Neural Networks

Variational Autoencoders
Part 2

(based in part on slides from Dan Schwartz and Tom Manzini)

Recap: Neural nets as generative models

- We've seen how neural nets can perform classification
  - Or regression
  - MLPs, CNNs, RNNs..
- And how they can generate data from Boltzmann distributions
  - Boltzmann machines
- Next step: NNs as generic generative models
  - Model the distribution of *any* data
  - Such that we can draw samples from it

Recap: Generative models and Maximum Likelihood Estimation

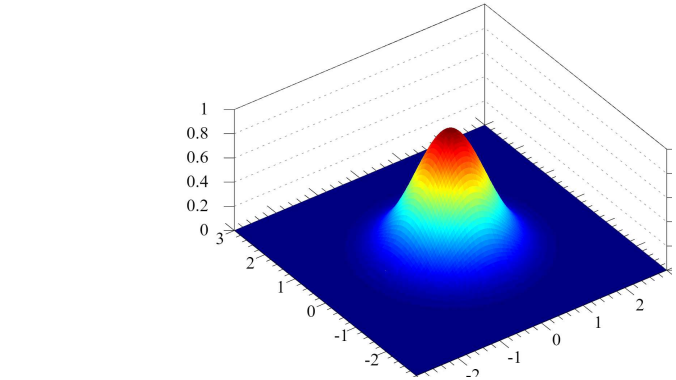
What is a generative model

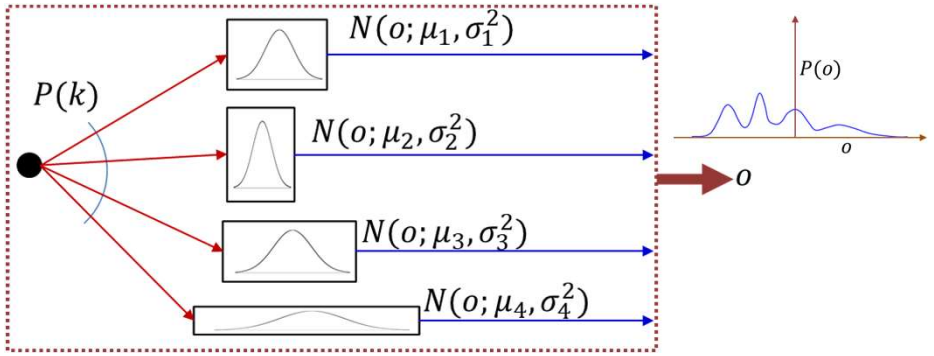
- In statistical estimation, a *generative model* is a functional or computational model for the probability distribution of a given data
  - Can be represented generically as $P(x;\theta)$, where x represents a data instance and θ are the *parameters* of the model
  - But actually encodes a *generative story* for how the data were produced

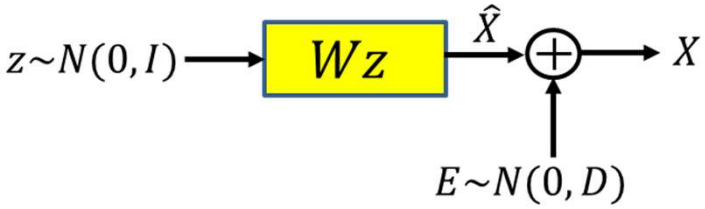
- Utility of the model
  - Can compute the probability of observing a given value x
  - Can also be used to *generate* samples of (or statistically similar to) the data

Recap: Examples of Generative Models

- Generative models can be simple, one step models of the generating
  - E.g. Gaussians, Multinomials
- Or a multi-step generating process
  - E.g. Gaussian Mixtures
  - E.g. Linear Gaussian Models







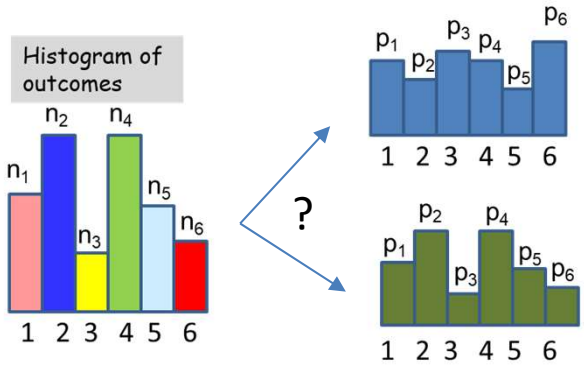
Recap: ML Estimation of Generative Models

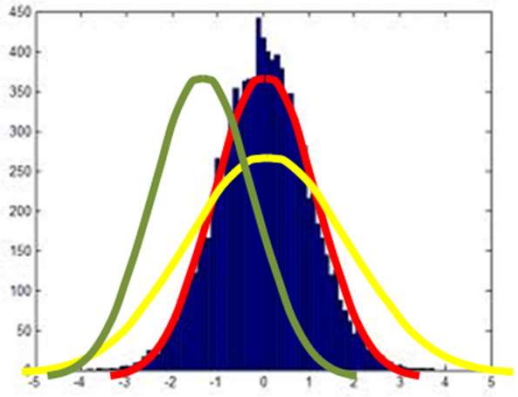
- Must estimate the parameters of the model from observed data

- Maximum likelihood estimation: Choose parameters to maximize the (log) likelihood of observed data

$$\theta^* = \underset{\theta}{\text{argmax}}\ \log(P(X;\theta))$$

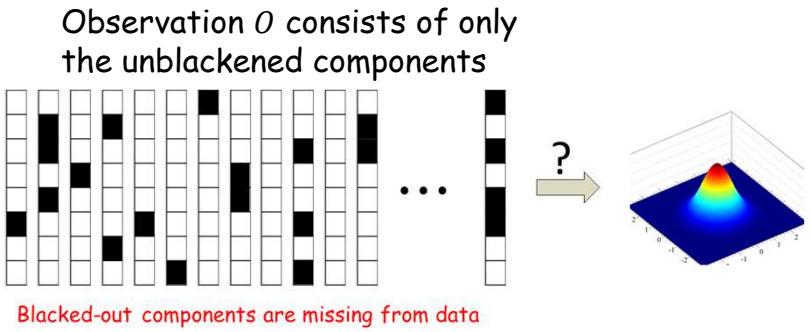
$$= \underset{\theta}{\text{argmax}} \sum_{x \in X} \log(P(x;\theta))$$





Recap: ML estimation from incomplete data

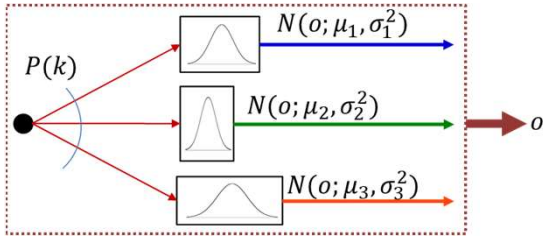
- In many situations, our observed data are missing information
  - E.g. components of the data
  - E.g. "inside" information about how the data are drawn by the model



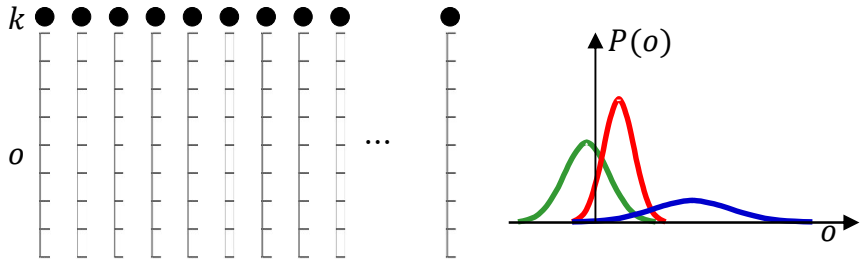
- In these cases, the ML estimate must only consider the *observed* data O

$$\underset{\theta}{\operatorname{argmax}} \sum_{o \in O} \log P(o;\theta)$$

  - But the observed data are incomplete



- Observation probability $P(o)$ must be obtained from the *complete* data probability, by marginalizing out missing components
  - This can cause ML estimation to become challenging



Recap: ML estimation from incomplete data

- ML estimate from *observed* data O

$$\underset{\theta}{\operatorname{argmax}} \sum_{o \in O} \log P(o;\theta)$$

- $P(o)$ is obtained by marginalizing out missing components

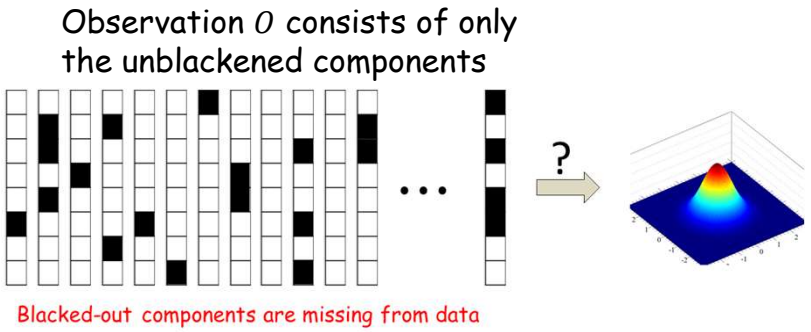
$$P(o;\theta) = \sum_{h} P(h,o;\theta)$$

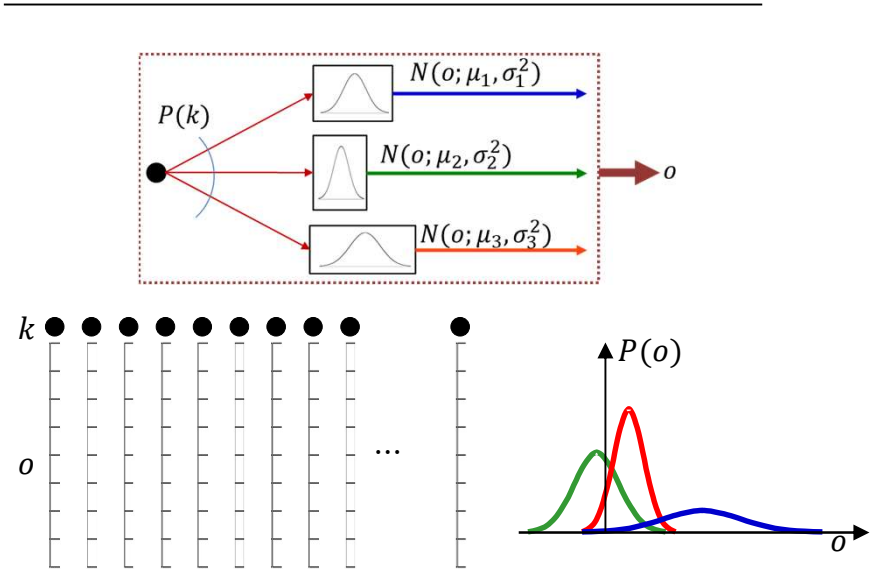
- The ML estimate becomes

$$\underset{\theta}{\operatorname{argmax}} \sum_{o \in O} \log \sum_{h} P(h,o;\theta)$$

  - h represent the hidden or missing components

- Minimizing the log of a sum of ugly functions usually doesn't have nice solutions





Recap: The ELBO function and EM

- We can define an *Empirical Lower Bound* (or ELBO) for the log probability $\log(P(o))$ as:

$$\log \sum_h P(h, o; \theta) \geq \sum_h q(h) \log P(h, o; \theta) - \sum_h q(h) \log q(h)$$

  - This bound holds for any probability distribution $q(h)$ but is tightest when $q(h) \cong P(h|o; \theta)$
    - For $q(h) = P(h|o; \theta)$ it actually works out to $P(o; \theta)$

- We get a nice iterative ML estimator if we maximize the ELBO instead of $\log(P(o))$ directly
  - If we use $q(h) = P(h|o; \theta^k)$ where θ^k is the kth estimate of θ, to obtain the (k+1)th estimate, this gives us the *Expectation Maximization* algorithm

Recap: The Expectation Maximization Algorithm

- Define the *auxiliary* function:

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

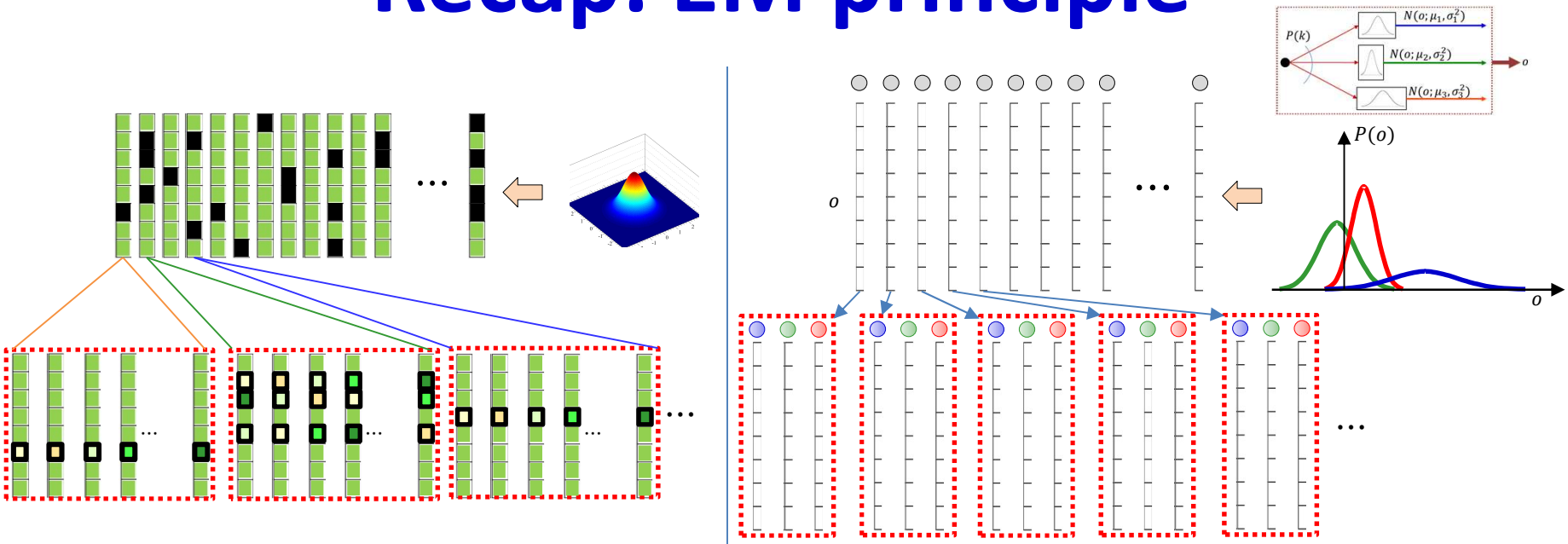
  - Which is the ELBO plus a term that doesn't depend on θ

- Iteratively compute

$$\theta^{k+1} \leftarrow \operatorname*{argmax}_{\theta} Q(\theta, \theta^k)$$

- Guaranteed to increase $\log P(o)$ with every iteration

Recap: EM principle

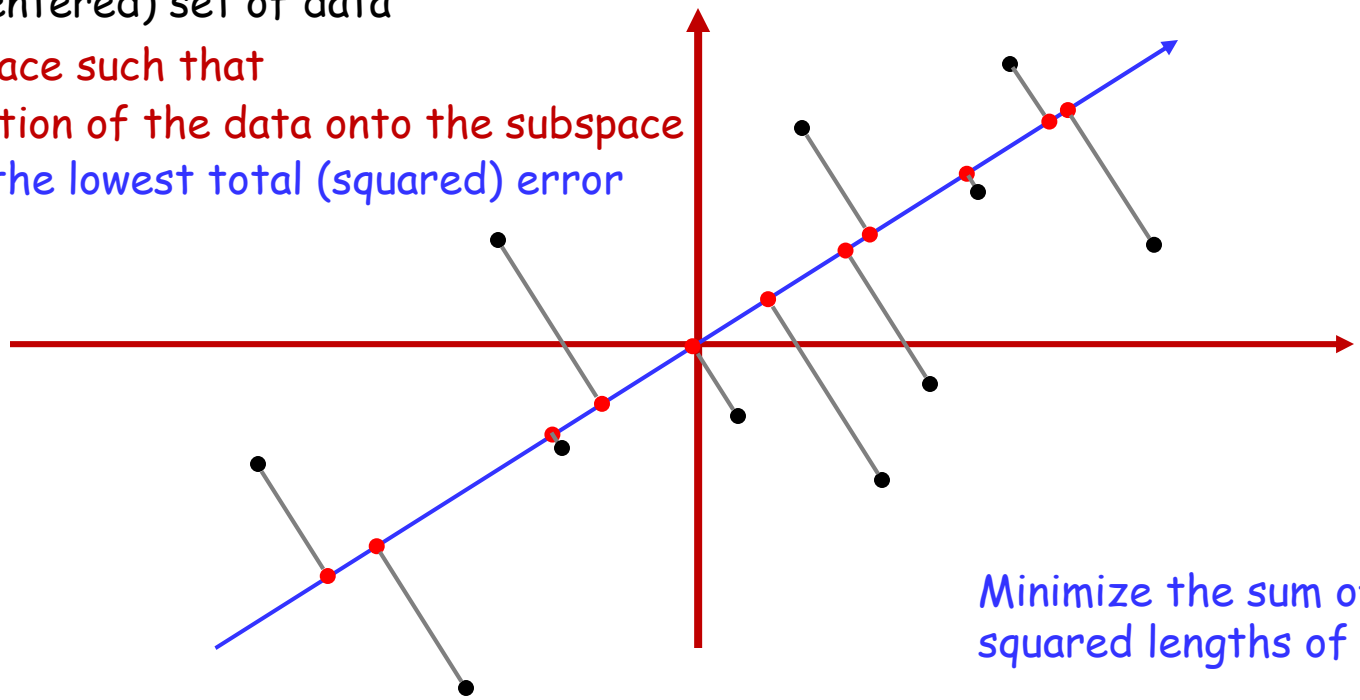


- Iteratively:
- **Complete the data according to the posterior probabilities $P(m|o)$ computed by the current model**
  - By explicitly considering every possible value, with its posterior-based proportionality
  - Or by sampling the posterior probability distribution $P(m|o)$
    - Upon completion each incomplete observation implicitly or explicitly becomes many (potentially infinite) complete observations
- ***Reestimate the model from completed data***

Principal Component Analysis

Given a (centered) set of data

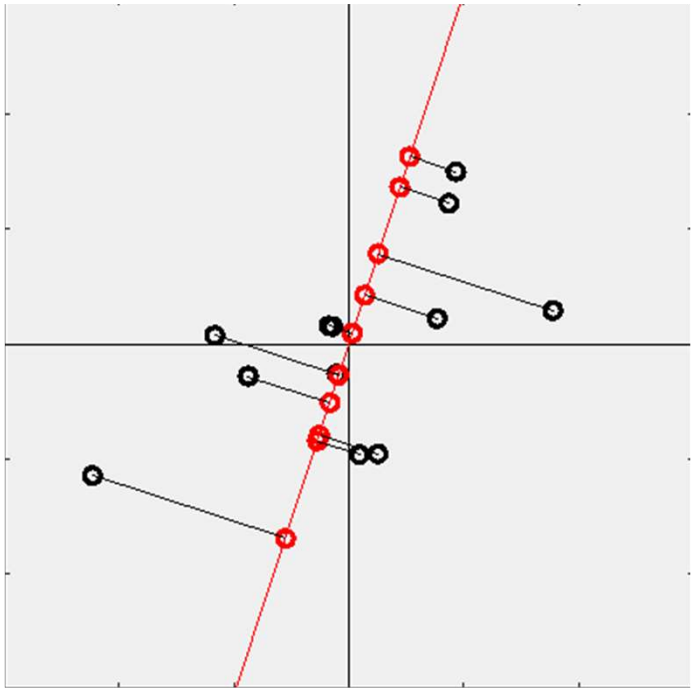
find subspace such that
the projection of the data onto the subspace
results in the lowest total (squared) error



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

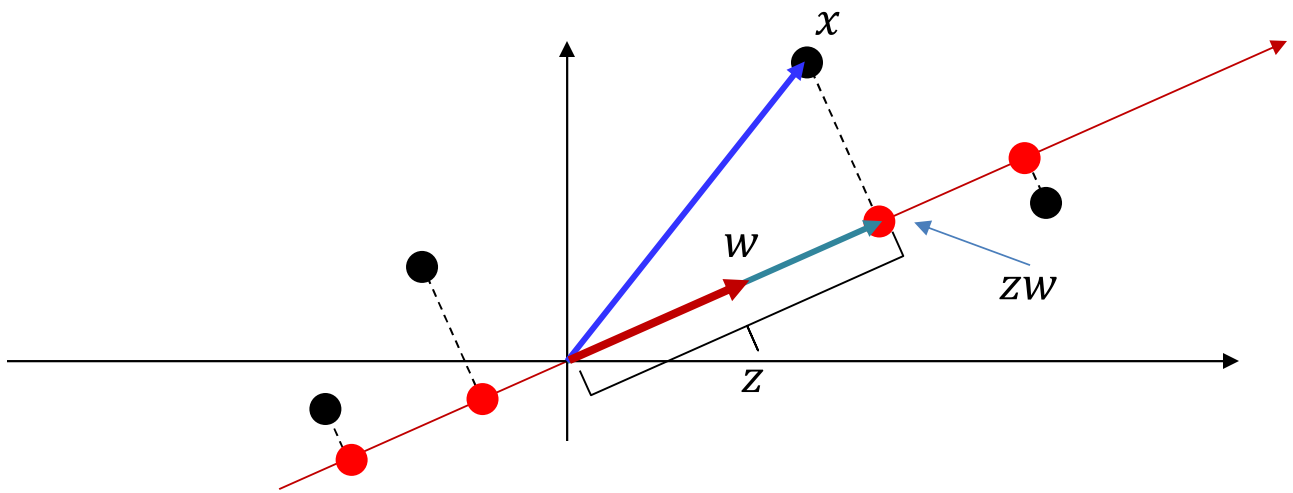
Principal Component Analysis



Search through all subspaces to find the one with minimum projection error

- 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

Recap: PCA Iterative Estimator

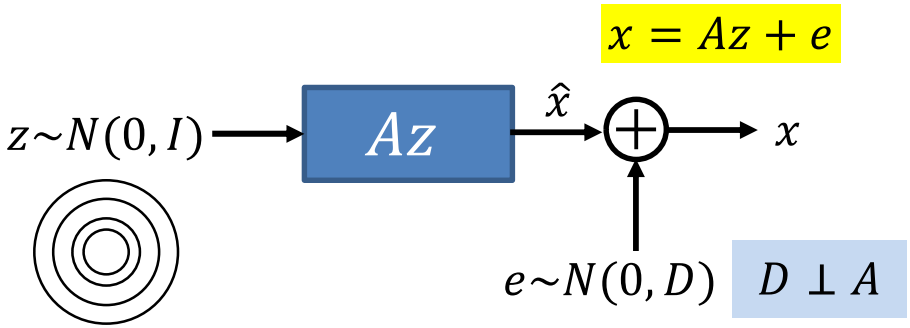


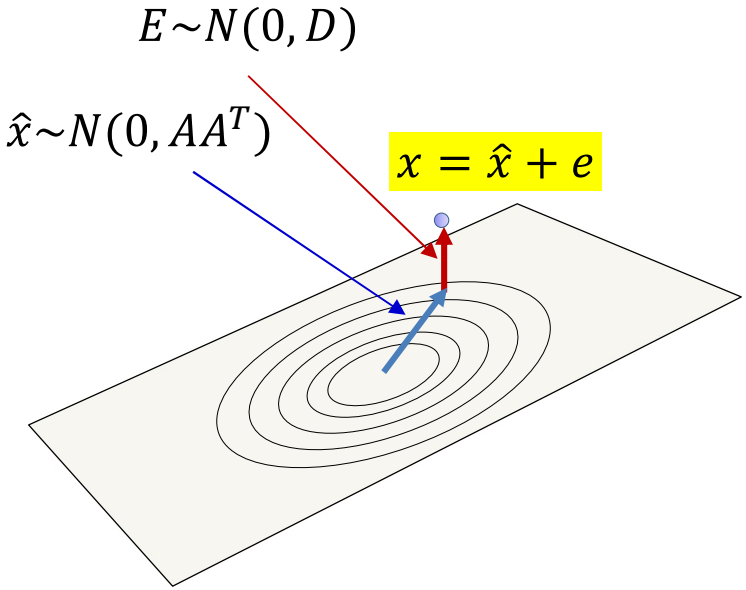
- Objective: find a vector (subspace) w and a *position* z on w such that $zw \approx x$ most closely (in an L_2 sense) for the entire (training) data

- Let $X = [x_1 x_2 \ldots x_N]$ be the entire training set (arranged as a matrix)
  - Objective: find vector bases (for the subspace) W and the set of *position vectors* $Z = [z_1 z_2 \ldots z_N]$ 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

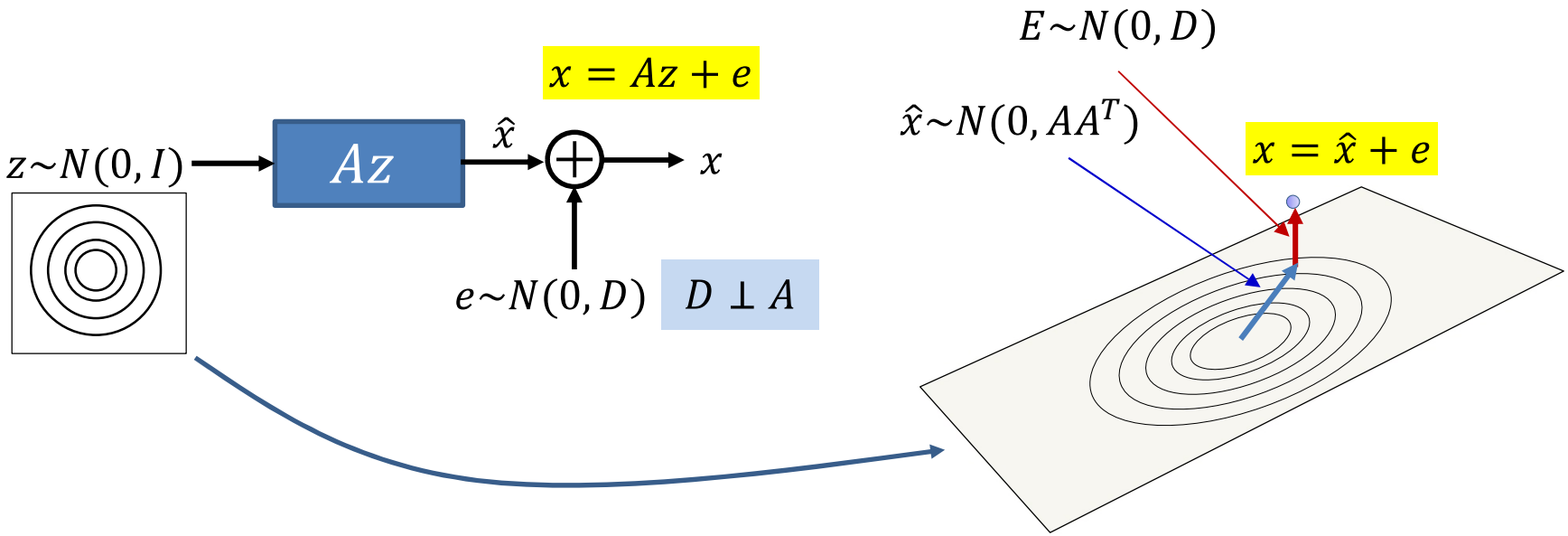
Recap: The *generative* story behind PCA





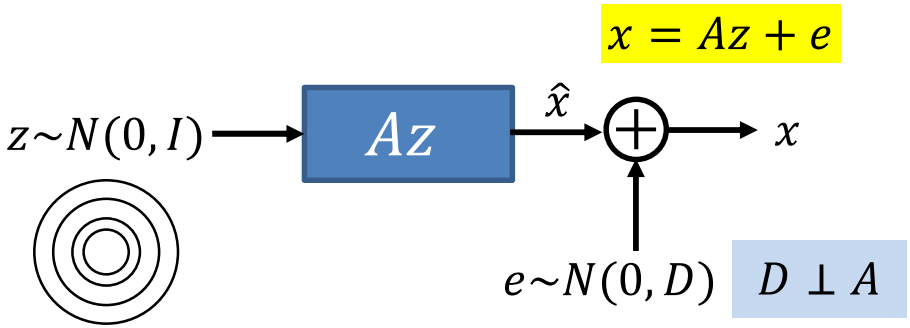
- **Generative story for PCA:**
  - z is drawn from a K-dim isotropic Gaussian
    - K is the dimensionality of the principal subspace
  - A is "basis" matrix
    - Matrix of principal Eigen vectors scaled by Eigen values
  - e is a 0-mean Gaussian noise that is orthogonal to the principal subspace
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

Recap: The *generative* story behind PCA



- Alternate view: Az stretches and rotates the K-dimensional planar space of z into a K-dimensional planar subspace (manifold) of the data space
- The circular distribution of z in the K-dimensional z space transforms into an ellipsoidal distribution on a K-dimensional hyperplane the data space
- Samples are drawn from the ellipsoidal distribution on the hyperplane, and noise is added to them

The probability modelled by PCA



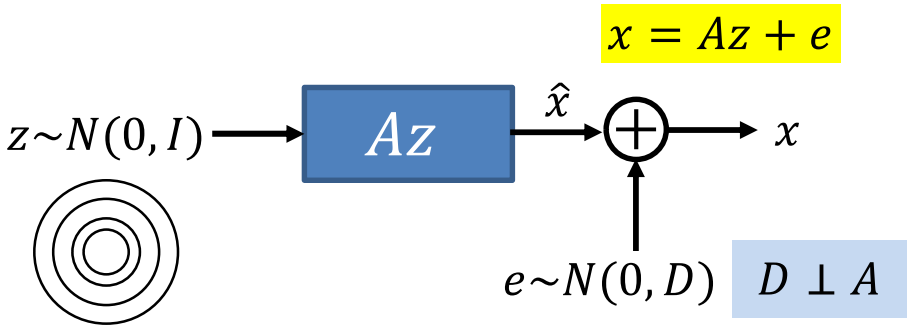
- **PCA models a Gaussian distribution:**

$$\hat{x} = Az \Rightarrow \qquad P(\hat{x}) = N(0, AA^T)$$
$$x = \hat{x} + E \Rightarrow \qquad P(x) = N(0, AA^T + D)$$

- The probability density of x is Gaussian lying mostly close to a hyperplane
  - With correlated structure on the plane
  - And uncorrelated components orthogonal to the plane
- Also

$$P(x|z) = N(Az, D)$$

ML estimation of PCA parameters



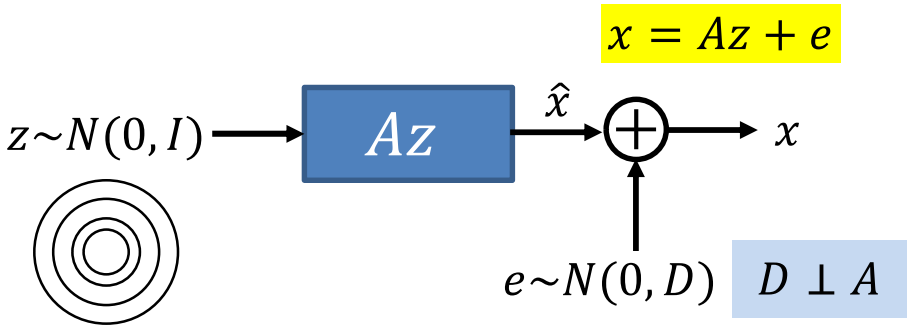
$$P(x) = N(0, AA^T + D)$$

- The parameters of the PCA generative model are A and D
- The ML estimator is

$$\underset{A,D}{\operatorname{argmax}} \sum_{x} \log \frac{1}{\sqrt{(2\pi)^d |AA^T + D|}} \exp(-0.5 x^T (AA^T + D)^{-1} x)$$

  - Where d is the dimensionality of the space
- Combined with the constraints on the number of columns in A (dimensions of principal subspace), and that $A^T D = 0$, this will give us the principal subspace

Missing information for PCA



- There is missing information about the observation X
  - Information about intermediate values drawn in generating X
  - We don't know z
    - Actually we don't know e either, but we'll work without it here and for the rest of this discussion
      - I.e. our notion of "complete" data is still incomplete in reality
      - But having guesses for both A and z is equivalent to knowing e, so it doesn't matter
- If we knew z for each X, estimating A (and D) would be simple

PCA with complete information

$$x = Az + E$$
$$P(x|z) = N(Az, D)$$

- Given complete information $(x_1, z_1), (x_2, z_2), \ldots$
  - Representing $X = [x_1, x_2, \ldots], \; Z = [z_1, z_2, \ldots]$

$$\underset{A,D}{\operatorname{argmax}} \sum_{(x,z)} \log P(x,z) = \underset{A,D}{\operatorname{argmax}} \sum_{(x,z)} \log P(x|z)$$

$$= \underset{A,D}{\operatorname{argmax}} \sum_{(x,z)} \log \frac{1}{\sqrt{(2\pi)^d |D|}} \exp(-0.5(x - Az)^T D^{-1}(x - Az))$$

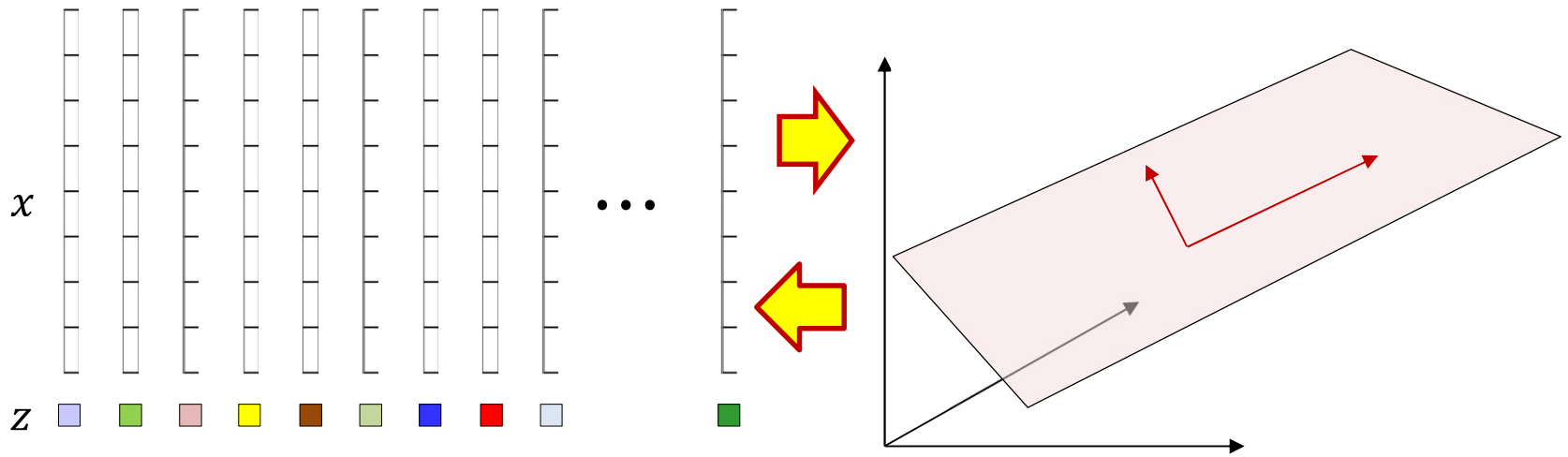
- Differentiating w.r.t A and equating to 0, we get the easy solution

$$A = XZ^+$$

  - (Some sloppy math (D is not invertible), but the solution is right)

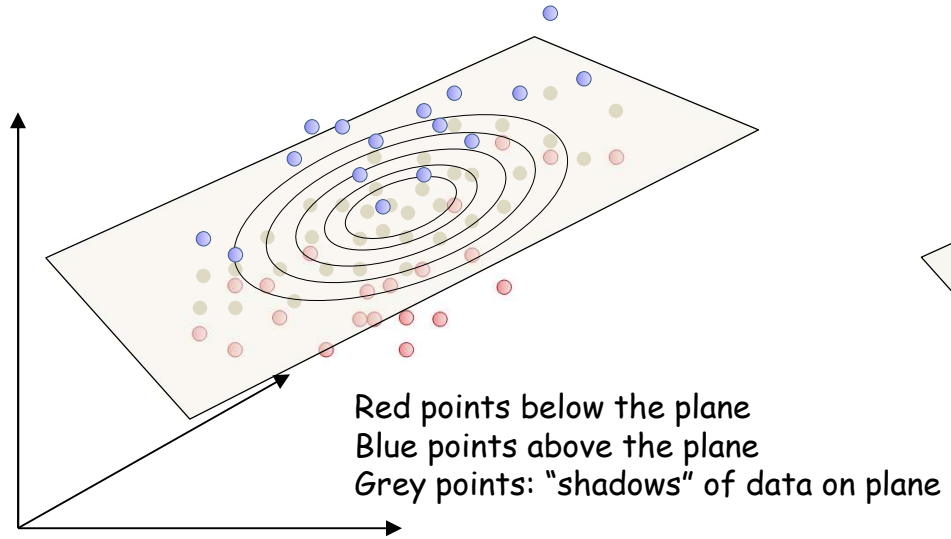
But we don't have z. It is missing

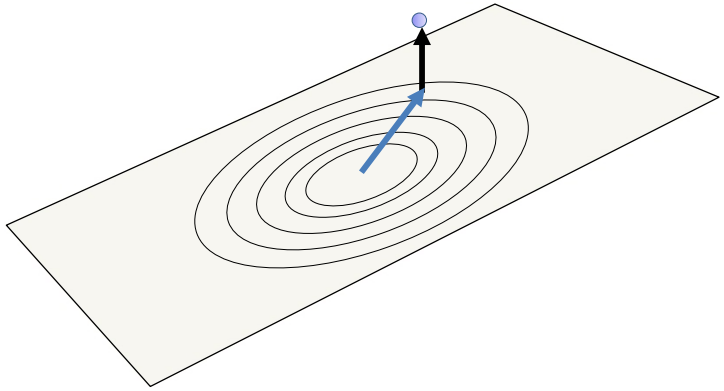
EM for PCA



- Initialize the plane
  - Or rather, the bases for the plane
- "Complete" the data by computing the appropriate zs for the plane
  - $P(z|X;\ A)$ is a delta, because E is orthogonal to A
- Reestimate the plane using the zs
- Iterate

Improving on PCA

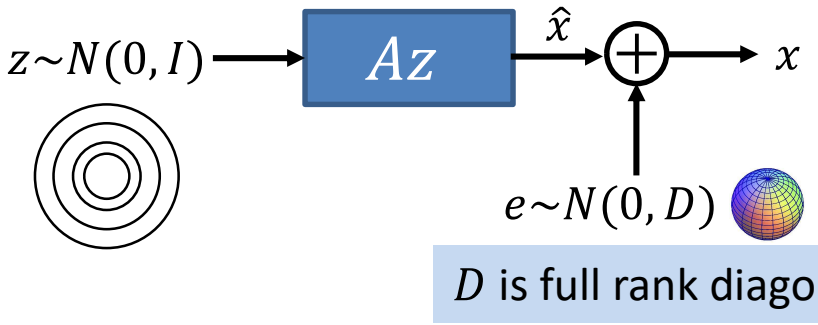


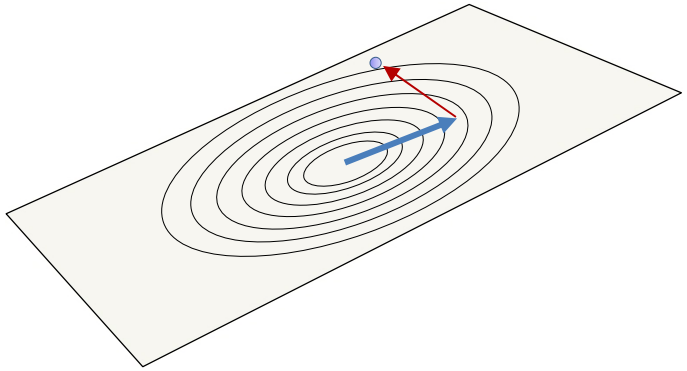


- PCA assumes the noise is always orthogonal to the data
  - Not always true
  - Noise in images can look like images, random noise can sound like speech, etc.
- Lets us generalize the model to permit non-orthogonal noise

The Linear Gaussian Model

$$x = Az + e$$

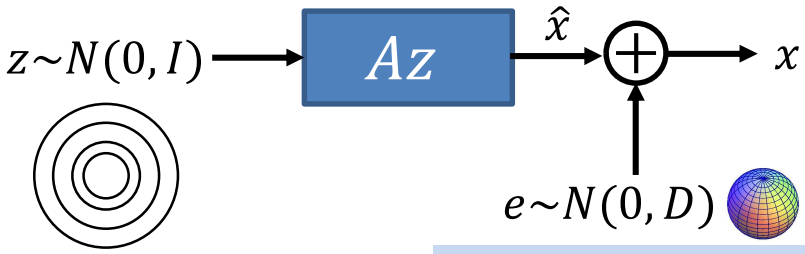




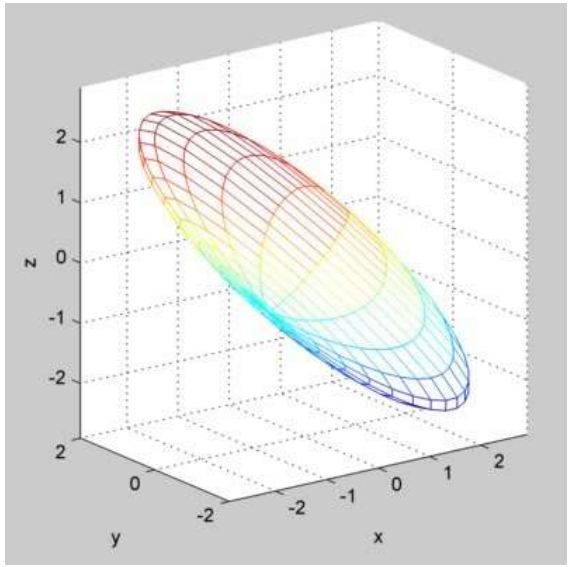
- The noise added to the output of the encoder can lie in *any* direction
  - Uncorrelated, but not just orthogonal to the principal subspace
- Generative model: to generate any point
  - Take a Gaussian step on the hyperplane
  - Add *full-rank* Gaussian uncorrelated noise ***that is independent of the position on the hyperplane***
    - Uncorrelated: diagonal covariance matrix
    - Direction of noise is unconstrained
      - Need not be orthogonal to the plane

The probability distribution modelled by the LGM

$x = Az + e$



D is full rank diagonal



- The noise added to the output of the encoder can lie in *any* direction

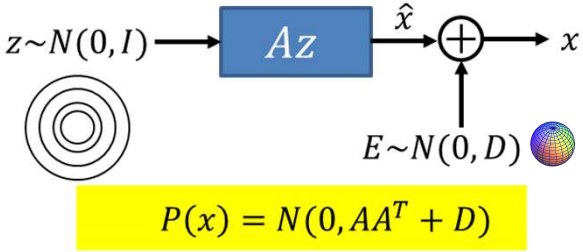
$$\hat{x} = Az \Rightarrow \qquad P(\hat{x}) = N(0, AA^T)$$

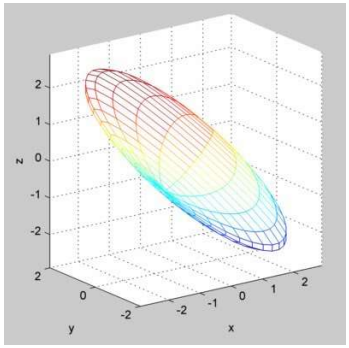
$$x = \hat{x} + E \Rightarrow \qquad P(x) = N(0, AA^T + D)$$

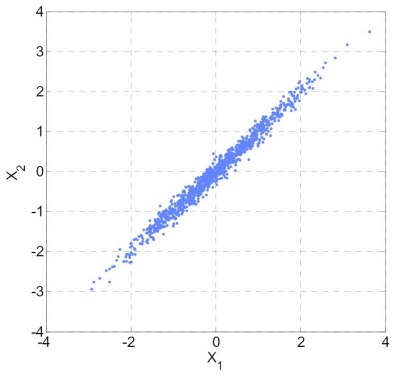
- The probability density of x is Gaussian lying mostly close to a hyperplane
  - With uncorrelated Gaussian
- Also

$$P(x|z) = N(Az, D)$$

The linear Gaussian model



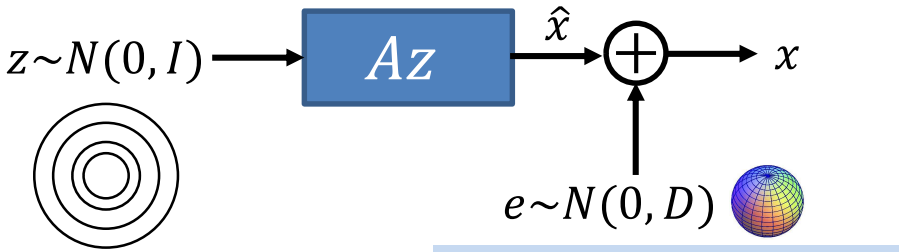




- Is a generative model for Gaussians
- Data distribution are Gaussian lying largely on a hyperplane with some Gaussian "fuzz"
  - Only components on the plane are correlated with one another
    - No correlations off the plane
  - Which allows us to model *some* correlations between components
    - Halfway between a Gaussian with a diagonal covariance, and one with a full covariance

ML estimation of LGM parameters

$$x = Az + e$$



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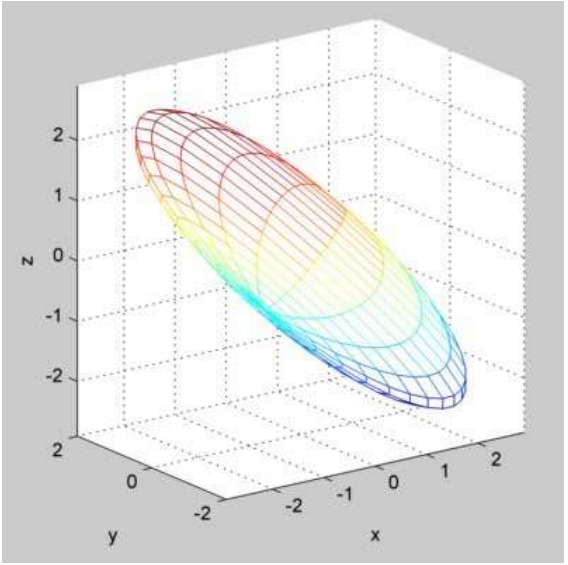


$$P(x) = N(0, AA^T + D)$$

- The parameters of the LGM generative model are A and D
- The ML estimator is

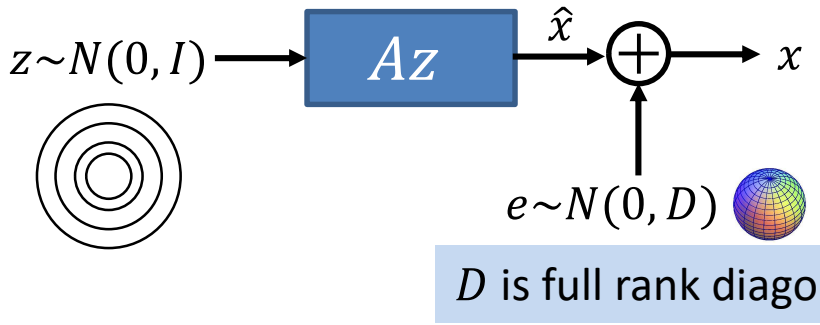
$$\underset{A,D}{\operatorname{argmax}} \sum_x \log \frac{1}{\sqrt{(2\pi)^d |AA^T + D|}} \exp(-0.5 x^T (AA^T + D)^{-1} x)$$

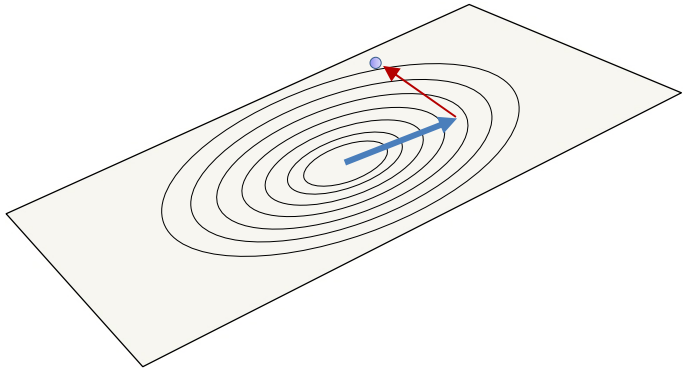
  - Where d is the dimensionality of the space

- As it turns out, this does *not* have a nice closed form solution
  - Because D is full rank

Missing information for LGMs

$$x = Az + e$$





- There is missing information about the observation X
  - Information about intermediate values drawn in generating X
  - We don't know z
- If we knew the z for each X, estimating A (and D) would be very simple

LGM with complete information

$$x = Az + e$$
$$P(x|z) = N(Az, D)$$

- Given complete information $X = [x_1, x_2, \dots]$, $Z = [z_1, z_2, \dots]$

$$\underset{A,D}{\operatorname{argmax}} \sum_{(x,z)} \log P(x,z) = \underset{A,D}{\operatorname{argmax}} \sum_{(x,z)} \log P(x|z)$$

$$= \underset{A,D}{\operatorname{argmax}} \sum_{(x,z)} \log \frac{1}{\sqrt{(2\pi)^d |D|}} \exp(-0.5(x - Az)^T D^{-1}(x - Az))$$

$$= \underset{A,D}{\operatorname{argmax}} \sum_{(x,z)} -\frac{1}{2}\log|D| - 0.5(x - Az)^T D^{-1}(x - Az)$$

- Differentiating w.r.t A and D equating to 0, we get an easy solution

LGM with complete information

$$\underset{A,D}{\operatorname{argmax}} \sum_{(x,z)} -\frac{1}{2}\log|D| - 0.5(x - Az)^T D^{-1}(x - Az)$$

- Differentiating w.r.t A and $D$and equating to 0, we get an easy solution
- Solution for A

$$\nabla_A \sum_{(x,z)} 0.5(x - Az)^T D^{-1}(x - Az) = 0 \quad \Rightarrow$$

$$\sum_{(x,z)} (x - Az)z^T = 0 \quad \Rightarrow \quad A = \left(\sum_{(x,z)} xz^T\right)\left(\sum_{z} zz^T\right)^{-1}$$

- Solution for D

$$\nabla_D \sum_{(x,z)} \frac{1}{2}\log|D| + 0.5(x - Az)^T D^{-1}(x - Az) = 0 \quad \Rightarrow$$

$$D = diag\left(\frac{1}{N}\left(\sum_{x} xx^T - A\sum_{(x,z)} xz^T\right)\right)$$

LGM with complete information

$$\underset{A,D}{\operatorname{argmax}} \sum_{(x,z)} -\frac{1}{2}\log|D| - 0.5(x - Az)^T D^{-1}(x - Az)$$

- Differentiating w.r.t A and $D$and equating to 0, we get an easy solution
- Solution for A

$$\nabla_A \sum_{(x,z)} 0.5(x - Az)^T D^{-1}(x - Az) = 0 \quad \Rightarrow$$

$$\sum_{(x,z)} (x - Az)z^T = 0 \quad \Rightarrow \quad A = \left(\sum_{(x,z)} xz^T\right)\left(\sum_{z} zz^T\right)^{-1}$$

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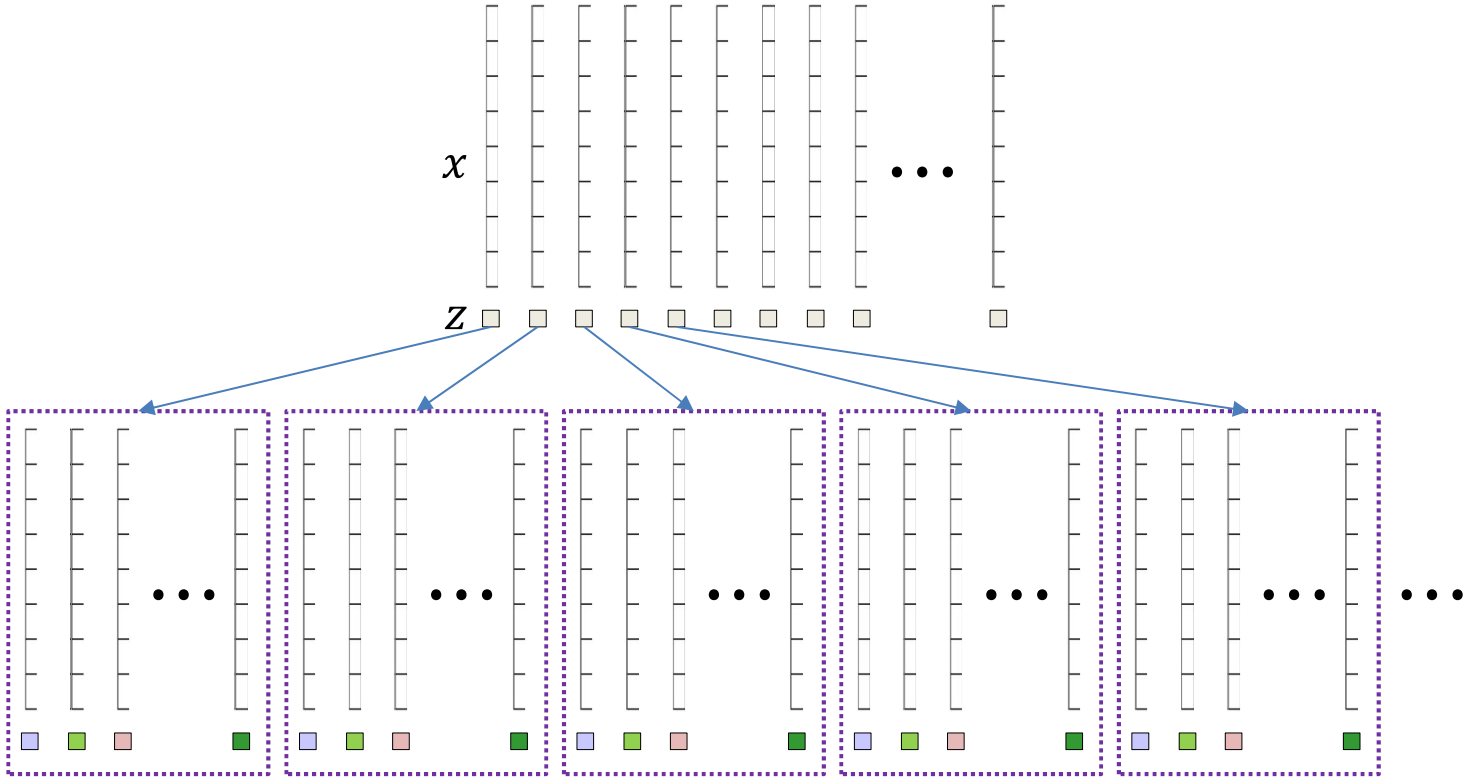
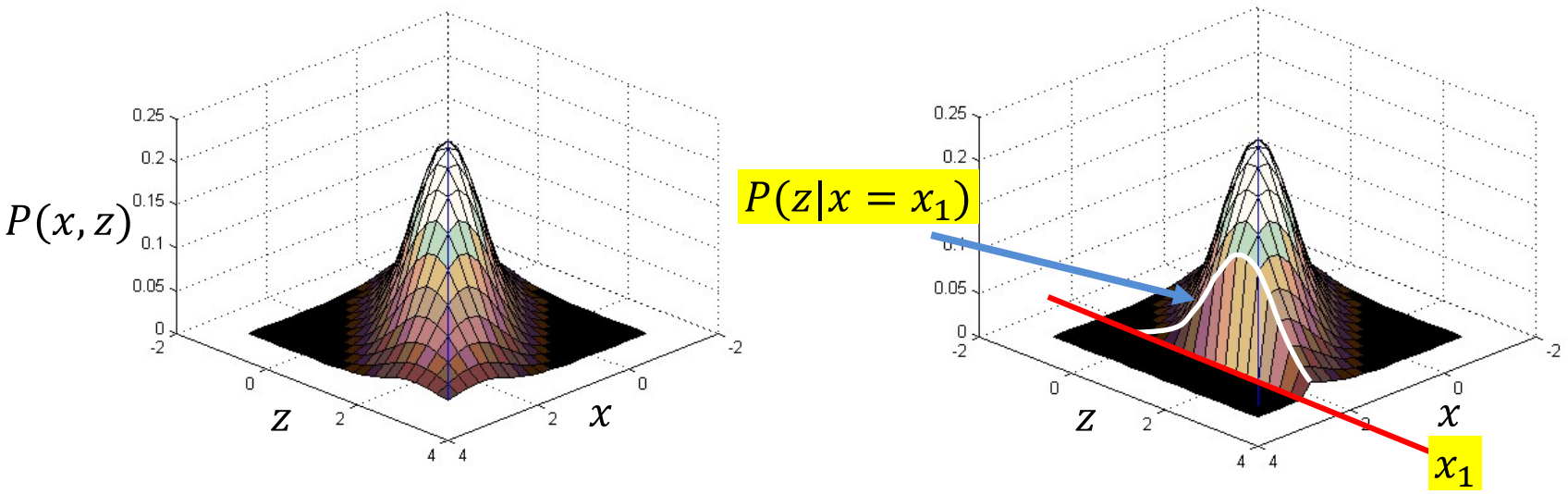
Unfortunately we do not observe z.
It is missing; the observations are incomplete

Expectation Maximization for LGM



- *Complete* the data
- Option 1:
  - In *every possible way* proportional to $P(z|x)$
  - Compute the solution from the completed data

The posterior $P(z|x)$

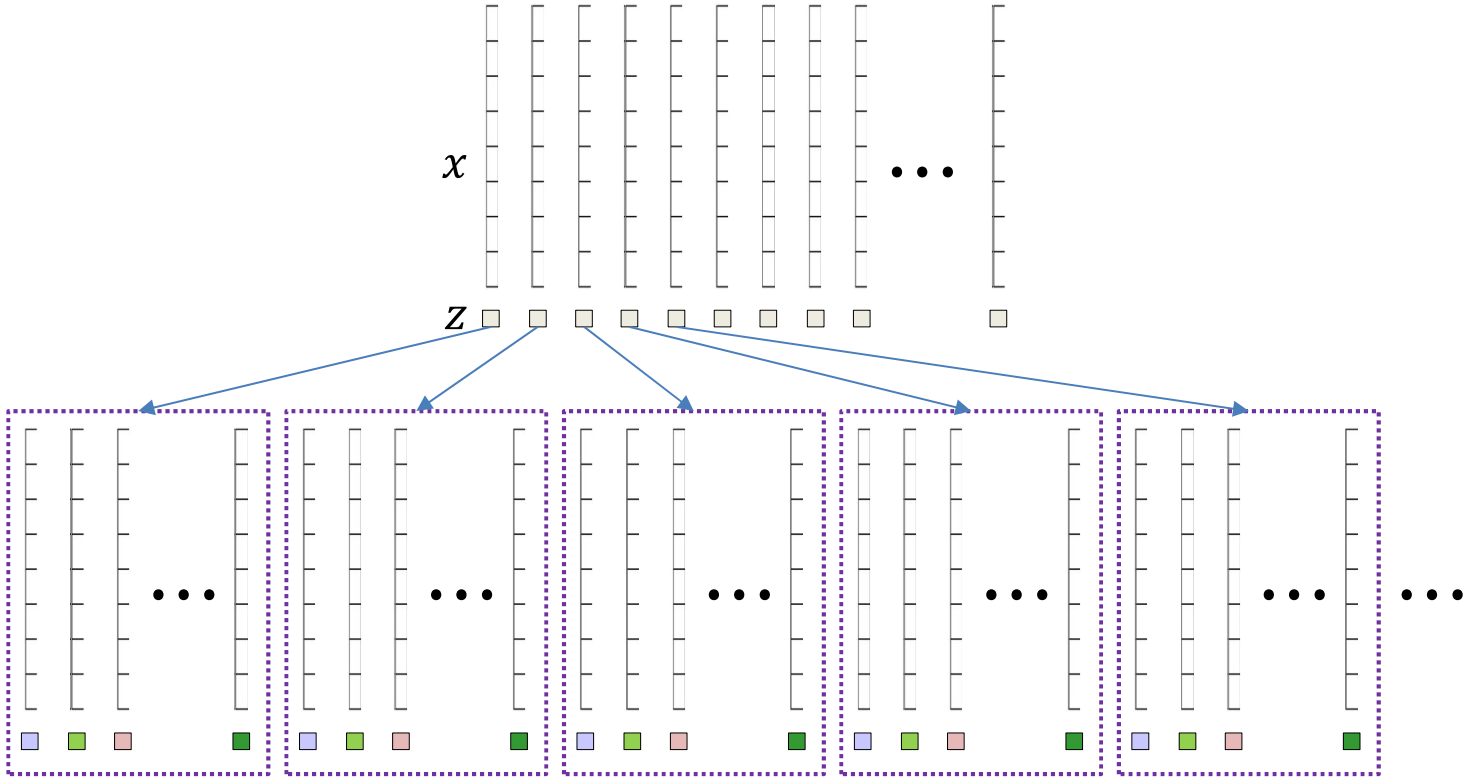


- $P(x)$ is Gaussian
  - We saw this
- The *joint* distribution of x and z is also Gaussian
  - Trust me
- The *conditional* distribution of z given x is also Gaussian

$$P(z|x) = N(z; A^T(AA^T + D)^{-1}x, I - A^T(AA^T + D)^{-1}A)$$

  - Trust me

Expectation Maximization for LGM



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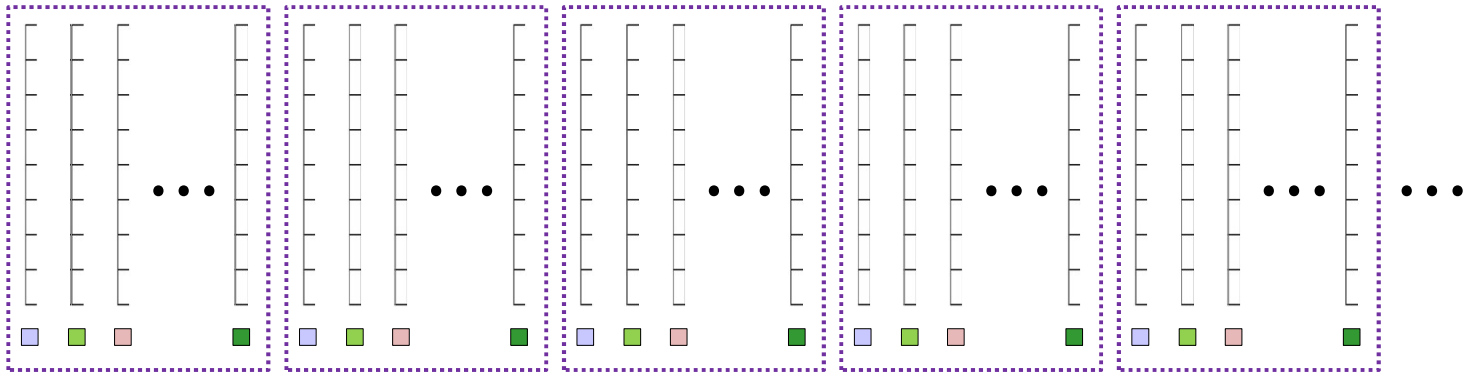
Expectation Maximization for LGM



- *Complete* the data in *every possible way* proportional to $P(z|x)$
  - Compute the solution from the completed data
  - $\underset{A,D}{\text{argmax}} \sum_{(x,z)} -\frac{1}{2}\log|D| - 0.5(x - Az)^T D^{-1}(x - Az)$
- The z values for each x are distributed according to $P(z|x)$. Segregating the summation by x

$$\underset{A,D}{\text{argmax}} \sum_{x} \int_{-\infty}^{\infty} p(z|x) \left(-\frac{1}{2}\log|D| - 0.5(x - Az)^T D^{-1}(x - Az) \right) dz$$

LGM with incomplete information

$$\underset{A,D}{\operatorname{argmax}} \sum_x \int_{-\infty}^{\infty} p(z|x) \left(-\frac{1}{2} \log|D| - 0.5(x - Az)^T D^{-1} (x - Az) \right) dz$$

- Differentiating w.r.t A and $D$and equating to 0, we get an easy solution
- Solution for A

$$\nabla_A \sum_x \int_{-\infty}^{\infty} p(z|x)(x - Az)^T D^{-1}(x - Az) dz = 0 \quad \Rightarrow$$

$$\sum_x \int_{-\infty}^{\infty} p(z|x)(x - Az) z^T dz = 0 \quad \Rightarrow \quad A = \left(\sum_x \int_{-\infty}^{\infty} p(z|x) x z^T dz \right) \left(\sum_x \int_{-\infty}^{\infty} p(z|x) z z^T dz \right)^{-1}$$

- Solution for D

$$\nabla_D \left(N \log|D| + \sum_x \int_{-\infty}^{\infty} p(z|x)(x - Az)^T D^{-1}(x - Az) dz \right) = 0 \quad \Rightarrow$$

$$D = diag\left(\frac{1}{N} \left(\sum_x x x^T - A \sum_x \int_{-\infty}^{\infty} p(z|x) x z^T dz \right) \right)$$

These are closed form solutions, the details of which are not relevant to us.

Key: All terms integrate over *all possible completion of incomplete observations*, where the proportionality attached to any completion of x is P(z|x)

LGM with incomplete information

- It is actually an iterative algorithm (EM):
- Solution for A

$$A^{k+1} = \left(\sum_x \int_{-\infty}^{\infty} p\left(z|x; A^k, D^k\right) x z^T dz\right)\left(\sum_x \int_{-\infty}^{\infty} p\left(z|x; A^k, D^k\right) z z^T dz\right)^{-1}$$

- Solution for D

$$D = diag\left(\frac{1}{N}\left(\sum_x x x^T - A \sum_x \int_{-\infty}^{\infty} p\left(z|x; A^k, D^k\right) x z^T dz\right)\right)$$

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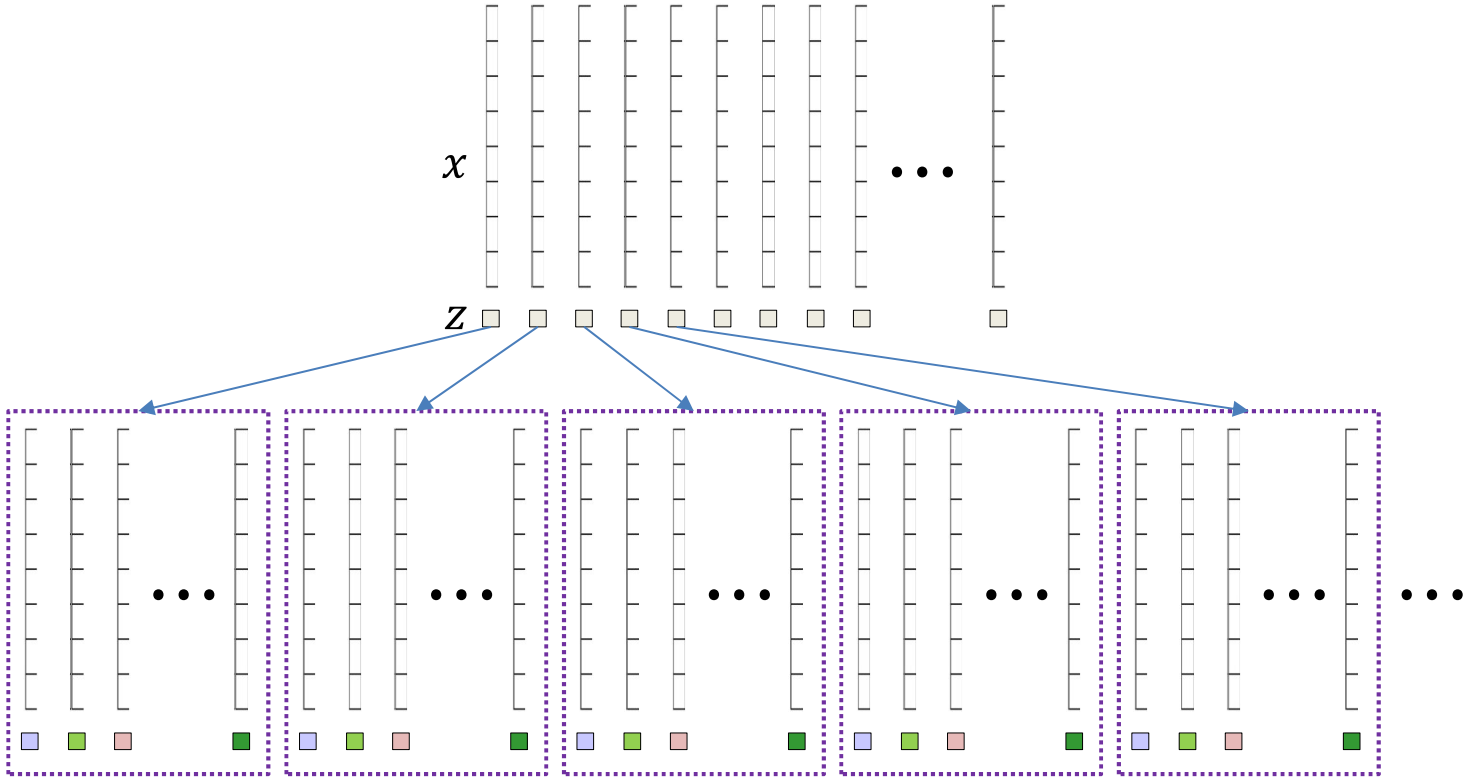
Expectation Maximization for LGM



- *Complete* the data

$$P(z|x) = N(z; A^T(AA^T + D)^{-1}x, I - A^T(AA^T + D)^{-1}A)$$

- Option 2:
  - ***By drawing samples from*** $P(z|x)$
  - Compute the solution from the completed data

LGM from drawn samples

- Since we now have a collection of *complete vectors,* we can use the usual complete-data formulae
- Solution for A

$$A^{k+1} = \left(\sum_{(x,z)} xz^T\right)\left(\sum_{z} zz^T\right)^{-1}$$

- Solution for D

$$A^{k+1} = diag\left(\frac{1}{N}\left(\sum_{x} xx^T - A^k \sum_{(x,z)} xz^T\right)\right)$$

These are closed form solutions

Draw missing components from P(z|x; A^k, D^k) to *complete the data*

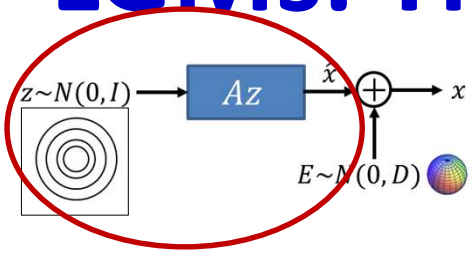
Estimate parameters from completed data

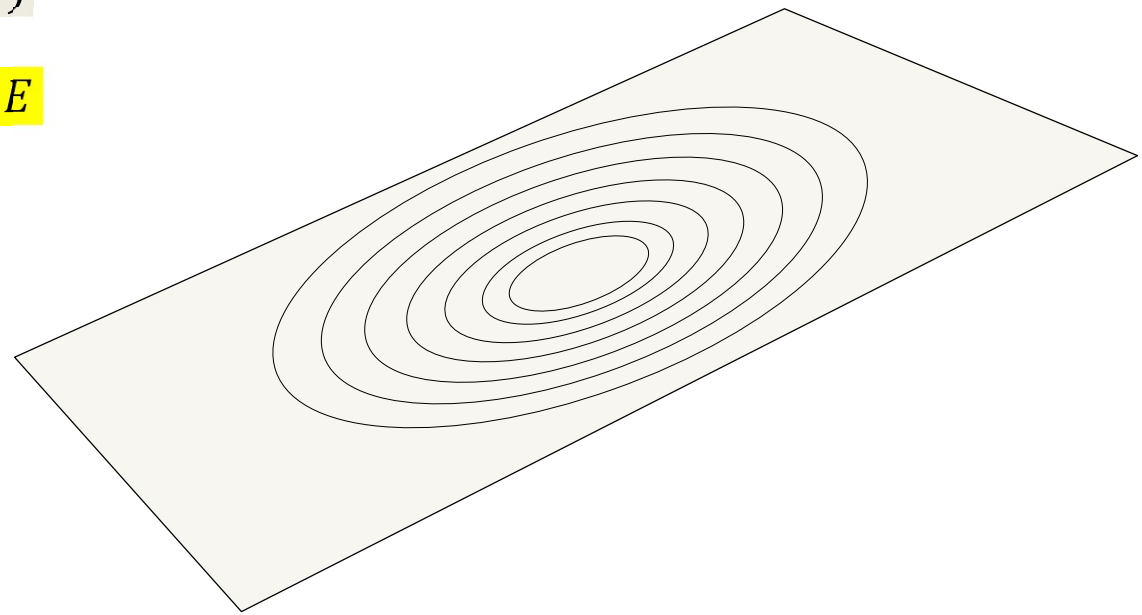
LGMs: The intuition

$z \sim N(0, I)$

$E \sim N(0, D)$

$x = Az + E$





- The linear transform stretches and rotates the K-dimensional input space onto a K-dimensional hyperplane in the data space
- The isotropic Gaussian in the input space becomes a stretched and rotated Gaussian on the hyperplane

LGMs: The intuition

$z \sim N(0, I)$

$E \sim N(0, D)$

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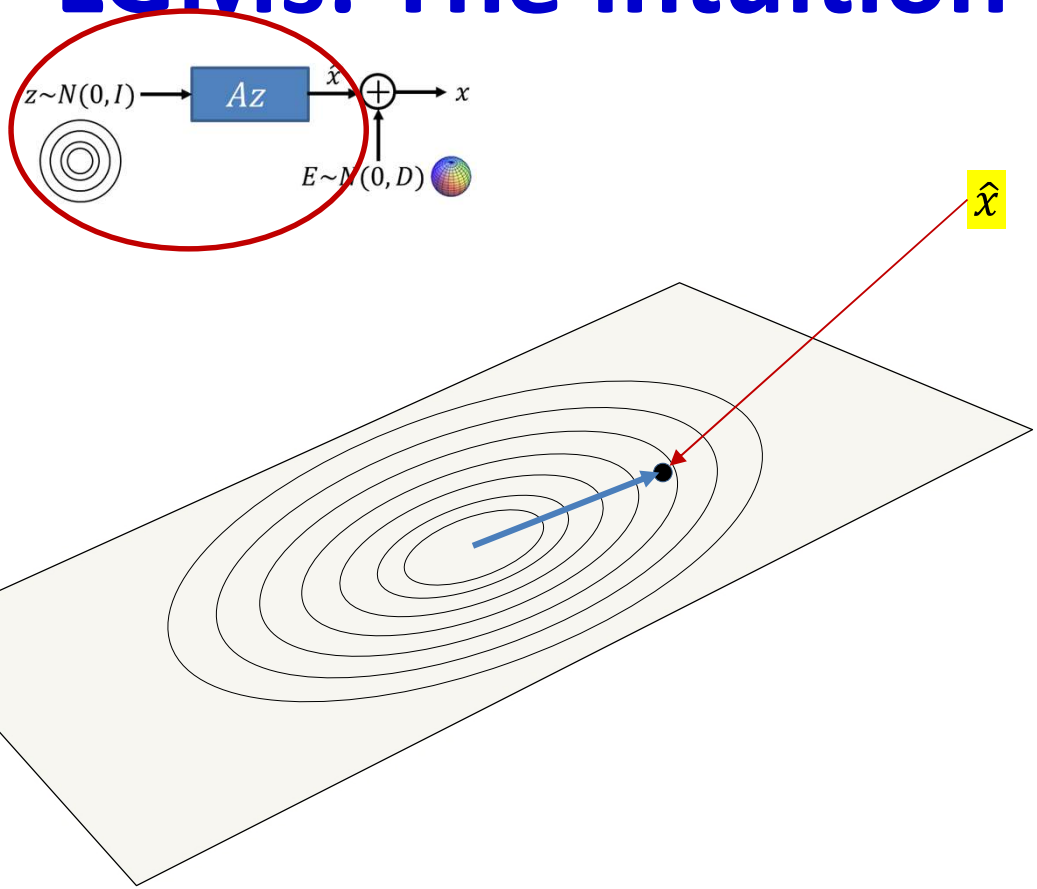

- Drawing samples: The first step places the z somewhere on the plane described by A
  - The distribution of points on the plane is also Gaussian

LGMs: The intuition

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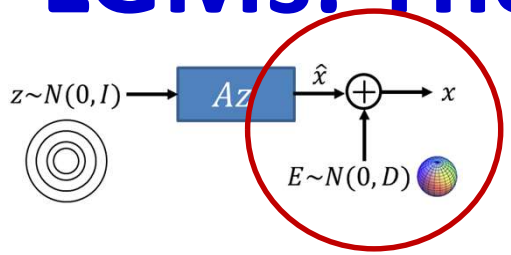
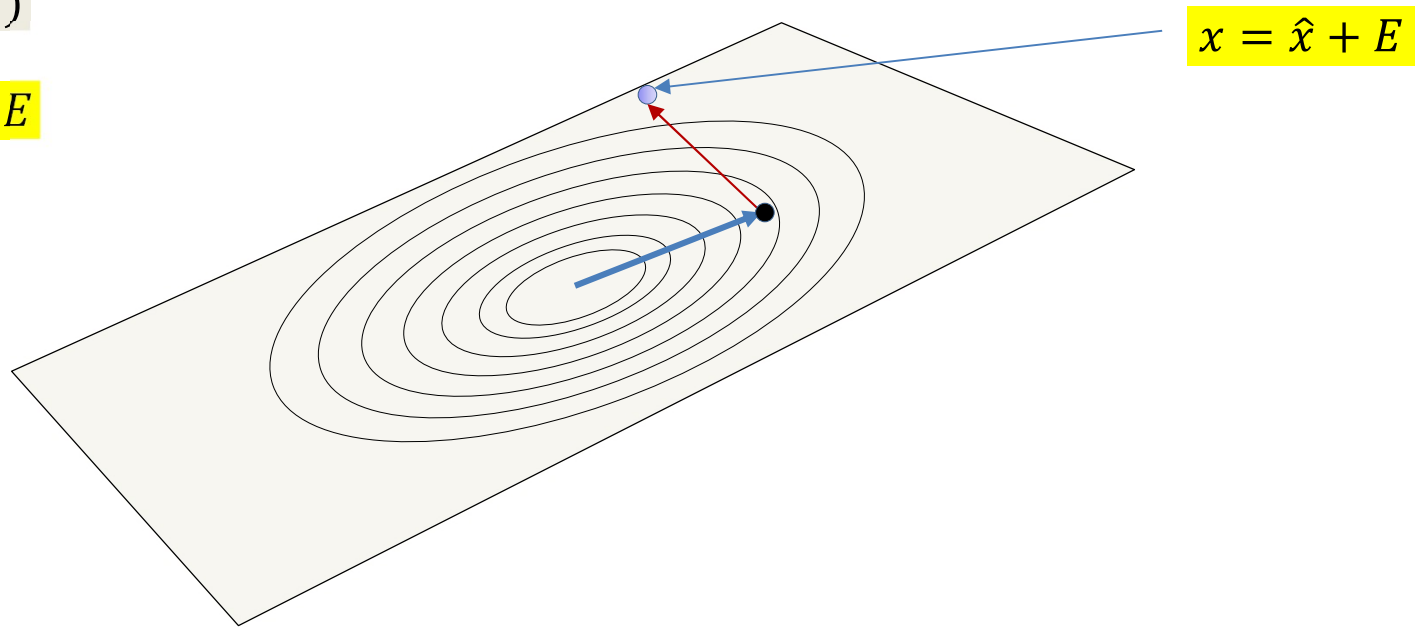




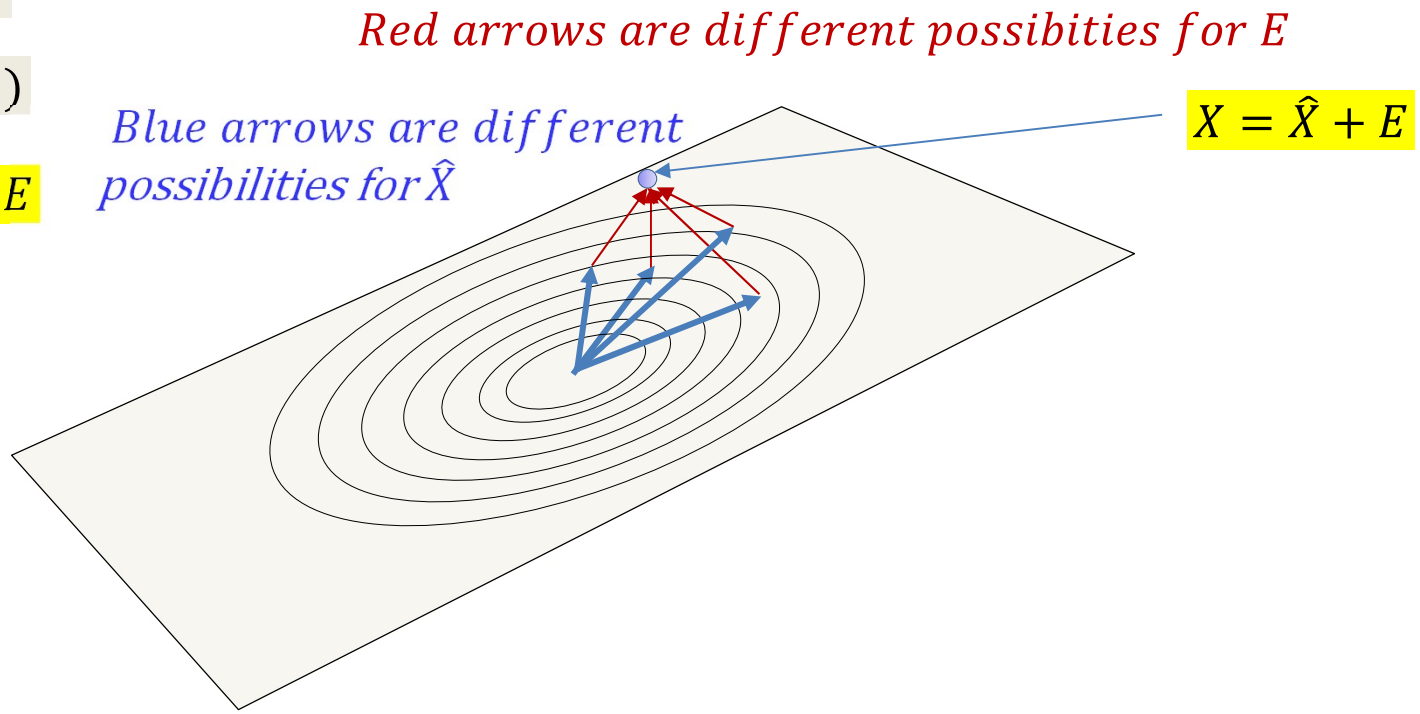
- LGM model: The first step places the z somewhere on the plane described by A
  - The distribution of points on the plane is also Gaussian
- Second step: Add Gaussian noise to produce points that aren't necessarily on the plane
  - Noise added is not revealed

EM for LGMs: The intuition

$z \sim N(0, I)$

$E \sim N(0, D)$

$X = Az + E$



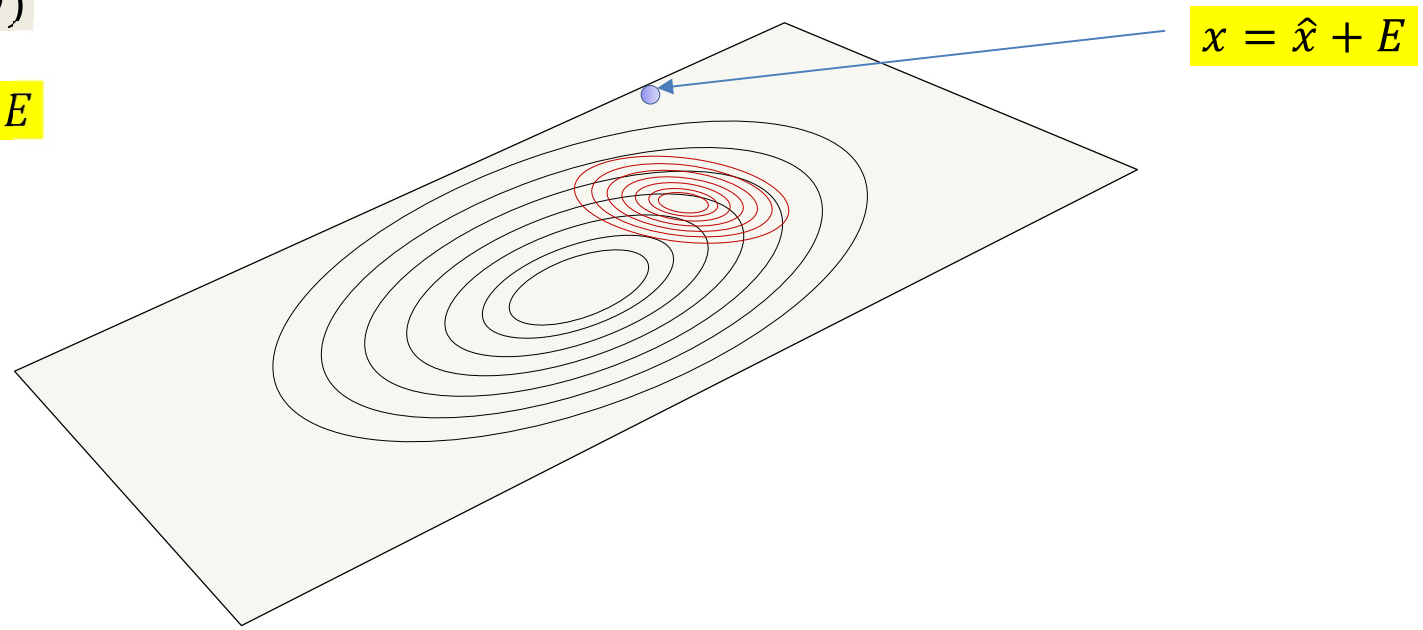
- In an LGM the way to produce any data instance is not unique
- Conversely, given only the data point, the "shadow" on the principal plane cannot be uniquely known

EM Solution

$z \sim N(0, I)$

$E \sim N(0, D)$

$x = Az + E$



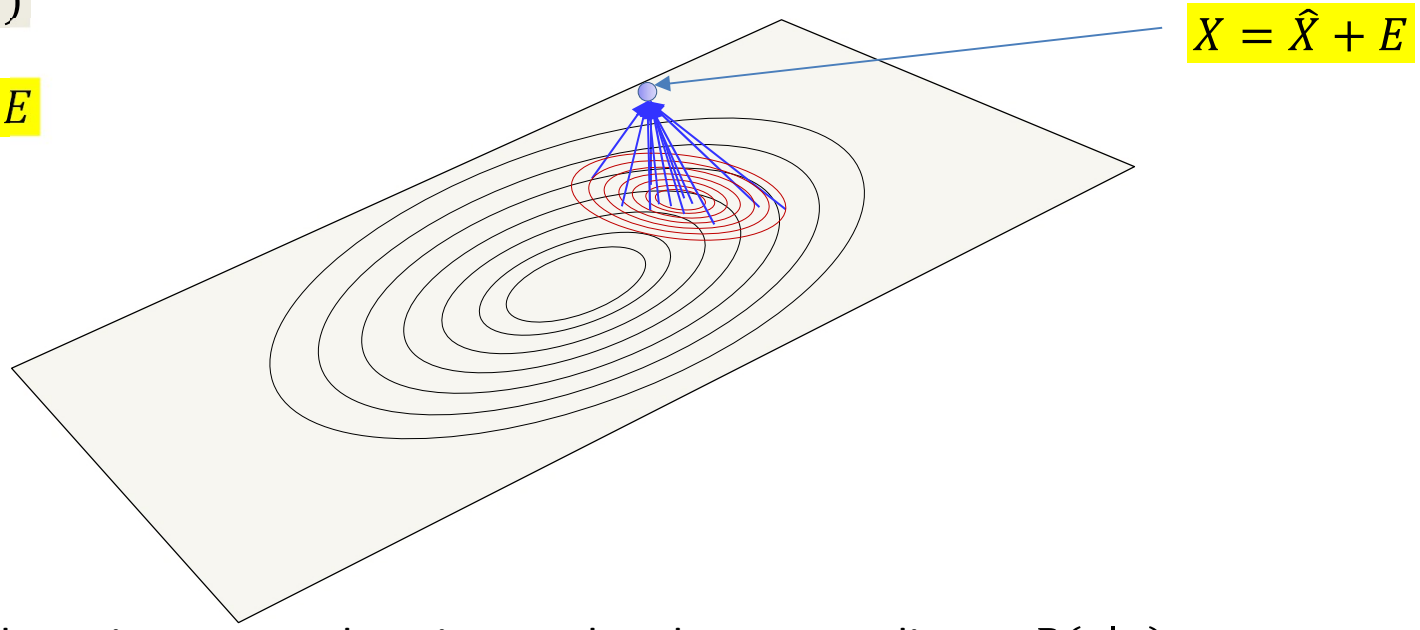
- The posterior probability $P(z|x)$ gives you the location of all the points on the plane that *could* have generated x and their probabilities

EM Solution

$z \sim N(0, I)$

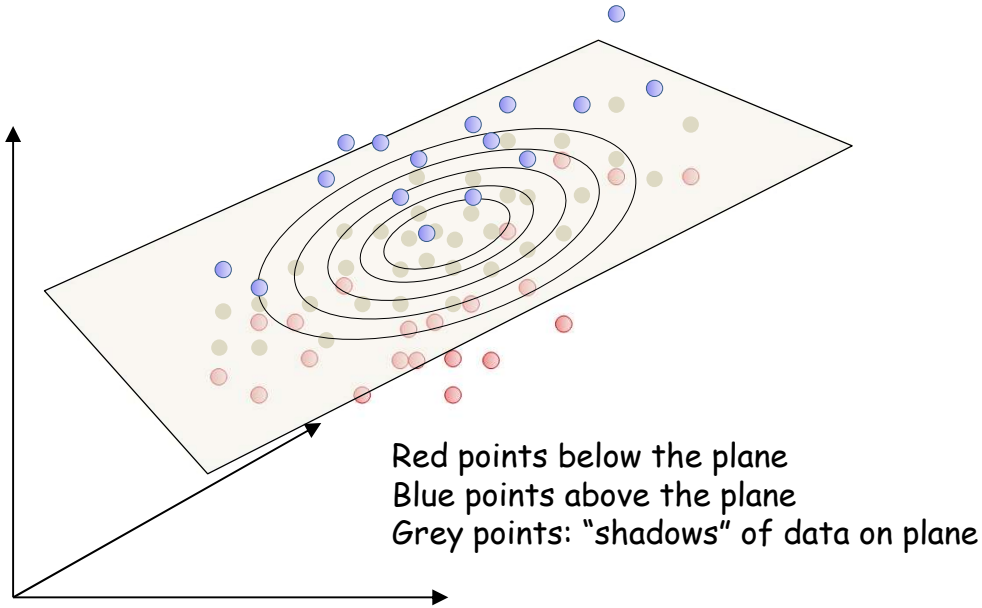
$E \sim N(0, D)$

$X = Az + E$



- Attach the point to *every* location on the plane, according to $P(z|x)$
  - Or to a sample of points on the plane drawn from $P(z|x)$
- There will be more attachments where $P(z|x)$ is higher, and fewer where it is lower

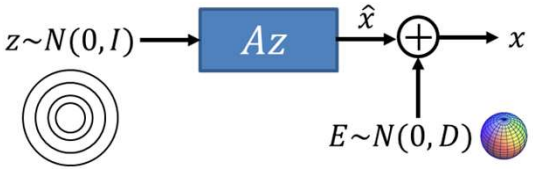
EM Solution

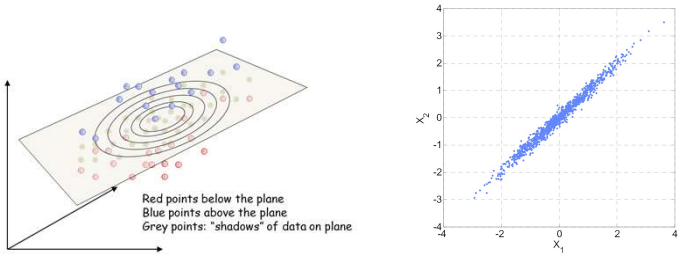


- Attach *every* training point in this manner
- Let the plane rotate and stretch until the total tension (sum squared length) of all the attachments is minimize
- Repeat attachment and rotation until convergence…

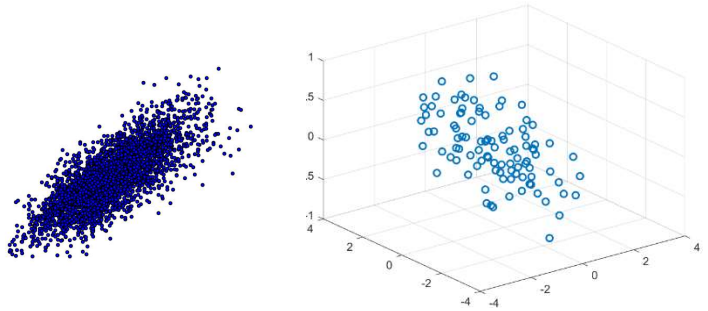
Summarizing LGMs

- LGMs are models for *Gaussian* distributions
- Specifically, they model the distribution of data as Gaussian, where most of the variation is along a *linear* manifold
  - They do this by transforming a Gaussian RV z through a linear transform $f(z) = Az$ that transforms the K-dim input space of z into a K-dimensional hyperplane (linear manifold) in the data space



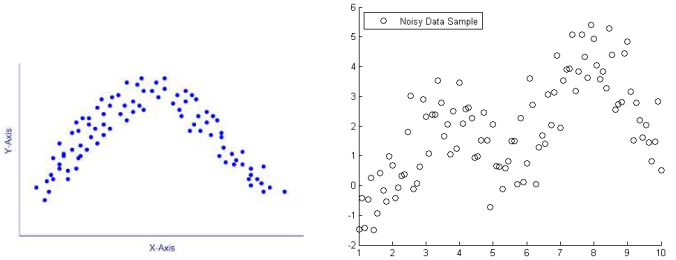


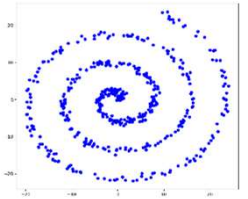
- They are excellent models for data that actually fit these assumptions
  - Often, we can simply assume that data lie near linear manifolds and model them with LGMs
  - PCA, an instance of LGMs, is very popular

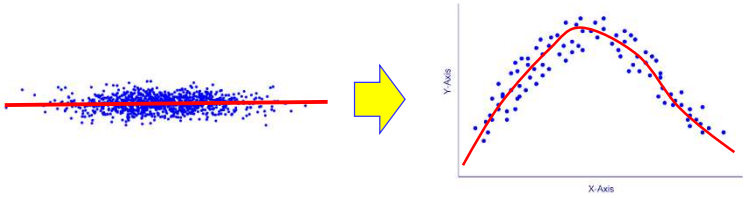


Where LGMs fail

- What about data that are not Gaussian distributed close to a plane
  - The distributions lie close to a curved or otherwise non-linear manifold?
- You can model these as Gaussian data centered on a plane that has been *warped into the observed shape*

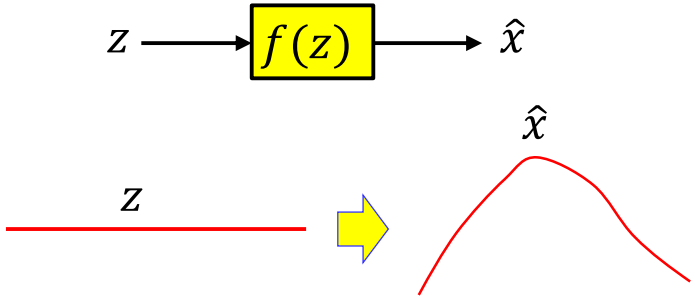






NLGMs

- **Step1:** Find a function that warps a lower-dimensional input plane to the target manifold in the data space
  - The non-linear version of the linear transform in the LGM



NLGMs

- **Step1:** Find a function that warps a lower-dimensional input plane to the target manifold in the data space
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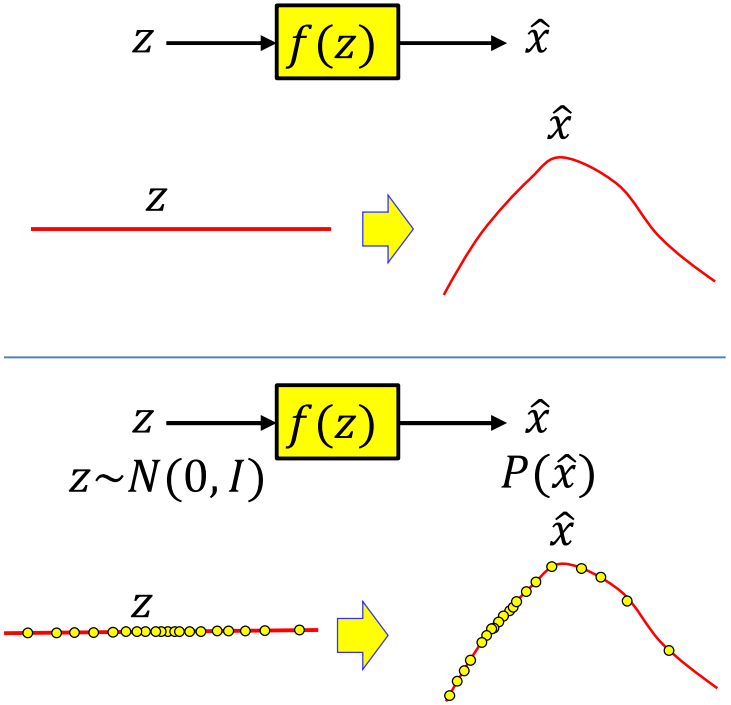
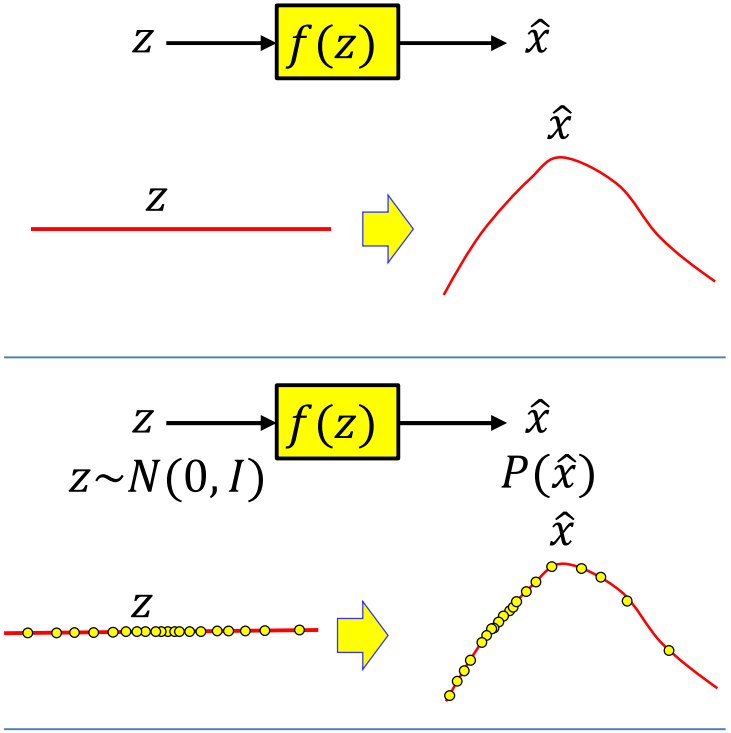
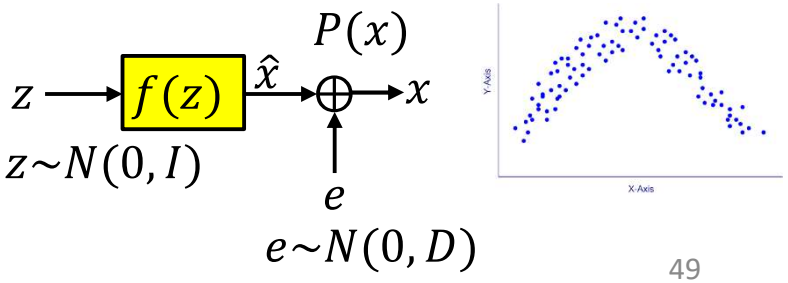
- **Step2:** Transform a Gaussian distribution on the input plane to a distribution on the curved manifold



NLGMs

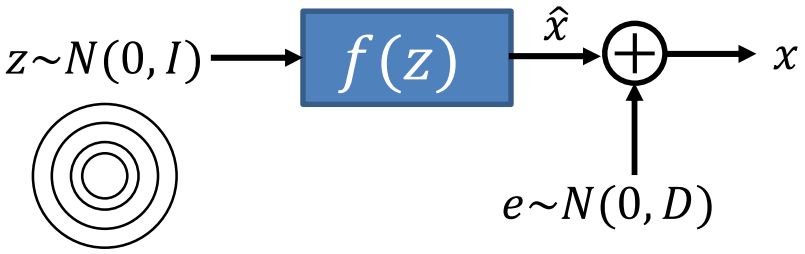
- **Step1:** Find a function that warps a lower-dimensional input plane to the target manifold in the data space
  - The non-linear version of the linear transform in the LGM
- **Step2:** Transform a Gaussian distribution on the input plane to a distribution on the curved manifold
- **Step3:** Add some uncorrelated Gaussian "fuzz" to account for off-manifold variations





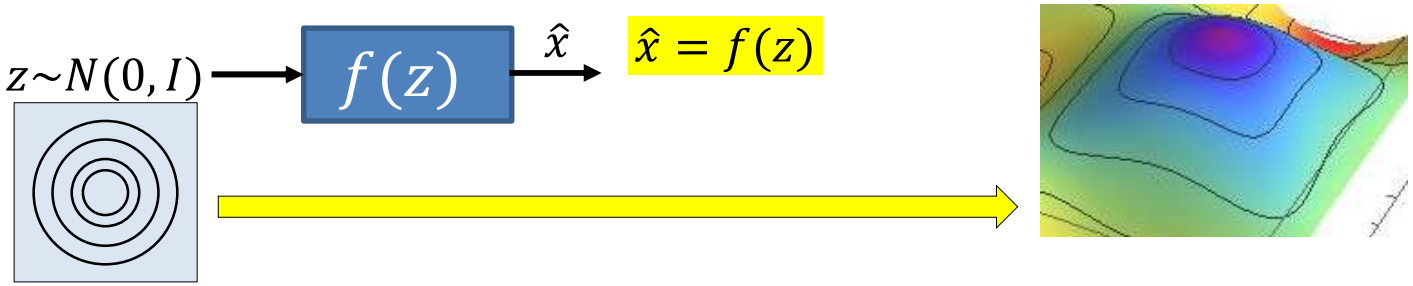
NLGMs

$$x = f(z) + e$$



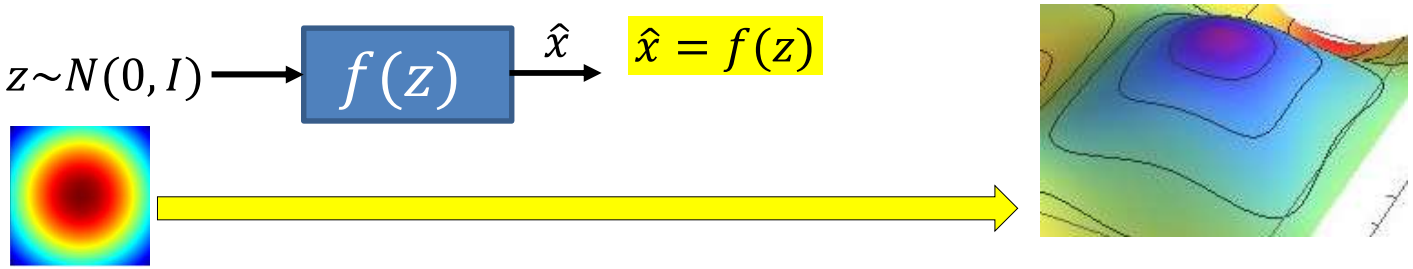
- The *non-linear* Gaussian model
- $f(z)$ is a *non-linear function* that produces a curved manifold
  - Like the decoder of a non-linear AE
- The samples of z are placed on this curved manifold
- The actual data are produced by adding noise to samples on the manifold

NLGMs



- The non-linear function warps the input space into a curved manifold in the data space

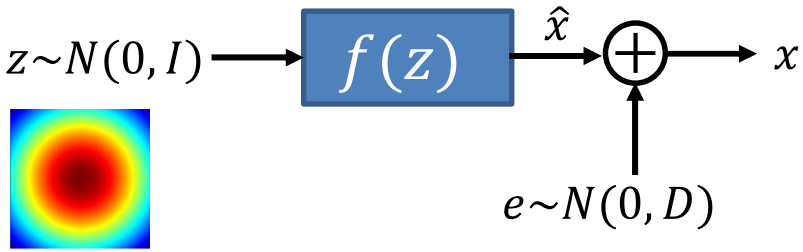
NLGMs

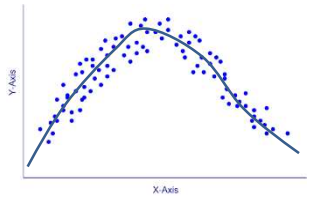


- The non-linear function warps the input space into a curved manifold in the data space
  - Samples drawn from z are placed on this manifold
  - The distribution of $\hat{x}$ on the manifold will follow the distribution of z
    - High-density regions of $\hat{x}$ correspond to high-density regions of z

NLGMs

$$x = f(z) + e$$





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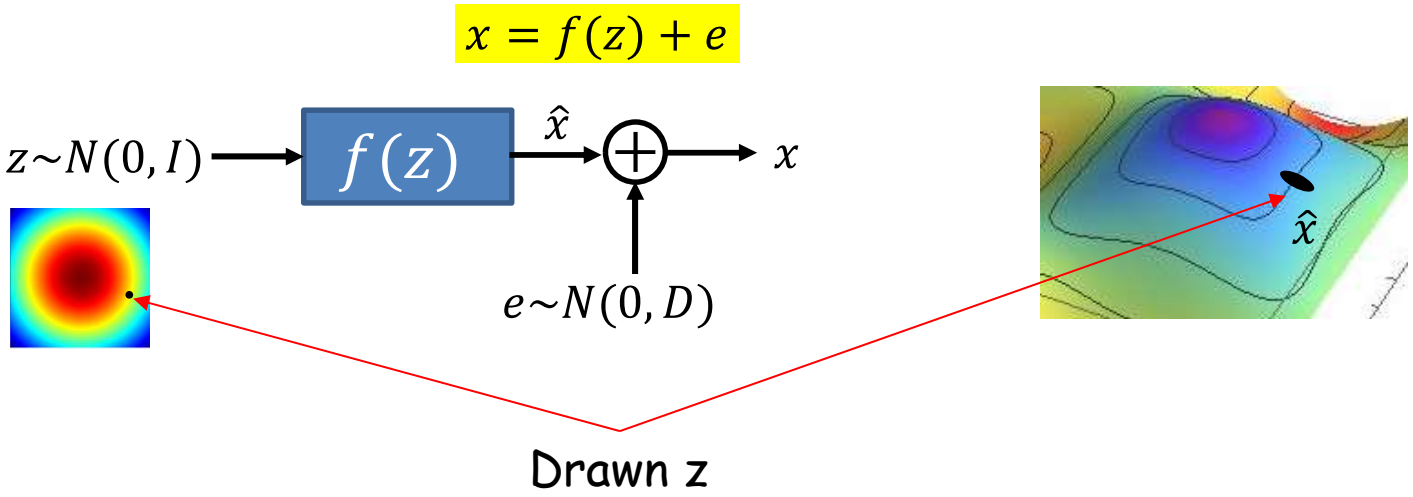
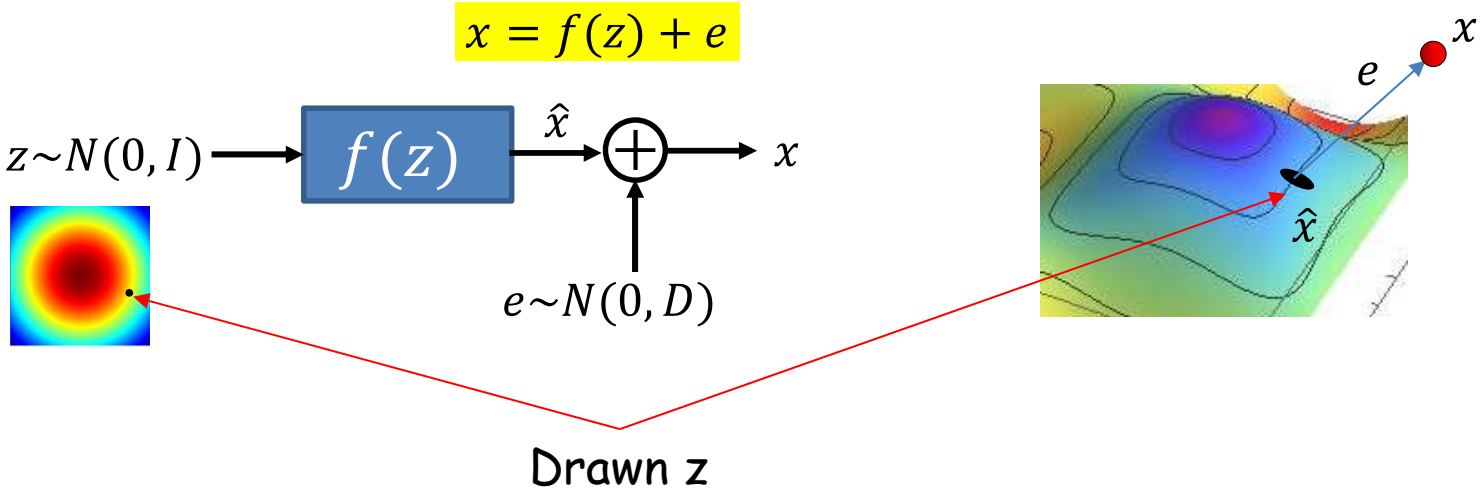
  - The distribution of $\hat{x}$ on the manifold will follow the distribution of z
    - High-density regions of $\hat{x}$ correspond to high-density regions of z
- The final observations are obtained by adding uncorrelated full-dimensional Gaussian noise to the samples

NLGM Generating Process



- Generating process:
  - Draw a sample z from a Uniform Gaussian
  - Transform z by $f(z)$
    - This places z on the curved manifold

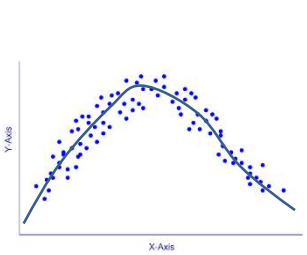
NLGMs Generating Process

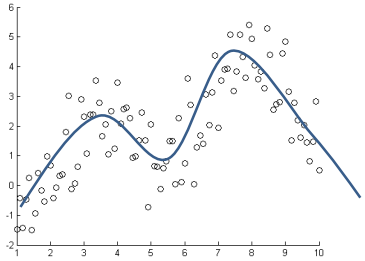


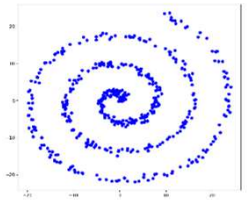
- Generating process: Draw a sample z from a Uniform Gaussian
  - Draw a sample z from a Uniform Gaussian
  - Transform z by $f(z)$
    - This places z on the curved manifold
  - Add uncorrelated Gaussian noise to get the final observation

NLGMs

$$x = f(z) + e$$

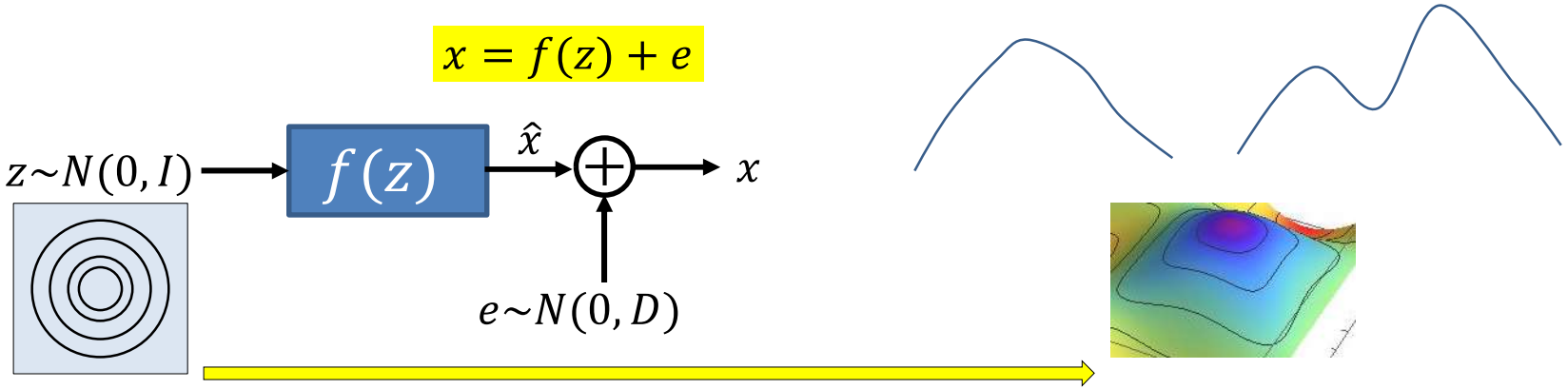






- The NLGM can model very complicated distributions
  - Distributions that may be viewed as lying close to a curved K-dimensional surface in the data space
    - Or even a linear surface: $f(z) = Az$ is a special case
    - K is the dimensionality of z

NLGMs



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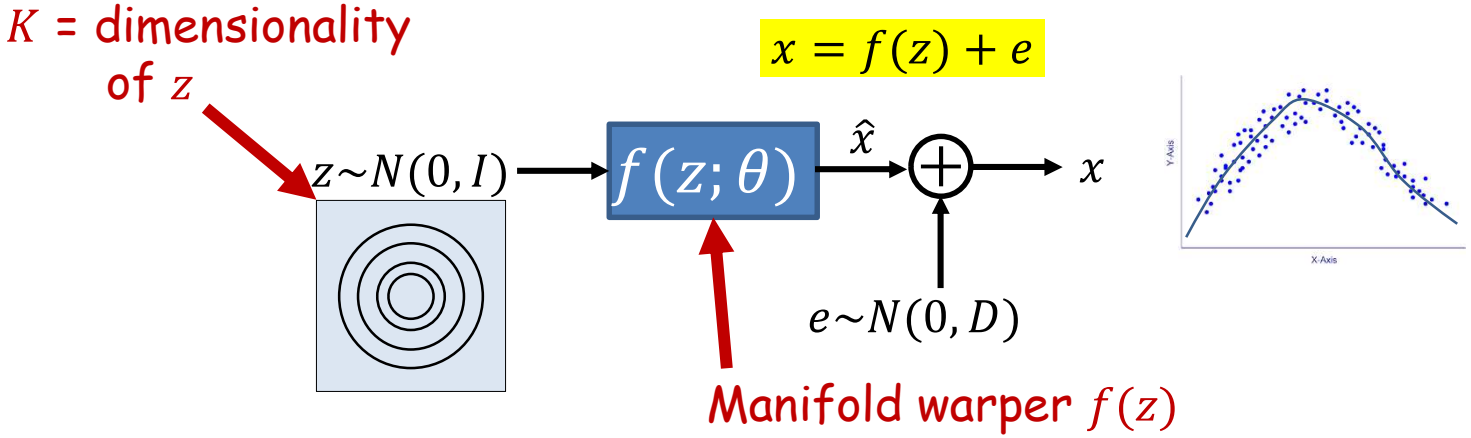
  - Distributions that may be viewed as lying close to a curved K-dimensional surface in the data space
    - Or even a linear surface: $f(z) = Az$ is a special case
    - K is the dimensionality of z

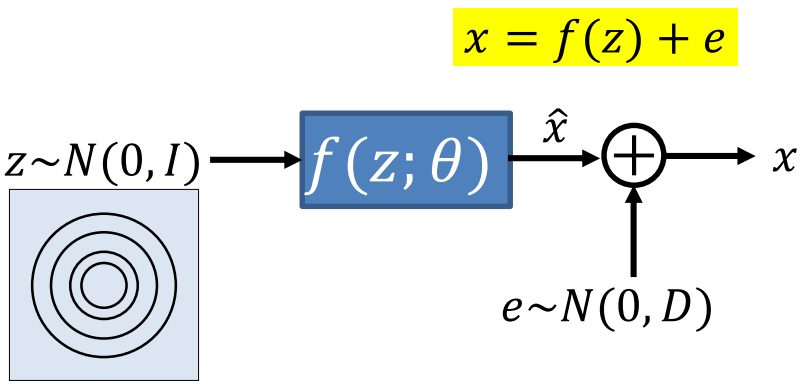
- Key requirement:
  - Identifying the dimensionality K of the curved manifold
  - Having a function $f(z)$ that can transform the (linear) K-dimensional input space (space of z) to the desired K-dimensional manifold in the data space

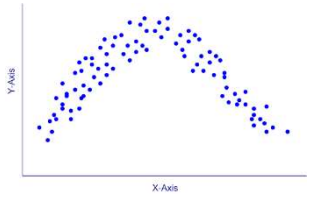
Designing NLGMs



- Key design issues:
  - Select (or guess) the dimensionality of the manifold
    - This is the dimensionality of z
  - Choosing the right function $f(z)$ that is capable of *learning* the shape of the manifold
    - We will choose a Neural Network $f(z; \theta)$

Learning the NLGM

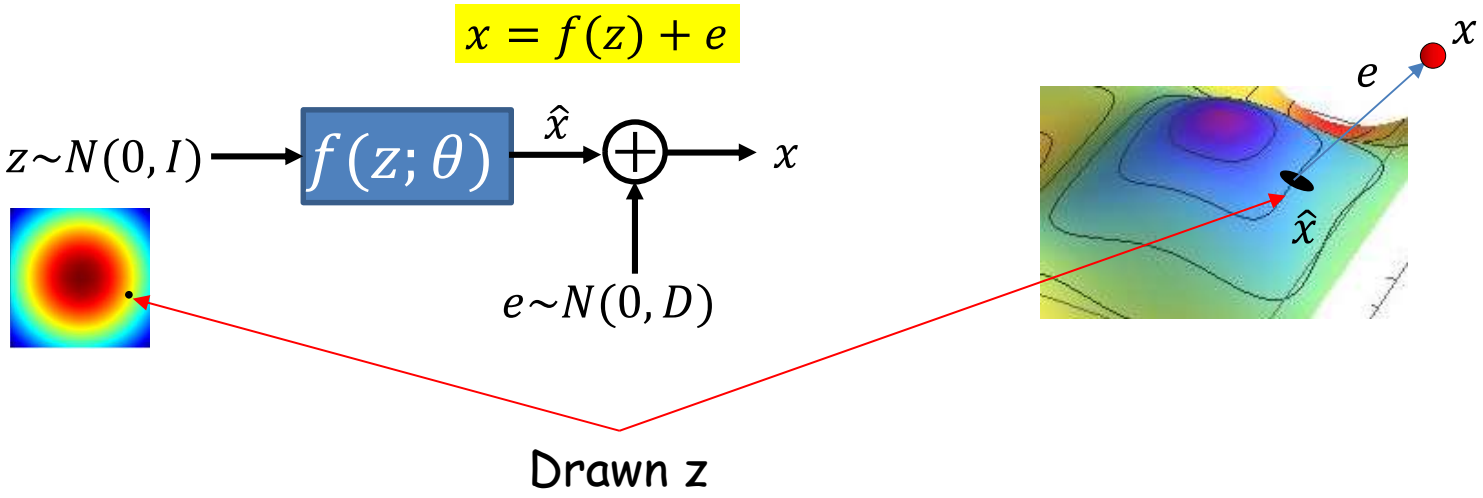




P(x)

- Given a collection of training data $X = \{x\}$
  - Estimate the parameters θ of $f(z;\theta)$
  - Estimate D
- The NLGM is a generative model that actually models a distribution
  - The distribution obtained when $N(0, I)$ is transformed by $f(z)$
- We will use ML estimation to learn its parameters to best match the training data

Probabilities modelled by the NLGM



- The conditional probability of x given z

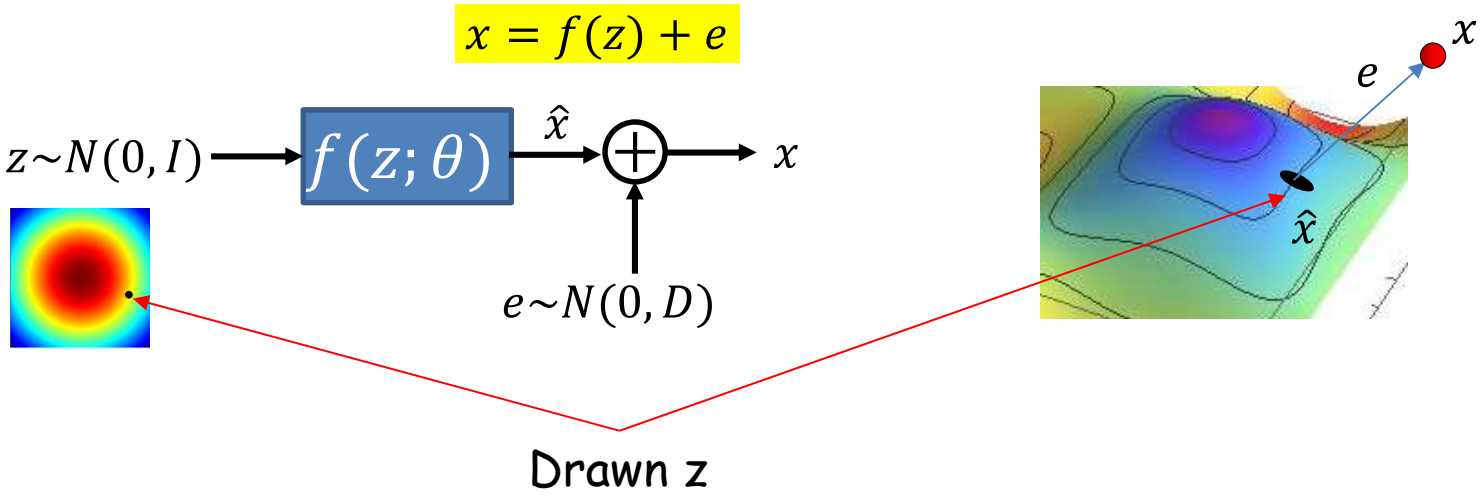
$$P(x|z) = N(x;\ f(z;\theta), D)$$

- The marginal probability of x

$$P(x) = \int_{-\infty}^{\infty} P(x|z)P(z)dz = \int_{-\infty}^{\infty} N(x;\ f(z;\theta), D)\ N(z;0,D)\ dz$$

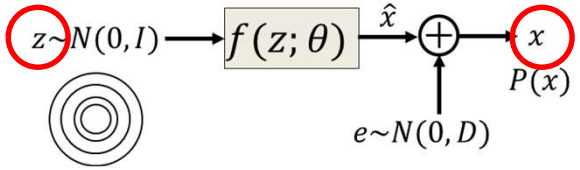
  - For most nonlinear functions $f(z;\theta)$ this math is not tractable, and we cannot get a closed form for $P(x)$
  - ***That won't prevent us from being able to estimate θ and D***

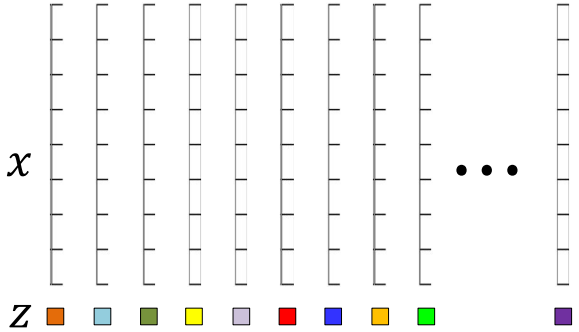
Learning the NLGM with *complete data*



- Drawing a sample from the NLGM is a two-step process
  - First a z is drawn
    - And transformed
  - Then an e is drawn
    - And added
- The complete data to describe any draw are the outcomes of every stage of the drawing process, i.e. (x, z)
  - Actually (x, e, z), but as before, we can work without e

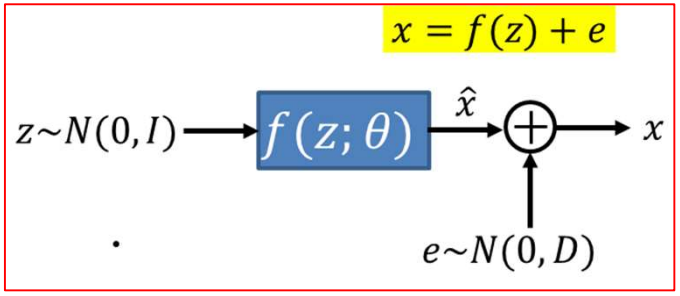
NLGM with complete data





- Let us first consider a *glass-box* process that gives us *complete* data
  - The output and the intermediate steps of the generation process
  - I.e. both the x and the z for every draw
- We will derive estimation rules for the model parameters using the complete data

ML estimation with complete information



$$x = f(z;\theta) + e$$
$$P(x|z) = N(f(z;\theta), D)$$

- Given complete information $X = [x_1, x_2, \dots]$, $Z = [z_1, z_2, \dots]$

$$\theta^*, D^* = \underset{\theta,D}{\operatorname{argmax}} \sum_{(x,z)} \log P(x,z) = \underset{\theta,D}{\operatorname{argmax}} \sum_{(x,z)} \log P(x|z)$$

$$= \underset{\theta,D}{\operatorname{argmax}} \sum_{(x,z)} \log \frac{1}{\sqrt{(2\pi)^d |D|}} \exp(-0.5(x - f(z;\theta))^T D^{-1} (x - f(z;\theta)))$$

$$= \underset{\theta,D}{\operatorname{argmax}} \sum_{(x,z)} -\frac{1}{2}\log|D| - 0.5(x - f(z;\theta))^T D^{-1} (x - f(z;\theta))$$

NLGM with complete information

$$\theta^*, D^* = \underset{\theta, D}{\operatorname{argmax}} \sum_{(x,z)} -\frac{1}{2}\log|D| - 0.5(x - f(z;\theta))^T D^{-1}(x - f(z;\theta))$$

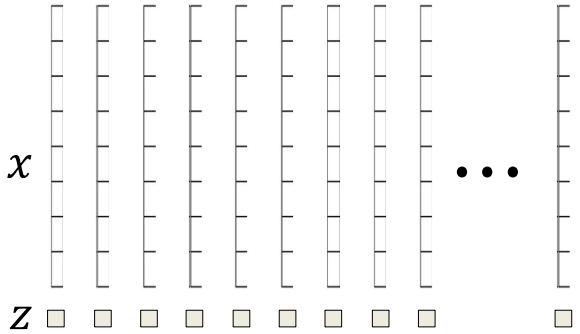
- There isn't a nice closed form solution, but we could learn the parameters using backpropagation, which minimizes the following loss

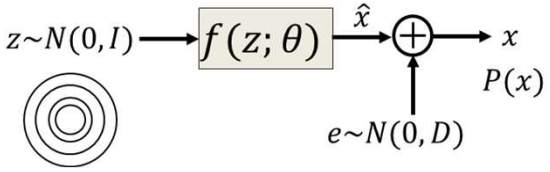
$$L(\theta, D) = \sum_{(x,z)} \frac{1}{2}\log|D| + 0.5(x - f(z;\theta))^T D^{-1}(x - f(z;\theta))$$

$$\theta^*, D^* = \underset{\theta, D}{\operatorname{argmin}}\, L(\theta, D)$$

Unfortunately we do not observe z.
It is missing; the observations are incomplete

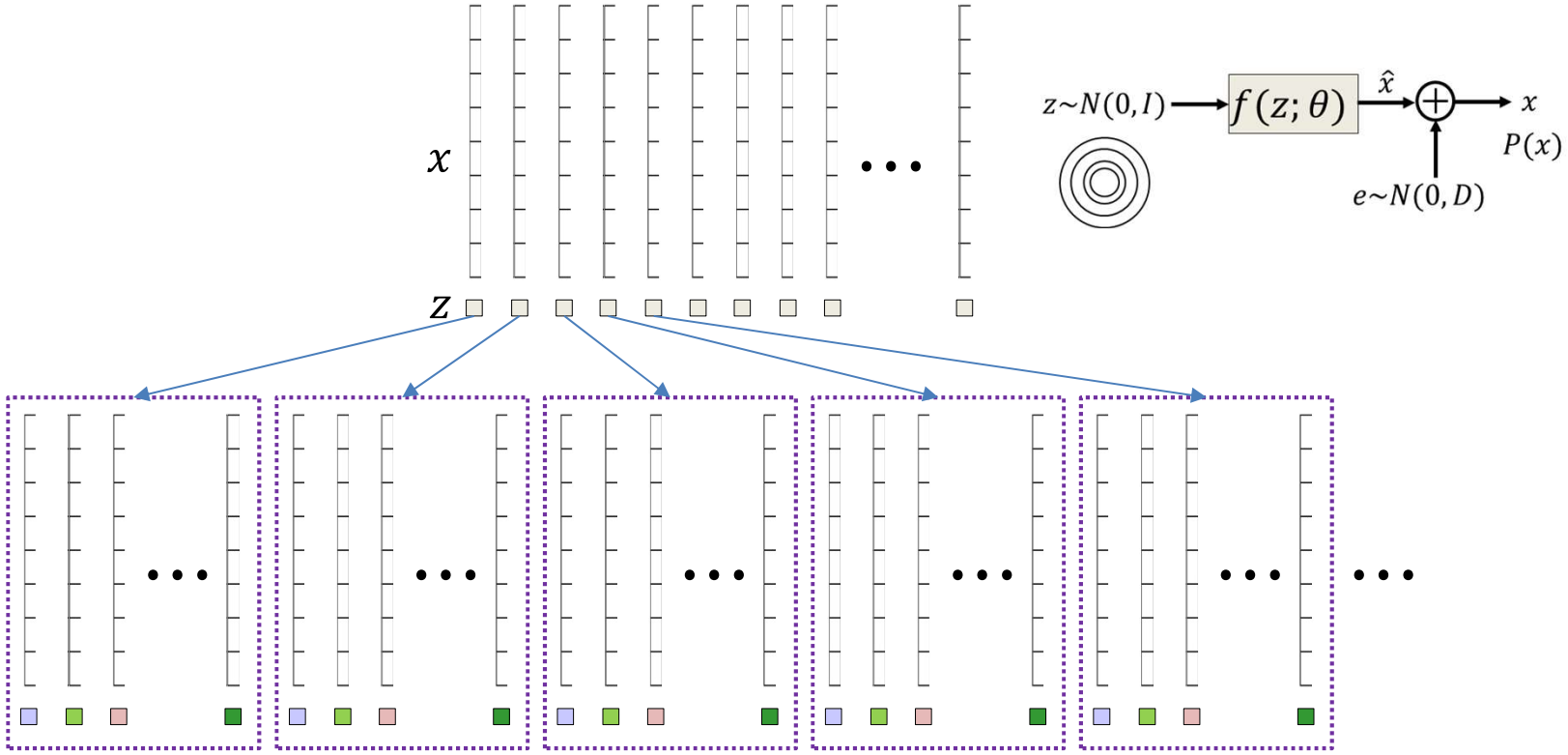
NLGM with incomplete data





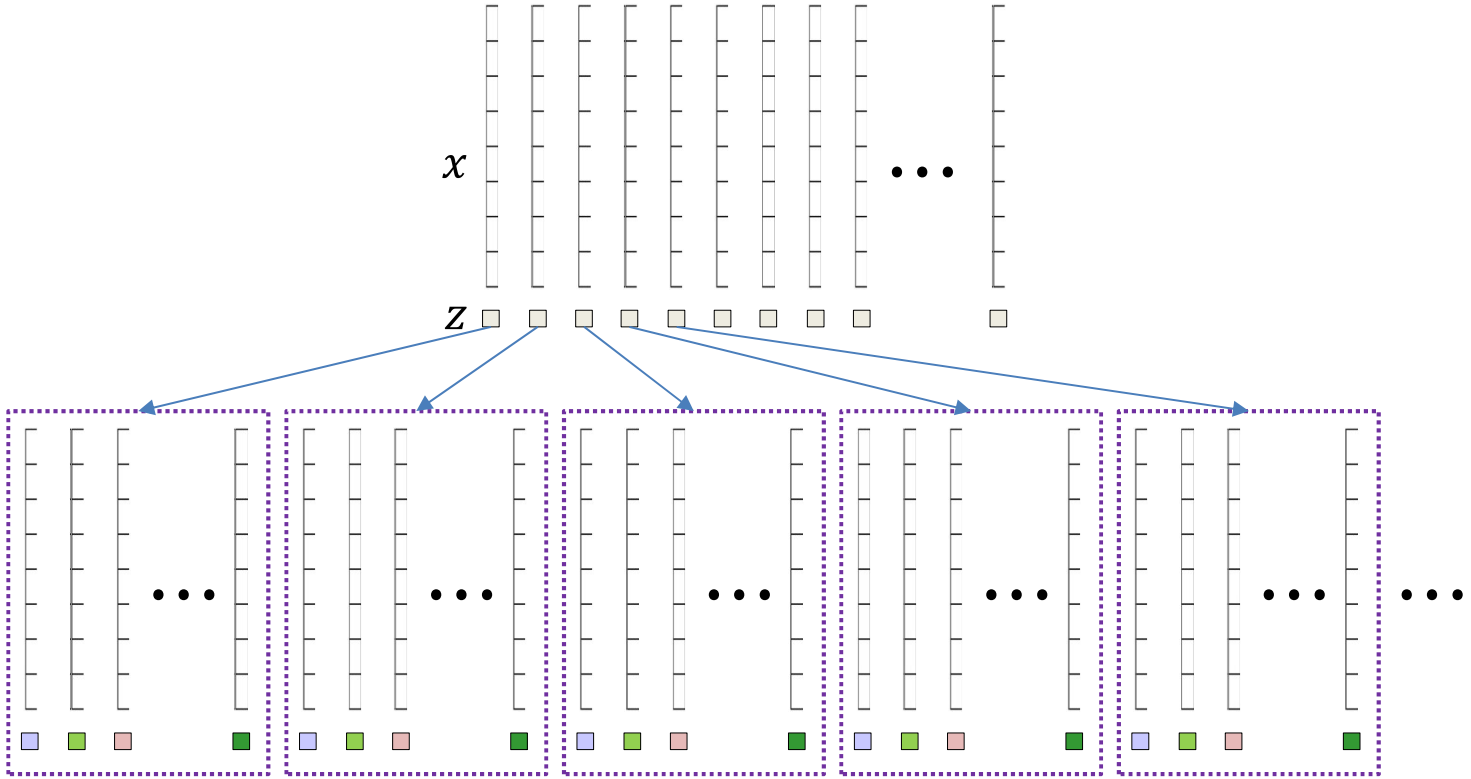
- We could estimate the model parameters if z were known for every data observation
  - I.e. if the data were complete
- Unfortunately we don't know z
  - The data are incomplete
- Solution: EM!
  - *Complete the data*

Expectation Maximization for NLGM



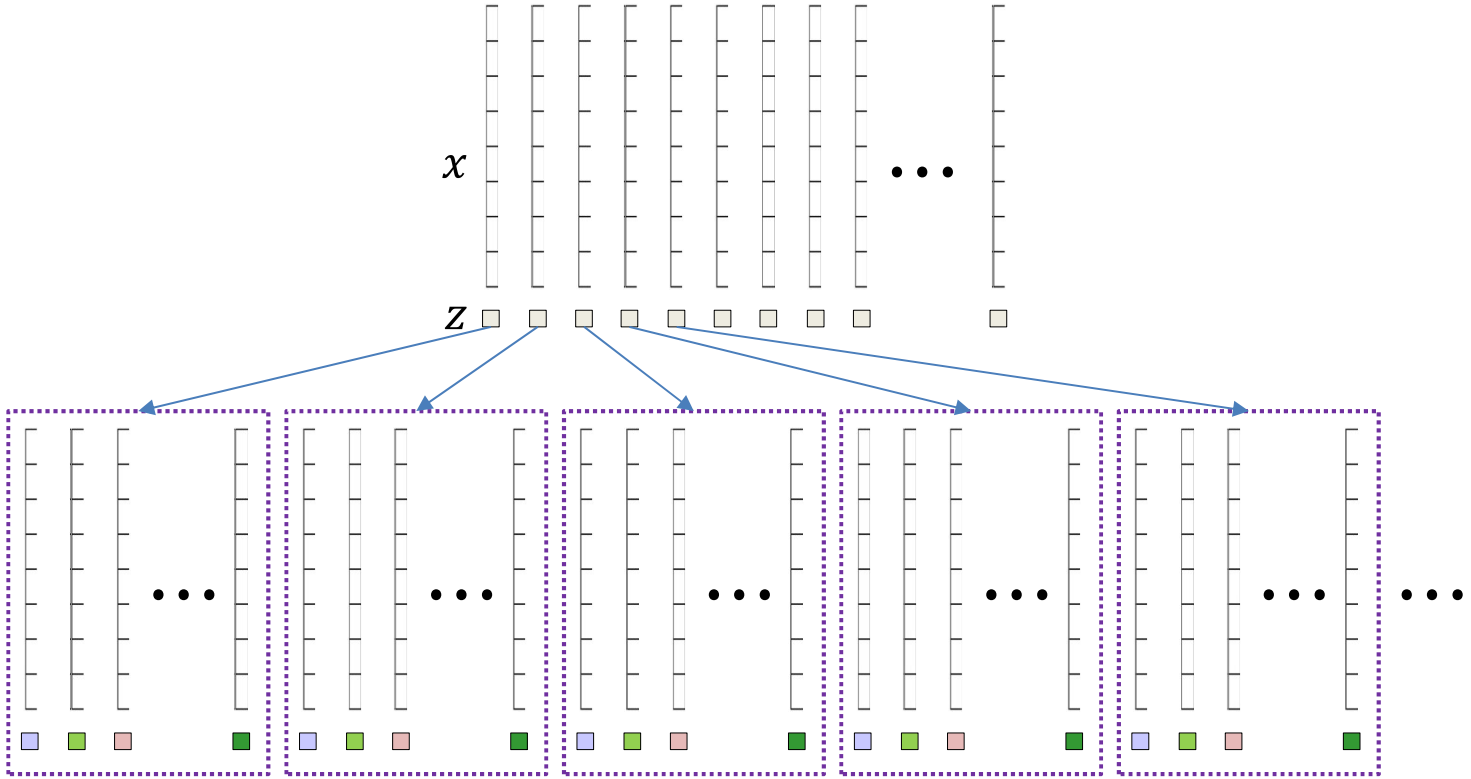
- *Complete* the data
- Option 1:
  - In *every possible way* proportional to $P(z|x)$
  - Compute the solution from the completed data

Expectation Maximization for LGM



- *Complete* the data
- Option 2:
  - ***By drawing samples from*** $P(z|x)$
  - Compute the solution from the completed data

Expectation Maximization for LGM



- *Complete* the data
- Option 2:
  - ***By drawing samples from*** $P(z|x)$
  - Compute the solution from the completed data

Using *every* possible value (option 1) is to be preferred over sampling (option 2) if the former produces tractable closed form solutions. Otherwise we must use option 2.

Problem with completing the data

- The posterior probability is given by

$$P(z|x) = \frac{P(x|z)P(z)}{P(x)}$$

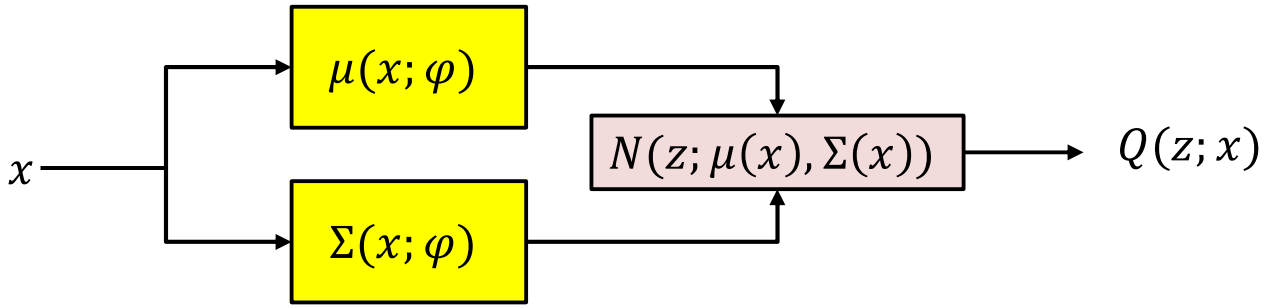
- The denominator

$$P(x) = \int_{-\infty}^{\infty} N(x;\ f(z;\theta), D)\ N(z;0,D)\ dz$$

  - This is intractable to compute in closed form for most $f(z;\theta)$

- $P(z|x)$ is intractable as a closed form solution
  - Makes it challenging to integrate over it or draw samples from it
  - But we could try to *approximate it*

Approximating $P(z|x)$



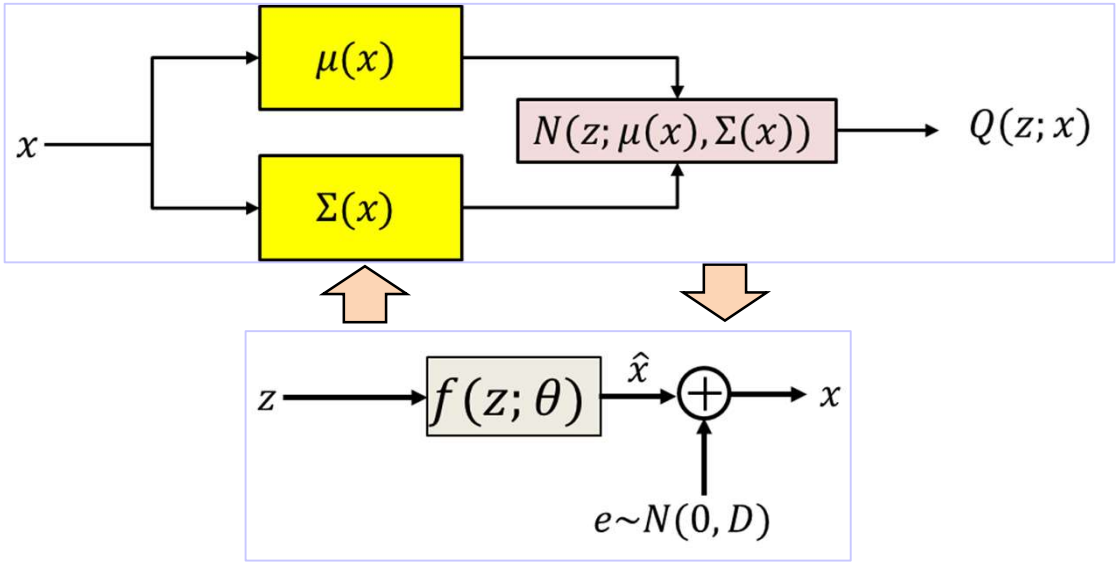
$\mu(x;\varphi)$ and $\Sigma(x;\varphi)$ are parametric functions of x, with parameters that we jointly represent as φ

- We will approximate $P(z|x)$ as

$$P(z|x) \approx Q(z,x) \;=\; Gaussian\; N(z;\mu(x),\Sigma(x))$$

  - where $\mu(x;\varphi)$ and $\Sigma(x;\varphi)$ are estimated such that $Q(z,x)$ approximates $P(z|x)$ as closely as possible
  - For convenience, we will assume $\Sigma(x;\varphi)$ is a diagonal matrix, represented entirely by its diagonal elements
- We will use $Q(z,x)$ as our proxy for $P(z|x)$

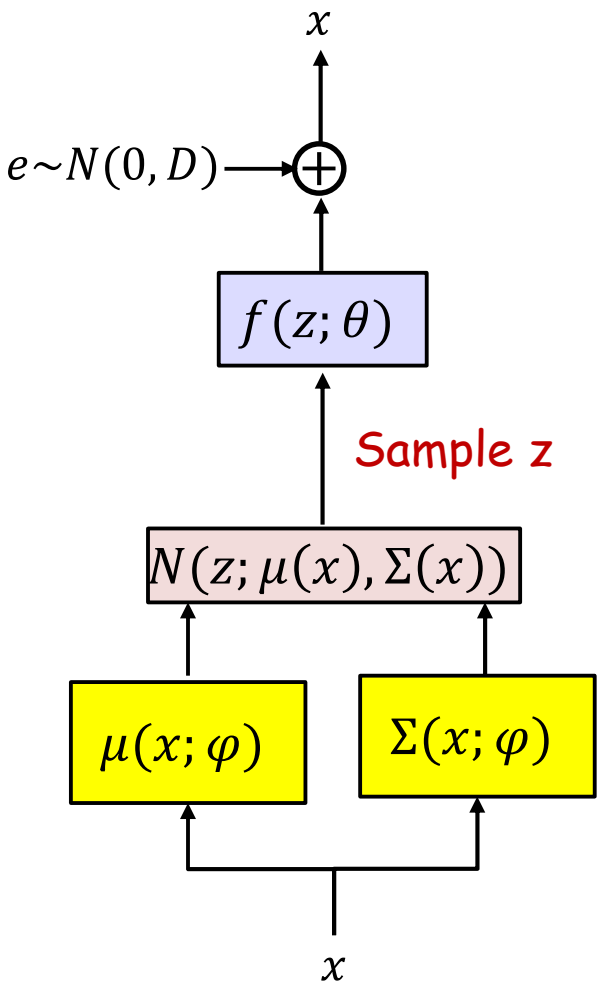
Overall Solution



- Initialize $f(z;\theta)$
- Iterate:
  - Estimate $\mu(x;\varphi)$ and $\Sigma(x;\varphi)$ to give you the best $Q(x,z)$
  - "Complete" the data using $Q(z,x)$
  - Reestimate $f(z;\theta)$

The complete pipeline

- Initialize θ and φ
- Iterate:
  - Sample z from $N(z; \mu(x; \varphi), \Sigma(x; \varphi))$ for each training instance
    - "Completing" the data
  - Reestimate θ from the entire "complete" data
  - Estimate φ using the entire "complete" data



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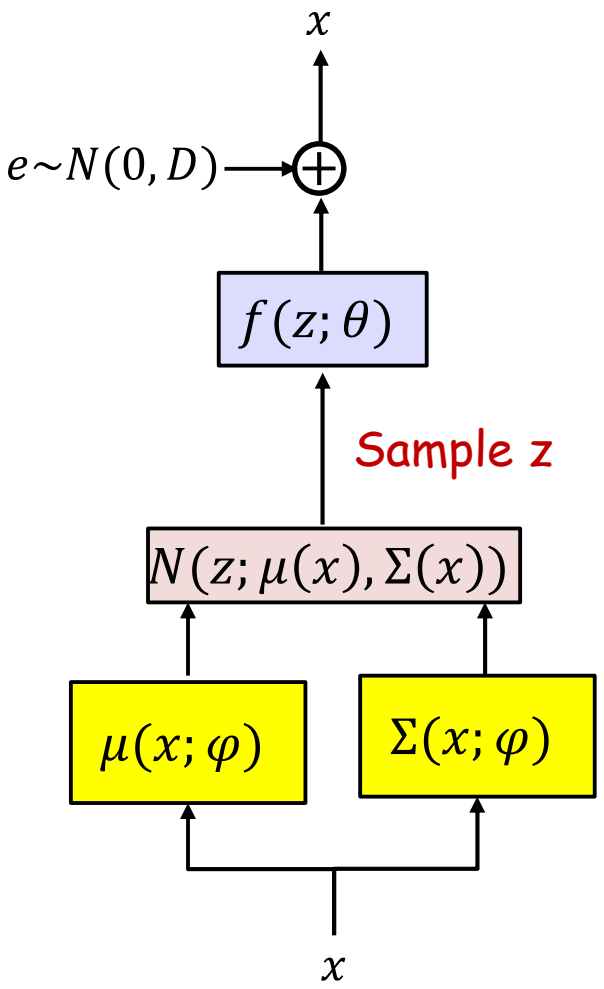

Sampling z

- *Sample z from $N(z; \mu(x; \varphi), \Sigma(x; \varphi))$ for each training instance*
  - *"Completing" the data*

- We use a standard "reparametrization" step to sample z
  - Sample z from a standard Gaussian, and scale and shift it such that it appears as a sample from $N(z; \mu(x; \varphi), \Sigma(x; \varphi))$

- For each training instance x
  - Compute $\mu(x; \varphi)$ and $\Sigma(x; \varphi)$
  - Draw one or more samples from the Gaussian $N(z; \mu(x; \varphi), \Sigma(x; \varphi))$
    - Draw K-dimensional vector ε from $N(0, I)$
    - Compute $z = \mu(x; \varphi) + \Sigma(x; \varphi)^{0.5}\varepsilon$

Sampling z

- *Sample z from $N(z; \mu(x;\varphi), \Sigma(x;\varphi))$ for each training instance*
  - *"Completing" the data*

- We use a standard "reparametrization" step to sample z
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- For each training instance x
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  - Draw one or more samples from the Gaussian $N(z; \mu(x;\varphi), \Sigma(x;\varphi))$
    - Draw K-dimensional vector ε from $N(0, I)$
    - Compute $z = \mu(x;\varphi) + \Sigma(x;\varphi)^{0.5}\varepsilon$

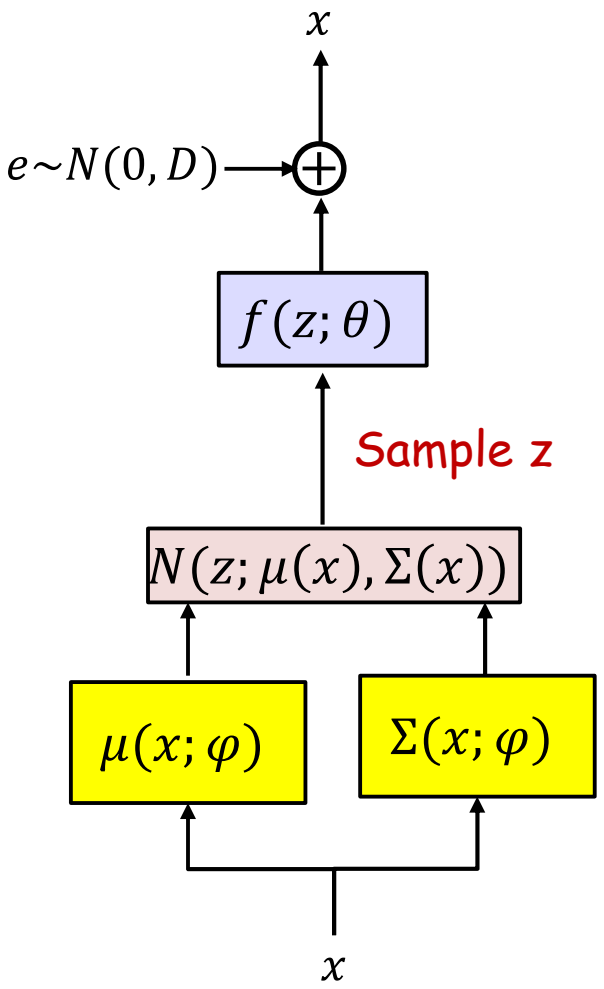
Remember this one $\quad \nabla_\varphi z = \nabla_\varphi \mu(x;\varphi) + diag(\varepsilon)\Sigma(x;\varphi)^{0.5}$

This will be specific to x and to the *specific sample of* z for that x (via ε)

The complete pipeline

- Initialize θ and φ
- Iterate:
  - Sample z from $N(z; \mu(x; \varphi), \Sigma(x; \varphi))$ for each training instance
    - "Completing" the data
  - Reestimate θ from the entire "complete" data
  - Estimate φ using the entire "complete" data

We know how to do this



NLGM with complete information

$$\theta^*, D^* = \underset{\theta, D}{\text{argmax}} \sum_{(x,z)} -\frac{1}{2}\log|D| - 0.5(x - f(z;\theta))^T D^{-1}(x - f(z;\theta))$$

- We can learn the parameters using backpropagation, which minimizes the following loss

$$L(\theta, D) = \sum_{(x,z)} \log|D| + (x - f(z;\theta))^T D^{-1}(x - f(z;\theta))$$

$$\theta^*, D^* = \underset{\theta, D}{\text{argmin}}\, L(\theta, D)$$

- It is common to assume that all the (diagonal) entries of D are identical, with value σ^2

$$L(\theta, \sigma^2) = d \log \sigma^2 + \sum_{(x,z)} \frac{1}{\sigma^2}\|x - f(z;\theta)\|^2$$

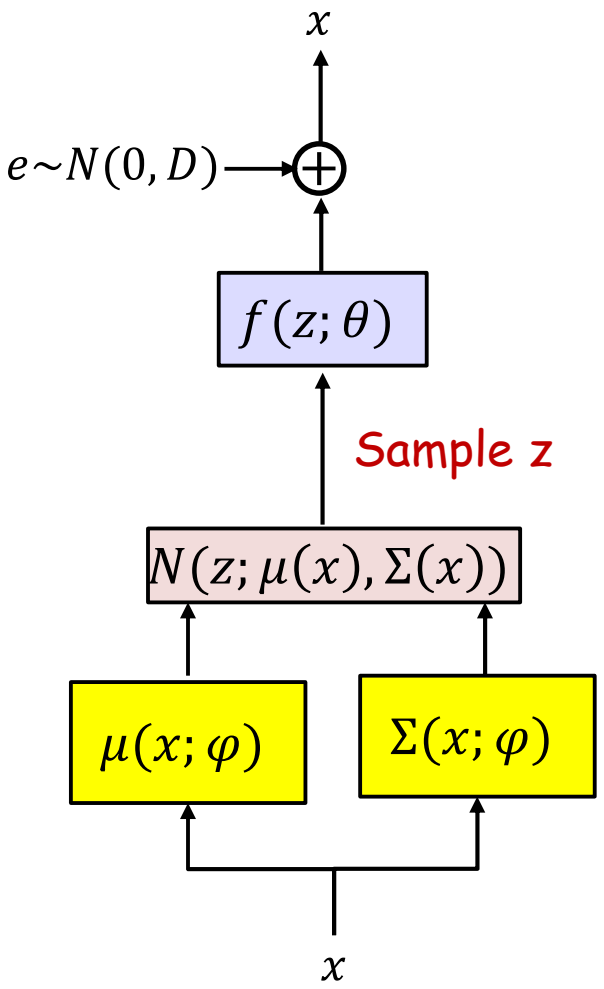
- The derivative of this w.r.t θ and σ^2 is trivially computed for backprop

The complete pipeline

- Initialize θ and φ
- Iterate:
  - Sample z from $N(z; \mu(x; \varphi), \Sigma(x; \varphi))$ for each training instance
    - "Completing" the data

    We know how to do this
  - Reestimate θ from the entire "complete" data

    We know how to do this
  - Estimate φ using the entire "complete" data



Approximating $P(z|x)$ by $Q(z,x)$

- Recall $Q(z,x) = N(z;\mu(x;\varphi),\Sigma(x;\varphi))$must approximate $P(z|x)$ as closely as possible

- Estimate φ to minimize the error between $Q(z,x)$ and $P(z|x)$
  - Define a divergence between $Q(z,x)$ and $P(z|x)$ and minimize it w.r.t. φ
  - Following the literature, we will use the KL divergence
    - Then I will give you a simpler explanation

Approximating $P(z|x)$ by $Q(z,x)$

$$KL(Q(z,x)P(z|x)) = E_{z\sim Q}\log\frac{Q(z,x)}{P(z|x)}$$
$$= E_{z\sim Q}\log Q(z,x) - E_{z\sim Q}\log P(z|x)$$
$$= E_{z\sim Q}\log Q(z,x) - E_{z\sim Q}\log\frac{P(z)P(x|z)}{P(x)}$$
$$= E_{z\sim Q}\log Q(z,x) - E_{z\sim Q}\log P(z) - E_{z\sim Q}\log P(x|z) - E_{z\sim Q}\log P(x)$$
$$= KL\big(Q(z,x),P(z)\big) - E_{z\sim Q}\log P(x|z) - E_{z\sim Q}\log P(x)$$

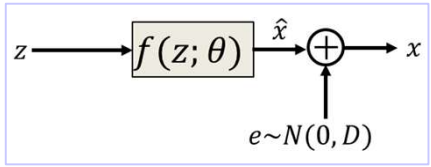
- $Q(z,x)$ is a function of φ. Minimizing the loss w.r.t. φ we get

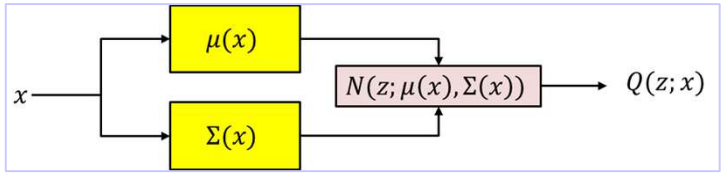
$$\varphi^* = \underset{\varphi}{\operatorname{argmin}}\, KL(Q(z,x)P(z|x))$$
$$= \underset{\varphi}{\operatorname{argmin}}\, KL\big(Q(z,x),P(z)\big) - E_{z\sim Q}\log P(x|z)$$

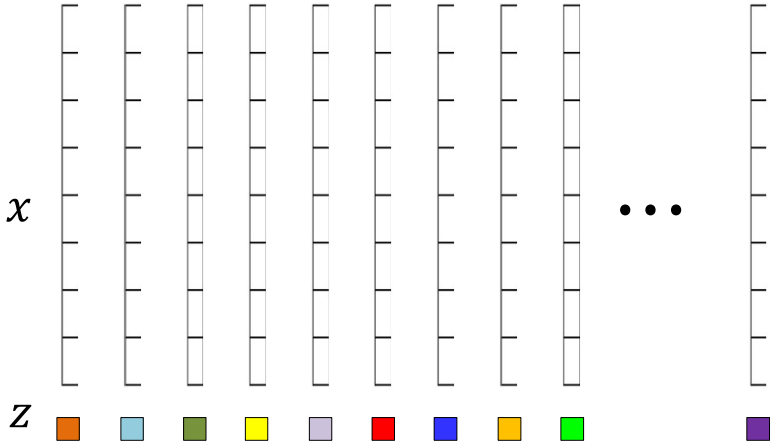
Find φ to minimize the (empirical estimate of the) KL divergence between Q(z,x) and P(z) while simultaneously maximizing the (empirical estimate of) the expectation of log P(x|z)

Lets try that again…

NLGM with complete data

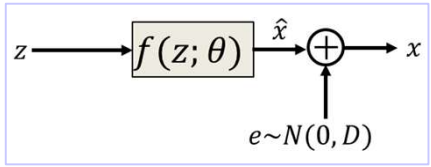


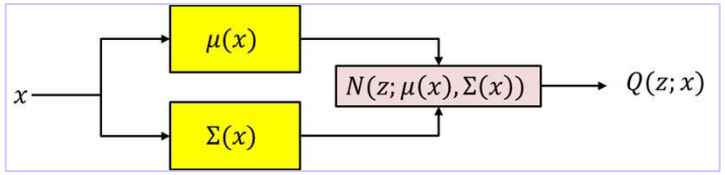


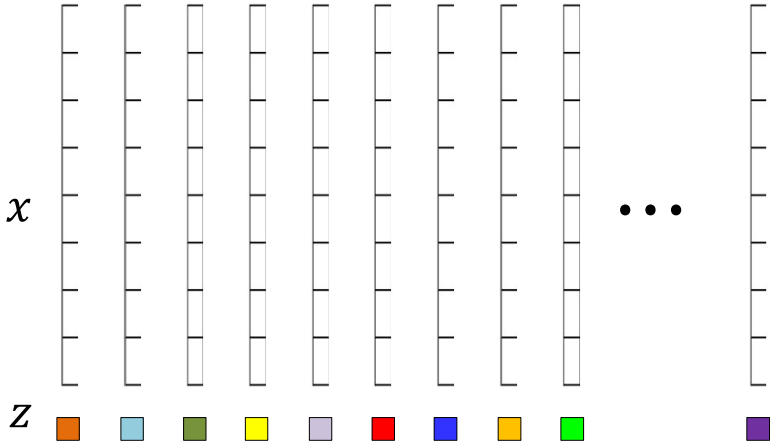


- Assume we have completed the data using $Q(z, x)$
  - We have a collection of (x, z) pairs
    - More precisely denoted as $(x, z_{x,j})$ since the value $z_{x,j}$ used to complete the observation is specific to x (subscript x)
      - Also, a single x may be completed in multiple ways (subscript j)
    - We will use (x, z) as our shorthand notation, though, with the implicit assumption that z is specific to x, and the x values in (x, z) are not unique
  - We can work with complete data!

NLGM with complete data







- Representing the completed data as $[X, Z] = \{(x, z)\}$, the actual posterior probability for Z given X as computed by the model is

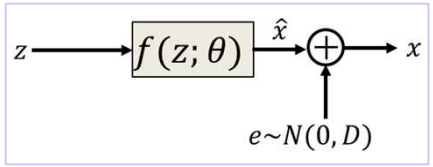
$$P(Z|X;\theta) = \prod_{(x,z)\in[X,Z]} P(z|x;\theta)\,, \qquad \log P(Z|X;\theta) = \sum_{(x,z)\in[X,Z]} \log P(z|x;\theta)$$

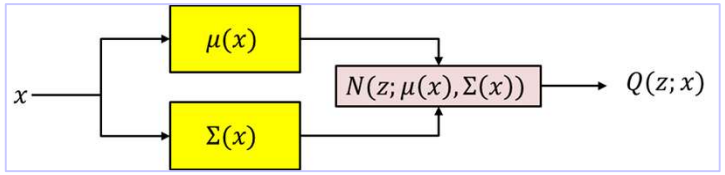
  - Because the observations are independent

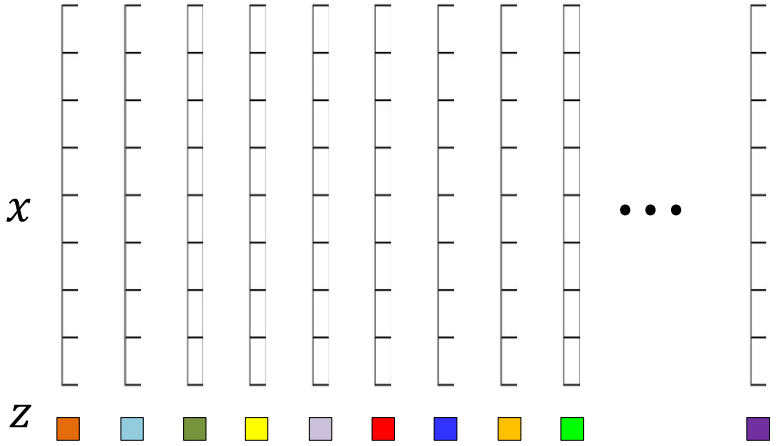
- The approximation using $Q(Z, X)$ is

$$Q(Z,X;\varphi) = \prod_{(x,z)\in[X,Z]} Q(z,x;\varphi)\,, \qquad \log Q(Z,X;\varphi) = \sum_{(x,z)\in[X,Z]} \log Q(z,x;\varphi)$$

NLGM with complete data







- Representing the completed data as $[X, Z] = \{(x, z)\}$, the actual posterior probability for Z given X as computed by the model is

We will estimate φ to minimize the discrepancy between these two probabilities

$$\log P(Z|X;\theta) = \sum_{(x,z)\in[X,Z]} \log P(z|x;\theta)$$

$$\log Q(Z,X;\varphi) = \sum_{(x,z)\in[X,Z]} \log Q(z,x;\varphi)$$

Estimating φ

- We will minimize the following error

$$\log Q(Z, X; \varphi) - \log P(Z|X; \theta)$$

$$= \sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z|x; \theta)$$

Estimating φ

- We will minimize the following error

$$\log Q(Z, X; \varphi) - \log P(Z|X; \theta)$$

$$= \sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z|x; \theta)$$

- By Bayes rule $P(z|x; \theta) = P(z)P(x|z)/P(x)$
- The error becomes

$$\sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z) - \log P(x|z; \theta) + \log P(x; \theta)$$

Estimating φ

- We will minimize the following error

$$\log Q(Z, X; \varphi) - \log P(Z|X; \theta)$$

$$= \sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z|x; \theta)$$

- By Bayes rule $P(z|x; \theta) = P(z)P(x|z)/P(x)$
- The error becomes

$$\sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z) - \log P(x|z; \theta) + \log P(x; \theta)$$

- φ influences $Q(z, x; \varphi)$ directly and z, because it is sampled from $Q(z, x; \varphi)$. $P(x; \theta)$ is not related to either φ or z and can be ignored.

Estimating φ

- We will minimize the following error

$$\log Q(Z, X; \varphi) - \log P(Z|X; \theta)$$

$$= \sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z|x; \theta)$$

- By Bayes rule $P(z|x; \theta) = P(z)P(x|z)/P(x)$
- The error becomes

$$\sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z) - \log P(x|z; \theta) + \log P(x; \theta)$$

- φ influences $Q(z, x; \varphi)$ directly and z, because it is sampled from $Q(z, x; \varphi)$.
- $P(x; \theta)$ is not related to either φ or z and can be ignored.
- This gives us the loss function

$$L_Q(\varphi) = \sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z) - \log P(x|z; \theta)$$

- This must be minimized w.r.t. φ

Estimating φ

- We will minimize the following error

$$\log Q(Z, X; \varphi) - \log P(Z|X; \theta)$$

$$= \sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z|x; \theta)$$

- By Bayes rule $P(z|x; \theta) = P(z)P(x|z)/P(x)$
- The error becomes

$$\sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z) - \log P(x|z; \theta) + \log P(x; \theta)$$

- φ influences $Q(z, x; \varphi)$ directly and z, because it is sampled from $Q(z, x; \varphi)$.
- $P(x; \theta)$ is not related to either φ or z and can be ignored.
- This giv

How do we complete the data?

$$L_Q(\varphi) = \sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z) - \log P(x|z; \theta)$$

- This must be minimized w.r.t. φ

Estimating φ

- The loss function

$$L_Q(\varphi) = \sum_{(x,z)\in[X,Z]} \log Q(z,x;\varphi) - \log P(z) - \log P(x|z;\theta)$$

- Multiple choices for data completion
- Simple option: Simply choose the samples you have already drawn
  - You can skip the next couple of slides if you do

$$\nabla_\varphi L_Q(\varphi) = \sum_{(x,z)\in[X,Z]} \nabla_\varphi \log Q(z,x;\varphi) + \nabla_z \log Q(z,x;\varphi)\,\nabla_\varphi z - \nabla_z \log P(z)\nabla_\varphi z - \nabla_z \log P(x|z;\theta)\,\nabla_\varphi z$$

Estimating φ

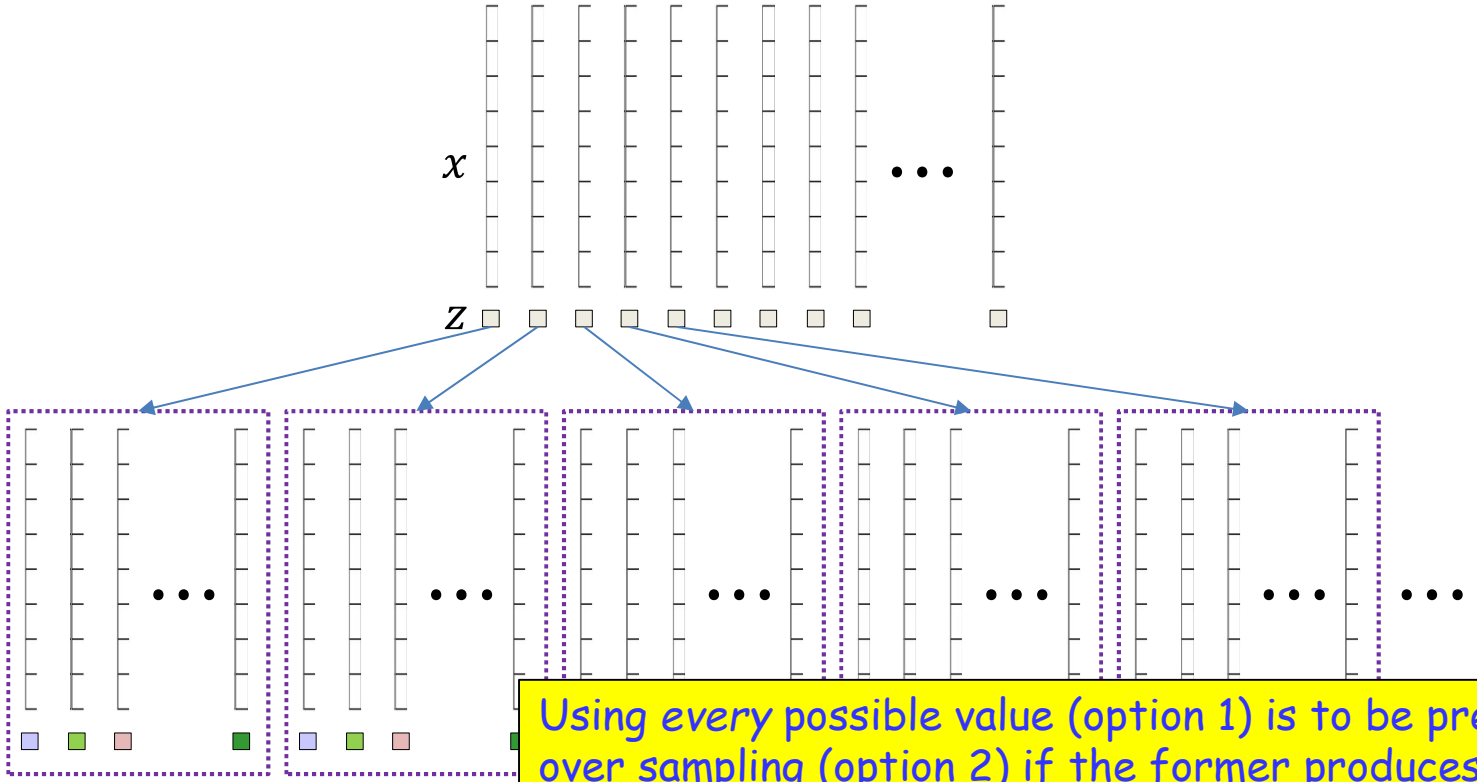
- The loss function

$$L_Q(\varphi) = \sum_{(x,z)\in[X,Z]} \log Q(z, x; \varphi) - \log P(z) - \log P(x|z; \theta)$$

- Multiple choices for data completion
- Simple option: Simply choose the samples you have already drawn
  - You can skip the next couple of slides if you do

- Orrrr try to be more precise….

Expectation Maximization for LGM



Using *every* possible value (option 1) is to be preferred over sampling (option 2) if the former produces tractable closed form solutions. Otherwise we must use option 2.

- *Complete* the data
  - Option 1 : Consider *every possible value for z*
  - Option 2: ***By drawing samples from*** $P(z|x)$
- Compute the solution from the completed data

Estimating φ

- The loss function

$$L_Q(\varphi) = \sum_{(x,z)\in[X,Z]} \underbrace{\log Q(z,x;\varphi) - \log P(z)}_{} - \underbrace{\log P(x|z;\theta)}_{}$$

- It turns out that the portion underlined in blue can be computed in closed form if you consider every possible value of z

- The portion underlined in red cannot

- So sum the first portion over all possible values of z from and the second one over only the drawn samples

$$L_Q(\varphi) = \sum_{(x)\in[X]} \int_{-\infty}^{\infty} Q(z,x;\varphi)(\log Q(z,x;\varphi) - \log P(z))\, dz - \sum_{(x,z)\in[X,Z]} \log P(x|z;\theta)$$

Estimating φ

- The loss function

$$L_Q(\varphi) = \sum_{(x,z)\in[X,Z]} \underbrace{\log Q(z,x;\varphi) - \log P(z)}_{} - \underbrace{\log P(x|z;\theta)}_{}$$

- It turns out that the portion underlined in blue can be computed in closed form if you consider every possible value of z

- The portion underlined in red cannot

- So sum the first portion over all possible values of z from and the second one over only the drawn samples

$$L_Q(\varphi) = \sum_{(x)\in[X]} \underbrace{\int_{-\infty}^{\infty} Q(z,x;\varphi)(\log Q(z,x;\varphi) - \log P(z))\, dz}_{KL(Q(z,x;\varphi),P(z))} - \sum_{(x,z)\in[X,Z]} \log P(x|z;\theta)$$

Estimating φ

- The loss function

$$L_Q(\varphi) = \sum_{x \in X} KL(Q(z, x; \varphi), P(z)) - \sum_{(x,z) \in [X,Z]} \log P(x|z; \theta)$$

- We have:

$$Q(z, x) = N\big(z; \mu(x; \varphi), \Sigma(x; \varphi)\big), \qquad P(z) = N(0, I)$$

- The KL between the two Gaussians works out to

$$KL\big(Q(z, x; \varphi), P(z)\big) = \frac{1}{2}\Big(tr\big(\Sigma(x; \varphi)\big) + \mu(x; \varphi)^T(\mu(x; \varphi) - d - \log|\Sigma(x; \varphi)|)\Big)$$

- We have

$$\log P(x|z; \theta) = \sum_{(x,z)} -\frac{1}{2}\log|D| - 0.5(x - f(z; \theta))^T D^{-1}(x - f(z; \theta))$$

- Plugging it all in:

$$L_Q(\varphi)$$
$$= \sum_{x \in X} \frac{1}{2}\Big(tr\big(\Sigma(x; \varphi)\big) + \mu(x; \varphi)^T(\mu(x; \varphi) - d - \log|\Sigma(x; \varphi)|)\Big)$$
$$+ \sum_{(x,z) \in [X,Z]} \frac{1}{2}\log|D| + 0.5(x - f(z; \theta))^T D^{-1}(x - f(z; \theta))$$

Estimating φ

- So we finally have the loss function (ignoring unnecessary terms and factors)

$$L_Q(\varphi)$$

$$= \sum_{x \in X} \Big(tr\big(\Sigma(x;\varphi)\big) + \mu(x;\varphi)^T \big(\mu(x;\varphi) - d - \log|\Sigma(x;\varphi)|\big) \Big)$$

$$+ \sum_{(x,z) \in [X,Z]} (x - f(z;\theta))^T D^{-1} (x - f(z;\theta))$$

- Assuming that $D$is diagonal with identical values σ^2 for the diagonal elements gives us the simplification

$$L_Q(\varphi) = \sum_{x \in X} \Big(tr\big(\Sigma(x;\varphi)\big) + \mu(x;\varphi)^T \big(\mu(x;\varphi) - d - \log|\Sigma(x;\varphi)|\big) \Big) + \frac{1}{\sigma^2} \sum_{(x,z) \in [X,Z]} \|(x - f(z;\theta))\|^2$$

- To estimate φ we will compute

$$\varphi^* = \underset{\varphi}{\operatorname{argmin}}\, L_Q(\varphi)$$

- To perform the minimization we will use gradient descent

Estimating φ

$$\varphi^* = \underset{\varphi}{\operatorname{argmin}}\, L_Q(\varphi)$$

- To perform the minimization we will use gradient descent

$$\nabla_\varphi L_Q(\varphi)$$

$$= \sum_{x \in X} \nabla_\varphi \left(tr\big(\Sigma(x;\varphi)\big) + \mu(x;\varphi)^T \big(\mu(x;\varphi) - d - \log|\Sigma(x;\varphi)|\big) \right)$$

$$+ \frac{1}{\sigma^2} \sum_{(x,z) \in [X,Z]} \nabla_z \|(x - f(z;\theta))\|^2 \nabla_\varphi z$$

The complete training pipeline

- Initialize θ and φ
- Iterate:
  - Sample $z_{x,\varepsilon}$ from $N(z;\mu(x;\varphi),\Sigma(x;\varphi))$ for each training instance
    - "Completing" the data
  - Reestimate θ from the entire "complete" data

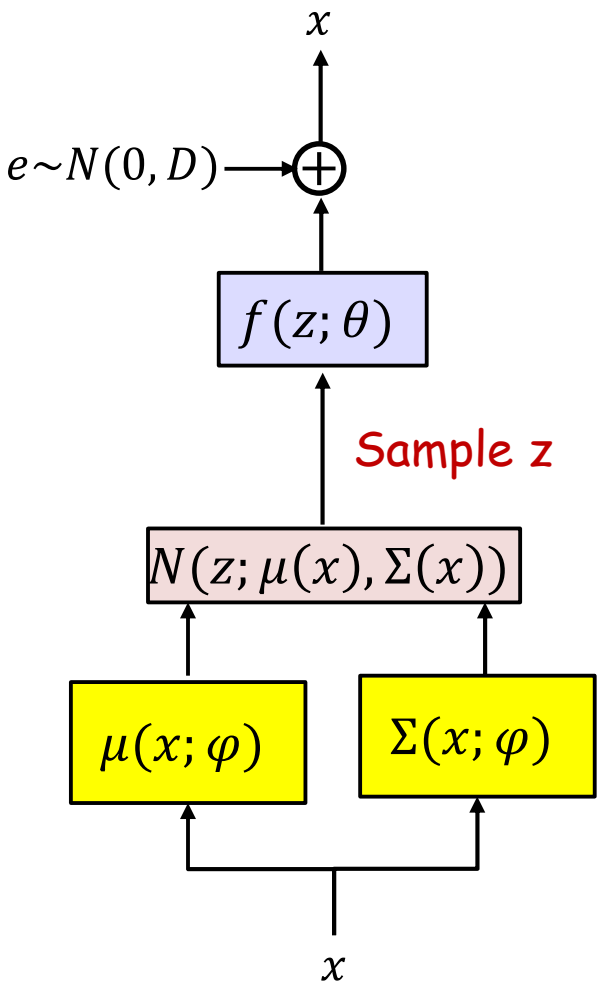
$$L(\theta,\sigma^2) = d\log\sigma^2 + \frac{1}{\sigma^2}\sum_{(x,z)}\|x - f(z;\theta)\|^2$$

  - Estimate φ using the entire "complete" data

$$L_Q(\varphi)$$

$$= \sum_{x\in X}\Big(tr\big(\Sigma(x;\varphi)\big) + \mu(x;\varphi)^T(\mu(x;\varphi) - d - \log|\Sigma(x;\varphi)|)\Big)$$

$$+\frac{1}{\sigma^2}\sum_{(x,z)\in[X,Z]}\|(x - f(z;\theta))\|^2$$



The complete training pipeline: Single step update

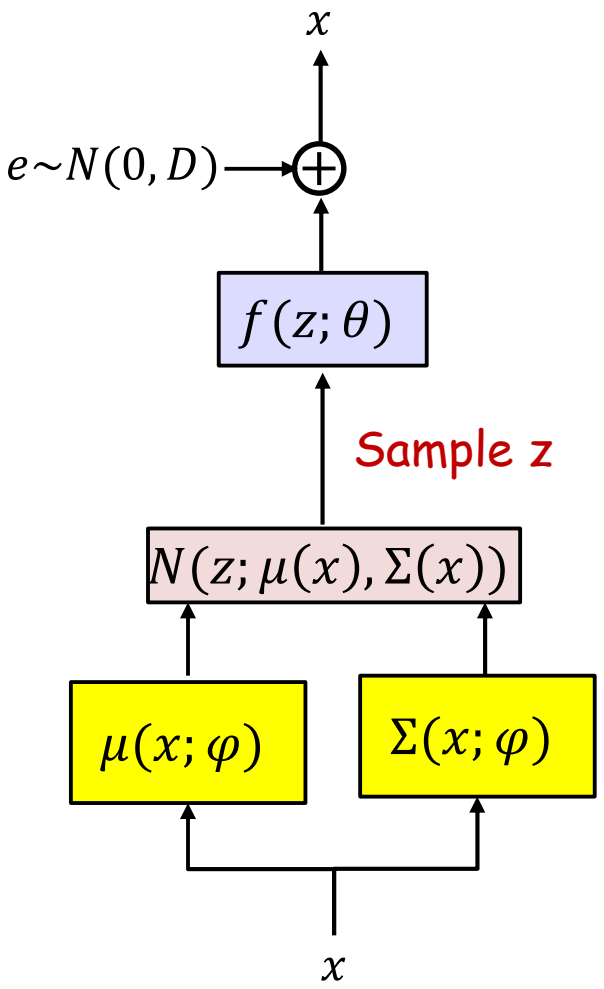
- Initialize θ and φ
- Iterate:
  - Sample $z_{x,\varepsilon}$ from $N(z;\mu(x;\varphi),\Sigma(x;\varphi))$ for each training instance
    - "Completing" the data
  - Reestimate θ and φ from the entire "complete" data

$$L(\theta,\sigma^2,\varphi)$$

$$= \sum_{x\in X}\Big(tr\big(\Sigma(x;\varphi)\big) + \mu(x;\varphi)^T(\mu(x;\varphi) - d - \log|\Sigma(x;\varphi)|)\Big)$$

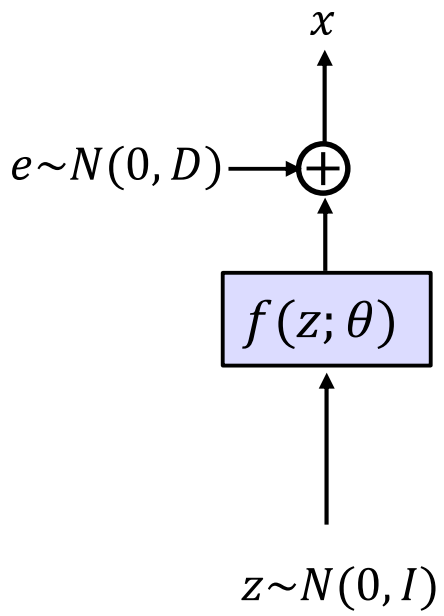
$$+ \frac{1}{\sigma^2}\sum_{(x,z)\in[X,Z]} \|(x - f(z;\theta))\|^2 + d\log\sigma^2$$

- (Merged the updates of θ and φ into a single step)
  - Gradient computation doesn't change



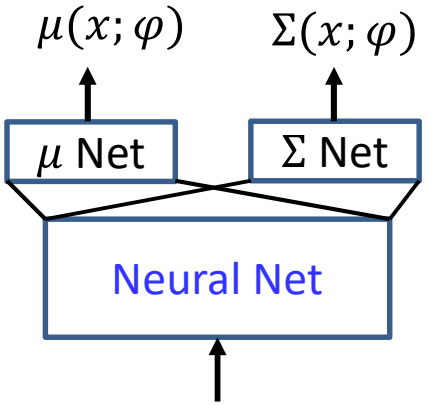
The complete training pipeline

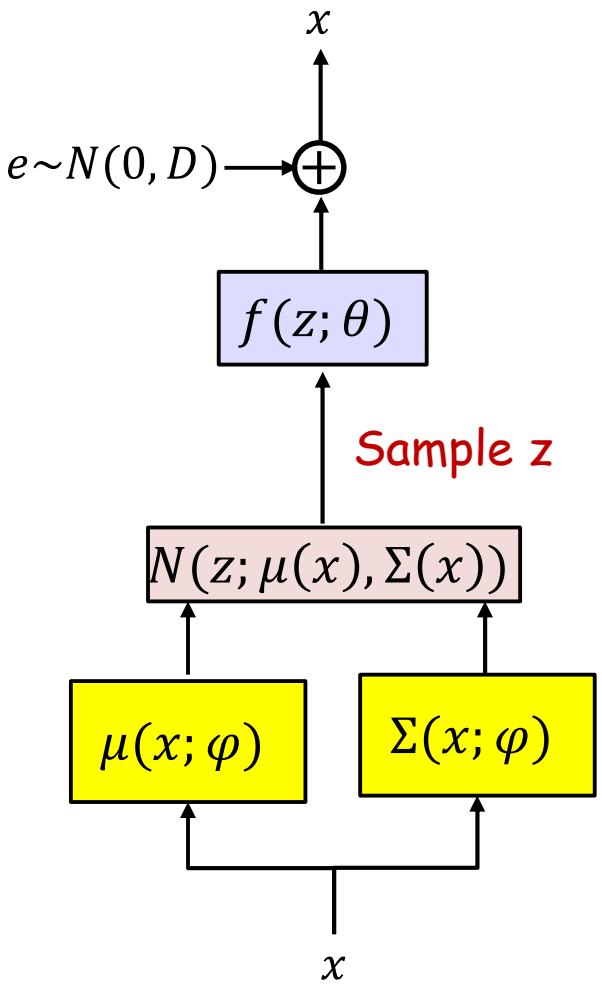
- Once trained the approximation function $Q(z, x)$ can be discarded
- The rest of the function gives us a *generative* model for x
- Generating data using this part of the model should (ideally) give us data similar to the training data



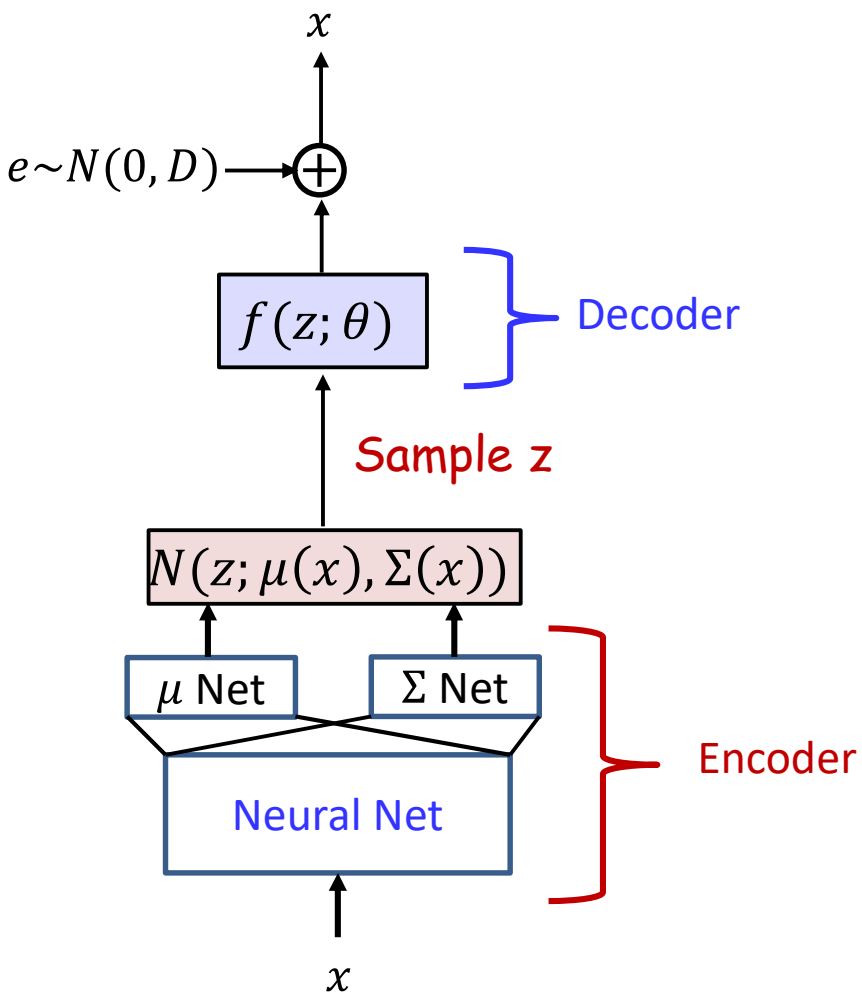
But where are the neural nets?

- $f(z;\theta)$ is generally modelled by a neural network
- $\mu(x;\varphi)$ and $\Sigma(x;\varphi)$ are generally modelled by a *common* network with two outputs
  - The combined parameters of the network are φ





The Variational AutoEncoder



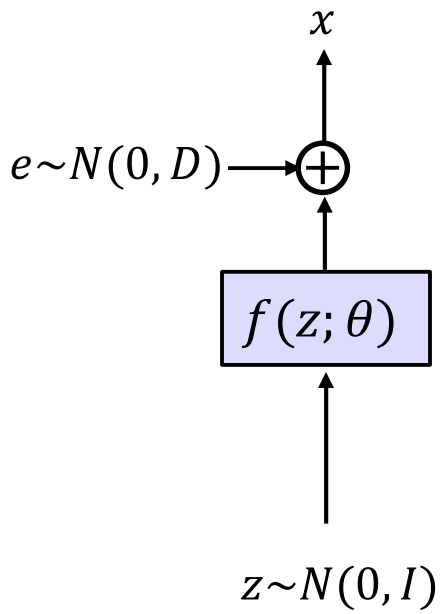
The decoder is the actual generative model

The encoder is primarily needed for training
It can also be used to generate the (approximate) distribution of latent space representations conditioned on specific inputs input
(much like a regular autoencoder)

z is a *latent-space* representation of the data
$\mu(x)$ can also be used as a *expected latent* representation of x

VAEs

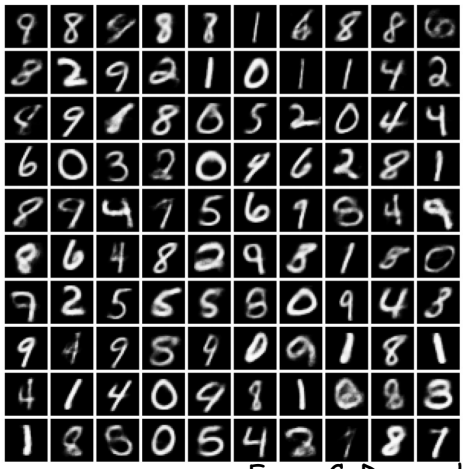
- VAEs are, unfortunately, *strictly* generative models
- They can be used to *generate samples* of the data
- But they cannot be used to *compute the likelihood* of data
  - At least not directly
  - Because $P(x;\theta)$ is generally intractable



- Nevertheless, they are highly effective as generators
  - They can learn highly complex distributions

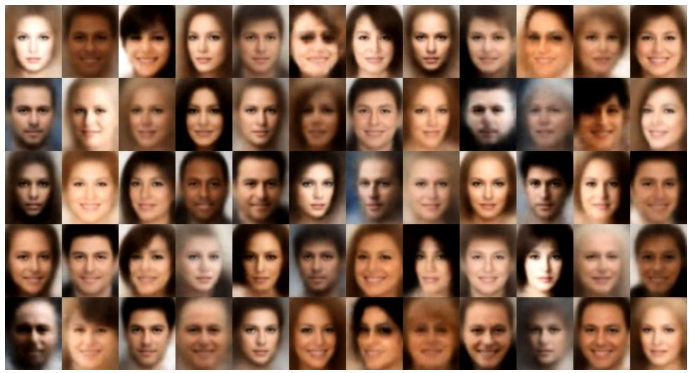
VAE examples

- Top: VAE trained on MNIST and used to generate new data



From C. Doersch

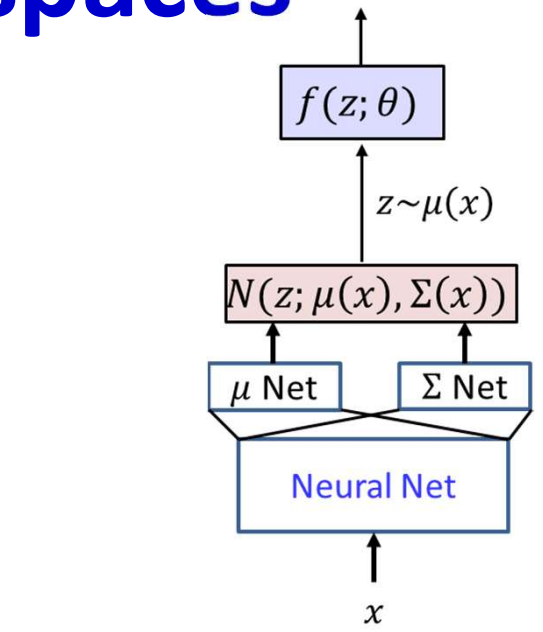
- Below: VAE trained on faces, and used to generate new data



From J. Rocco

VAE and latent spaces

- The latent space z often captures underlying structure in the data x in a smooth manner
- Varying z continuously in different directions can result in plausible variations in the drawn output
  - Typically manipulations are performed by wiggling z around its expected value $\mu(x)$
- Typically, in these draws, you do not add the noise e
  - The output is the *expected* generation for a given latent value z



VAE conclusions

- Simple non-linear extensions of linear Gaussian models
- Excellent generative models for the distribution of data $P(x)$
  - Various extensions such as Conditional VAEs, which model *conditional* distributions, such as $P(x|y)$
    - Straight-forward extension where the conditioning variable y is an additional input to the encoder and decoder
- Have also been successfully embedded into dynamical system models
  - $P(z)$ now becomes a mixture, or a Markov model instead of $N(0, I)$
- In all cases, the arithmetic for learning is similar to that presented here
- Read the literature on the topic, it is vase