Data thinning to overcome double dipping

Anna Neufeld

April, 2023

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Double Dipping: Using the same data for two tasks, such as:

1. Generating and testing a null hypothesis.
2. Fitting and evaluating a model.

One possible solution: sample splitting

	Feature 1	Feature 2
Obs. 1	12	6
Obs. 2	31	8
Obs. 3	11	31
Obs. 4	22	34

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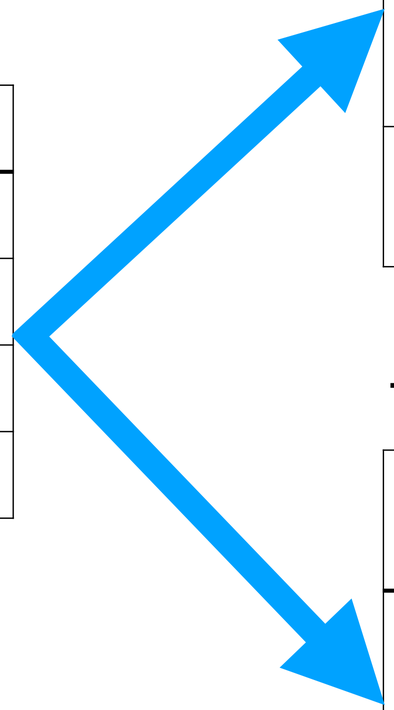

Train

	Feature 1	Feature 2
Obs. 1	12	6
Obs. 2	31	8

Test

	Feature 1	Feature 2
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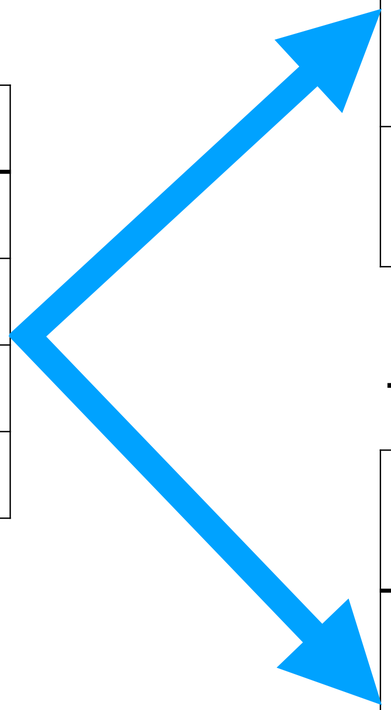

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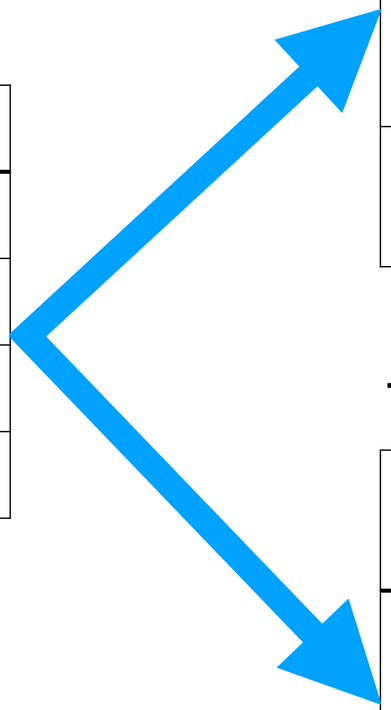

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Test

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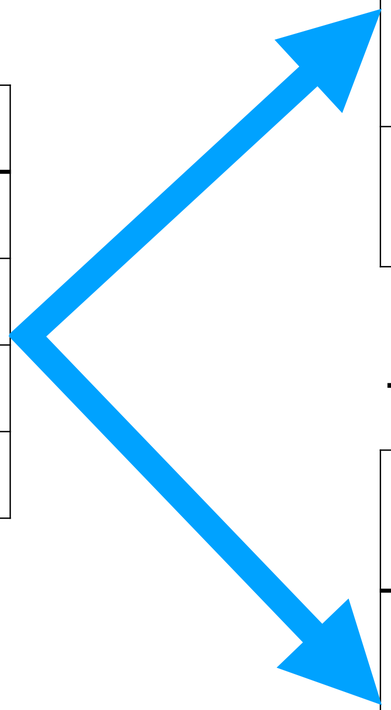

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Fit model.

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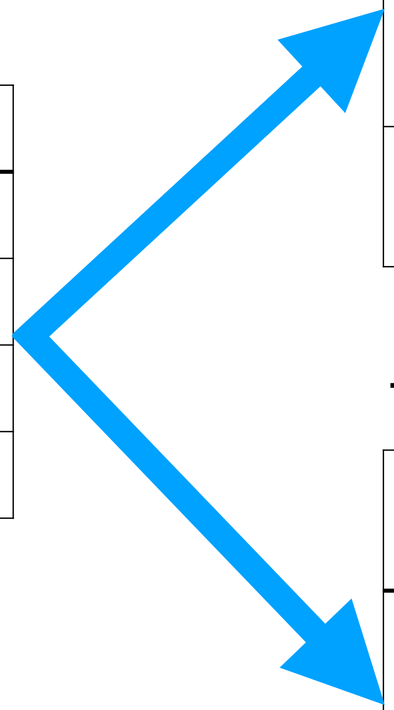

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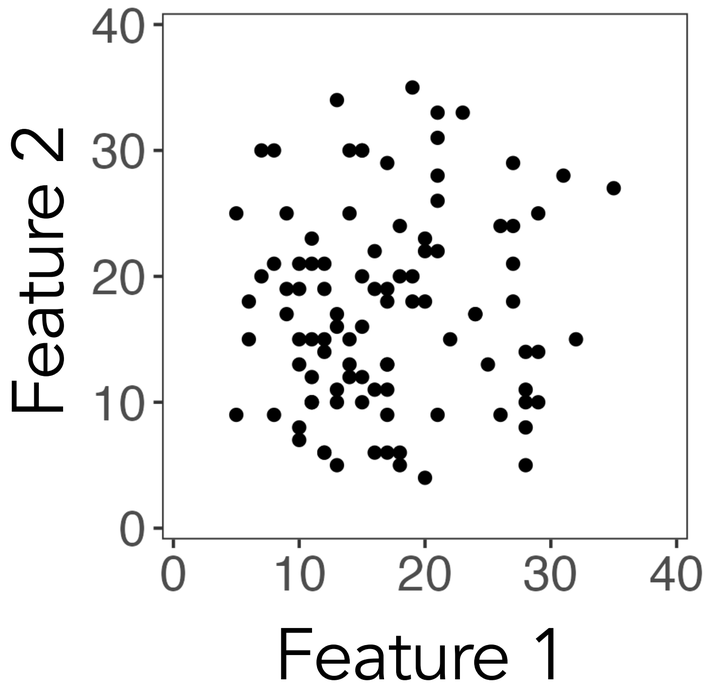
Evaluate model.

Outline

1. **Motivation: sample splitting doesn’t always work**
2. Poisson thinning
3. Data thinning
4. Generalized data thinning
5. Application to changepoint validation
6. Ongoing work

Example 1: using the same data to generate and test a hypothesis



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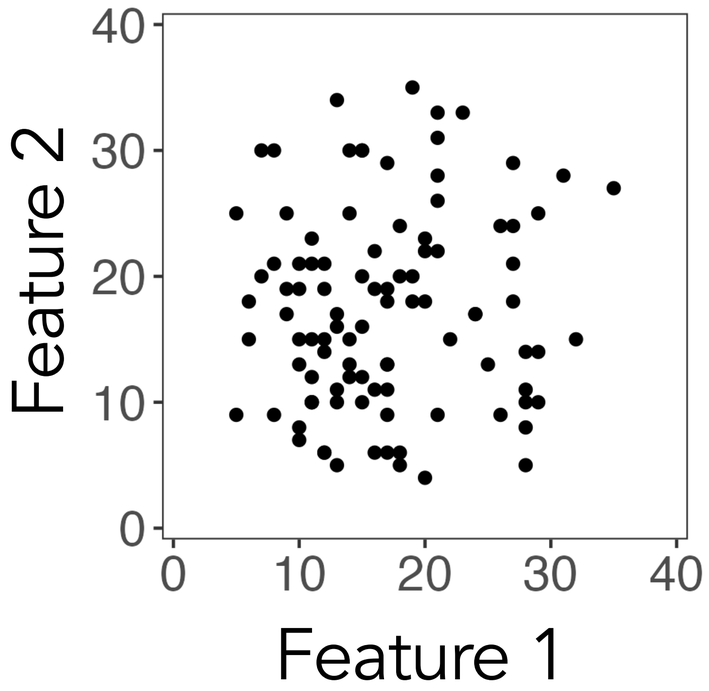

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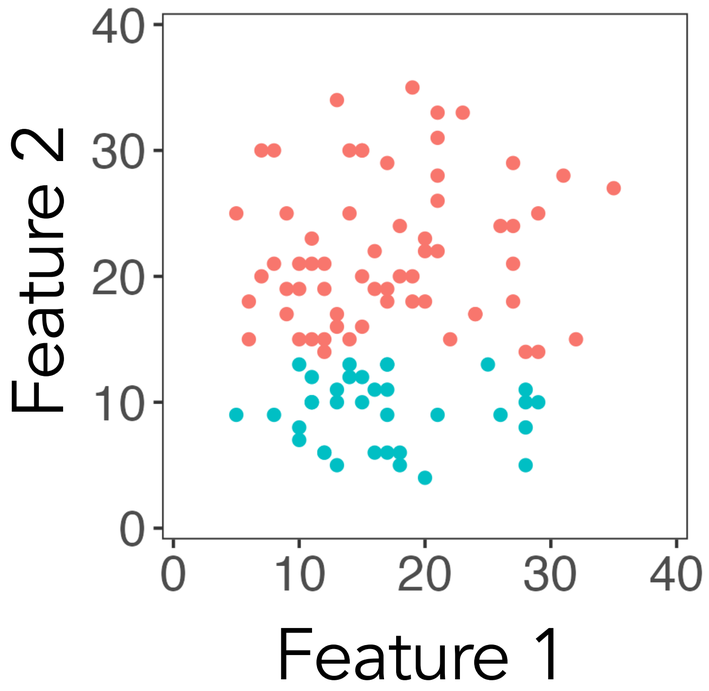

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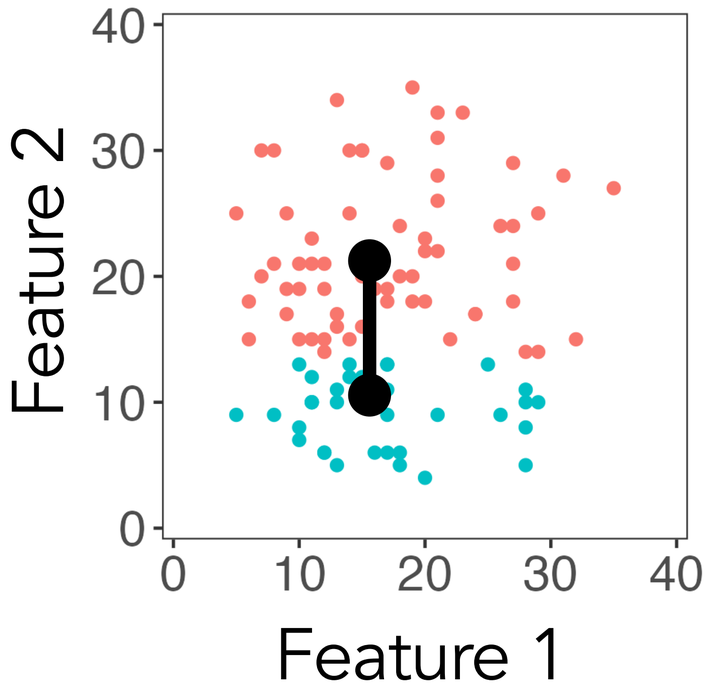

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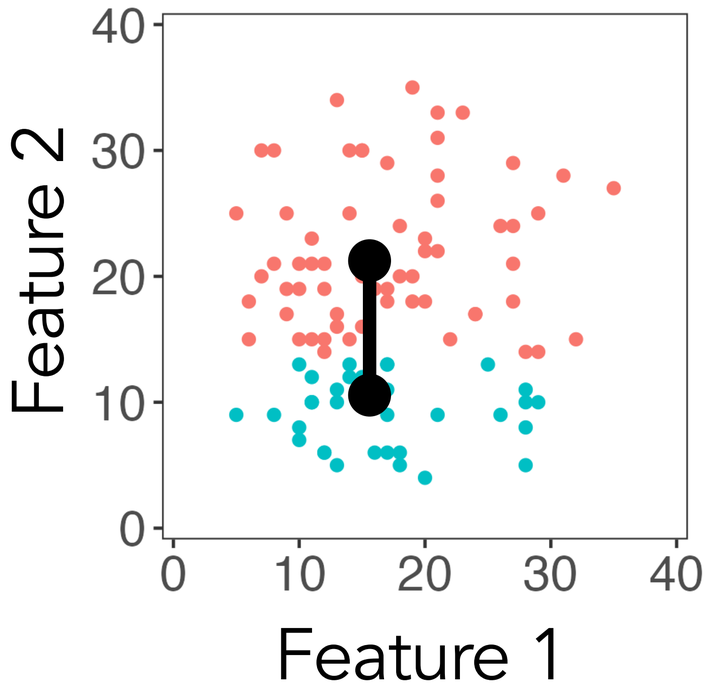

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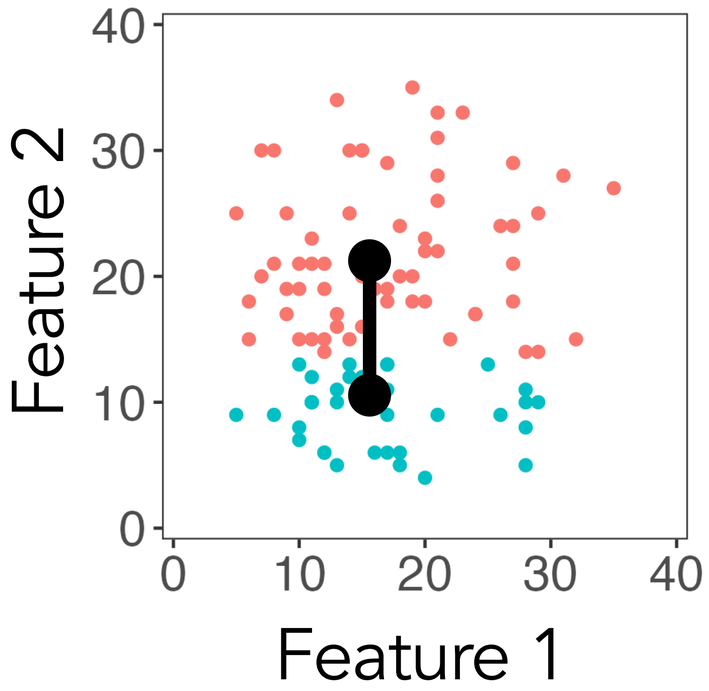

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$p < 10^{-10}$ 😱

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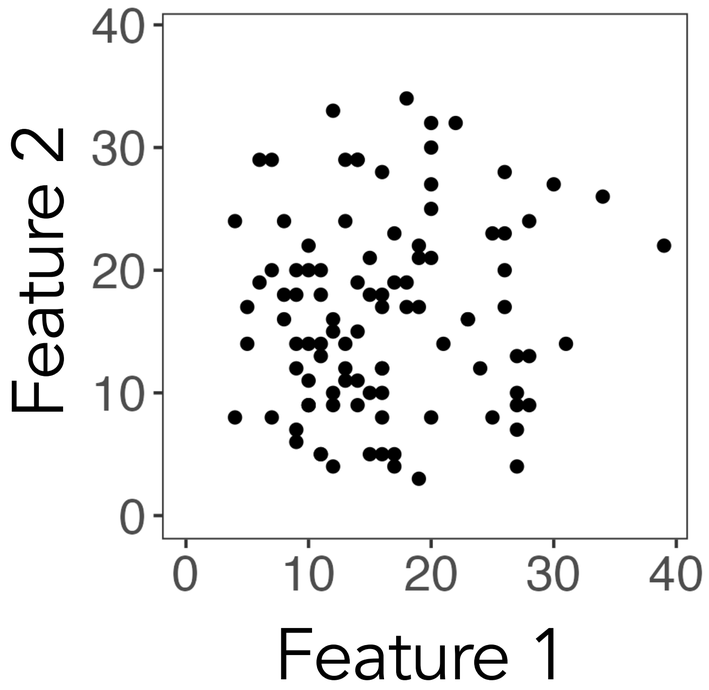

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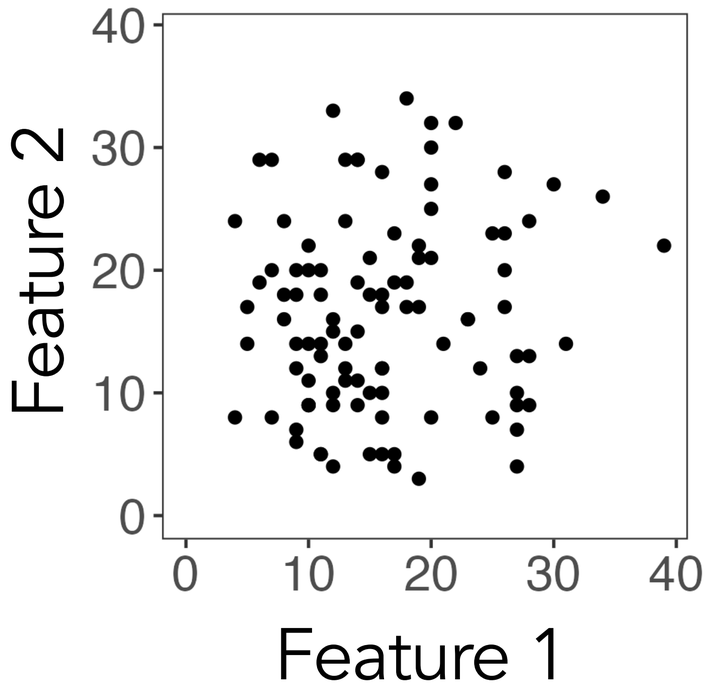

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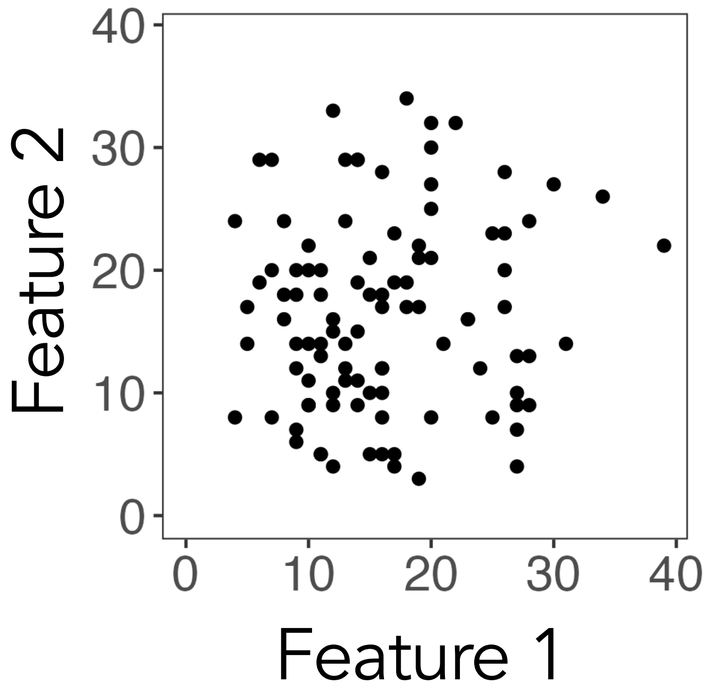

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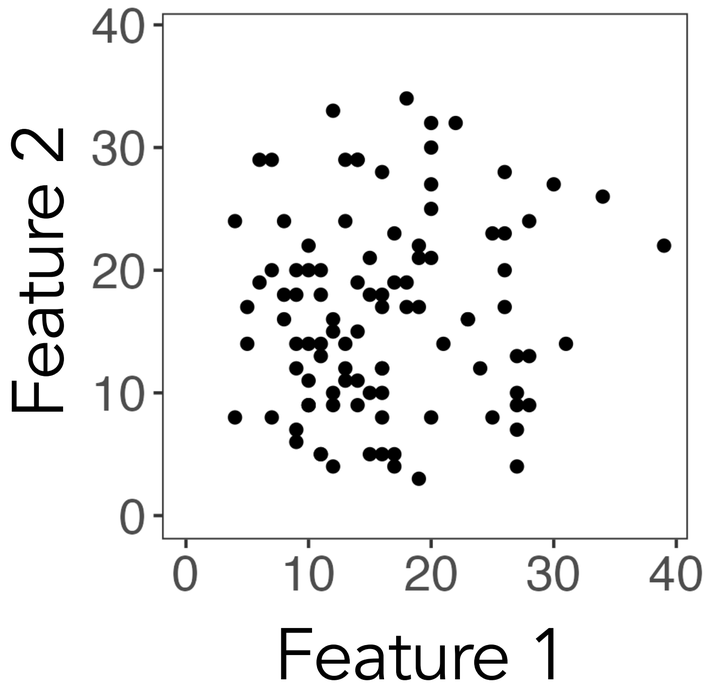

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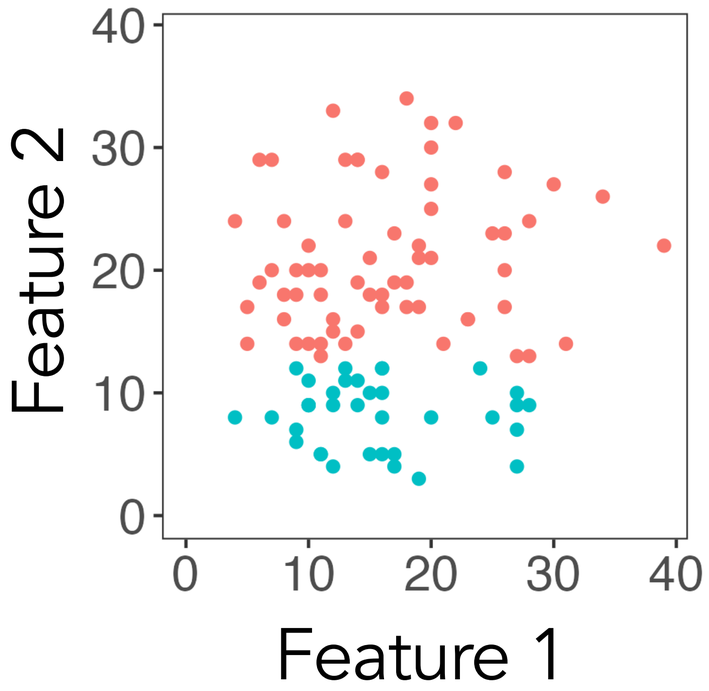

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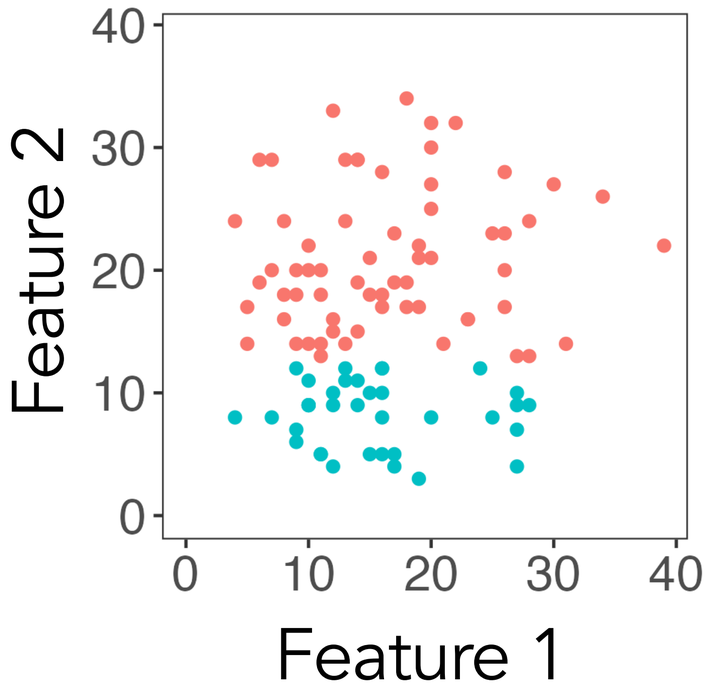

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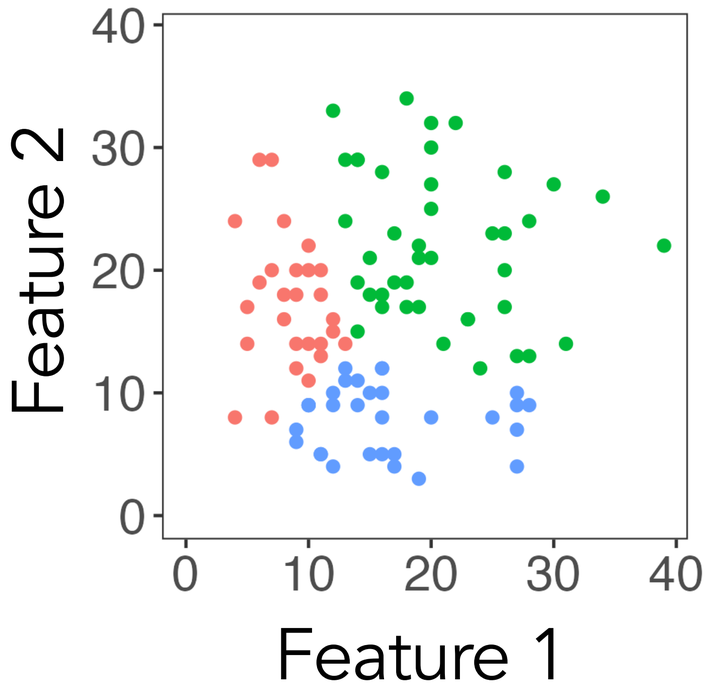

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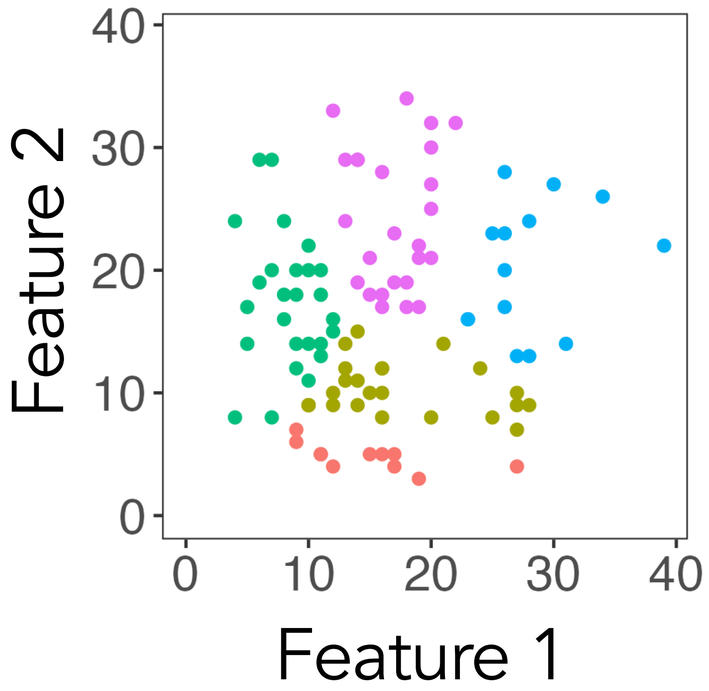

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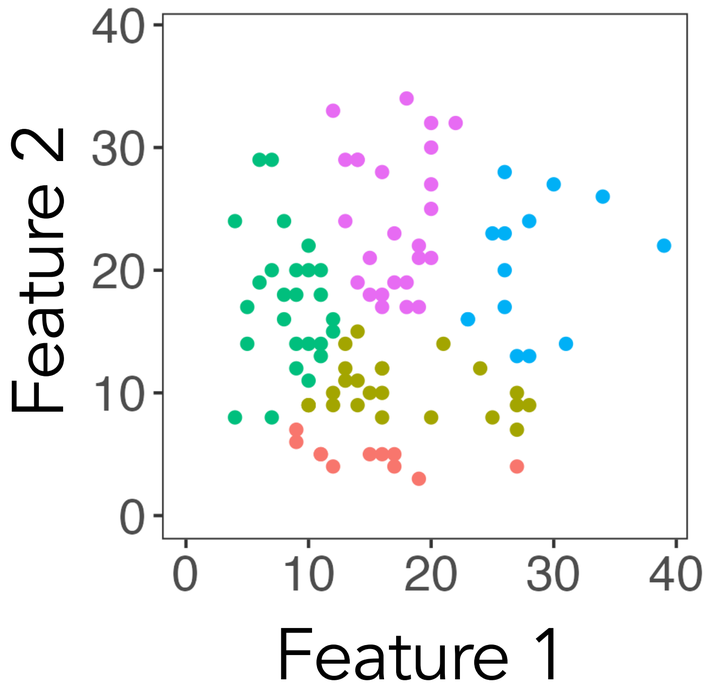

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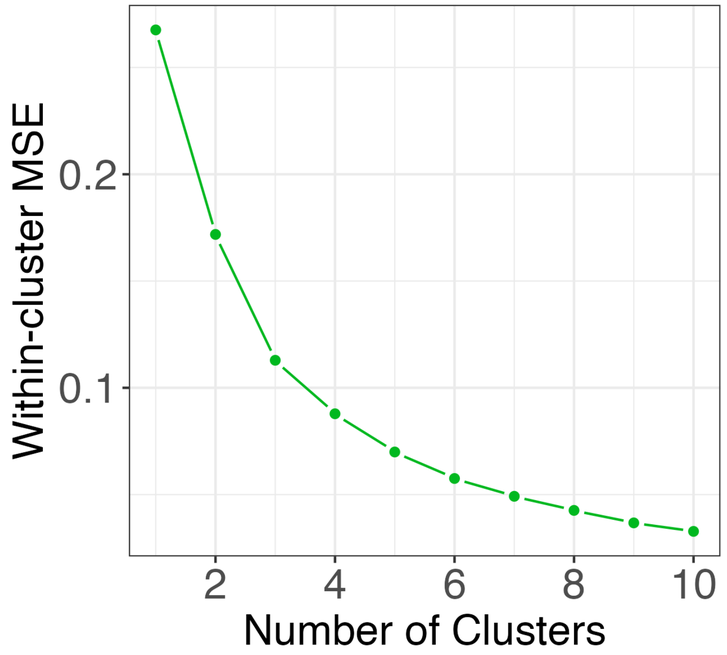
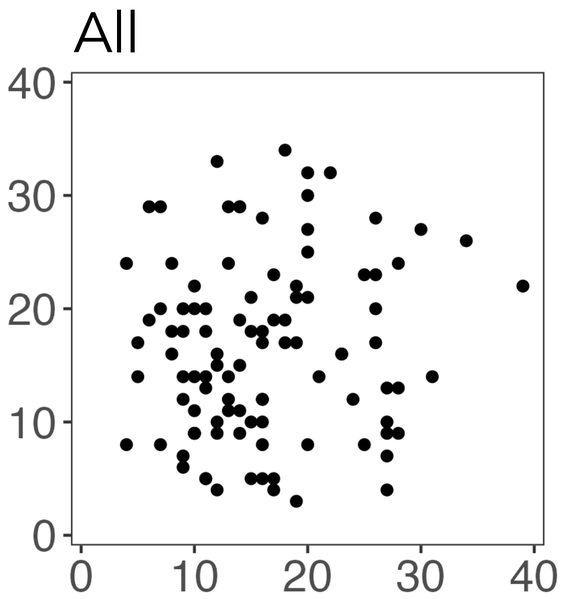


Sample splitting cannot be used for our motivating examples



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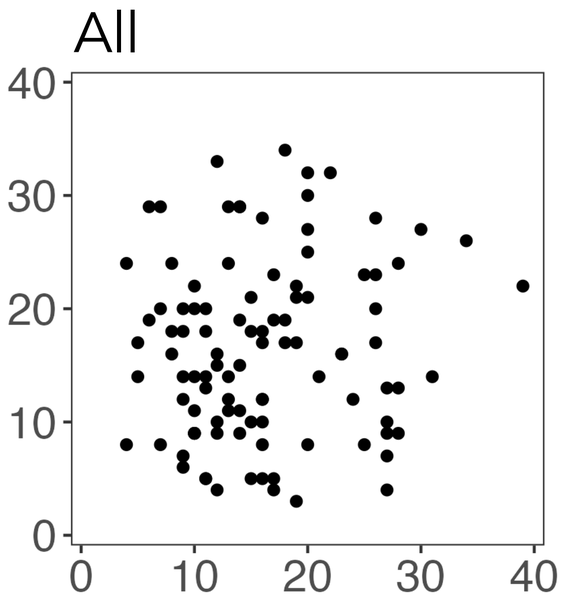

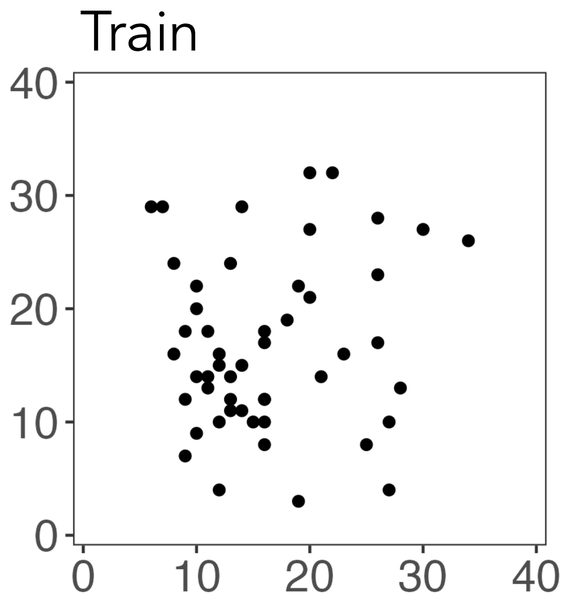

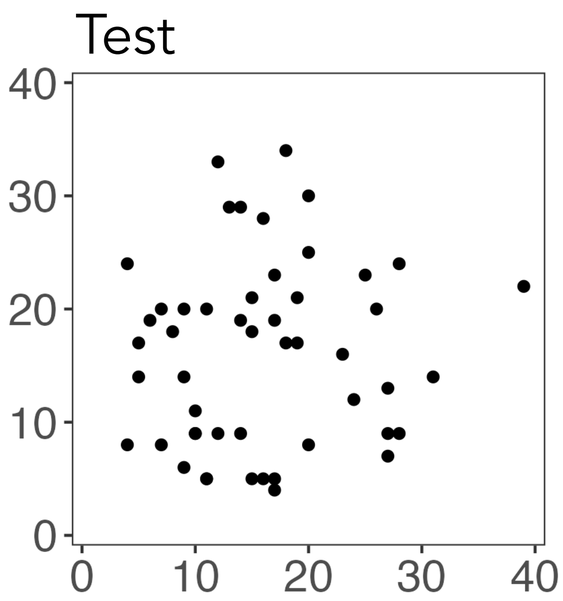

Step 1: split observations into train/test.

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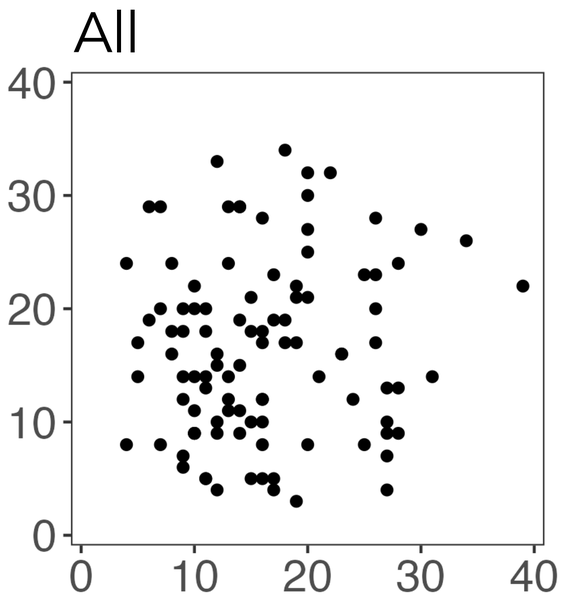

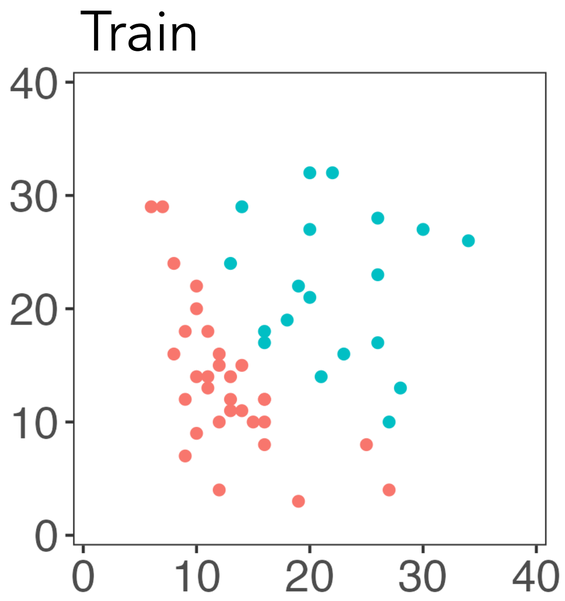

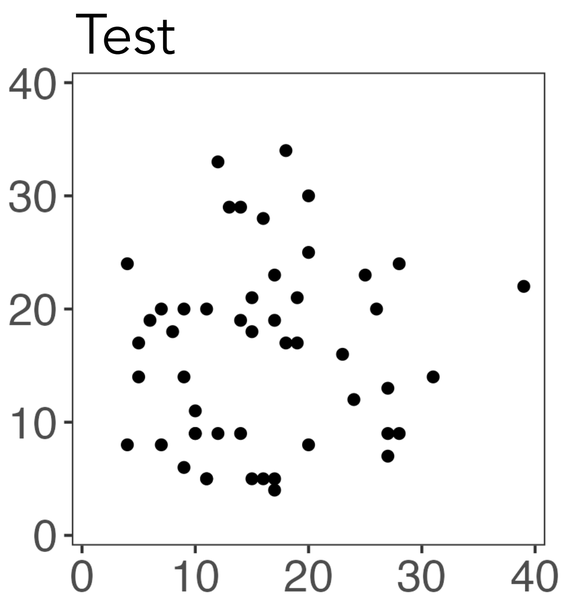

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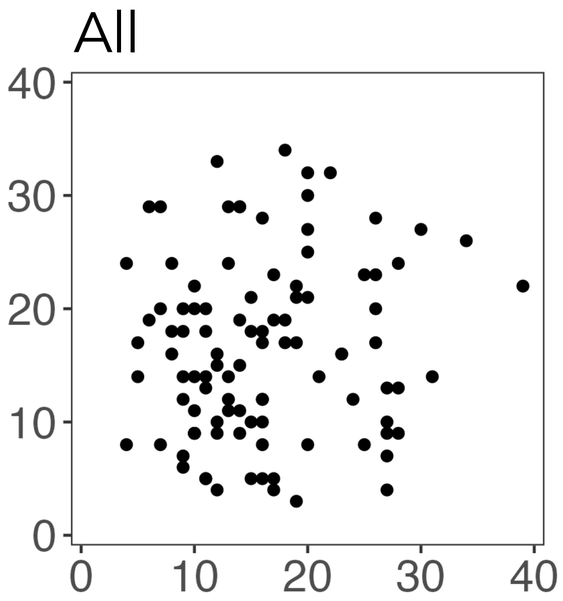

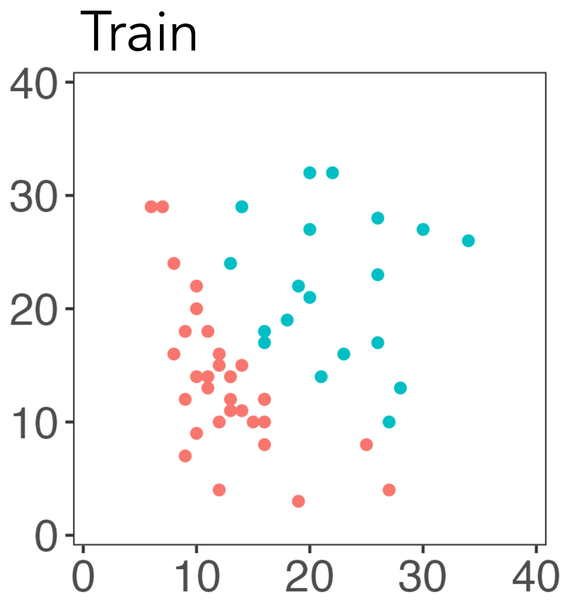

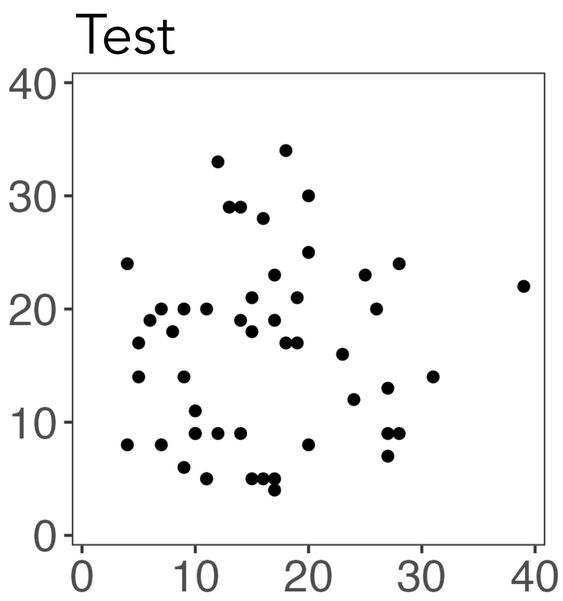

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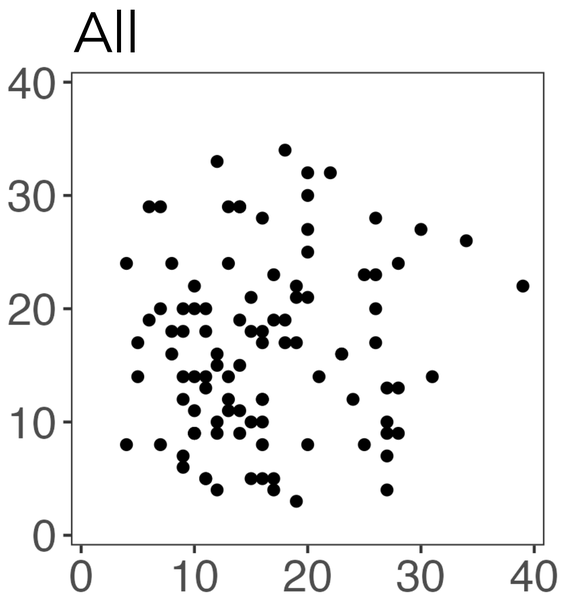

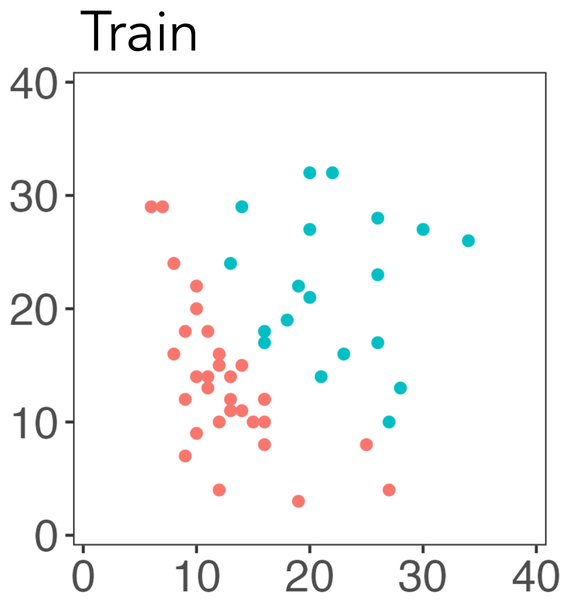

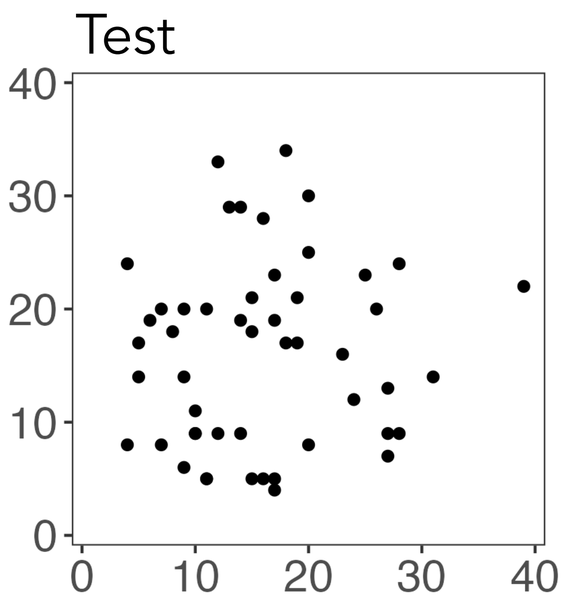

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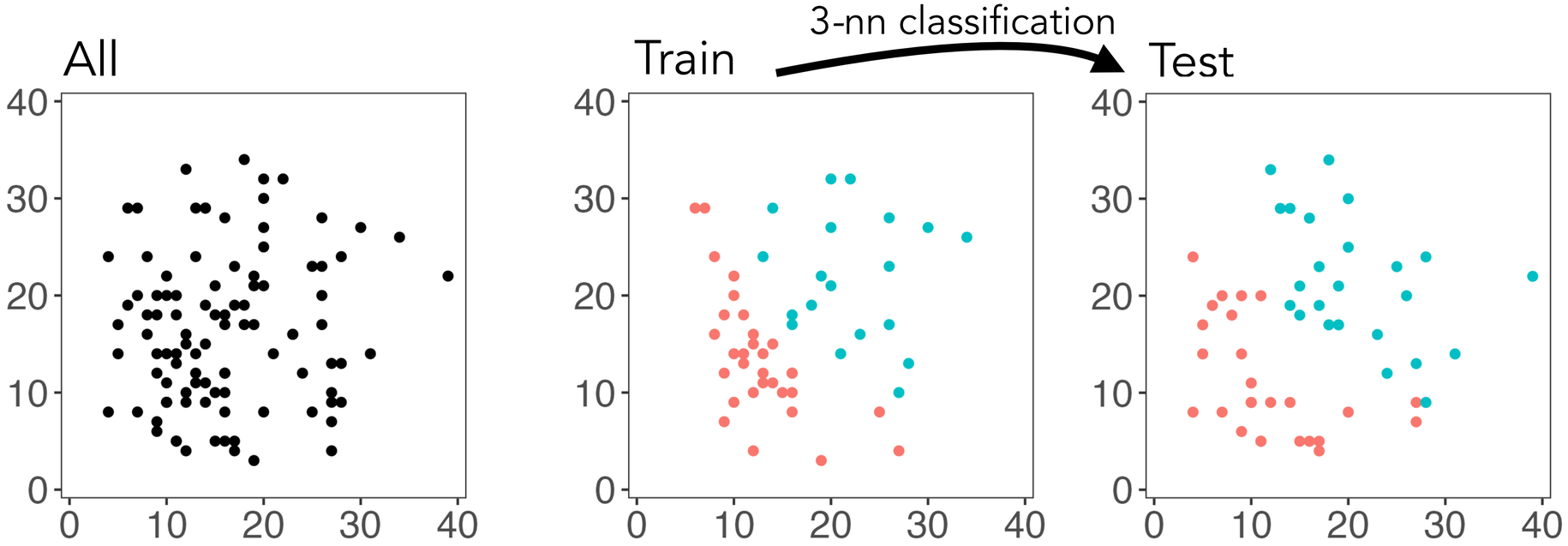

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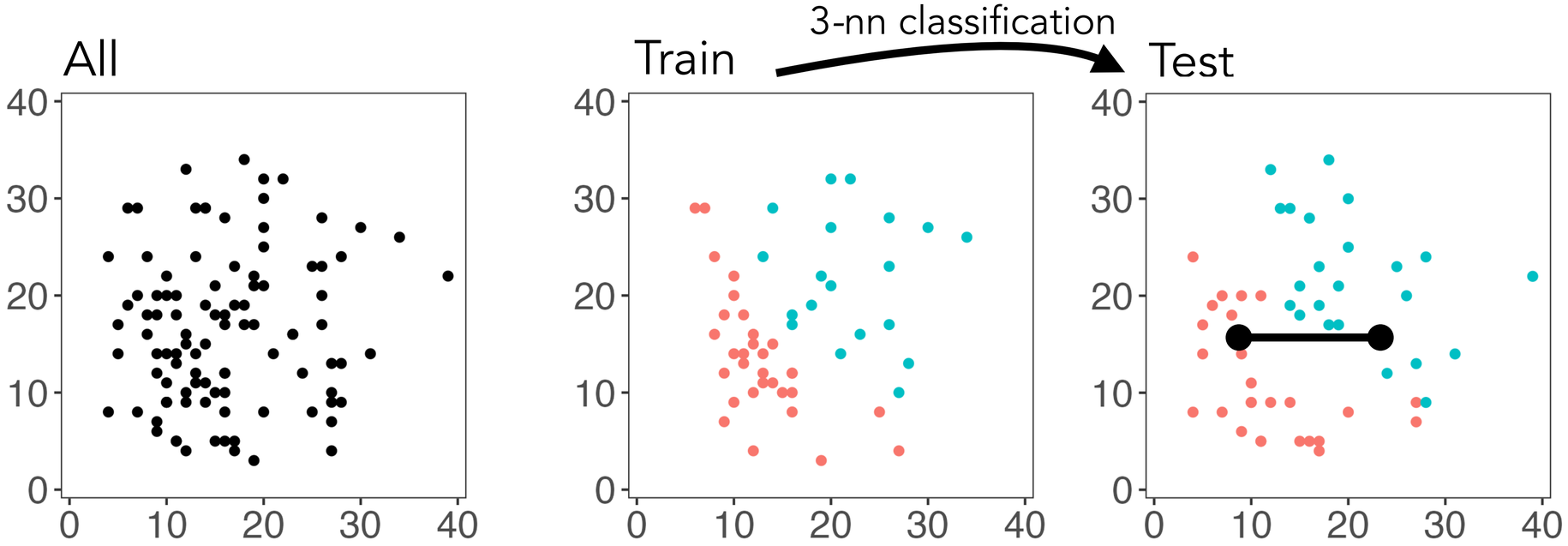

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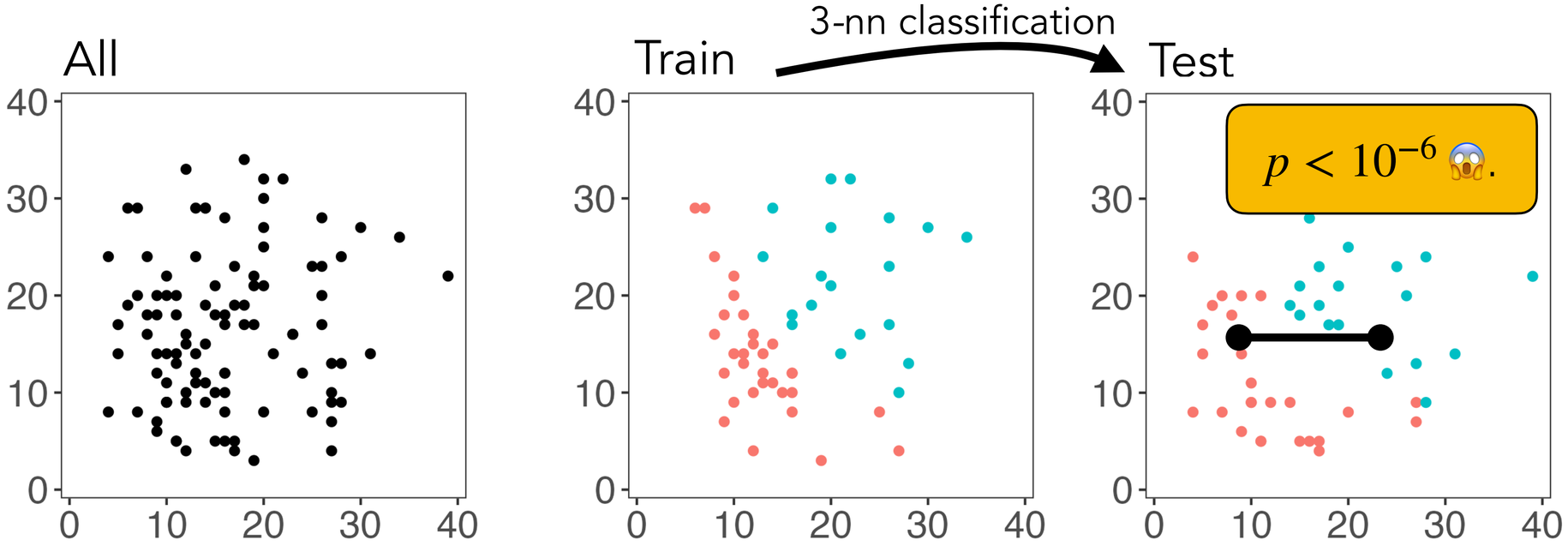

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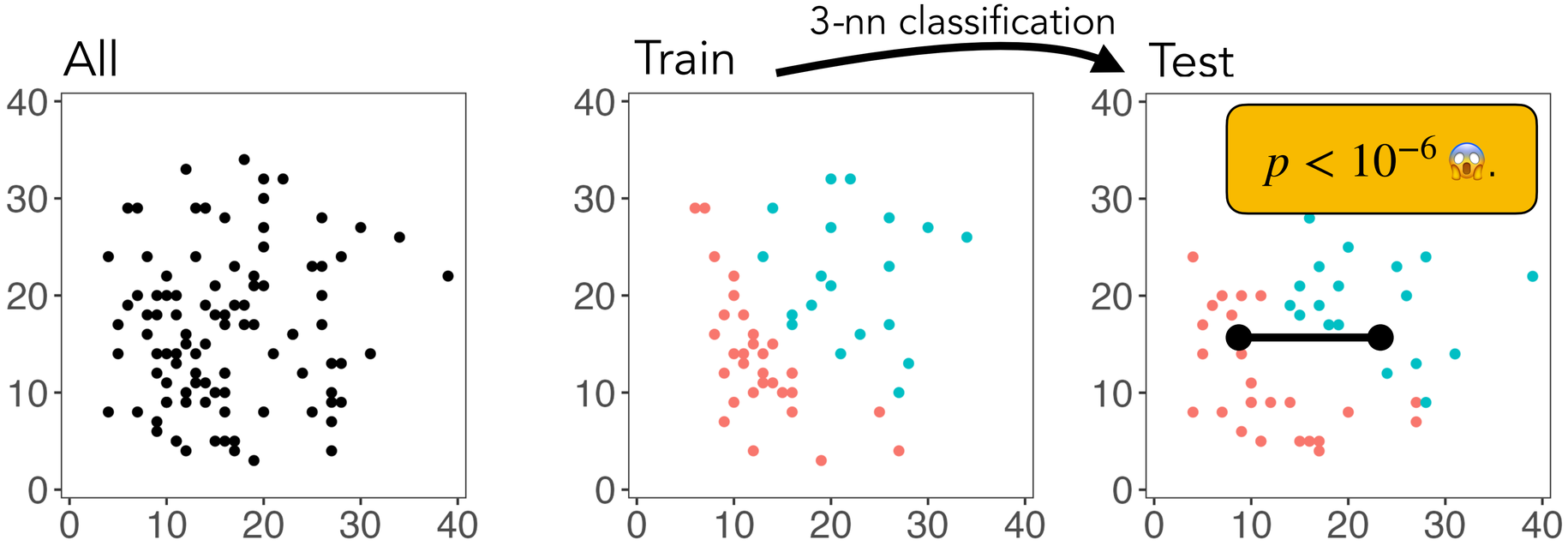

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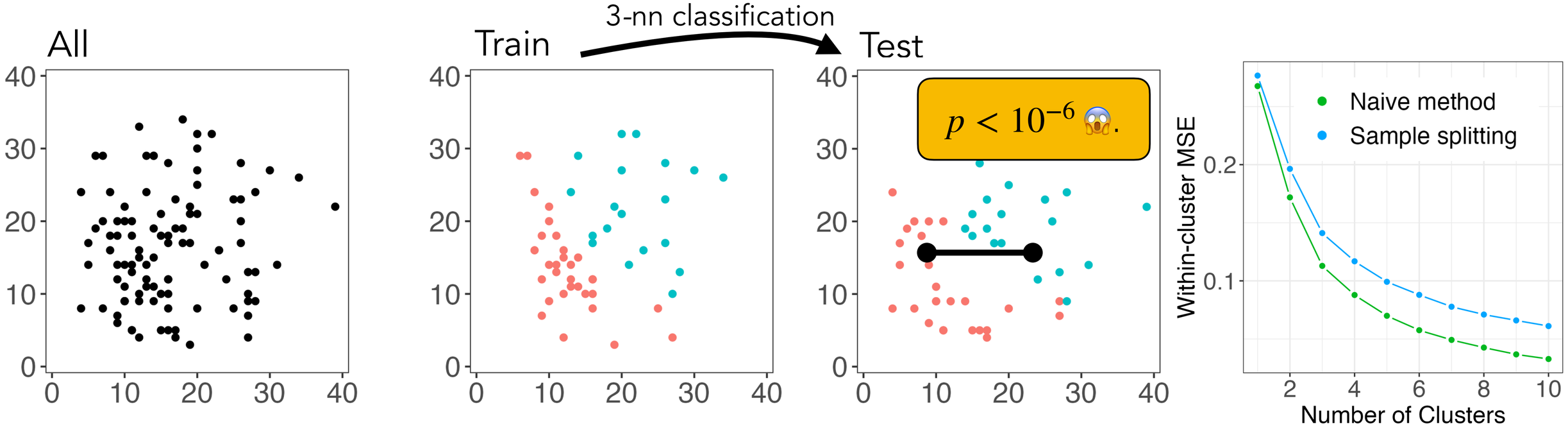

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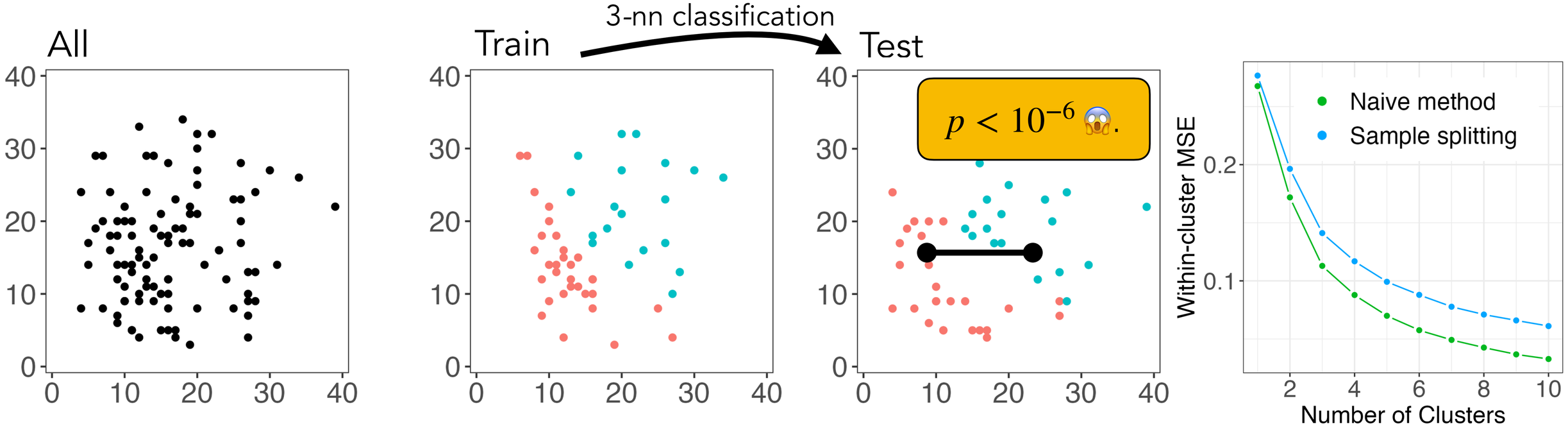

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Gao, Bien, and Witten, 2022 (JASA).
Fu and Perry, 2020 (JCGS).

Other situations in which sample splitting is not a good option

1. Fixed-X regression settings.

2. Non-IID data.

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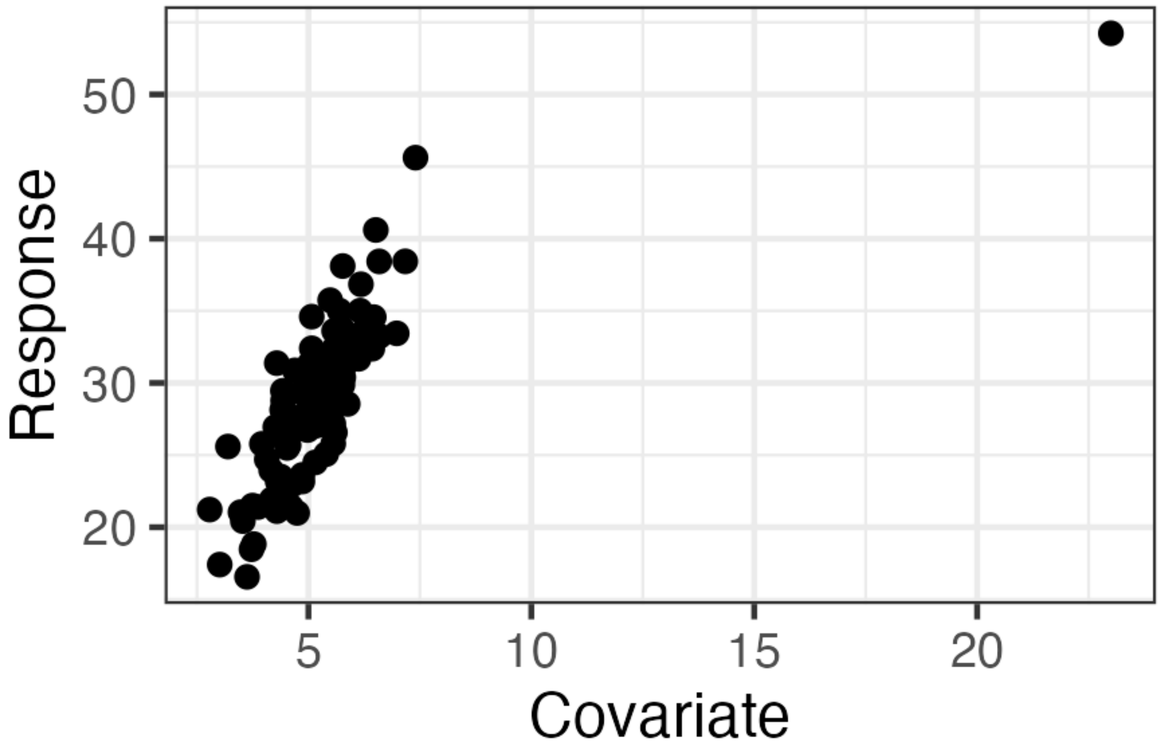

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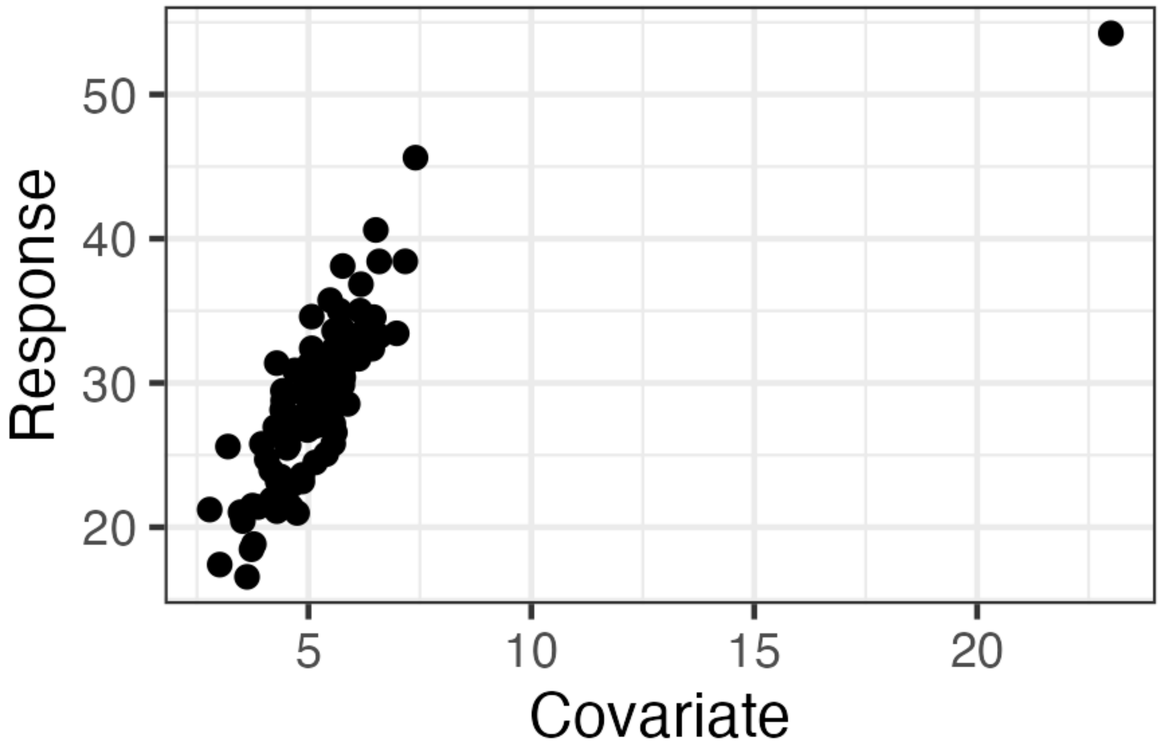
Application later: changepoint detection.



Outline

1. Motivation: sample splitting doesn’t always work
2. **Poisson thinning**
3. Data thinning
4. Generalized data thinning
5. Application to changepoint validation
6. Ongoing work

Poisson thinning

X

	Feature 1	Feature 2
Obs. 1	18	6
Obs. 2	31	8
Obs. 3	11	31
Obs. 4	22	34

Poisson thinning

X

	Feature 1	Feature 2
Obs. 1	18	6
Obs. 2	31	8
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$X^{(1)}$

	Feature 1	Feature 2
Obs. 1	14	1
Obs. 2	10	6
Obs. 3	5	17
Obs. 4	6	25

$X^{(2)}$

	Feature 1	Feature 2
Obs. 1	4	5
Obs. 2	21	2
Obs. 3	6	14
Obs. 3	16	9

Poisson thinning

X

	Feature 1	Feature 2
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	Feature 1	Feature 2
Obs. 1	14	1
Obs. 2	[illegible]	6
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$$X_{ij}^{(1)} \mid X_{ij} = x_{ij} \sim \text{Binomial}(x_{ij}, \epsilon)$$

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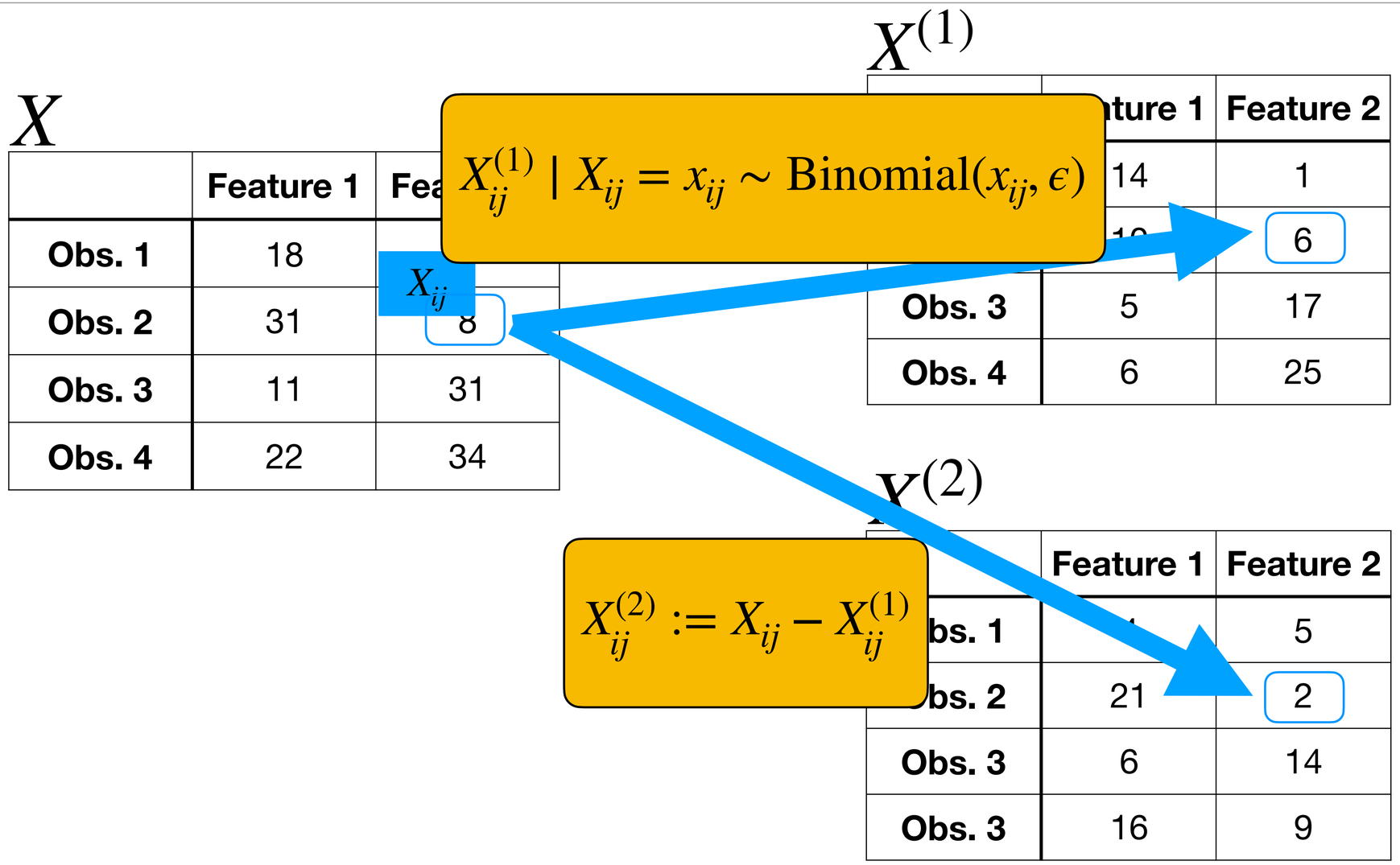

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$$X_{ij}^{(2)} := X_{ij} - X_{ij}^{(1)}$$

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If $X_{ij} \sim \text{Poisson}(\Lambda_{ij})$, then:

1. $X_{ij}^{(1)} \sim \text{Poisson}(\epsilon\Lambda_{ij})$
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A very well-known result: binomial thinning of the Poisson distribution.

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Select hypothesis.

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Test hypothesis.

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Fit model.

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Evaluate model.

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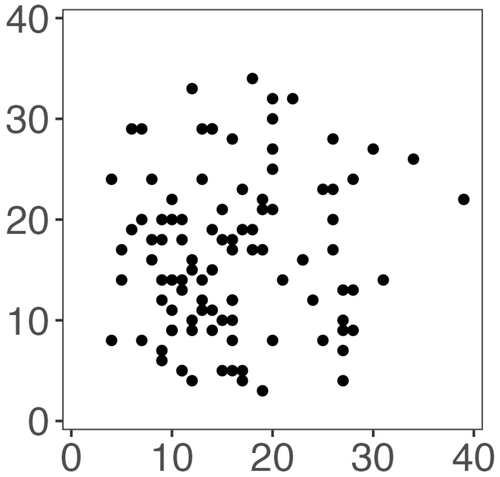
Thinning avoids the pitfall of sample splitting on our motivating examples



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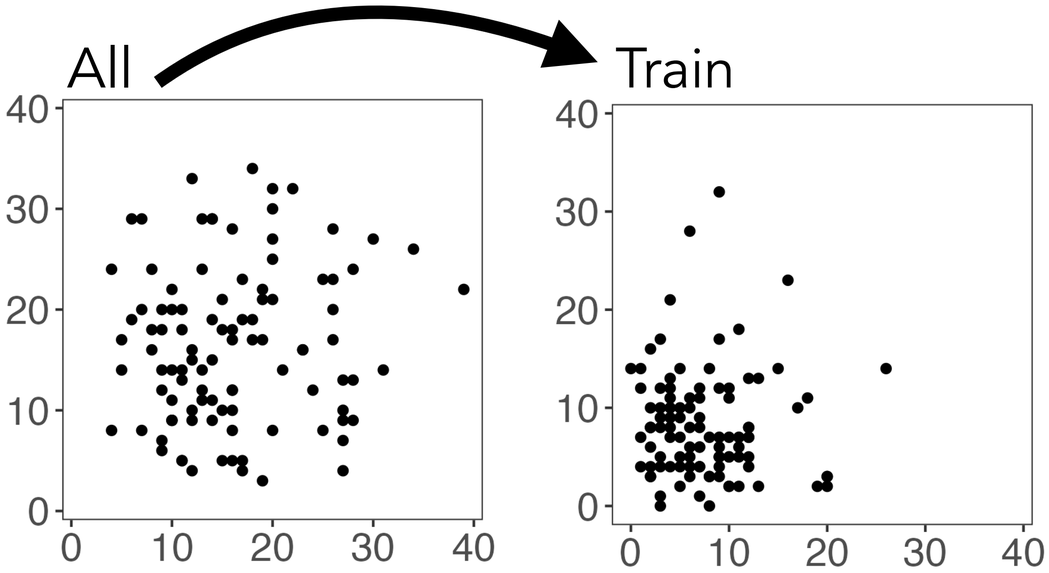

Step 1: thin observations into train/test.

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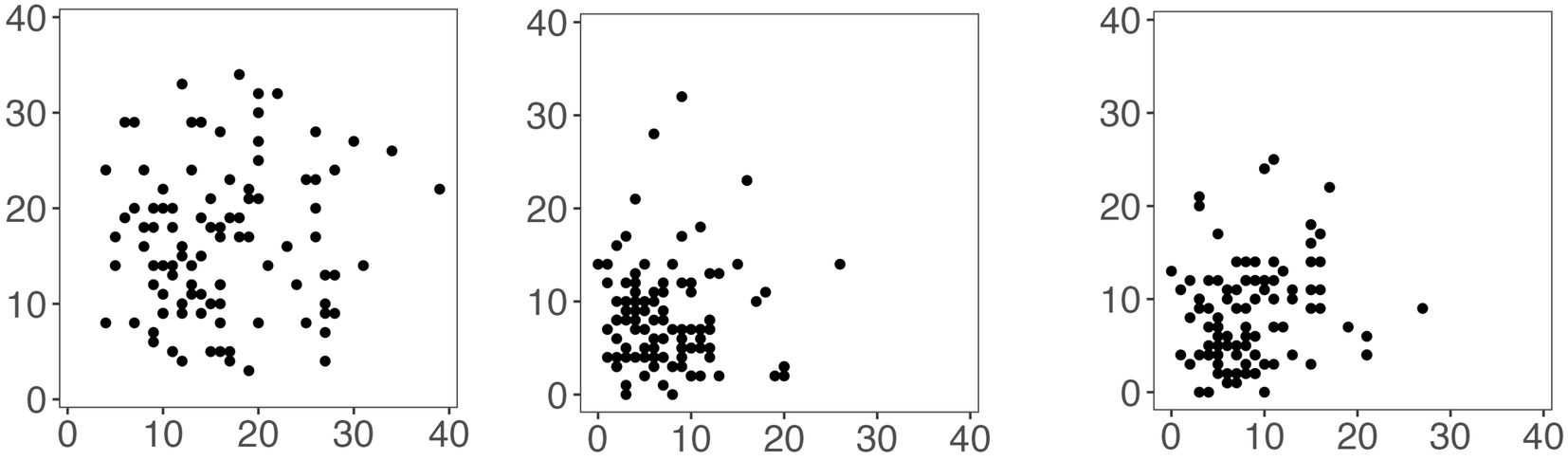

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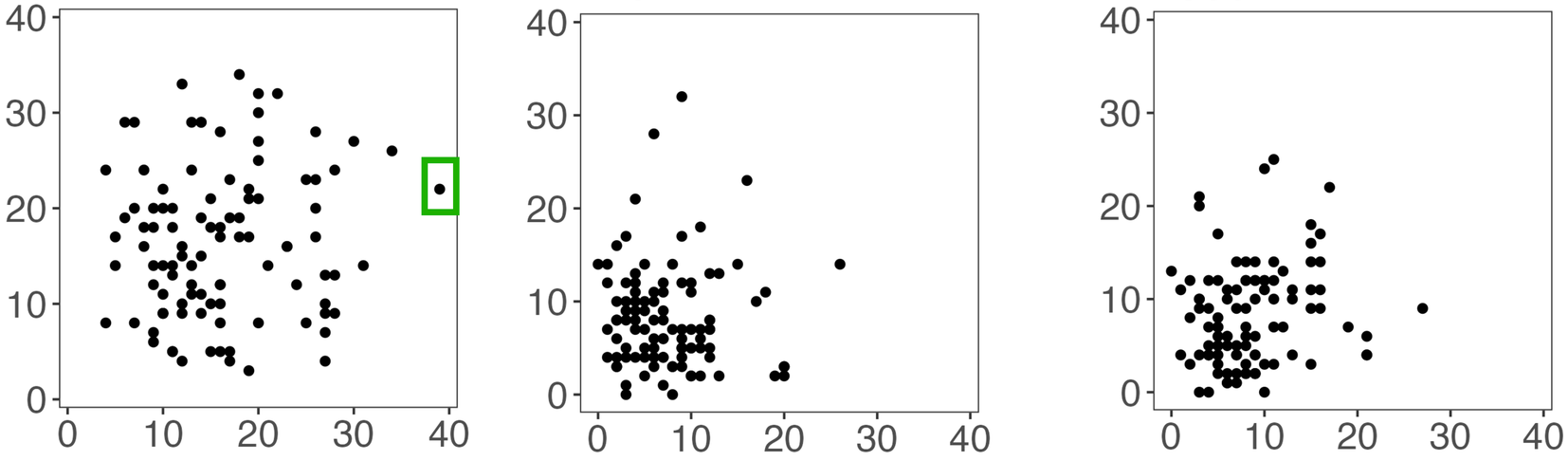

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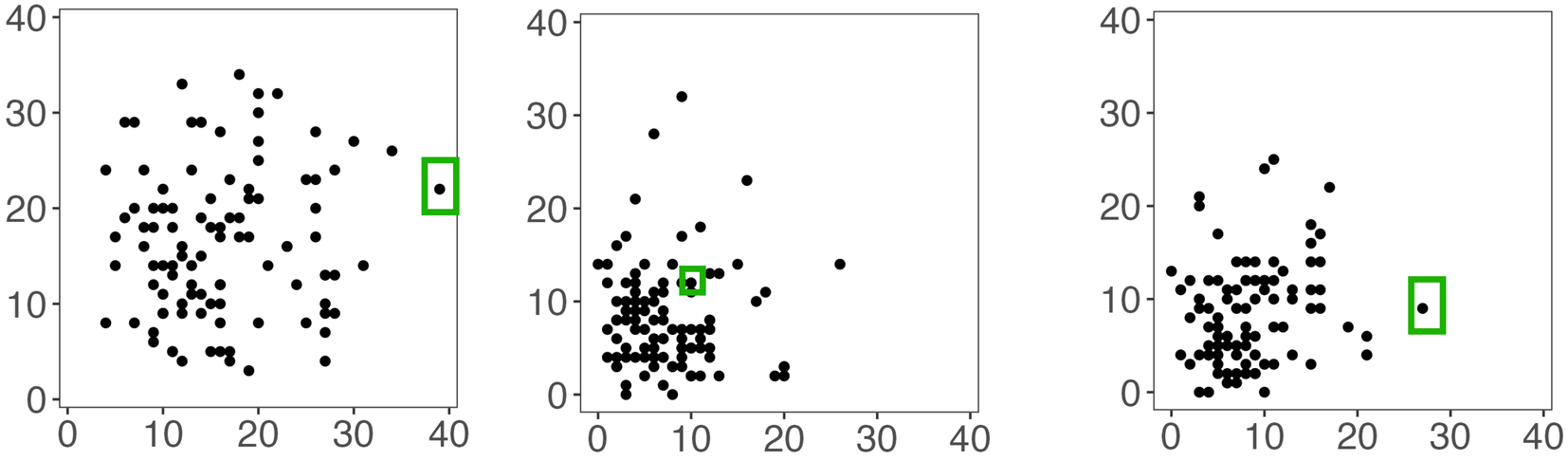

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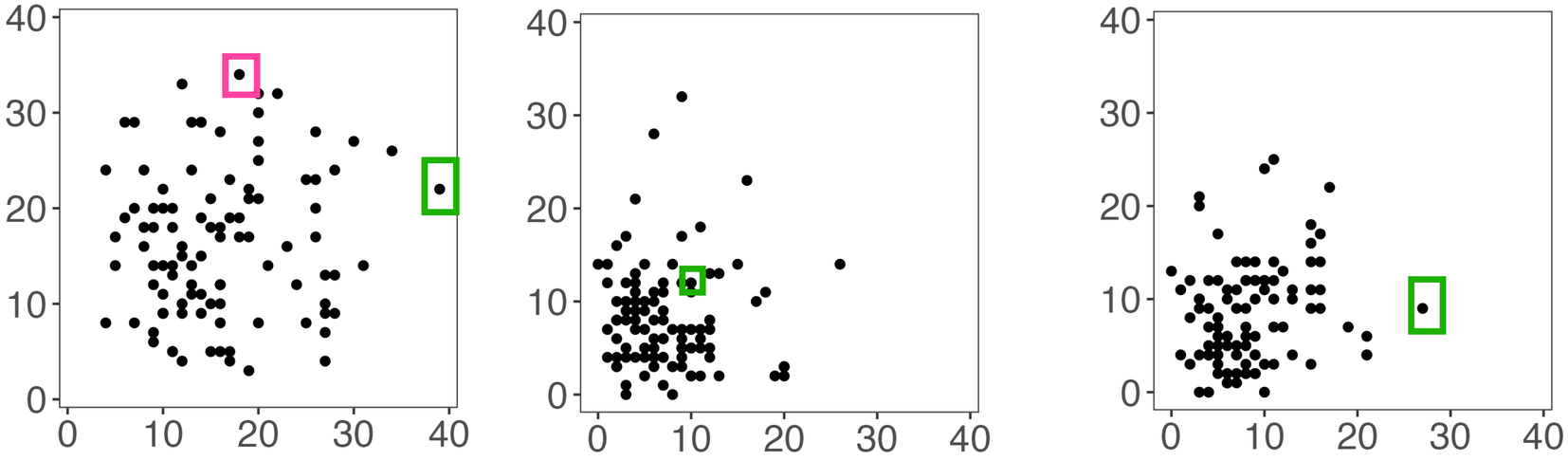

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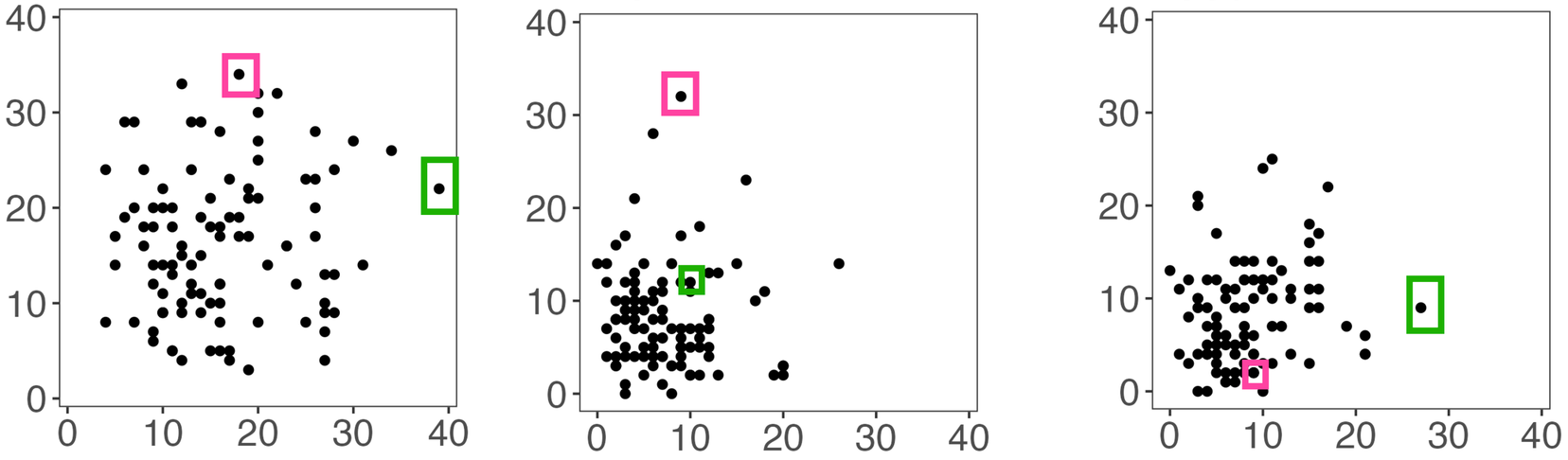

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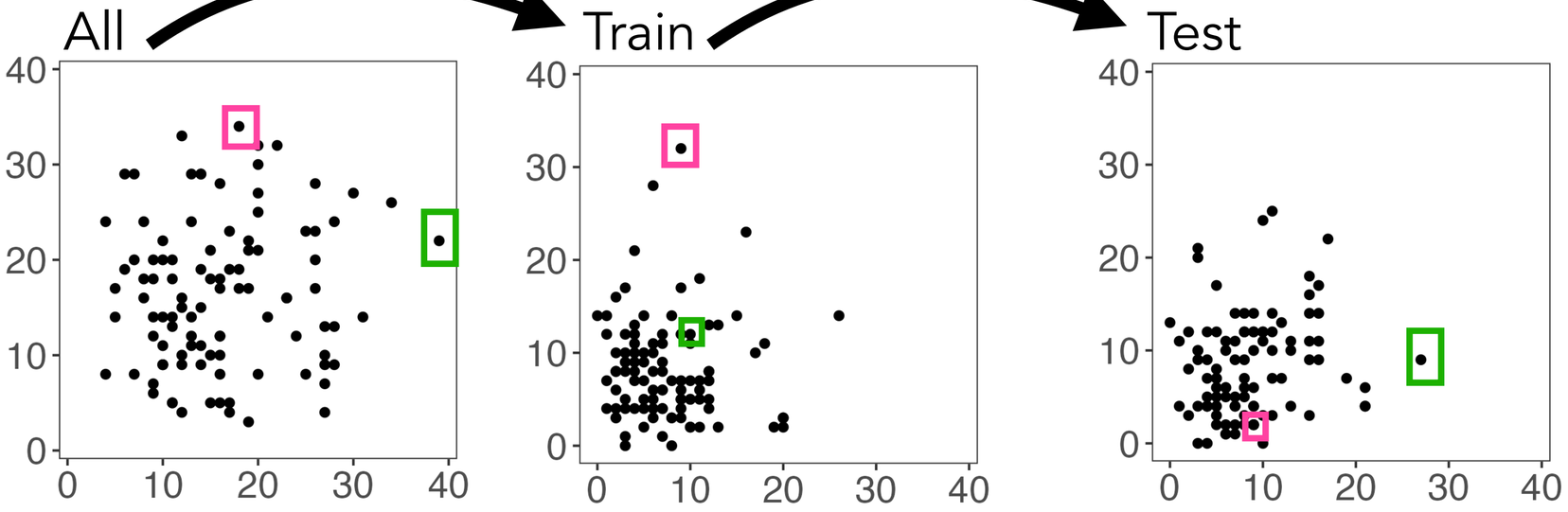

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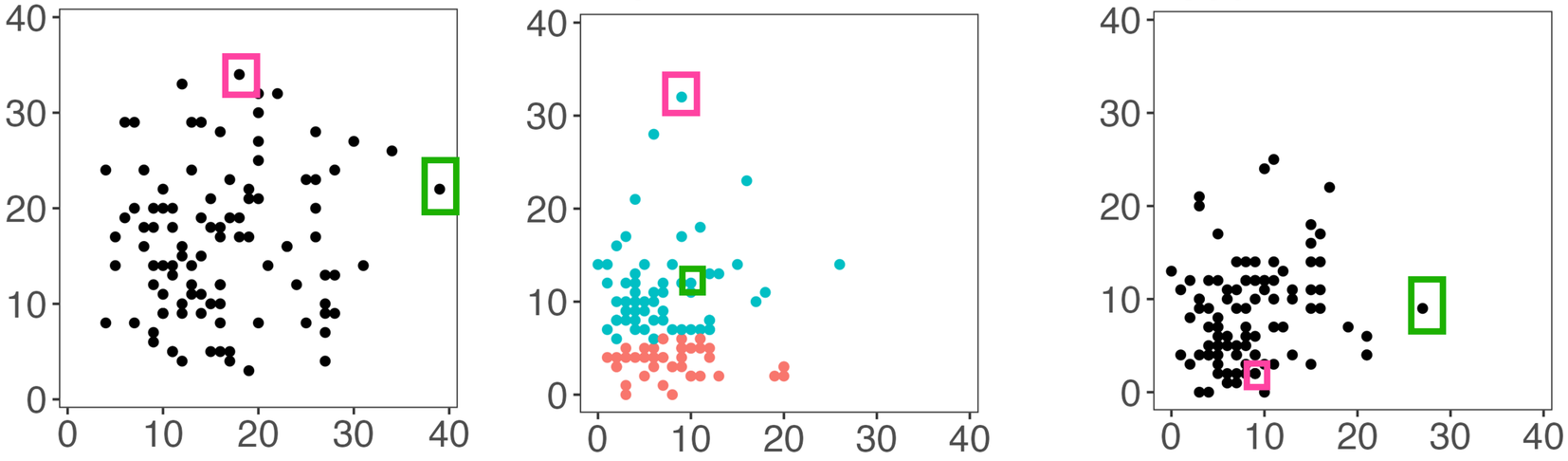

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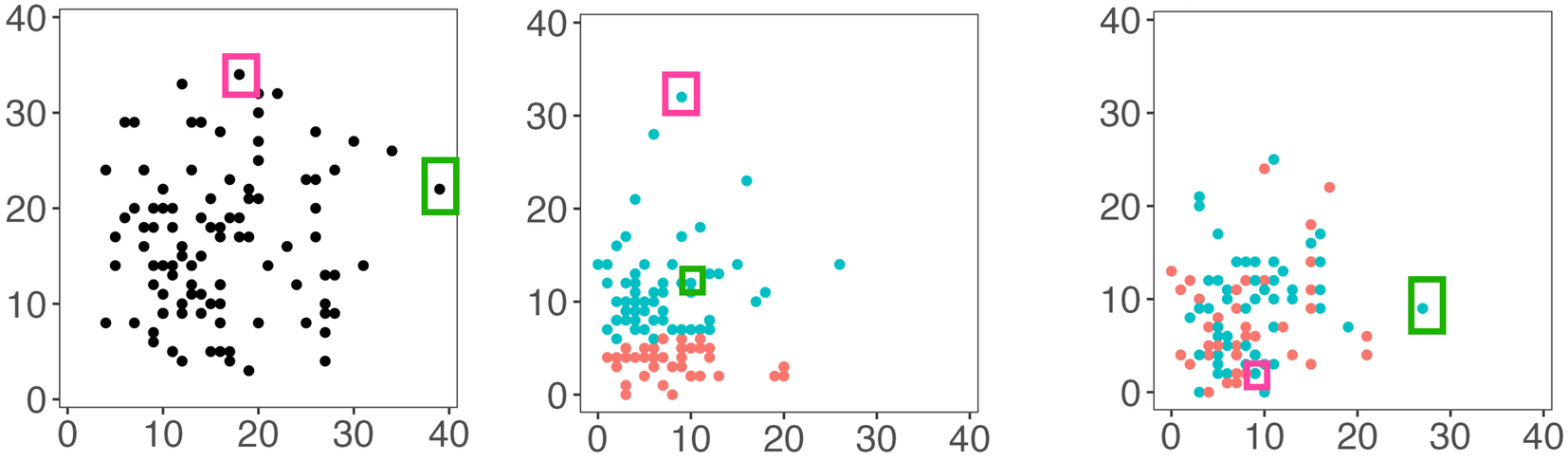

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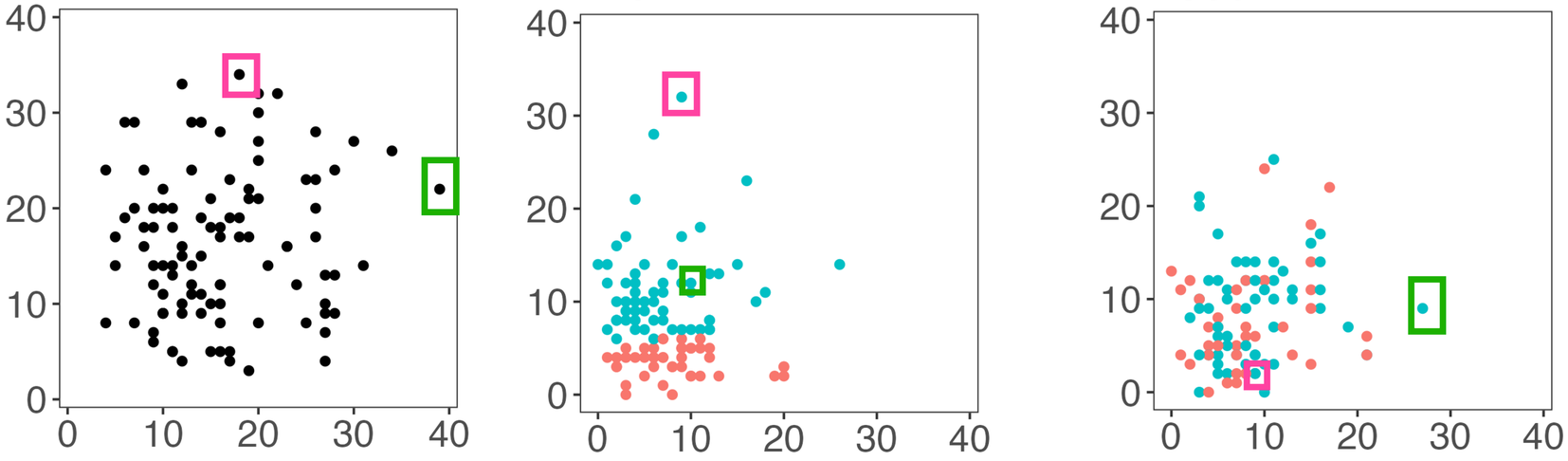

Step 1: thin observations into train/test.

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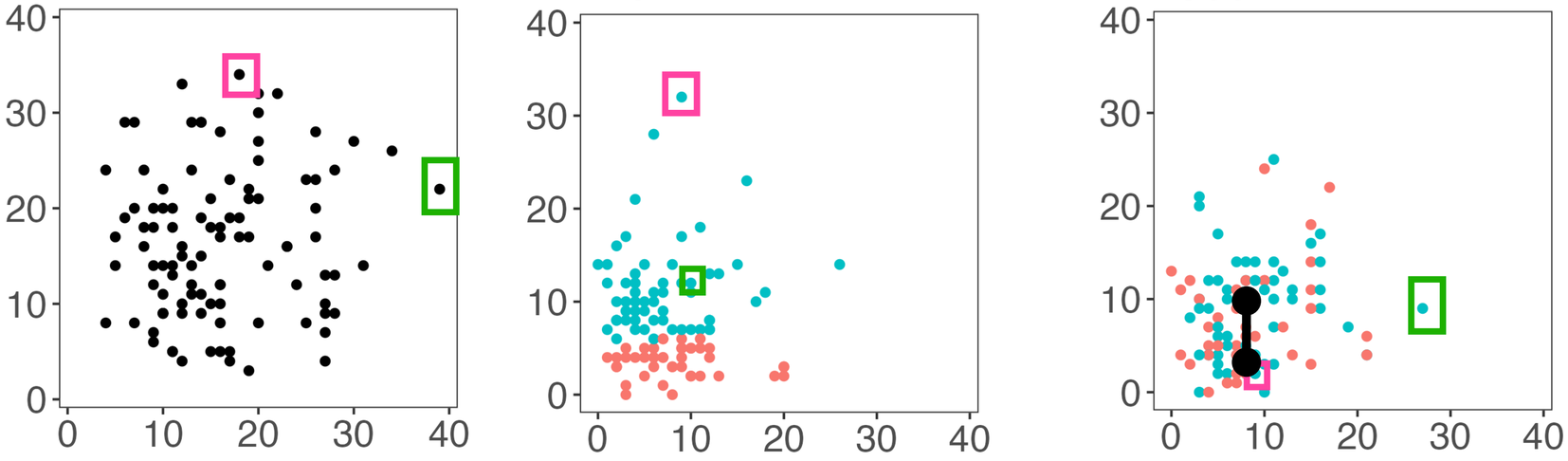

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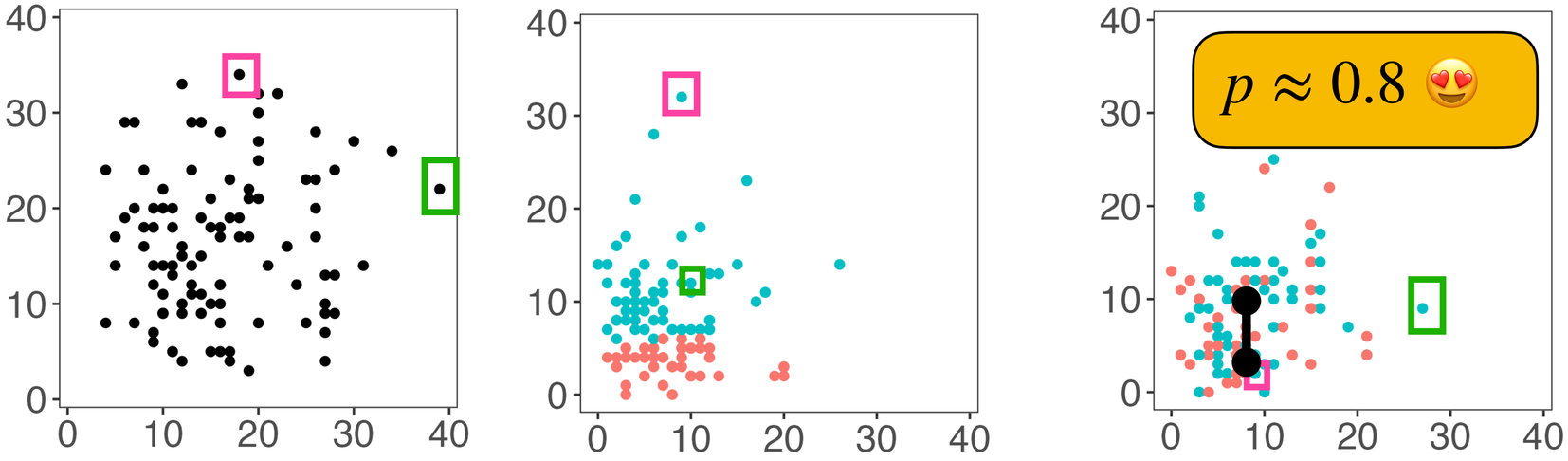

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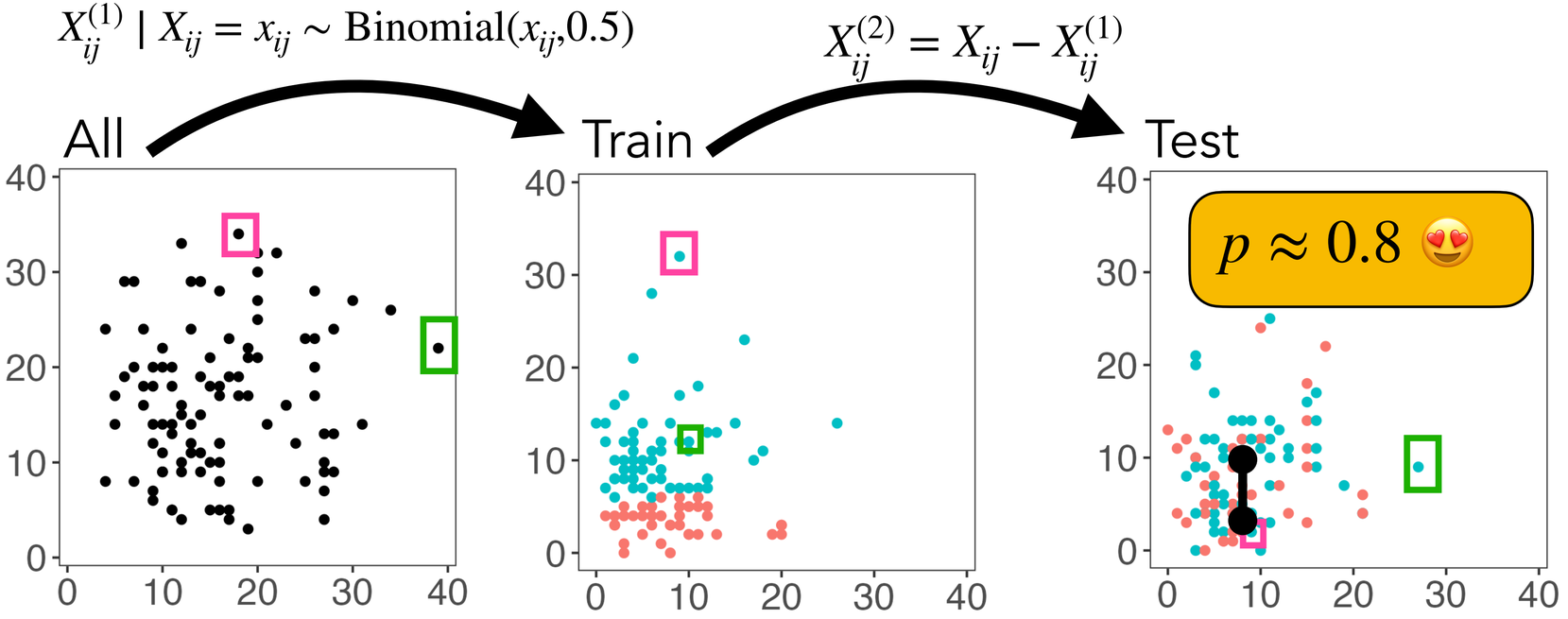

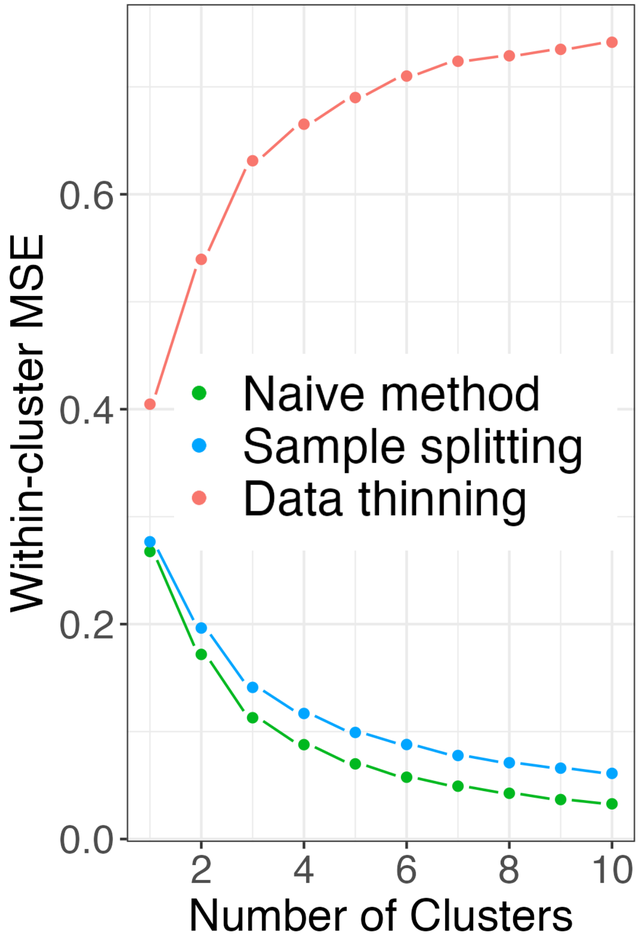

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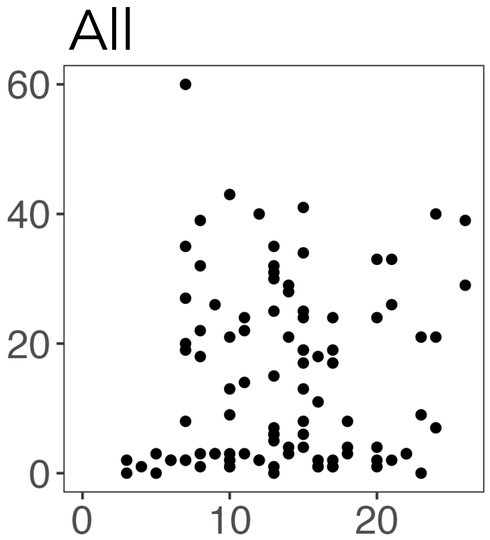

$$X_{i2} \sim \begin{cases} \text{Poisson}(3) & \text{if } i \leq 50 \\ \text{Poisson}(25) & \text{if } i > 50 \end{cases}$$

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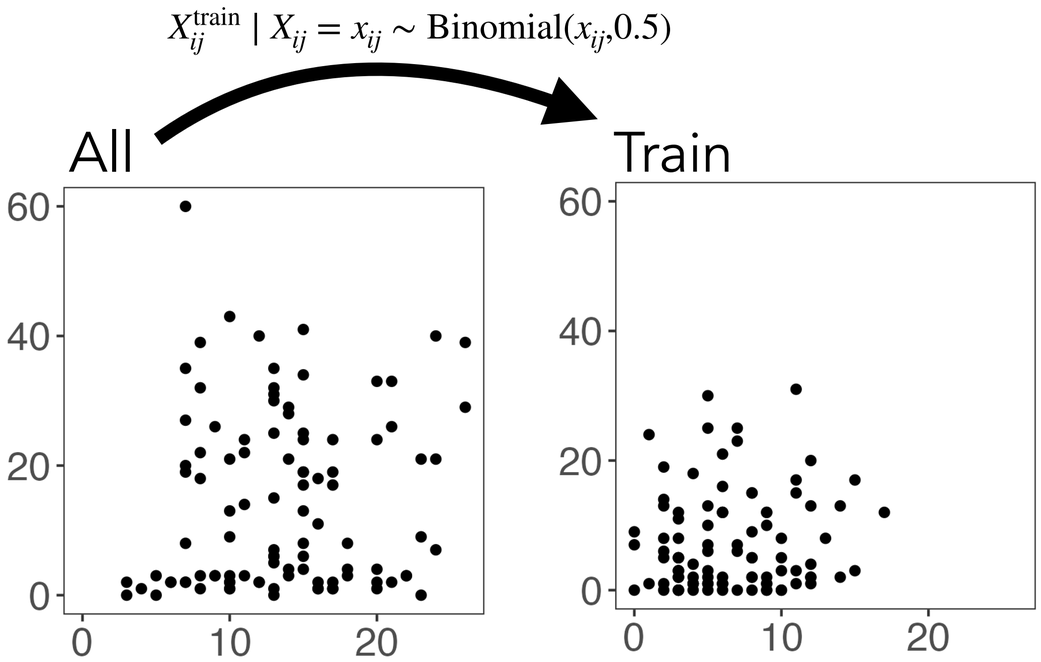

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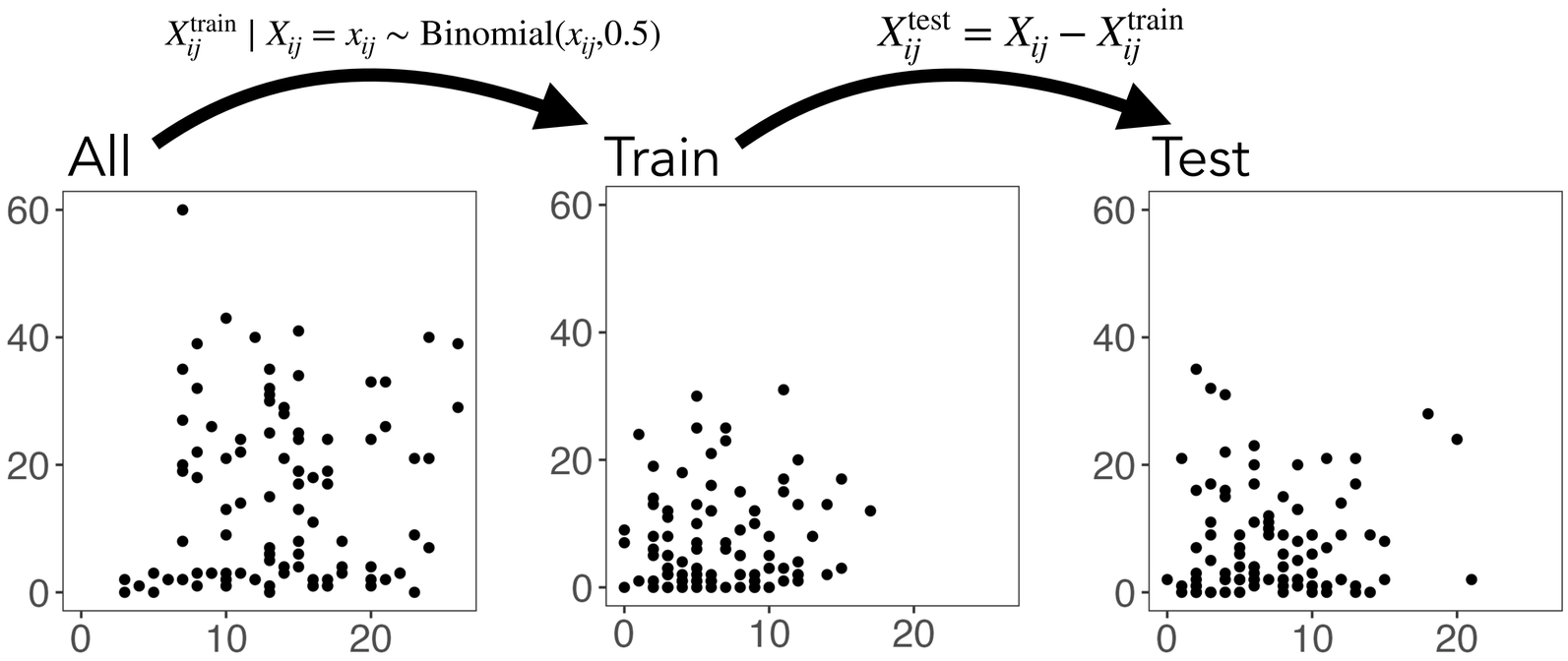

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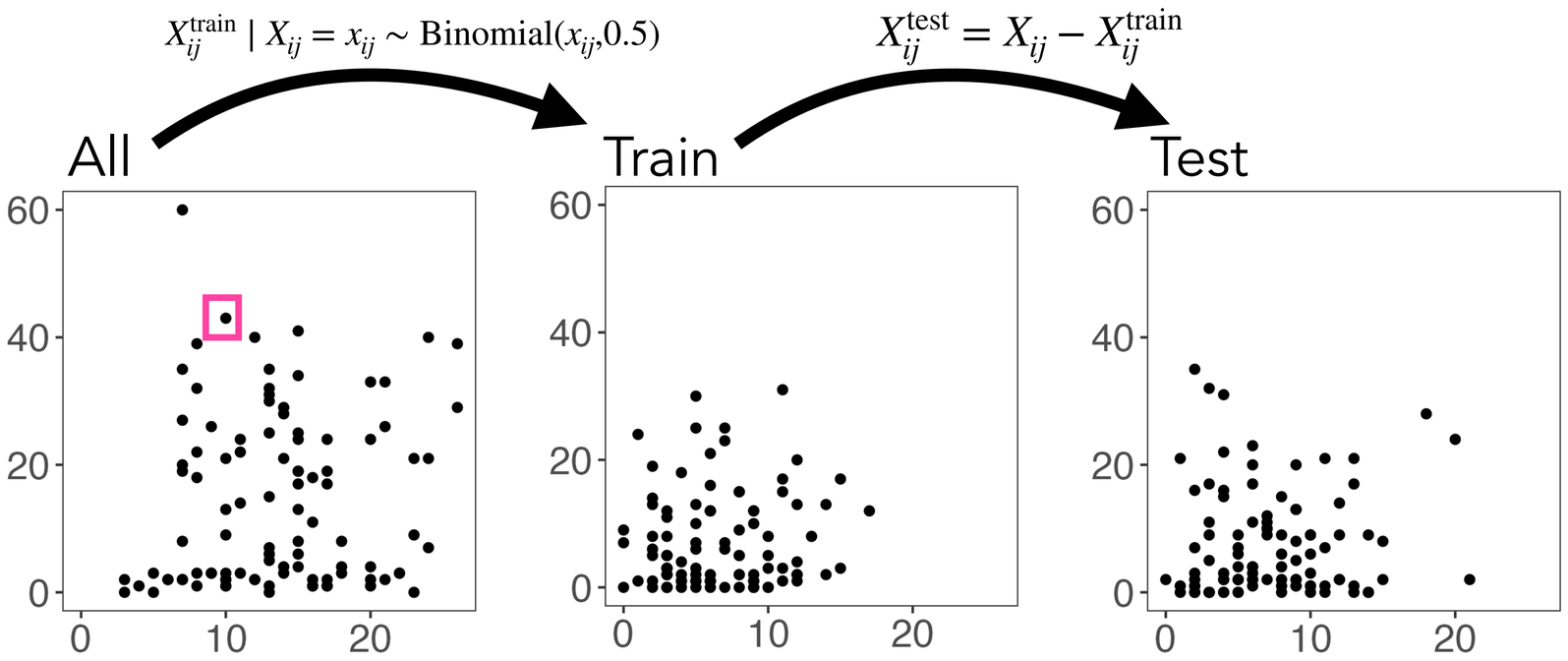

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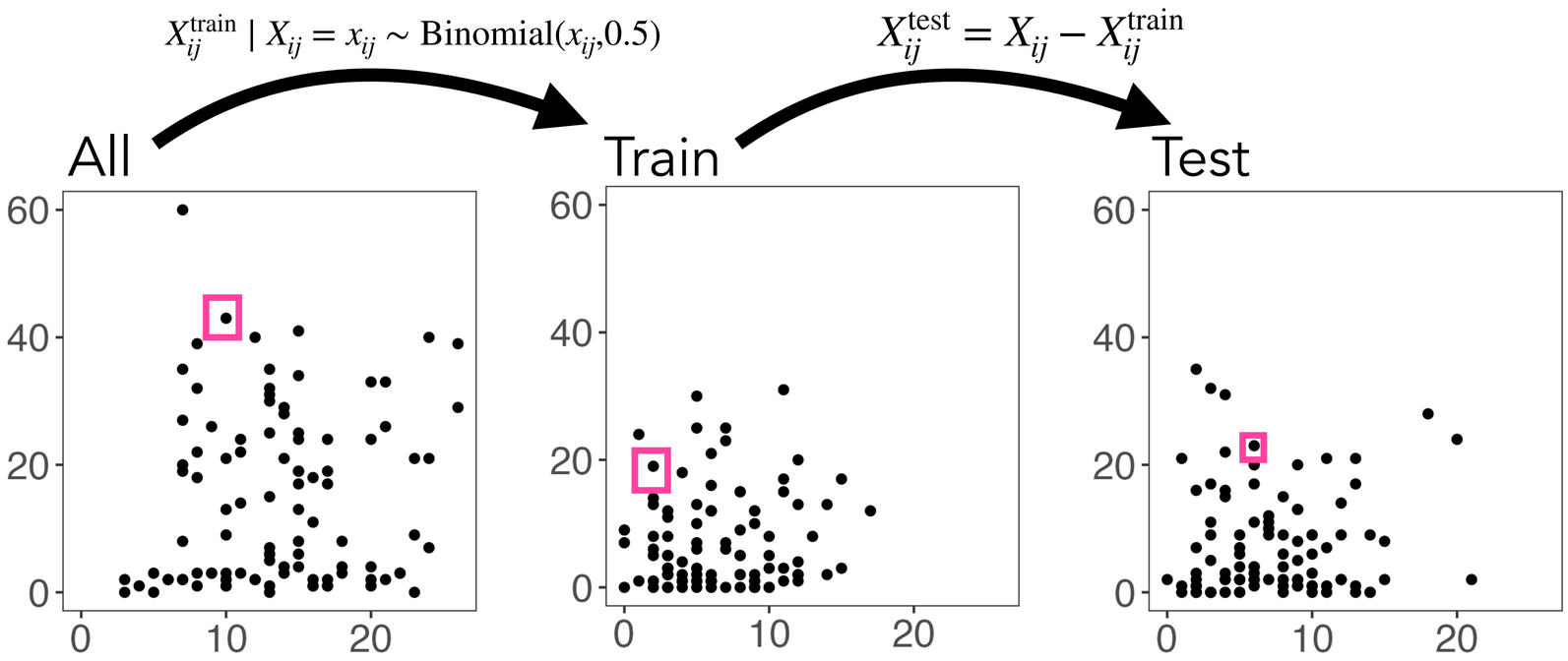

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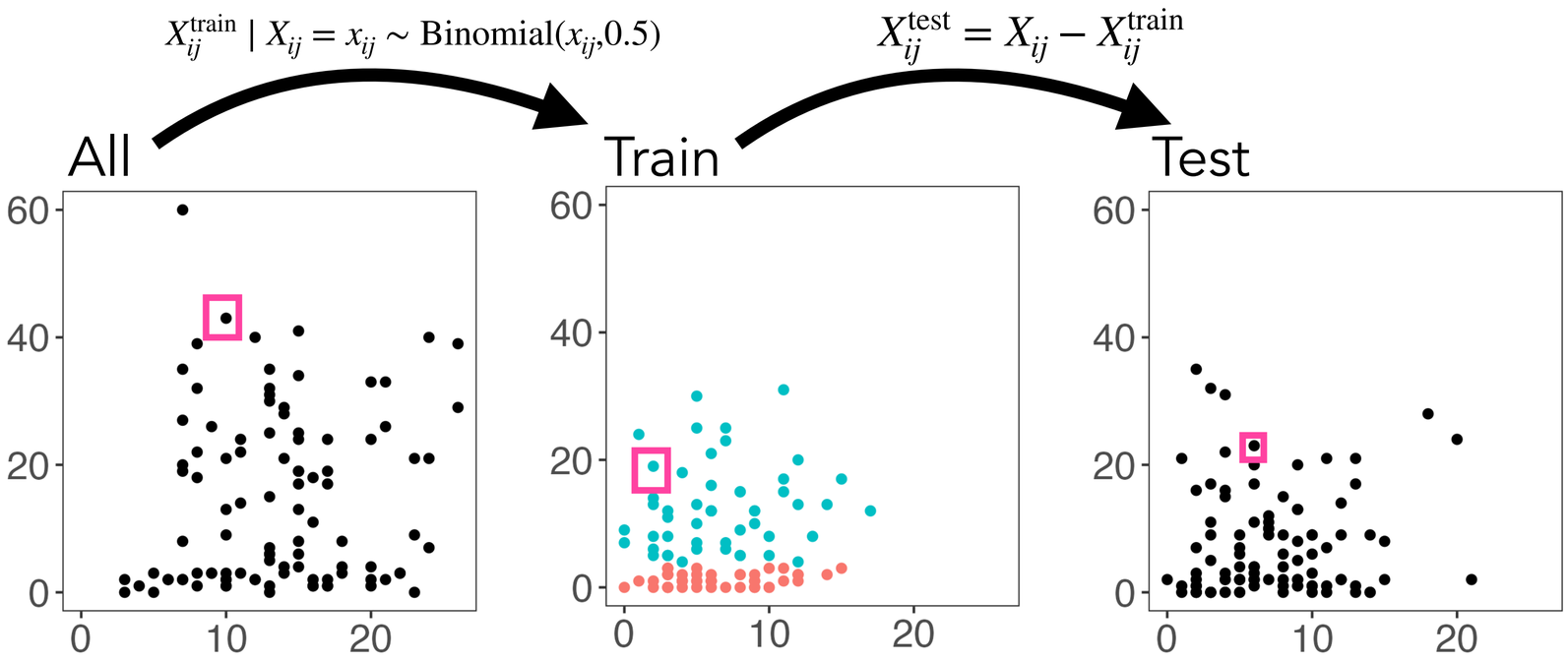

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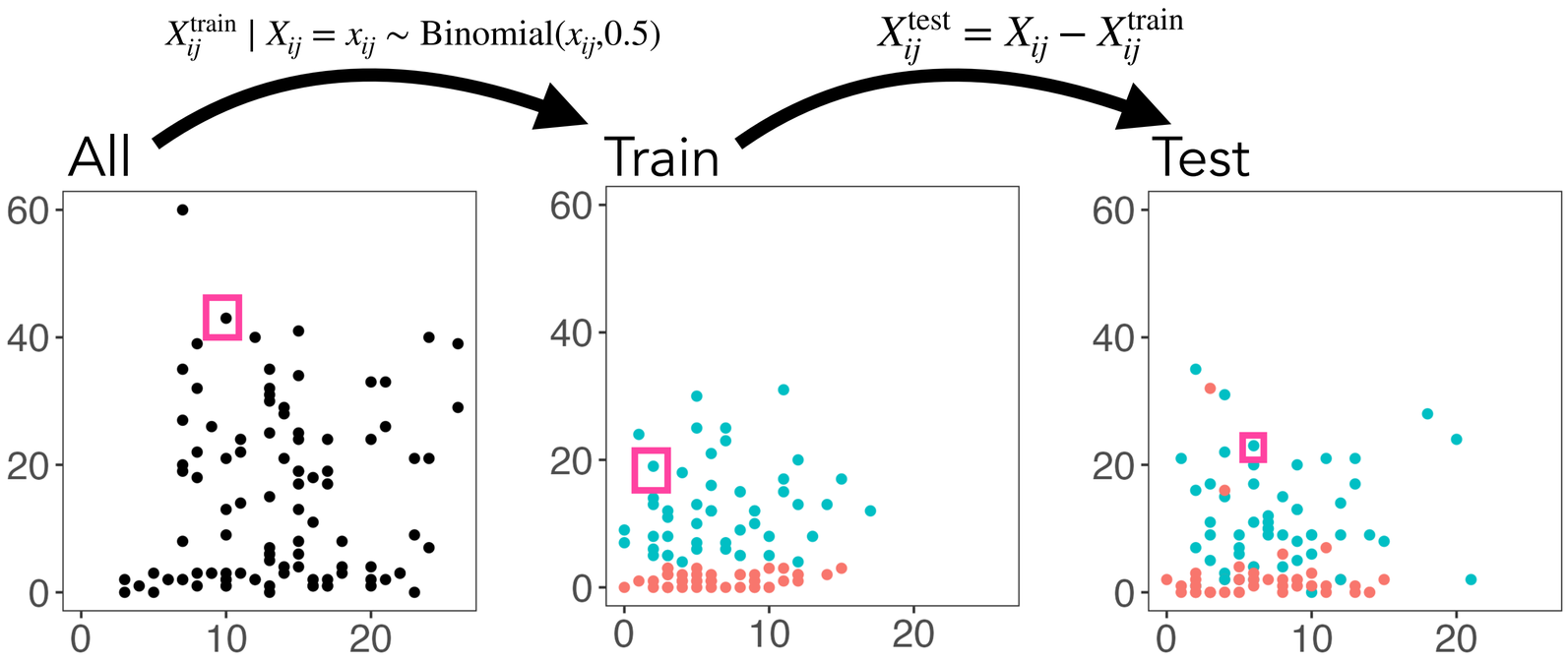

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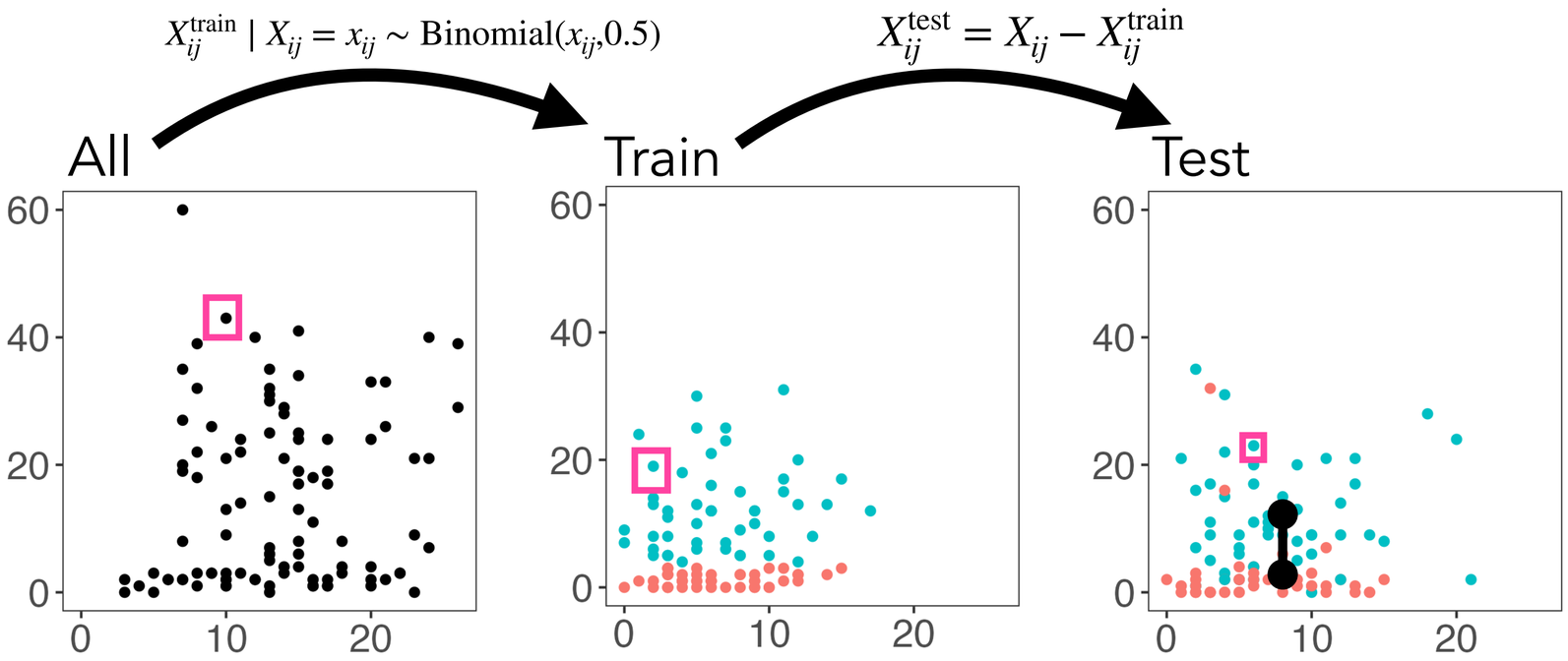

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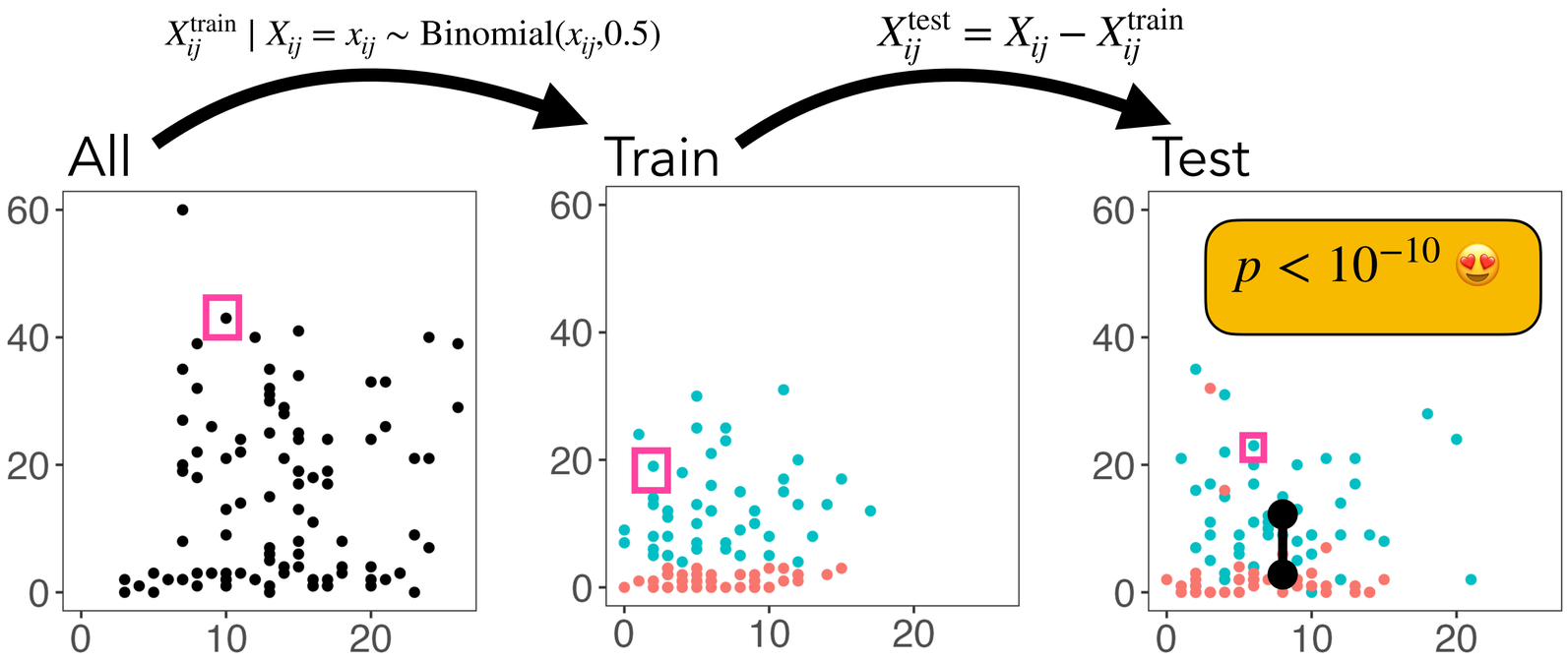

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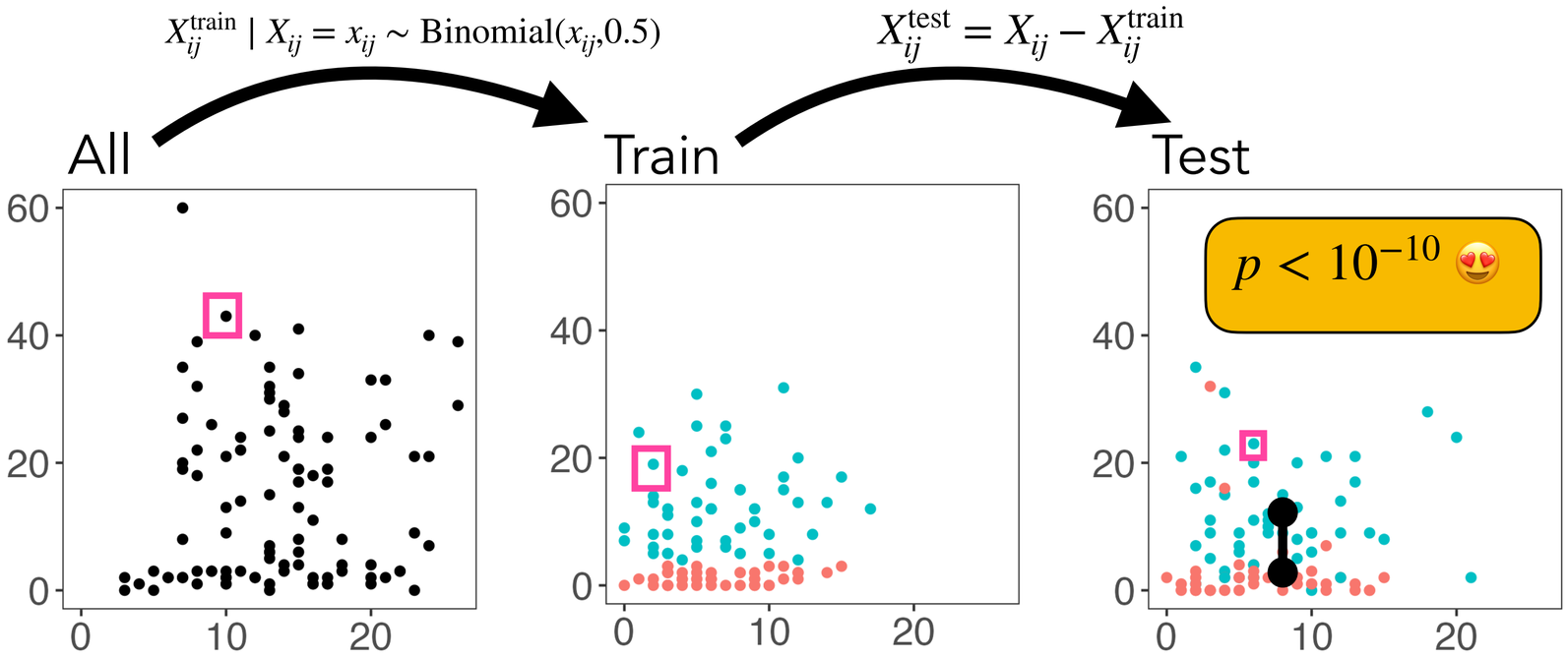

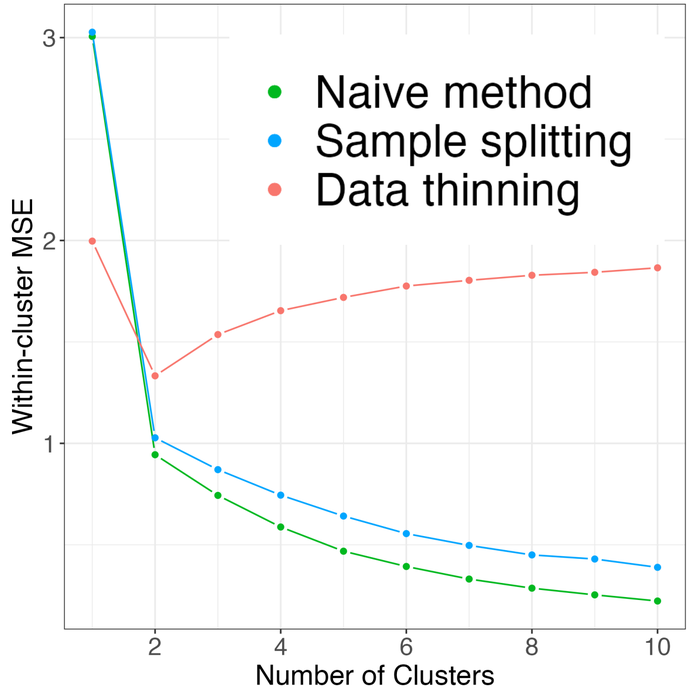

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Outline

1. Motivation: sample splitting doesn’t always work
2. Poisson thinning
3. **Data thinning**
4. Generalized data thinning
5. Application to changepoint validation
6. Ongoing work

What did we like about Poisson thinning?

We split a single observation X into $X^{(1)}$ and $X^{(2)}$ such that:

(1) $X^{(1)}$ and $X^{(2)}$ have the same distribution as X, up to a parameter scaling.

(2) $X^{(1)} \perp\!\!\!\perp X^{(2)}$.

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Can we achieve these same properties when X is not Poisson?

Data thinning

Goal: split a single observation X into $X^{(1)}$ and $X^{(2)}$ such that:

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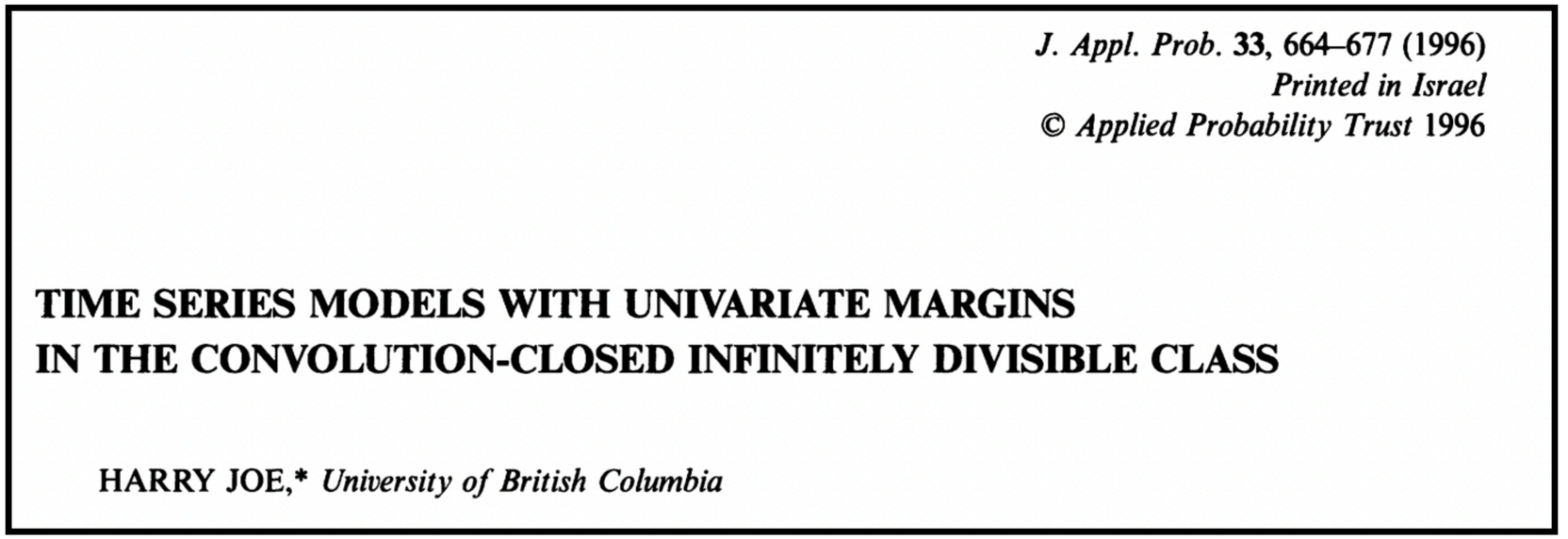

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Printed in Israel

TIME SERIES MODELS WITH UNIVARIATE MARGINS IN THE CONVOLUTION-CLOSED INFINITELY DIVISIBLE CLASS

HARRY JOE,* *University of British Columbia*

Convolution-closed distributions

A family of distributions F_λ is "convolution-closed" in parameter λ if

- $X' \sim F_{\lambda_1}$,
- $X'' \sim F_{\lambda_2}$,
- $X' \perp\!\!\!\perp X''$

together imply that $X' + X'' \sim F_{\lambda_1+\lambda_2}$.

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Distribution	Convolution-closed in:
$X \sim \text{Poisson}(\lambda)$	λ
$X \sim \text{N}(\mu, \sigma^2)$	(μ, σ^2)
$X \sim \text{NegativeBinomial}(\mu, b)$	(μ, b)
$X \sim \text{Gamma}(\alpha, \beta)$	α, if β is fixed
$X \sim \text{Binomial}(r, p)$	r, if p is fixed
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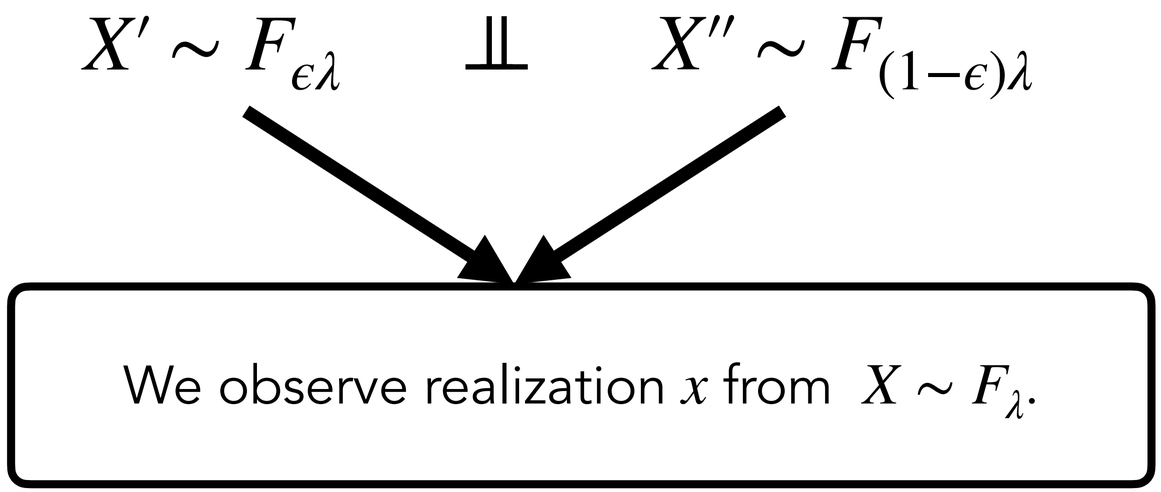
Jorgensen and Song (1998, Journal of Applied Probability) unify notation for any **exponential dispersion family.**

Data thinning for convolution-closed distributions

We observe realization x from $X \sim F_\lambda$.

Data thinning for convolution-closed distributions

We know x could have arisen as $x' + x''$, where



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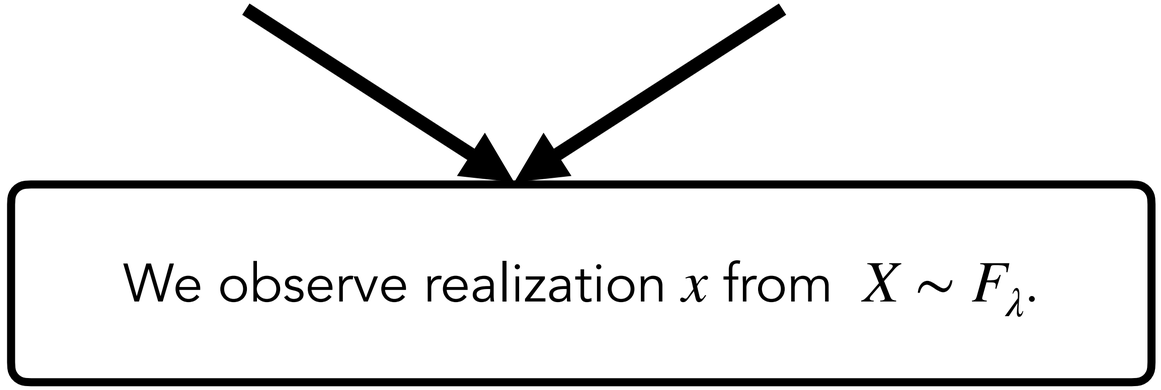

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If we had observed x' and x'', we would have satisfied our goal of data thinning!

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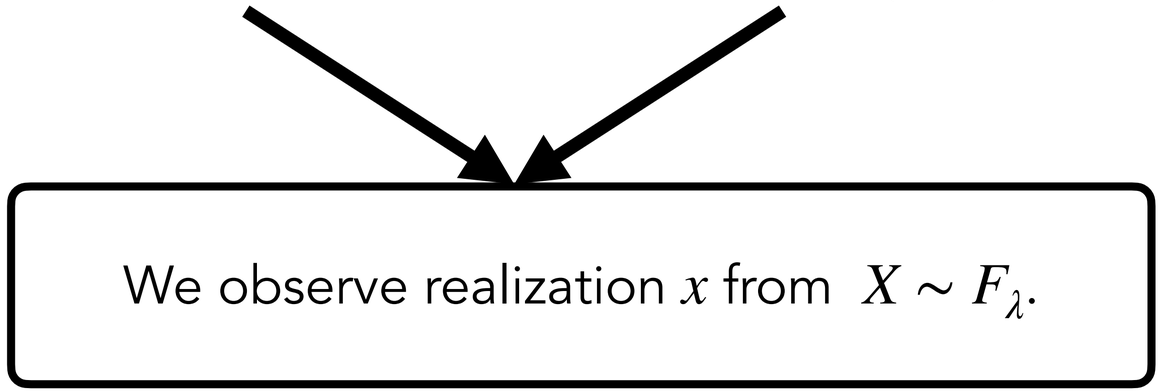

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Let $G_{\epsilon,x}$ be the conditional distribution of $X' \mid X = x$.

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Data thinning recipe for the Poisson distribution

We observe realization x from $X \sim \text{Poisson}(\lambda)$.

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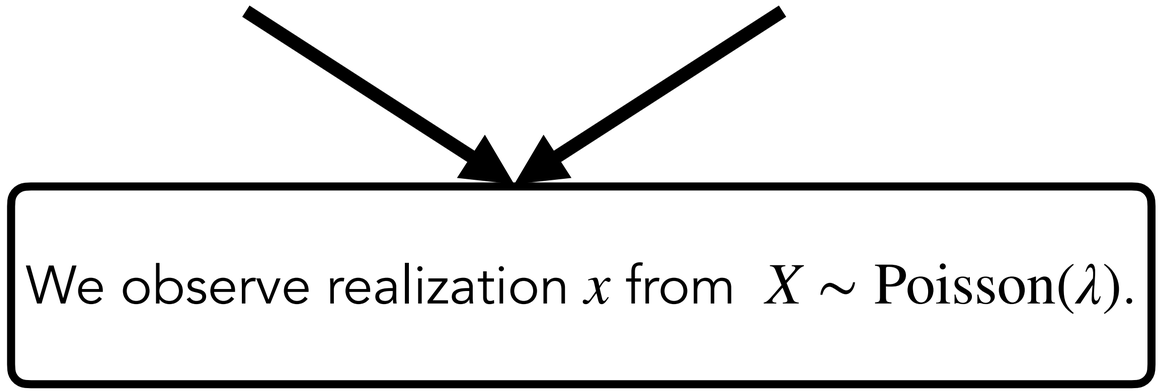

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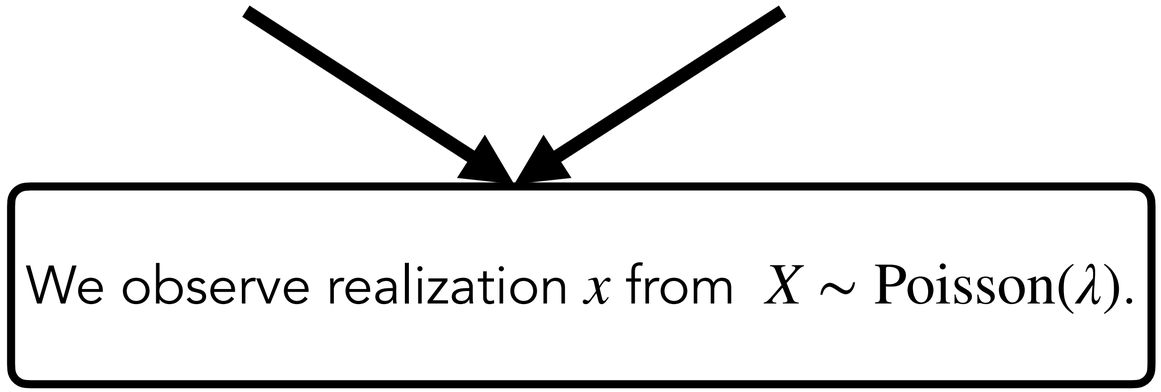

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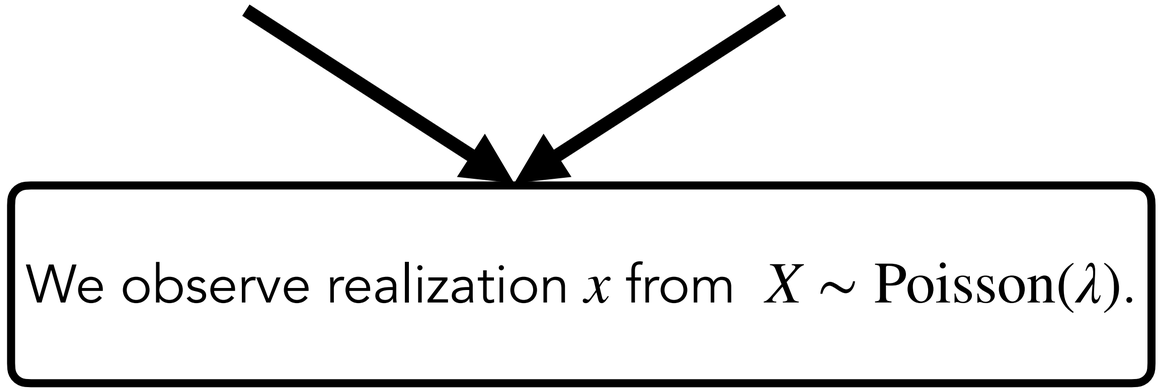

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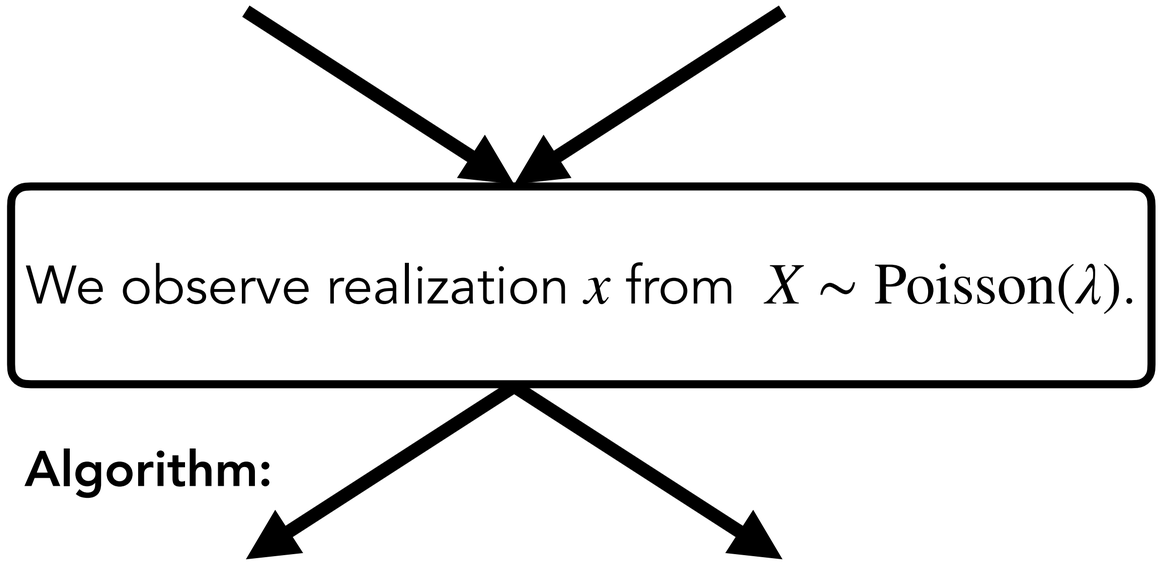

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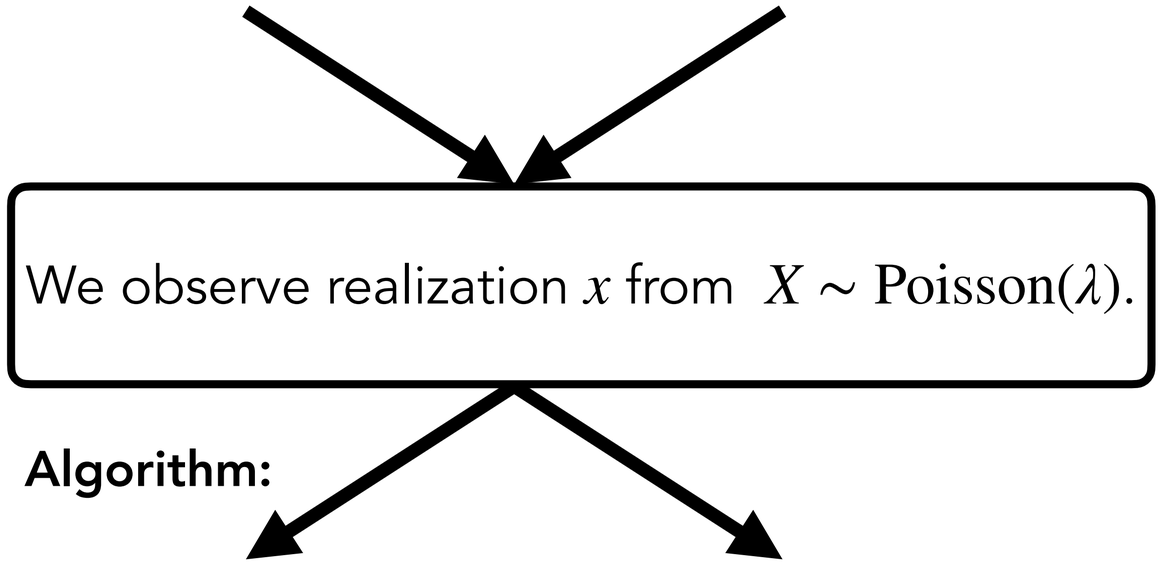

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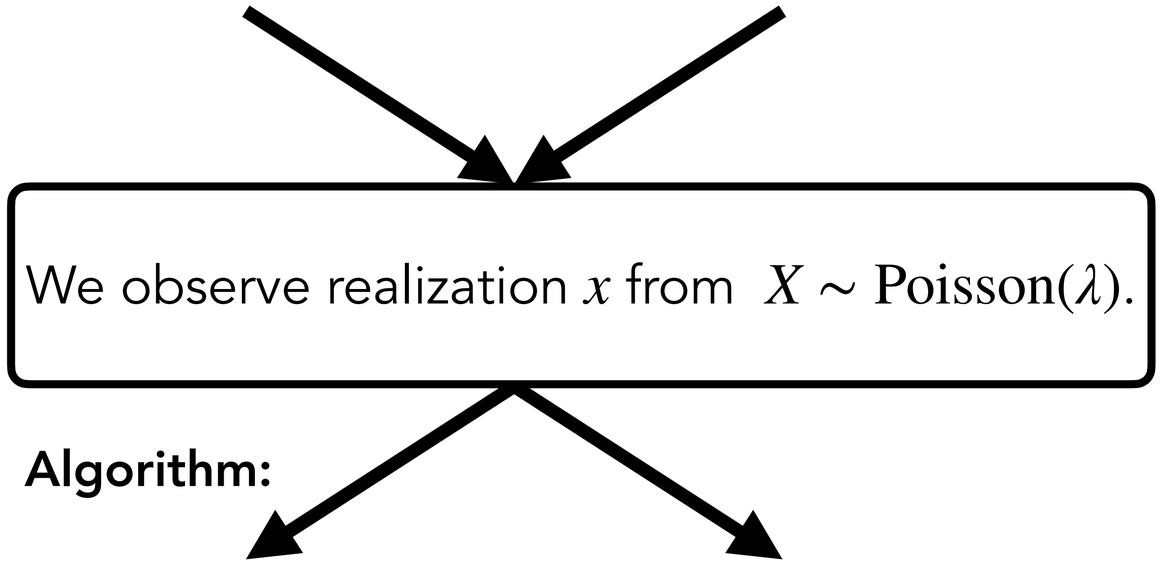

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We recover the well-known Poisson thinning recipe.

Data thinning recipe for the Gaussian distribution

We observe realization x from $X \sim \mathrm{N}(\mu, \sigma^2)$.

Data thinning recipe for the Gaussian distribution

We know x could have arisen as $x' + x''$, where

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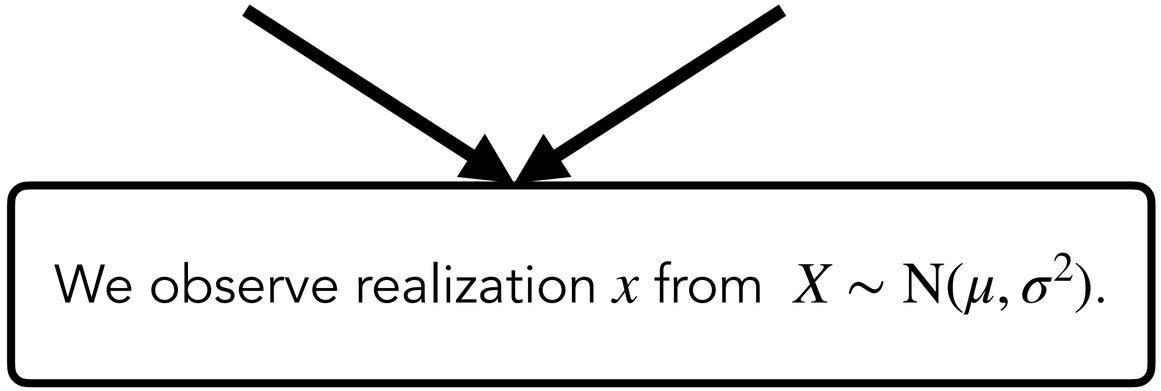

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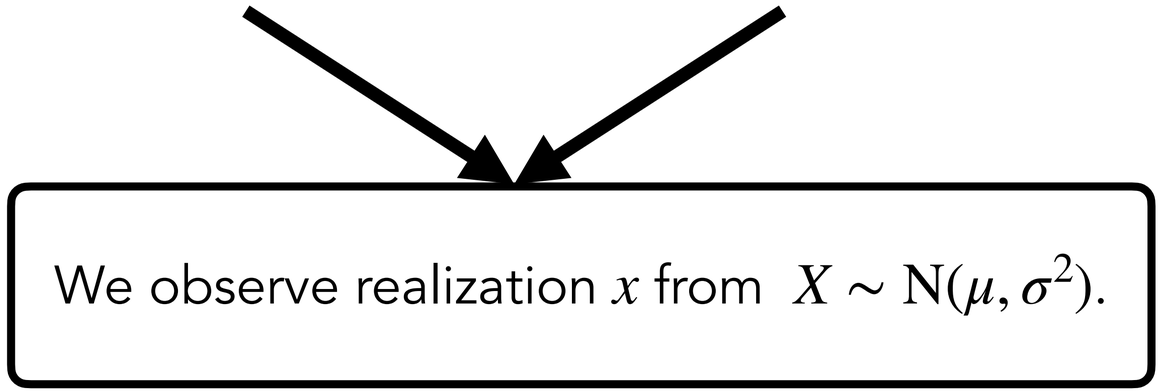

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We know x could have arisen as $x' + x''$, where

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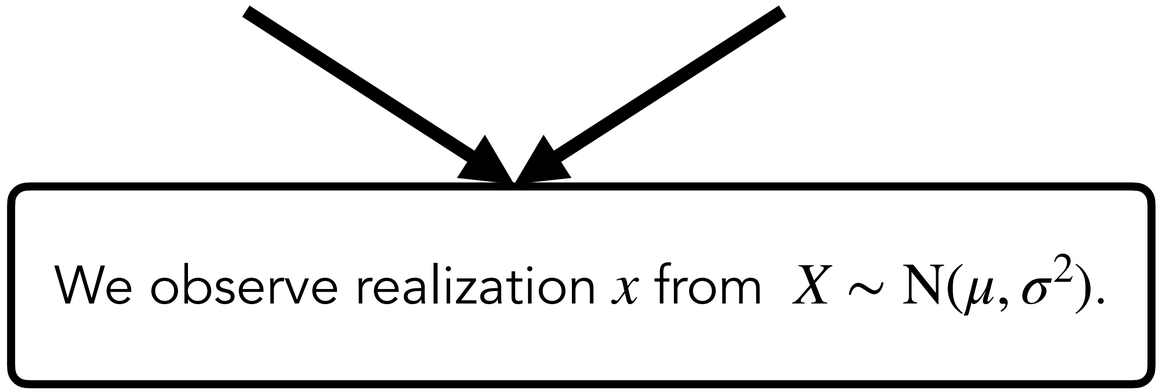

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Can show that the conditional distribution of $X' \mid X = x$ is $\mathrm{N}(\epsilon x, \epsilon(1-\epsilon)\sigma^2)$.

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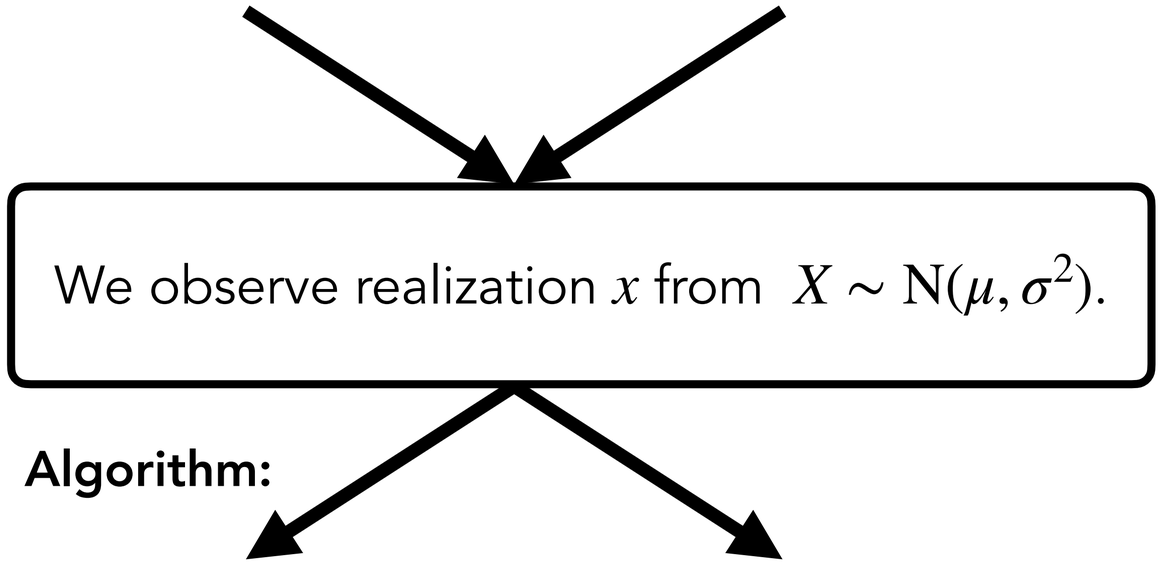

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We observe realization x from $X \sim \mathrm{N}(\mu, \sigma^2)$.

Algorithm:

Draw $X^{(1)} \mid X = x \sim \mathrm{N}(\epsilon x, \epsilon(1-\epsilon)\sigma^2)$. Let $X^{(2)} = X - X^{(1)}$.

Theorem:

$X^{(1)} \sim \mathrm{N}(\epsilon\mu, \epsilon\sigma^2)$, $X^{(2)} \sim \mathrm{N}((1-\epsilon)\mu, (1-\epsilon)\sigma^2)$, $X^{(1)} \perp\!\!\!\perp X^{(2)}$.

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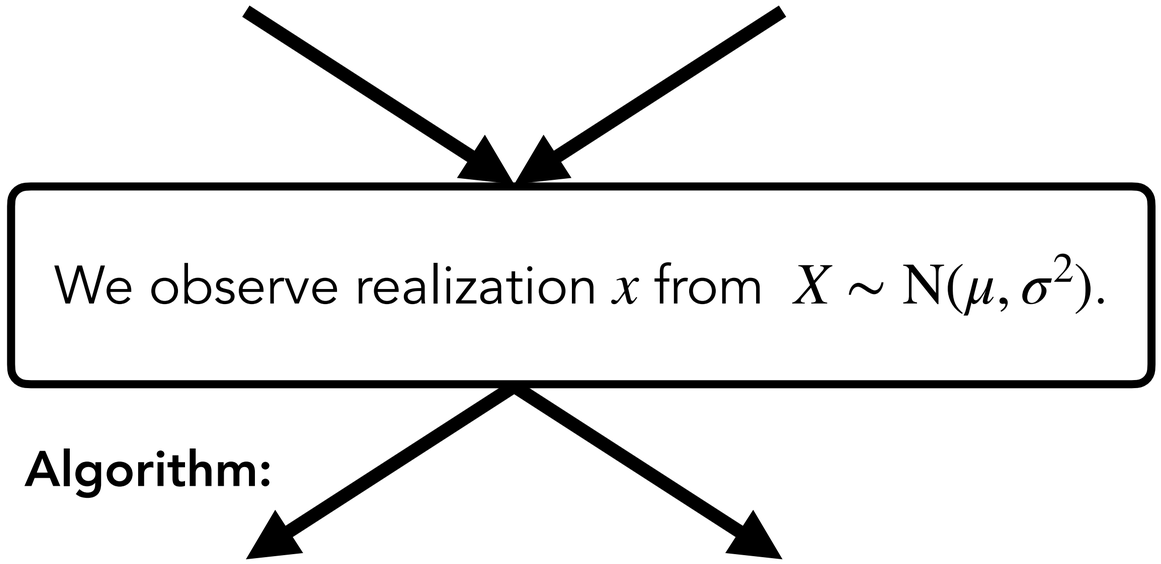

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Can we work backwards to recover x' and x''?

Can show that the conditional distribution of $X' \mid X = x$ is $\mathrm{N}(\epsilon x, \epsilon(1-\epsilon)\sigma^2)$.

Recovers a scaled version of another well-known result.

Data thinning recipe for the negative binomial distribution

We observe realization x from $X \sim \text{NB}(\mu, b)$.

Data thinning recipe for the negative binomial distribution

We know x could have arisen as $x' + x''$, where

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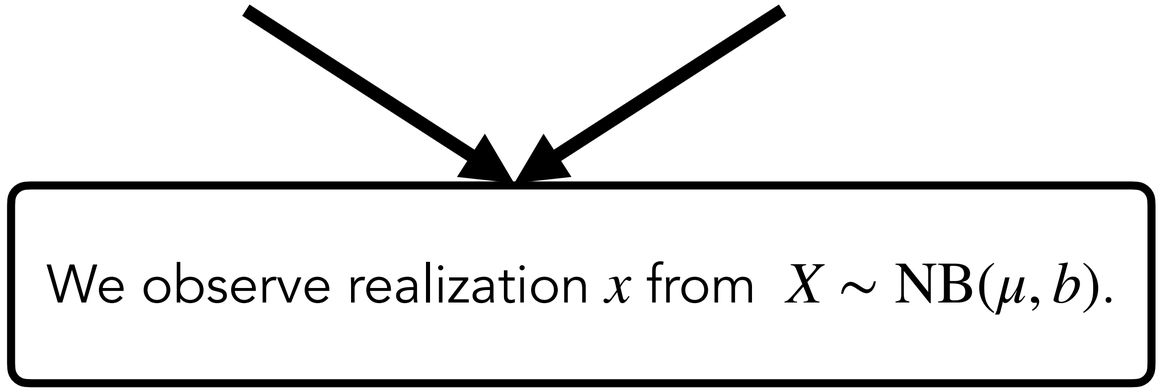

Data thinning recipe for the negative binomial distribution

We know x could have arisen as $x' + x''$, where

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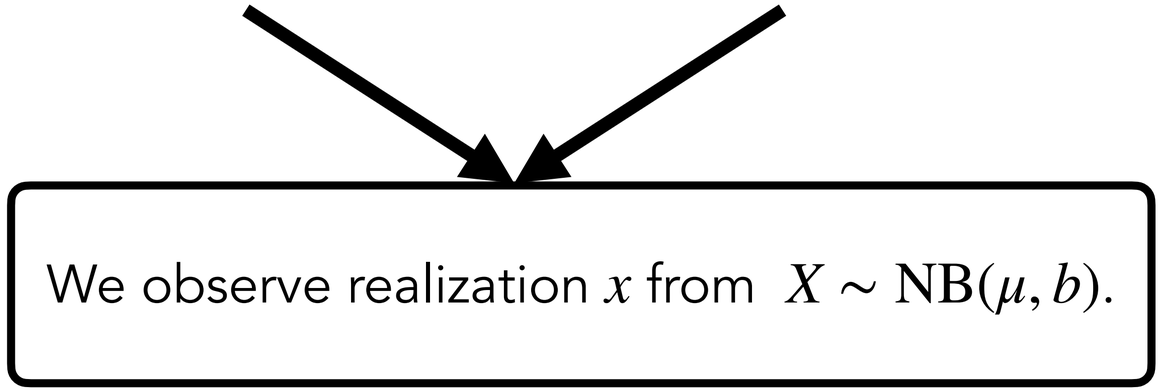

Can we work backwards to recover x' and x''?

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Can we work backwards to recover x' and x''?

Can show that the conditional distribution of $X' \mid X = x$ is $\text{BetaBinomial}(x, \epsilon b, (1-\epsilon)b)$.

Data thinning recipe for the negative binomial distribution

We know x could have arisen as $x' + x''$, where

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Algorithm:

Draw
$X^{(1)} \mid X = x \sim \text{BetaBin}(x, \epsilon b, (1-\epsilon)b)$.

Let $X^{(2)} = X - X^{(1)}$.

Can we work backwards to recover x' and x''?

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Data thinning recipe for the negative binomial distribution

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Can we work backwards to recover x' and x''?

Can show that the conditional distribution of $X' \mid X = x$ is $\text{BetaBinomial}(x, \epsilon b, (1-\epsilon)b)$.

Data thinning recipe for the negative binomial distribution

We know x could have arisen as $x' + x''$, where

$X' \sim \text{NB}(\epsilon\mu, \epsilon b) \quad \perp\!\!\!\perp \quad X'' \sim \text{NB}((1-\epsilon)\mu, (1-\epsilon)b)$

We observe realization x from $X \sim \text{NB}(\mu, b)$.

Algorithm:

Draw
$X^{(1)} \mid X = x \sim \text{BetaBin}(x, \epsilon b, (1-\epsilon)b)$.

Let $X^{(2)} = X - X^{(1)}$.

Theorem:

$X^{(1)} \sim \text{NB}(\epsilon\mu, \epsilon b)$, $X^{(2)} \sim \text{NB}((1-\epsilon)\mu, (1-\epsilon)b)$, $X^{(1)} \perp\!\!\!\perp X^{(2)}$.

Can we work backwards to recover x' and x''?

Can show that the conditional distribution of $X' \mid X = x$ is $\text{BetaBinomial}(x, \epsilon b, (1-\epsilon)b)$.

This is a new result!

For many common distributions, the distribution $G_{\epsilon,x}$ has a simple form

Distribution of X:	Draw $X^{(1)} \mid X = x$ from $G_{\epsilon,x}$, where $G_{\epsilon,x}$ is:	Distribution of $X^{(1)}$:	Distribution of $X^{(2)}$, where $X^{(2)} = X - X^{(1)}$:
$\text{Poisson}(\lambda)$	$\text{Binomial}(x, \epsilon)$	$\text{Poisson}(\epsilon\lambda)$	$\text{Poisson}((1-\epsilon)\lambda)$

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Related work on Poisson thinning:

- Sarkar and Stephens, 2021, Nature Genetics.
- Chen et al., 2021, arXiv:2108.03336
- Leiner et al., 2021, arXiv:2112.11079.
- Neufeld et al., 2022, Biostatistics.
- Oliveira, Lei, and Tibshirani, 2022, arXiv:2212.01943.

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$\text{N}(\mu, \sigma^2)$	$\text{N}(\epsilon x, \epsilon(1-\epsilon)\sigma^2)$	$\text{N}(\epsilon\mu, \epsilon\sigma^2)$	$\text{N}((1-\epsilon)\mu, (1-\epsilon)\sigma^2)$

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Related work on Gaussian thinning:

- Tian and Taylor, 2018, Annals of Statistics.
- Rasines and Young, 2022, Biometrika.
- Leiner et al., 2021, arXiv:2112.11079.
- Tian, 2020, Annals of Statistics.
- Oliveira, Lei, and Tibshirani, 2021, arXiv:2111.09447.

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Distribution of X:	Draw $X^{(1)} \mid X = x$ from $G_{\epsilon,x}$, where $G_{\epsilon,x}$ is:	Distribution of $X^{(1)}$:	Distribution of $X^{(2)}$, where $X^{(2)} = X - X^{(1)}$:
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$\text{N}(\mu, \sigma^2)$	$\text{N}(\epsilon x, \epsilon(1-\epsilon)\sigma^2)$	$\text{N}(\epsilon\mu, \epsilon\sigma^2)$	$\text{N}((1-\epsilon)\mu, (1-\epsilon)\sigma^2)$
$\text{NegativeBinomial}(\mu, b)$	$\text{BetaBinomial}(x, \epsilon b, (1-\epsilon)b)$.	$\text{NegativeBinomial}(\epsilon\mu, \epsilon b)$	$\text{NegativeBinomial}((1-\epsilon)\mu, (1-\epsilon)b)$

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$\text{NegativeBinomial}(\mu, b)$	$\text{BetaBinomial}(x, \epsilon b, (1-\epsilon)b)$.	$\text{NegativeBinomial}(\epsilon\mu, \epsilon b)$	$\text{NegativeBinomial}((1-\epsilon)\mu, (1-\epsilon)b)$
$\text{Binomial}(r, p)$	$\text{Hypergeometric}(\epsilon r, (1-\epsilon)r, x)$.	$\text{Binomial}(\epsilon r, p)$	$\text{Binomial}((1-\epsilon)r, p)$

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$\text{Gamma}(\alpha, \beta)$	$x \cdot \text{Beta}(\epsilon\alpha, (1-\epsilon)\alpha)$.	$\text{Gamma}(\epsilon\alpha, \beta)$	$\text{Gamma}((1-\epsilon)\alpha, \beta)$
$\text{Exponential}(\lambda)$	$x \cdot \text{Beta}(\epsilon, (1-\epsilon))$.	$\text{Gamma}(\epsilon, \lambda)$	$\text{Gamma}(1-\epsilon, \lambda)$
$\text{N}_k(\mu, \Sigma)$	$\text{N}(\epsilon x, \epsilon(1-\epsilon)\Sigma)$.	$\text{N}_k(\epsilon\mu, \epsilon\Sigma)$	$\text{N}_k((1-\epsilon)\mu, (1-\epsilon)\Sigma)$
$\text{Multinomial}_k(r, p)$	$\text{MultivarHypergeom}(x_1, \ldots, x_K, \epsilon r)$	$\text{Multinom}_k(\epsilon r, p)$	$\text{Multinomial}_k((1-\epsilon)r, p)$
$\text{Wishart}_p(n, \Sigma)$.	$x^{1/2} Z x^{1/2}$, where . $Z \sim \text{MatrixBeta}_p(\epsilon n/2, (1-\epsilon)n/2)$	$\text{Wishart}_p(\epsilon n, \Sigma)$	$\text{Wishart}_p((1-\epsilon)n, \Sigma)$

What if we get a nuisance parameter wrong?

Gaussian thinning algorithm

Suppose $X \sim \mathrm{N}\left(\mu, \sigma^2\right)$.

Draw
$X^{(1)} \sim \mathrm{N}(\epsilon x, \epsilon(1-\epsilon)\,\sigma^2)$ and
$X^{(2)} = X - X^{(1)}$.
Then:

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2) $X^{(2)} \sim \mathrm{N}\left((1-\epsilon)\mu, (1-\epsilon)^2\sigma^2 + \epsilon(1-\epsilon)\tilde{\sigma}^2\right)$
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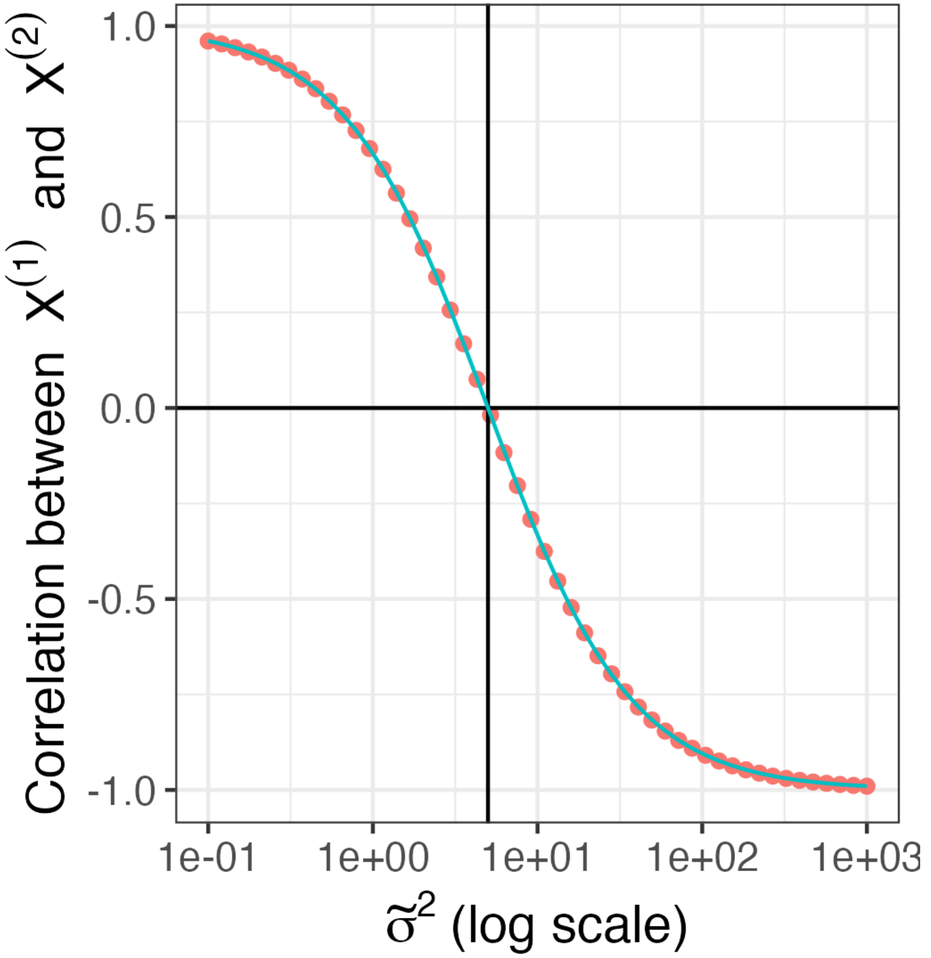

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Suppose $X \sim \text{NegBin}\left(\mu, b\right)$.

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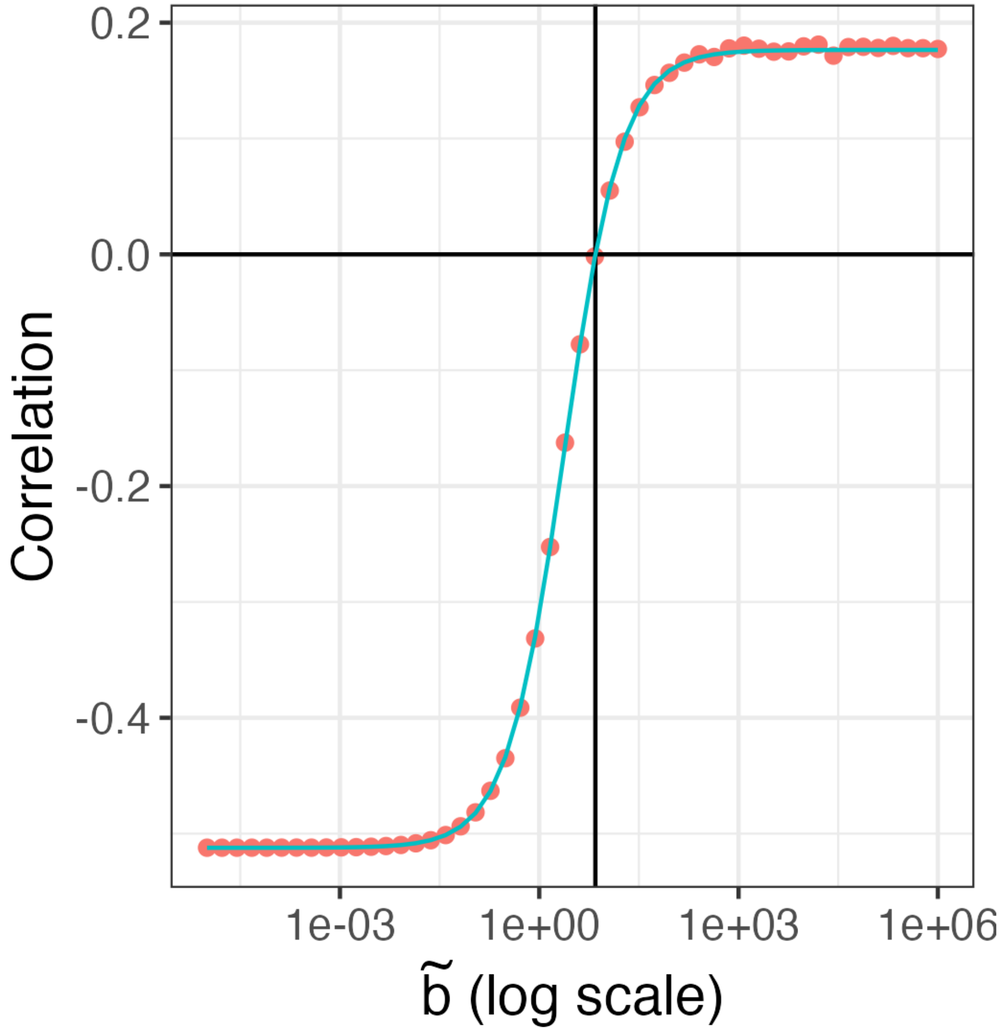

The tuning parameter ϵ governs an information tradeoff

Gaussian thinning algorithm

Suppose $X \sim \mathrm{N}\left(\mu, \sigma^2\right)$.

Draw
$X^{(1)} \sim \mathrm{N}(\epsilon x, \epsilon(1-\epsilon)\,\sigma^2)$ and
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Theorem: Fisher Information in X about μ is divided between $X^{(1)}$ and $X^{(2)}$ with proportions ϵ and $1-\epsilon$.

The tuning parameter ϵ governs an information tradeoff

Gaussian thinning algorithm

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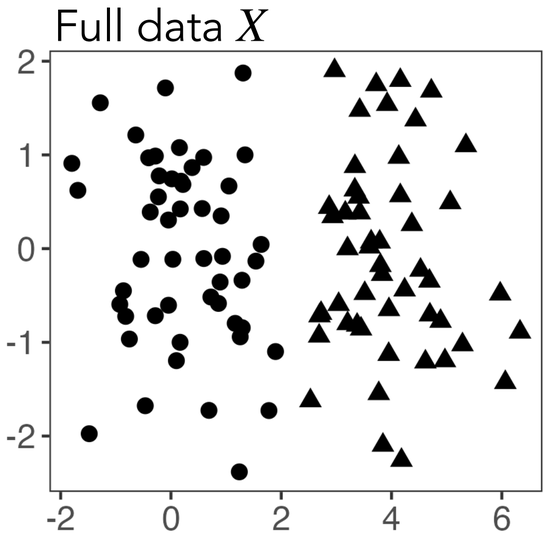
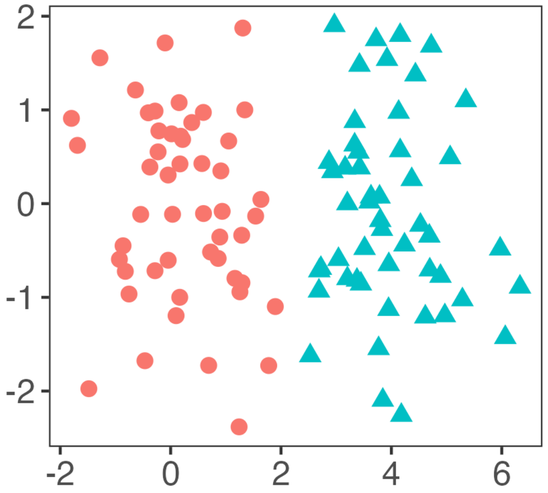
Similar results can be derived for other decompositions.

Visualizing the role of ϵ



Visualizing the role of ϵ

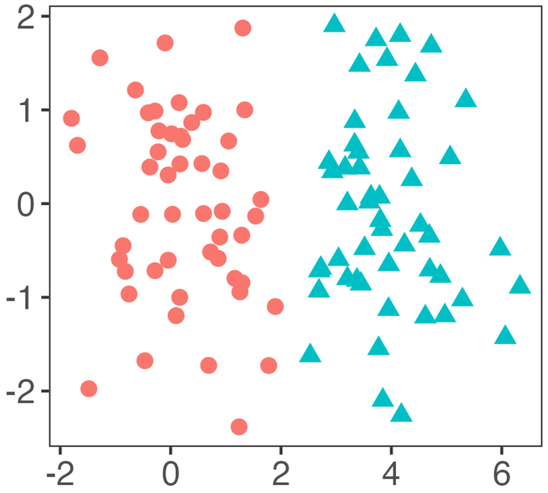
Full data X



Adjusted Rand index = 1

Visualizing the role of ϵ

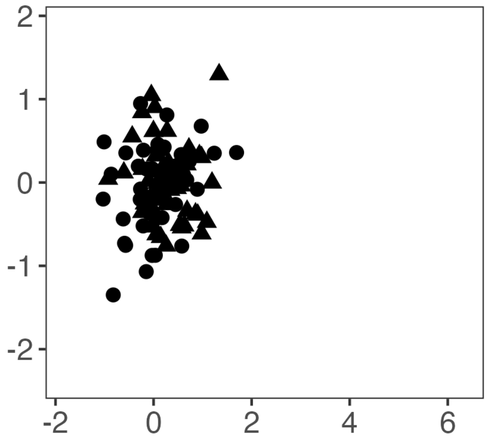
Full data X



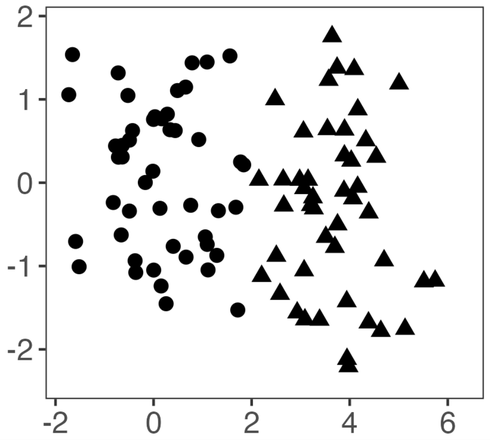
Adjusted Rand index = 1

$\epsilon = 0.1$

$X^{(1)}$



$X^{(2)}$



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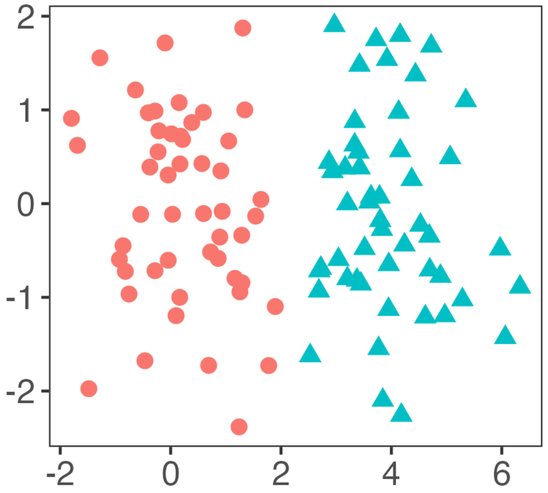

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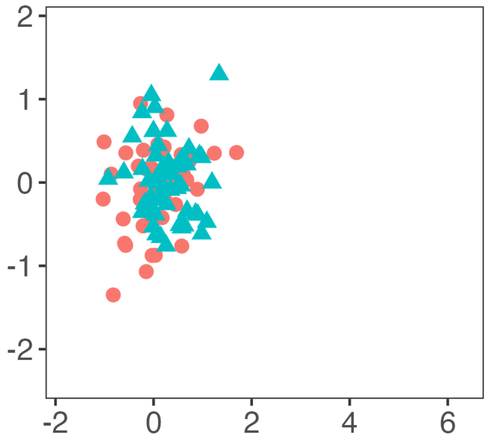

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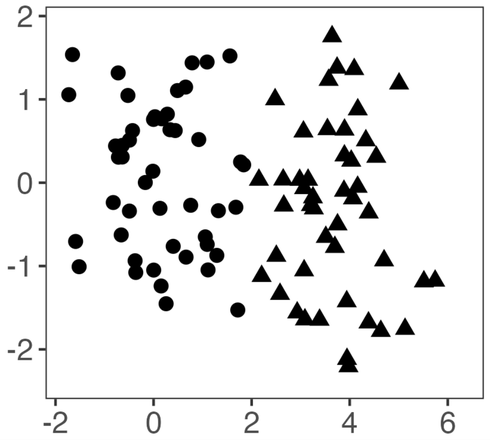
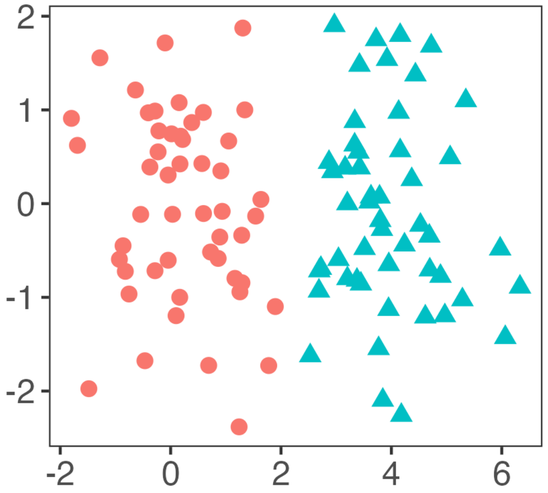


Visualizing the role of ϵ

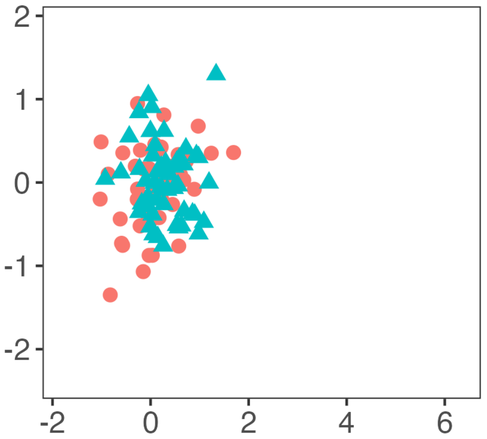
Full data X



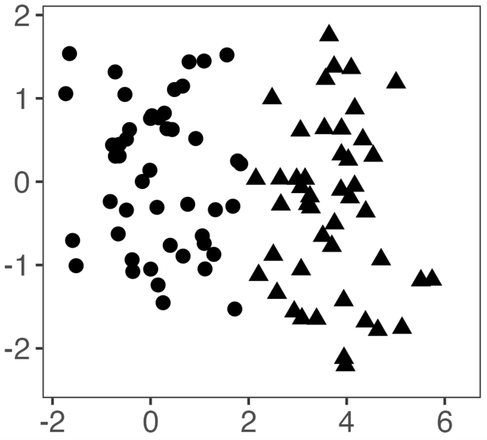
Adjusted Rand index = 1

$\epsilon = 0.1$

$X^{(1)}$, ARI = 0.03

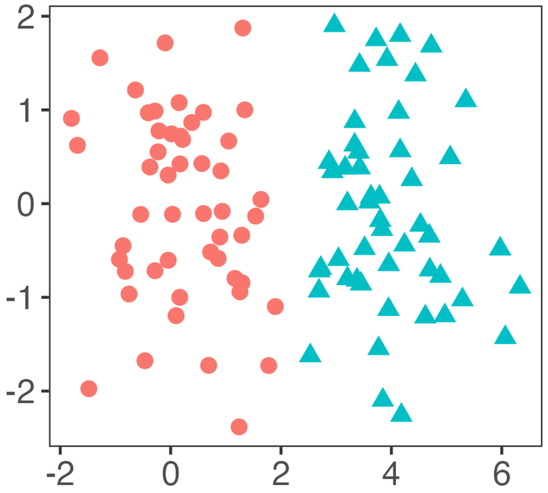


$X^{(2)}$



Visualizing the role of ϵ

Full data X



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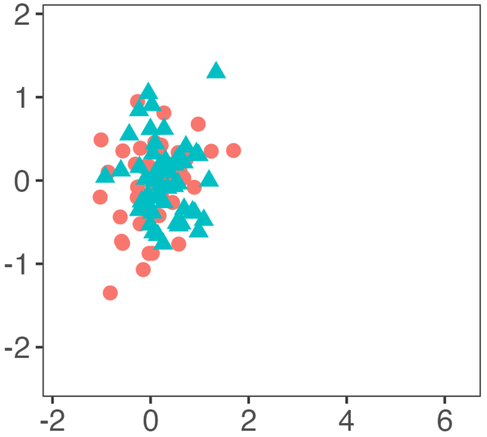
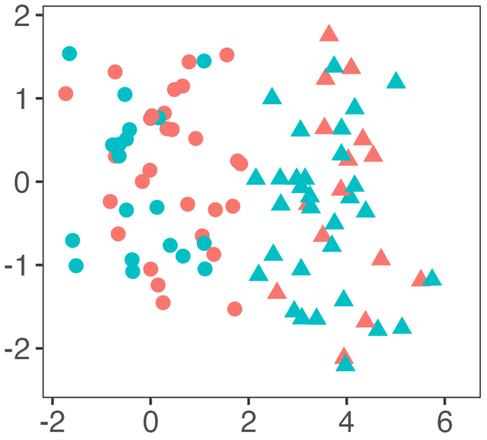


$X^{(2)}$



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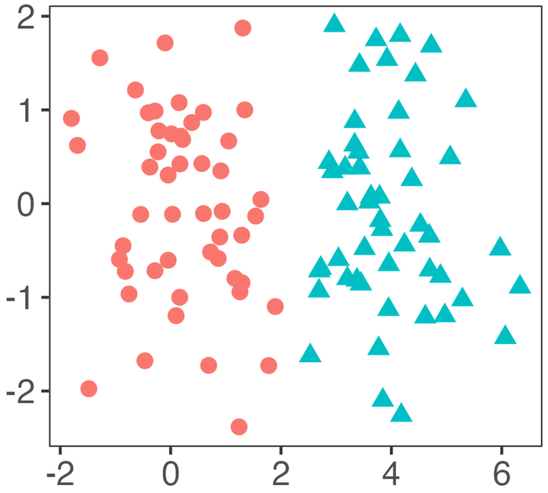

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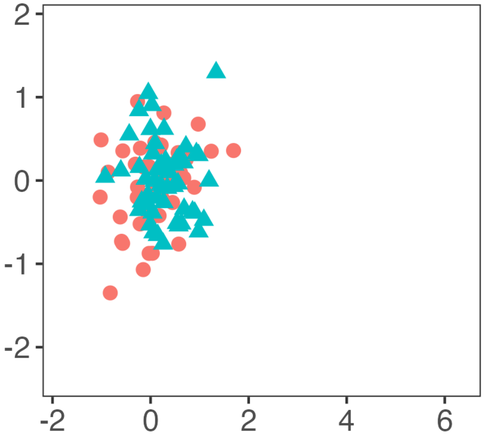
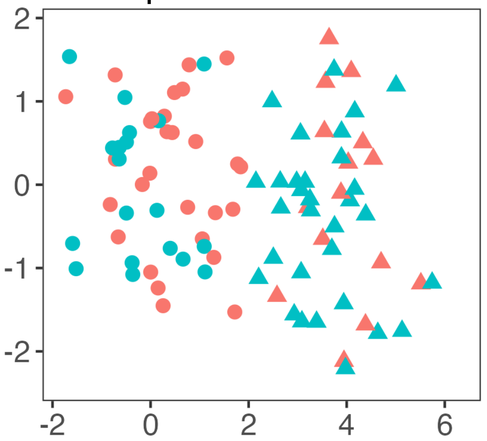
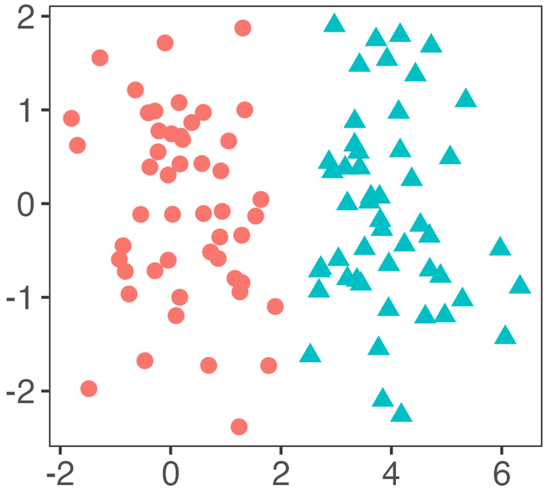


$X^{(2)}$, p-value = 0.36



Visualizing the role of ϵ

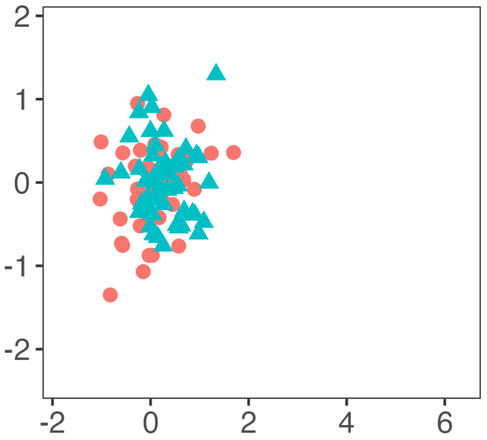
Full data X



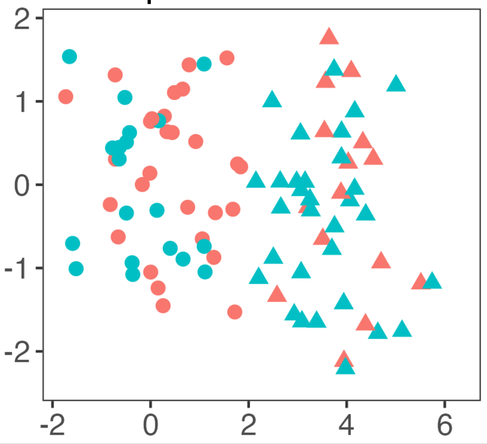
Adjusted Rand index = 1

$\epsilon = 0.1$

$X^{(1)}$, ARI = 0.03

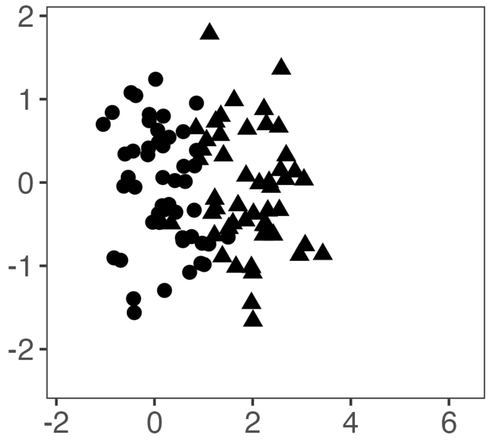


$X^{(2)}$, p-value = 0.36

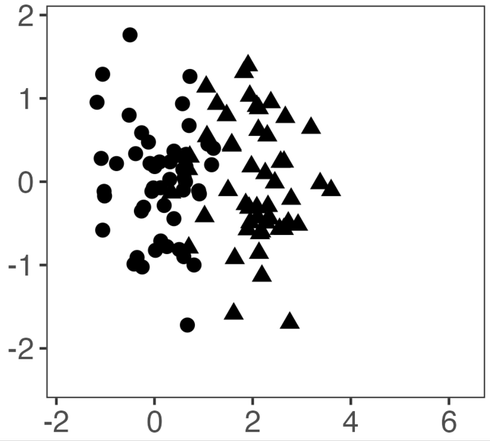


$\epsilon = 0.5$

$X^{(1)}$

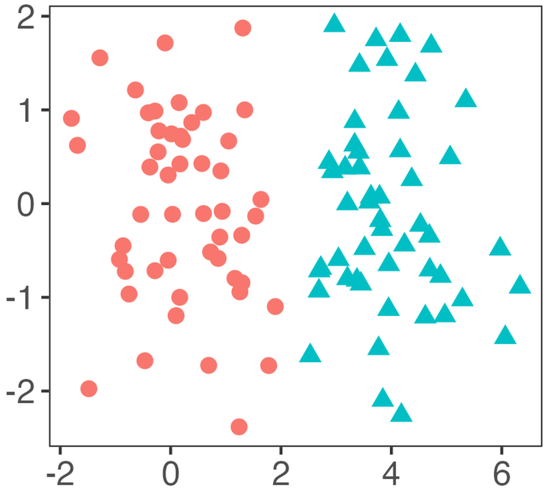


$X^{(2)}$



Visualizing the role of ϵ

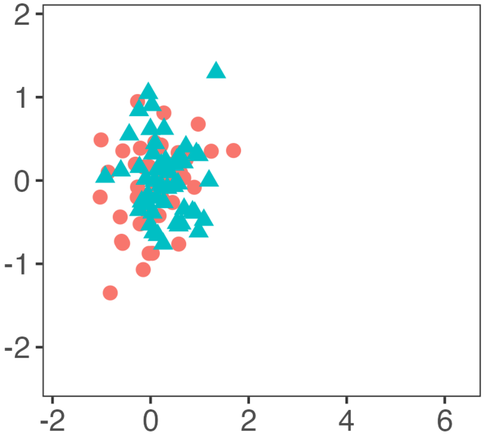
Full data X



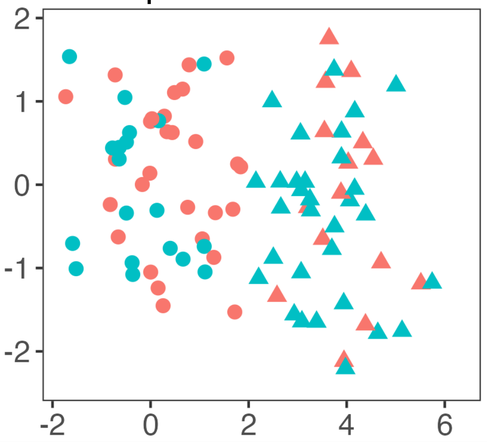
Adjusted Rand index = 1

$\epsilon = 0.1$

$X^{(1)}$, ARI = 0.03

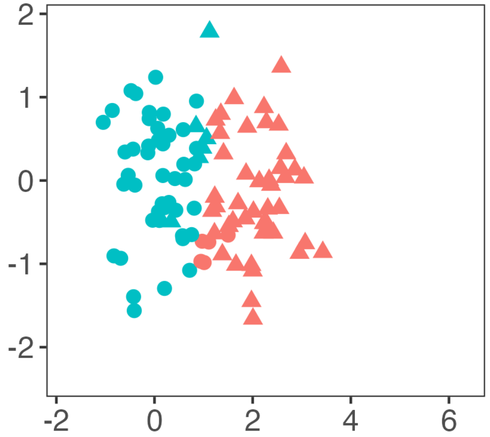


$X^{(2)}$, p-value = 0.36

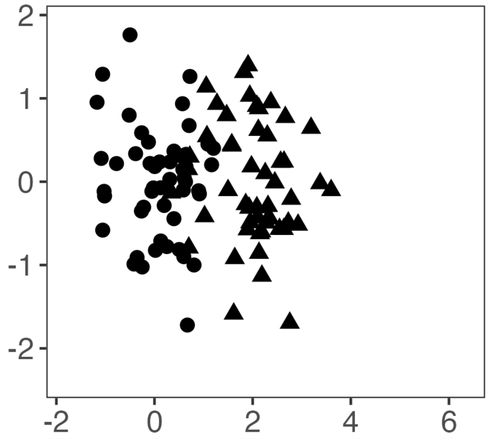


$\epsilon = 0.5$

$X^{(1)}$, ARI = 0.65

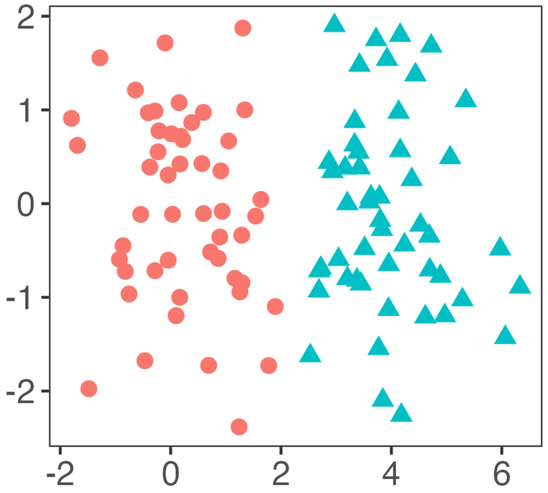


$X^{(2)}$



Visualizing the role of ϵ

Full data X



Adjusted Rand index = 1

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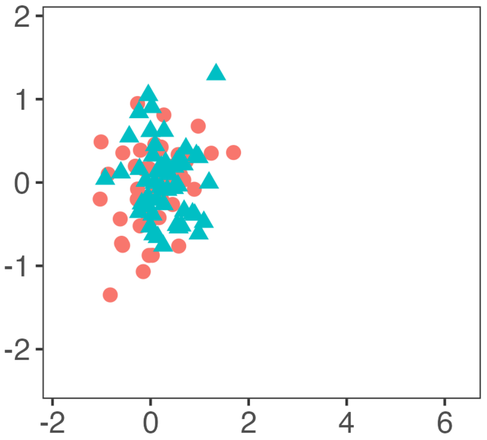
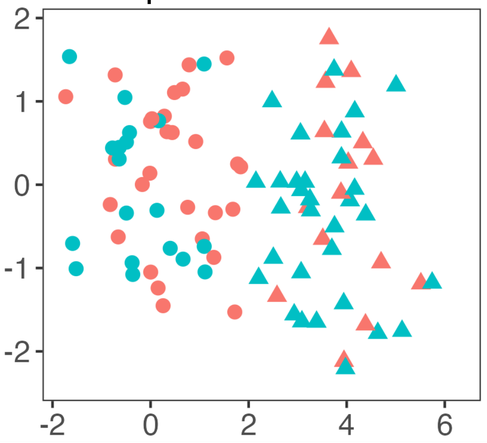
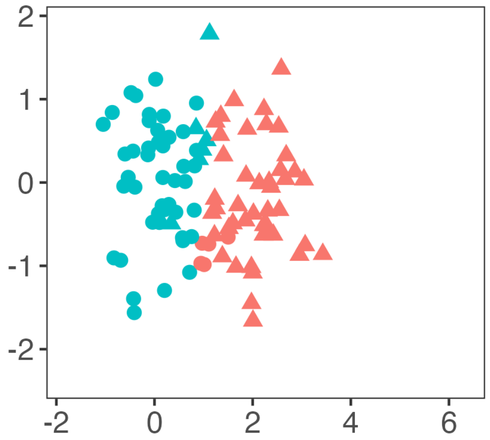


$X^{(2)}$, p-value = 0.36

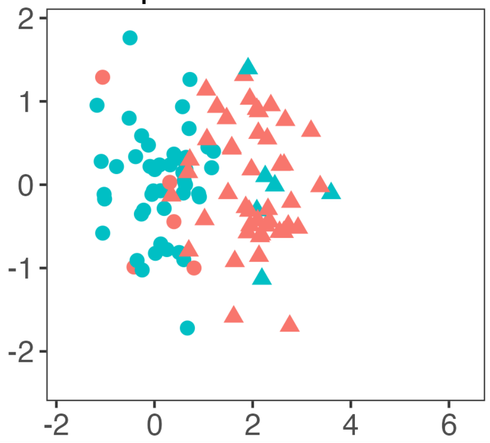


$\epsilon = 0.5$

$X^{(1)}$, ARI = 0.65

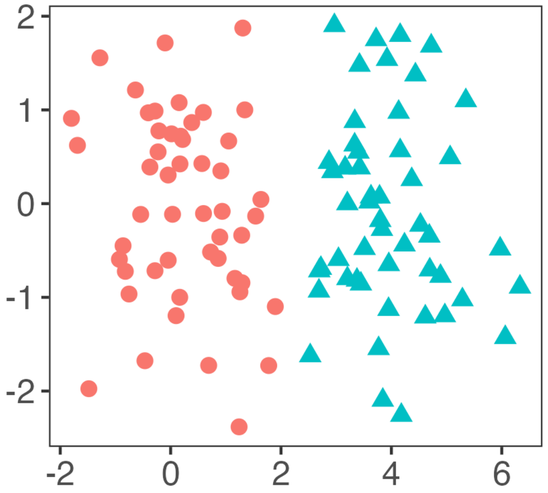


$X^{(2)}$, p-value = 0.02



Visualizing the role of ϵ

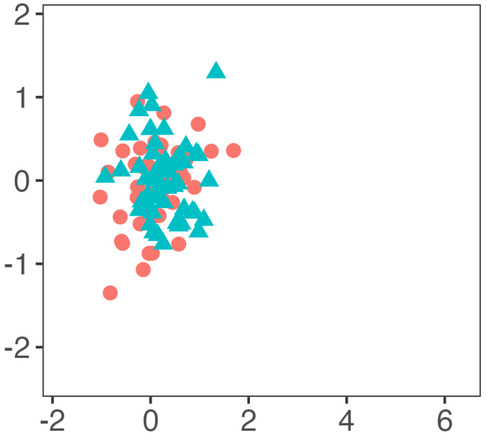
Full data X



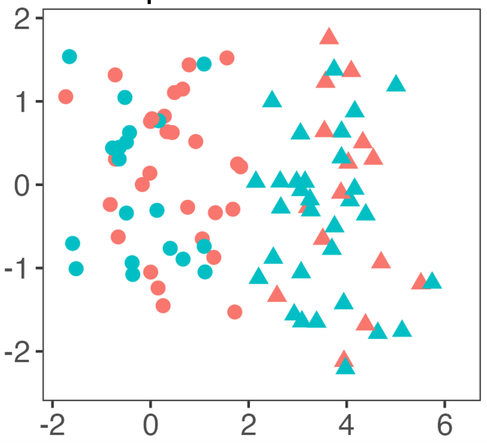
Adjusted Rand index = 1

$\epsilon = 0.1$

$X^{(1)}$, ARI = 0.03

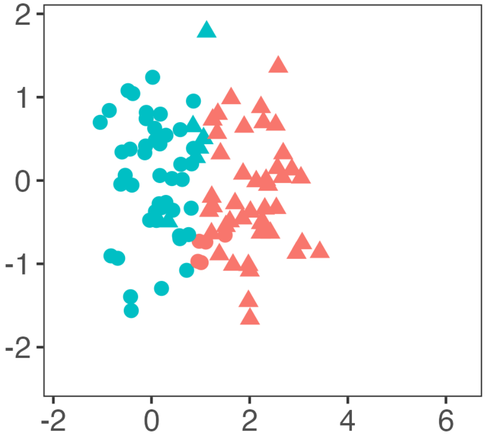


$X^{(2)}$, p-value = 0.36

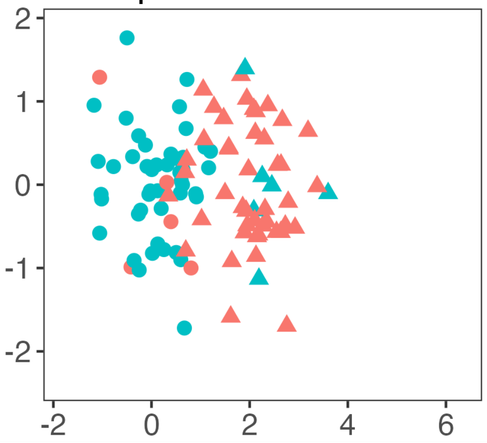


$\epsilon = 0.5$

$X^{(1)}$, ARI = 0.65

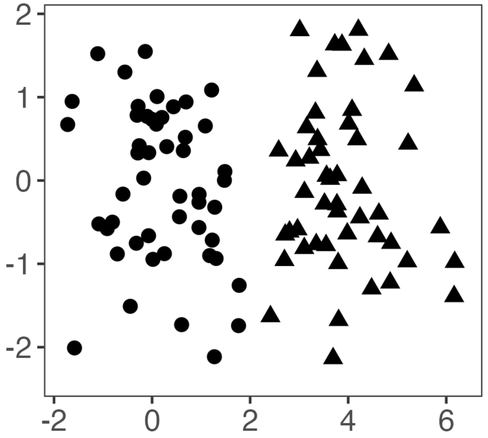


$X^{(2)}$, p-value = 0.02

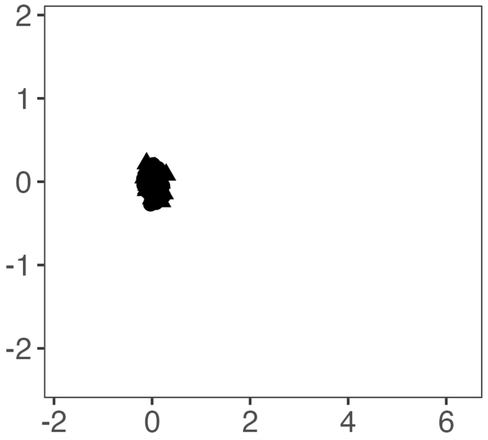


$\epsilon = 0.99$

$X^{(1)}$

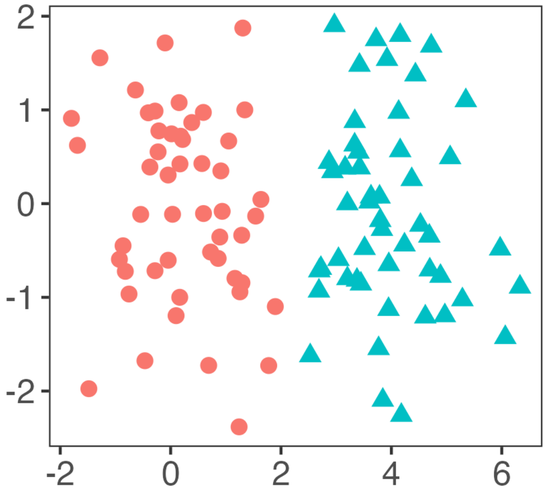


$X^{(2)}$



Visualizing the role of ϵ

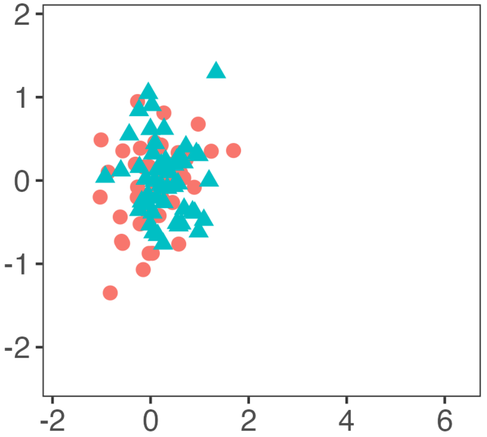
Full data X



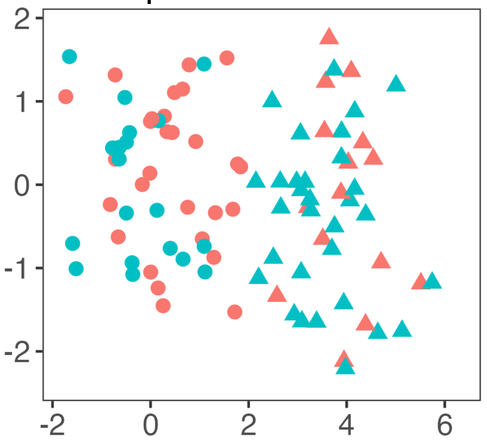
Adjusted Rand index = 1

$\epsilon = 0.1$

$X^{(1)}$, ARI = 0.03



$X^{(2)}$, p-value = 0.36



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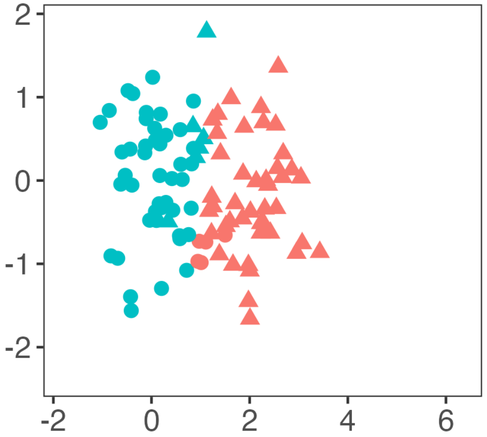
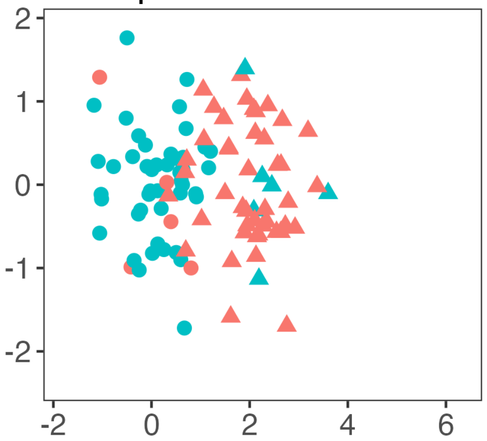
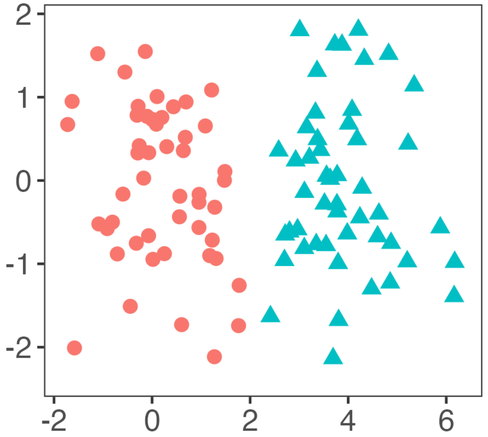


$X^{(2)}$, p-value = 0.02

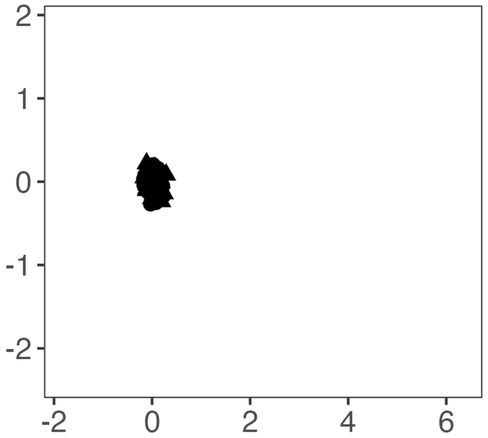


$\epsilon = 0.99$

$X^{(1)}$, ARI = 1

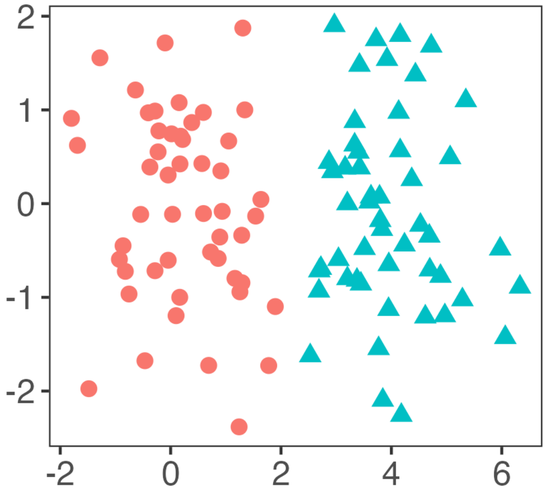


$X^{(2)}$



Visualizing the role of ϵ

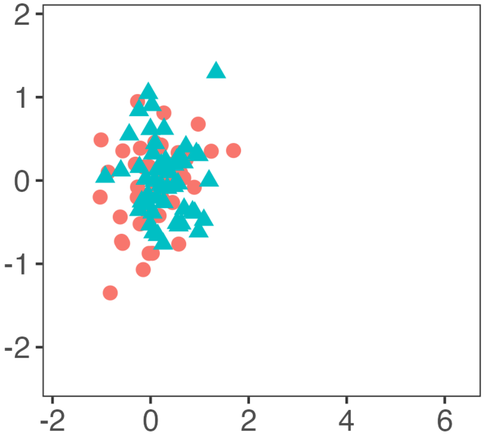
Full data X



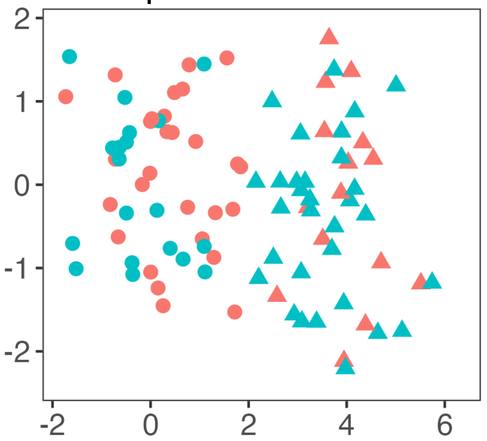
Adjusted Rand index = 1

$\epsilon = 0.1$

$X^{(1)}$, ARI = 0.03



$X^{(2)}$, p-value = 0.36



$\epsilon = 0.5$

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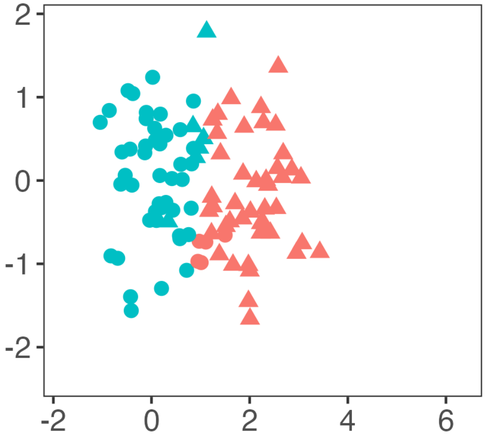
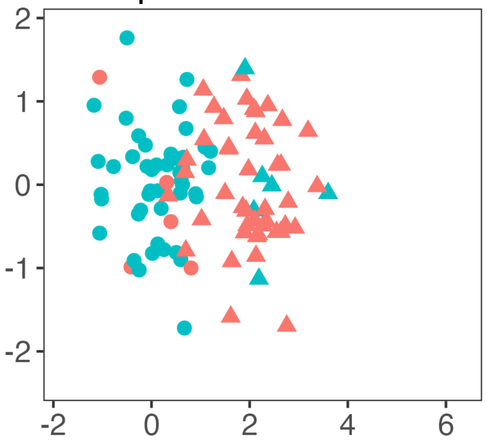
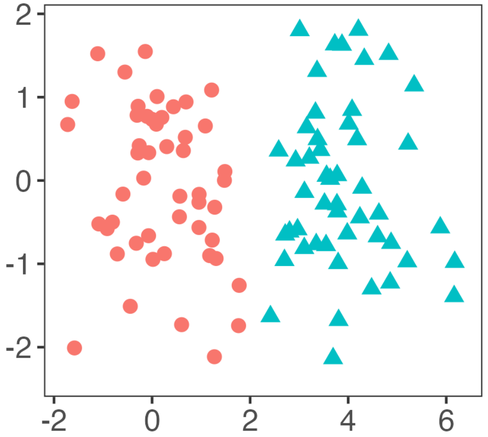


$X^{(2)}$, p-value = 0.02

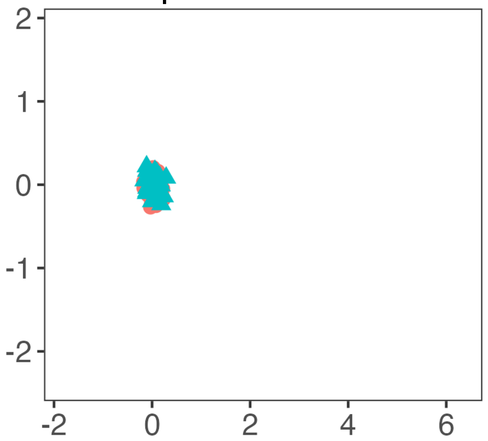


$\epsilon = 0.99$

$X^{(1)}$, ARI = 1



$X^{(2)}$, p-value = 0.11



Our recipe extends naturally to splitting into M>2 folds

Goal: split a single observation X into $\left(X^{(1)}, \ldots, X^{(M)}\right)$ such that:

(1) Each $X^{(m)}$ has the same distribution as X, up to a parameter scaling.

(2) The $X^{(m)}$ are mutually independent.

For many distributions, the multifold recipe has a simple form

Distribution of X	Draw $\left(X^{(1)}, \ldots, X^{(M)}\right) \mid X = x$ from:	Distribution of $X^{(m)}$
$\text{Poisson}(\lambda)$	$\text{Multinomial}(x, \epsilon_1, \ldots, \epsilon_M)$	$\text{Poisson}(\epsilon_m \lambda)$

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$\text{N}(\mu, \sigma^2)$	$\text{N}_M(\epsilon\mu, \sigma^2 \text{diag}(\epsilon) - \sigma^2 \epsilon\epsilon^T)$.	$\text{N}(\epsilon_m \mu, \epsilon_m \sigma^2)$

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Distribution of X	Draw $\left(X^{(1)}, \ldots, X^{(M)}\right) \mid X = x$ from:	Distribution of $X^{(m)}$
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$\text{N}(\mu, \sigma^2)$	$\text{N}_M(\epsilon\mu, \sigma^2 \text{diag}(\epsilon) - \sigma^2 \epsilon\epsilon^T)$.	$\text{N}(\epsilon_m \mu, \epsilon_m \sigma^2)$
$\text{NegativeBinomial}(\mu, b)$	$\text{DirichletMultinomial}(x, \epsilon_1 b, \ldots, \epsilon_M b)$.	$\text{NegativeBinomial}(\epsilon_m \mu, \epsilon_m b)$

For many distributions, the multifold recipe has a simple form

Distribution of X	Draw $\left(X^{(1)}, \ldots, X^{(M)}\right) \mid X = x$ from:	Distribution of $X^{(m)}$
$\text{Poisson}(\lambda)$	$\text{Multinomial}(x, \epsilon_1, \ldots, \epsilon_M)$	$\text{Poisson}(\epsilon_m \lambda)$
$\text{N}(\mu, \sigma^2)$	$\text{N}_M(\epsilon\mu, \sigma^2 \text{diag}(\epsilon) - \sigma^2 \epsilon\epsilon^T)$.	$\text{N}(\epsilon_m \mu, \epsilon_m \sigma^2)$
$\text{NegativeBinomial}(\mu, b)$	$\text{DirichletMultinomial}(x, \epsilon_1 b, \ldots, \epsilon_M b)$.	$\text{NegativeBinomial}(\epsilon_m \mu, \epsilon_m b)$
$\text{Gamma}(\alpha, \beta)$	$x \cdot \text{Dirichlet}\left(\epsilon_1 \alpha, \ldots, \epsilon_M \alpha\right)$	$\text{Gamma}(\epsilon_m \alpha, \beta)$
$\text{Exponential}(\lambda)$	$x \cdot \text{Dirichlet}\left(\epsilon_1, \ldots, \epsilon_M\right)$	$\text{Gamma}(\epsilon_m, \lambda)$
$\text{Binomial}(r, p)$	$\text{MultivariateHypergeometric}(\epsilon_1 r, \ldots, \epsilon_M r, x)$.	$\text{Binomial}(\epsilon_m r, p)$

Statistics > Methodology

[Submitted on 18 Jan 2023]

Data thinning for convolution-closed distributions

Anna Neufeld, Ameer Dharamshi, Lucy L. Gao, Daniela Witten

We propose data thinning, a new approach for splitting an observation into two or more independent parts that sum to the original observation, and that follow the same distribution as the original observation, up to a (known) scaling of a parameter. This proposal is very general, and can be applied to any observation drawn from a "convolution closed" distribution, a class that includes the Gaussian, Poisson, negative binomial, Gamma, and binomial distributions, among others. It is similar in spirit to -- but distinct from, and more easily applicable than -- a recent proposal known as data fission. Data thinning has a number of applications to model selection, evaluation, and inference. For instance, cross-validation via data thinning provides an attractive alternative to the "usual" approach of cross-validation via sample splitting, especially in unsupervised settings in which the latter is not applicable. In simulations and in an application to single-cell RNA-sequencing data, we show that data thinning can be used to validate the results of unsupervised learning approaches, such as k-means clustering and principal components analysis.

R package and tutorials: https://anna-neufeld.github.io/datathin/

Outline

1. Motivation: sample splitting doesn’t always work
2. Poisson thinning
3. Data thinning
4. **Generalized data thinning**
5. Application to changepoint validation
6. Ongoing work

Revisiting the goals of data thinning

Goal: split a single observation X into $X^{(1)}$ and $X^{(2)}$ such that:

(1) $X^{(1)}$ and $X^{(2)}$ have the same distribution as X, up to a parameter scaling.

(2) $X^{(1)} \perp\!\!\!\perp X^{(2)}$.

Revisiting the goals of data thinning

Goal: split a single observation X into $X^{(1)}$ and $X^{(2)}$ such that:

(1) $X^{(1)}$ and $X^{(2)}$ have the same distribution as X, up to a parameter scaling.

(2) $X^{(1)} \perp\!\!\!\perp X^{(2)}$.

In our previous recipe:

(3) $X = X^{(1)} + X^{(2)}$.

Revisiting the goals of data thinning

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In our previous recipe:

~~**(3)** $X = X^{(1)} + X^{(2)}$.~~

Revisiting the goals of data thinning

Goal: split a single observation X into $X^{(1)}$ and $X^{(2)}$ such that:

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In our previous recipe:

~~**(3)** $X = X^{(1)} + X^{(2)}$.~~ **(3)** $X = T(X^{(1)}, X^{(2)})$.

Revisiting the goals of data thinning

Goal: split a single observation X into $X^{(1)}$ and $X^{(2)}$ such that:

~~**(1)** $X^{(1)}$ and $X^{(2)}$ have the same distribution as X, up to a parameter scaling.~~

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In our previous recipe:

~~**(3)** $X = X^{(1)} + X^{(2)}$.~~ **(3)** $X = T(X^{(1)}, X^{(2)})$.

Revisiting the goals of data thinning

Goal: split a single observation X into $X^{(1)}$ and $X^{(2)}$ such that:

~~**(1)** $X^{(1)}$ and $X^{(2)}$ have the same distribution as X, up to a parameter scaling.~~

(2) $X^{(1)} \perp\!\!\!\perp X^{(2)}$.

In our previous recipe:

~~**(3)** $X = X^{(1)} + X^{(2)}$.~~ **(3)** $X = T(X^{(1)}, X^{(2)})$.

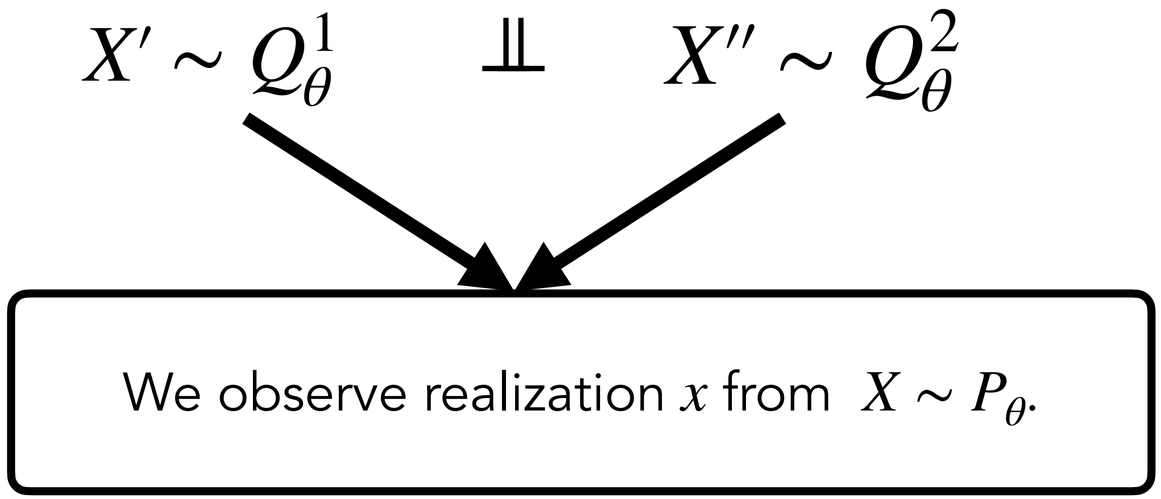
Suppose we know that, if $(X', X'') \sim Q_\theta^1 \times Q_\theta^2$, then $T(X', X'') \sim P_\theta$.
Then we can "unwind" this transformation.

Generalized thinning with non-additive decompositions

We observe realization x from $X \sim P_\theta$.

Generalized thinning with non-additive decompositions

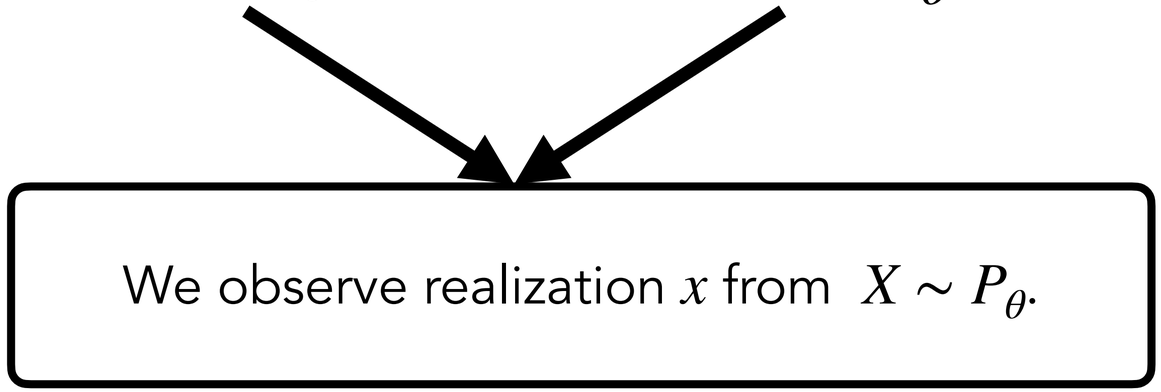
We know x could have arisen as $T(x', x'')$, where



Generalized thinning with non-additive decompositions

We know x could have arisen as $T(x', x'')$, where

$$X' \sim Q_\theta^1 \quad \perp\!\!\!\perp \quad X'' \sim Q_\theta^2$$



Can we work backwards to recover x' and x''?

Generalized thinning with non-additive decompositions

We know x could have arisen as $T(x', x'')$, where

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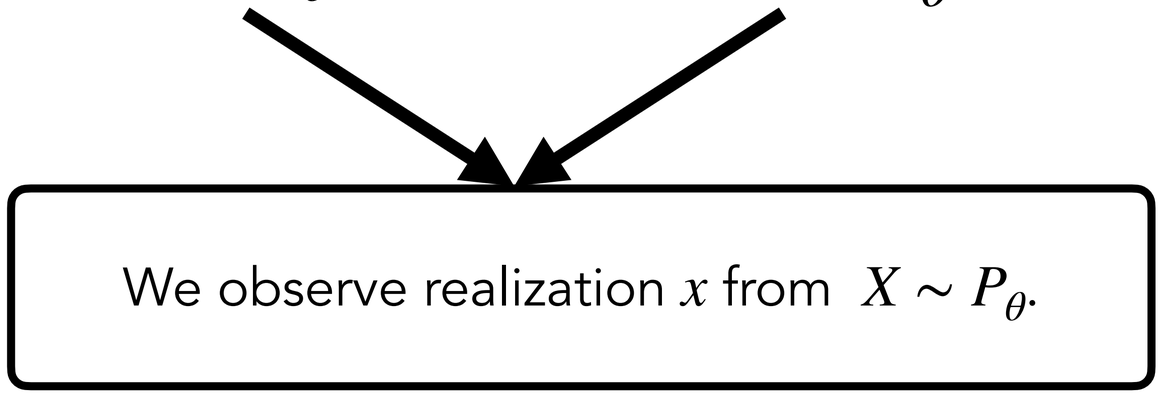

Can we work backwards to recover x' and x''?

Let $G_{\theta,x}$ be the conditional distribution of $(X', X'') \mid X = x$.

Generalized thinning with non-additive decompositions

We know x could have arisen as $T(x', x'')$, where

$$X' \sim Q_\theta^1 \quad \perp\!\!\!\perp \quad X'' \sim Q_\theta^2$$

We observe realization x from $X \sim P_\theta$.

Algorithm:

Draw $\left(X^{(1)}, X^{(2)}\right) \mid X = x$ from $G_{\theta,x}$.

Can we work backwards to recover x' and x''?

Let $G_{\theta,x}$ be the conditional distribution of $(X', X'') \mid X = x$.

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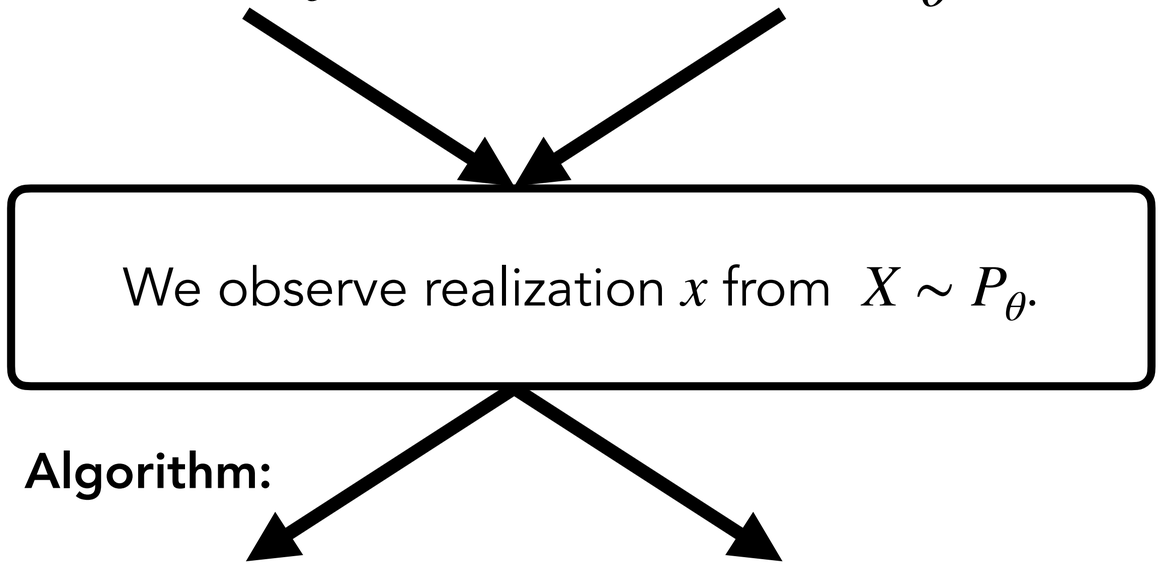

Theorem:

$X^{(1)} \sim Q_\theta^1, \quad X^{(2)} \sim Q_\theta^2, \quad X^{(1)} \perp\!\!\!\perp X^{(2)}$.

Can we work backwards to recover x' and x''?

Let $G_{\theta,x}$ be the conditional distribution of $(X', X'') \mid X = x$.

Generalized thinning with non-additive decompositions

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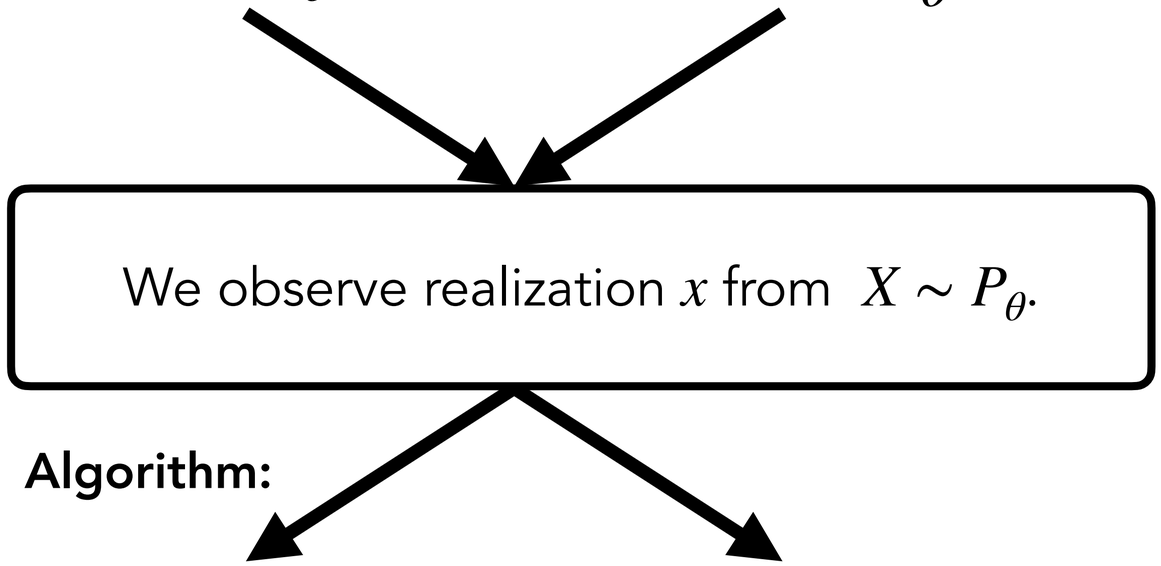

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Can we work backwards to recover x' and x''?

Let $G_{\theta,x}$ be the conditional distribution of $(X', X'') \mid X = x$.

Key idea: If $X = T(X', X'')$ is sufficient for θ in the joint of (X', X''), then $G_{\theta,x}$ does not depend on θ.

The list of distributions we can thin is extensive

Family	Distribution P_θ, where $X \sim P_\theta$.	Distribution $Q_\theta^{(k)}$ where $X^{(k)} \overset{ind.}{\sim} Q_\theta^{(k)}$.	Sufficient statistic T (sufficient for θ)
Natural exponential family (in parameter θ)	$N(\theta, \sigma^2)$	$\mathrm{N}(\epsilon_k\theta, \epsilon_k\sigma^2)$	$\sum_{k=1}^K X^{(k)}$
	$\mathrm{Poisson}(\theta)$	$\mathrm{Poisson}(\epsilon_k\theta)$	
	$\mathrm{NegBin}(r, \theta)$	$\mathrm{NegBin}(\epsilon_k r, \theta)$	
	$\mathrm{Binomial}(r, \theta)$	$\mathrm{Binomial}(\epsilon_k r, \theta)$	
	$\mathrm{Gamma}(\alpha, \theta)$	$\mathrm{Gamma}(\epsilon_k\alpha, \theta)$	
	$\mathrm{N}_p(\boldsymbol{\theta}, \Sigma)$	$N_p(\epsilon_k\boldsymbol{\theta}, \epsilon_k\Sigma)$	
	$\mathrm{Multinomial}_p(r, \boldsymbol{\theta})$	$\mathrm{Multinomial}_p(\epsilon_k r, \boldsymbol{\theta})$	
	$\mathrm{Gamma}(K/2, \theta)$	$N(0, \frac{1}{2\theta})$	$\sum_{k=1}^K \left(X^{(k)}\right)^2$
	$\mathrm{Gamma}(K, \theta)$	$\mathrm{Weibull}(\theta^{-\frac{1}{\nu}}, \nu)$	$\sum_{k=1}^K \left(X^{(k)}\right)^\nu$
General exponential family (in parameter θ)	$\mathrm{Beta}(\theta, \beta)$	$\mathrm{Beta}\left(\frac{1}{K}\theta + \frac{k-1}{K}, \frac{1}{K}\beta\right)$	$\left(\Pi_{k=1}^K X^{(k)}\right)^{1/K}$
	$\mathrm{Beta}(\alpha, \theta)$	$\mathrm{Beta}\left(\frac{1}{K}\alpha, \frac{1}{K}\theta + \frac{k-1}{K}\right)$	$\left(\Pi_{k=1}^K \left(1 - X^{(k)}\right)\right)^{1/K}$
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	$\mathrm{Weibull}(\theta, \nu)$	$\mathrm{Gamma}(\frac{1}{K}, \theta^{-\nu})$	$\left(\sum_{k=1}^K X^{(k)}\right)^{1/\nu}$
	$\mathrm{Pareto}(\nu, \theta)$	$\mathrm{Gamma}(\frac{1}{K}, \theta)$	$\nu \times \mathrm{Exp}\left(\sum_{k=1}^K X^{(k)}\right)$
	$\mathrm{N}(0,\theta)$	$\mathrm{Gamma}(\frac{1}{2K}, \frac{1}{2\theta})$	$X^2 = \sum_{k=1}^K X^{(k)}$
	$\mathrm{N}_K(\theta_1 1_K, \theta_2 I_K)$	$N(\theta_1, \theta_2)$	sample mean and variance
Truncated support family	$\mathrm{Unif}(0, \theta)$	$\theta \cdot \mathrm{Beta}(\frac{1}{K}, 1)$	$\max\left(X^{(1)}, \ldots, X^{(K)}\right)$
	$\theta \cdot \mathrm{Beta}(\alpha, 1)$	$\theta \cdot \mathrm{Beta}(\frac{\alpha}{K}, 1)$	
	$\theta + \mathrm{Exp}(\lambda)$	$\theta + \mathrm{Exp}(\lambda/\mathrm{K})$	$\min\left(X^{(1)}, \ldots, X^{(K)}\right)$
Non-parametric	F^n	F^{n_k}	$\mathrm{sort}(X^{(1)}, \ldots, X^{(K)})$

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Statistics > Methodology

[Submitted on 22 Mar 2023]

Generalized Data Thinning Using Sufficient Statistics

Ameer Dharamshi, Anna Neufeld, Keshav Motwani, Lucy L. Gao, Daniela Witten, Jacob Bien

Outline

1. Motivation: sample splitting doesn’t always work
2. Poisson thinning
3. Data thinning
4. Generalized data thinning
5. **Application to changepoint validation**
6. Ongoing work

Application: changepoint detection

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Goal: Identify points in a sequence where the distribution changes.

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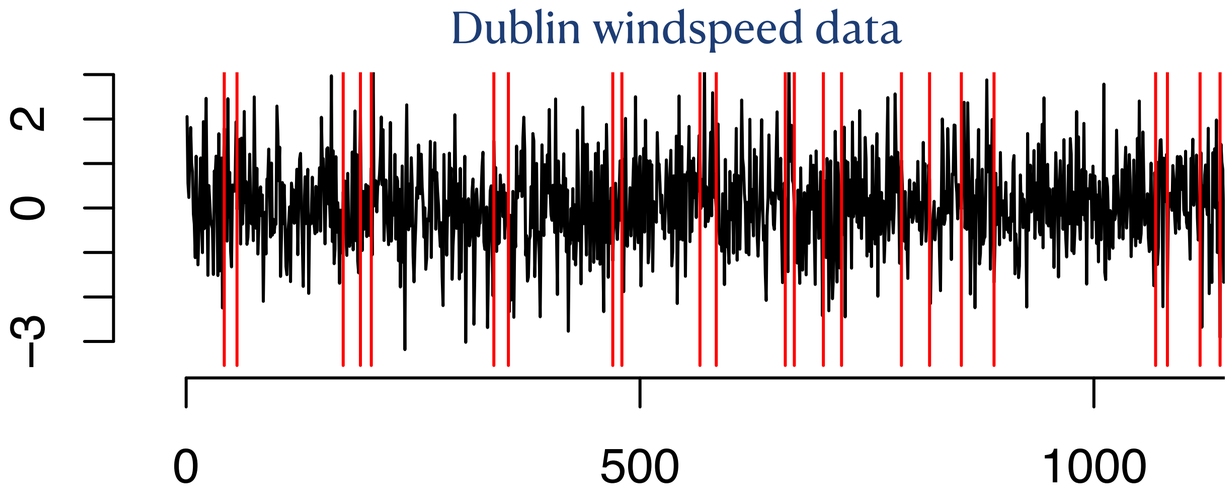
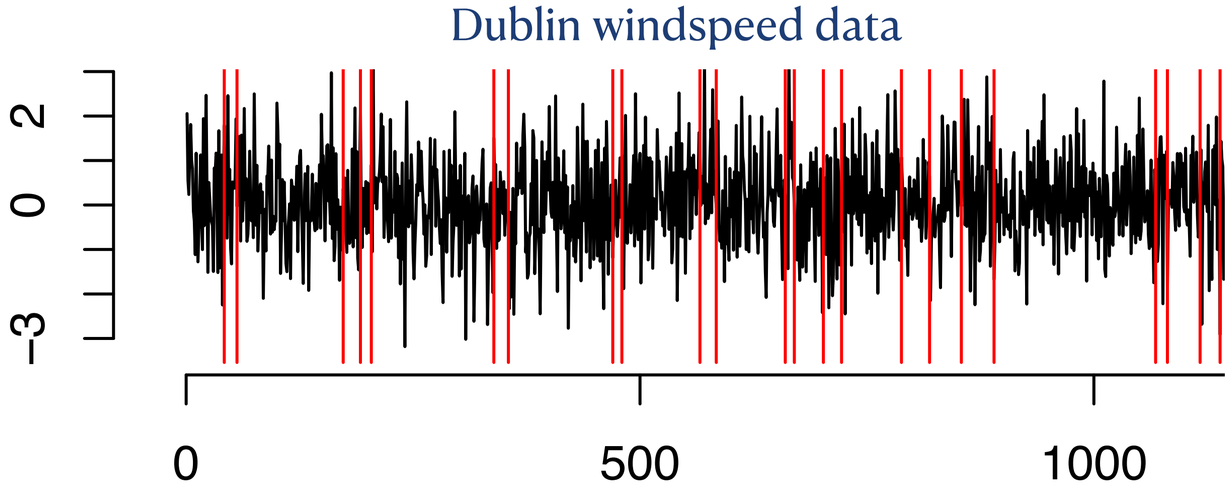


Application: changepoint detection

Goal: Identify points in a sequence where the distribution changes.

Setting: Differences in wind speeds have previously been modeled as $X_i \sim N(0, \theta_i)$. How can we validate an estimated changepoint?



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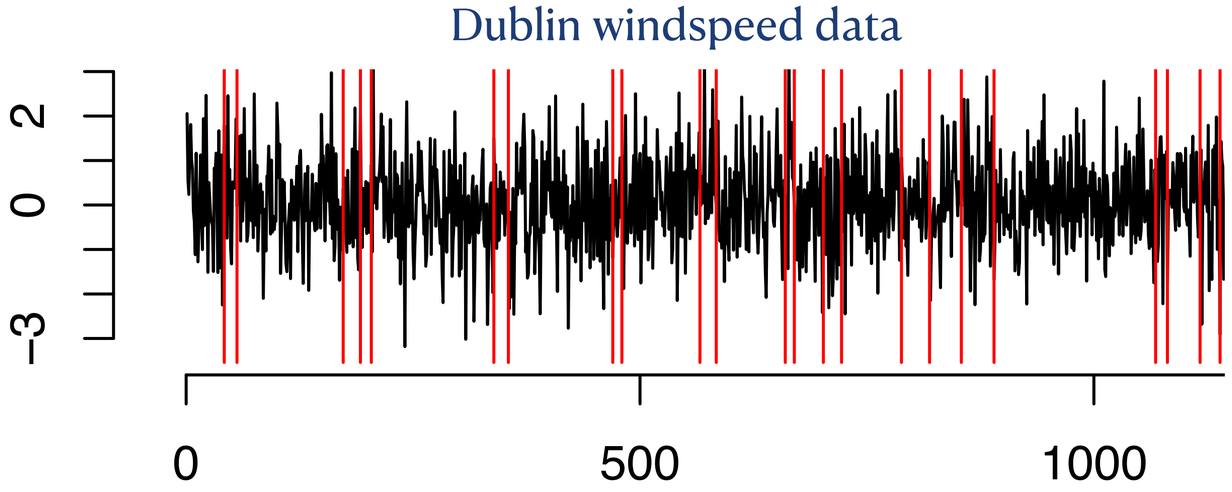

Can we thin a Gaussian with unknown variance?

We can't apply this because the variance is unknown

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Non-parametric	F^n	F^{n_k}	$\mathrm{sort}(X^{(1)}, \ldots, X^{(K)})$

But, we do know how to thin a Gamma!

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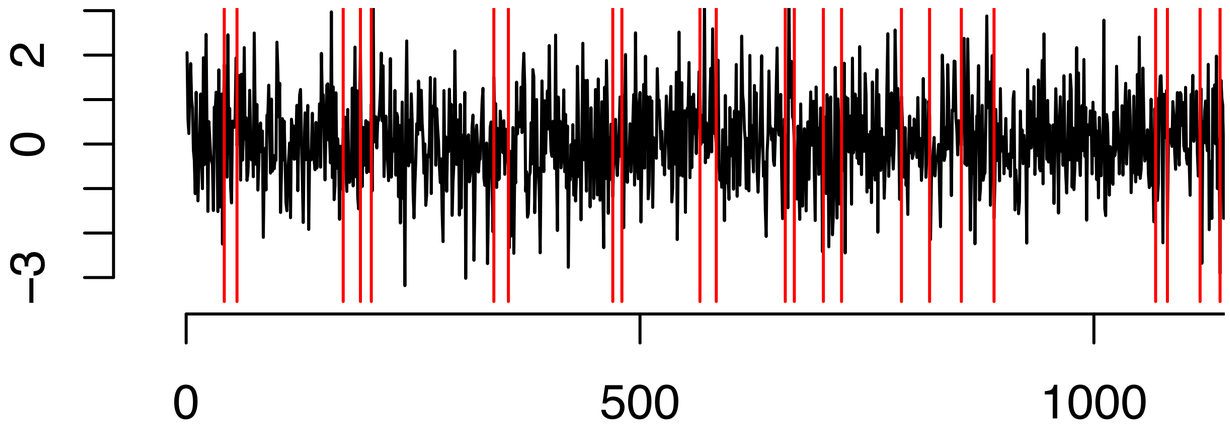
Fact: if $X_i \sim N(0,\theta_i)$, then

$$X_i^2 \sim \mathrm{Gamma}(\frac{1}{2}, \frac{1}{2\theta_i^2}).$$

Application: changepoint detection

Goal: Identify points in a sequence where the distribution changes.

Setting: Differences in wind speeds have previously been modeled as $X_i \sim N(0, \theta_i)$. How can we validate an estimated changepoint?



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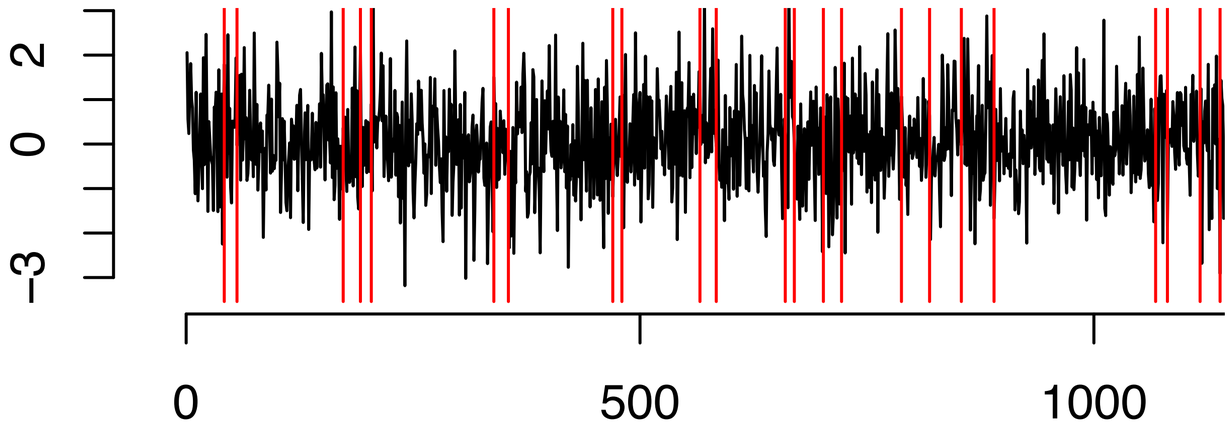
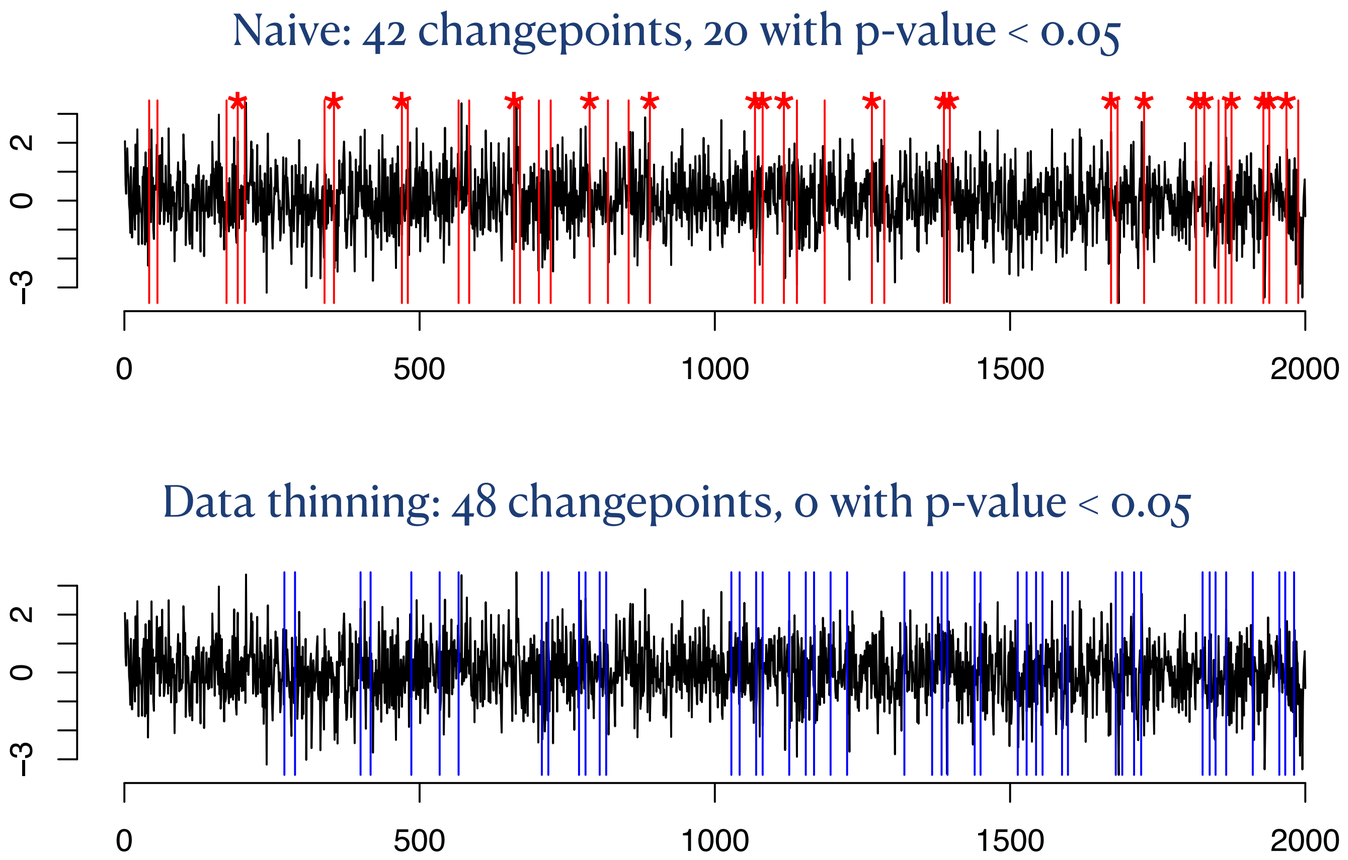


Define $Z_i := X_i^2$. Note that $Z_i \sim \text{Gamma}\left(0.5, 0.5/\theta_i^2\right)$.

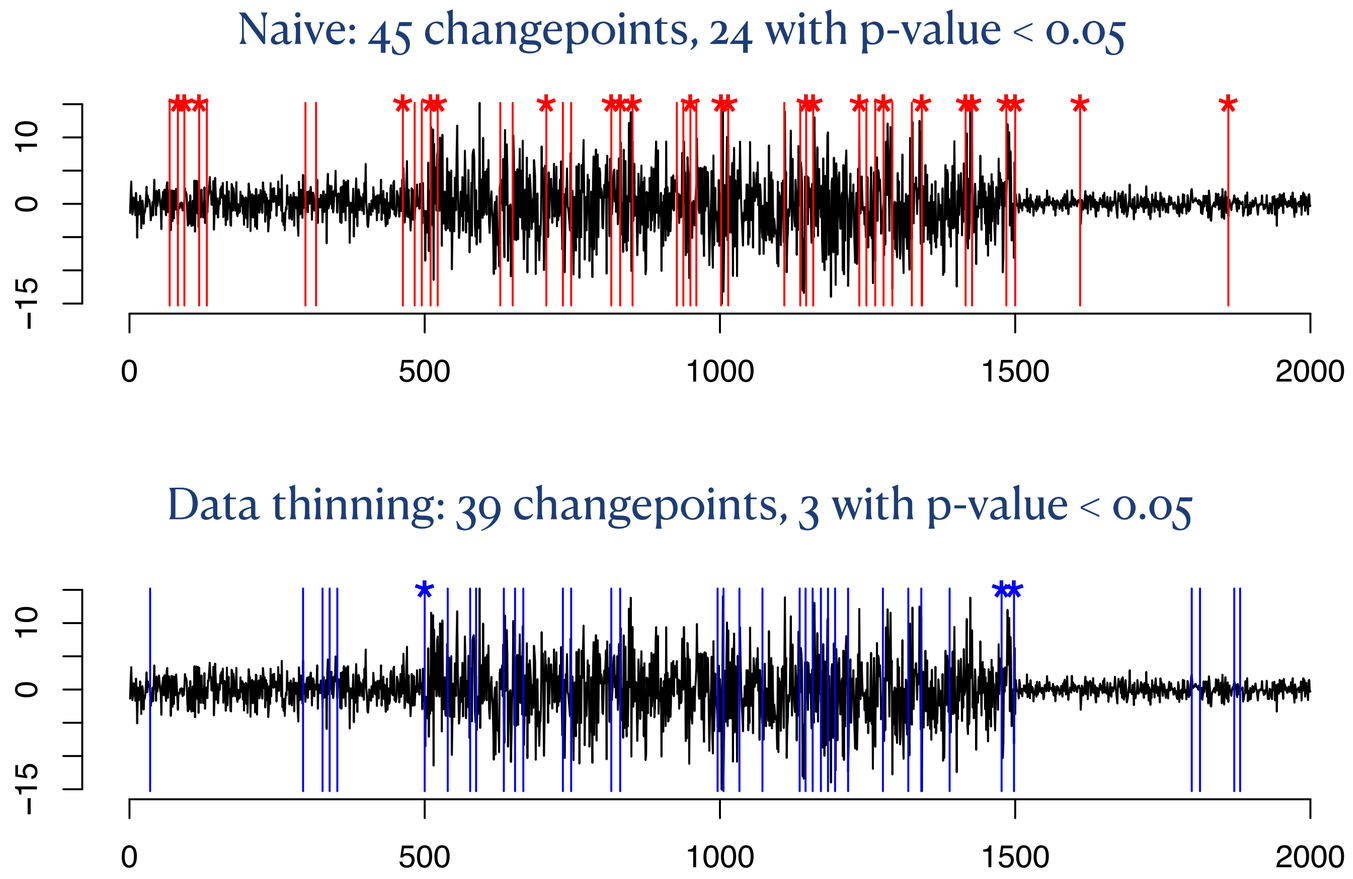
Option 1: Estimate and test changepoints on Z_i.

Option 2: Thin Z_i into $Z_i^{(1)} \sim \text{Gamma}\left(0.25, 0.5/\theta_i^2\right)$ and $Z_i^{(2)} \sim \text{Gamma}\left(0.25, 0.5/\theta_i^2\right)$.
Identify changepoints using $Z_i^{(1)}$, and test using $Z_i^{(2)}$.

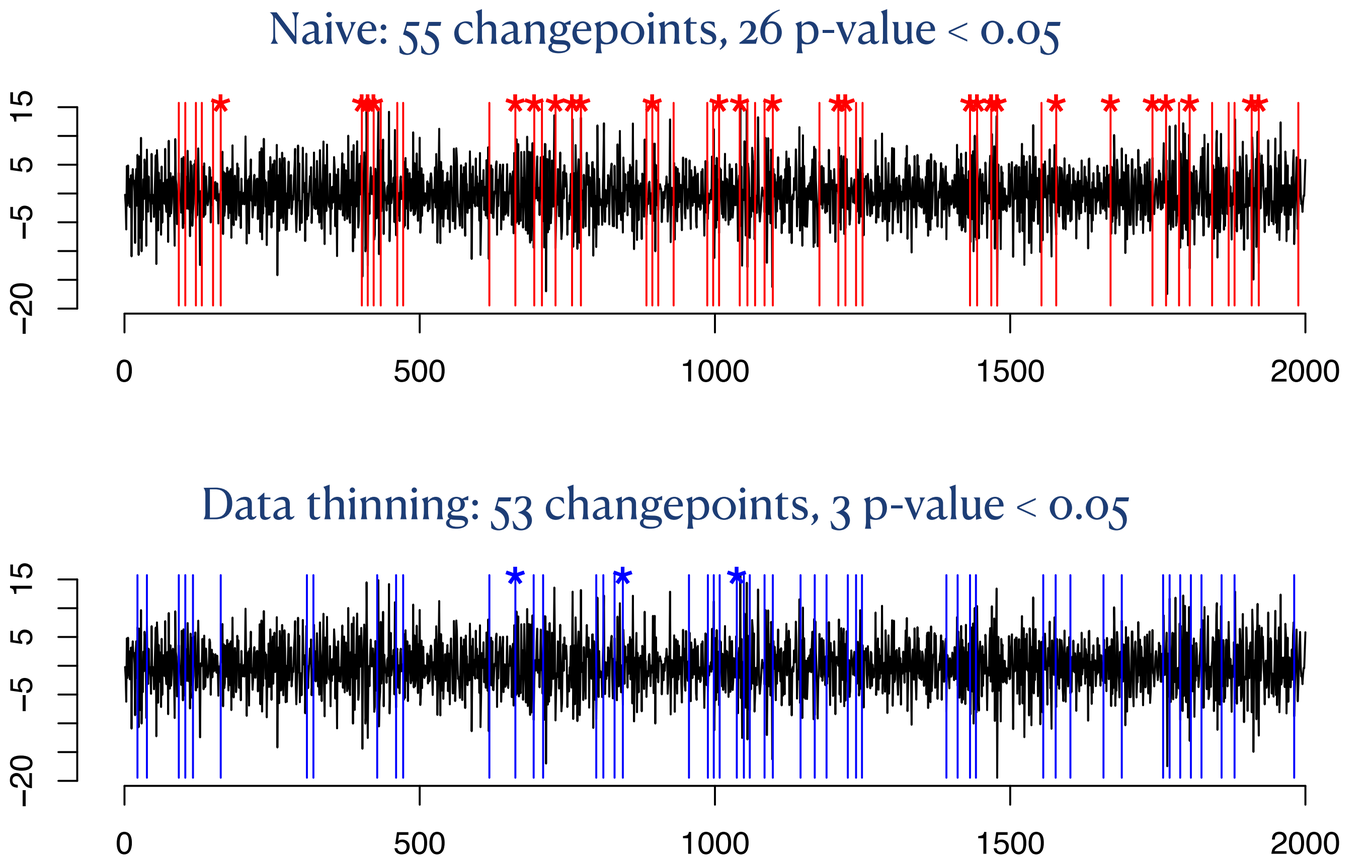
Quick detour to simulated data with no changepoints



Quick detour to simulated data with two true changepoints



Dublin wind speed data

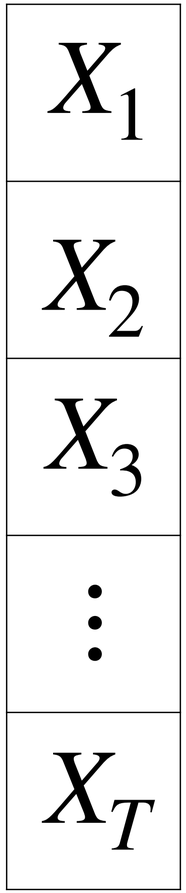


Outline

1. Motivation: sample splitting doesn’t always work
2. Poisson thinning
3. Data thinning
4. Generalized data thinning
5. Application to changepoint validation
6. **Ongoing work**

What if we want to thin time series data?

$$X_t \sim N(\mu_t, \sigma^2)$$



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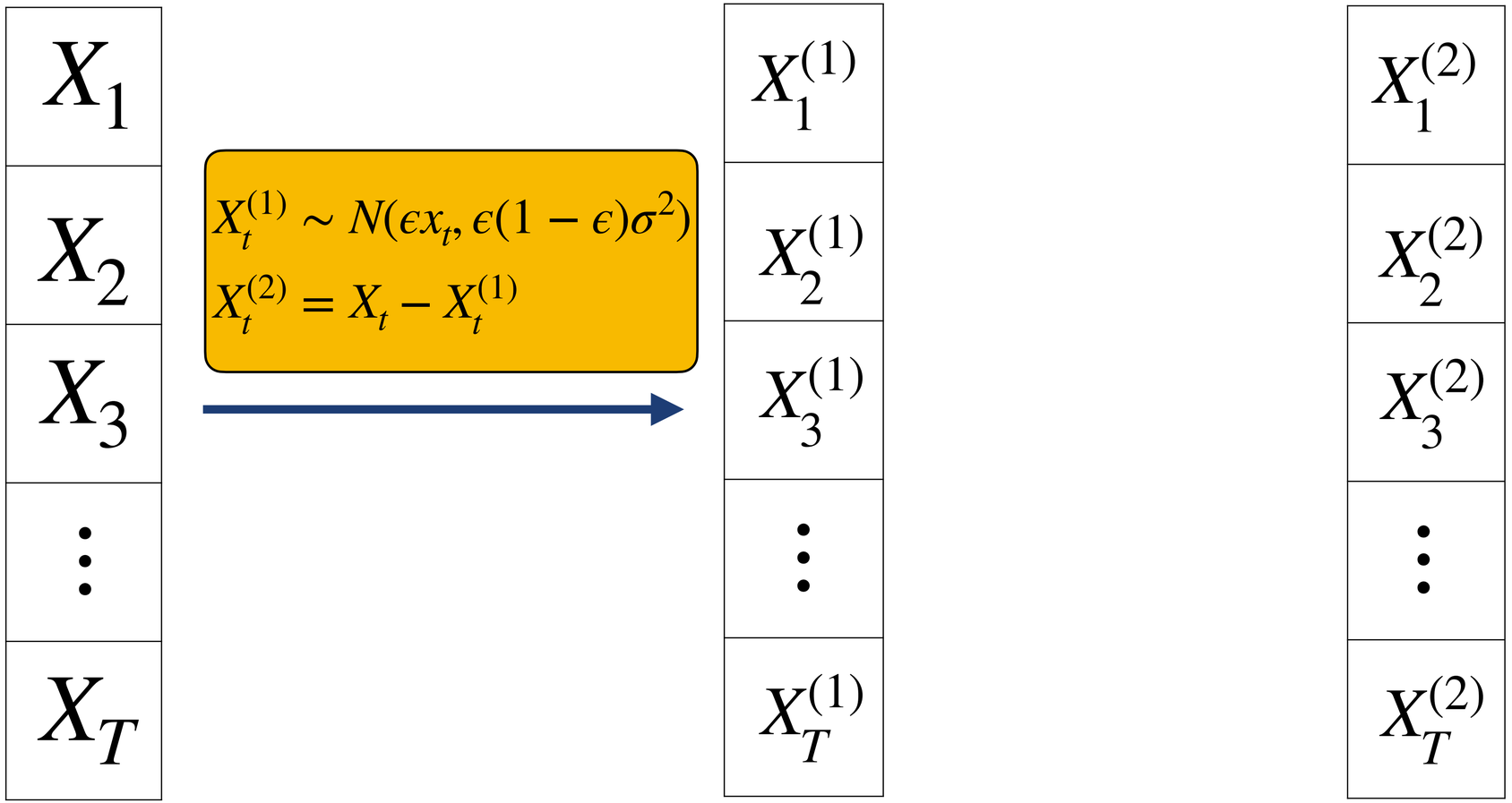

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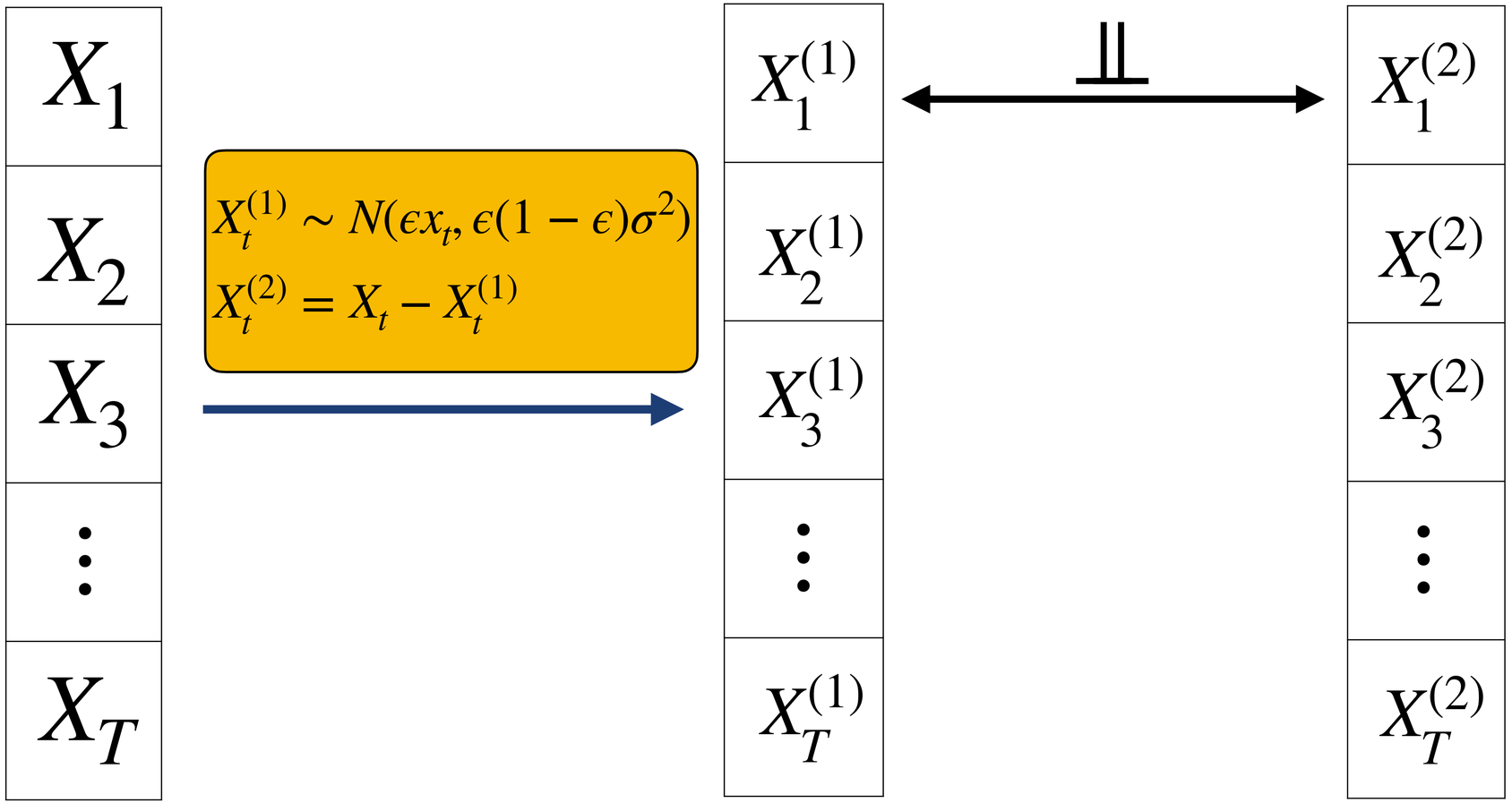

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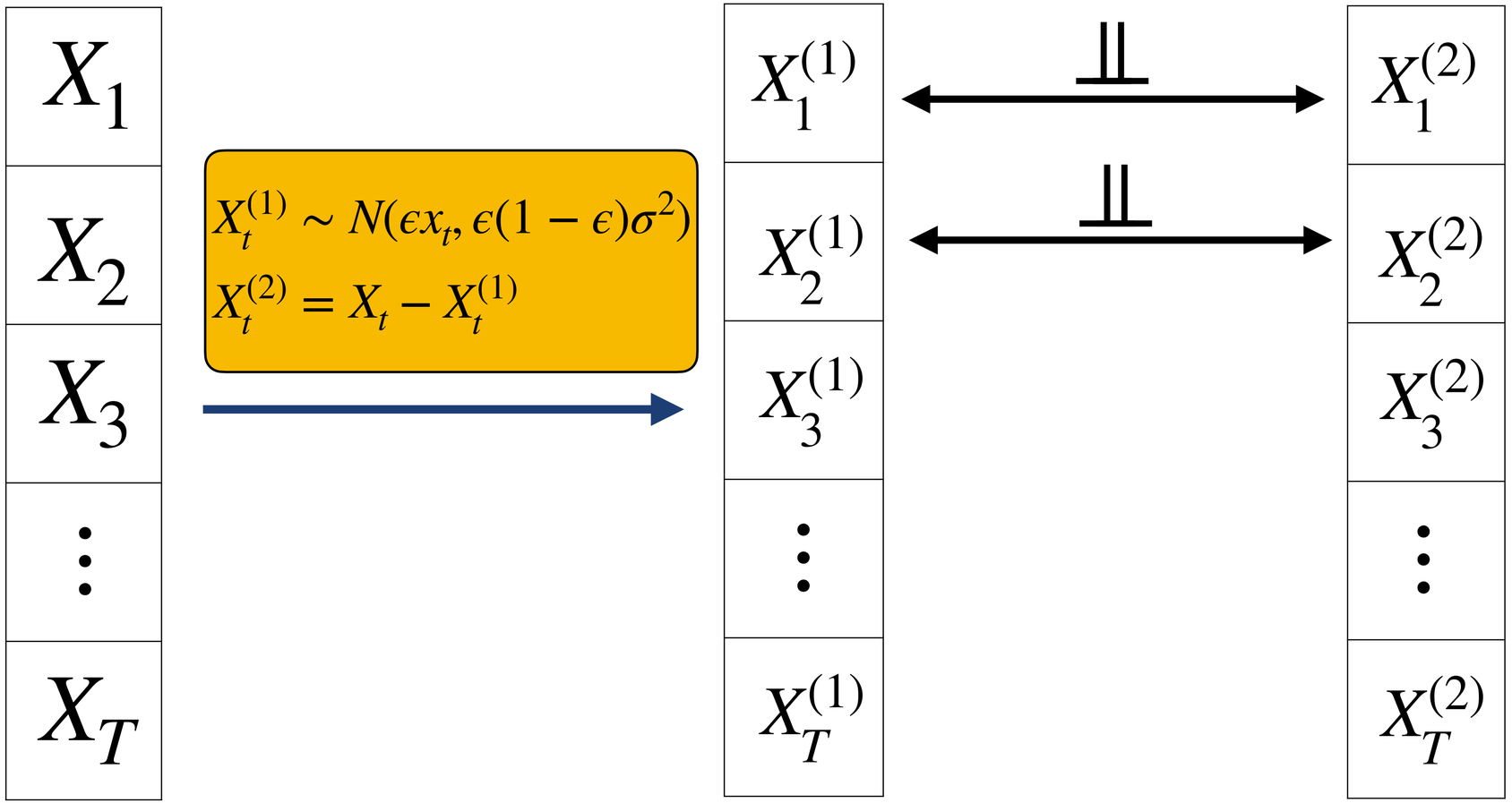

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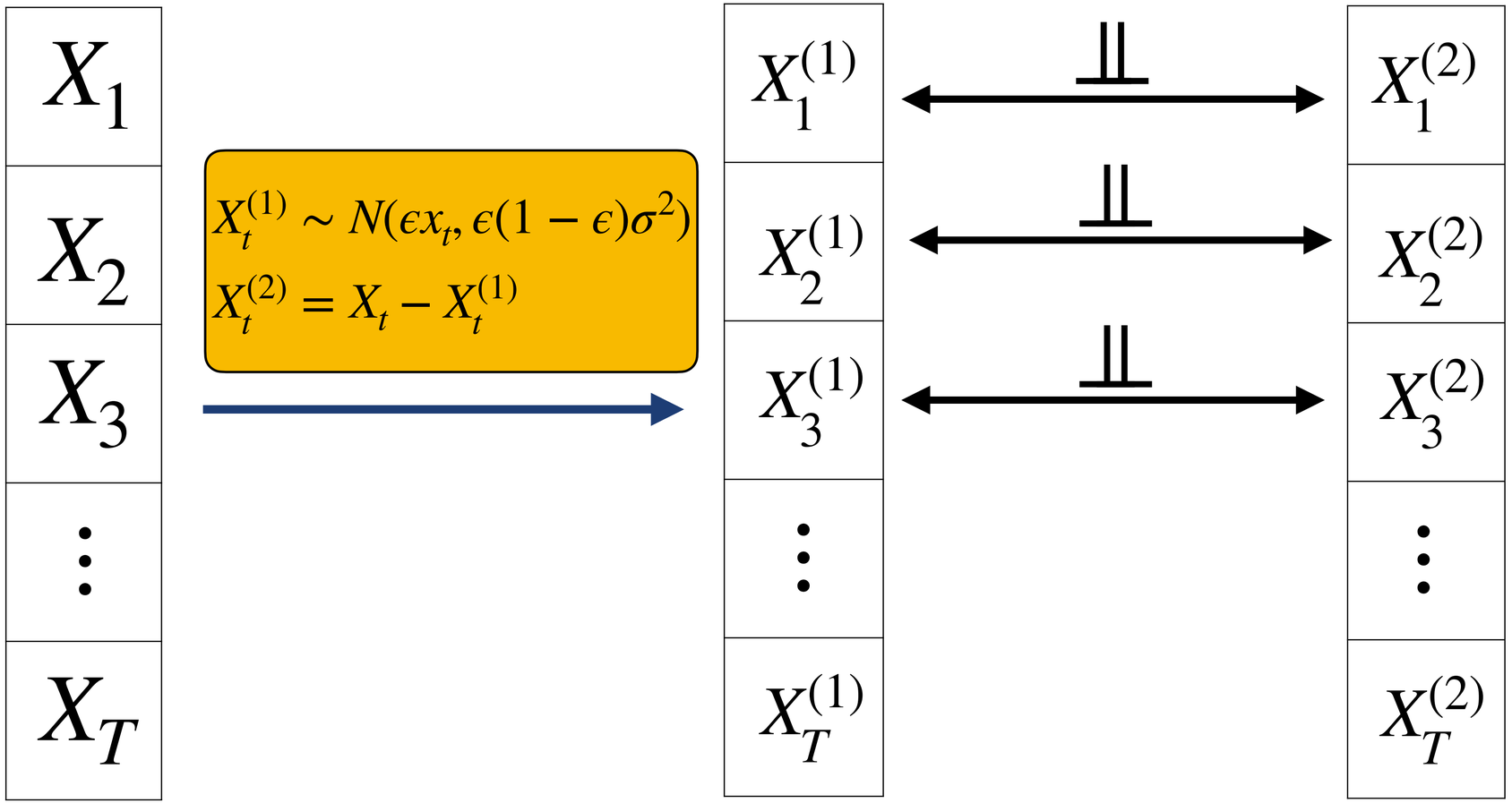

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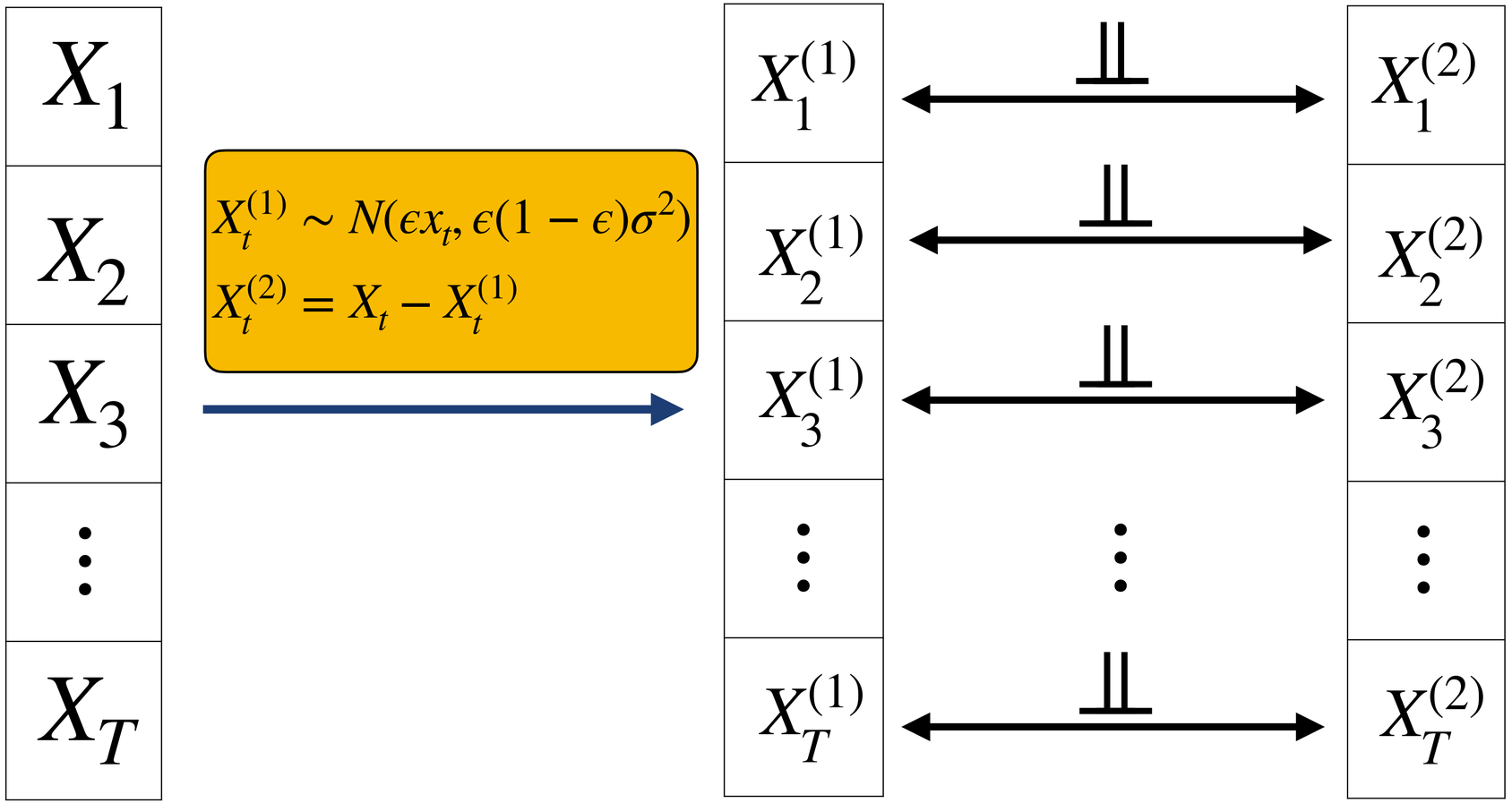

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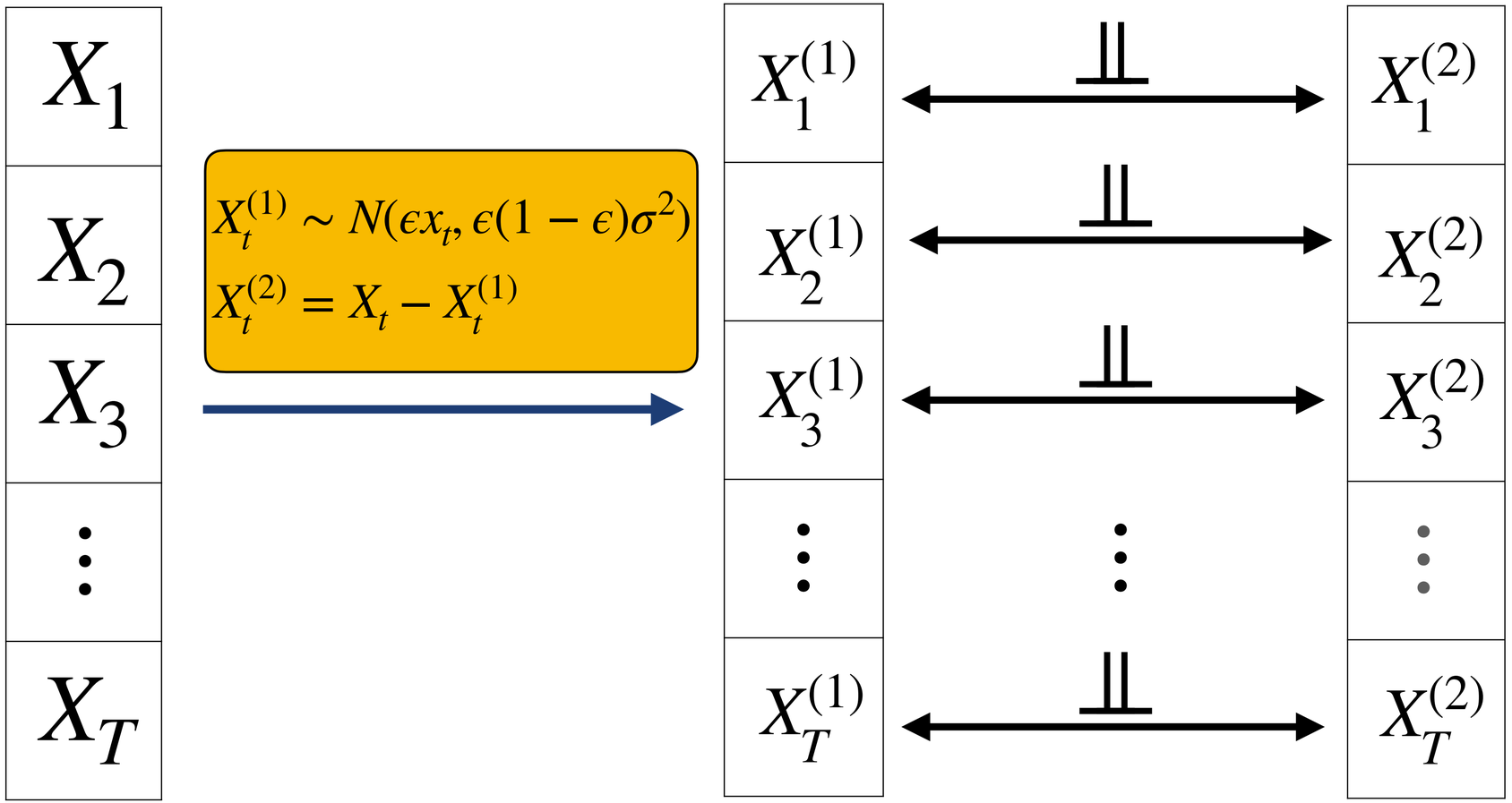

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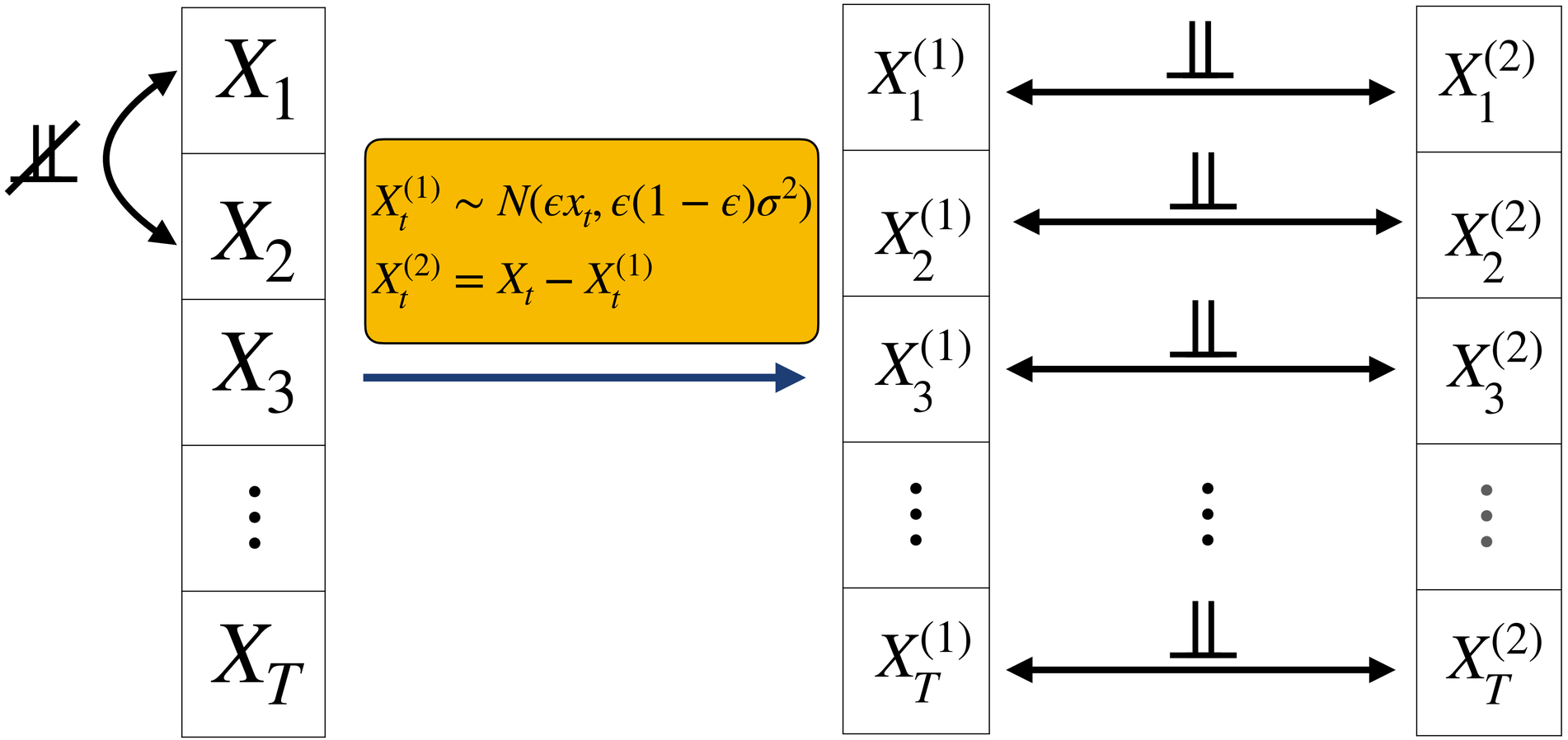

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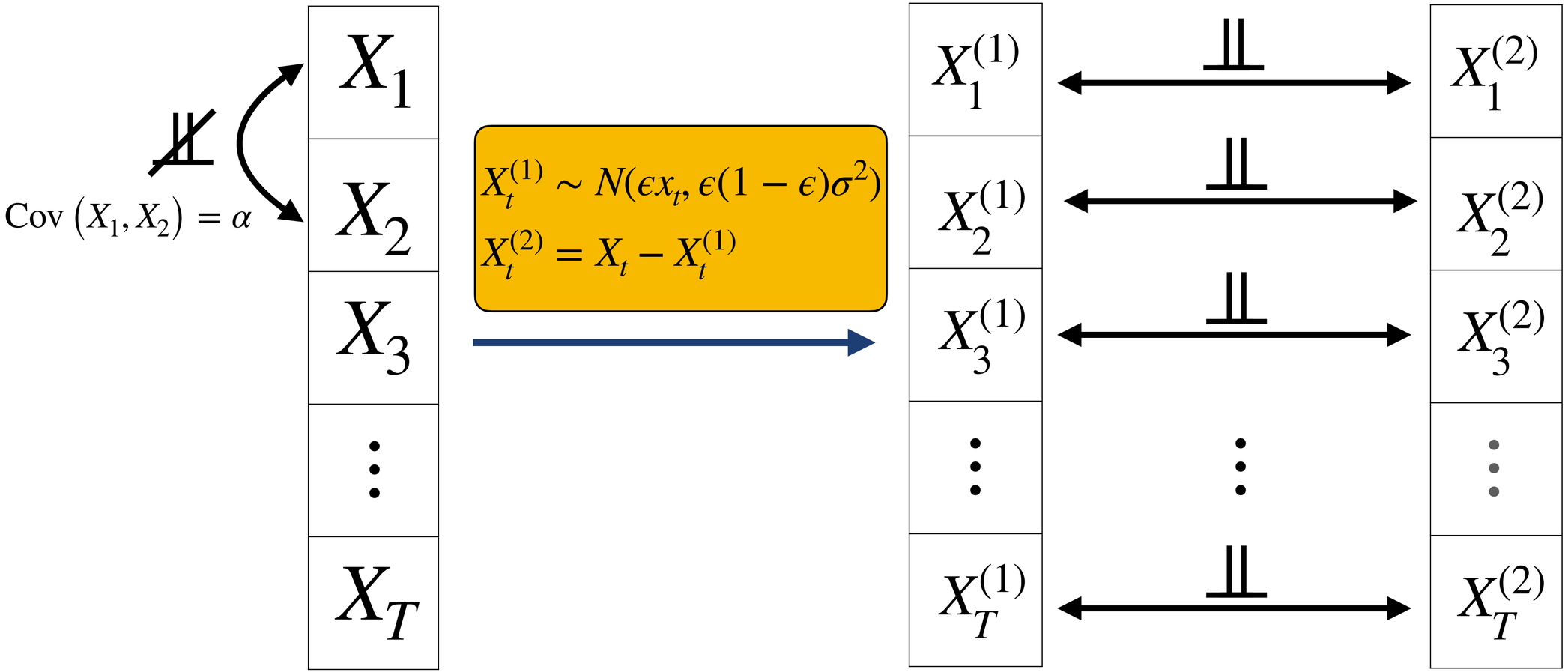

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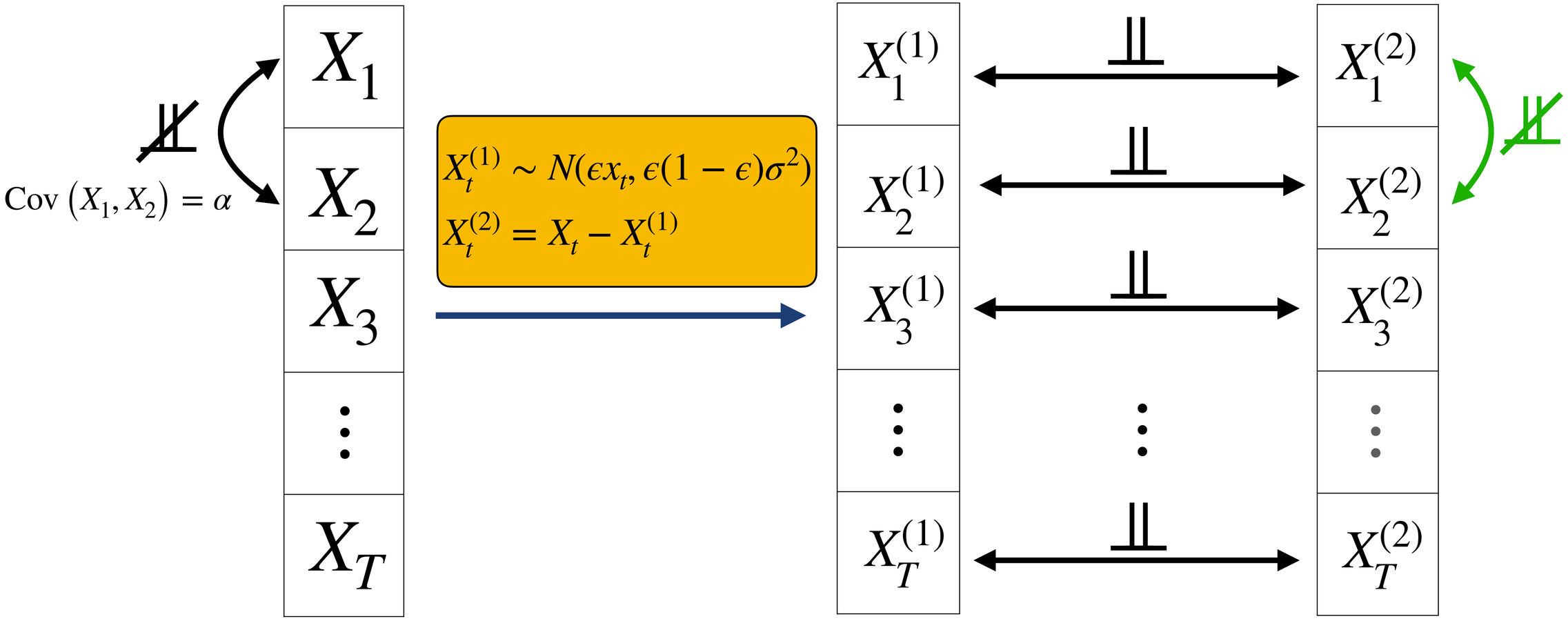

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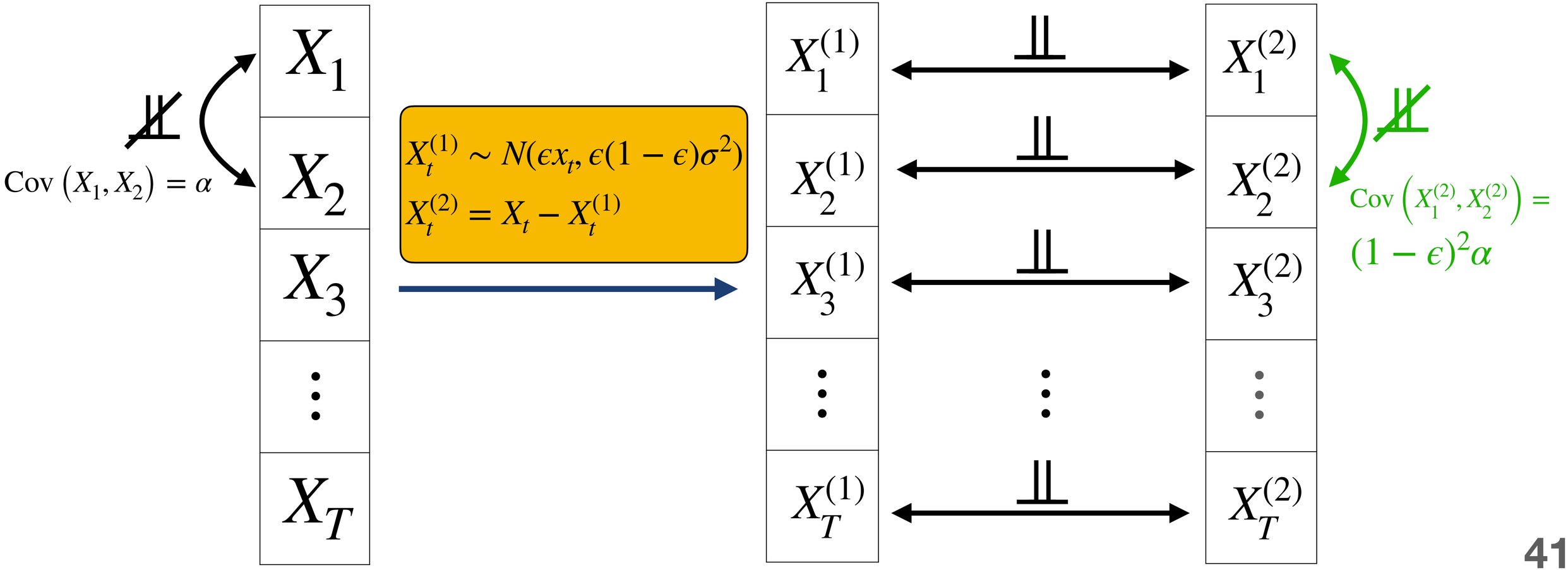

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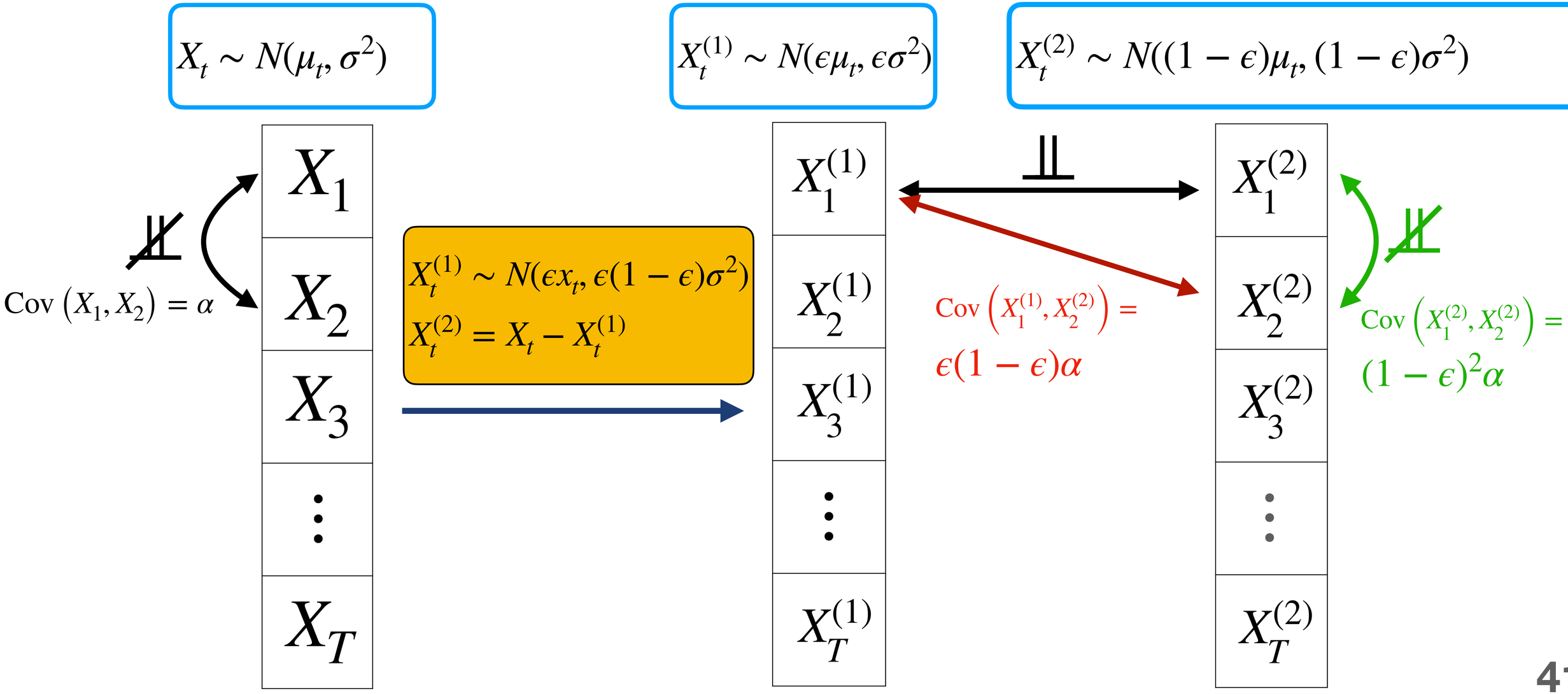

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   - **Challenge:** this is a singular Wishart, and it's hard to work with.

Acknowledgements

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University of Washington

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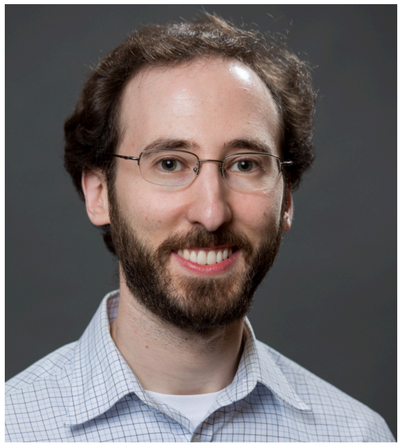
Johns Hopkins



Jacob Bien
USC

Questions?

Are the results of our data analysis stable?