Neural Networks

Variational Autoencoders

(based on slides from Dan Schwarts and Tom Manzini)
Neural nets as generative models

• We’ve seen how neural nets can perform classification
  – Or regression
  – MLPs, CNNs, RNNs..

• Next step: NNs as generic generative models
  – Model the distribution of *any* data
  – Such that we can draw samples from it
But first...
The story of generative models

• What are generative models
• How to estimate them
  – *Expectation maximization*
What is a generative model

• A model for the probability distribution of a data $x$
  – E.g. a multinomial, Gaussian etc.

• Computational equivalent: a model that can be used to “generate” data with a distribution similar to the given data $x$
  – Typical setting: a box that takes in random seeds and outputs random samples like $x$
  – Question: how do we generate the random seeds...
Its turtles all the way down (kinda)…
Some “simple” generative models

• The multinomial PMF
  \[ P(x = v) = P(v) \]
  – For discrete data
    • \( v \) belongs to a discrete set
  – Can be expressed as a table of probabilities if the set of possible \( v \)s is finite
  – Else, requires a parametric form, e.g. Poisson
    \[ P(x = k) = \frac{\lambda^k e^{-\lambda}}{k!} \text{ for } k \geq 0 \]
    • \( \lambda \) is the Poisson parameter

• The Gaussian PDF
  \[ P(x = v) \]
  \[ = \frac{1}{\sqrt{2\pi|\Sigma|}} \exp\left(-0.5(x - \mu)^T \Sigma^{-1}(x - \mu)\right) \]
  – For continuous-valued data
  – \( \mu \) is the mean of the distribution
  – \( \Sigma \) is the Covariance matrix
Learning a generative model for data

- You are given some set of observed data $X = \{x\}$.
- You choose a model $P(x; \theta)$ for the distribution of $x$
  - $\theta$ are the parameters of the model
- Estimate the $\theta$ such that $P(x; \theta)$ best “fits” the observations $X = \{x\}$
  - Hoping it will also represent data outside the training set.
An example: Multinomials

- A dice roller rolls dice and you plot the histogram of outcomes
  - Shown to right
- The distribution is a multinomial
  - Parameters to be learned: $p_1, p_2, p_3, p_4, p_5, p_6$
- Which of the two multinomial PDFs shown to the right is more likely to be the PDF for the dice?
  - Why?
An example

- The left figure shows the histogram of a collection of observations
- We decide to model the distribution as Gaussian
  - Parameters: Mean $\mu$ and variance $\sigma^2$

- Which of the three Gaussians shown in the right figure is most likely to be the actual PDF of the RV?
  - Why?
Defining “Best Fit”: Maximum likelihood

• The data are generated by draws from the distribution
  – I.e. the generating process draws from the distribution

• Assumption: The world is a boring place
  – The data you have observed are very typical of the process

• Consequent assumption: The distribution has a high probability of generating the observed data
  – Not necessarily true

• Select the distribution that has the highest probability of generating the data
  – Should assign lower probability to less frequent observations and vice versa
Maximum likelihood

- The maximum likelihood principle:
  \[ \argmax_{\theta} P(X; \theta) = \argmax_{\theta} \log(P(X; \theta)) \]
The maximum likelihood principle:

\[ \underset{\theta}{\text{argmax}} \, P(X; \theta) = \underset{\theta}{\text{argmax}} \log(P(X; \theta)) \]

For the histogram:

\[ \underset{\{p_1, p_2, p_3, p_4, p_5, p_6\}}{\text{argmax}} \log(\prod_{x \in X} P(x)) \]

For the Gaussian:

\[ \underset{\mu, \sigma^2}{\text{argmax}} \log(\prod_{x \in X} P(x)) \]
Maximum likelihood

- The maximum likelihood principle:
  \[ \argmax_{\theta} P(X; \theta) = \argmax_{\theta} \log(P(X; \theta)) \]

- For the histogram
  \[ \argmax_{\theta} \log(\prod_{x \in X} P(x)) \]
  Can be grouped by value (every instance of \( i \) has the same probability)

- For the Gaussian
  \[ \argmax_{\mu, \sigma^2} \log(\prod_{x \in X} P(x)) \]
  This probability is a Gaussian
Maximum likelihood

• The maximum likelihood principle:

\[ \arg\max_{\theta} P(X; \theta) = \arg\max_{\theta} \log(P(X; \theta)) \]

• For the histogram

\[ \arg\max \log\left(\prod_i p_i^{n_i}\right) \quad \{p_1, p_2, p_3, p_4, p_5, p_6\} \]

• For the Gaussian

\[ \arg\max_{\mu, \sigma^2} \log(\prod_{x \in X} \text{Gaussian}(x; \mu, \sigma^2)) \]
Maximum likelihood

- The maximum likelihood principle:
  \[ \argmax_{\theta} P(X; \theta) = \argmax_{\theta} \log(P(X; \theta)) \]
- For the histogram
  \[ \argmax_{\{p_1, p_2, p_3, p_4, p_5, p_6\}} \sum_i n_i \log(p_i) \]
  \[ \Rightarrow p_i = \frac{n_i}{N} \text{ (N is the total number of observations)} \]

- For the Gaussian
  \[ \argmax_{\mu, \sigma^2} \sum_{x \in X} \log \text{Gaussian}(x; \mu, \sigma^2) \]
  \[ \Rightarrow \mu = \frac{1}{N} \sum_{x \in X} x ; \quad \sigma^2 = \frac{1}{N} \sum_{x \in X} (x - \mu)^2 \]
Maximum Likelihood Estimation

• Sometimes the data provided may be incomplete
  – Insufficient to estimate your model parameters directly

• This could be because the data themselves have missing components
  – E.g. Data vectors have some missing components

• Or because of the structure of the network
  – Mixture models, multi-stage Generative models
Maximum Likelihood Estimation

• Sometimes the data provided may be incomplete
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• Or because of the structure of the network
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Examples of incomplete data: missing data

- Objective: Estimate a Gaussian distribution from a collection of vectors
- Problem: Several of the vector components are missing
- Must estimate the mean and covariance of the Gaussian with these incomplete data
  - What would be a good way of doing this?
Maximum likelihood estimation with incomplete data

- Original problem: Estimate the Gaussian given a collection $X = \{x\}$ of complete vectors

$$\arg\max_{\mu, \sigma^2} \log(P(X)) \quad \text{where } X \text{ is the entire data}$$

$$= \arg\max_{\mu, \sigma^2} \sum_{x \in X} \log P(x) \quad \text{where } P() \text{ is a Gaussian}$$

- Unfortunately, many components of each vector are missing in our data
Maximum likelihood estimation with incomplete data

- These are the actual data we have: A set $O = \{o_1, ..., o_N\}$ of incomplete vectors
  - Comprising only the observed components of the data
Maximum likelihood estimation with incomplete data

- These are the actual data we have: A set $O = \{o_1, \ldots, o_N\}$ of *incomplete* vectors
  - Comprising only the *observed* components of the data

- We are *missing* the data $M = \{m_1, \ldots, m_N\}$
  - Comprising the *missing* components of the data
Maximum likelihood estimation with incomplete data

- These are the actual data we have: A set $O = \{o_1, ..., o_N\}$ of incomplete vectors
  - Comprising only the observed components of the data

- We are missing the data $M = \{m_1, ..., m_N\}$
  - Comprising the missing components of the data

- The complete data includes both the observed and missing components
  \[ X = \{x_1, ..., x_N\}, \quad x_i = (o_i, m_i) \]
  - Keep in mind that at the complete data are not available (the missing components are missing)
Maximum likelihood estimation with incomplete data

- Maximum likelihood estimation: Maximize the likelihood of the observed data
  - That is all we really have

\[
\arg\max_{\mu, \sigma^2} \log(P(O)) = \arg\max_{\mu, \sigma^2} \sum_{o \in O} \log P(o)
\]

- Unfortunately, the Gaussian is defined on the complete vector:
  - \( P(x) = \text{Gaussian}(x; \mu, \sigma^2) \)
  - In order to compute \( P(o) \) we must derive it from \( P(x) \)
The log likelihood of incomplete data

- The probability of any vector $x$ with observed and missing parts $o$ and $m$
  
  $$P(x) = P(o, m)$$

- Compute the probability of the observed components by marginalizing out the missing components

  $$P(o) = \int_{-\infty}^{\infty} P(x)dm = \int_{-\infty}^{\infty} P(o, m)dm$$

- The log probability of the entire observed training data:

  $$\sum_{o \in O} \log \int_{-\infty}^{\infty} P(o, m)dm$$
Maximum likelihood estimation with incomplete data

- Maximum likelihood estimation: Maximize the likelihood of the observed data

\[
\arg\max_{\mu, \sigma^2} \log(P(O)) = \arg\max_{\mu, \sigma^2} \sum_{o \in O} \log \int_{-\infty}^{\infty} P(o, m) dm
\]

- This requires the maximization of the log of an integral!
  - No closed form
  - Challenging on a good day, impossible on a bad one
Maximum Likelihood Estimation

• Sometimes the data provided may be incomplete
  – Insufficient to estimate your model parameters directly

• This could be because the data themselves have missing components
  – E.g. Data vectors have some missing components

• Or because of the structure of the network
  – Mixture models, multi-stage Generative models
Examples of incomplete data:
missing information in Gaussian mixtures

- The generative model characterizes the data as the outcome of a two-level process
  - In the first step the process chooses a Gaussian from a collection
  - In the second, it draws the vector $o$ from the chosen Gaussian
  - The overall model is a mixture Gaussian

- Objective: Learn the parameters of all the Gaussians from training data
  - Learn the means and variances of the individual Gaussians
    - And also the probability with which each Gaussian is selected for the draw

\[ P(o) = \sum_k P(k)N(o; \mu_k, \sigma_k^2) \]
The Gaussian Mixture generative model

- Note, the process actually draws two variables for each observation, $k$ and $o$.

- The probability of a particular draw is actually the joint probability of both variables
  \[ P(k, o) = P(k)P(o|k) = P(k)N(o; \mu_k, \sigma_k^2) \]

- To compute the probability of obtaining any observation $o$, we are marginalizing out the Gaussian index variable
  \[ P(o) = \sum_k P(k, o) = \sum_k P(k)N(o; \mu_k, \sigma_k^2) \]
The complete data needed to precisely learn the model

- Ideal data: Each training instance includes both the data vector $o$ and the Gaussian $k$ it was drawn from
  - In order to estimate the parameters of any Gaussian, you only need to segregate the training instances from that Gaussian, and compute the mean and variance from them
Learning a GMM with “complete” data
The GMM problem of incomplete data: missing information

- Problem: We are not given the actual Gaussian for each observation
  - Our data are incomplete

- What we want: \((o_1, k_1), (o_2, k_2), (o_3, k_3)\) ...
- What we have: \(o_1, o_2, o_3\) ...
ML estimation with only observed data

• The maximum likelihood estimation problem:
  – Given observed data \( O = \{o_1, o_2, o_3 \ldots \} \),
  – estimate \( \{(\mu_k, \sigma_k^2), \forall k \} \) – the parameters of all the Gaussians

\[
\text{argmax}_{\{(\mu_k, \sigma_k^2), \forall k \}} \log(P(O)) = \text{argmax}_{\{(\mu_k, \sigma_k^2), \forall k \}} \sum_{o \in O} \log P(o)
\]
**ML estimation with only observed data**

- The maximum likelihood estimation problem:
  - Given *observed data* \( O = \{ o_1, o_2, o_3 ... \} \),
  - estimate \( \{(\mu_k, \sigma_k^2), \forall k\} \) – the parameters of all the Gaussians

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\text{argmax}_{\{(\mu_k, \sigma_k^2), \forall k\}} \log(P(O)) = \text{argmax}_{\{(\mu_k, \sigma_k^2), \forall k\}} \sum_{o \in O} \log P(o)
\]

- The probability of an individual vector:

\[
P(o) = \sum_k P(k, o)
\]
The maximum likelihood estimation problem:
- Given observed data $O = \{o_1, o_2, o_3 \ldots\}$,
- estimate $\{(\mu_k, \sigma^2_k), \forall k\}$ – the parameters of all the Gaussians

$$\arg\max_{\{(\mu_k, \sigma^2_k), \forall k\}} \log(P(O)) = \arg\max_{\{(\mu_k, \sigma^2_k), \forall k\}} \sum_{o \in O} \log P(o)$$

The probability of an individual vector:

$$P(o) = \sum_k P(k, o) = \sum_k P(k)N(o; \mu_k, \sigma^2_k)$$
ML estimation with only observed data

- The maximum likelihood estimation problem:
  - Given observed data $O = \{o_1, o_2, o_3 \ldots \}$,
  - estimate $\{(\mu_k, \sigma^2_k), \forall k\}$ – the parameters of all the Gaussians

$$ \arg\max \log(P(O)) = \arg\max \sum_{o \in O} \log P(o) $$

- The probability of an individual vector:

$$ P(o) = \sum_k P(k)N(o; \mu_k, \sigma^2_k) $$

- The maximum likelihood estimation again

$$ \arg\max \sum_{o \in O} \log \sum_k P(k)N(o; \mu_k, \sigma^2_k) $$
The maximum likelihood estimation problem:

- Given observed data \( O = \{ o_1, o_2, o_3 \ldots \} \),
- estimate \( \{ (\mu_k, \sigma_k^2), \forall k \} \) – the parameters of all the Gaussians

\[
\arg\max_{\{ (\mu_k, \sigma_k^2), \forall k \}} \log(P(O)) = \arg\max_{\{ (\mu_k, \sigma_k^2), \forall k \}} \sum_{o \in O} \log P(o)
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The probability of an individual vector:

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P(o) = \sum_k P(k)N(o; \mu_k, \sigma_k^2)
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The maximum likelihood estimation again

\[
\arg\max_{\{ (\mu_k, \sigma_k^2), \forall k \}} \sum_{o \in O} \log \sum_k P(k)N(o; \mu_k, \sigma_k^2)
\]

This includes the log of a sum, which defies direct optimization
The general form of the problem

• The “presence” of missing data or variables requires them to be marginalized out of your probability
  – By summation or integration

• This results in a maximum likelihood estimate of the form

\[ \hat{\theta} = \arg\max_{\theta} \sum_{o} \log \sum_{h} P(h, o; \theta) \]

  – The inner summation may also be an integral in some problems
  – Explicitly introducing \( \theta \) in the RHS to show that the probability is computed by a model with parameter \( \theta \) which must be estimated

• The log of a sum (or integral) makes estimation challenging
  – No closed form solution
  – Need efficient iterative algorithms
The general form of the problem

• The “presence” of missing data or variables requires them to be marginalized out of your probability
  – By summation or integration

Can we get an approximation to this that is more tractable? (i.e. without a summation or integral within the log)

\[
\hat{\theta} = \arg\max_{\theta} \sum_o \log \sum_h P(h, o)
\]

–– The inner summation may also be an integral in some problems

• The log of a sum (or integral) makes estimation challenging
  – No closed form solution
  – Need efficient iterative algorithms
The variational lower bound

• We can rewrite

\[ \log P(o) = \log \sum_h P(h, o) = \log \sum_h Q(h) \frac{P(h, o)}{Q(h)} \]

  – Where \( Q(h) \) is some function such that \( Q(h) \geq 0 \) and \( \sum_h Q(h) = 1 \)
    • i.e. a probability distribution

• The logarithm is a concave function, therefore

\[ \log \sum_h Q(h) \frac{P(h, o)}{Q(h)} \geq \sum_h Q(h) \log \frac{P(h, o)}{Q(h)} \]
The logarithm is a concave function

- For any $x_1$ and $x_2$, for any $0 \leq q \leq 1$,
  $$\log(qx_1 + (1-q)x_2) \geq q \log(x_1) + (1-q)\log(x_2)$$

- More generally for any set of $\{x_i\}$, and any weights $\{q_i\}$ s.t. $q_i \geq 0$ and $\sum_i q_i = 1$
  $$\log\left(\sum_i q_i x_i \right) \geq \sum_i q_i \log(x_i)$$
The variational lower bound

• By the concavity of the log function

$$\log \sum_h Q(h) \frac{P(h, o)}{Q(h)} \geq \sum_h Q(h) \log \frac{P(h, o)}{Q(h)}$$

  – For any $Q(h) \geq 0$ and $\sum_h Q(h) = 1$
  – Note, the LHS is exactly equal to $\log P(o)$

• This is the *variational lower bound* on $\log P(o)$
  – Also called the Evidence Lower BOund, or ELBO
Or more explicitly

• By the concavity of the log function

\[ \log P(o; \theta) \geq \sum_h Q(h) \log \frac{P(h, o; \theta)}{Q(h)} \]

– Explicitly showing that the probability is computed by a model with parameter \( \theta \)
  • We must maximize \( P(o; \theta) \) w.r.t \( \theta \)

• This is the \textit{variational lower bound} or ELBO on \( \log P(o; \theta) \)
The (variational) lower bound

- The lower bound is always at or below the original function
- If it is a tight lower bound, the max of the lower bound can be expected to be near the max of the function

lowerbound: $f'(\theta) \leq f(\theta)$

• The lower bound is always at or below the original function
The (variational) lower bound

- The lower bound is always at or below the original function.
- If it is a tight lower bound, the max of the lower bound can be expected to be near the max of the function.
  - To make the lower bound tight, we need to choose $Q(h)$ properly.

$tight lower bound: f'(\theta) \leq f(\theta)$
Choosing a good $Q(h)$

- Let $Q(h) = P(h|o; \theta')$

$$\log P(o; \theta) \geq \sum_h P(h|o; \theta') \log \frac{P(h, o; \theta)}{P(h|o; \theta')}$$

- Let

$$J(\theta, \theta') = \sum_h P(h|o; \theta') \log \frac{P(h, o; \theta)}{P(h|o; \theta')}$$

- We get

$$\log P(o; \theta) \geq J(\theta, \theta')$$

- And

$$\log P(o; \theta) = J(\theta, \theta)$$
Choosing a good $Q(h)$

- Let $Q(h) = P(h|o; \theta')$

$$\log P(o; \theta) \geq \sum_h P(h|o; \theta') \log \frac{P(h, o; \theta)}{P(h|o; \theta')}$$

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- We get

$$\log P(o; \theta) \geq J(\theta, \theta')$$

- And

$$\log P(o; \theta) = J(\theta, \theta)$$
\[ P(o; \theta) = J(\theta, \theta) \]

\[
J(\theta, \theta) = \sum_h P(h|o; \theta) \log \frac{P(h,o; \theta)}{P(h|o; \theta)}
\]

\[
= \sum_h P(h,o; \theta) \log P(o; \theta)
\]

\[
\log P(o; \theta) \sum_h P(h|o; \theta) = \log P(o; \theta)
\]
Expectation Maximization

• We have

\[ J(\theta, \theta') = \sum_h P(h|o; \theta') \log \frac{P(h, o; \theta)}{P(h|o; \theta')} \]

• where

\[ \log P(o; \theta) \geq J(\theta, \theta') \]

• And

\[ \log P(o; \theta) = J(\theta, \theta) \]

• This gives us the following iterative algorithm that guarantees non-decreasing \( P(o; \theta) \) with iterations:

\[ \theta^{k+1} \leftarrow \arg\max_{\theta} J(\theta, \theta^k) \]
\(\theta^{k+1} \leftarrow \underset{\theta}{\text{argmax}} J(\theta, \theta')\)

- Initialize \(\theta^0\)
- Construct \(J(\theta, \theta^0)\)
  - It touches \(\log P(o; \theta)\) at \(\theta^0\) because \(\log P(o; \theta^0) = J(\theta^0, \theta^0)\)
\[ \theta^{k+1} \leftarrow \operatorname{argmax}_\theta J(\theta, \theta') \]

- Find \( \theta^1 = \operatorname{argmax}_\theta J(\theta, \theta^0) \)
  - \( J(\theta^1, \theta^0) \geq J(\theta^0, \theta^0) \) (since you’re maximizing \( J(\theta, \theta^0) \) w.r.t \( \theta \))
\[ \theta^{k+1} \leftarrow \arg\max_{\theta} J(\theta, \theta') \]

- Find \( \theta^1 = \arg\max_{\theta} J(\theta, \theta^0) \)
  - \( J(\theta^1, \theta^0) \geq J(\theta^0, \theta^0) \) (since you’re maximizing \( J(\theta, \theta^0) \) w.r.t \( \theta \))
- \( \log P(o; \theta^1) \geq J(\theta^1, \theta^0) \)
  - since \( J(\theta, \theta^0) \) is a lower bound on \( \log P(o; \theta) \)
- So the iteration increases \( \log P(o; \theta) \)
\[ \theta^{k+1} \leftarrow \text{argmax}_{\theta} J(\theta, \theta') \]

- Construct \( J(\theta, \theta^1) \)
  - It touches \( \log P(o; \theta) \) at \( \theta^1 \) because \( \log P(o; \theta^1) = J(\theta^1, \theta^1) \)
Find $\theta^2 = \arg\max_{\theta} J(\theta, \theta^1)$

- $J(\theta^2, \theta^1) \geq J(\theta^1, \theta^1)$ (since you’re maximizing $J(\theta, \theta^1)$ w.r.t $\theta$)
\( \theta^{k+1} \leftarrow \text{argmax}_\theta J(\theta, \theta') \)

- Find \( \theta^2 = \text{argmax}_\theta J(\theta, \theta^1) \)
  - \( J(\theta^2, \theta^1) \geq J(\theta^1, \theta^1) \) (since you’re maximizing \( J(\theta, \theta^1) \) w.r.t \( \theta \))
- \( \log P(o; \theta^2) \geq J(\theta^2, \theta^1) \)
  - Since \( J(\theta, \theta^1) \) is a lower bound on \( \log P(o; \theta) \)
- So the iteration increases \( \log P(o; \theta) \)
\[ \theta^{k+1} \leftarrow \arg\max_{\theta} J(\theta, \theta') \]

- Repeat the steps:
  - Compose \( J(\theta, \theta^k) \) to “touch” \( \log P(o; \theta) \) at the current estimate \( \theta^k \)
  - Set \( \theta^{k+1} \leftarrow \arg\max_{\theta} J(\theta, \theta^k) \)

- Each step is guaranteed to increase (or at least not decrease) \( \log P(o; \theta) \)
  - Stop when \( \log P(o; \theta) \) stops increasing
\( \theta^{k+1} \leftarrow \underset{\theta}{\text{argmax}} J(\theta, \theta') \)

- Repeat the steps:
  - Compose \( J(\theta, \theta^k) \) to “touch” \( \log P(o; \theta) \) at the current estimate \( \theta^k \)
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Repeat the steps:

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- Each step is guaranteed to increase (or at least not decrease) \( \log P(o; \theta) \)
  - Stop when \( \log P(o; \theta) \) stops increasing
Expectation Maximization

- Initialize $\theta^0$
- $k = 0$
- Iterate (over $k$) until $\log P(O; \theta)$ converges:
  - Construct ELBO function
    \[ J(\theta, \theta^k) = \sum_{o \in O} \sum_{h} P(h|o; \theta^k) \log \frac{P(h,o; \theta)}{P(h|o; \theta^k)} \]
  - Maximization step
    \[ \theta^{k+1} \leftarrow \arg\max_{\theta} J(\theta, \theta^k) \]
- Let’s simplify a bit
Expectation Maximization

• Initialize $\theta^0$
• $k = 0$
• Iterate (over $k$) until $\log P(O; \theta)$ converges:
  – Construct ELBO function

$$J(\theta, \theta^k) = \sum_{o \in O} \sum_{h} P(h|o; \theta^k) \log P(h, o; \theta) - \sum_{o \in O} \sum_{h} P(h|o; \theta^k) \log P(h|o; \theta^k)$$

  – Maximization step

$$\theta^{k+1} \leftarrow \underset{\theta}{\text{argmax}} J(\theta, \theta^k)$$
Expectation Maximization

- Initialize $\theta^0$
- $k = 0$
- Iterate (over $k$) until $\log P(O; \theta)$ converges:
  - Construct ELBO function
    $$J(\theta, \theta^k) = \sum_{o \in O} \sum_{h} P(h|o; \theta^k) \log P(h, o; \theta) - \sum_{o \in O} \sum_{h} P(h|o; \theta^k) \log P(h|o; \theta^k)$$
  - Maximization step
    $\theta^{k+1} \leftarrow \arg \max_{\theta} J(\theta, \theta^k)$

Not a function of $\theta$

Can be ignored for maximization
**Expectation Maximization**

- **Initialize** $\theta^0$
- $k = 0$
- **Iterate** (over $k$) until $\log P(O; \theta)$ converges:
  - **Expectation Step:**
    
    Compute $P(h|o; \theta^k)$ for all $o \in O$ for all $k$
  
  - **Maximization step**
    
    $$
    \theta^{k+1} \leftarrow \operatorname{argmax}_\theta \sum_{o \in O} \sum_h P(h|o; \theta^k) \log P(h, o; \theta)
    $$
Expectation Maximization for Maximum Likelihood Estimation

- Objective: Estimate

$$\theta^* = \arg\max_{\theta} \sum_{o \in O} \log \sum_{h} P(h, o; \theta)$$

- Solution: Iteratively perform the following optimization instead

$$\theta^{k+1} \leftarrow \arg\max_{\theta} \sum_{o \in O} \sum_{h} P(h|o; \theta^k) \log P(h, o; \theta)$$

- This maximizes an Empirical Lower Bound (ELBO) and guarantees increasing log likelihood with iterations
  - Giving you a local maximum log likelihood estimate for $\theta^*$
Expectation Maximization: In summary

- Construct an *Empirical Lower Bound* function $J(\theta, \theta^k)\]

\[
J(\theta, \theta^k) = \sum_{o \in O} \sum_h P(h|o; \theta^k) \log P(h, o; \theta) - \sum_{o \in O} \sum_h P(h|o; \theta^k) \log P(h|o; \theta^k)
\]

- Iteratively maximize the ELBO function

\[
\theta^{k+1} \leftarrow \arg\max_{\theta} J(\theta, \theta^k)
\]
Expectation Maximization

• Initialize $\theta^0$
• $k = 0$
• Iterate (over $k$) until $\sum_{o \in O} \log P(o; \theta)$ converges:
  – Expectation Step:
    Compute $P(h|o; \theta^k)$ for all $o \in O$ for all $k$
  – Maximization step

$$\theta^{k+1} \leftarrow \arg\max_\theta \sum_{o \in O} \sum_h P(h|o; \theta^k) \log P(h, o; \theta)$$
That’s so much math, but what does it really do?

• What does EM practically do when we have missing data?
  – What is the intuition behind how it resolves the problem?
Recap: Maximum Likelihood Estimation

• Sometimes the data provided may be incomplete
  – Insufficient to estimate your model parameters directly

• This could be because the data themselves have missing components
  – E.g. Data vectors have some missing components

• Or because of the structure of the network
  – Mixture models, multi-stage Generative models
Recall this: Gaussian estimation with incomplete vectors

- These are the actual data we have: A set $O = \{o_1, \ldots, o_N\}$ of incomplete vectors
  - Comprising only the observed components of the data

- We are missing the data $M = \{m_1, \ldots, m_N\}$
  - Comprising the missing components of the data

- The complete data includes both the observed and missing components
  $X = \{x_1, \ldots, x_N\}$, $x_i = (o_i, m_i)$
  - Keep in mind that at the complete data are not available (the missing components are missing)
Let's look at a single vector

- These are the actual data we have: A set $O = \{o_1, \ldots, o_N\}$ of incomplete vectors
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- The complete data includes both the observed and missing components

\[ X = \{x_1, \ldots, x_N\}, \quad x_i = (o_i, m_i) \]

- Keep in mind that at the complete data are not available (the missing components are missing)
Let's look at a single vector

- We will try to complete the vector by filling in the missing value with \textit{plausible} values that match the observed components

- Plausible: Values that “go with” the observed values, according to the distribution of the data
• Question: If we have a very large number of vectors from the Gaussian, all with the same observed components $o$, what would their missing components be?
• Question: If we have a very large number of vectors from the Gaussian, all with the same observed components \( o \), what would their missing components be?

• We would see every possible value, but in proportion to their probability: \( P(m|o) \) (conditioned on the observations)
Completing incomplete vectors

• Complete vector by filling up the missing components with every possible value
  – I.e. make many complete “clones” of the incomplete vector

• But assign a proportion to each value
  – Proportion is $P(m|o)$
    • Which can be computed if we know $P(x) = P(o, m)$

\[\text{in proportion: } P(\ast|o)\]
Gaussian estimation with incomplete vectors

- “Expand” every incomplete vector out into all possibilities
  - In appropriate proportions \( P(m|o) \)
  - For already complete observations, there is no expansion
- Estimate the statistics from the expanded data
Gaussian estimation with incomplete vectors

- "Expand" every incomplete vector out into all possibilities
  - In appropriate proportions $P(m|o)$
  - For already complete observations, there is no expansion
- Estimate the statistics from the expanded data

From a previous estimate of the model
Estimating the Gaussian Parameters

- Compute the statistics from the (proportionately) expanded set
- Let $x_i(m)$ be the “completed” version of the observation $o_i$, when the missing components are filled with value $m$
  
  $$x_i(m) = (m, o_i)$$
  - There will be one such vector for every value of $m$

- Estimate the statistics from the expanded data

  $$\mu^{k+1} = \frac{1}{N} \sum_{o \in O} \int_{-\infty}^{\infty} P(m|o; \theta^k)x_i(m)dm$$

  $$\Sigma^{k+1} = \frac{1}{N} \sum_{o \in O} \int_{-\infty}^{\infty} P(m|o; \theta^k)(x_i(m) - \mu^{k+1})(x_i(m) - \mu^{k+1})^T dm$$
EM for computing the Gaussian Parameters

- Initial $\theta^0 = (\mu^0, \Sigma^0)$
- Until $P(O; \theta)$ converges:

$$
\mu^{k+1} = \frac{1}{N} \sum_{o \in O} \int_{-\infty}^{\infty} P(m|o; \theta^k)x_i(m)dm \\
\Sigma^{k+1} = \frac{1}{N} \sum_{o \in O} \int_{-\infty}^{\infty} P(m|o; \theta^k)(x_i(m) - \mu^{k+1})(x_i(m) - \mu^{k+1})^T dm
$$

Where $x_i(m) = (m, o_i)$ and the parameters of $P(m|o; \theta^k)$ are derived from the $P(x; \theta^k) = \text{Gaussian}(x; \mu^k, \Sigma^k)$
Recap: Maximum Likelihood Estimation

- Sometimes the data provided may be incomplete
  - Insufficient to estimate your model parameters directly

- This could be because the data themselves have missing components
  - E.g. Data vectors have some missing components

- Or because of the structure of the network
  - Mixture models, multi-stage Generative models
The GMM problem of incomplete data: missing information

- Problem: We are not given the actual Gaussian for each observation
  - Our data are incomplete

- What we want: \((o_1, k_1), (o_2, k_2), (o_3, k_3)\) ...

- What we have: \(o_1, o_2, o_3\) ...
Consider a single vector

- *Every* Gaussian is capable of generating this vector
  - With different probabilities
Consider a single vector

- Every Gaussian is capable of generating this vector
  - With different probabilities

- If we saw a large number of these vectors, how many of these would have come from each Gaussian?
Consider a single vector

- Every Gaussian is capable of generating this vector
  - With different probabilities

- If we saw a large number of these vectors, how many of these would have come from each Gaussian

- All of them, but in proportion to \( P(k|o) \)
Completing incomplete vectors

- Complete the data by attributing to every Gaussian
  - i.e. make many complete “clones” of the data

- But assign a proportion to each completed vector
  - Proportion is $P(k|o)$
    - Which can be computed if we know $P(k)$ and $P(o|k)$

- Then estimate the parameters using the complete data
Completing incomplete vectors

- Complete the data by attributing to *every Gaussian*
  - I.e. make many complete “clones” of the data

- But assign a *proportion* to each completed vector
  - Proportion is $P(k|o)$
    - Which can be computed if we know $P(k)$ and $P(o|k)$

- Then estimate the parameters using the complete data
EM for GMMs

- “Complete” each vector in every possible way:
  - assign each vector to every Gaussian
  - In proportion $P(k|o; \theta^i)$ (computed from current model estimate)
- Compute statistics from “completed” data
EM for GMMs

In proportion to

Now you can segregate the vectors by Gaussian

- The number of segregated complete vectors from each observation will be in proportion to $P(k|o; \theta^l)$
Now you can segregate the vectors by Gaussian

- The number of segregated complete vectors from each observation will be in proportion to \( P(k|o; \theta^l) \)

\[
\begin{align*}
\mu_{k}^{l+1} &= \frac{1}{\sum_{o} P(k|o; \theta^l)} \sum_{o} P(k|o; \theta^l) o \\
\Sigma_{k}^{l+1} &= \frac{1}{\sum_{o} P(k|o; \theta^l)} \sum_{o} P(k|o; \theta^l) (o - \mu_{k}^{l+1})(o - \mu_{k}^{l+1})^T
\end{align*}
\]
EM for GMMs

• Initialize $\mu_k^0$ and $\Sigma_k^0$ for all $k$
• Iterate (over $l$):
  – Compute $P(k|o; \theta^l)$ for all $o$
    • Compute the proportions by which $o$ is assigned to all Gaussians
  – Update:
    - $\mu_k^{l+1} = \frac{1}{\sum_o P(k|o; \theta^l)} \sum_o P(k|o; \theta^l) o$
    - $\Sigma_k^{l+1} = \frac{1}{\sum_o P(k|o; \theta^l)} \sum_o P(k|o; \theta^l) (o - \mu_k^{l+1})(o - \mu_k^{l+1})^T$
General EM principle

• “Complete” the data by considering *every* possible value for missing data/variables
  – In proportion to their posterior probability, given the observation, $P(m|o)$ (or $P(k|o)$)

• Reestimate parameters from the “completed” data
General EM principle

• “Complete” the data by considering every possible value for missing data/variables
  – In proportion to their posterior probability, given the observation, $P(m|o)$ (or $P(k|o)$)

• Reestimate parameters from the “completed” data
**General EM principle**

- “Complete” the data by considering *every* possible value for missing data/variables
  - In proportion to their posterior probability, given the observation, $P(m|o)$ (or $P(k|o)$)

Sufficient to “complete” the data by *sampling* missing values from the posterior $P(m|o)$ (or $P(k|o)$) instead
Alternate EM principle

• “Complete” the data by *sampling* possible value for missing data/variables from $P(m|o)$ (or $P(k|o)$)

• Reestimate parameters from the “completed” data
Overall EM principle: Remember this

- Initially, some data/information are missing
Overall EM principle: Remember this

• Initially, some data/information are missing
  • *Initialize model parameters*
Overall EM principle: Remember this

- Initially, some data/information are missing
- Initialize model parameters
- Iterate:

\[ P(m|o) \] computed by the current model

- By explicitly considering every possible value, with its posterior-based proportionality
- Or by sampling the posterior probability distribution

\[ P(o) \]
Overall EM principle: Remember this

• Initially, some data/information are missing
• Initialize model parameters
• Iterate
  – Complete the data according to the posterior probabilities $P(m|o)$ computed by the current model
    • By explicitly considering every possible value, with its posterior-based proportionality
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Overall EM principle: Remember this

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  - Reestimate the model
Overall EM principle: Remember this

• Initially, some data/information are missing
• Initialize model parameters
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  – Complete the data according to the posterior probabilities $P(m|o)$ computed by the current model
    • By explicitly considering every possible value, with its posterior-based proportionality
    • Or by sampling the posterior probability distribution $P(m|o)$
  – Reestimate the model
And now for something completely different...

Principal Component Analysis
Principal Component Analysis

Given a (centered) set of data

• Find the principal subspace such that when all vectors are approximated as lying on that subspace, the approximation error is minimal
  – Assuming “centered” (zero-mean) data
Principal Component Analysis

Given a (centered) set of data
find subspace such that

- Find the principal subspace such that when all vectors are approximated as lying on that subspace, the approximation error is minimal
  - Assuming “centered” (zero-mean) data
Principal Component Analysis

*Given a (centered) set of data find subspace such that the projection of the data onto the subspace*

- Find the principal subspace such that when all vectors are approximated as lying on that subspace, the approximation error is minimal
  - Assuming “centered” (zero-mean) data
Principal Component Analysis

Given a (centered) set of data
find subspace such that
the projection of the data onto the subspace
results in the lowest total (squared) error

Minimize the sum of the
squared lengths of these lines

- Find the principal subspace such that when all vectors are approximated
  as lying on that subspace, the approximation error is minimal
  - Assuming “centered” (zero-mean) data
Principal Component Analysis

- Find the principal subspace such that when all vectors are approximated as lying on that subspace, the approximation error is minimal
  - Assuming “centered” (zero-mean) data
Principal Component Analysis

- Find the principal subspace such that when all vectors are approximated as lying on that subspace, the approximation error is minimal
  - Assuming “centered” (zero-mean) data
Principal Component Analysis

- Find the principal subspace such that when all vectors are approximated as lying on that subspace, the approximation error is minimal
  - Assuming “centered” (zero-mean) data
Can be done in closed form

• Since we’re minimizing quadratic L$_2$ error, we can find a closed form solution
Can be done in closed form

Since we’re minimizing quadratic $L_2$ error, we can find a closed form solution.
Can be done in closed form

- Since we’re minimizing quadratic $L_2$ error, we can find a closed form solution
Can be done in closed form

• Since we’re minimizing quadratic $L_2$ error, we can find a closed form solution
Can be done in closed form

• Since we’re minimizing quadratic L₂ error, we can find a closed form solution
• Total projection error for all data:

\[ L = \sum_x x^T x - w T x x^T w \]

• Minimizing this w.r.t \( w \) (subject to \( w = \) unit vector) gives you the Eigenvalue equation

\[ \left( \sum_x x^T x \right) w = \lambda w \]

• This can be solved to find the principal subspace
There’s also an iterative solution

- Objective: find a vector (subspace) $w$ and a position $z$ on $w$ such that $zw \approx x$ most closely (in an $L_2$ sense) for the entire (training) data

- Let $X = [x_1, x_2, ..., x_N]$ be the entire training set (arranged as a matrix)
  - Objective: find vector bases (for the subspace) $W$ and the set of position vectors $Z = [z_1, z_2, ..., z_N]$ for all vectors in $X$ such that $WZ \approx X$

- Initialize $W$
- Iterate until convergence:
  - Given $W$, find the best position vectors $Z$: $Z \leftarrow W^+X$
  - Given position vectors $Z$, find the best subspace: $W \leftarrow XZ^+$
  - Guaranteed to find the principal subspace
The iterative algorithm

- Initialize a subspace (the basis $w$)
The iterative algorithm

- Initialize a subspace (the basis $w$)
- Iterate until convergence:
  - Find the best position vectors $Z$ on the $W$ subspace for each training instance
    - Find the location on $W$ that is closest to each instance, i.e. the perpendicular projection

This individually minimizes the length of lines from the points to the plane.
The iterative algorithm

- Initialize a subspace (the basis $w$)
- Iterate until convergence:
  - Find the best position vectors $Z$ on the $W$ subspace for each training instance
    - Find the location on $W$ that is closest to each instance, i.e. the perpendicular projection
  - Let $W$ rotate and stretch/shrink, keeping the arrangement of $Z$ locations fixed
    - Minimize the total square length of the lines attaching the projection on the plane to the instance

This jointly minimizes the total squared length of lines from the points to their “attachments” on the plane.
The iterative algorithm

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  - Find the best position vectors $Z$ on the $W$ subspace for each training instance
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    - Minimize the total square length of the lines attaching the projection on the place to the instance
A failed attempt at animation

• Someone with animated-gif generation skills, help me...
A cartoon view of Iterative PCA

- Note that the real problem in estimating $Z$ is computing $W^+$
  - If you know $W^+$, $Z$ is obtained by a direct matrix multiply
Drawing this differently

- Look familiar?
- An autoencoder with linear activations
- Backprop actually works by simultaneously updating $Z$ (implicitly) and $W$ in tiny increments
A minor issue: Scaling invariance

- The estimation is scale invariant
- We can increase the length of $w$, and compensate for it by reducing $z$
- The solution is not unique!
Rotation/scaling invariance

\[ \mathbf{v} = a \mathbf{w}_1 + b \mathbf{w}_2 \]
\[ \mathbf{z} = \begin{bmatrix} a \\ b \end{bmatrix} \]

\[ \mathbf{v} = a' \mathbf{w}_1' + b' \mathbf{w}_2' \]
\[ \mathbf{z} = \begin{bmatrix} a' \\ b' \end{bmatrix} \]

\[ \mathbf{v} = a'' \mathbf{w}_1'' + b'' \mathbf{w}_2'' \]
\[ \mathbf{z} = \begin{bmatrix} a'' \\ b'' \end{bmatrix} \]

• We can rotate and scale the vectors in \( W \) without changing the actual subspace they compose.
• The representation of any point in the hyperspace in terms of these vectors will also change.
  – The \( \mathbf{z}s \) in the two cases will be related through a linear transform.
• The subspace is invariant to transformations of \( \mathbf{z} \).
Resolving this issue

• A unique solution can be found by either
  – Requiring the vectors in $W$ to be unit length and orthogonal
    • Standard “closed” form PCA
    – Constraining the variance of $Z$ to be unity

• While the $W$'s estimated with the two solutions will be different, the resulting discovered principal subspace will be the same
Resolving this issue

- A unique solution can be found by either
  - Requiring the vectors in $W$ to be unit length and orthogonal
    - Standard “closed” form PCA
    - Constraining the variance of $Z$ to be unity

- While the $W$s estimated with the two solutions will be different, the resulting discovered principal subspace will be the same
Constraining the linear AE

• The linear AE can be constrained to give you a unique(ish) solution

• Impose a unity constraint on the variance of $Z$ — How?
So what are we doing in the iterative solution?

- For every training vector \( x \), we are missing the information \( z \) about where the vector lies on the principal subspace hyperplane.
- If we had \( z \), we could uniquely identify the plane.
Iterative solution

- Initialize the plane
  - Or rather, the bases for the plane
Iterative solution

- Initialize the plane
  - Or rather, the bases for the plane
- “Complete” the data by computing the appropriate zs for the plane
Iterative solution

- Initialize the plane
  - Or rather, the bases for the plane
- “Complete” the data by computing the appropriate zs for the plane
- Reestimate the plane using the zs
Iterative solution

- Initialize the plane
  - Or rather, the bases for the plane
- “Complete” the data by computing the appropriate zs for the plane
- Reestimate the plane using the zs
- Iterate
Iterative solution

- Initialize the plane
  - Or rather, the bases for the plane
- "Complete" the data
- Reesti
- Iterate

Look Familiar?
Iterative solution

- This looks like EM
  - In fact it is
- But what is the generative model?
- And what distribution is this encoding?
Constraining the linear AE

- Imposing the constraint that $z$ must have unit variance is the same as assuming that $z$ is drawn from a standard Gaussian – 0 mean, unit variance!

- The decoder of the AE with the unit-variance constraint on $z$ is in fact a Generative model
The *generative* story behind PCA (linear AEs)

- Linear AEs actually have a generative story
- In order to generate any point
  - We first take a Gaussian step on the principal plane
  - Then we take an orthogonal *Gaussian* step from where we land to generate a point
  - PCA / Linear AEs find the plane and the characteristics of the Gaussian steps from the data
The *generative* story behind PCA (linear AEs)

- **Generative story for PCA:**
  - $z$ is drawn from a $K$-dim isotropic Gaussian
    - $K$ is the dimensionality of the principal subspace
  - $A$ is “basis” matrix
    - Matrix of principal Eigen vectors scaled by Eigen values
  - $E$ is a 0-mean Gaussian noise that is orthogonal to the principal subspace
    - The covariance of the Gaussian is low-rank and orthogonal to the principal subspace!
The generative story behind PCA (linear AEs)

- Generative story for PCA:
  - \( z \) is drawn from a \( K \)-dim isotropic Gaussian
    - \( K \) is the dimensionality of the principal subspace
  - \( A \) is “basis” matrix
    - Matrix of principal Eigen vectors scaled by Eigen values
  - \( E \) is a 0-mean Gaussian noise that is orthogonal to the principal subspace
    - The covariance of the Gaussian is low-rank and orthogonal to the principal subspace!

\[
\begin{align*}
  z \sim &\ N(0, I) \\
  E \sim &\ N(0, D) \\
  X = &\ Az + E \\
  \hat{X} \sim &\ N(0, \Sigma) \\
  X = &\ \hat{X} + E
\end{align*}
\]

PCA implicitly obtains maximum likelihood estimate of \( A \) and \( D \), from training data \( X \)
The generative (PCA) story of linear AEs

- The decoder weights are just the PCA basis matrix

\[ V^T = A \]
\[ \hat{X} = Az \]

Note: the generative model is the decoder

\[ z \sim N(0, I) \]
\[ \hat{X} = V^T z \]

\[ E \sim N(0, D) \]

- The decoder weights are just the PCA basis matrix
The generative (PCA) story of linear AEs

- The decoder weights are just the PCA basis matrix
- The encoder only projects the data into latent Gaussian position variable $z$
- Encoder: transforms input $X$ into Gaussian $z$
- Decoder: transforms Gaussian $z$ into principal subspace reconstruction $\hat{X}$

Note: the generative model is the decoder

The encoder finds the specific $z$ for any input $x$

$z \sim N(0, I)$
$\hat{X} = V^T z$
$z = WX$

$V^T = A$
$\hat{X} = Az$

Changed notation
The distribution modelled by PCA

If \( z \) is Gaussian, \( \hat{X} \) is Gaussian
\( \hat{X} \) and \( E \) are Gaussian \( \Rightarrow \) \( X \) is Gaussian

PCA model: The observed data are Gaussian
- Gaussian data lying very close to a principal subspace
- Comprising “clean” Gaussian data on the subspace plus orthogonal noise
Can we do better?

• PCA assumes the noise is always orthogonal to the data
  – Not always true
  – Noise in images can look like images, random noise can sound like speech, etc.
• Lets us generalize the model to permit non-orthogonal noise
The Linear Gaussian Model

\[ z \sim N(0, I) \]
\[ E \sim N(0, D) \]
\[ X = Az + E \]

- **Update the model:** The noise added to the output of the encoder can lie in any direction
  - Uncorrelated, but not just orthogonal to the principal subspace

- **Generative model:** to generate any point
  - Take a Gaussian step on the hyperplane
  - Add *full-rank* Gaussian uncorrelated noise that is independent of the position on the hyperplane
    - Uncorrelated: diagonal covariance matrix
    - Direction of noise is unconstrained
      - Need not be orthogonal to the plane
The linear Gaussian model

- $z \sim N(0, I)$
- $E \sim N(0, D)$
- $X = Az + E$

Red arrows are different possibilities for $E$

Blue arrows are different possibilities for $\hat{X}$

- The way to produce any data instance is no longer unique
  - though different corrections may have different probabilities
Revisiting the linear Gaussian model

- The way to produce any data instance is no longer unique
  - though different corrections may have different probabilities
- This is still a parametric model for a Gaussian distribution
  - Parameters are $A$ and $D$ (assuming 0 mean)

$z \sim N(0, I)$

$E \sim N(0, D)$

$X = Az + E$

$P(X) = N(X; 0, AA^T + D)$

Red arrows are different possibilities for $E$

Blue arrows are different possibilities for $\hat{X}$

$X = \hat{X} + E$
Revisiting the linear Gaussian model

- The way to produce any data instance is no longer unique—though different corrections may have different probabilities.

- This is in fact a parametric model for a Gaussian distribution.

- Parameters are $A$ and $D$ (assuming 0 mean).

- Also known as Factor Analysis:
  - $A$ is the loading matrix
  - $z$ are the factors
  - $D$ is diagonal

- Blue arrows are different possibilities for $\hat{X}$

- Red arrows are different possibilities for $E$

- $X = A z + E$

- $P(X) = N(X; 0, AA^T + D)$
Story for the day

• EM: An iterative technique to estimate probability models for data with missing components or information
  – By iteratively “completing” the data and reestimating parameters

• PCA: Is actually a generative model for Gaussian data
  – Data lie close to a linear manifold, with orthogonal noise

• Factor Analysis: Also a generative model for Gaussian data
  – Data lie close to a linear manifold
  – Like PCA, but without directional constraints on the noise

• Will continue with FA and Variational AutoEncoders in the next class