

Linear prediction with **NA**, Imputation versus specific methods

Alexis Ayme

Under the supervision of:

Claire Boyer, Aymeric Dieuleveut and Erwan Scornet



Background

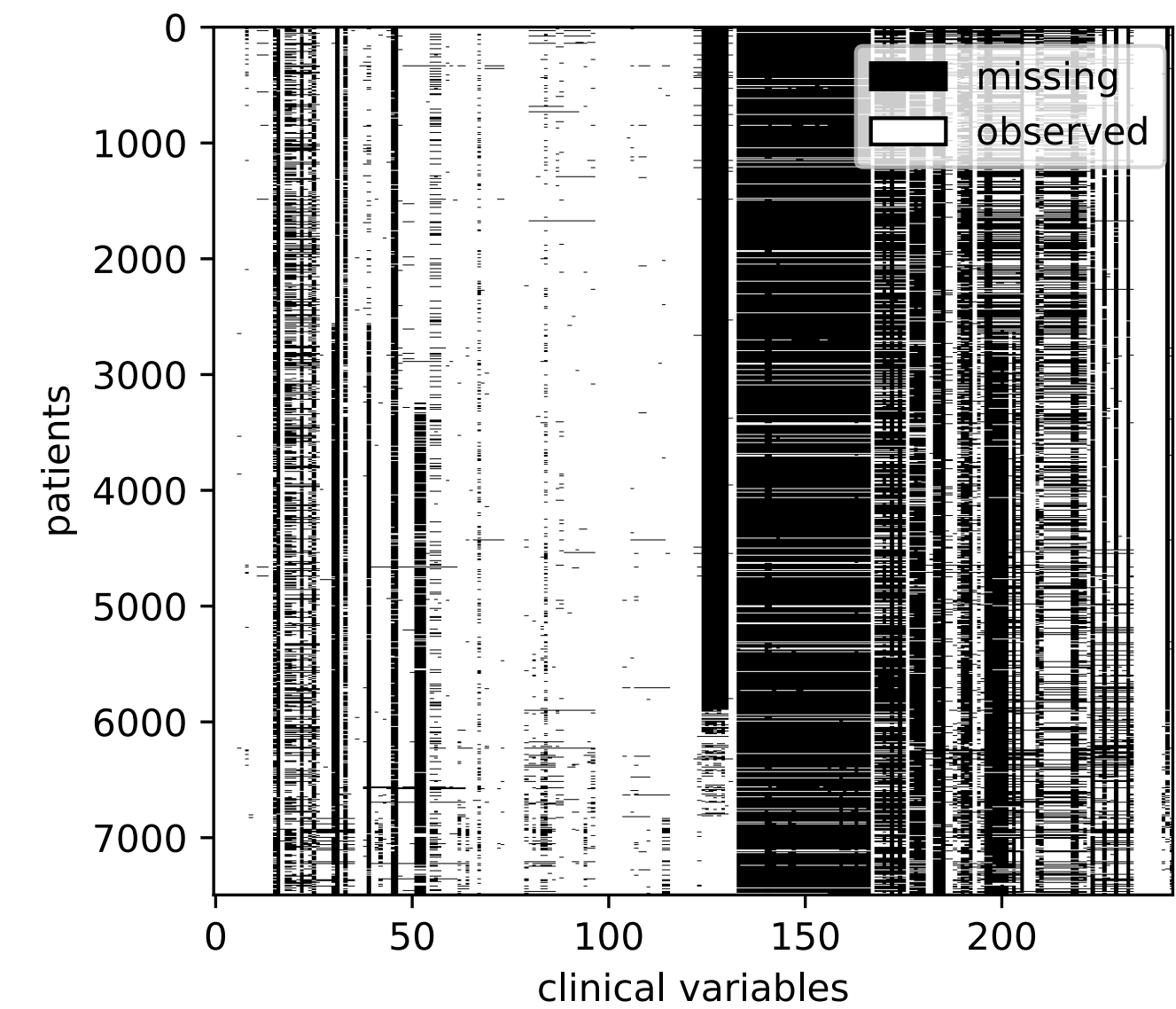
- Growing mass of data => **NA** (not attributed)/missing values

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○ Different sources:

1. Bugs
2. Cost, sensitive data
3. **Multiplication of sources** (i.e. merging)

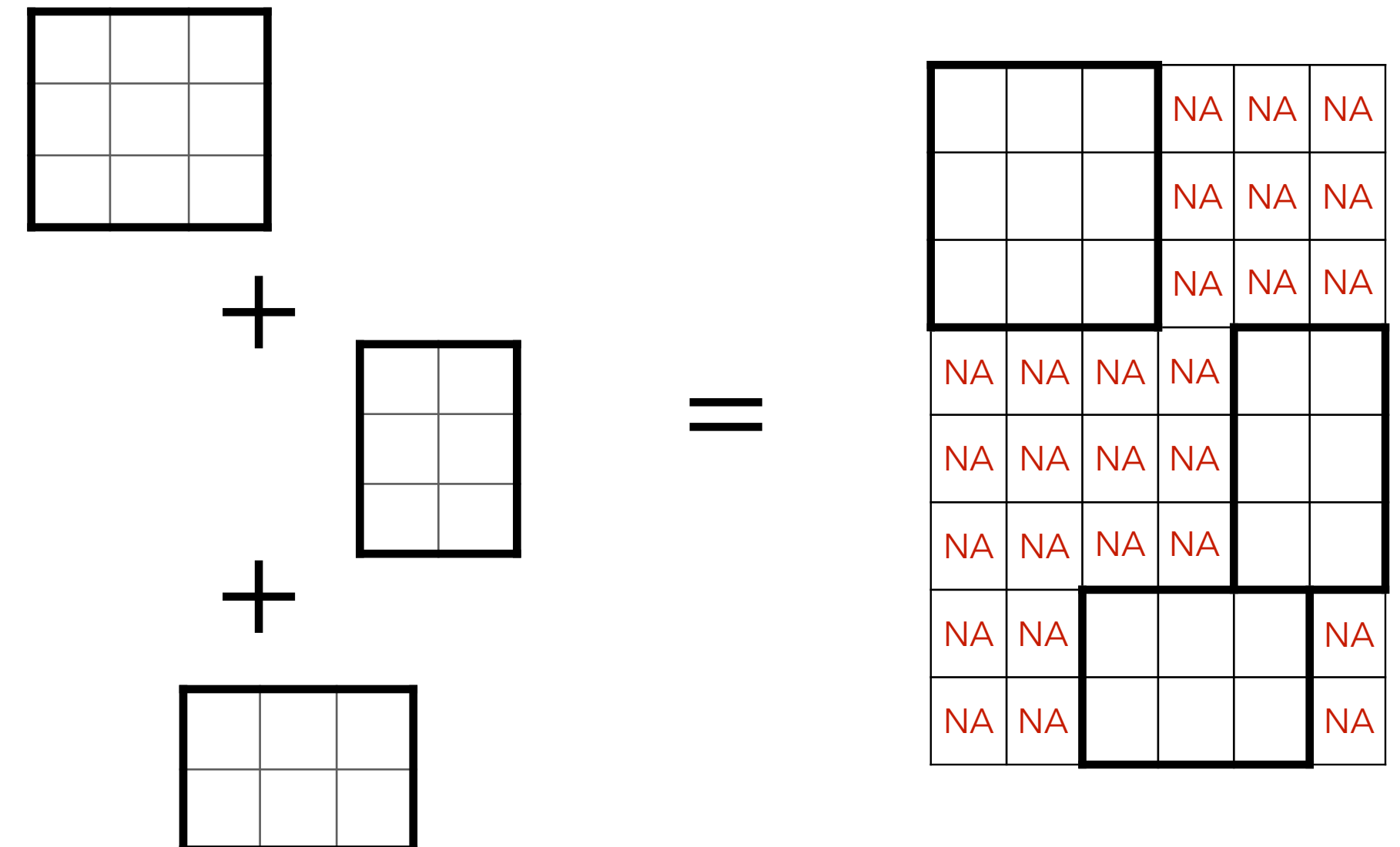
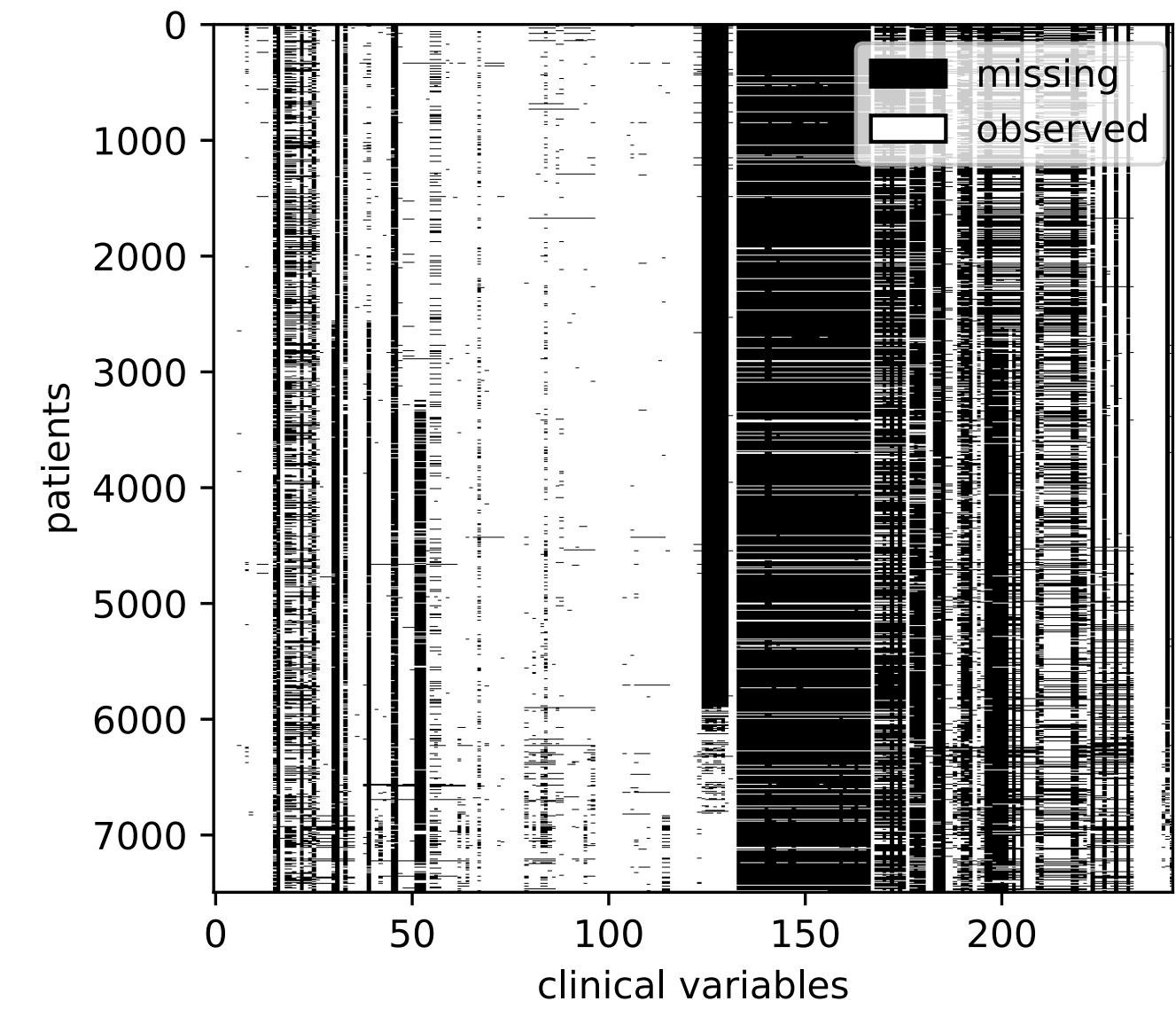


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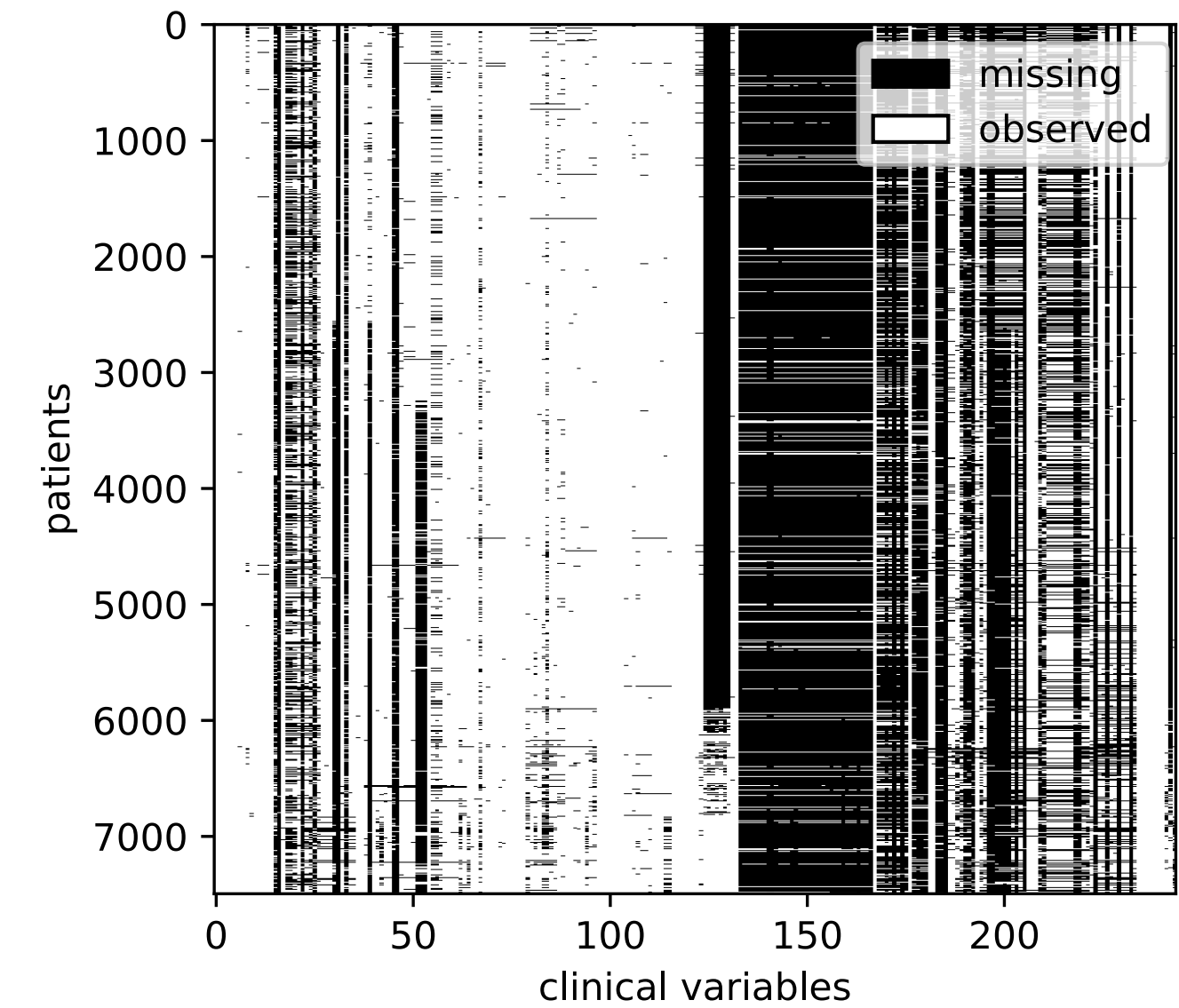


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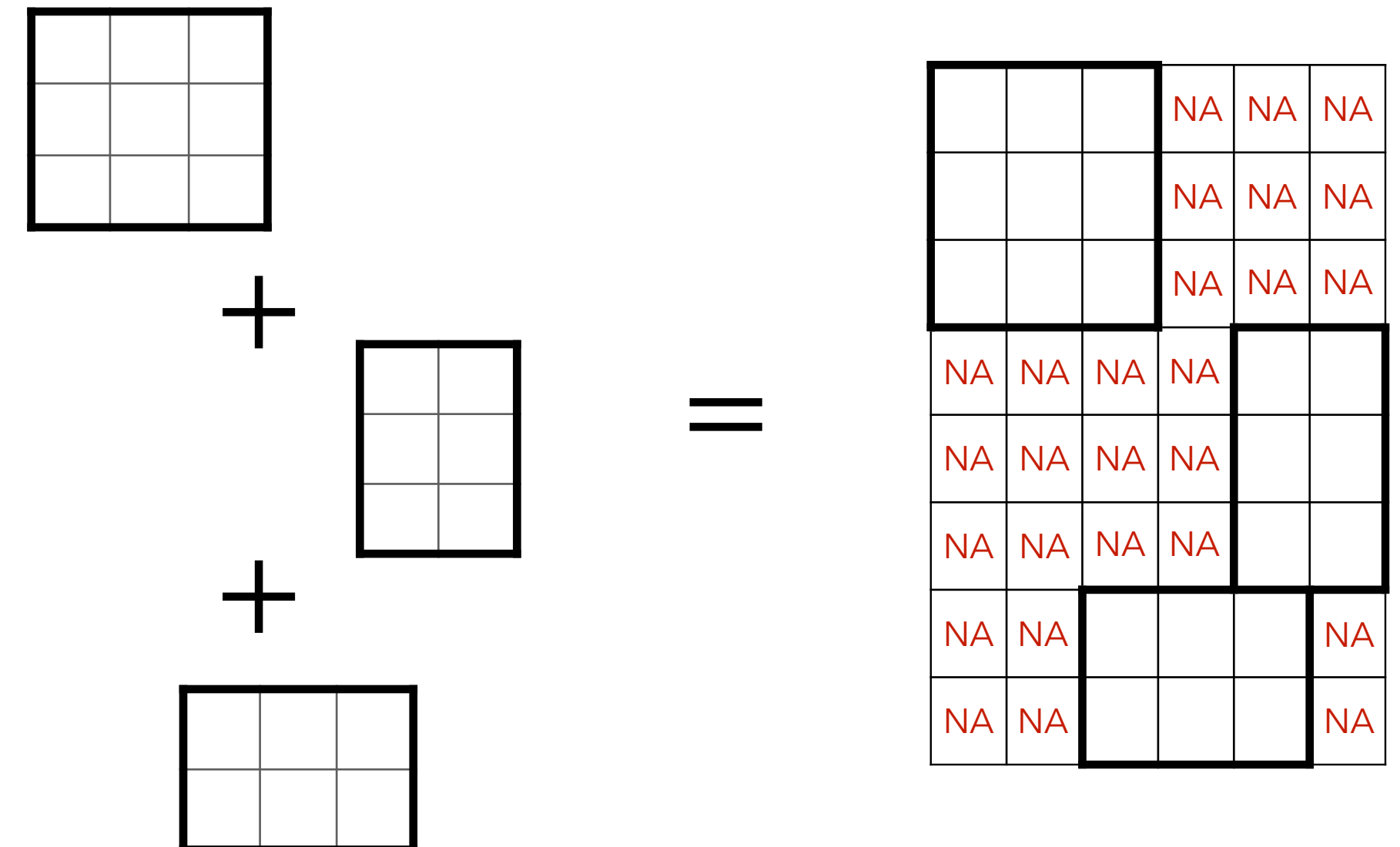
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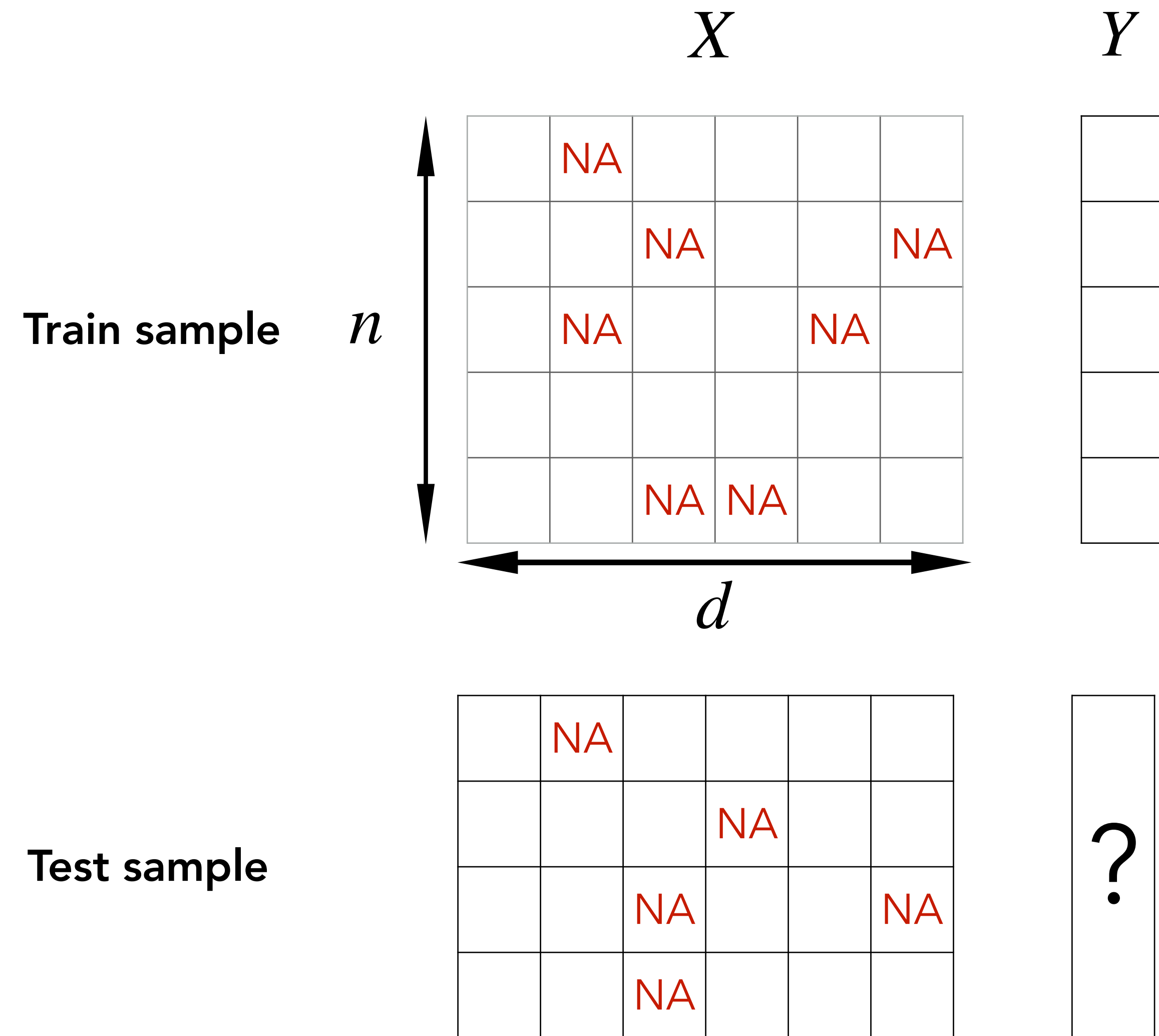


○ Growing mass of data => **High-dimensional** dataset

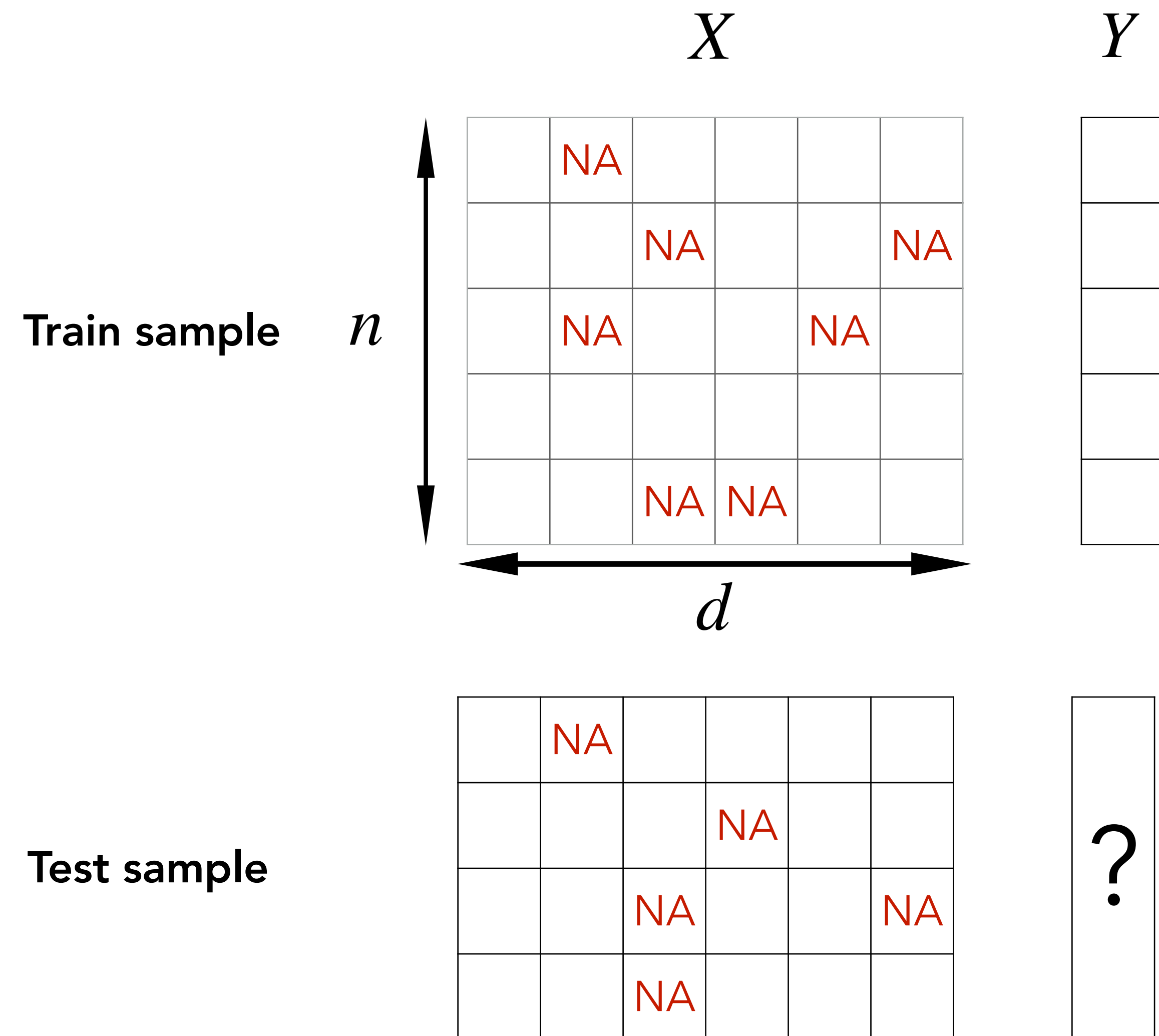
1. Cost
2. **Multiplication of sources** (i.e. merging)
3. Genotype, text



Supervised learning with missing values (NA)



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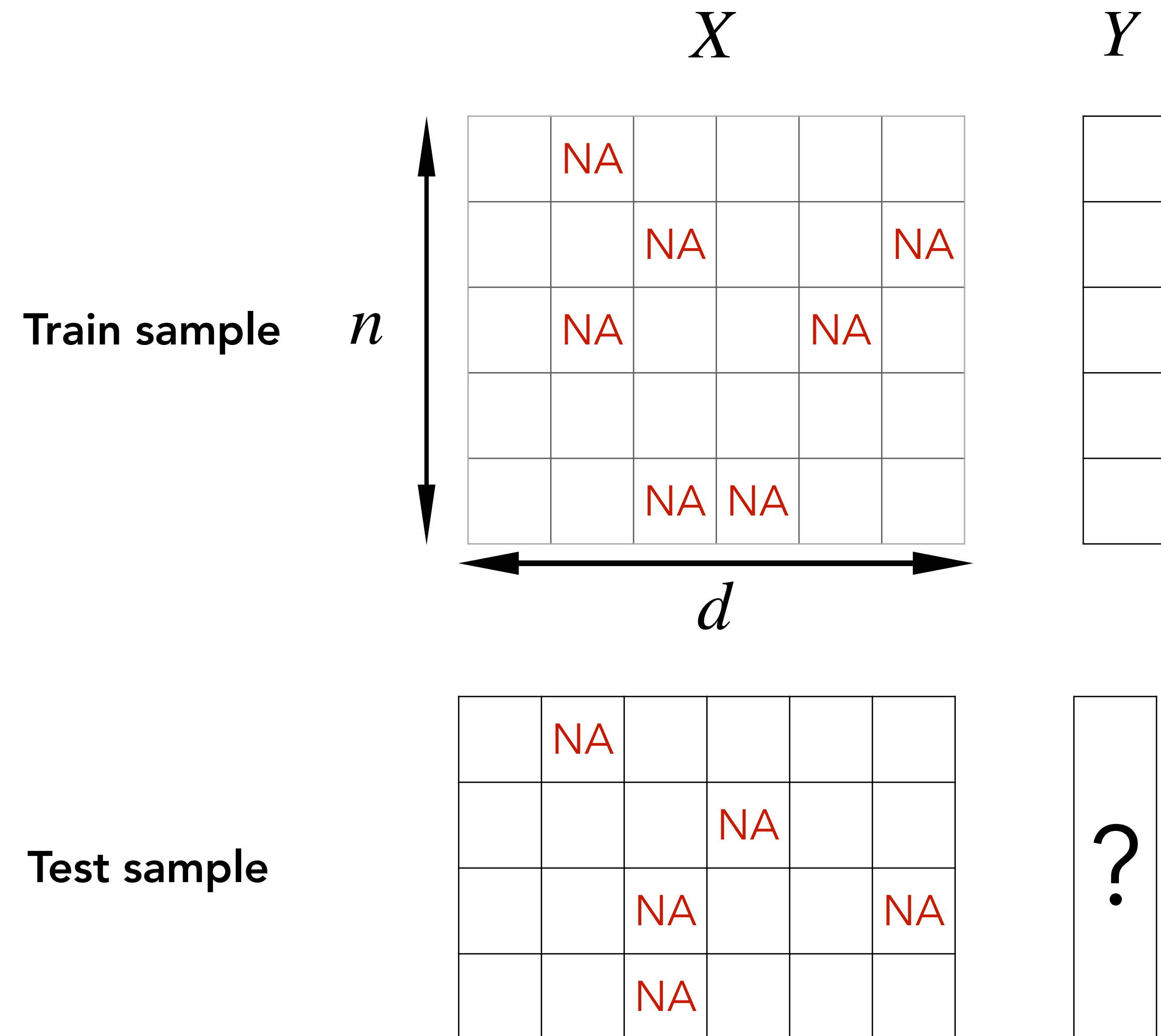
○ Missing pattern: $M_i \in \{0,1\}^d$

$$X_i = (\text{NA}, 8, 0, \text{NA}, 6, 2)$$



$$M_i = (1, 0, 0, 1, 0, 0)$$

Supervised learning with missing values (NA)



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○ Input: $Z = (X_{\text{obs}}, M)$

○ Output: $Y \in \mathbb{R}$

Goal: Predict on **test sample** minimizing

$$R_{\text{missing}}(f) = \mathbb{E}_{Z,Y} \left[(Y - f(Z))^2 \right]$$

Supervised learning vs inference

- **Linear model** for complete inputs

$$Y_i = \beta^\top X_i + \epsilon_i$$

with $\mathbb{E}[\epsilon_i^2] = \sigma^2$ and:

- if model is well specified: $\mathbb{E}[\epsilon_i | X_i] = 0$
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Supervised learning vs inference

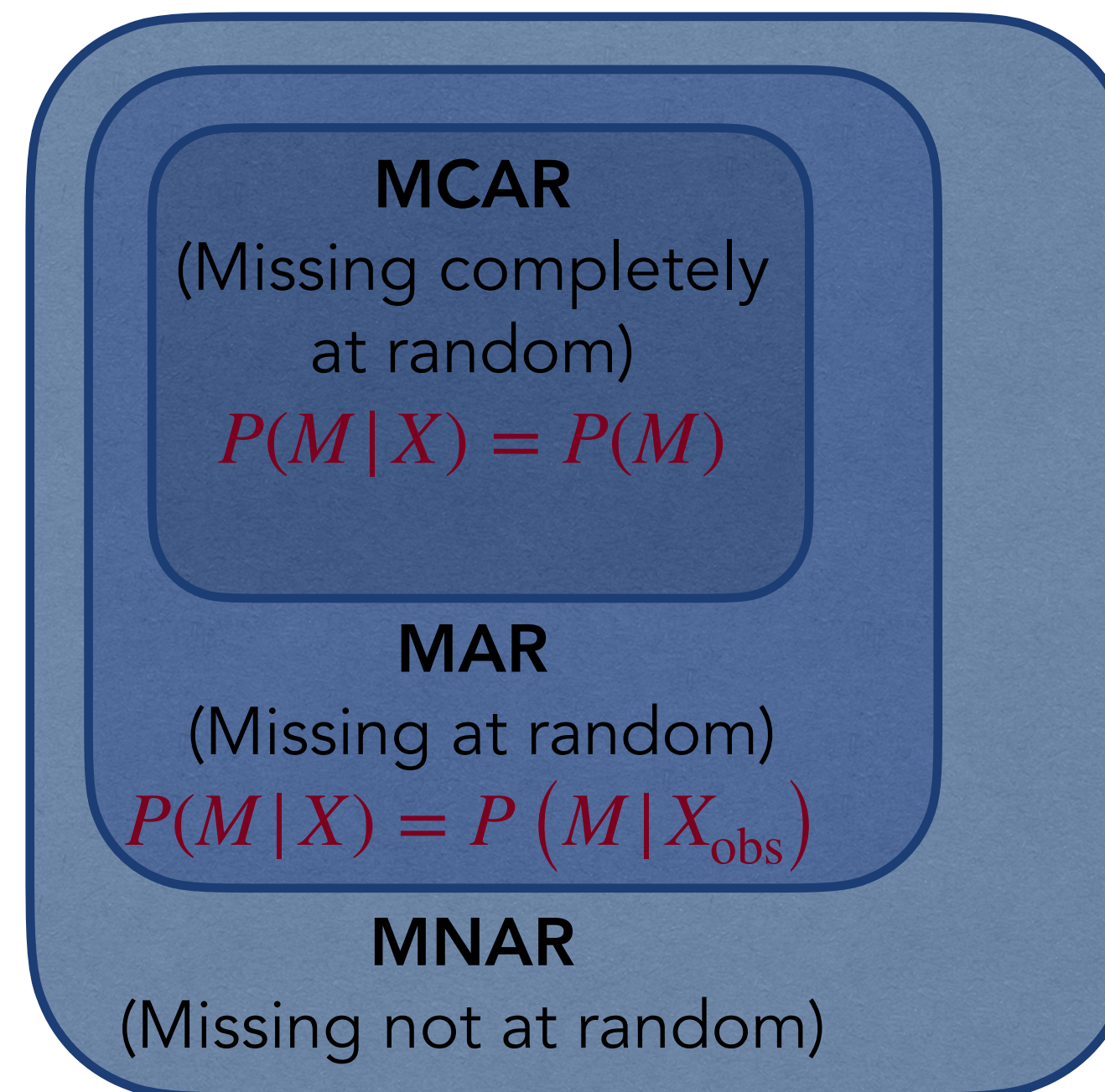
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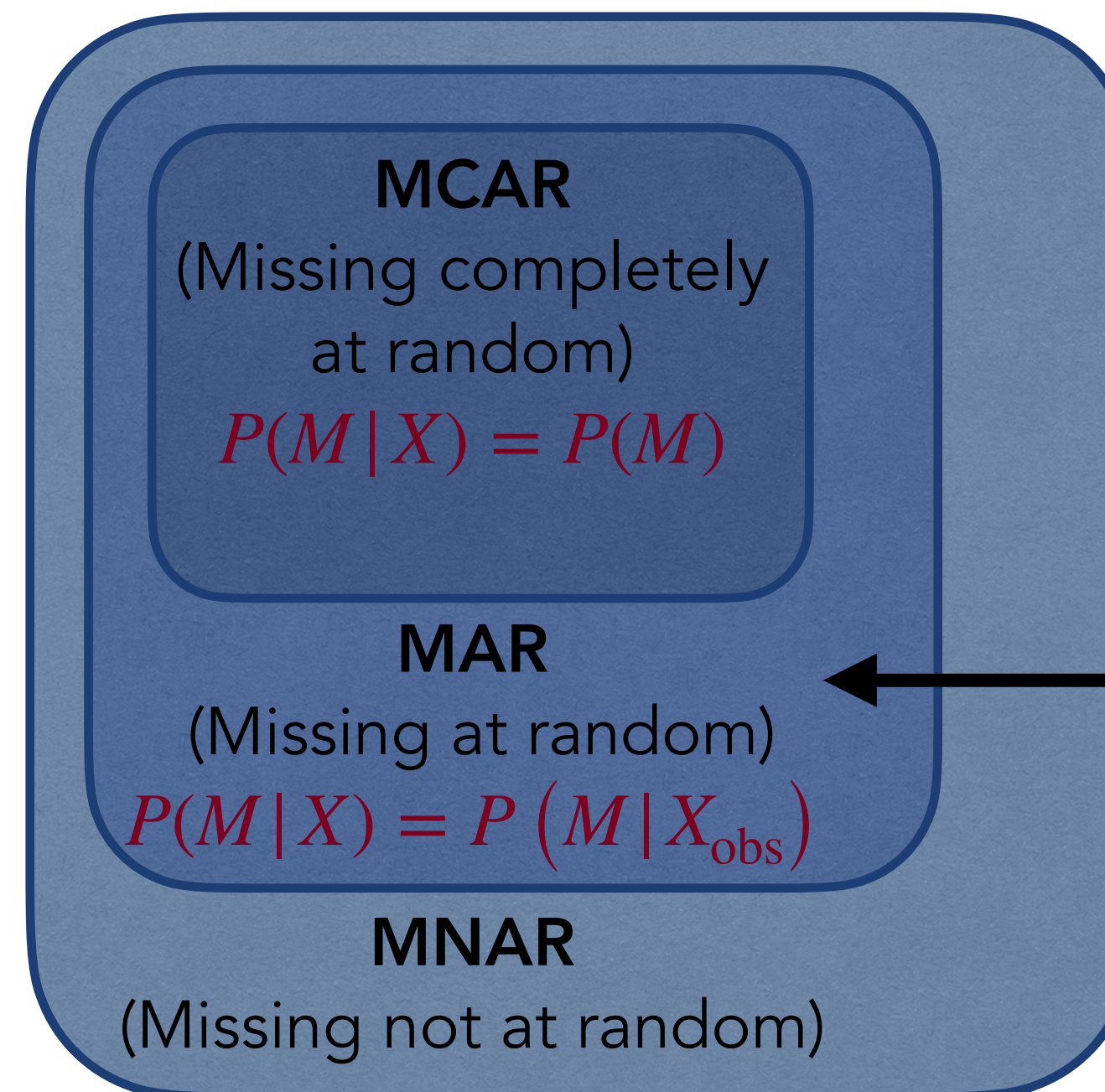
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Rubin 76, Little 92,
Jones 96; Robins et al 94

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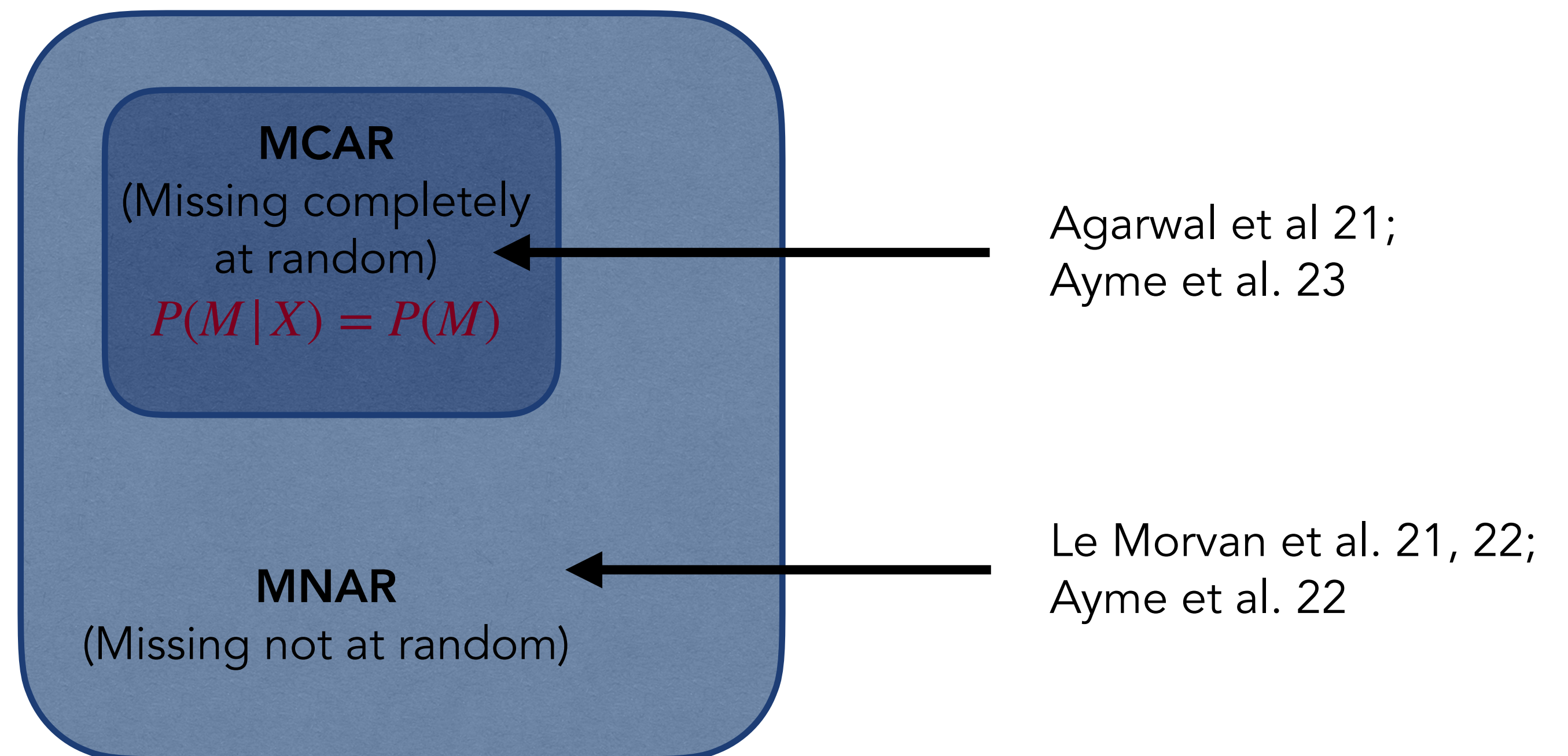
- **Inference**: estimate the model parameter β

- **Prediction**: predict Y on a new observation X

Estimation of β is not sufficient

$$X = (\text{NA}, 8, 0, \text{NA}, 6, 2)$$

- **Missing data mechanism**



Introduction: Handle missing values

- **Handle missing values with:**

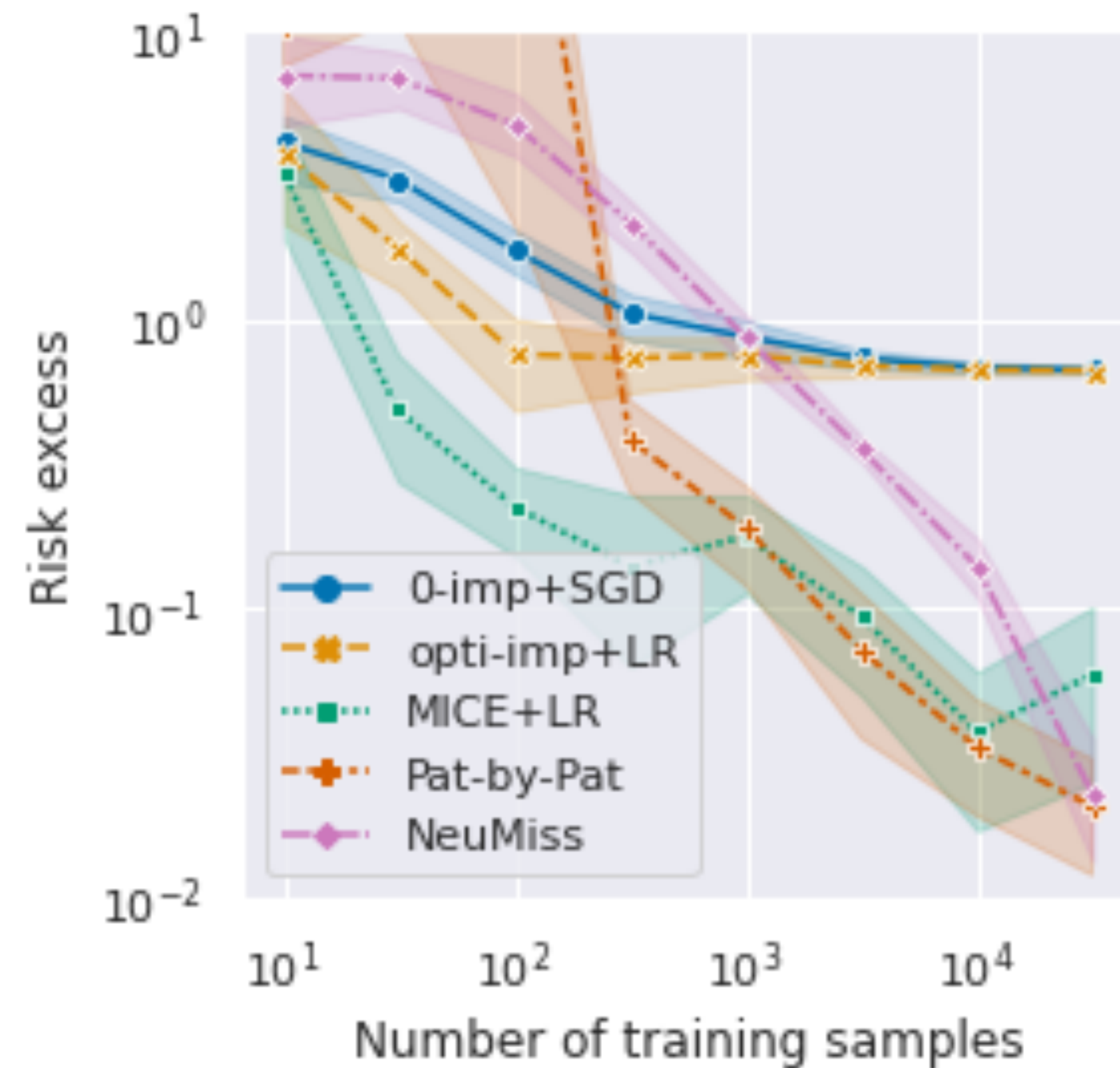
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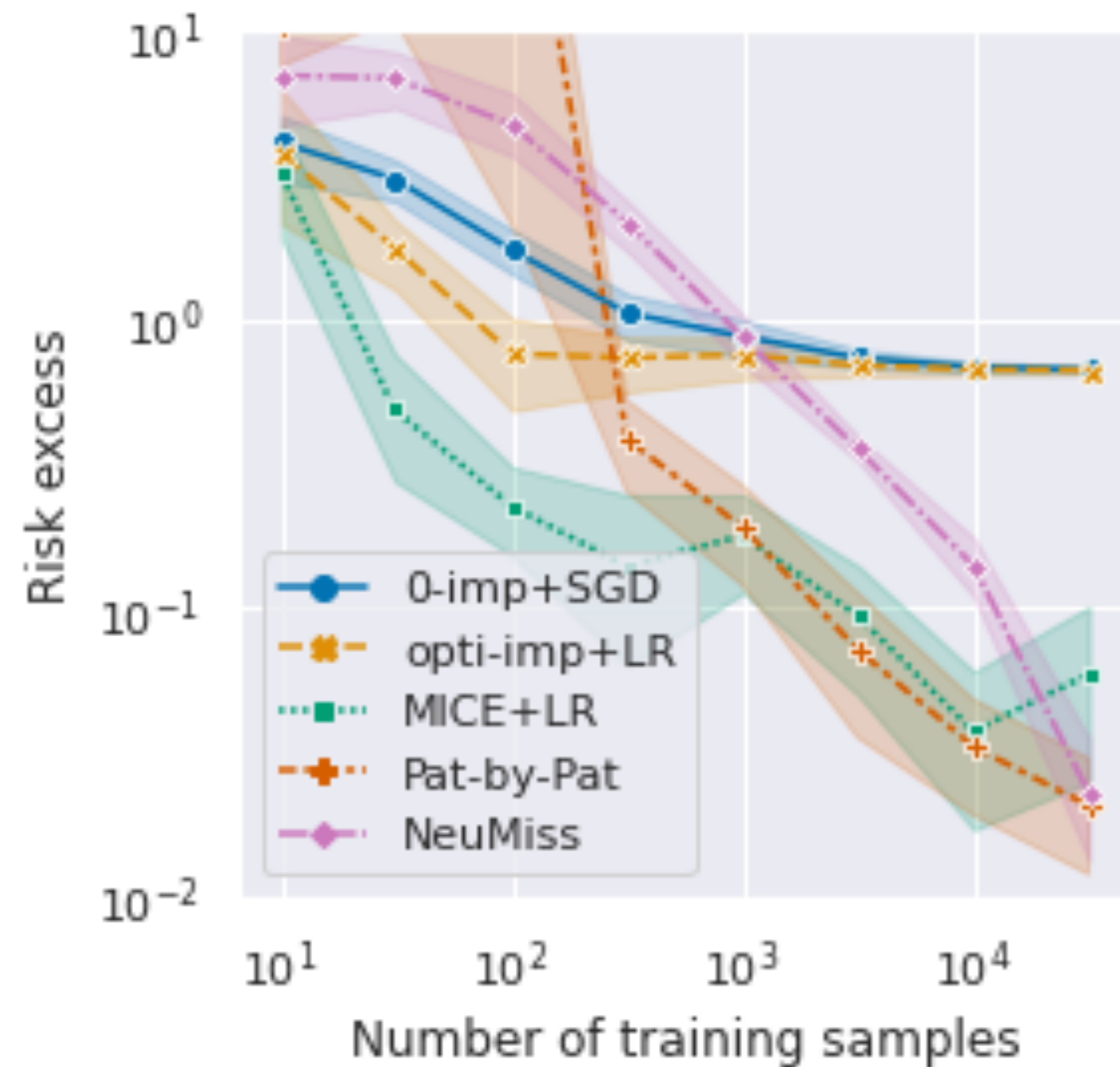


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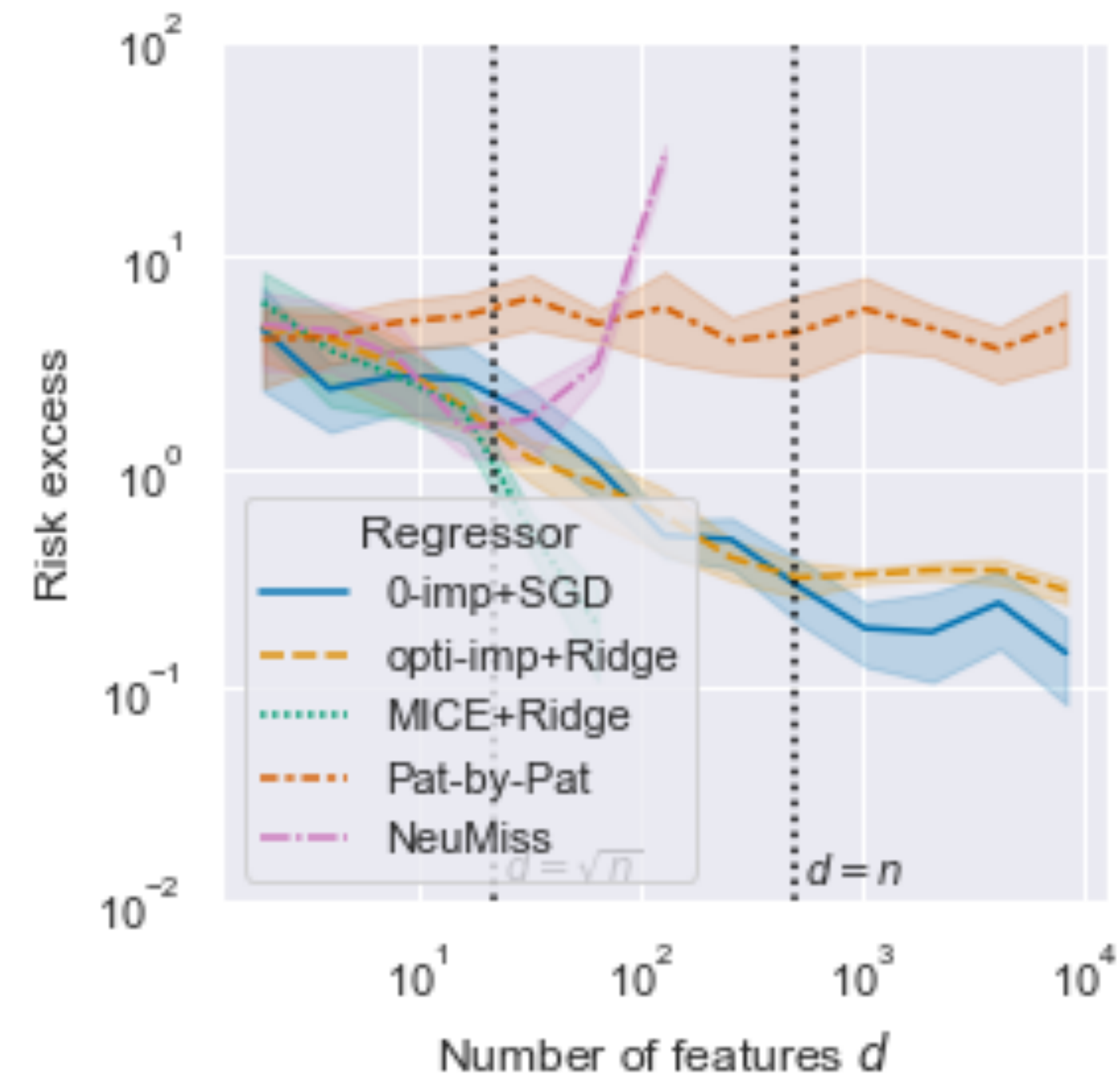
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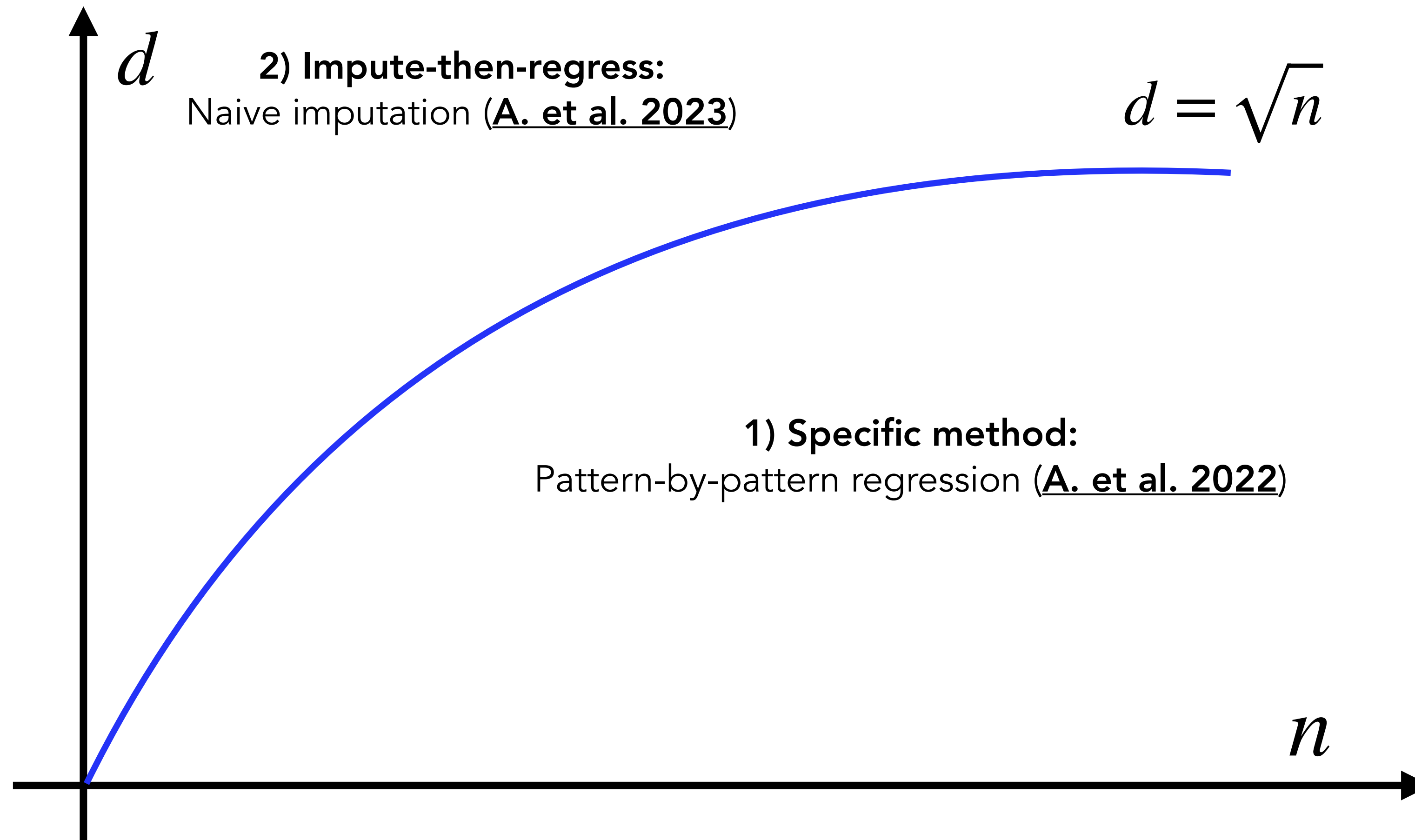
○ Low dimension $n \rightarrow +\infty$



○ High dimension $d \rightarrow +\infty$



In this talk



1) Specific method: Pattern-by-Pattern regression

- Bayes predictor decomposition

$$f^*(Z) = \sum_{m \in \{0,1\}^d} f_m^*(X_{\text{obs}(m)}) \mathbf{1}_{M=m}$$

Local **Bayes prediction** for the missing pattern ($M = m$)

Proposition: (Le Morvan et al. 2020)

Under **linear model** and several **missing data scenarios** (including MNAR), f_m^* are **linear**

- Pattern-by-pattern predictor

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Local **Least-Square** regression on
 $\{(X_{i,\text{obs}}, Y_i), M_i = m\}$

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- Definition: excess risk

$$\mathcal{E}(\hat{f}) = \mathbb{E} \left[\left(\hat{f}(Z) - f^*(Z) \right)^2 \right]$$

- Definition: missing pattern **complexity**

$$\mathfrak{C}_p \left(\frac{d}{n} \right) = \sum_{m \in \{0,1\}^d} p_m \wedge \frac{d}{n}$$

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Under Lipschitz and Sub-Gaussian assumptions

$$\mathcal{E}(\hat{f}) \leq A \log(n) \mathfrak{C}_p \left(\frac{d}{n} \right) + \text{Approx}$$

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Examples:

1. **Uniform** distribution: $\mathfrak{C}_p \left(\frac{d}{n} \right) = 2^d \frac{d}{n}$

2. **Bernoulli** distribution: $M_j \sim \mathcal{B}(1 - \rho)$ and $1 - \rho \leq \frac{d}{n}$

$$\mathfrak{C}_p \left(\frac{d}{n} \right) \leq \frac{d^2}{n}$$

1) Specific method: Pattern-by-Pattern regression

- Minimax risk

Worst case on a class of problem \mathcal{P}_p

$$\mathcal{E}_{\text{mini}}(p) = \inf_{\tilde{f}} \sup_{\mathbb{P} \in \mathcal{P}_p} \mathbb{E}_{\mathbb{P}} \left[(\tilde{f}(Z) - f^*(Z))^2 \right]$$

Best algorithm

where \mathcal{P}_p represents a class of data distributions

- for which the missing pattern distribution is p
- under Lipschitz and Sub-Gaussian assumptions

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Theorem:

$$\sigma^2 \mathfrak{C}_p \left(\frac{1}{n} \right) \lesssim \mathcal{E}_{\text{mini}}(p) \leq \underbrace{\mathcal{E}(\hat{f})}_{\text{previous thm}} \leq A \log(n) \mathfrak{C}_p \left(\frac{d}{n} \right)$$

- Lower bound still holds when \mathcal{P}_p includes **MAR** missing values

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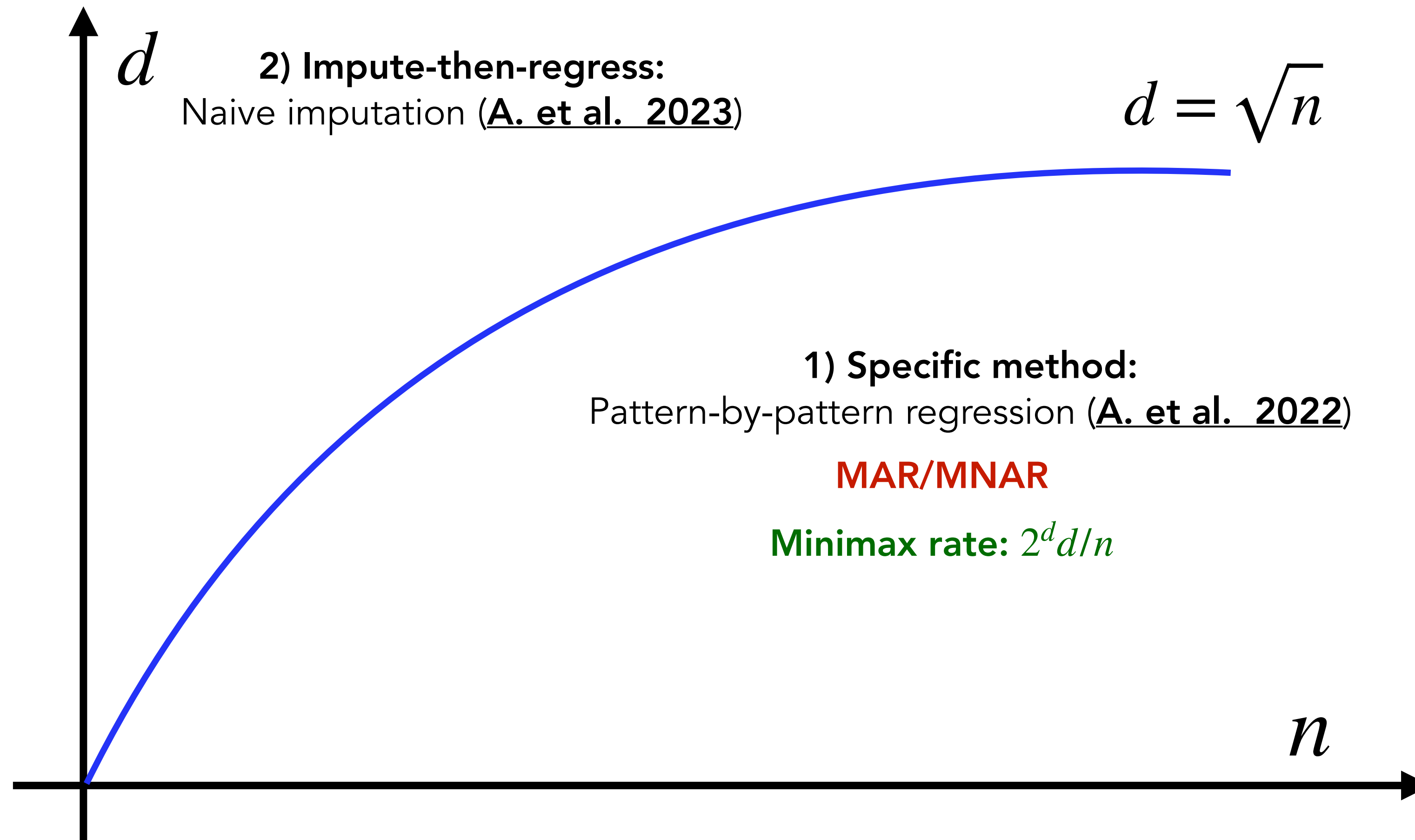
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Examples

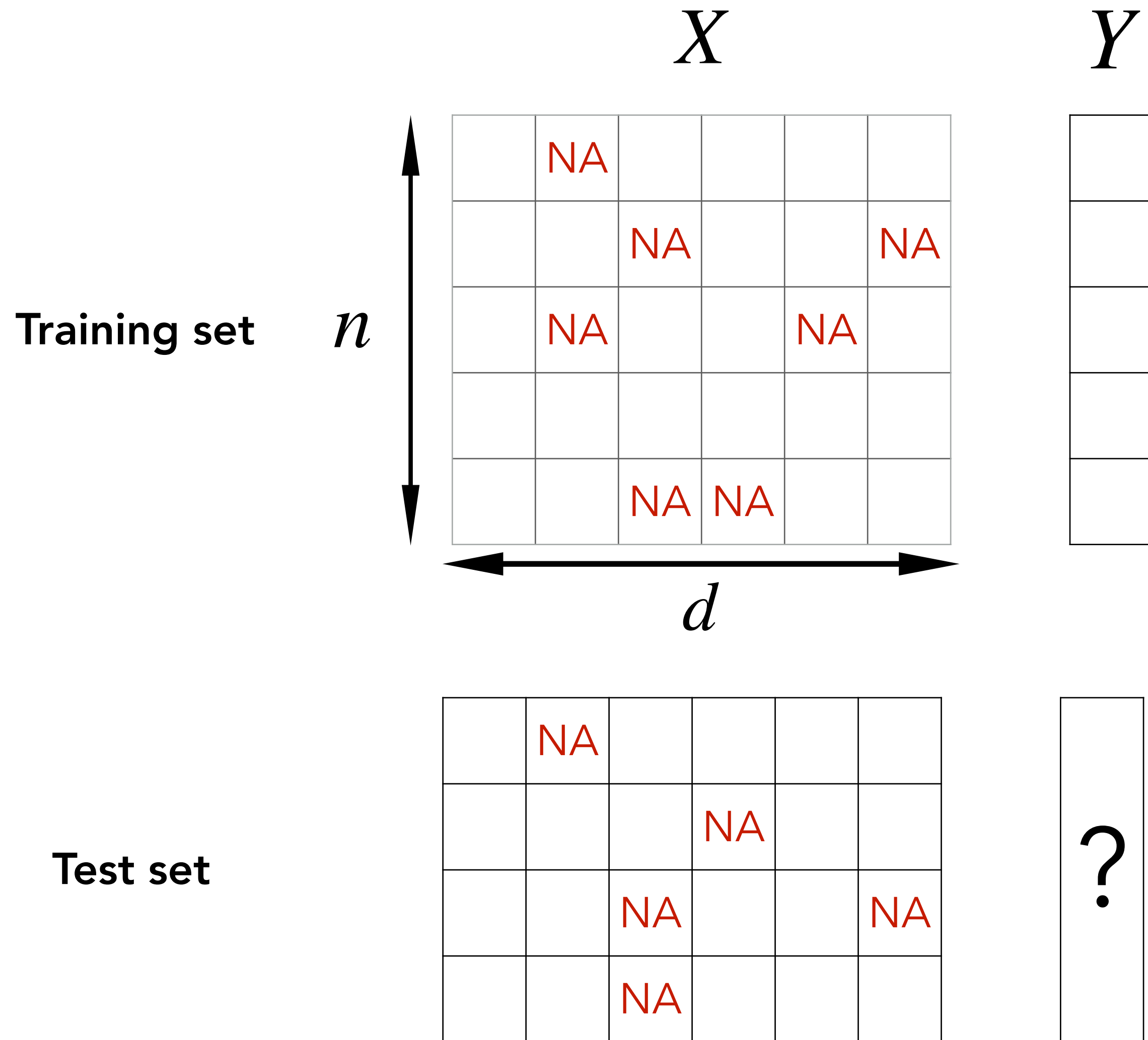
- Uniform** distribution: $\mathfrak{C}_p \left(\frac{1}{n} \right) = \frac{2^d}{n}$, $\mathfrak{C}_p \left(\frac{d}{n} \right) = 2^d \frac{d}{n}$
- Bernoulli** distribution: $\mathfrak{C}_p \left(\frac{1}{n} \right) = \frac{d}{n}$, $\mathfrak{C}_p \left(\frac{d}{n} \right) = \frac{d^2}{n}$

- without stronger assumption, best rate can be exponential!

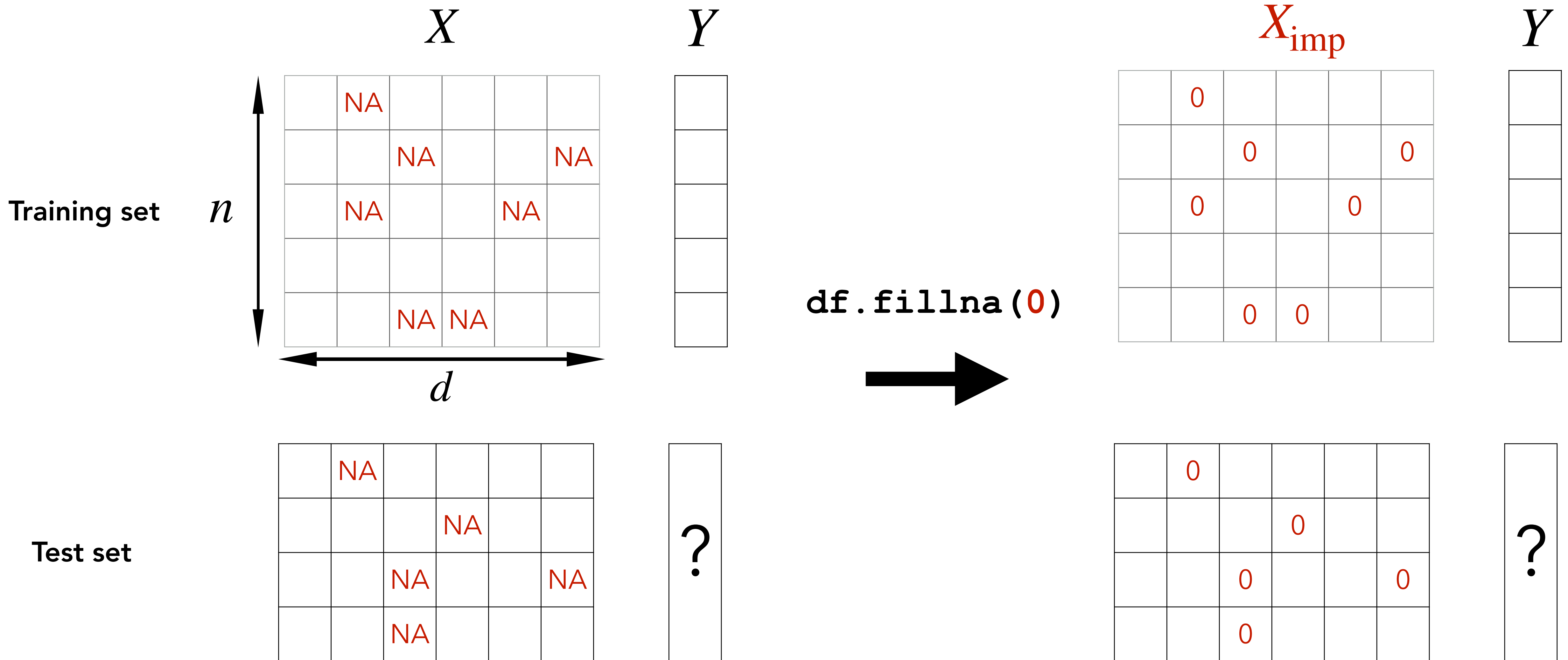
1) Specific method:



2) Imputation by 0



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2) Imputation by 0: Framework

- o Linear prediction risk on **imputed data**:

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- o **Imputation Bias**:

Risk of the optimal **linear** predictor on **complete** data



$$B_{\text{imp}} = R_{\text{imp}}^* - R^*$$



Risk of the optimal **linear** predictor on **0-imputed** data

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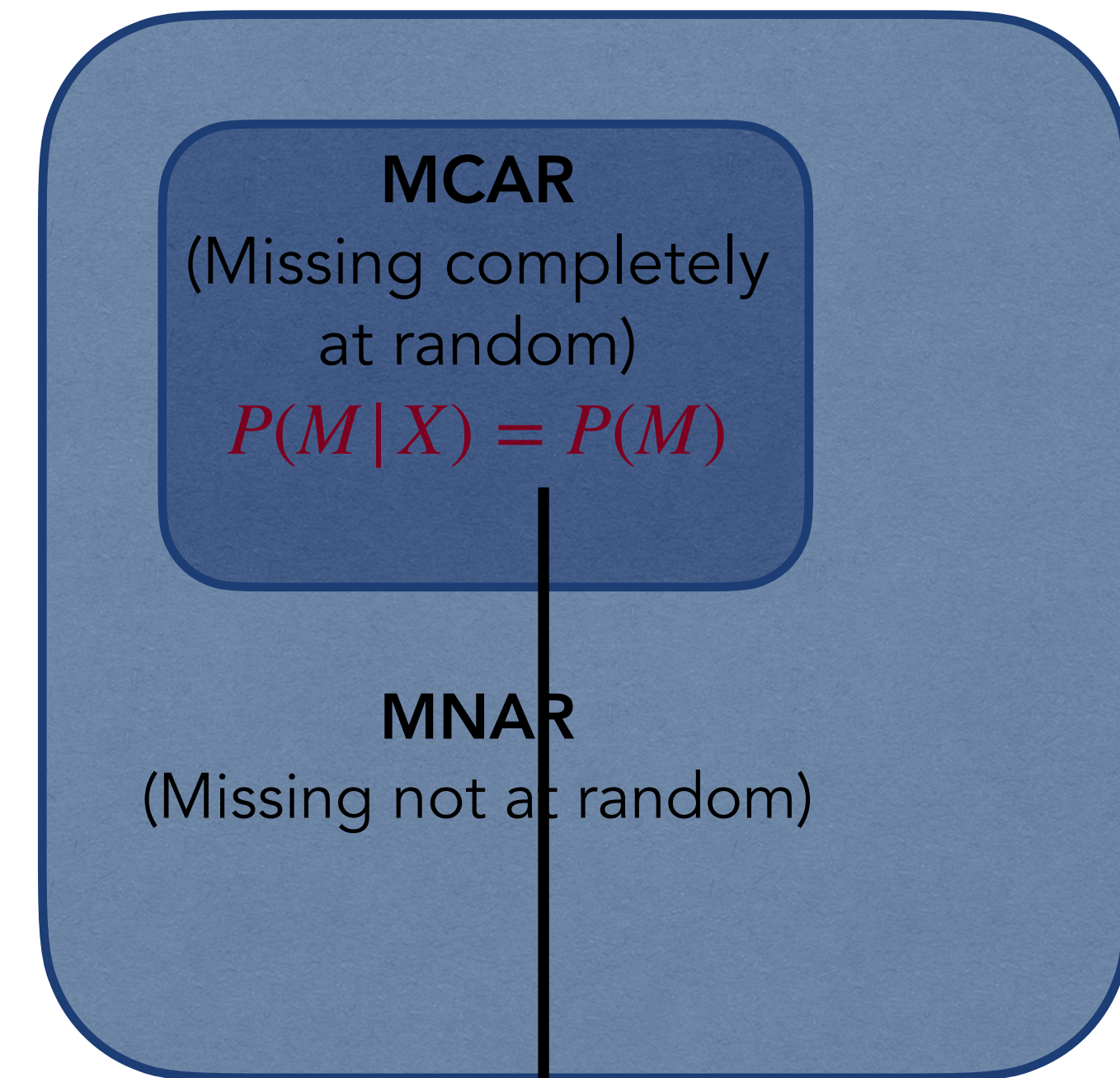


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Risk of the optimal **linear** predictor on **0-imputed** data

- Missing values



Bernoulli Model: Missing values i.i.d

$$M_1, \dots, M_d \sim \mathcal{B}(1 - \rho)$$

2) Imputation by 0: Toy example

○ Complete Model:

$$Y = X_1 .$$

$$X = (X_1, X_1, \dots, X_1)$$

$$\theta^* = (1, 0, \dots, 0)^\top$$

$$R^* = 0$$

○ With imputed missing values: $M_1, \dots, M_d \sim \mathcal{B}(1/2)$

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$$\theta_1 = (1, 0, \dots, 0)^\top$$



$$\theta_1^\top X_{\text{imp}} = X_1 M_1$$



$$R(\theta_1) = \frac{1}{2} \mathbb{E}[X_1^2]$$

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○ With imputed missing values: $M_1, \dots, M_d \sim \mathcal{B}(1/2)$

$$\theta_1 = (1, 0, \dots, 0)^\top$$

$$\theta_2 = 2(1/d, 1/d, \dots, 1/d)^\top$$

$$\theta_1^\top X_{\text{imp}} = X_1 M_1$$

$$\theta_2^\top X_{\text{imp}} = \frac{2X_1}{d} \sum_j M_j$$

$$R(\theta_1) = \frac{1}{2} \mathbb{E}[X_1^2]$$

$$R(\theta_2) = \frac{1}{d} \mathbb{E}[X_1^2]$$

$$B_{\text{imp}} = R^* - R_0^* \leq \frac{1}{d} \mathbb{E}[X_1^2]$$

2) Imputation by 0 = implicit ridge?

- Ridge penalization

$$R_\lambda(\theta) = R(\theta) + \lambda \|\theta\|_2^2$$

Theorem: Under Bernoulli model and $\sum_{j,j} = 1$ for all $j \in [d]$,

$$R_{\text{imp}}(\theta) = R(\rho\theta) + \rho(1 - \rho) \|\theta\|_2^2$$

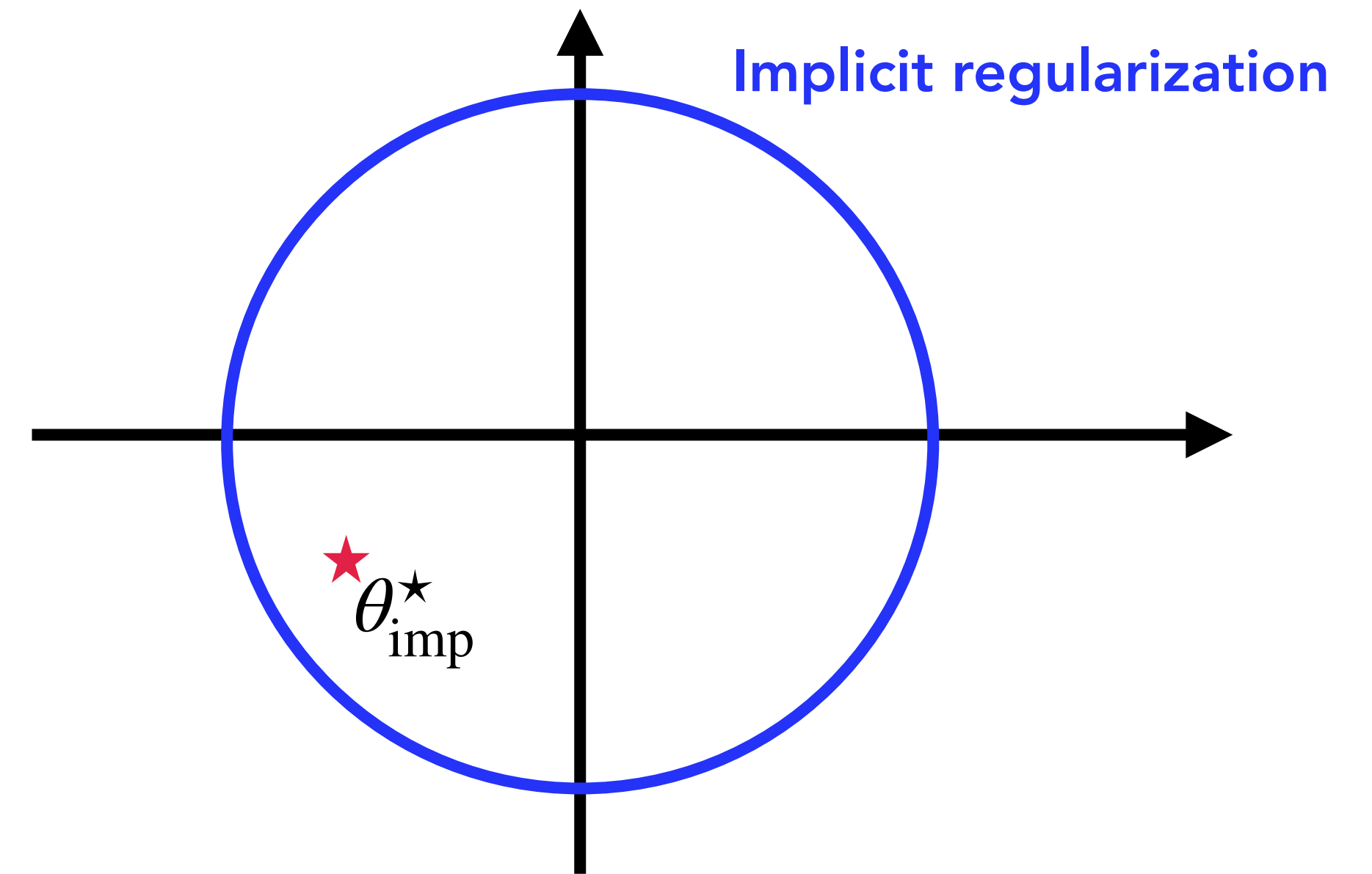
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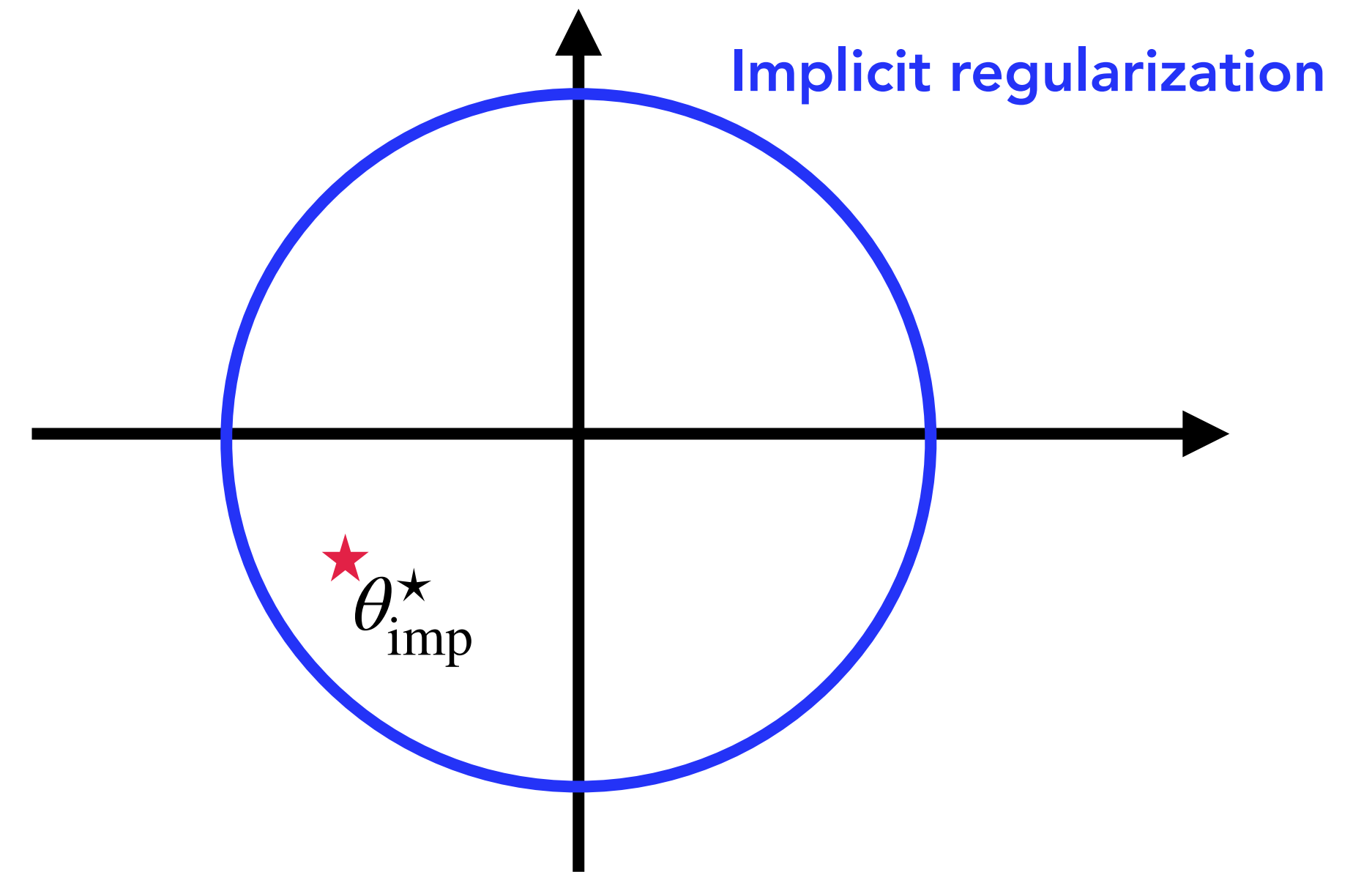
$$R_{\text{imp}}(\theta) = R(\rho\theta) + \rho(1 - \rho)\|\theta\|_2^2$$

○ Ridge bias

$$B_{\text{ridge},\lambda} = \inf_{\theta} \{R(\theta) - R(\theta_\star) + \lambda \|\theta\|_2^2\}$$

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where $\lambda_{\text{imp}} = \frac{\rho}{1 - \rho}$ $B_{\text{imp}} = B_{\text{ridge},\lambda_{\text{imp}}}$



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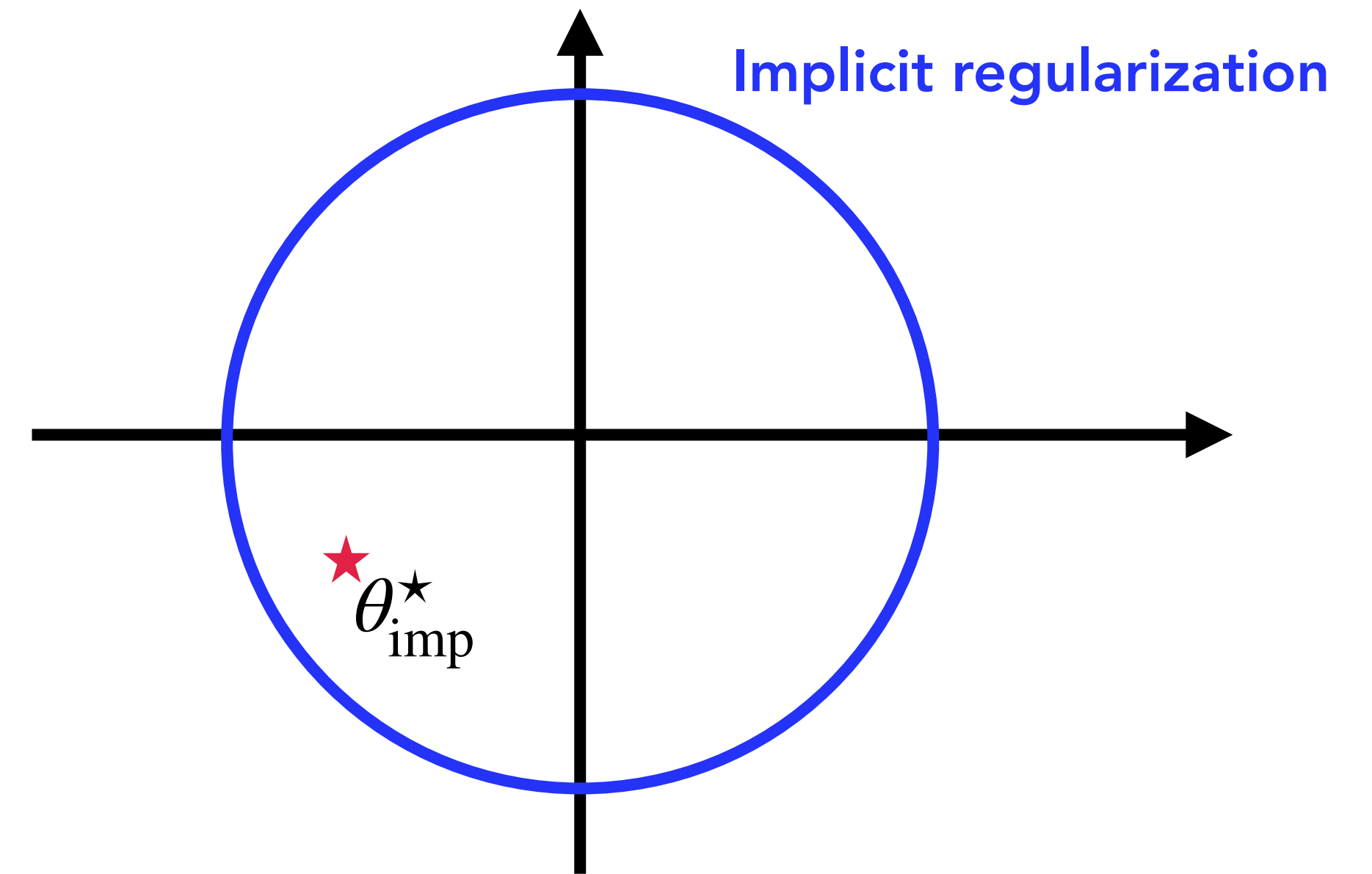
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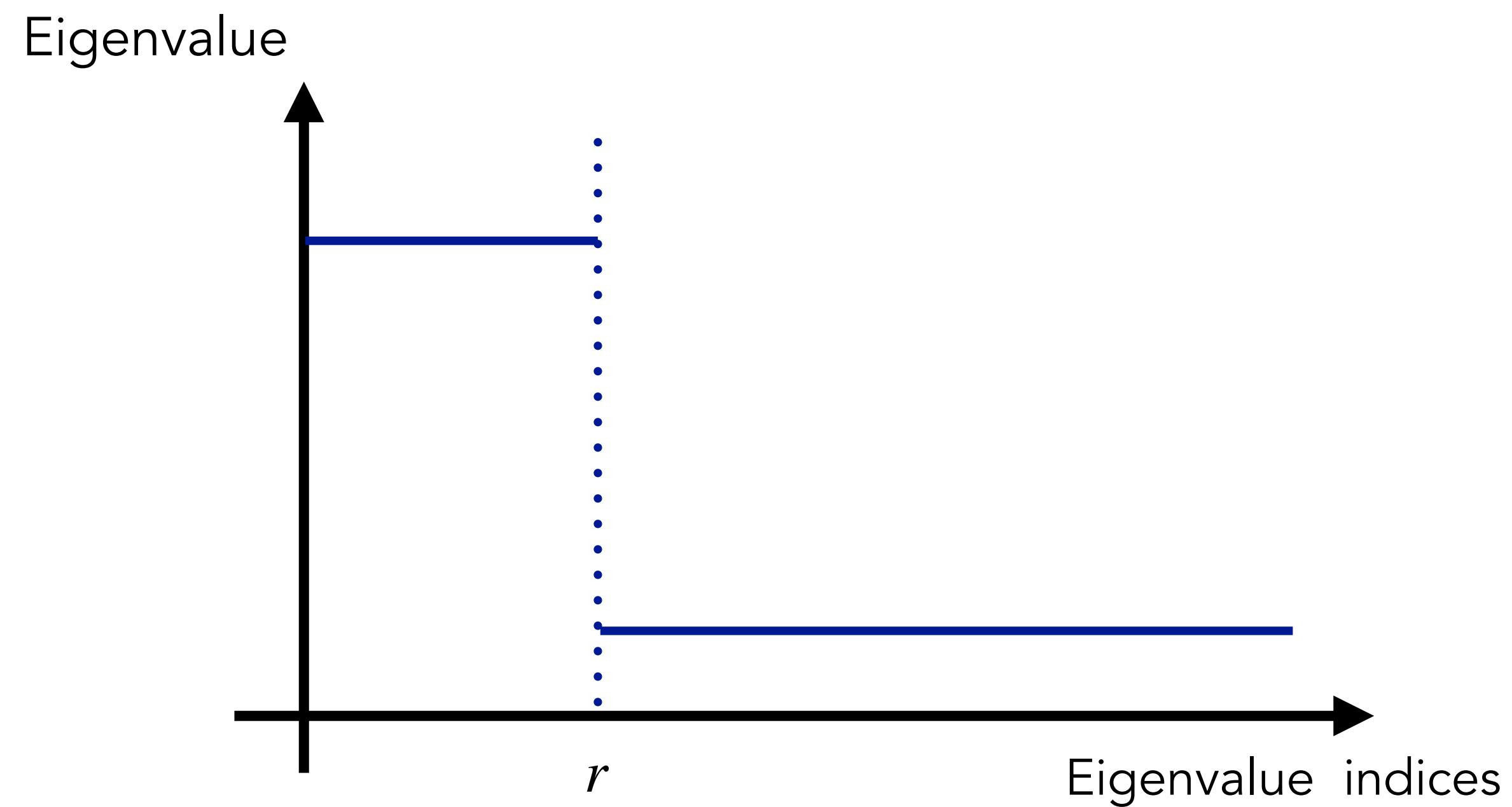


1. **Imputation induce a ridge penalization** (Optimal predictor has a small norm)
2. **Imputation by 0 seem to be at the same price of ridge penalization**
3. Penalization parameter λ_{imp} depends only on $1 - \rho$ the proportion of missing values.
4. Available for all MCAR setting with another λ_{imp}

2) Imputation by 0: Illustration on low rank data

○ Low rank data (or spiked): $\text{rank}(\Sigma) \approx r$

$$B_{\text{imp}} \lesssim \frac{r}{d} \mathbb{E}Y^2$$

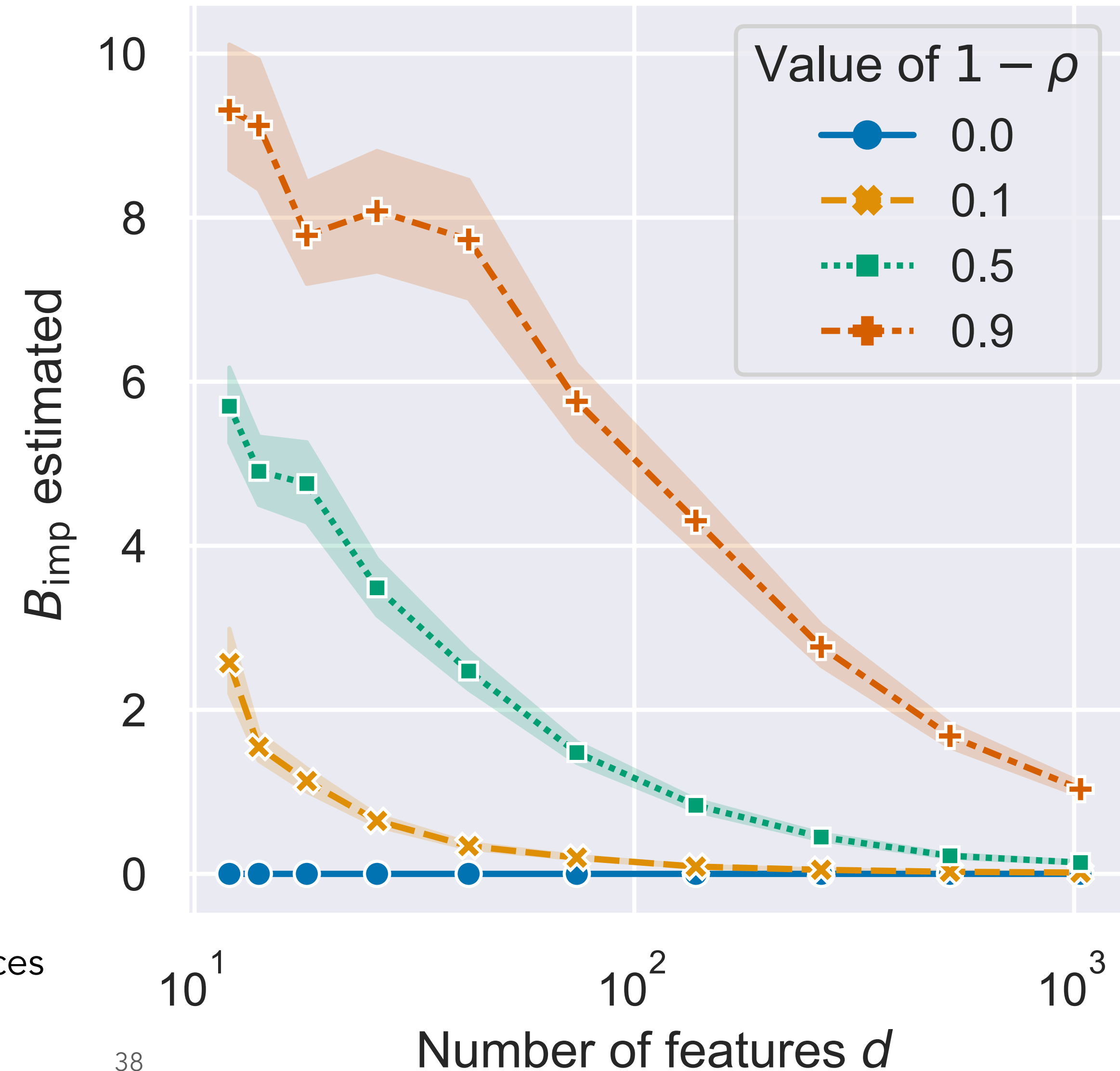
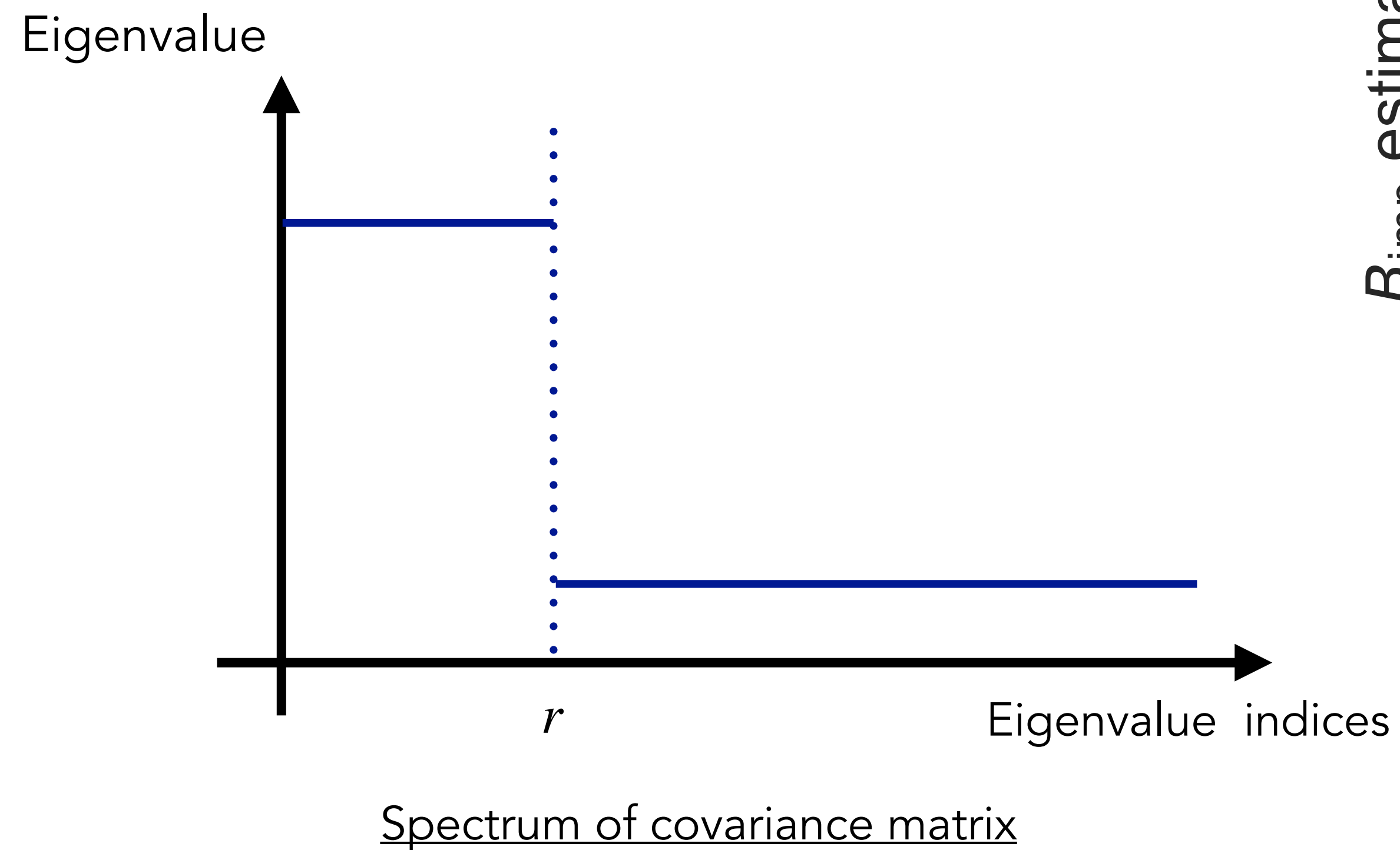


Spectrum of covariance matrix

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2) Imputation by 0: Learn imputed data with SGD

○ **SGD recursion:** with **constant** learning rate $\gamma = \frac{1}{d\sqrt{n}}$

$$\begin{cases} \theta_0 = 0 \\ \theta_{\text{imp},t} = \left[I - \gamma X_{\text{imp},t} X_{\text{imp},t}^\top \right] \theta_{\text{imp},t-1} + \gamma Y_t X_{\text{imp},t} \end{cases}$$

○ Polyak Ruppert average:

$$\bar{\theta}_{\text{imp},n} = \frac{1}{n+1} \sum_{t=1}^n \theta_{\text{imp},t}$$

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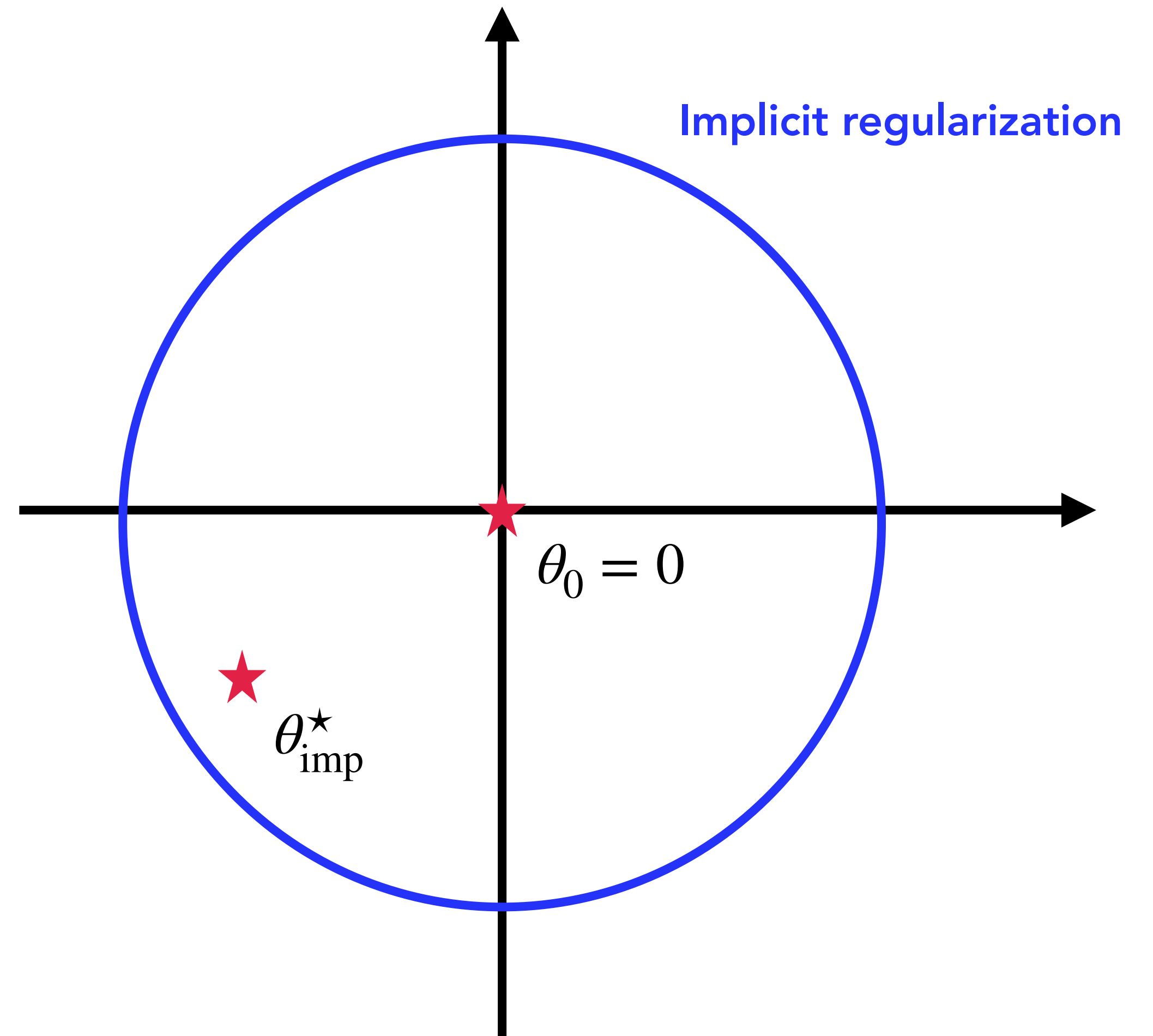
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Theorem: Under classical SGD assumptions,

$$\mathbb{E} \left[R_{\text{imp}} \left(\bar{\theta}_{\text{imp},n} \right) \right] - R^* \leq B_{\text{imp}} + \frac{d}{\sqrt{n}} \|\theta_{\text{imp}}^*\|_2^2 + \frac{\sigma^2}{\sqrt{n}}$$



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$$\mathbb{E} \left[R_{\text{imp}} \left(\bar{\theta}_{\text{imp},n} \right) \right] - R^* \leq \left(\frac{1}{\rho\sqrt{n}} + \frac{1-\rho}{d} \right) \frac{r}{\rho} \mathbb{E} Y^2 + \frac{\sigma^2}{\sqrt{n}}$$

Theorem: Under classical SGD assumptions,

$$\mathbb{E} \left[R_{\text{imp}} \left(\bar{\theta}_{\text{imp},n} \right) \right] - R^* \leq B_{\text{imp}} + \frac{d}{\sqrt{n}} \|\theta_{\text{imp}}^*\|_2^2 + \frac{\sigma^2}{\sqrt{n}}$$

2) Imputation by 0: Learn imputed data with SGD

○ SGD recursion:

$$\begin{cases} \theta_0 = 0 \\ \theta_{\text{imp},t} = \left[I - \gamma X_{\text{imp},t} X_{\text{imp},t}^\top \right] \theta_{\text{imp},t-1} + \gamma Y_t X_{\text{imp},t} \end{cases}$$

○ Polyak Ruppert average:

$$\bar{\theta}_{\text{imp},n} = \frac{1}{n+1} \sum_{t=1}^n \theta_{\text{imp},t}$$

Theorem: Under classical SGD assumptions,

$$\mathbb{E} \left[R_{\text{imp}} \left(\bar{\theta}_{\text{imp},n} \right) \right] - R^* \leq B_{\text{imp}} + \frac{d}{\sqrt{n}} \|\theta_{\text{imp}}^*\|_2^2 + \frac{\sigma^2}{\sqrt{n}}$$

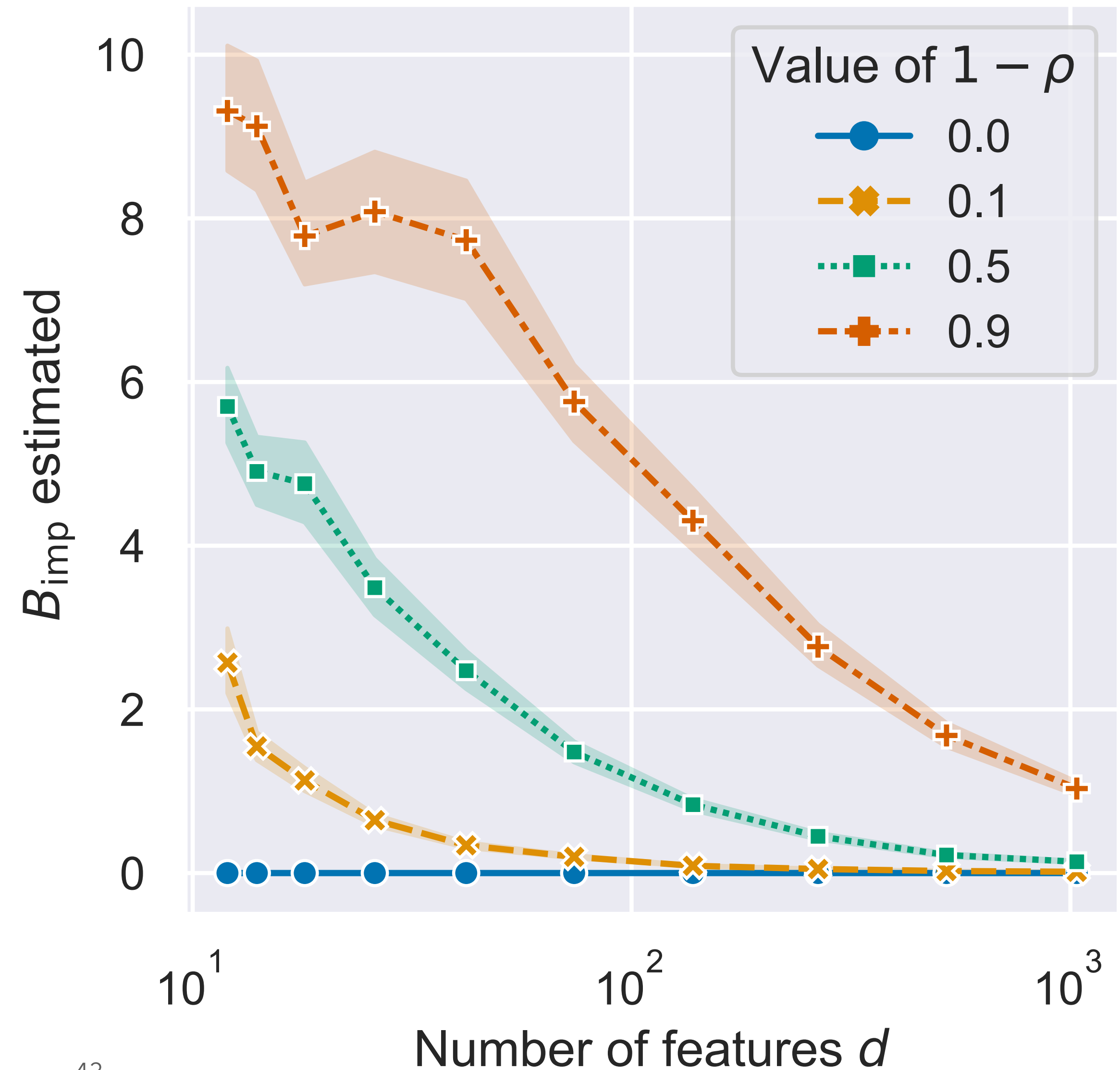
○ Illustration on low rank:

$$\mathbb{E} \left[R_{\text{imp}} \left(\bar{\theta}_{\text{imp},n} \right) \right] - R^* \leq \left(\frac{1}{\rho\sqrt{n}} + \frac{1-\rho}{d} \right) \frac{r}{\rho} \mathbb{E} Y^2 + \frac{\sigma^2}{\sqrt{n}}$$

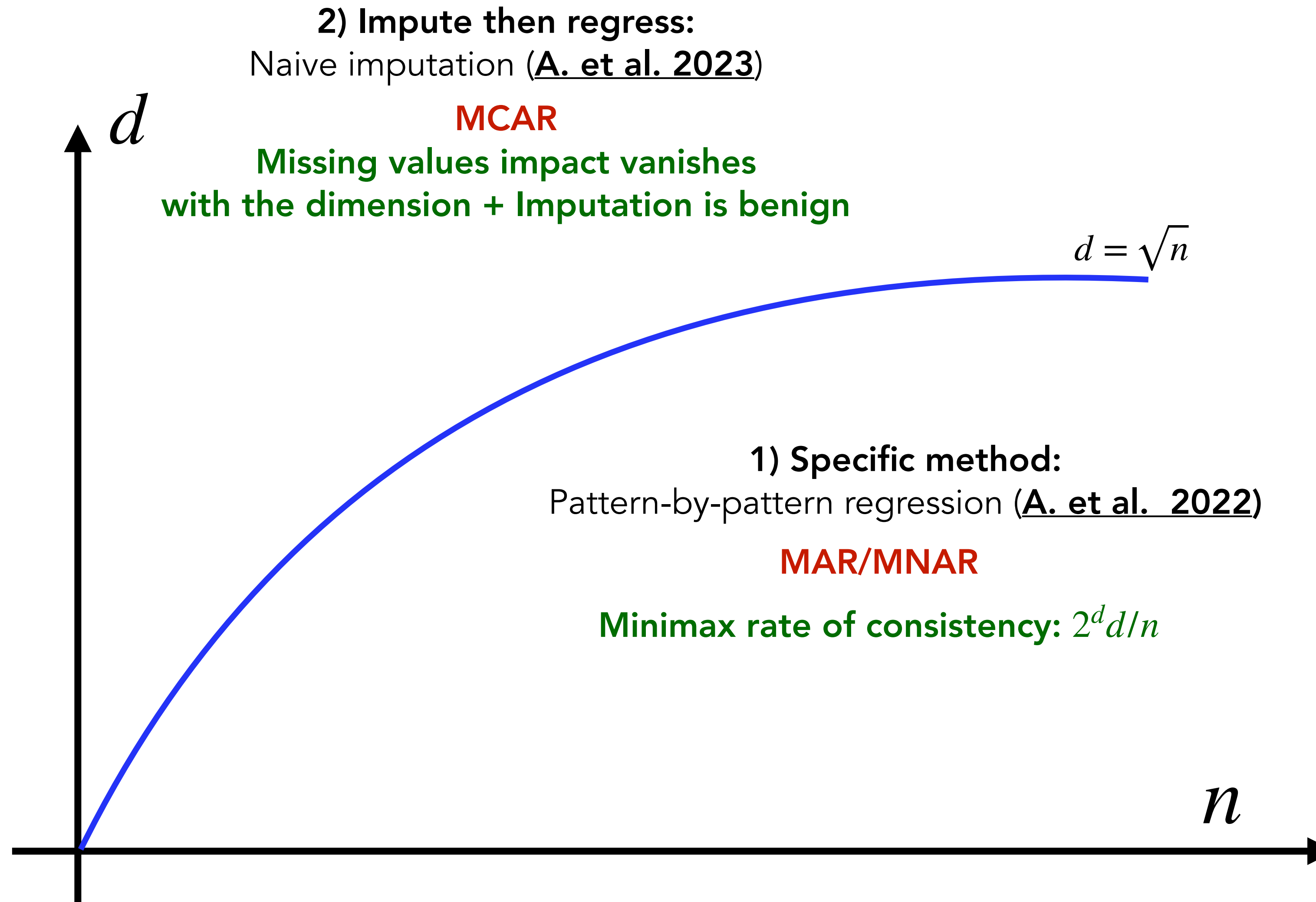
1. We leverage on implicit regularization.
2. Streaming online (one passe)
3. Trade-off between imputation bias and initial condition.
4. **Imputation bias vanishes for $d \gg \sqrt{n}$**

2) Imputation by 0: Conclusion

1. In practice: In high-dimension imputation (even naive) out performs specific methods designed to handle missing values.
2. Imputation by 0 induces a **Ridge penalization**.
3. Imputation bias **vanishes** with dimension. As a consequence missing values are not an issue in high dimension (correlated setting).
4. The regime $d \gg \sqrt{n}$ leads to **slow rates** of consistency.



Conclusion



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