelihood $\iff$ maximise log likelihood

**Goal:** find $\mu$ and $\Sigma$ that maximise log likelihood:

$$
\mathcal{L} = \log \prod_{n=1}^{N} p(x_n | \mu, \Sigma) = \sum_{n} \log p(x_n | \mu, \Sigma)
$$

$$
= -\frac{N}{2} \log |2\pi \Sigma| - \frac{1}{2} \sum_{n} (x_n - \hat{\mu})^\top \Sigma^{-1} (x_n - \hat{\mu})
$$

**Note:** equivalently, minimise $-\mathcal{L}$, which is **quadratic** in $\mu$

**Procedure:** take derivatives and set to zero:

$$
\frac{\partial \mathcal{L}}{\partial \mu} = 0 \quad \Rightarrow \quad \hat{\mu} = \frac{1}{N} \sum_{n} x_n \quad \text{(sample mean)}
$$

$$
\frac{\partial \mathcal{L}}{\partial \Sigma} = 0 \quad \Rightarrow \quad \hat{\Sigma} = \frac{1}{N} \sum_{n} (x_n - \hat{\mu}) (x_n - \hat{\mu})^\top \quad \text{(sample covariance)}
$$
modelling correlations
\[\Leftrightarrow\]
maximising likelihood of a Gaussian model
\[\Leftrightarrow\]
minimising a squared error cost function
\[\Leftrightarrow\]
minimising data coding cost in bits (assuming Gaussian distributed)
MVN Limitations

Gaussians are fundamental and widespread, but not every distribution of interest is Gaussian.

- Not all random processes fit the central limit theorem.
- Some processes produce outliers.
- Some data has higher-order or non-linear structure.
- Even if data are Gaussian, if $D$ is large the full MVN model may be difficult to handle. There are $D(D + 1)/2$ parameters in the MVN covariance.
What about these data?

- joint distribution $p(x_{i1}, x_{i2})$ is not Normal.
- conditional distributions $p(x_{i1} | x_{i2})$ and $p(x_{i2} | x_{i1})$ vary, and are difficult to codify.
- easier to describe by an latent tri-valued discrete process

\[
s_i \sim \text{Discrete}[1/3, 1/3, 1/3] \\
x_i \sim \mathcal{N} (\mu_{s_i}, \Sigma)
\]
Latent Variable Models

Explain correlations in $x$ by assuming some latent variables $y$

$$y \sim \mathcal{P}[\theta_y]$$

$$x \mid y \sim \mathcal{P}[\theta_x]$$

$$p(x, y; \theta_x, \theta_y) = p(x \mid y; \theta_x)p(y; \theta_y)$$

$$p(x; \theta_x, \theta_y) = \int d\mathbf{y} \ p(x \mid \mathbf{y}; \theta_x)p(\mathbf{y}; \theta_y)$$
The data were measured in 3D, but are mostly specified by position on a 2D surface.
Data such as these are often modelled using Principal Components Analysis (PCA).

Assume data $\mathcal{D} = \{x_i\}$ have zero mean (if not, subtract it!).

- Find direction of greatest variance – $\lambda_{(1)}$.

$$
\lambda_{(1)} = \arg\max_{\|v\|=1} \sum_n (x_n^T v)^2
$$

- Find direction orthogonal to $\lambda_{(1)}$ with greatest variance – $\lambda_{(2)}$

  $\vdots$

- Find direction orthogonal to $\{\lambda_{(1)}, \lambda_{(2)}, \ldots, \lambda_{(n-1)}\}$ with greatest variance – $\lambda_{(n)}$.

- Terminate when remaining variance drops below a threshold.
Eigendecomposition of a Covariance Matrix

The eigendecomposition of a covariance matrix makes finding the PCs easy. Recall that $u$ is an eigenvector, with scalar eigenvalue $\omega$, of a matrix $C$ if

$$C u = \omega u$$

$u$ can have any norm, but we will define it to be unity (i.e., $u^T u = 1$).

For a covariance matrix $C = \langle xx^T \rangle$ (which is $D \times D$, symmetric, positive semi-definite):

- In general there are $D$ eigenvector-eigenvalue pairs $(u(i), \omega(i))$, except if two or more eigenvectors share the same eigenvalue (in which case the eigenvectors are degenerate — any linear combination is also an eigenvector).
- The $D$ eigenvectors are orthogonal (or orthogonalisable, if $\omega(i) = \omega(j)$). Thus, they form an orthonormal basis. $\sum_i u(i) u(i)^T = I$.
- Any vector $v$ can be written as

$$v = \left( \sum_i u(i) u(i)^T \right) v = \sum_i (u(i)^T v) u(i) = \sum_i v(i) u(i)$$

- The original matrix $C$ can be written:

$$C = \sum_i \omega(i) u(i) u(i)^T = USU^T$$

where $U = [u(1), u(2), \ldots, u(D)]$ collects the eigenvectors and $S = \text{diag} [(\omega(1), \omega(2), \ldots, \omega(D))]$. 
PCA and Eigenvectors

• The variance in direction $u_i$ is
  \[
  \langle (x^T u_i)^2 \rangle = \langle u_i^T x x^T u_i \rangle = u_i^T C u_i = u_i^T \omega_i u_i = \omega_i
  \]

• The variance in an arbitrary direction $v$ is
  \[
  \langle (x^T v)^2 \rangle = \langle \left( x^T \left( \sum_i v_i u_i \right) \right)^2 \rangle = \sum_{ij} v_i u_i^T C u_j v_j
  \]
  \[
  = \sum_{ij} v_i \omega_j v_j u_i^T u_j = \sum_{i} v_i^2 \omega_i
  \]

• If $v^Tv = 1$, then $\sum_i v_i^2 = 1$ and so $\arg\max_{\|v\|=1} \langle (x^T v)^2 \rangle = u_{(\text{max})}$
  The direction of greatest variance is the eigenvector the largest eigenvalue.

• In general, the PCs are exactly the eigenvectors of the empirical covariance matrix, ordered by decreasing eigenvalue.

• The eigenspectrum shows how the variance is distributed across dimensions
PCA subspace

The $K$ principle components define the $K$-dimensional subspace of greatest variance.

- Each data point $\mathbf{x}_n$ is associated with a projection $\tilde{\mathbf{x}}_n$ into the principle subspace.

\[
\tilde{\mathbf{x}}_n = \sum_{k=1}^{K} x_{n(k)} \lambda_{(k)}
\]

- This can be used for lossy compression, denoising, recognition, . . .
Example of PCA: Eigenfaces

from www-white.media.mit.edu/vismod/demos/facerec/basic.html
Another view of PCA: Mutual Information

**Problem:** Given \( x \), find \( y = Ax \) with columns of \( A \) unit vectors, s.t. \( I(y; x) \) is maximised (assuming that \( P(x) \) is Gaussian).

\[
I(y; x) = H(y) + H(x) - H(y, x) = H(y)
\]

So we want to maximise the entropy of \( y \). What is the entropy of a Gaussian?

\[
H(z) = - \int d\mathbf{z} \ p(\mathbf{z}) \ln p(\mathbf{z}) = \frac{1}{2} \ln |\Sigma| + \frac{D}{2}(1 + \ln 2\pi)
\]

Therefore we want the distribution of \( y \) to have largest volume (i.e. det of covariance matrix).

\[
\Sigma_y = A\Sigma_x A^\top = AU S_x U^\top A^\top
\]

So, \( A \) should be aligned with the columns of \( U \) which are associated with the largest eigenvalues (variances).

Projection to the principal component subspace preserves the most information about the (Gaussian) data.
Network Interpretations
and Encoder-Decoder Duality
A linear autoencoder neural network trained to minimise squared error learns to perform PCA (Baldi & Hornik, 1989).
Probabilistic PCA

We could think of the projection $\tilde{x}_n$ as a latent variable, but it is more usual to construct a standard normal latent $y$.

Observed vector data $D = \{x_1, x_2, \ldots, x_N\}; x_i \in \mathbb{R}^D$

Assumed latent variables $\{y_1, y_2, \ldots, y_N\}; y_i \in \mathbb{R}^K$

Linear generative model: $x_d = \sum_{k=1}^{K} \Lambda_{dk} y_k + \epsilon_d$

- $y_k$ are independent $\mathcal{N}(0, 1)$ Gaussian factors
- $\epsilon_d$ are independent $\mathcal{N}(0, \psi)$ Gaussian noise
- $K < D$

So, model for observations $x$ is still Gaussian with:

$$p(y) = \mathcal{N}(0, I)$$
$$p(x|y) = \mathcal{N}(\Lambda y, \psi I)$$

$$p(x) = \int p(y)p(x|y)dy = \mathcal{N}(0, \Lambda \Lambda^T + \psi I)$$

where $\Lambda$ is a $D \times K$ matrix.

This is Probabilistic PCA (pPCA). The maximum-likelihood parameter $\Lambda$, for fixed $\psi$, lies in the $K$-principal subspace.
Probabilistic PCA

- Two panels show the data distribution in the original $x$-$y$ space.
- The second panel illustrates the projection of the data onto the principal components in the $x$-$y$ space.
PCA and pPCA

- In PCA the “noise” is orthogonal to the subspace, and we can project $x_n \rightarrow \tilde{x}_n$ trivially.
- In pPCA, the noise is more sensible (equal in all directions). But what is the projection? Find the expected value of $y_n| x_n$ and then take $\tilde{x}_n = \Lambda \bar{y}_n$.
- **Tactic:** write $p(y_n, x_n|\theta)$, consider $x_n$ to be fixed. What is this as a function of $y_n$?

\[
p(y_n, x_n) = p(y_n) p(x_n| y_n)
= (2\pi)^{-K/2} \exp\{-\frac{1}{2} y_n^\top y_n\} |2\pi \Psi|^{-1/2} \exp\{-\frac{1}{2} (x_n - \Lambda y_n)^\top \Psi^{-1} (x_n - \Lambda y_n)\}
= c \times \exp\{-\frac{1}{2} [y_n^\top y_n + (x_n - \Lambda y_n)^\top \Psi^{-1} (x_n - \Lambda y_n)]\}
= c' \times \exp\{-\frac{1}{2} [y_n^\top (I + \Lambda^\top \Psi^{-1} \Lambda)y_n - 2y_n^\top \Lambda^\top \Psi^{-1} x_n]\}
= c'' \times \exp\{-\frac{1}{2} [y_n^\top \Sigma^{-1} y_n - 2y_n^\top \Sigma^{-1} \mu + \mu^\top \Sigma^{-1} \mu]\}
\]

So $\Sigma = (I + \Lambda^\top \Psi^{-1} \Lambda)^{-1} = I - \beta \Lambda$ and $\mu = \Sigma \Lambda^\top \Psi^{-1} x_n = \beta x_n$. Where $\beta = \Sigma \Lambda^\top \Psi^{-1}$.
- Thus, $\tilde{x}_n = \Lambda (I + \Lambda^\top \Psi^{-1} \Lambda)^{-1} \Lambda^\top \Psi^{-1} x_n = x_n - \Psi (\Lambda \Lambda^\top + \Psi)^{-1} x_n$
- This is not the same projection. pPCA takes into account noise in the principal subspace.
- As $\psi \rightarrow 0$, pPCA $\rightarrow$ PCA.
Factor Analysis

If dimensions are not equivalent, equal variance makes no sense.

Observed vector data $D = \{x_1, x_2, \ldots, x_N\}; x_i \in \mathbb{R}^D$
Assumed latent variables $\{y_1, y_2, \ldots, y_N\}; y_i \in \mathbb{R}^K$

Linear generative model: $x_d = \sum_{k=1}^{K} \Lambda_{dk} y_k + \epsilon_d$

- $y_k$ are independent $\mathcal{N}(0, 1)$ Gaussian factors
- $\epsilon_d$ are independent $\mathcal{N}(0, \Psi_{dd})$ Gaussian noise
- $K < D$

So, model for observations $x$ is still Gaussian with:

$$p(y) = \mathcal{N}(0, I)$$
$$p(x|y) = \mathcal{N}(\Lambda y, \Psi)$$

$$p(x) = \int p(y)p(x|y)dy = \mathcal{N}(0, \Lambda\Lambda^\top + \Psi)$$

where $\Lambda$ is a $D \times K$ matrix, and $\Psi$ is $K \times K$ and diagonal.

**Dimensionality Reduction:** Finds a low-dimensional projection of high dimensional data that captures the correlation structure of the data.
ML learning finds $\Lambda$ and $\Psi$ given data

parameters (corrected for symmetries): $DK + D - \frac{K(K-1)}{2}$

If number of parameters $> \frac{D(D+1)}{2}$ model is not identifiable

no closed form solution for ML params: $\mathcal{N}(0, \Lambda\Lambda^\top + \Psi)$

[Bayesian treatment would also have priors over $\Lambda$ and $\Psi$ and would average over them for prediction.]
Our analysis for pPCA still applies:

\[ \tilde{x}_n = \Lambda (I + \Lambda^T \Psi^{-1} \Lambda)^{-1} \Lambda^T \Psi^{-1} x_n = x_n - \Psi (\Lambda \Lambda^T + \Psi)^{-1} x_n \]

but now \( \Psi \) is diagonal but not spherical.

Note, though, that \( \Lambda \) is generally different from that found by pPCA.
Gradient Methods of Learning FA

Write down negative log likelihood:

\[ \frac{1}{2} \log |2\pi (\Lambda\Lambda^T + \Psi)| + \frac{1}{2} \mathbf{x}^T (\Lambda\Lambda^T + \Psi)^{-1} \mathbf{x} \]

Optimise w.r.t. \( \Lambda \) and \( \Psi \) (need matrix calculus) subject to constraints

We will soon see an easier way to learn latent variable models...
FA vs PCA

- PCA and pPCA are rotationally invariant; FA is not
  
  If $x \rightarrow Ux$ for unitary $U$, then $\lambda^{PCA}_i \rightarrow U\lambda^{PCA}_i$

- FA is measurement scale invariant; PCA and pPCA are not
  
  If $x \rightarrow Sx$ for diagonal $S$, then $\lambda^{FA}_i \rightarrow S\lambda^{FA}_i$

- FA and pPCA define a probabilistic model; PCA does not
Limitations of Gaussian, FA and PCA models

- Gaussian, FA and PCA models are easy to understand and use in practice.
- They are a convenient way to find interesting directions in very high dimensional data sets, e.g., as preprocessing.
- Their problem is that they make very strong assumptions about the distribution of the data, only the mean and variance of the data are taken into account.

The class of densities which can be modelled is too restrictive.

By using *mixtures* of simple distributions, such as Gaussians, we can expand the class of densities greatly.
A mixture distribution has a single discrete latent variable:

\[ s_i \overset{iid}{\sim} \text{Discrete}[\pi] \]
\[ x_i \mid s_i \sim P_{s_i}[\theta_{s_i}] \]

Mixtures arise naturally when observations from different sources have been collated. They can also be used to approximate arbitrary distributions.
The Mixture Likelihood

The mixture model is

\[ s_i \overset{iid}{\sim} \text{Discrete}[\pi] \]
\[ x_i \mid s_i \sim P_{s_i}[\theta_{s_i}] \]

Under the discrete distribution

\[ P(s_i = m) = \pi_m; \quad \pi_m \geq 0, \quad \sum_{m=1}^{k} \pi_m = 1 \]

Thus, the probability (density) at a single data point \( x_i \) is

\[ P(x_i) = \sum_{m=1}^{k} P(x_i \mid s_i = m)P(s_i = m) \]
\[ = \sum_{m=1}^{k} \pi_m P_m(x_i; \theta_m) \]

The mixture distribution (density) is a convex combination (or weighted average) of the component distributions (densities).
Approximation with a Mixture of Gaussians (MoG)

The component densities may be viewed as elements of a *basis* which can be combined to approximate arbitrary distributions.

Here are examples where non-Gaussian densities are modelled (approximated) as a mixture of Gaussians. The red curves show the (weighted) Gaussians, and the blue curve the resulting density.

Given enough mixture components we can model (almost) any density (as accurately as desired), but still only need to work with the well-known Gaussian form.
Clustering with a MoG
In clustering applications, the latent variable $s_i$ represents the (unknown) identity of the cluster to which the $i$th observation belongs.

Thus, the latent distribution gives the *prior* probability of a data point coming from each cluster.

$$P(s_i = m \mid \pi) = \pi_m$$

Data from the $m$th cluster are distributed according to the $m$th component:

$$P(x_i \mid s_i = m) = P_m(x_i)$$

Once we observe a data point, the *posterior* probability distribution for the cluster it belongs to is

$$P(s_i = m \mid x_i) = \frac{P_m(x_i)\pi_m}{\sum_m P_m(x_i)\pi_m}$$

This is often called the *responsibility* of the $m$th cluster for the $i$th data point.
The MoG likelihood

Each component of a MoG is a Gaussian, with mean $\mu_m$ and covariance matrix $\Sigma_m$. Thus, the probability density evaluated at a set of $n$ iid observations, $\mathcal{D} = \{x_1 \ldots x_n\}$ (i.e. the likelihood) is

$$p(\mathcal{D} | \{\mu_m\}, \{\Sigma_m\}, \pi) = \prod_{i=1}^{n} \sum_{m=1}^{k} \pi_m N(x_i | \mu_m, \Sigma_m)$$

$$= \prod_{i=1}^{n} \sum_{m=1}^{k} \pi_m |2\pi \Sigma_m|^{-1/2} \exp \left[ -\frac{1}{2}(x_i - \mu_m)^T \Sigma_m^{-1} (x_i - \mu_m) \right]$$

The log of the likelihood is

$$\log p(\mathcal{D} | \{\mu_m\}, \{\Sigma_m\}, \pi) = \sum_{i=1}^{n} \log \sum_{m=1}^{k} \pi_m |2\pi \Sigma_m|^{-1/2} \exp \left[ -\frac{1}{2}(x_i - \mu_m)^T \Sigma_m^{-1} (x_i - \mu_m) \right]$$

Note that the logarithm fails to simplify the component density terms. A mixture distribution does not lie in the exponential family. Direct optimisation is not easy.
Maximum Likelihood for a Mixture Model

The log likelihood is:

\[ \mathcal{L} = \sum_{i=1}^{n} \log \left( \sum_{m=1}^{k} \pi_m P_m(x_i; \theta_m) \right) \]

Its partial derivative wrt \( \theta_m \) is

\[ \frac{\partial \mathcal{L}}{\partial \theta_m} = \sum_{i=1}^{n} \frac{\pi_m}{\sum_{m=1}^{k} \pi_m P_m(x_i; \theta_m)} \frac{\partial P_m(x_i; \theta_m)}{\partial \theta_m} \]

or, using \( \frac{\partial P}{\partial \theta} = P \times \frac{\partial \log P}{\partial \theta} \),

\[ = \sum_{i=1}^{n} \frac{\pi_m P_m(x_i; \theta_m)}{\sum_{m=1}^{k} \pi_m P_m(x_i; \theta_m)} \frac{\partial \log P_m(x_i; \theta_m)}{\partial \theta_m} \]

\[ = \sum_{i=1}^{n} r_{im} \frac{\partial \log P_m(x_i; \theta_m)}{\partial \theta_m} \]

And its partial derivative wrt \( \pi_m \) is

\[ \frac{\partial \mathcal{L}}{\partial \pi_m} = \sum_{i=1}^{n} \frac{P_m(x_i; \theta_m)}{\sum_{m=1}^{k} \pi_m P_m(x_i; \theta_m)} = \sum_{i=1}^{n} \frac{r_{im}}{\pi_m} \]
For a MoG, with $\theta_m = \{ \mu_m, \Sigma_m \}$ we get

$$
\frac{\partial L}{\partial \mu_m} = \sum_{i=1}^{n} r_{im} \Sigma_m^{-1} (x_i - \mu_m)
$$

$$
\frac{\partial L}{\partial \Sigma_m^{-1}} = \frac{1}{2} \sum_{i=1}^{n} r_{im} (\Sigma_m - (x_i - \mu_m)(x_i - \mu_m)^T)
$$

These equations can be used (along with the derivatives wrt to $\pi_m$) for gradient based learning; e.g., taking small steps in the direction of the gradient (or using conjugate gradients).
The K-means Algorithm

The K-means algorithm is a limiting case of the mixture of Gaussians (c.f. PCA and Factor Analysis).

Take \( \pi_m = 1/k \) and \( \Sigma_m = \sigma^2 I \), with \( \sigma^2 \to 0 \). Then the responsibilities become binary

\[
  r_{im} \to \delta(m, \arg\min_l \| x_i - \mu_l \|^2)
\]

with 1 for the component with the closest mean and 0 for all other components. We can then solve directly for the means by setting the gradient to 0.

The k-means algorithm iterates these two steps:

- assign each point to its closest mean \( \left( \text{set } r_{im} = \delta(m, \arg\min_l \| x_i - \mu_l \|^2) \right) \)
- update the means to the average of their assigned points \( \left( \text{set } \mu_m = \frac{\sum_i r_{im} x_i}{\sum_i r_{im}} \right) \)

This usually converges within a few iterations, although the fixed point depends on the initial values chosen for \( \mu_m \). The algorithm has no learning rate, but the assumptions are quite limiting.
A preview of the EM algorithm

We wrote the k-means algorithm in terms of binary responsibilities. Suppose, instead, we used the fractional responsibilities from the full (non-limiting) MoG, but still neglected the dependence of the responsibilities on the parameters. We could then solve for both \( \mu_m \) and \( \Sigma_m \).

The **EM algorithm** for MoGs iterates these two steps:

- Evaluate the responsibilities for each point given the current parameters.
- Optimise the parameters assuming the responsibilities stay fixed:

\[
\mu_m = \frac{\sum_i r_{im} x_i}{\sum_i r_{im}} \quad \text{and} \quad \Sigma_m = \frac{\sum_i r_{im} (x_i - \mu_m)(x_i - \mu_m)^T}{\sum_i r_{im}}
\]

Although this appears *ad hoc*, we will see (later) that it is a special case of a general algorithm, and is actually guaranteed to increase the likelihood at each iteration.
There are several problems with the new algorithms:

- slow convergence for the gradient based method
- gradient based method may develop invalid covariance matrices
- local minima; the end configuration may depend on the starting state
- how do you adjust $k$? Using the likelihood alone is no good.
- singularities; components with a single data point will have their covariance going to zero and the likelihood will tend to infinity.