# COMPSCI 689
# Lecture 19: Latent Linear Models

Benjamin M. Marlin

College of Information and Computer Sciences
University of Massachusetts Amherst

Slides by Benjamin M. Marlin (marlin@cs.umass.edu).

# Probabilistic Unsupervised Learning

- In probabilistic unsupervised learning, our goal is to model multivariate data $\mathbf{x} = [x_1, ..., x_D]$ generated by an unknown probabilistic process using a probabilistic model learned from a data set $\mathcal{D} = \{\mathbf{x}_n | 1 \leq n \leq N\}$.
- Since the data are vectors, we use vector-valued random variables to model them $\mathbf{X} = [X_1, ..., X_D]$.
- Each data dimension $d$ takes values from a potentially different set $\mathcal{X}_d$. We have $\mathbf{x} \in \mathcal{X}$. $\mathcal{X} = \mathcal{X}_1 \times ... \times \mathcal{X}_D$.

# Joint Distributions

- A probability distribution over the joint settings of multiple random variables is referred to as a *joint distribution*.
- When all dimensions of $\mathbf{x}$ are discrete, the joint distribution is represented by a *joint probability mass* function $P(\mathbf{X} = \mathbf{x}) = P(X_1 = x_1, ..., .X_D = x_d)$.
- When all dimensions of $\mathbf{x}$ are continuous, the joint distribution is represented by a *joint probability density* function $p(\mathbf{X} = \mathbf{x}) = p(X_1 = x_1, ..., .X_D = x_d)$.

# Multivariate Normal

- The multivariate normal (or Gaussian) distribution is a fundamental building block for unsupervised learning with vector-valued random variables $\mathbf{X} \in \mathbb{R}^D$.

- The distribution has two parameters $\theta = [\mu, \Sigma]$. $\mu$ is the mean vector and $\Sigma$ is the covariance matrix.

- The probability density is given below (assuming $\mathbf{x}$ and $\mu$ are column vectors):

$$\mathcal{N}(\mathbf{x}; \mu, \Sigma) = \frac{1}{|2\pi\Sigma|^{1/2}} \exp\left( -\frac{1}{2}(\mathbf{x}-\mu)^T \Sigma^{-1} (\mathbf{x}-\mu) \right)$$

- We have $\mu \in \mathbb{R}^D$ and $\Sigma \in \mathbb{S}^D_+$, the space of symmetric, positive definite $D \times D$ matrices.

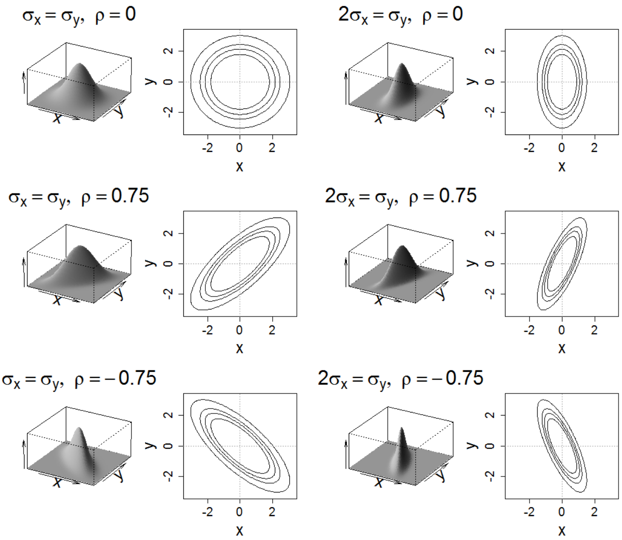
# Example: Bivariate Normal

- The bivariate normal distribution is a special case of the multivariate normal where $D = 2$ so that $\mathbf{X} = [X_1, X_2]$.
- In this case the mean vector $\mu = [\mu_1, \mu_2]$ specifies a location in 2D real space.
- The covariance matrix can be represented either directly or via the marginal standard deviations and the correlation between $X_1$ and $X_2$:

$$\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{12} & \Sigma_{22} \end{bmatrix} = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}$$

- The level sets of the bivariate normal density are ellipses whose axes are determined by the eigenvalues and eigenvectors of the covariance matrix.

# Example: Bivariate Normal



# MLE for the Multivariate Normal

- Given a data set $\mathcal{D} = \{\mathbf{x}_n\}_{1:N}$, the MLE for the multivariate normal is found by solving the optimization problem:

$$\mu^*, \Sigma^* = \arg\min_{\mu,\Sigma} - \sum_{n=1}^{N} \log \mathcal{N}(\mathbf{x}_n; \mu, \Sigma)$$

- The solutions are:

$$\hat{\mu} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n, \qquad \hat{\Sigma} = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_n - \hat{\mu})(\mathbf{x}_n - \hat{\mu})^T$$

# Other Special Cases of MVNs

- Consider the general case for arbitrary $D$.
- If $\mu = [0, ..., 0]$ and $\Sigma = I$ is the identity matrix, $\mathcal{N}(\mathbf{x}; \mu, \Sigma)$ is called a “a standard multivariate normal".
- If $\Sigma = \sigma I$, $\mathcal{N}(\mathbf{x}; \mu, \Sigma)$ is called an “isotropic Gaussian."
- If $\Sigma$ is a diagonal matrix, $\mathcal{N}(\mathbf{x}; \mu, \Sigma)$ is called a “diagonal Gaussian" or “axis-aligned Gaussian"

# Marginalization

- Suppose we have a joint distribution on a vector-valued random variable $\mathbf{X} \in \mathbb{R}^D$. Let $A \subseteq \{1, ..., D\}$, $M = |A|$, and $\mathbf{X}_A = [X_{A_1}, ..., X_{A_M}]$.
- The probability distribution $P(\mathbf{X}_A = \mathbf{x}_A)$ is called the *marginal distribution* of $\mathbf{X}_A$.
- Let $B = \{1, ..., D\}/A$. The marginal distribution of $\mathbf{X}_A$ is then given by:

$$P(\mathbf{X}_A = \mathbf{x}_A) = \int_{\mathcal{X}_B} P(\mathbf{X}_A = \mathbf{x}_A, \mathbf{X}_B = \mathbf{x}_B) d\mathbf{x}_B$$

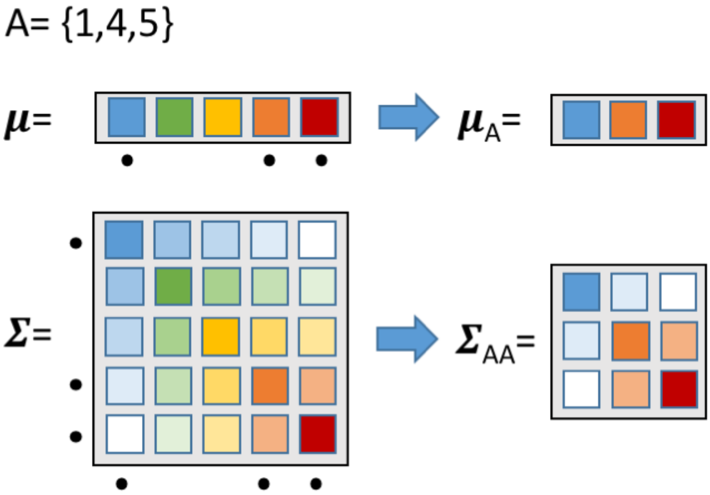
# Marginalization for MVNs

- The multivariate normal distribution has the remarkable (and convenient) property of being closed under marginalization.
- Suppose we have an MVN $P(\mathbf{X}|\theta) = \mathcal{N}(\mathbf{X}; \mu, \Sigma)$ for $\mathbf{X} \in \mathbb{R}^D$. Let $A \subseteq \{1, ..., D\}$, $B = \{1, ..., D\}/A$, and $M = |A|$. We have:

  $$P(\mathbf{X}_A = \mathbf{x}_A) = \mathcal{N}(\mu_A, \Sigma_{AA})$$

  where $\mu_A = [\mu_{A_1}, ..., \mu_{A_M}]$ and $(\Sigma_{AA})_{ij} = \Sigma_{A_i, A_j}$.
- In other words, we get the marginal distribution on a subset of $\mathbf{X}$ just by discarding the elements of $\mu$ that correspond to $B$, and the rows and columns of $\Sigma$ that correspond to $B$.

# Marginalization for MVNs: Example



# Conditioning for MVNs

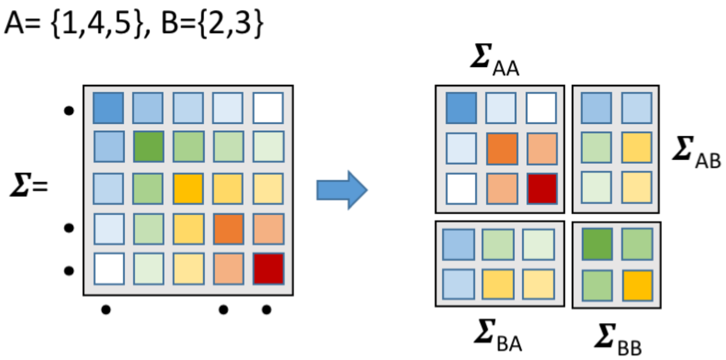
- The multivariate normal distribution has the remarkable (and convenient) property of also being closed under conditioning.
- Suppose we have an MVN $p(\mathbf{X}|\theta) = \mathcal{N}(\mathbf{X}; \mu, \Sigma)$ for $\mathbf{X} \in \mathbb{R}^D$. Let $A \subseteq \{1, ..., D\}$, $B = \{1, ..., D\} \backslash A$. We have:

$$p(\mathbf{X}_A = \mathbf{x}_A | \mathbf{X}_B = \mathbf{x}_B) = \mathcal{N}(\mathbf{x}_A; \mu_{A|B}, \Sigma_{AA|B})$$

$$\mu_{A|B} = \mu_A + \Sigma_{AB}(\Sigma_{BB})^{-1}(\mathbf{x}_B - \mu_B)$$

$$\Sigma_{AA|B} = \Sigma_{AA} - \Sigma_{AB}(\Sigma_{BB})^{-1}\Sigma_{BA}$$

# Conditioning for MVNs: Example



# Factor Analysis

- Factor analysis is a classical statistical model for linear manifolds based on the multivariate normal distribution.

- The model asserts that real-valued data $\mathbf{x} \in \mathbb{R}^D$ are generated in a two stage process that starts by first generating a low-dimensional latent factor vector $\mathbf{z} \in \mathbb{R}^K$ from a multivariate normal distribution.
- The observed $\mathbf{x}$'s are then generated by a linear combination of basis vectors weighted by the latent factor values: $\mathbf{Wz}$ with independent Gaussian noise added.

- The matrix $\mathbf{W}$ has size $D \times K$. Each column of $\mathbf{W}$ corresponds to a basis vector.

# Factor Analysis: Probabilistic Model

- The probabilistic model/generative process for factor analysis is shown below:

$$
\begin{aligned}
p(\mathbf{X}=\mathbf{x}, \mathbf{Z}=\mathbf{z}) &= p(\mathbf{X}=\mathbf{x}|\mathbf{Z}=\mathbf{z})p(\mathbf{Z}=\mathbf{z}) \\
p(\mathbf{Z}=\mathbf{z}) &= \mathcal{N}(\mathbf{z}; 0, I) \\
p(\mathbf{X}=\mathbf{x}|\mathbf{Z}=\mathbf{z}) &= \mathcal{N}(\mathbf{x}; \mathbf{W}\mathbf{z}+\mu, \Psi)
\end{aligned}
$$

- $\Psi$ is restricted to be a positive, diagonal matrix. We can learn $\mu$, or simply remove the data set mean and require $\mu = 0$. We will assume the data mean has been removed and thus the optimal value of $\mu$ is 0.

# Factor Analysis: Marginal Distribution

- The marginal distribution of **X** is is given by:

$$
\begin{aligned}
P(\mathbf{X} = \mathbf{x}) &= \int \mathcal{N}(\mathbf{x}; \mathbf{W}\mathbf{z}, \Psi)\mathcal{N}(\mathbf{z}; 0, I)d\mathbf{z} \\
&= \mathcal{N}(\mathbf{x}; 0, \mathbf{W}\mathbf{W}^T + \Psi)
\end{aligned}
$$

# Factor Analysis: Learning

- To learn the factor analysis model, we need to minimize the negative log marginal likelihood:

$$
\begin{aligned}
\mathrm{nlml}(\mathcal{D}, \theta) &= -\sum_{n=1}^{N} \log \mathcal{N}(\mathbf{x}_n; 0, \mathbf{W}\mathbf{W}^T + \Psi) \\
&= \frac{N}{2}\log(|2\pi(\mathbf{W}\mathbf{W}^T + \Psi)|) + \frac{1}{2}\sum_{n=1}^{N} \mathbf{x}_n^T(\mathbf{W}\mathbf{W}^T + \Psi)^{-1}\mathbf{x}_n
\end{aligned}
$$

- Question: To learn the model via direct NLML minimization, what parameter constraints do we need to enforce?

# Factor Analysis: Generation/Decoding

- A learned factor analysis model can be used as a *generator*.
- We can choose any vector $\mathbf{z}$, plug it in to the model, and obtain the mean of $p(\mathbf{x}|\mathbf{z})$ as $\mathbf{W}\mathbf{z}$.
- If we want a probabilistic generator, we can sample from $p(\mathbf{x}|\mathbf{z})$.
- This generate a new data case $\mathbf{x}$ based on the latent code $\mathbf{z}$ that we supplied.
- This process is also referred to a *decoding*

# Factor Analysis: Dimensionality Reduction/Encoding

- A learned factor analysis model can be used as a probabilistic dimensionality reduction model.
- Given a centered value for $\mathbf{x}$, we need to infer the probability distribution on the low-dimensional code $\mathbf{z}$. We have:

$$
\begin{aligned}
p(\mathbf{z}|\mathbf{x}) &= \mathcal{N}(\mathbf{z}; \bar{\mathbf{z}}, \mathbf{S}) \\
\mathbf{S} &= (I + \mathbf{W}^T \Psi \mathbf{W})^{-1} \\
\bar{\mathbf{z}} &= \mathbf{S}\mathbf{W}^T \Psi^{-1} \mathbf{x}
\end{aligned}
$$

- $\bar{\mathbf{z}}$ is obtained via a linear projection from $D$ dimensional space to $K$ dimensional space. This process is referred to as *encoding*.

# Factor Analysis: Reconstruction

- A learned factor analysis model can be used to “reconstruct" an input $\mathbf{x}$ by first encoding $\mathbf{x}$ into $\bar{\mathbf{z}}$, then decoding it back into $\mathbf{x}'$.
- This process can be useful for solving unsupervised de-noising tasks.