Selected Topics in Mathematics of Learning

High-Dimensional Statistics

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Part V: Large Inverse Covariance Matrices

Objectives:

1. **Understand the Concept of the Precision Matrix**
   - Define the precision matrix and explain its relationship to the inverse of the covariance matrix.
   - Explore its role in capturing conditional independencies in multivariate distributions.

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   - Interpret the structure of graphical models and their connection to the precision matrix.
   - Distinguish between independence and conditional independence in the context of graphs.

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2. **Analyze Graphical Representations of Relationships in Data**
   - Interpret the structure of graphical models and their connection to the precision matrix.
   - Distinguish between independence and conditional independence in the context of graphs.
3. **Deepen Knowledge of the Multivariate Normal Distribution**
   - Examine the role of the precision matrix within the multivariate normal framework.
   - Relate matrix theory concepts to covariance and precision matrices.

4. **Evaluate Methods for Estimating the Precision Matrix**
   - Discuss the limitations of directly using $\widehat{\Sigma}^{-1}$ (the inverse of the sample covariance matrix).
   - Introduce and explain the graphical LASSO as a sparsity-inducing method for precision matrix estimation.

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   - Compare and contrast covariance matrices with precision matrices in practical contexts.
6. **Explore Regularization and Model Selection Techniques**
   - Understand the role of regularization in estimating sparse precision matrices.
   - Learn criteria and strategies for selecting the optimal regularization parameter.

Outline

1. Precision matrix
   1. Graphs
   2. Independence vs uncorrelatedness
   3. Independence vs conditional independence
   4. Multivariate normal
   5. Some more matrix theory

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1. Precision Matrix

What is the Precision Matrix?

- The precision matrix, denoted by: $\Theta = (\Theta_{ij})_{i,j=1,\ldots,p} = \Sigma^{-1}$ is the inverse of the covariance matrix.
- Many statistical procedures focus on estimating Θ rather than Σ.
- Why? Θ reveals **conditional independence relationships**, providing insights into the underlying structure of the data.

Why is the Precision Matrix Important?

- It helps uncover relationships between variables by describing how they depend on one another after accounting for all other variables.
- This makes Θ a fundamental tool in learning data structures and interpreting dependencies.

To interpret the precision matrix properly, we will need to learn more about

- **Undirected Graphs**
- **Independence vs Conditional Independence**
- **Multivariate Normal Distribution**
- **Matrix Theory**

1.1 Undirected Graph

- A **graph** G consists of:
  - **Vertices** (V): A set of points (nodes).
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- **Subgraph**:
  - A subset $U \subseteq V$, along with all edges between vertices in U.

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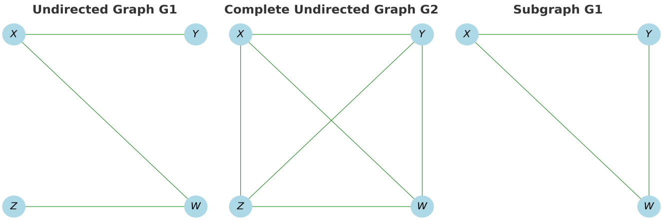

Notice that G1 is a subgraph to graph G2 but not to graph G1.

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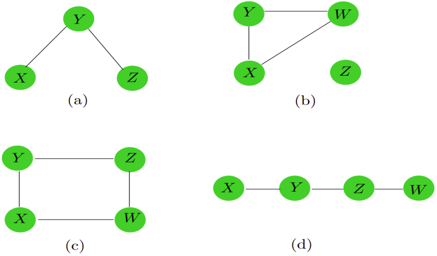

The adjacency matrix A corresponding to the graph in (b) is given by:

$$A = \begin{bmatrix} xx & xy & xz & xw \\ yx & yy & yz & yw \\ zx & zy & zz & zw \\ wx & wy & wz & ww \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix}$$

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For **Continuous** independent random variables (denoted $X \perp\!\!\!\perp Y$):

we have: $f_{X,Y}(x,y) = f_X(x) \cdot f_Y(y)$

where $\quad F_{X,Y}(x,y) = \mathbb{P}(X \leq x, Y \leq y) \quad$ and $\quad f_{X,Y}(x,y) = \dfrac{\partial^2 F_{X,Y}(x,y)}{\partial x \, \partial y}$

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The marginal distribution of a single variable is obtained by summing or integrating out the other variable(s) from the joint distribution:

$$f_X(x) = \int_{-\infty}^{\infty} f_{X,Y}(x, y) \, dy \quad f_Y(y) = \int_{-\infty}^{\infty} f_{X,Y}(x, y) \, dx$$

In terms of events we can formulate: Two events A and B are **independent** if and only if $\mathbb{P}(A \cap B) = \mathbb{P}(A) \cdot \mathbb{P}(B)$.

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Example:

- Rolling a die: Getting a 6 on the first roll (A) and getting a 6 on the second roll (B) are independent events.
- By contrast, the event of getting a 6 the first time a die is rolled and the event that the sum of the numbers seen on the first and second trial is 8 are not independent.

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- Let W be a random variable such that:

$$\mathbb{P}(W = 1) = \mathbb{P}(W = -1) = \frac{1}{2}.$$

- Let $X \sim N(0, 1)$ (standard normal random variable).
- Define $Y := WX$.

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Analysis:

$$\begin{aligned}
\mathrm{Cov}(X, Y) &= \mathbb{E}[XY] = \mathbb{E}[X \cdot WX] = \mathbb{E}[X^2 W] \\
&= \mathbb{E}[X^2] \cdot \mathbb{E}[W] && \text{(since } X^2 \text{ and } W \text{ are independent)} \\
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Calculation of $\mathbb{E}[W]$: $\mathbb{E}[W]=1\cdot\mathbb{P}(W=1)+(-1)\cdot\mathbb{P}(W=-1)=\frac{1}{2}-\frac{1}{2}=0.$

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Calculation of $\mathbb{E}[W]$: $\mathbb{E}[W] = 1 \cdot \mathbb{P}(W = 1) + (-1) \cdot \mathbb{P}(W = -1) = \frac{1}{2} - \frac{1}{2} = 0.$
Conclusion: $\mathrm{Cov}(X, Y) = 0$. Thus, although $\mathrm{Cov}(X, Y) = 0$, X and Y are **not** independent because Y is defined as a function of X ($Y = WX$).

1.3 Independence vs conditional independence

Two variables X and Y are conditionally independent given variable Z, if and only if their conditional distribution factorizes as:

$$f_{X,Y|Z=z}(x,y) = f_{X|Z=z}(x)f_{Y|Z=z}(y)$$

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Notation: $X \perp\!\!\!\perp Y | Z$. (For continuous random variables.)
Let A, B and C be events. Then, A and B are conditionally independent given C, if and only if $P(C) > 0$ and ,

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In that case we have $\mathbb{P}(A|B, C) = \mathbb{P}(A|C)$, i.e. in light of information C, B provides no (further) information about A.

$$\mathbb{P}(A \mid C) = \frac{\mathbb{P}(A \cap C)}{\mathbb{P}(C)}$$

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- **Independent Events:**
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  - This extra information restricts the possible outcomes of the second die to odd numbers.

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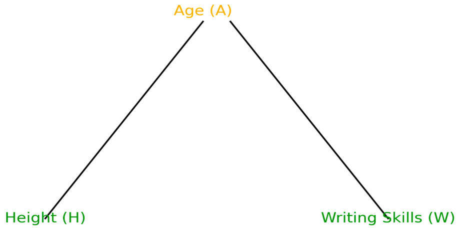
  - Observing the result of one die gives no information about the result of the other die.
- **Conditionally Dependent Events:**
  - Suppose the result of the first die is 3.
  - Someone tells you a third event: "The sum of the two results is even."
  - This extra information restricts the possible outcomes of the second die to odd numbers.
- **Conclusion:** While the two dice are independent, they are **not conditionally independent** given the sum is even.

1.3 Independence vs conditional independence: Conditioning Example

Observations:

- Random sample of school kids.
- Age (A) correlates with both height (H) and writing skills (W).



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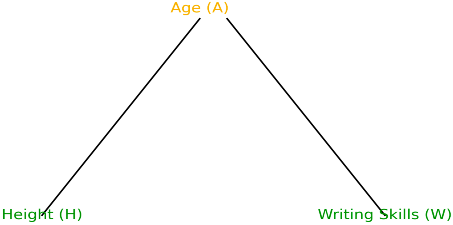

Conditioning:

- Fix $A = 10$ (e.g., consider only one age group).
- **Effect:** Removes correlation between H and W that is due to age as a common factor.

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Conditional Probability:

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$$P(H \leq 170 \cap W \leq 80 \mid A = 10) = P(H \leq 170 \mid A = 10)P(W \leq 80 \mid A = 10)$$

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Adding Another Variable:

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Adding Another Variable:

$$P(H \cap W \mid V, A) = P(H \mid V, A)P(W \mid V, A)$$

- **Assumption:** H and W are conditionally independent given both V and A.

1.4 Multivariate normal

Uncorrelated and independent
Suppose that $X = (X_1, \dots, X_p)^\top \sim \mathcal{N}(\mu, \Sigma)$.
Partition the multivariate normal distribution:

$$X = \begin{pmatrix} Y_a \\ Y_b \end{pmatrix}$$

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The two random vectors Y_a and Y_b are independent if and only if they are uncorrelated.

$$\mathrm{Cov}(X) = \mathbb{E}\left[\begin{pmatrix} Y_a \\ Y_b \end{pmatrix} \begin{pmatrix} Y_a' & Y_b' \end{pmatrix} \right] = \begin{pmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{pmatrix}$$

Marginal distribution

Partition the multivariate normal distribution:

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Conveniently, the marginal distributions are exactly what you would intuitively think they should be:

$$Y_a \sim \mathcal{N}(\mu_a, \Sigma_{aa}).$$

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Conditional

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A more complicated question: what is the distribution of Y_a given Y_b?

This gets messy if Σ is singular, but if Σ is full rank, then

$$Y_a | Y_b = y_b \sim \mathcal{N}(\mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(y_b - \mu_b), \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}),$$

where $\Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba} = \mathrm{Cov}(Y_a | Y_b = y_b)$.

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where $\Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba} = \mathrm{Cov}(Y_a | Y_b = y_b)$.

Note that if $\Sigma_{ab} = 0$, then Y_a and Y_b are independent and $Y_a | Y_b \sim \mathcal{N}(\mu_a, \Sigma_{aa})$.

1.5. Some more matrix theory

Inverse of a 2×2 block matrix

Suppose we have a block matrix

$$\mathbf{M} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}$$

with $\mathbf{D}$ and $\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}$ invertible.

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with $\mathbf{D}$ and $\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}$ invertible. Then, the inverse of the matrix $\mathbf{M}$ is given by

$$\mathbf{M}^{-1} = \begin{bmatrix} \left(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}\right)^{-1} & -\left(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}\right)^{-1}\mathbf{B}\mathbf{D}^{-1} \\ -\mathbf{D}^{-1}\mathbf{C}\left(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}\right)^{-1} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{C}\left(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}\right)^{-1}\mathbf{B}\mathbf{D}^{-1} \end{bmatrix}.$$