# Selected Topics in Mathematics of Learning

**High-Dimensional Statistics**

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## Part I

### Why high-dimensional statistics?

**Objectives:**

- **Understand the importance of high-dimensional statistics:**
  - Explain why high-dimensional data is critical in modern data science and machine learning.

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- **Identify common challenges in high dimensions:**
  - Discuss computational and statistical difficulties in high-dimensional data.

## Part I

### Why high-dimensional statistics?

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- **Understand the importance of high-dimensional statistics:**
  - Explain why high-dimensional data is critical in modern data science and machine learning.
- **Identify common challenges in high dimensions:**
  - Discuss computational and statistical difficulties in high-dimensional data.
- **Explore specific examples**
- **Discuss solutions:**
  - Present methods like dimension reduction to handle challenges.

# Outline

# 1. Why High-Dimensional Statistics?

## High-dimensional data: Motivation

- **Intensive data collection with increasing number of features measured per individual.**
    - Biotech data (e.g., genetics: millions of genes and combinations per observation).
    - High-resolution imaging (millions of pixels/voxels).
    - Finance (e.g., stock indices).
    - Climate studies.
    - Web data.
    - Crowdsourcing data, etc

# 1.1 High-Dimensional Data: Blessing or Curse?

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## Curse

- Separating the signal from the noise is in general almost impossible in high-dimensional data, computations can rapidly exceed the available resources, volumes can unexpectedly vanish.

# 1.2 Classical vs. High-Dimensional Statistical Theories

## 1. Classical Theory

- Assumption: $N \gg p$ (number of observations $N$ is much larger than the number of features $p$).
- Asymptotic assumption: $p$ is fixed while $N \to \infty$.
- Key tools:
  - Law of Large Numbers (LLN)
  - Central Limit Theorem (CLT)

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## 2. High-Dimensional Theory

- Assumptions:
  - $N \sim p$, e.g., $\frac{N}{p} \to \alpha$ (finite ratio as $N, p \to \infty$).
  - $p \gg N$, e.g., $p \sim e^N$ (exponential growth of $p$ relative to $N$).
- Often non-asymptotic (finite-sample) analysis such as concentration inequalities.

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## 3. Challenges in High Dimensions

- Number of features $p$ may exceed the number of observations $N$. E.g., 104 genes per only 50 samples.
- Not all features are relevant for answering a specific question.
- Classical methods often fail (e.g., linear regression, covariance estimation) due to the "curse of dimensionality."

## 2. What can go wrong in high dimensions?
### High-dimensional ball and volume concentration

- In high-dimensional spaces, the volume of a ball is concentrated near its surface.
- Let $B_p(0, r)$ represent an Euclidean ball of radius $r$ in $p$-dimensions.
- The volume of such a ball is: $V_p(r) = r^p V_p(1)$ where $V_p(1)$ is the volume of a unit ball in $p$-dimensions.

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### Crust of a High-Dimensional Ball

- Define the “crust" as the thin outer layer: $C_p(r) = B_p(0, r) \setminus B_p(0, 0.99r)$
- The fraction of the volume in the crust is: $\frac{\text{volume}(C_p(r))}{\text{volume}(B_p(0,r))} = 1 - 0.99^p$

- As $p \to \infty$, $1 - 0.99^p$ approaches 1, meaning almost all the volume is concentrated in the crust. Thus, a ball is essentially a sphere in high dimensions.

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**Takeaway**

In high dimensions, most of the volume is located near the surface, which defies low-dimensional intuition. This result shows that our usual intuition about shapes doesn't hold in high dimensions, which has significant implications for understanding high-dimensional data and probability distributions.

1. **Volume of a unit ball in $\mathbb{R}^p$:** $V_p(1) := \frac{\pi^{p/2}}{\Gamma\left(\frac{p}{2}+1\right)}$.

   where $\Gamma$ is the gamma function, a generalization of the factorial function such that $\Gamma(p) = (p-1)! \quad$ for positive integers $p$.

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2. **By Stirling's approximation for large $p$:** That is $p! \approx \sqrt{2\pi p}\left(\frac{p}{e}\right)^p$, we get: $\Gamma\left(\frac{p}{2}+1\right) \sim \sqrt{2\pi\frac{p}{2}}\left(\frac{p}{2e}\right)^{\frac{p}{2}}$.

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3. **Asymptotic behavior of $V_p(1)$:** $V_p(1) \sim \left(\frac{2\pi e}{p}\right)^{p/2} (p\pi)^{-1/2}$.

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4. **Volume of a ball with radius $r$ in $\mathbb{R}^p$:** $V_p(r) = r^p V_p(1)$.

   This volume also vanishes as $p \to \infty$.

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### Unreliable empirical covariance matrix

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- When $p$ (number of features) is large relative to $n$ (number of observations), the empirical (observed) covariance $\hat{\Sigma}$ may not accurately represent the true (theoretical) covariance.

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**Takeaway**

Be cautious with empirical covariance matrices in high dimensions; alternative techniques or regularization may be needed.

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### Unreliable empirical covariance matrix

Empirical covariance in High-Dimension

. Let $x_1, \dots, x_m \overset{iid}{\sim} \mathcal{N}(0, \underbrace{\Sigma}_{p \times p})$ with $\Sigma = I_p$.

. $Sp(\Sigma) = (1, \dots, 1)$ (p times)

. Empirical covariance

$$\hat{\Sigma} = \frac{1}{m} \sum_{i=1}^{m} x_i x_i^T .$$

We have $\operatorname{rank}(\hat{\Sigma}) = m$ so

$$\begin{aligned} m\, \mathbb{E}[|\hat{\Sigma}|_{op}] &\geq \mathbb{E}[Tr(\hat{\Sigma})] \\ &= Tr(\mathbb{E}[\hat{\Sigma}]) \\ &= Tr\Big(\frac{1}{m} \sum_{i=1}^{m} \underbrace{\mathbb{E}[x_i x_i^T]}_{= \Sigma}\Big) \\ &= Tr(\Sigma) = p \end{aligned}$$

So $\mathbb{E}[|\hat{\Sigma}|_{op}] \geq \frac{p}{m} \underset{\text{if } p \gg m}{\gg} 1 = |\Sigma|_{op}$

. Furthermore, we can prove (later) that

$$\mathbb{E}[|\hat{\Sigma}|_{op}] \leq \Big(1 + \sqrt{\frac{p}{m}}\Big)^2 \underset{p \gg m}{=} \frac{p}{m}(1 + o(1))$$

So

$$Sp(\hat{\Sigma}) \underset{p \gg m}{\approx} \Big(\underbrace{\frac{p}{m}(1+o(1)), \dots, \frac{p}{m}(1+o(1))}_{m \text{ times}}\Big)$$

$\leadsto$ very different from $sp(\Sigma)$,

so we cannot rely on $\hat{\Sigma}$ when $p \gg m$.

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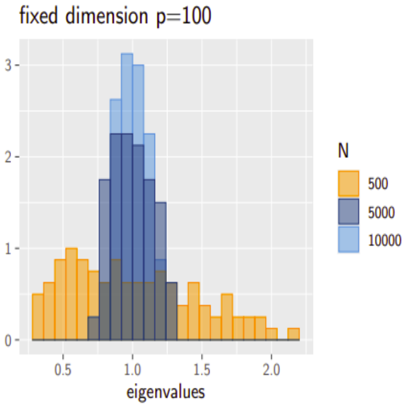
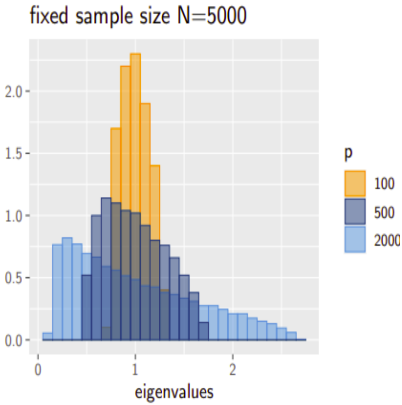
### Unreliable empirical covariance matrix




Left: For fixed and small $p$, eigenvalues of $\Sigma$ peak at 1 as $N \to \infty$.
Right: For fixed $N$, eigenvalues of $\hat{\Sigma}$ does not peak at 1 as $p \to \infty$.

## 2. What can go wrong in high dimensions?
### Unbounded distribution of the pairwise distances between points (Lost in high-dimensional spaces)

Let the random variables $X^{(1)}, X^{(2)}, \dots, X^{(n)}$ be i.i.d with $\sim \mathcal{U}([0,1]^p)$ distribution, i.e., independent and uniformly distributed in the hypercube $[0,1]^p$.

**Pairwise Distances:** The distance between two points $X^{(i)}$ and $X^{(j)}$ is given by:

$$d_{ij} = \|X^{(i)} - X^{(j)}\| = \sqrt{\sum_{k=1}^{p} \left(X_k^{(i)} - X_k^{(j)}\right)^2}.$$

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**Expected Value of Squared Distances:**

$$\mathbb{E}\left[\|X^{(i)} - X^{(j)}\|^2\right] = \sum_{k=1}^{p} \mathbb{E}\left[\left(X_k^{(i)} - X_k^{(j)}\right)^2\right] = p \cdot \mathbb{E}\left[(U - U')^2\right] \stackrel{?}{=} \frac{p}{6}.$$

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**Standard Deviation of Squared Distances:**

$$\text{Std}\left[\|X^{(i)} - X^{(j)}\|^2\right] = \sqrt{\sum_{k=1}^{p} \text{Var}\left[\left(X_k^{(i)} - X_k^{(j)}\right)^2\right]} = \sqrt{p \cdot \text{Var}\left[(U - U')^2\right]} \overset{?}{\approx} 0.2\sqrt{p}.$$

where $U$ and $U'$ are two i.i.d. random variables with $\sim \mathcal{U}([0,1])$ distribution.

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## (Lost in high-dimensional spaces)

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As the dimension $p \to \infty$, both the mean and variance of squared distances grow, causing distances to become increasingly large on average. This makes tasks like clustering or nearest neighbor classification challenging, as points become relatively far from each other, making it difficult to define meaningful similarities or groups based on distance metrics.

## Take Home Message (so far)

In high-dimensional spaces, be careful not to be mislead by your low-dimensional intuitions !!

## 2. What can go wrong in high dimensions?
### Curse 1 of Dimensionality: Fluctuations cumulate

Let $X^{(1)}, \dots, X^{(n)} \in \mathbb{R}^p$ be i.i.d. random vectors with $\mathrm{cov}(X) = \sigma^2 I_p$. We want to estimate the expected value $\mathbb{E}[X]$ using the sample mean:

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**Variance of the Sample Mean:**

$$\mathbb{E}\left[\|\overline{X}_n - \mathbb{E}[X]\|^2\right] = \sum_{j=1}^{p} \mathbb{E}\left[\left(\overline{X}_{n,j} - \mathbb{E}[X_j]\right)^2\right] = \sum_{j=1}^{p} \text{Var}(\overline{X}_{n,j}).$$

Since $\text{Var}(\overline{X}_{n,j}) = \frac{\sigma^2}{n}$, we get:

$$\mathbb{E}\left[\|\overline{X}_n - \mathbb{E}[X]\|^2\right] = \frac{p\sigma^2}{n}.$$

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**Implication:** When $p \gg n$, the error in estimating the mean grows with the dimensionality $p$, making it difficult to accurately estimate $\mathbb{E}[X]$.

**Observations:** $(Y_i, X^{(i)}) \in \mathbb{R} \times [0,1]^p$ for $i = 1, \ldots, n$.

**Model:** $Y_i = f(X^{(i)}) + \epsilon_i$, where $f$ is smooth and the $\epsilon_i$ are noise terms.

Assume that $(Y_i, X^{(i)})_{i=1,\ldots,n}$ are i.i.d., and that $X^{(i)} \sim \mathcal{U}([0,1]^p)$.

**Local averaging:** Estimate $f$ using local averaging:

$$\hat{f}(x) = \text{average of } \{Y_i : X^{(i)} \text{ close to } x\}.$$

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- The **union bound** (Boole's Inequality) states that for any events $A_1, A_2, \dots, A_n$:

$$\mathbb{P}\left(\bigcup_{i=1}^{n} A_i\right) \leq \sum_{i=1}^{n} \mathbb{P}(A_i).$$

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### Curse 2 of Dimensionality: Local averaging is ineffective

**Observations:** $(Y_i, X^{(i)}) \in \mathbb{R} \times [0,1]^p$ for $i = 1, \ldots, n$.

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- The event $\exists i \in \{1, \ldots, n\} : \|x - X^{(i)}\| \leq \delta$ is equivalent to the union of the events $A_i$:

$$\exists i \in \{1, \ldots, n\} : \|x - X^{(i)}\| \leq \delta \quad \Leftrightarrow \quad \bigcup_{i=1}^{n} \left\{\|x - X^{(i)}\| \leq \delta\right\}.$$

- Applying the union bound to this union of events gives:

$$\mathbb{P}\left[\bigcup_{i=1}^{n}\left\{\|x - X^{(i)}\| \leq \delta\right\}\right] \leq \sum_{i=1}^{n}\mathbb{P}\left[\|x - X^{(i)}\| \leq \delta\right].$$

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- Since the $X^{(i)} \overset{i.i.d}{\sim} \mathcal{U}([0,1]^p)$ , each term in the sum is equal:

$$\mathbb{P}\left[\|x - X^{(1)}\| \leq \delta\right] = \mathbb{P}\left[\|x - X^{(2)}\| \leq \delta\right] = \ldots = \mathbb{P}\left[\|x - X^{(n)}\| \leq \delta\right].$$

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- Thus, the sum simplifies to:

$$\sum_{i=1}^{n} \mathbb{P}\left[\|x - X^{(i)}\| \leq \delta\right] = n\,\mathbb{P}\left[\|x - X^{(1)}\| \leq \delta\right].$$

**Problem:** For $x \in [0,1]^p$, we have:

$$\mathbb{P}\left[\exists i \in \{1, \ldots, n\} : \|x - X^{(i)}\| \leq \delta\right] \leq n\mathbb{P}\left[\|x - X^{(1)}\| \leq \delta\right] \leq nV_p(\delta),$$

where $V_p(\delta)$ is the volume of a ball of radius $\delta$ in $\mathbb{R}^p$.

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As $p \to \infty$: The volume $V_p(\delta) \approx \left(\frac{2\pi e}{p}\right)^{p/2} \delta^p \sqrt{\pi p}$, and the probability decreases rapidly:

$$nV_p(\delta) \to 0 \text{ as } p \to \infty.$$

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**Conclusion:** In high dimensions, finding enough data points close to $x$ becomes extremely unlikely, making local averaging ineffective.

**Question: Which sample size is needed to avoid the loss of locality?**

Number $n$ of points $x_1, \ldots, x_n$ required for having at least one observation at distance $\delta = 1$ with probability $1/2$:

$$n \geq \frac{1}{2V_p(1)} \quad \text{where} \quad V_p(1) = \text{Volume of a unit ball in } \mathbb{R}^p.$$

As $p \to \infty$: The volume $V_p(\delta) \approx \left(\frac{2\pi e}{p}\right)^{p/2} \delta^p \sqrt{\pi p}$, and the probability decreases rapidly:

$$nV_p(\delta) \to 0 \text{ as } p \to \infty.$$

**Conclusion:** In high dimensions, finding enough data points close to $x$ becomes extremely unlikely, making local averaging ineffective.

**Question: Which sample size is needed to avoid the loss of locality?**

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**Asymptotic Behavior:** For large $p$, we have: $V_p(1) \sim \left(\frac{2\pi e}{p}\right)^{p/2} \sqrt{\pi p}$.
**Implications for Sample Size:**

- As $p \to \infty$, $V_p(1)$ decreases rapidly, leading to: $n \geq \left(\frac{p}{2\pi e}\right)^{p/2} \sqrt{\frac{p\pi}{4}}$.

### Which sample size is needed to avoid the loss of locality?

**Example:** For different values of $p$:

| Dimension $p$ | Estimated Sample Size $n$ |
|---|---|
| 20 | 39 |
| 30 | 45630 |
| 50 | $5.7 \times 10^{12}$ |
| 100 | $4.2 \times 10^{39}$ |
| 200 | Larger than the estimated number of particles in the observable universe |

- This required sample size grows exponentially with $p$, making it impractically large for high dimensions.

**Threshold for Detection Increases:**

- In high-dimensional spaces, detecting a weak signal $\theta_j$ becomes challenging because the signal must be significantly larger than the noise.
- Suppose $Z_j \sim N(\sqrt{n}\theta_j, \sigma^2)$, where:
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- As $p$ increases, the signal $\theta_j$ needs to be stronger (larger) to stand out against the noise.
- This makes it harder for weak signals to be detected, as they become obscured by the noise in high-dimensional data.

## Curse 4 of Dimensionality: Multicollinearity (ill-conditioning) of matrices

In high-dimensional data, where the number of predictors $p$ is large, linear regression faces significant computational challenges. These challenges can affect both the feasibility and stability of the model.

The linear regression model is defined as:

$$y = X\beta + \epsilon,$$

where: $y \in \mathbb{R}^n$ (response vector), $X \in \mathbb{R}^{n\times p}$ (design matrix with $n$ observations and $p$ predictors), $\beta \in \mathbb{R}^p$ (coefficient vector) and $\epsilon \in \mathbb{R}^n$ (error vector).

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- When $p$ is large, the $O(p^3)$ complexity becomes computationally expensive, making the inversion step a bottleneck.
- This complexity arises from performing *Gaussian elimination* or using other matrix decomposition methods (e.g., *LU decomposition*).

**2. Numerical Stability:**

- When $p$ is large, multicollinearity (high correlation between predictors) is common.

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- High-dimensional linear regression may become infeasible without sufficient computational resources.
- Optimized algorithms and specialized hardware (e.g., GPUs) can help mitigate some of these challenges.
- Reducing the dimensionality of data through methods like PCA before fitting the model can make computations more manageable.

## 2. What can go wrong in high dimensions?
### Some other curses of dimensionality

- Curse 5: An accumulation of rare events may not be rare (false discoveries, etc). In high-dimensional data, each dimension or variable can be associated with a certain type of "rare event." For example, detecting an anomaly in one variable might be rare, but when you have many variables, the chances that at least one of these variables will exhibit a rare event increase. This is because the probability of encountering at least one rare event grows with the number of variables.

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- Curse 6: Algorithmic complexity must remain low. When $p$ is large, an algorithmic complexity larger than $O(p^2)$ is computationally prohibitive. For very large $p$, even a complexity $O(p^2)$ can be an issue.
- etc

**Hopeless?**

High-dimensional data are often concentrated around low-dimensional structures, reflecting the (relatively) small complexity of the systems producing the data. Examples of low-dimensional structures:

- Geometrical structures in images.
- Regulation networks of a biological system.
- Social structures in marketing data.
- Human technologies have limited complexity, etc

**Dimension Reduction:**

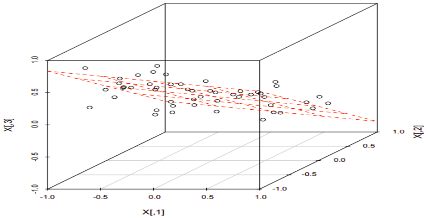
- **Unsupervised**: Principal Component Analysis (PCA).
- **Supervised**: Methods that utilize labeled data.

For any data points $X^{(1)}, \ldots, X^{(n)} \in \mathbb{R}^p$ and any dimension $d \leq p$, PCA computes the linear subspace $V_d$ such that:

$$V_d \in \arg \min_{\mathrm{dim}(V) \leq d} \sum_{i=1}^{n} \|X^{(i)} - \mathrm{Proj}_V X^{(i)}\|^2,$$

where $\mathrm{Proj}_V$ is the orthogonal projection matrix onto the subspace $V$.

**Example:** $V_2$ in dimension $p = 3$.




**Recap on PCA:** PCA finds a lower-dimensional representation of the data that preserves the directions with the most variance, allowing us to approximate the data using fewer dimensions.

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Key questions:
What embedded low-dimensional structures are present in data?
How can they be exploited?