

Data thinning for convolution-closed distributions

Anna Neufeld
June, 2023

We often wish that we had access to two independent datasets, drawn from the same data-generating mechanism

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

	Feature 1	Feature 2
Obs. 1	9	3
Obs. 2	33	9
Obs. 3	12	29
Obs. 4	25	41

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Test

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Obs. 1	9	3
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Fit model.

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Validate model.

As we typically have access to only one dataset, a common solution is sample splitting

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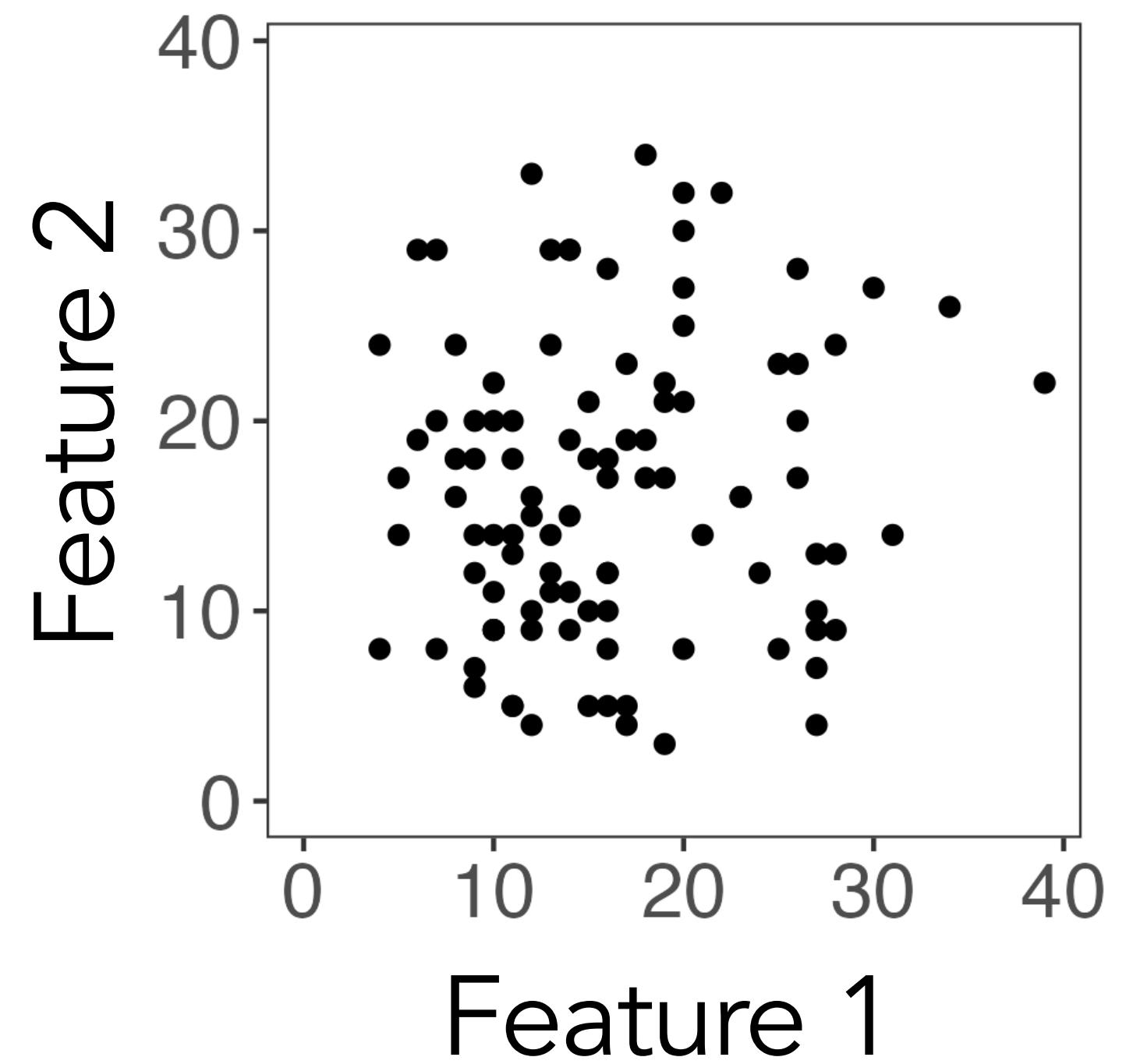
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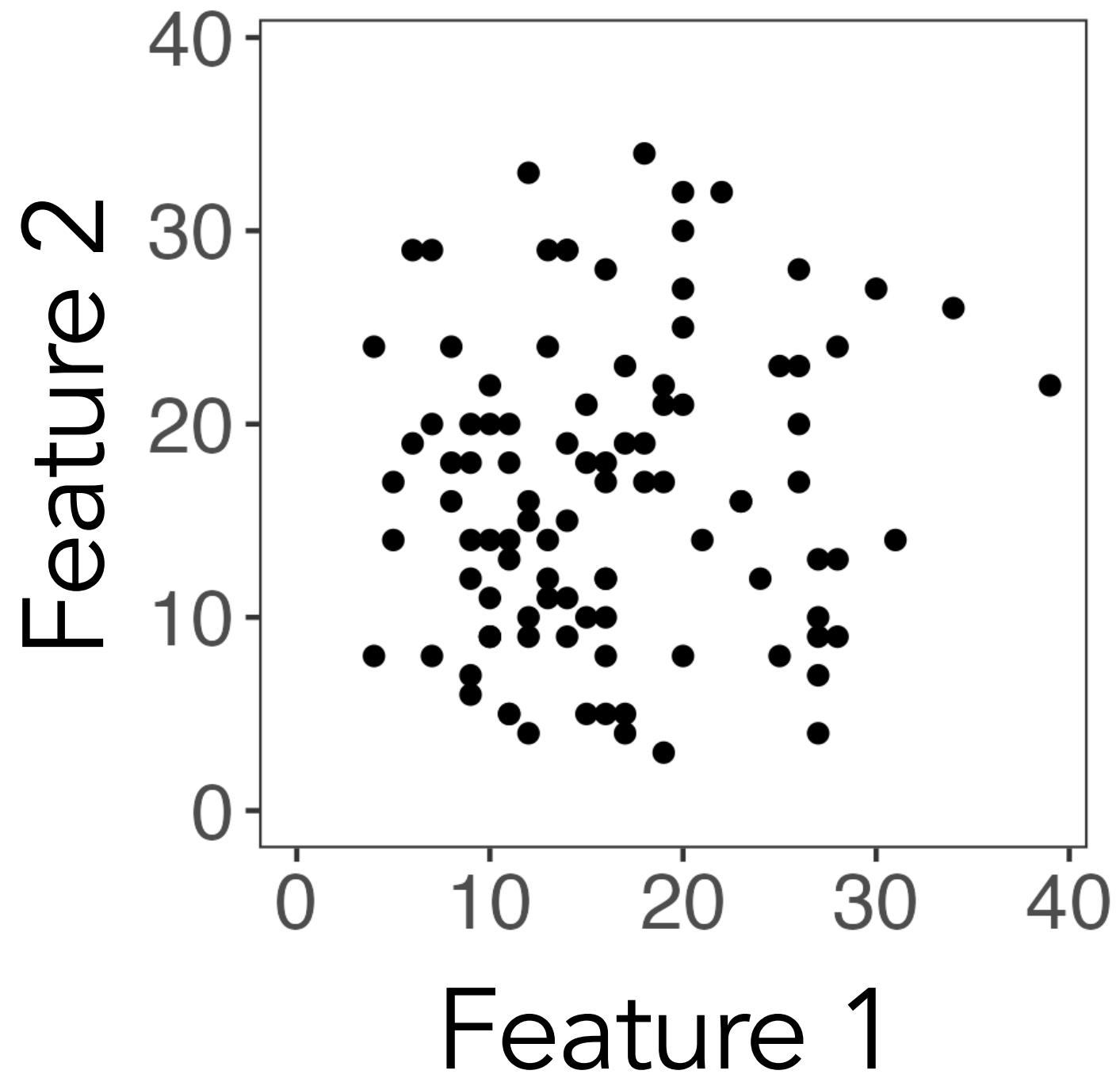
Outline

1. **Motivation: sample splitting doesn't always work**
2. Poisson thinning
3. Data thinning
4. Application to changepoint detection
5. Generalized data thinning

Example: how many clusters are in this data?



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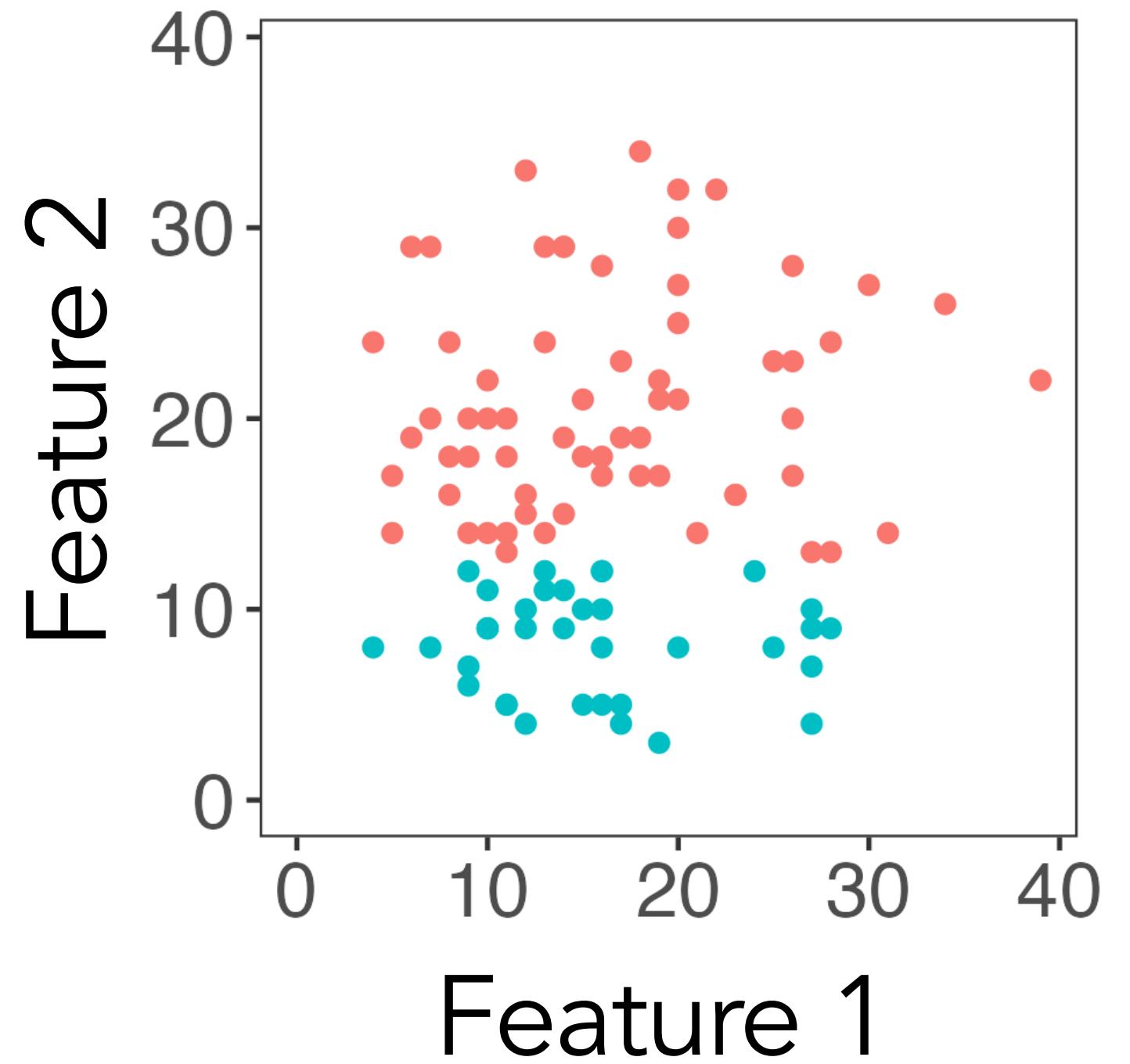


For several values of k :

Step 1: fit a model
with k clusters.

Step 2: evaluate
model using a loss
function.

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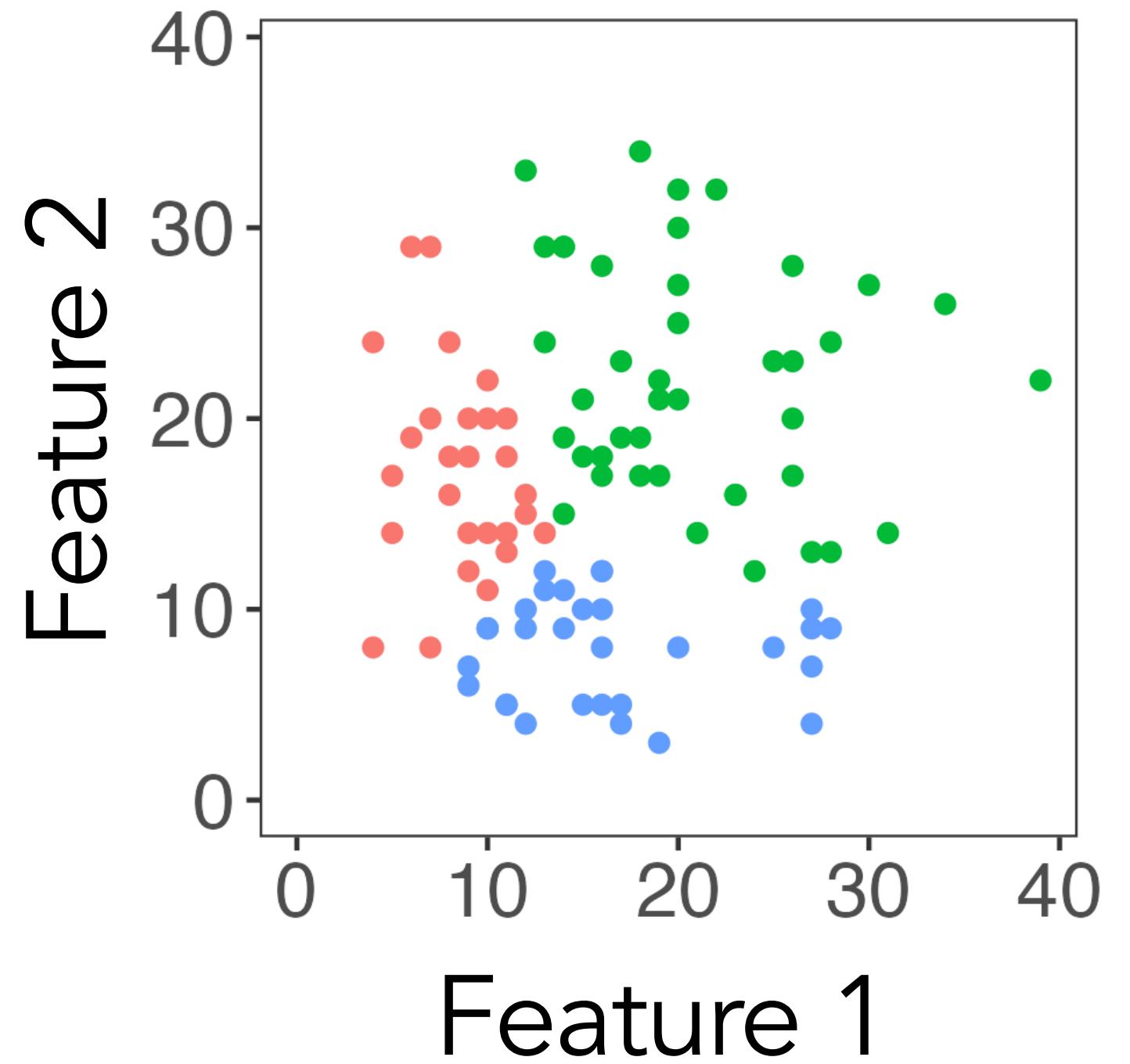


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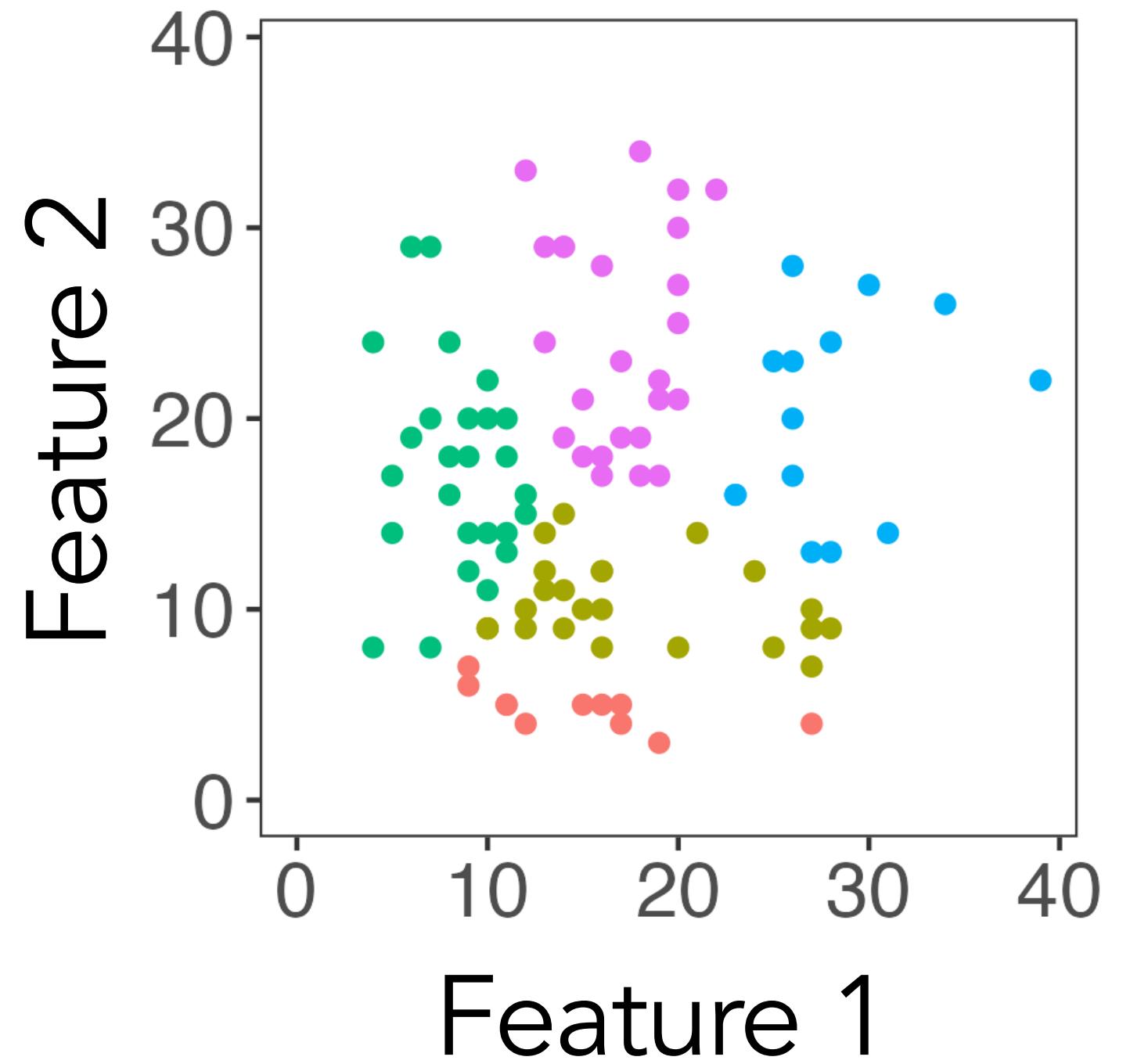


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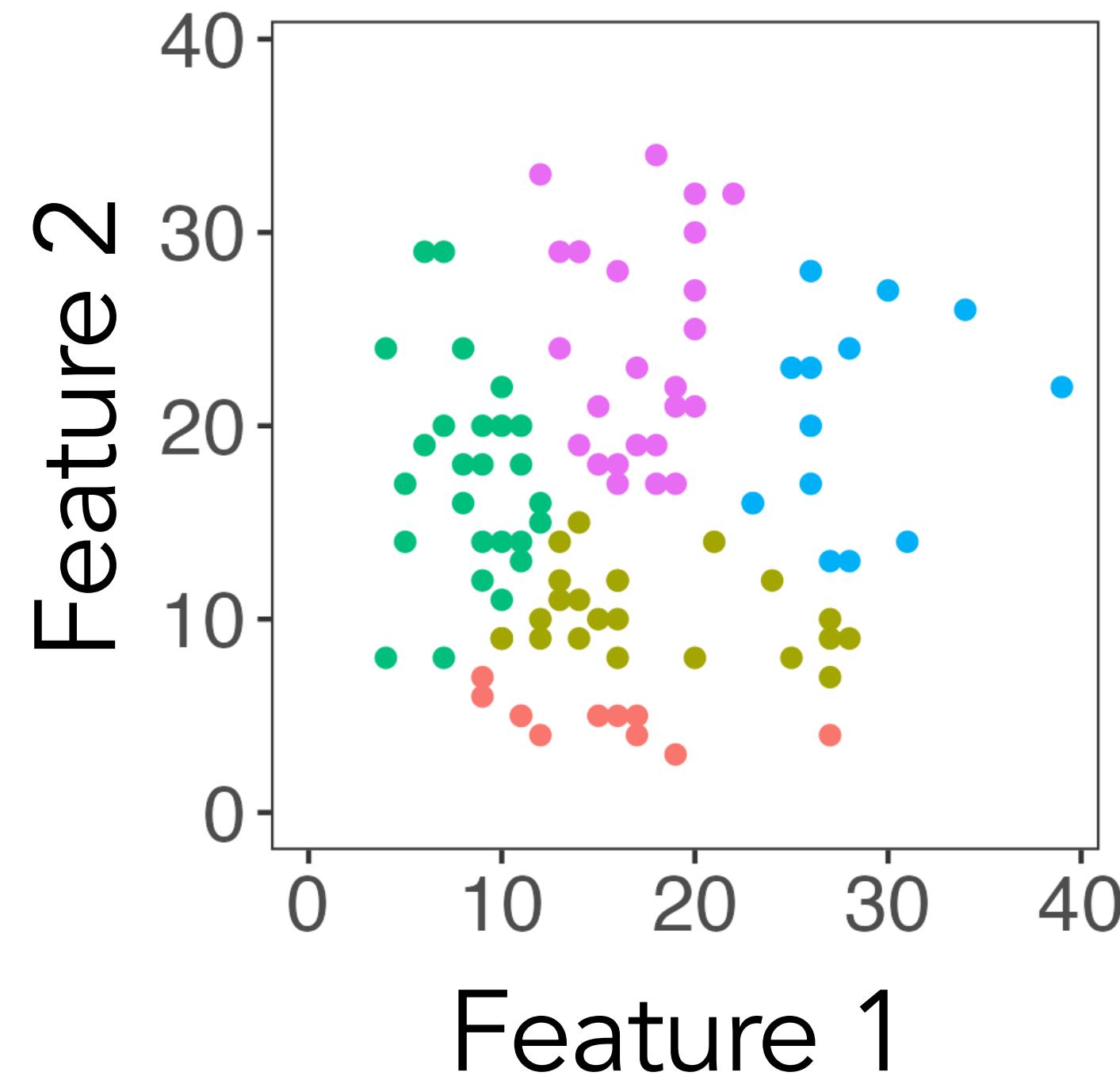


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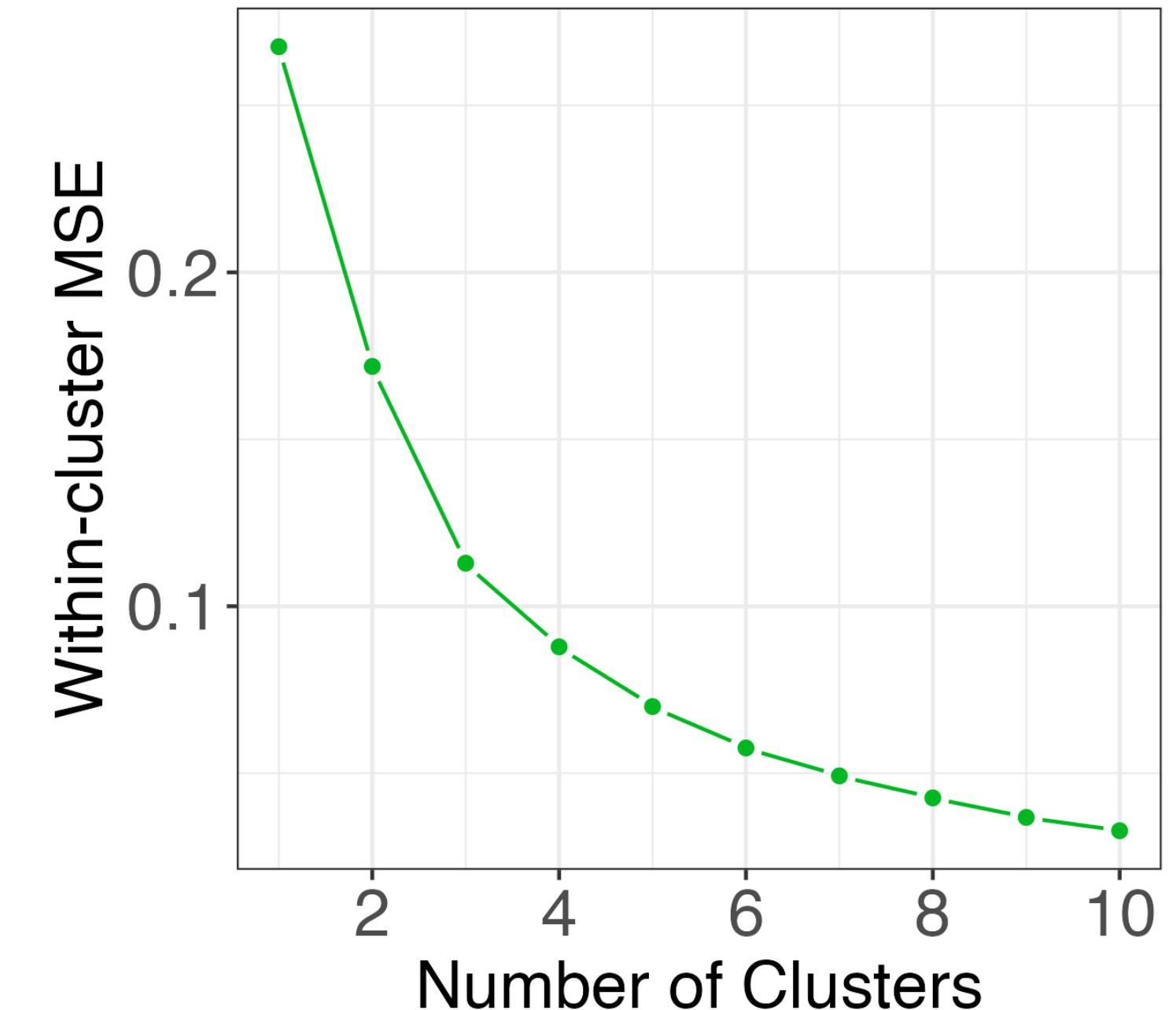
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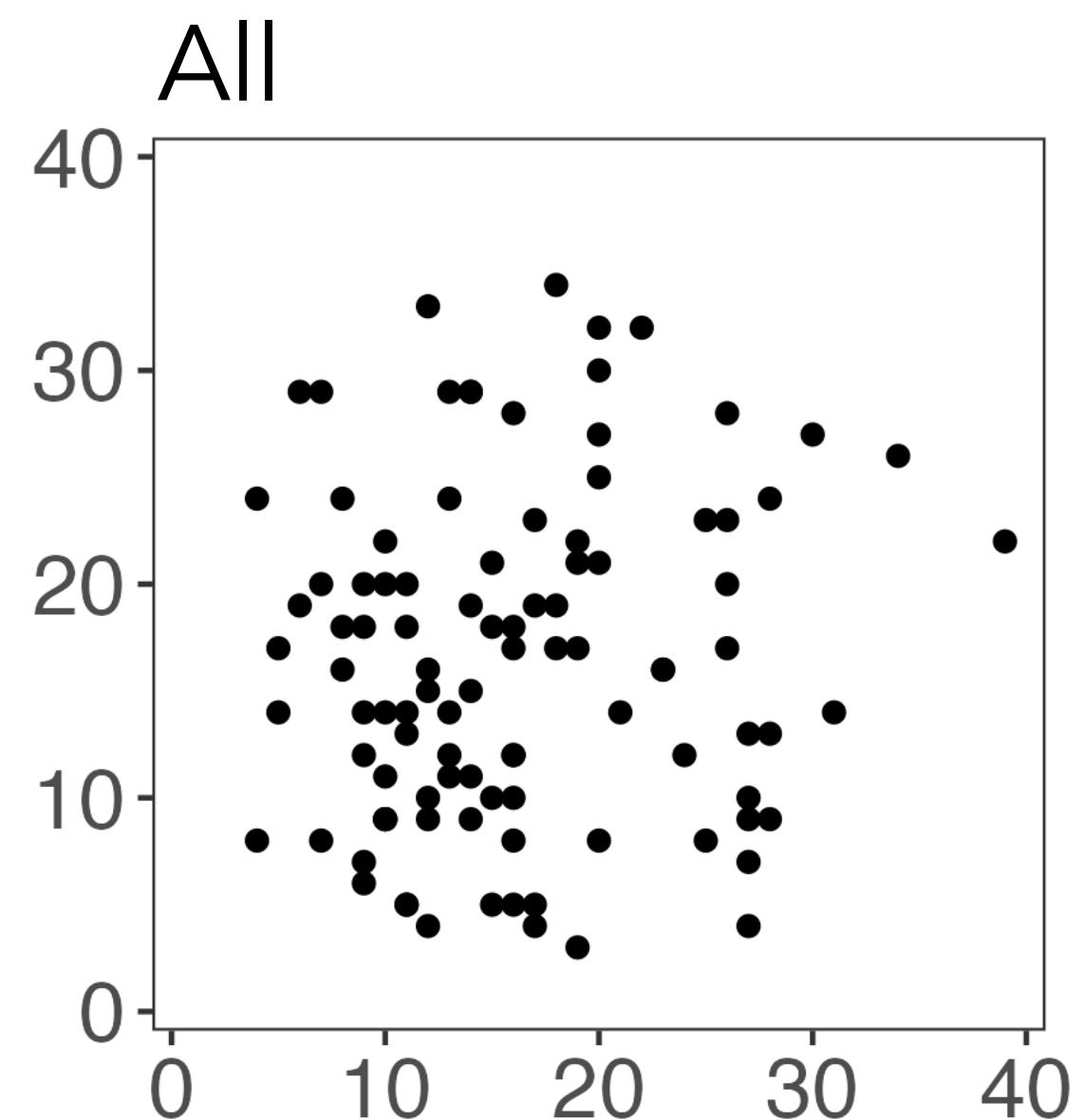
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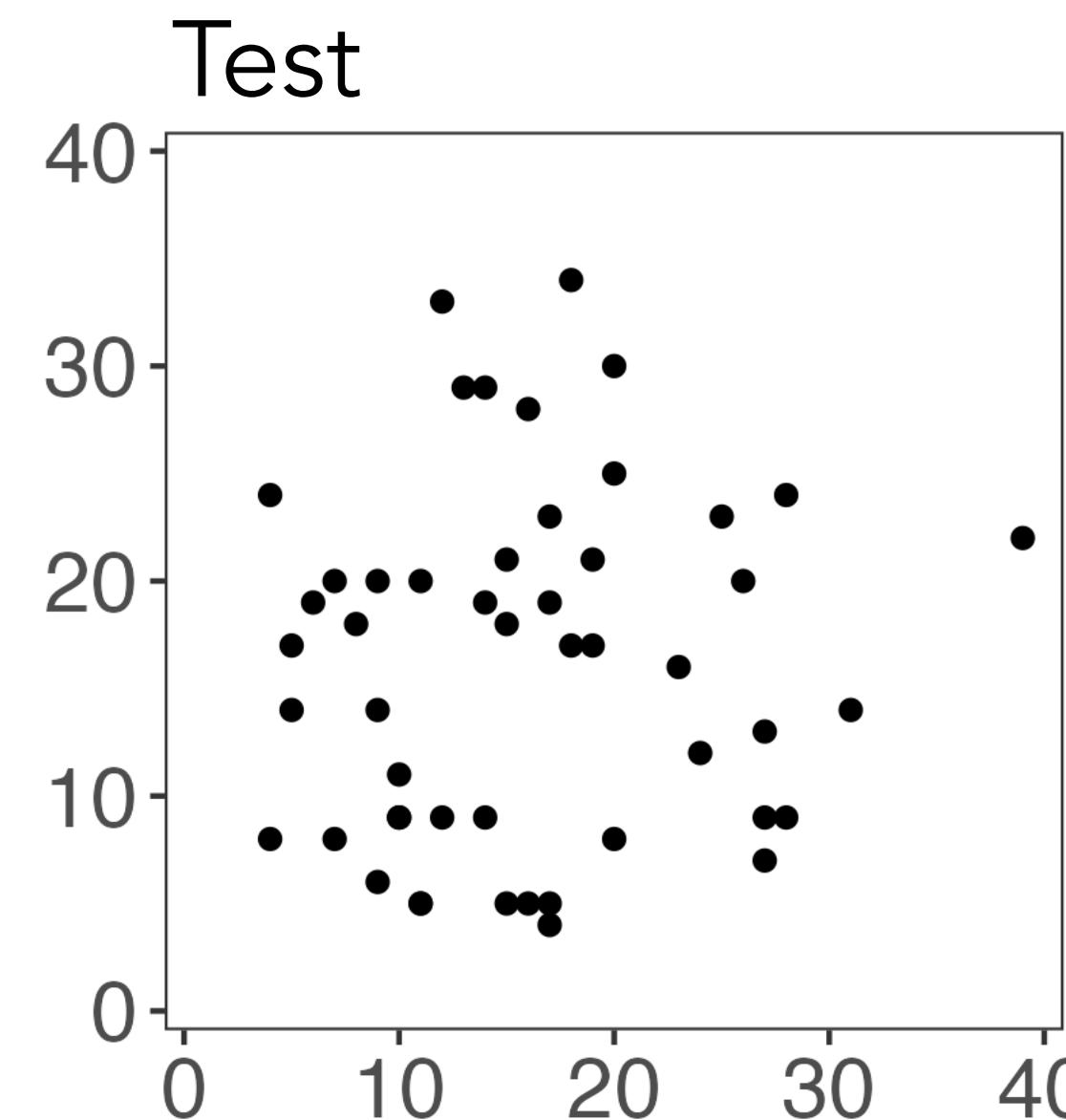
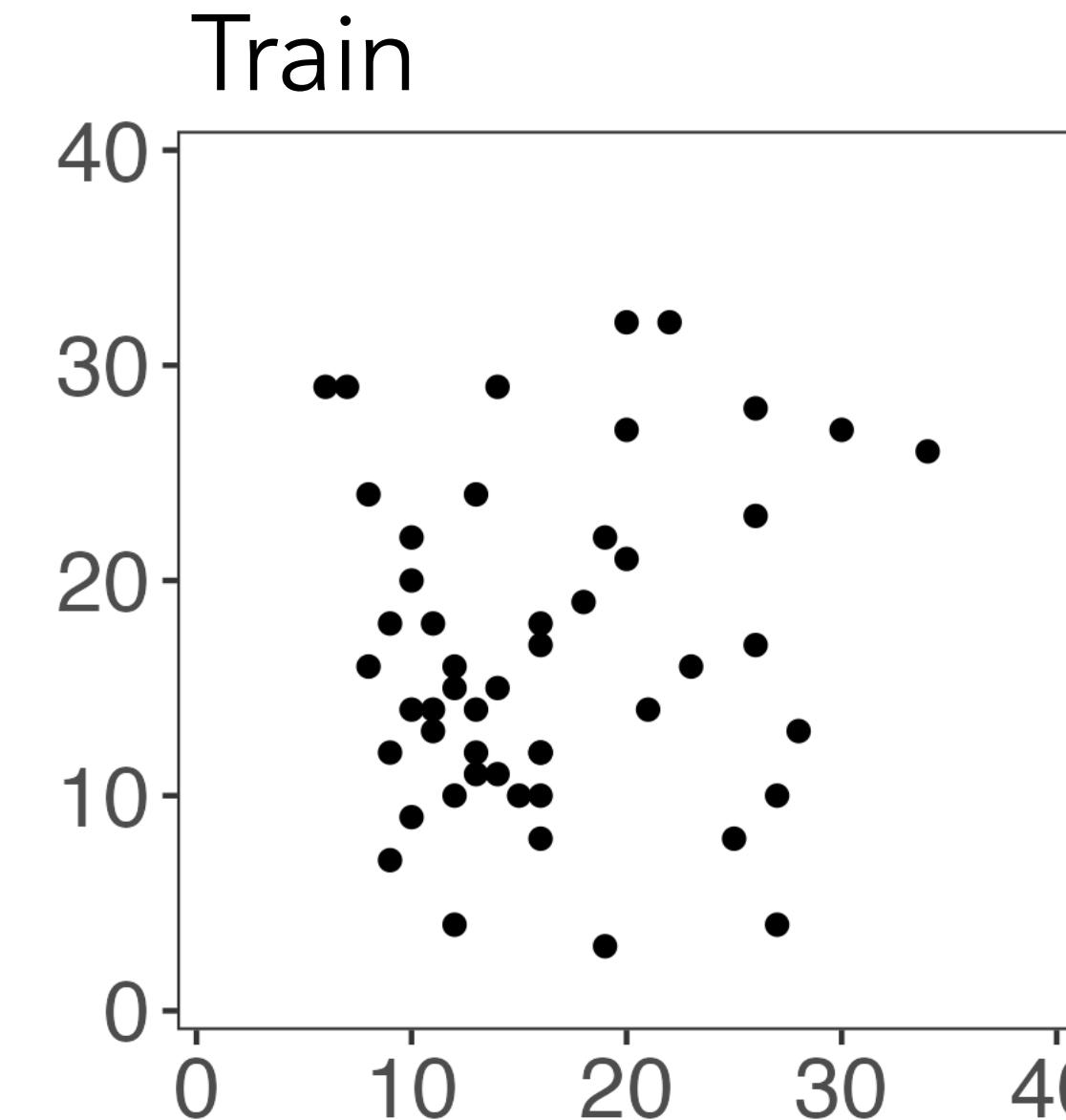
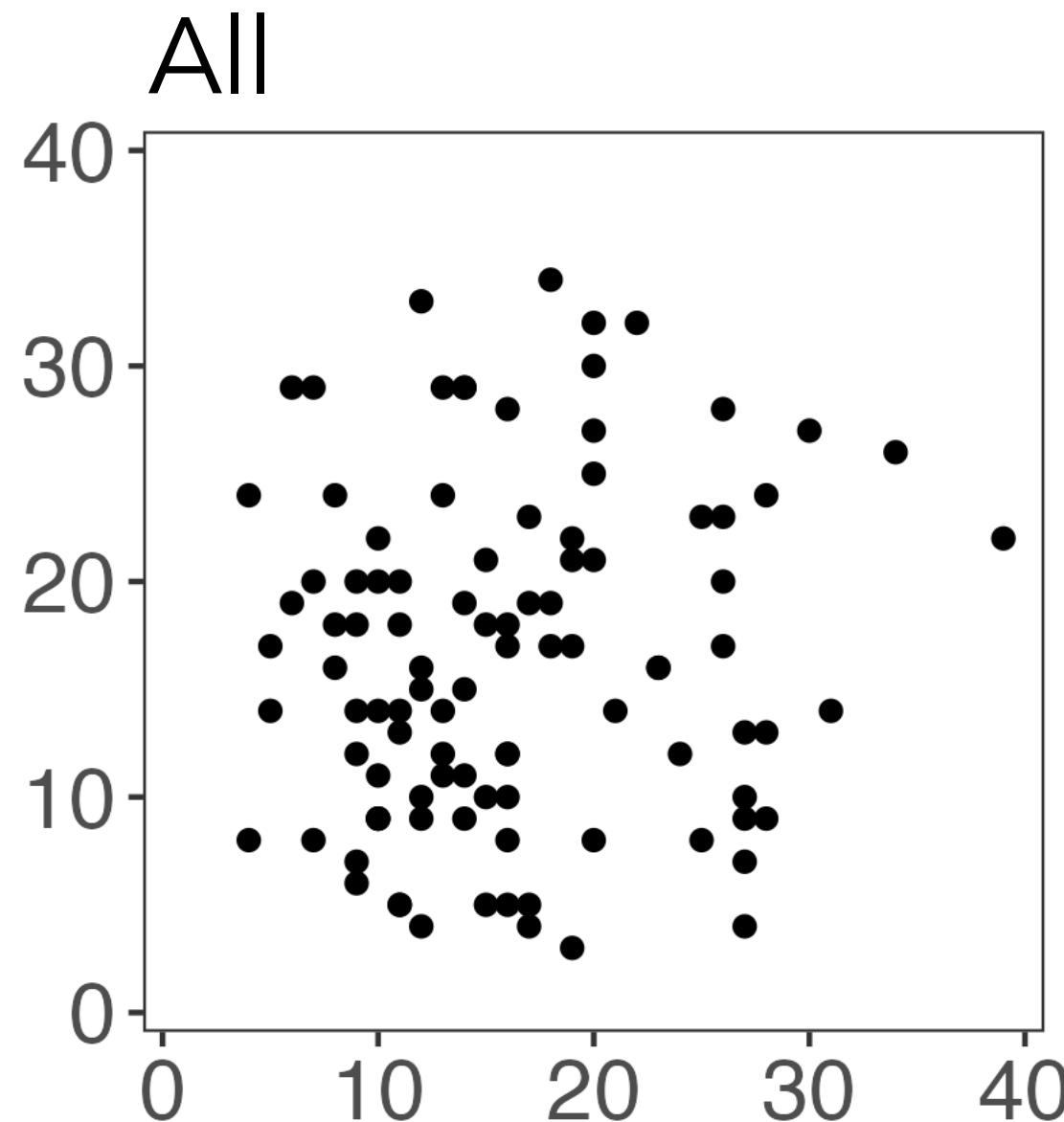
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Sample splitting cannot be used to validate the results of clustering

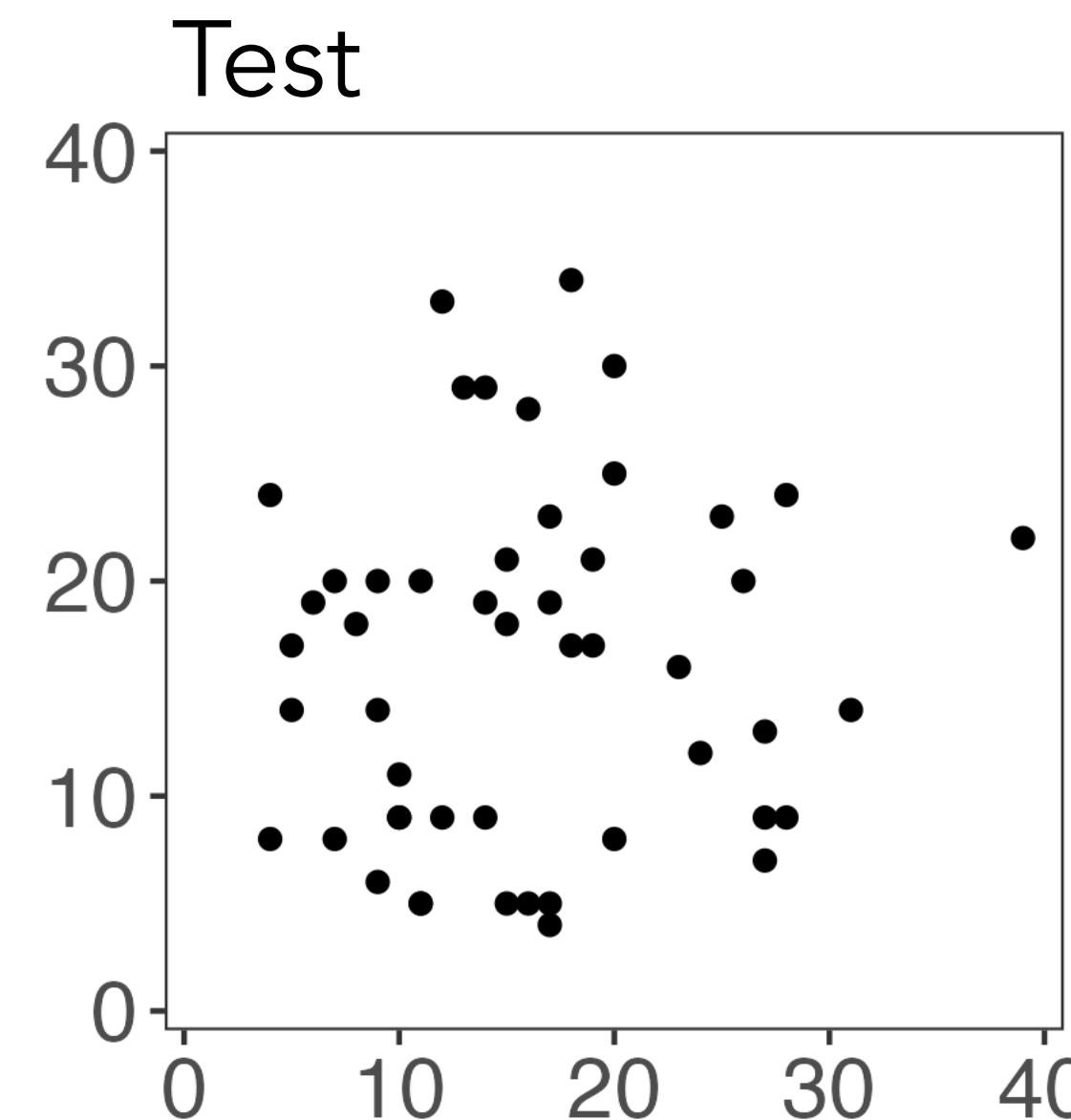
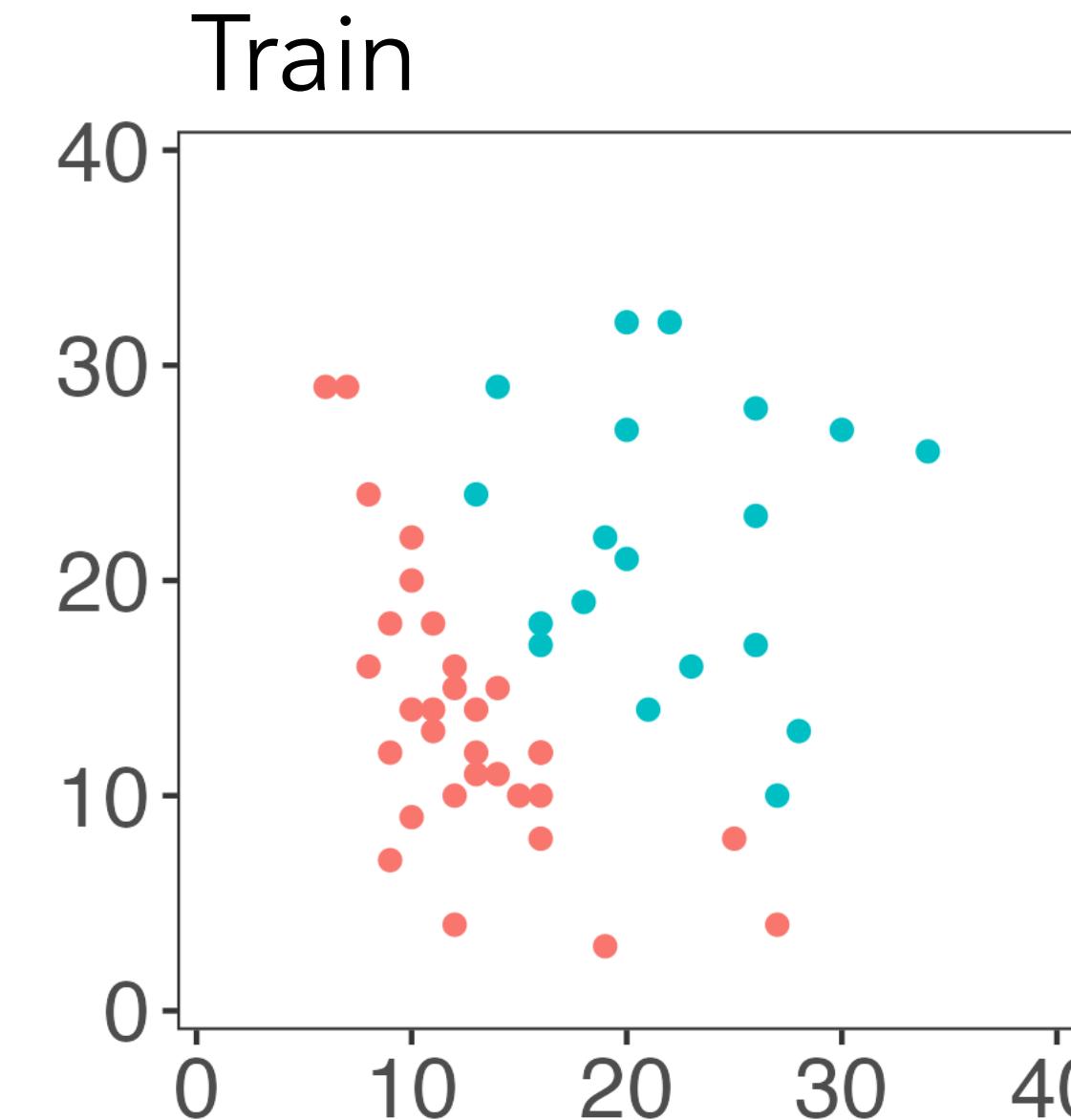
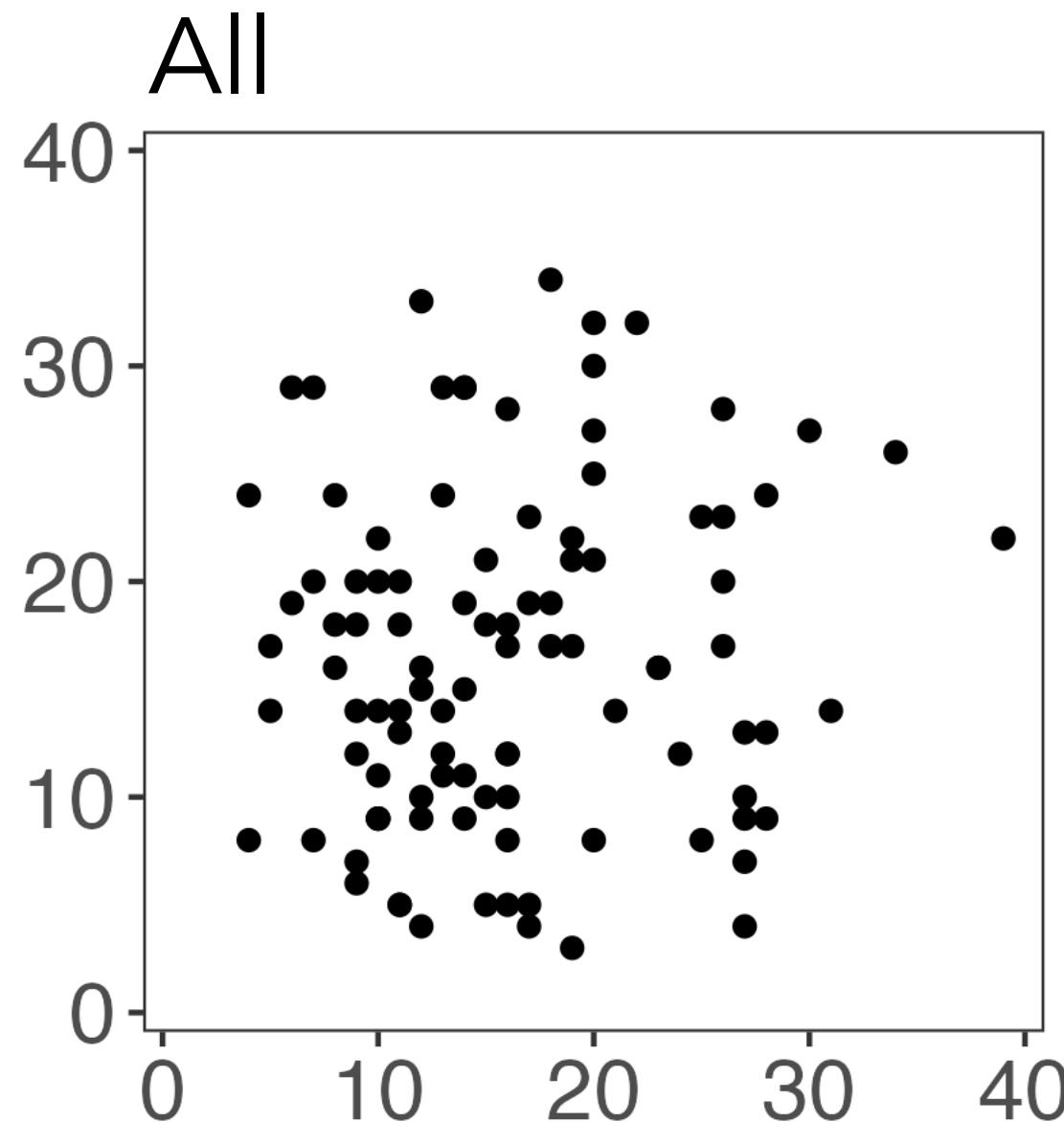


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Step 1: split
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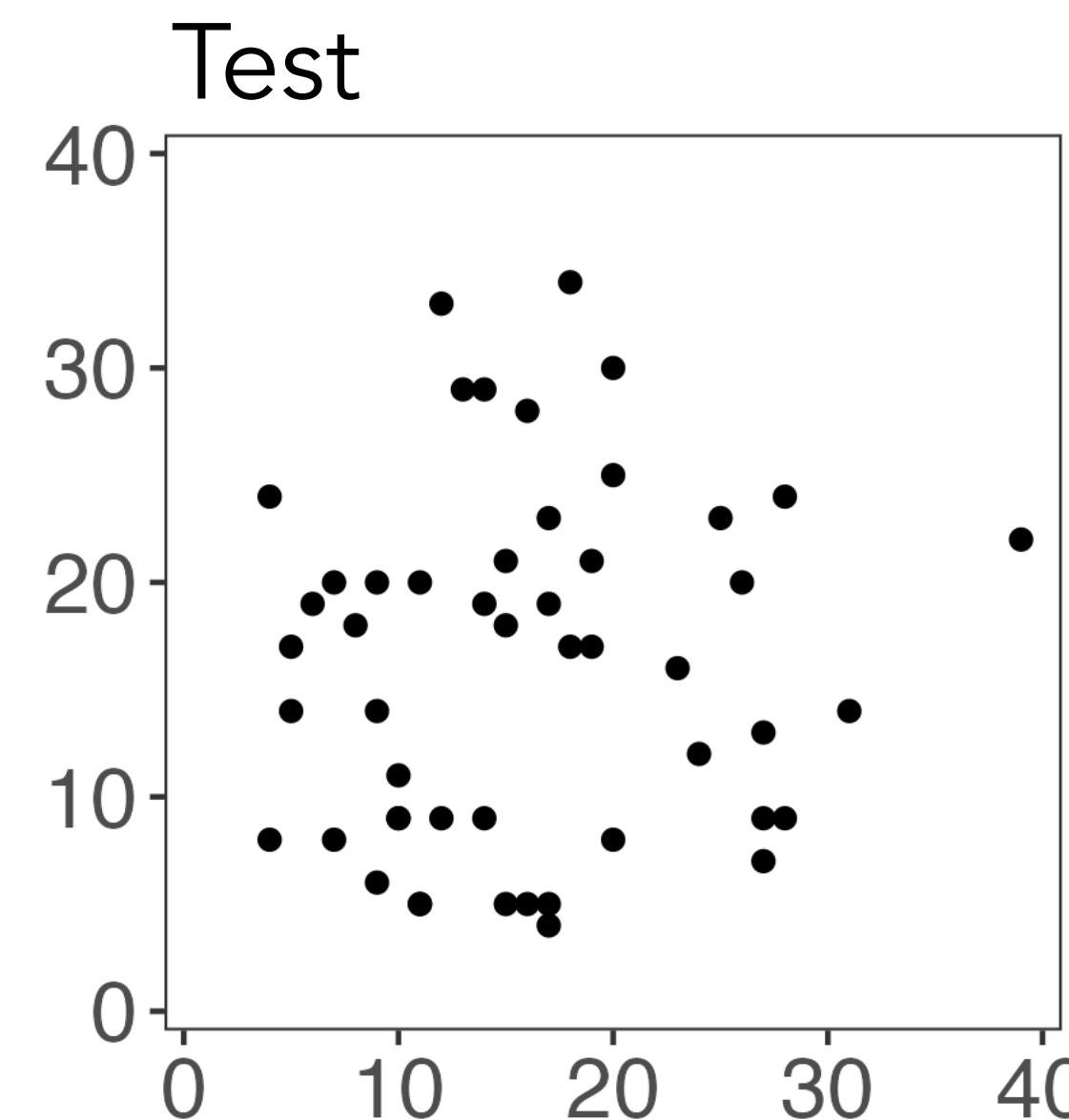
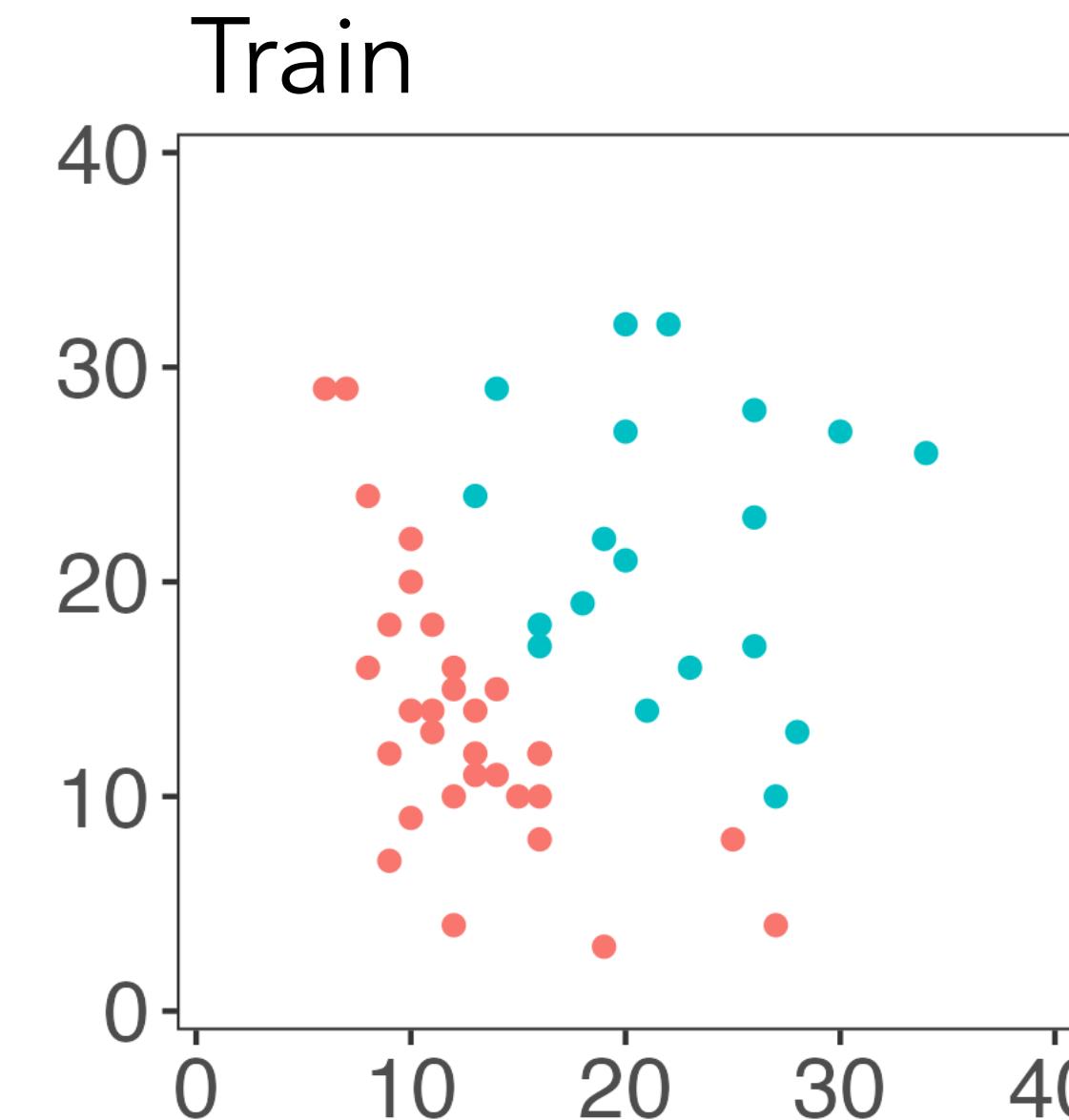
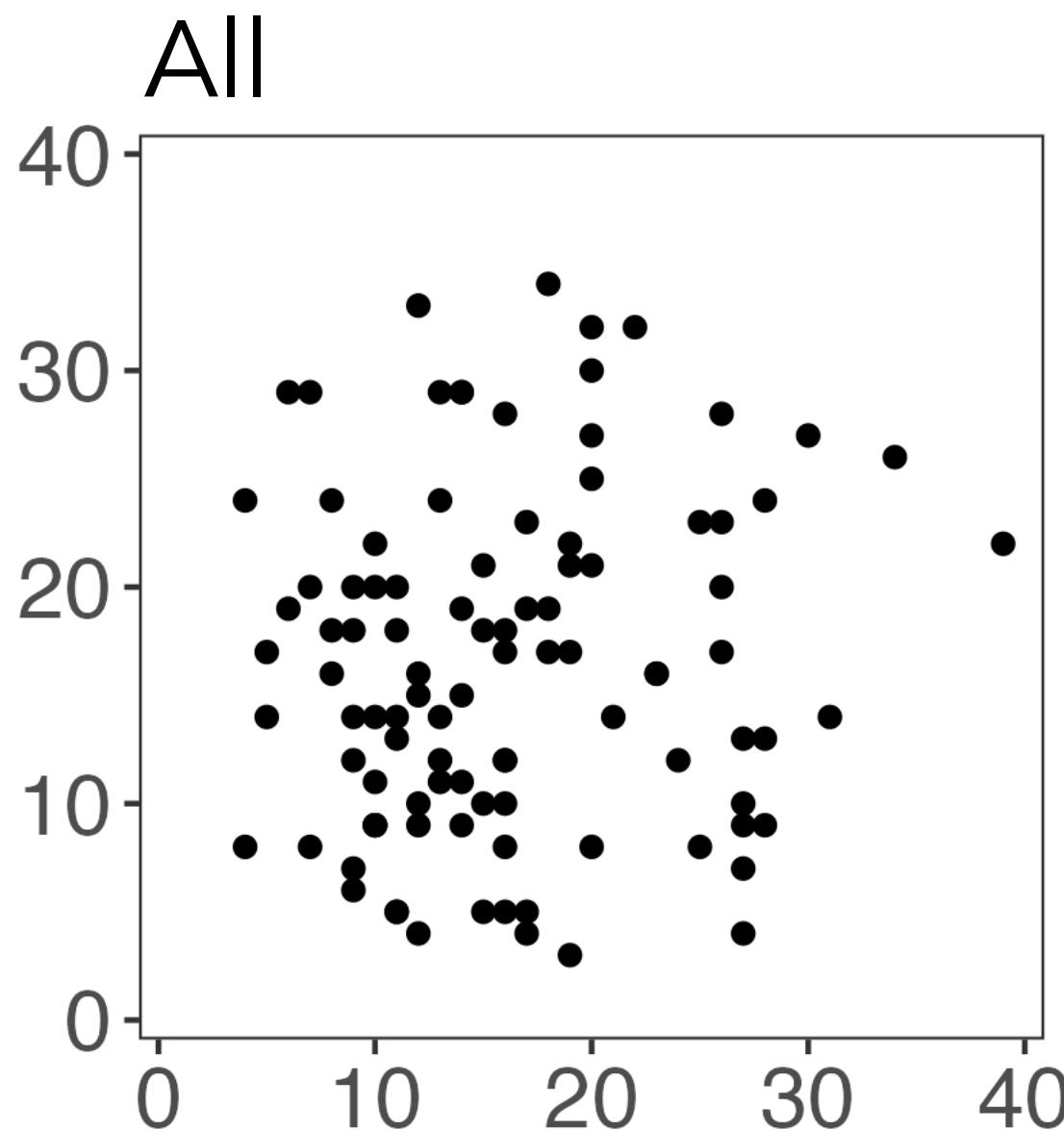
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Step 1: split observations into train/test.

Step 2: cluster the training set.

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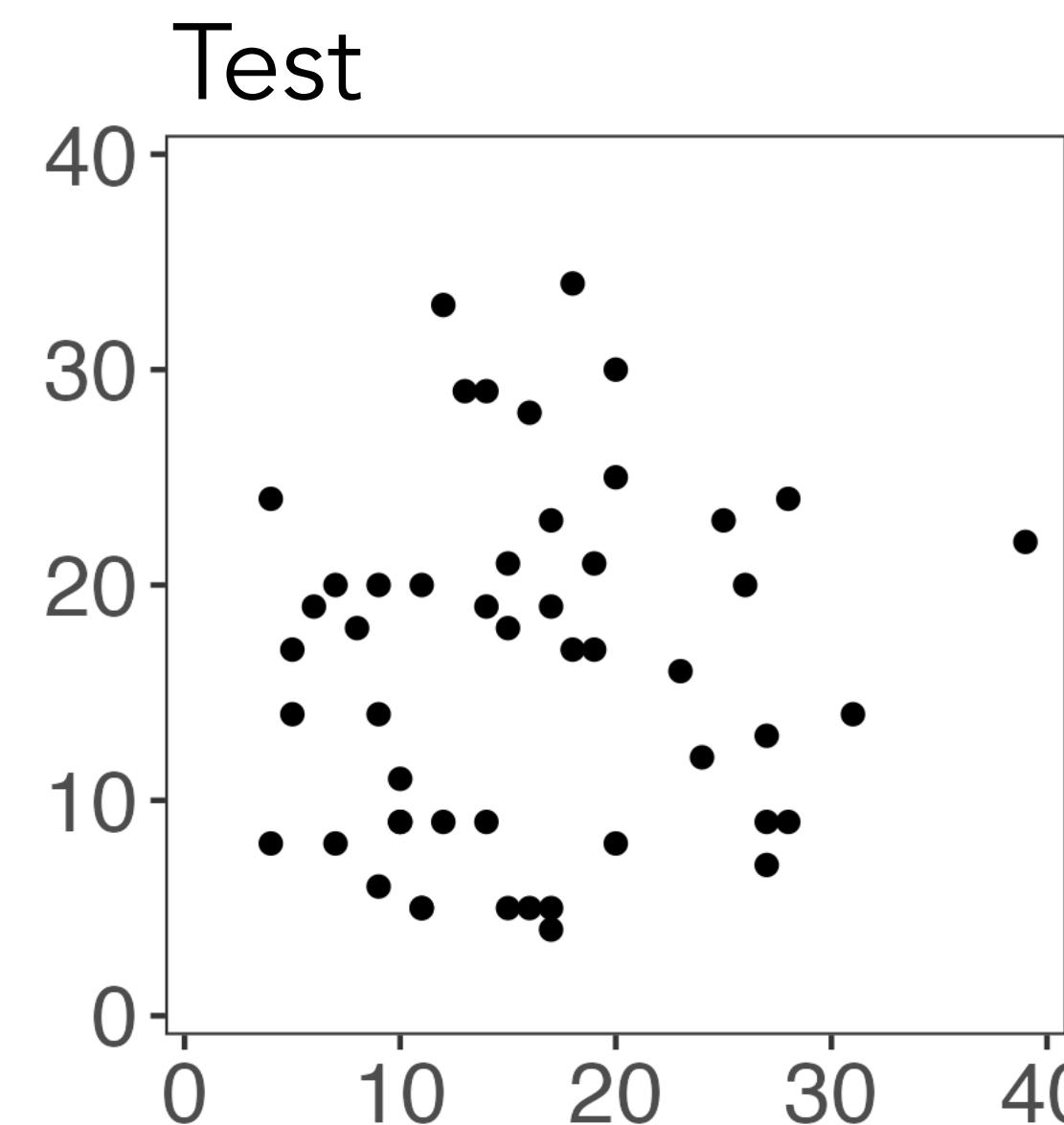
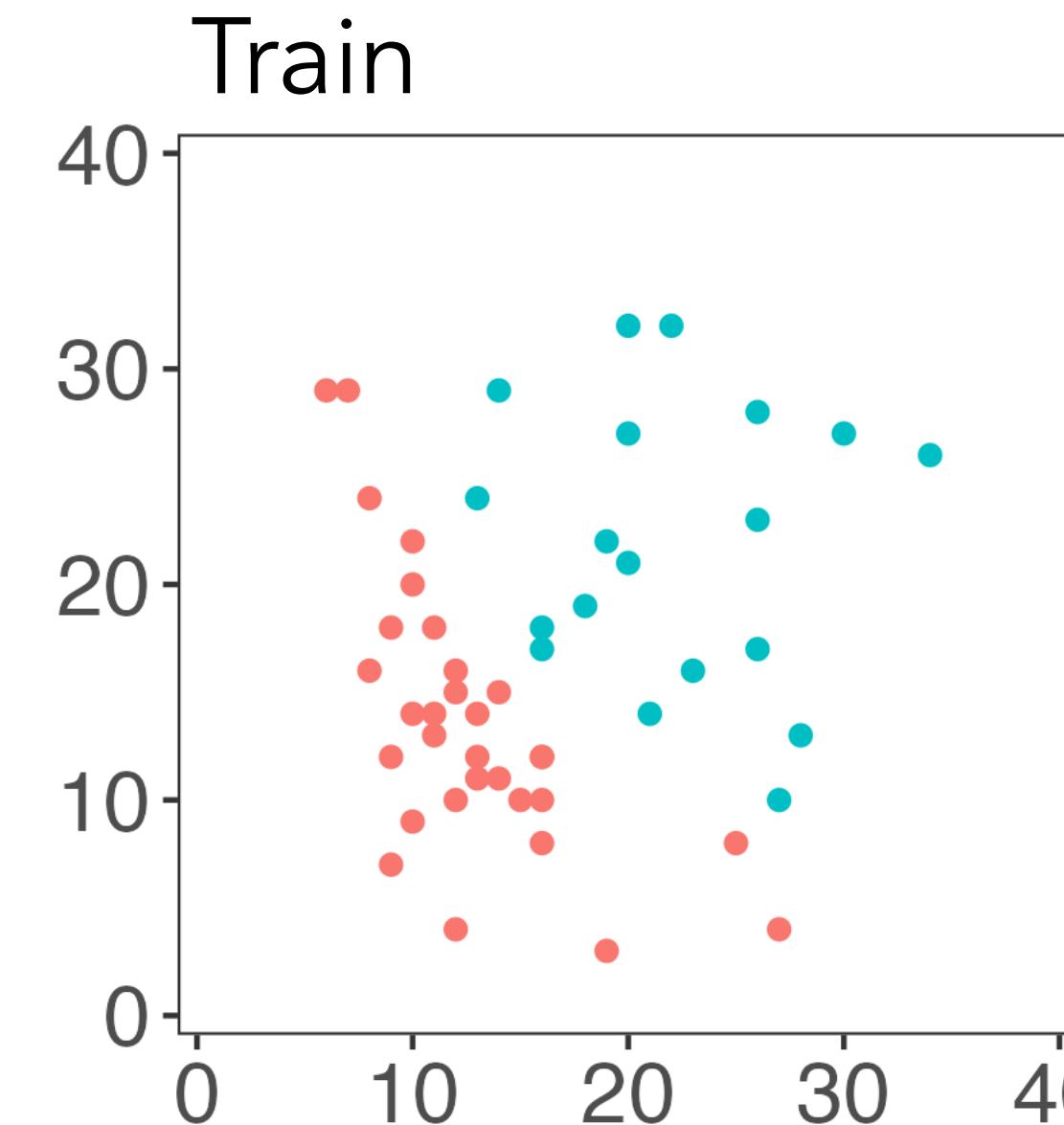
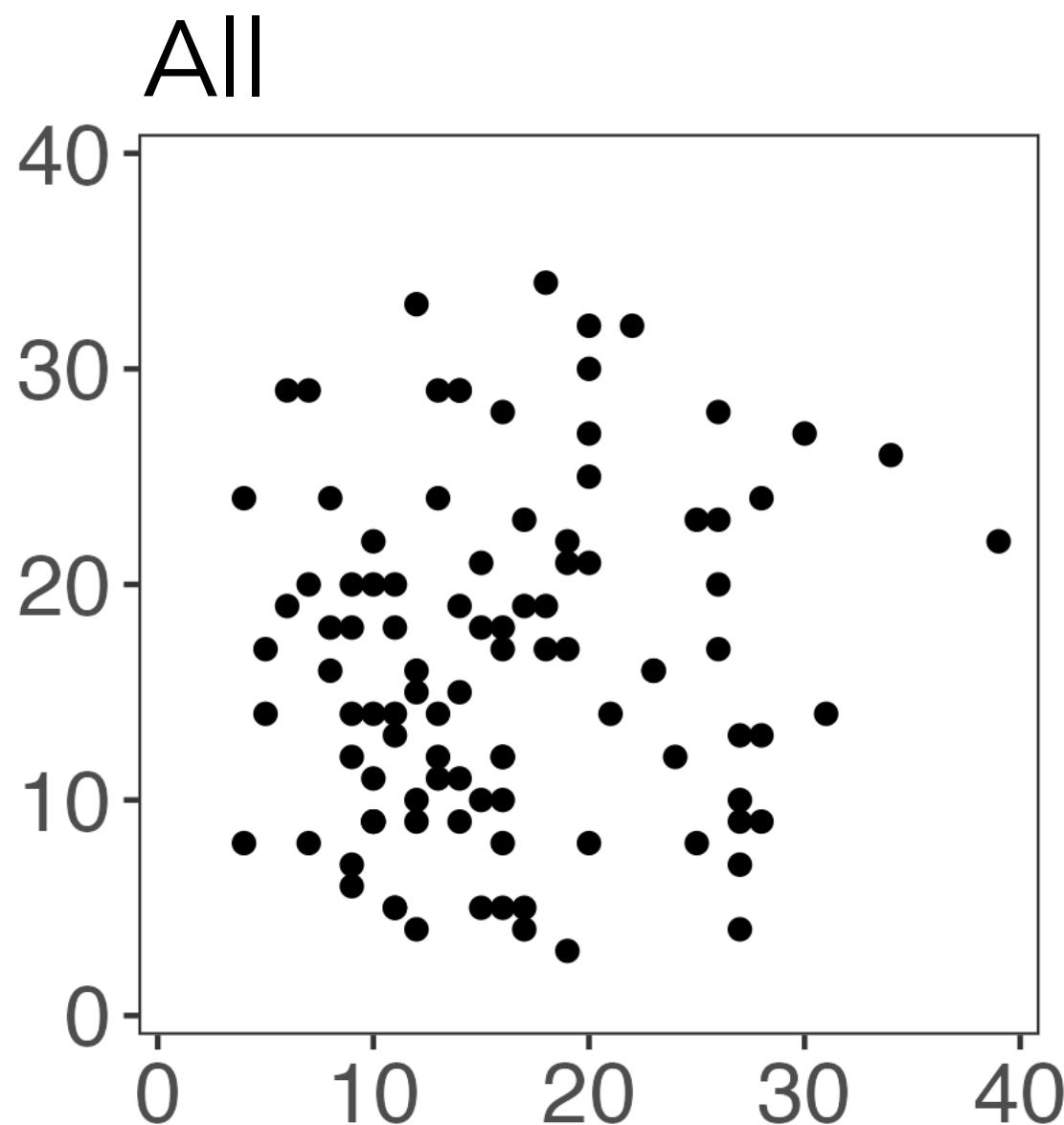


Step 1: split observations into train/test.

Step 2: cluster the training set.

Step 3: evaluate clusters using test set.

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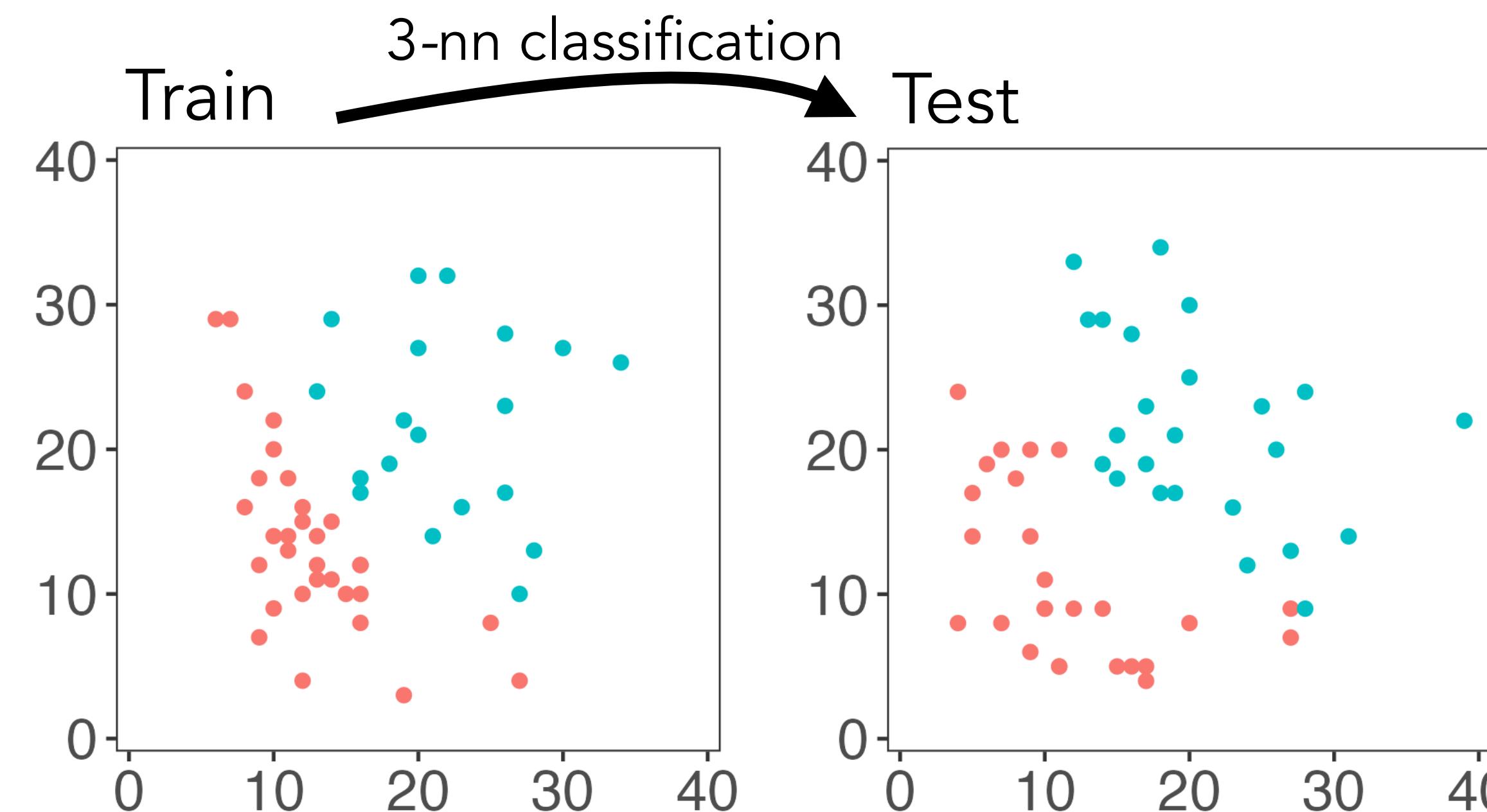
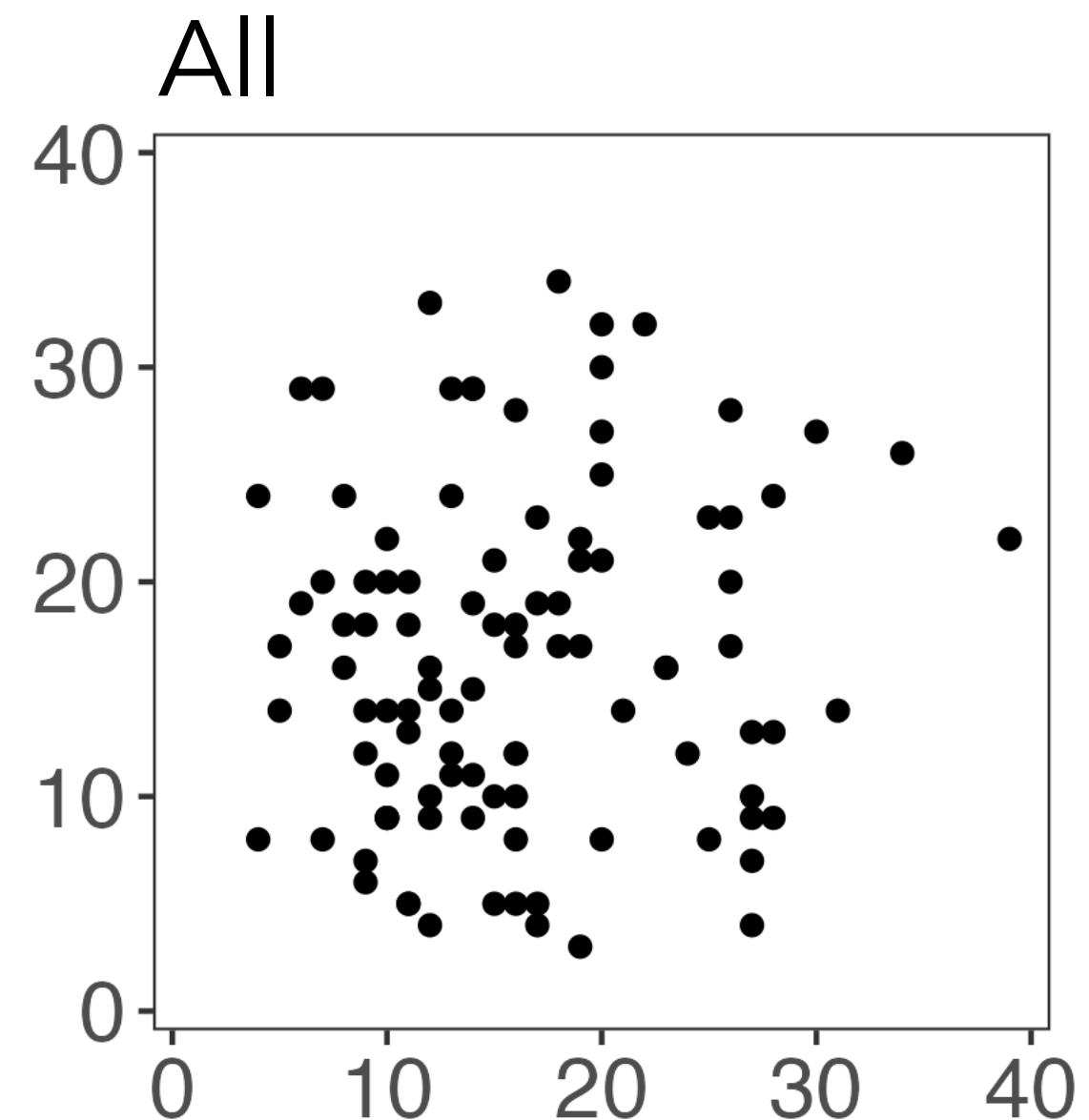
Step 1: split observations into train/test.

Step 2: cluster the training set.

Step 2.5: assign labels to observations in test set.

Step 3: evaluate clusters using test set.

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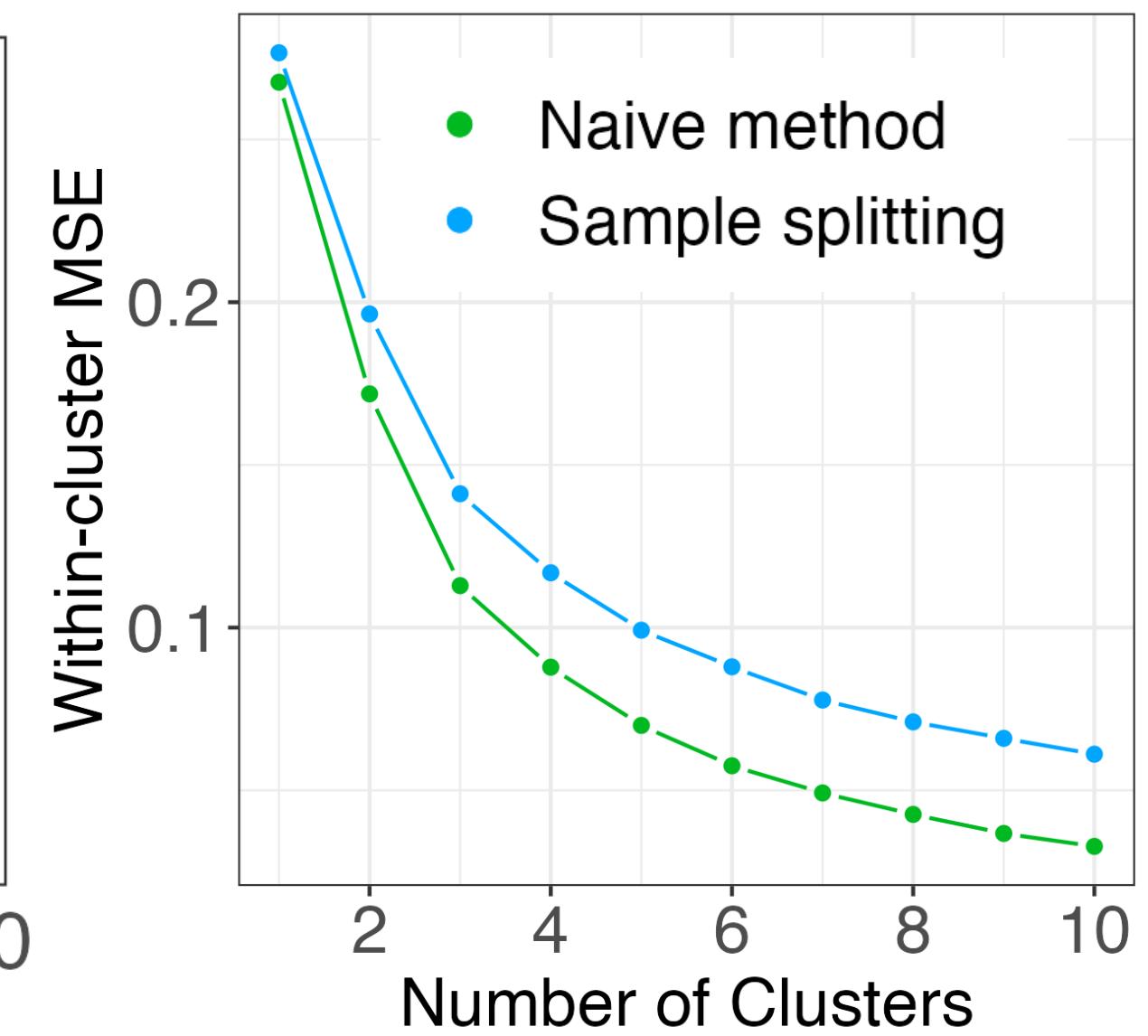
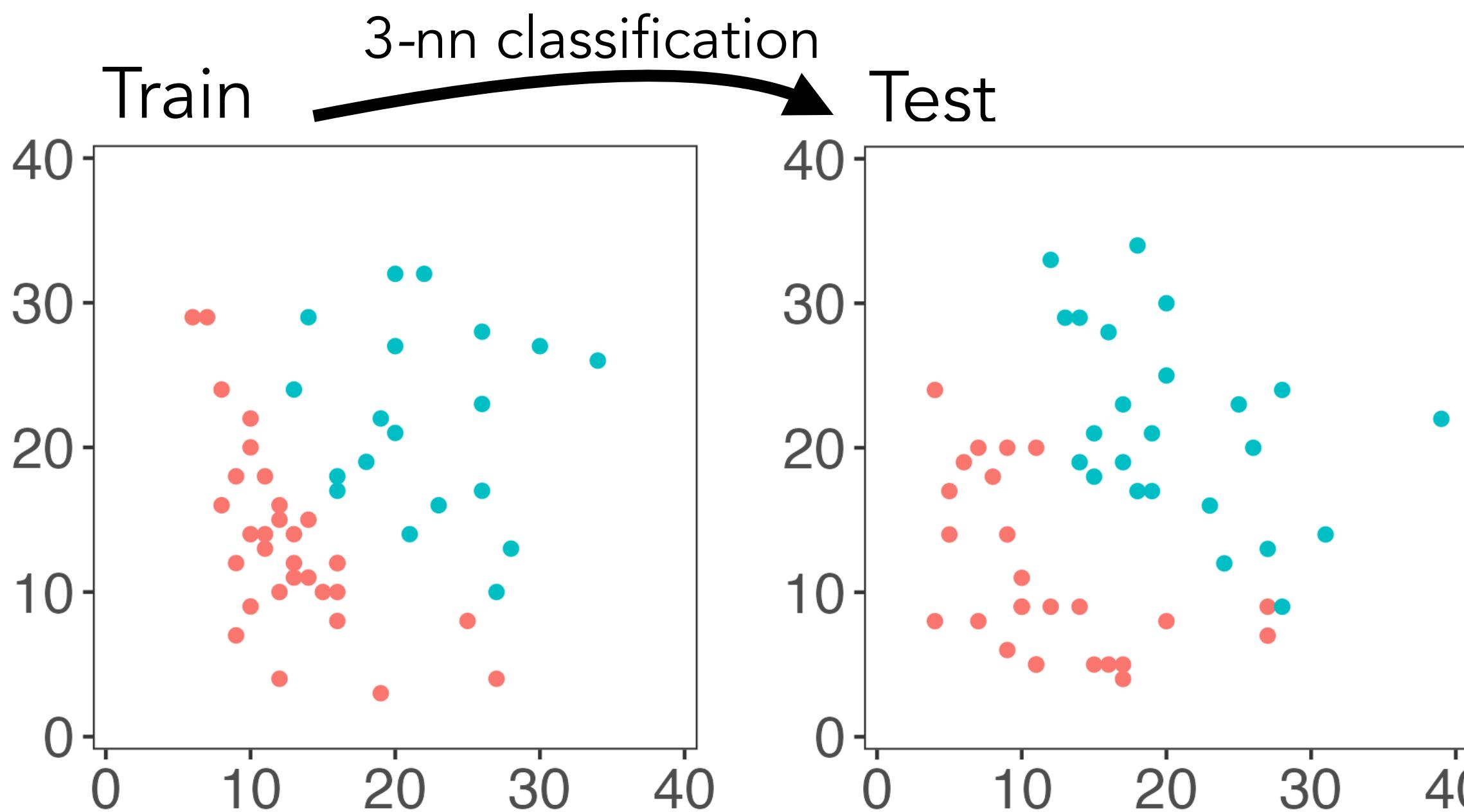
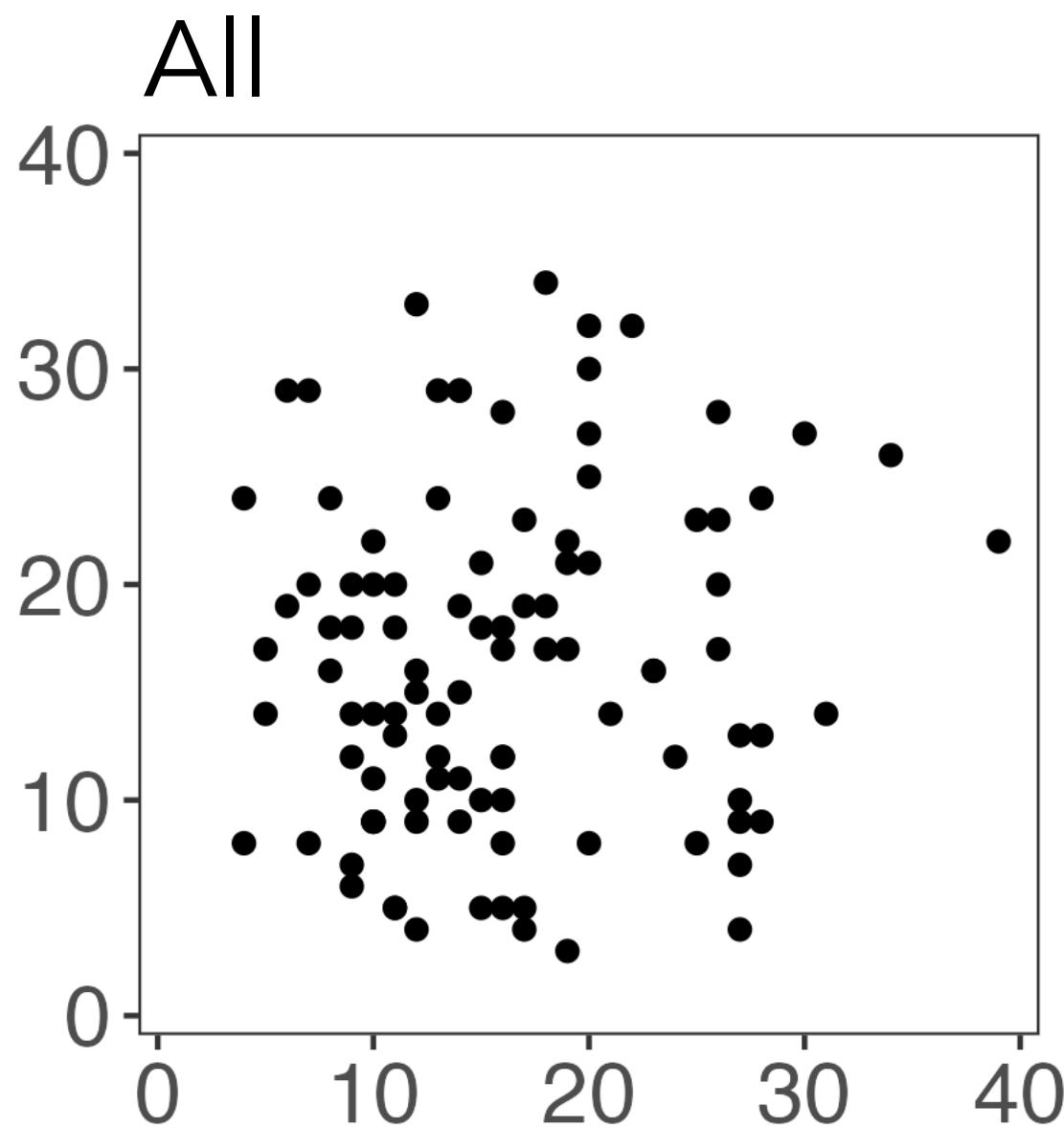
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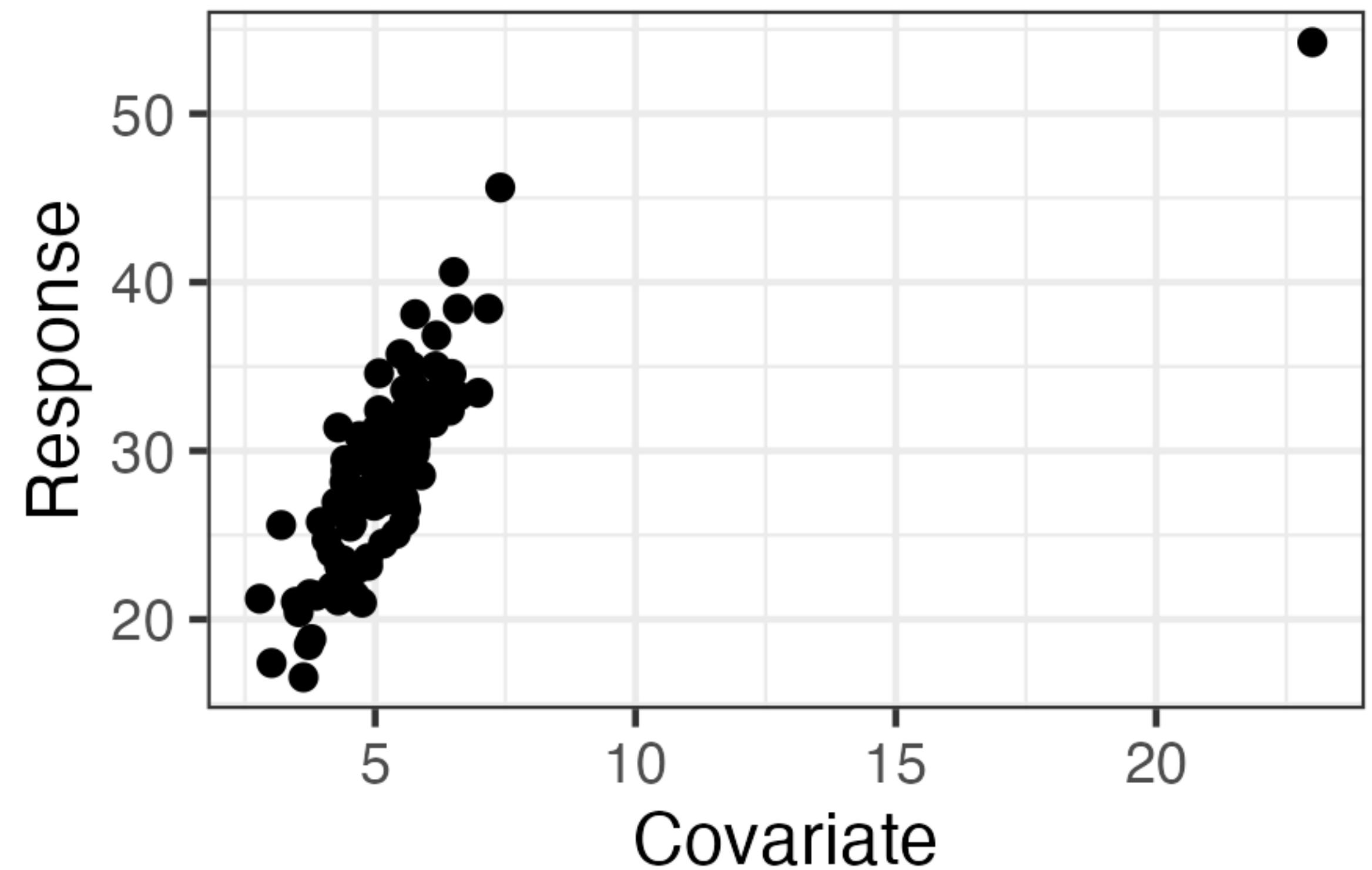
Step 2: cluster the training set.

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Other situations in which sample splitting is not a good option

1. Fixed-X regression settings.
2. Non-IID data.
3. Data with outliers or influential points.



Outline

1. Motivation: sample splitting doesn't always work
2. **Poisson thinning**
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Poisson thinning

X

	Feature 1	Feature 2
Obs. 1	18	6
Obs. 2	31	8
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Poisson thinning

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	Feature 1	Feature 2
Obs. 1	18	6
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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. 4	16	9

Poisson thinning

X

	Feature 1	Feature 2
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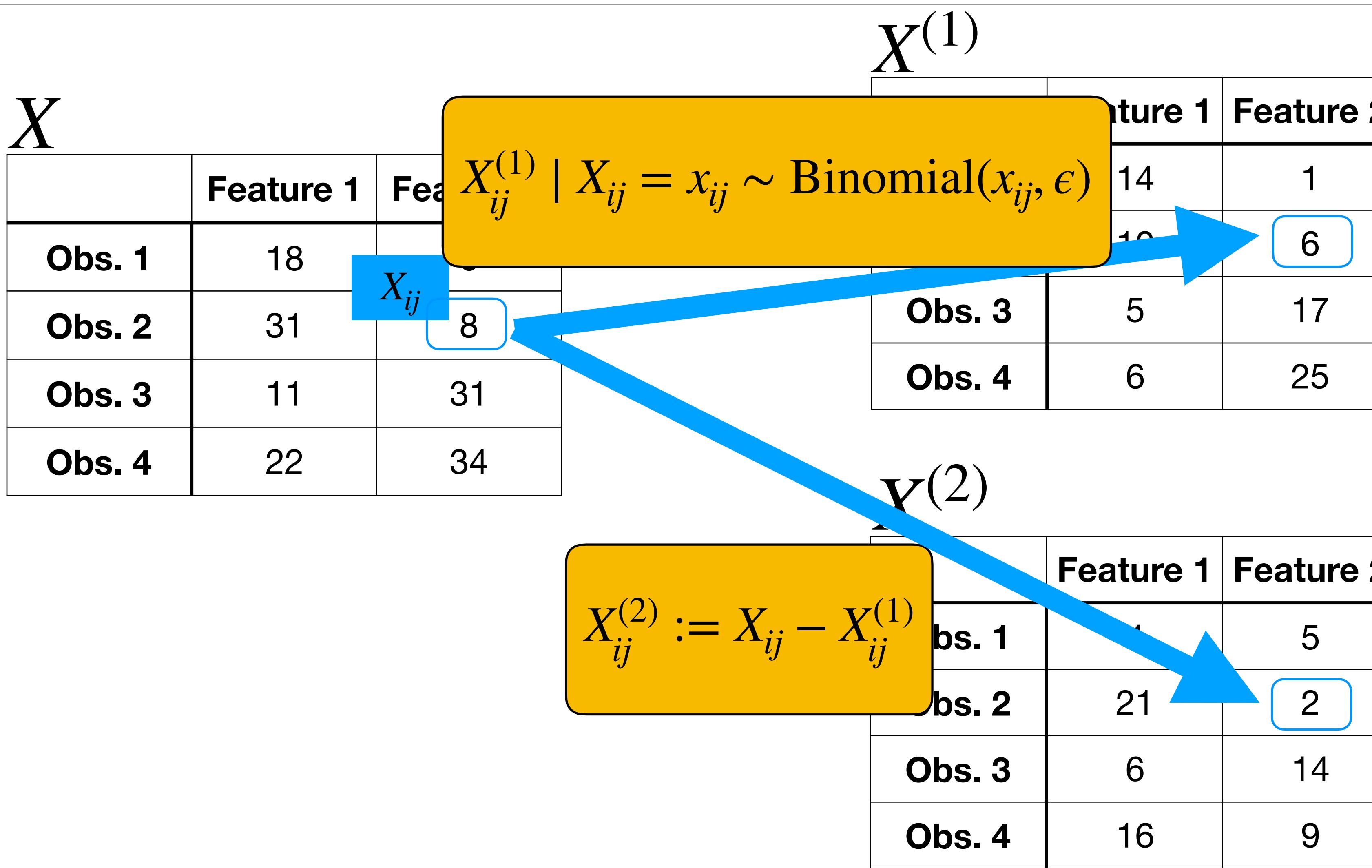
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$X^{(2)}$

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Poisson thinning



Poisson thinning

X			$X^{(1)}$	$X^{(2)}$
	Feature 1	Feature 2		
Obs. 1	18	X_{ij}	$X_{ij}^{(1)} \mid X_{ij} = x_{ij} \sim \text{Binomial}(x_{ij}, \epsilon)$	14
Obs. 2	31	8		10
Obs. 3	11	31		5
Obs. 4	22	34		25

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

1. $X_{ij}^{(1)} \sim \text{Poisson}(\epsilon \Lambda_{ij})$
2. $X_{ij}^{(2)} \sim \text{Poisson}((1 - \epsilon) \Lambda_{ij})$
3. $X_{ij}^{(1)} \perp\!\!\!\perp X_{ij}^{(2)}$

	$X^{(1)}$	$X^{(2)}$
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Obs. 1	14	5
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A very well-known result.

Poisson thinning

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	$X^{(2)}$	Feature 1	Feature 2
Obs. 1	4	1	5
Obs. 2	21	2	2
Obs. 3	6	14	14
Obs. 4	16	9	9

A very well-known result.

Poisson thinning

	$X^{(1)}$	$X^{(2)}$
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	8	17
	31	25

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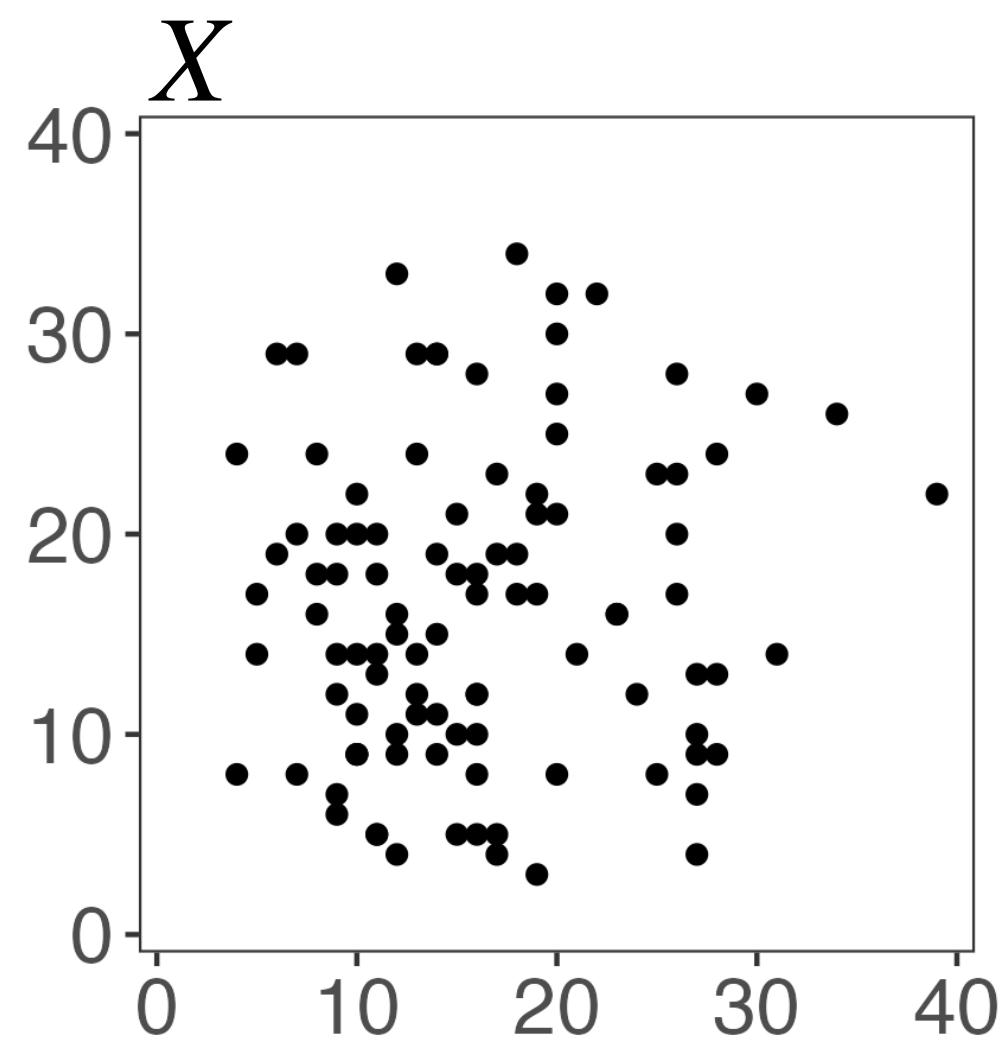
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$X_{ij}^{(2)} := X_{ij} - X_{ij}^{(1)}$

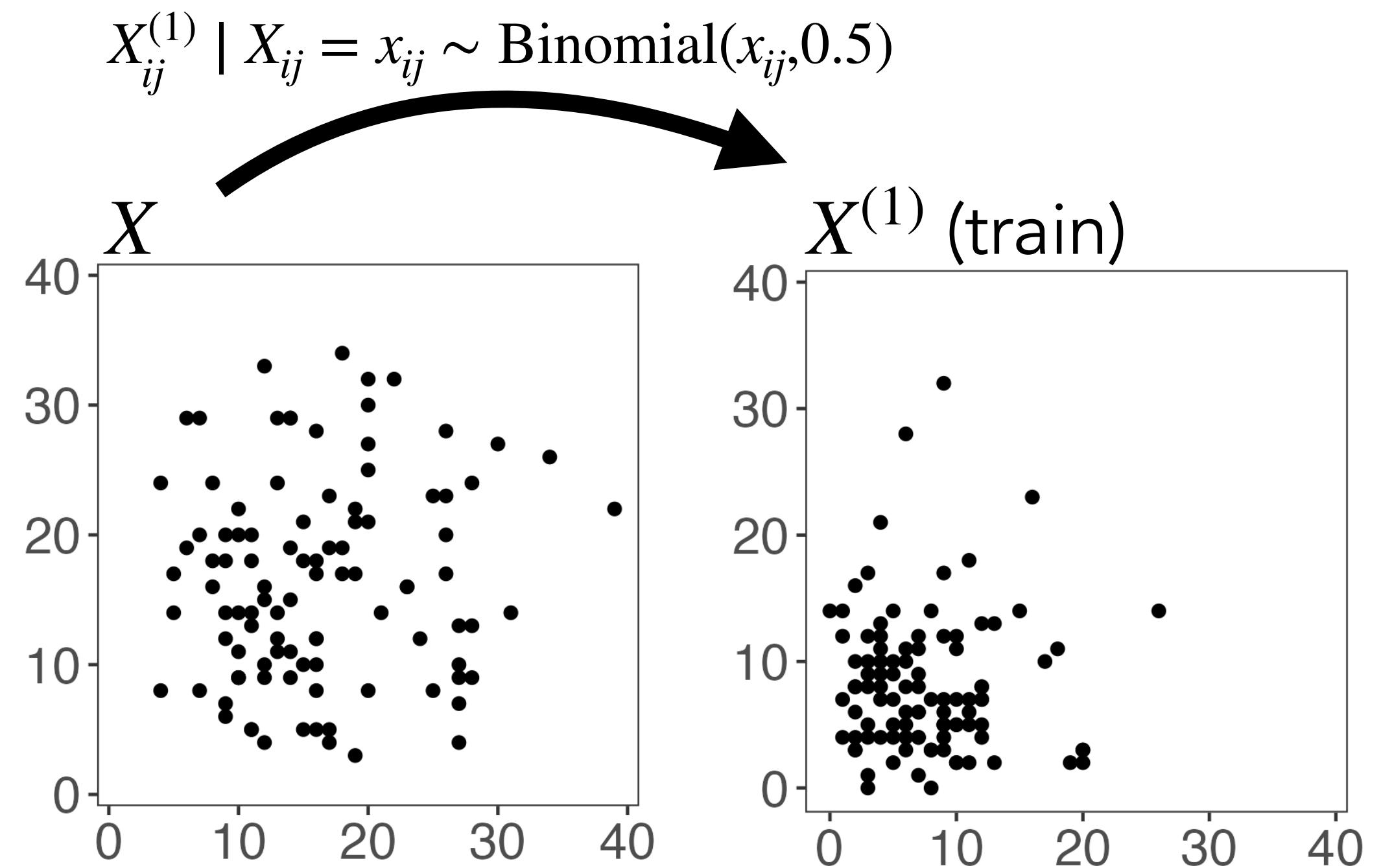
Validate model.

A very well-known result.

Thinning avoids the pitfall of sample splitting on our motivating example

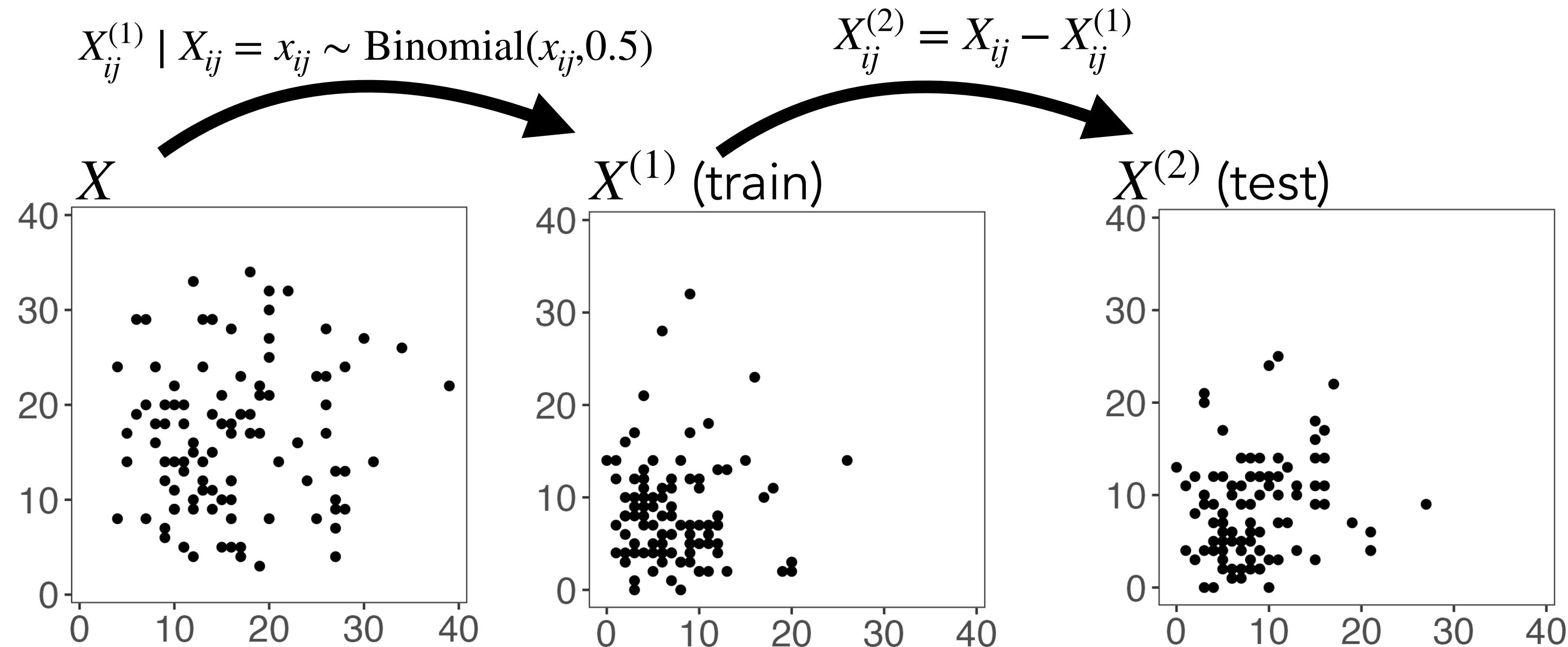


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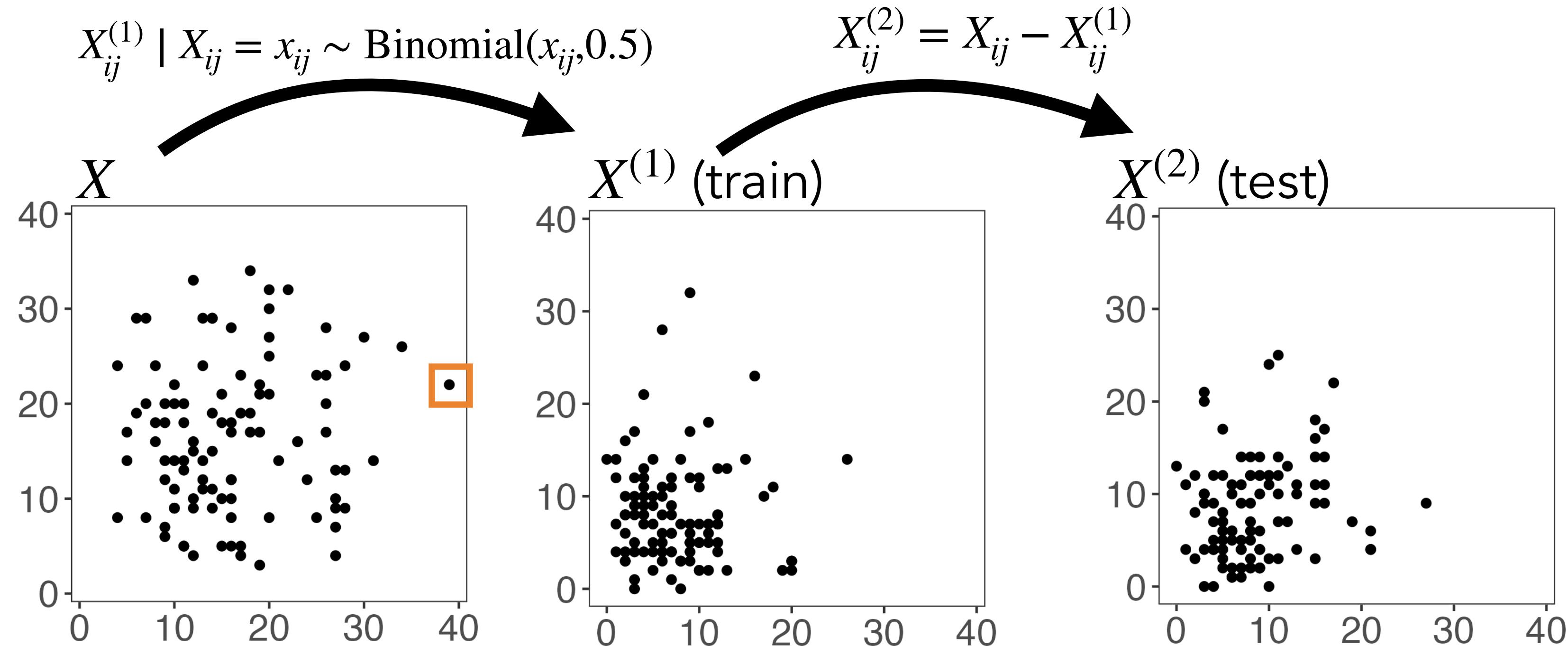
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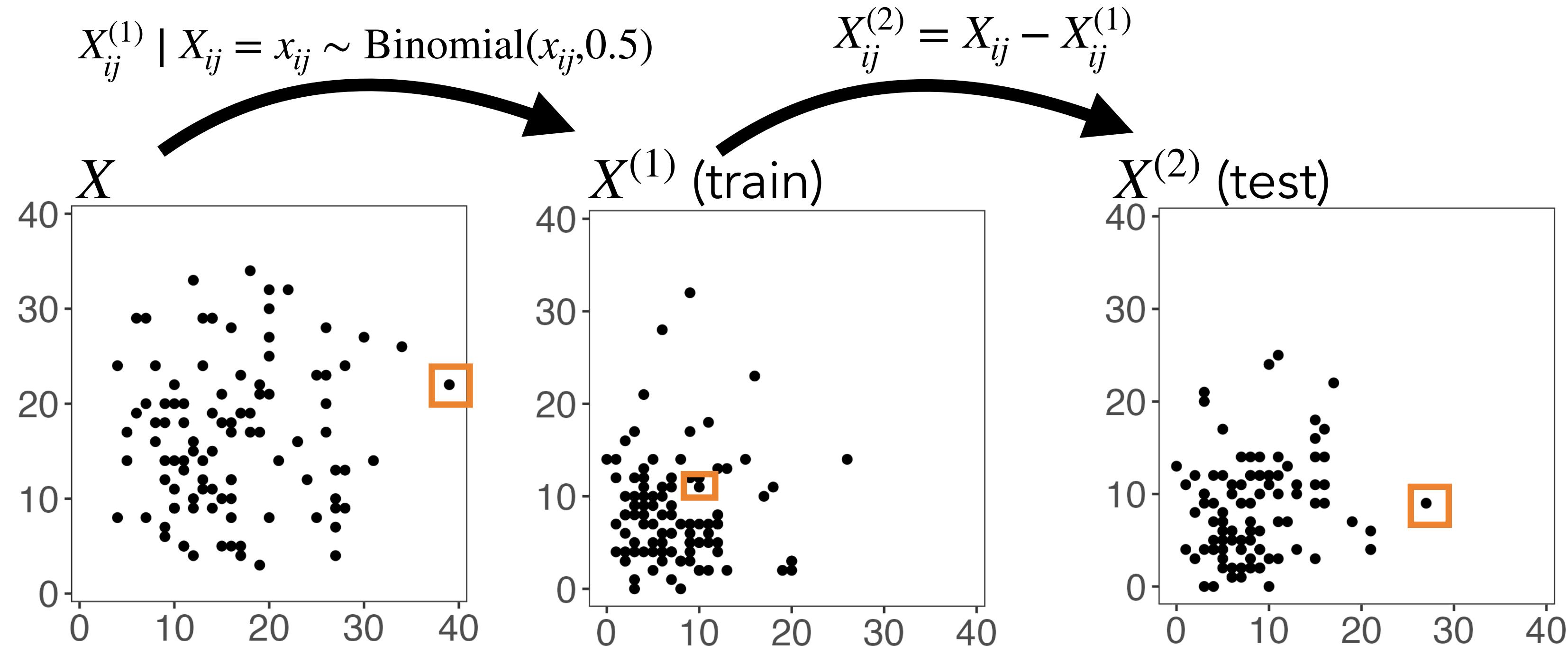
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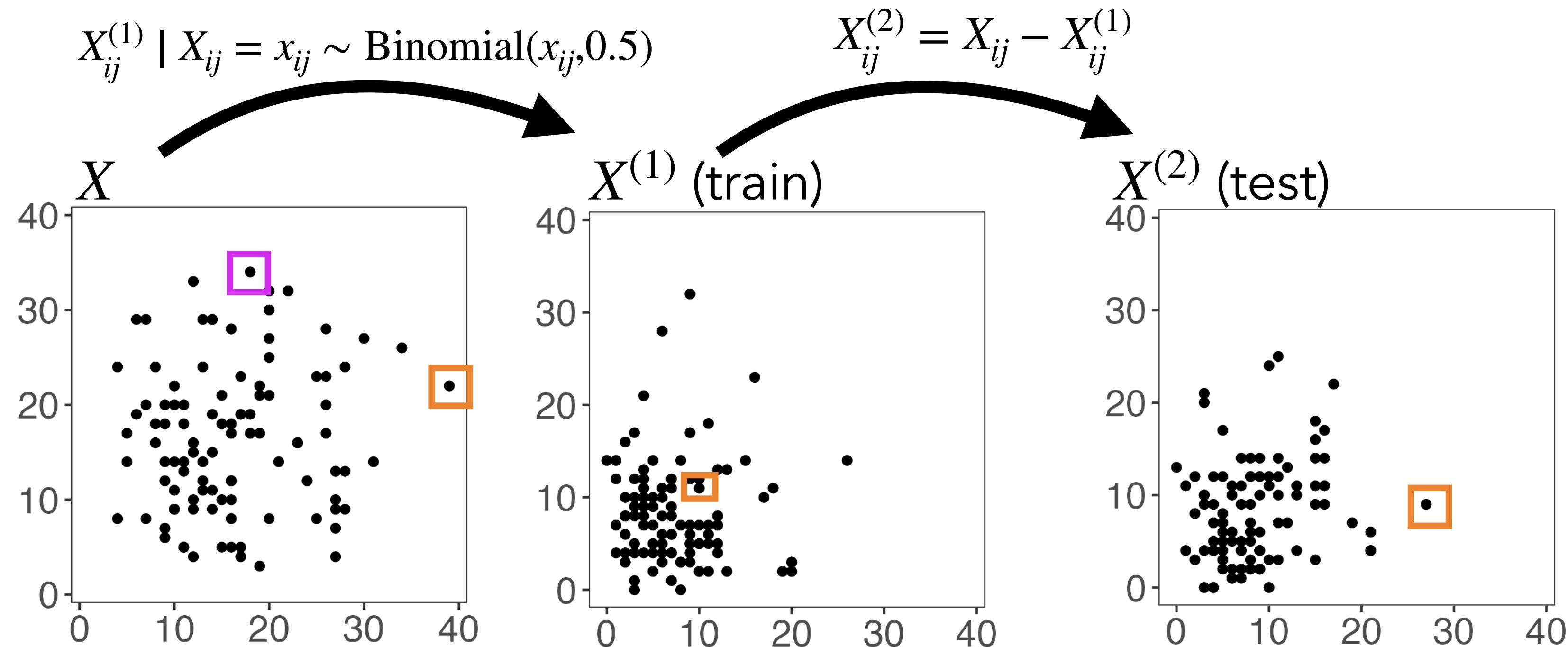
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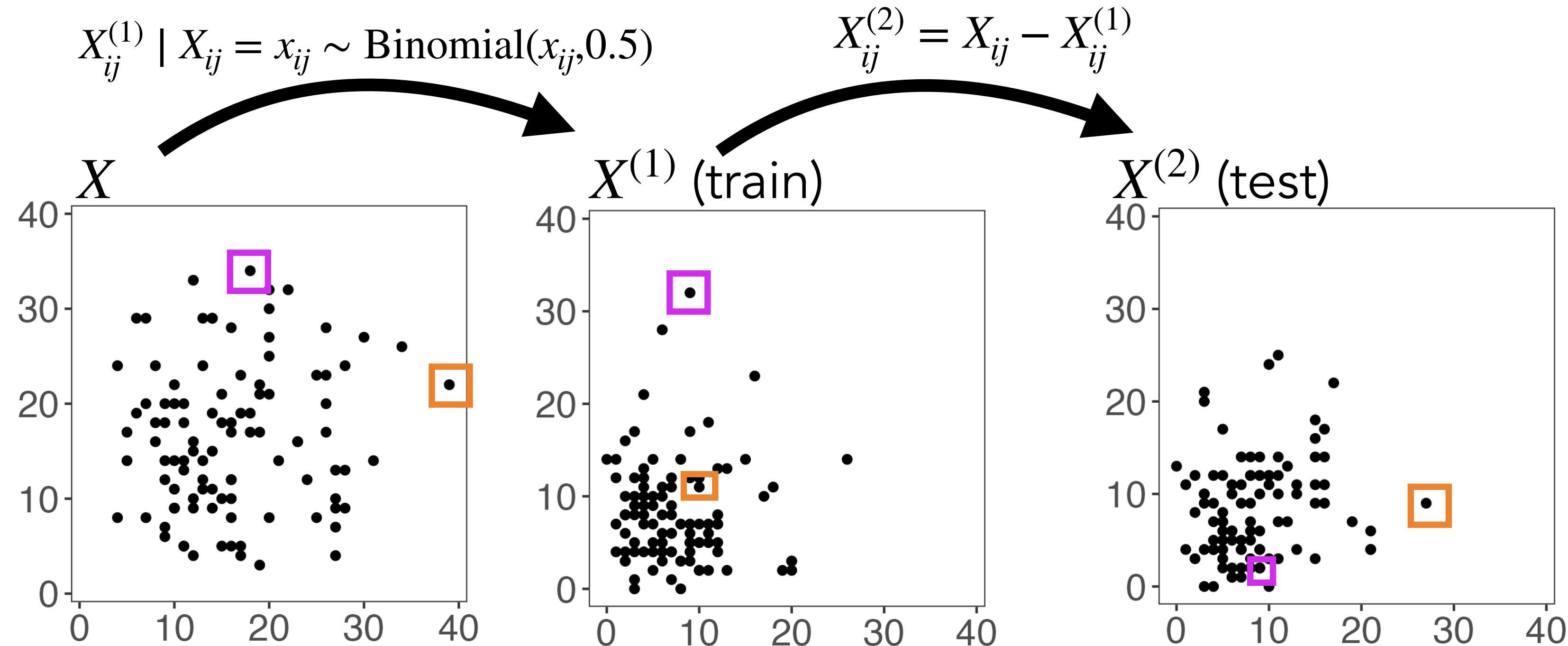
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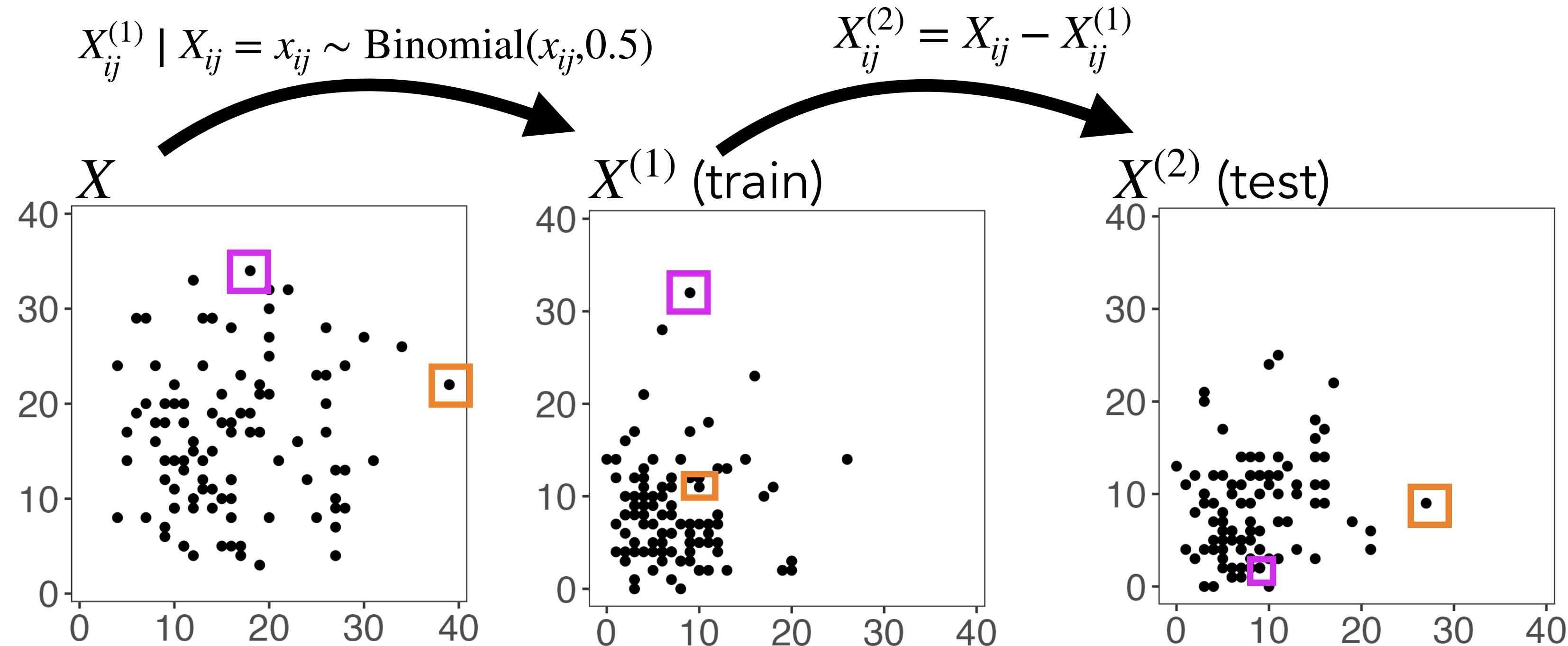
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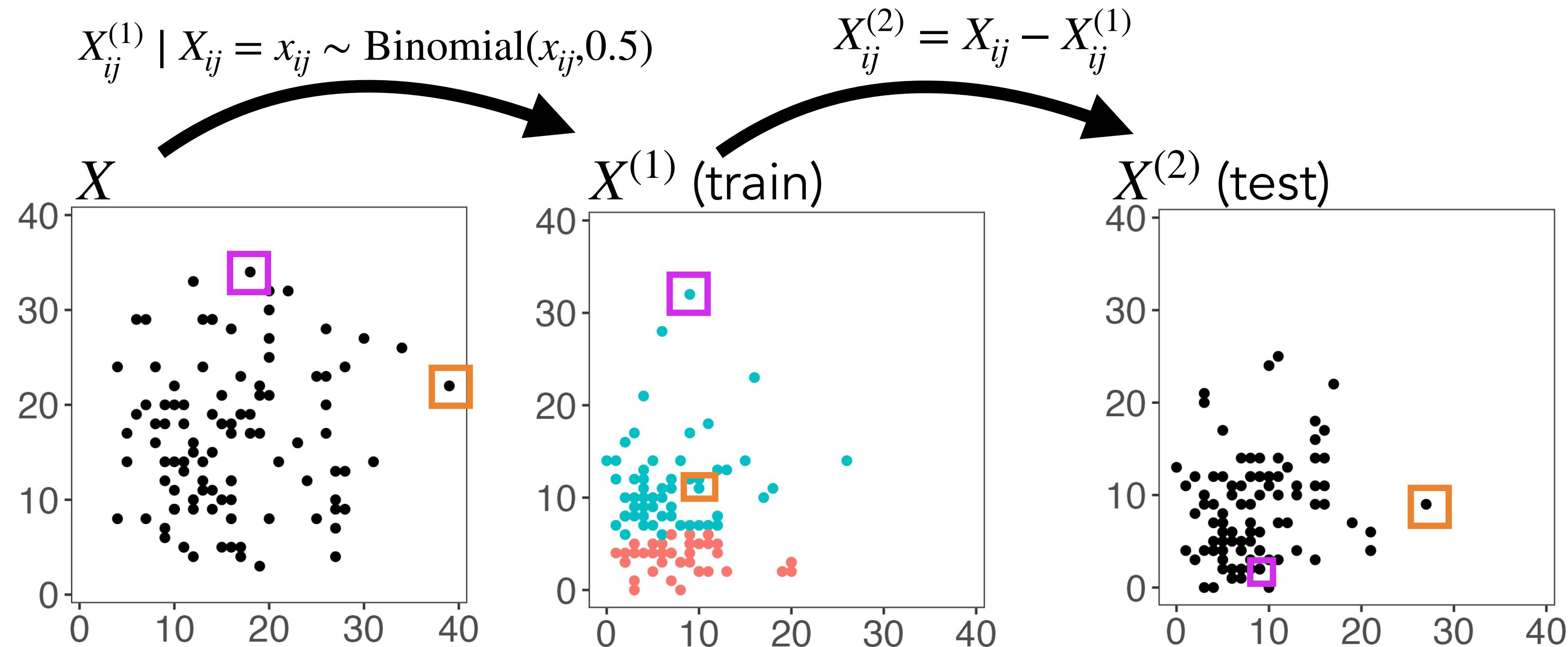
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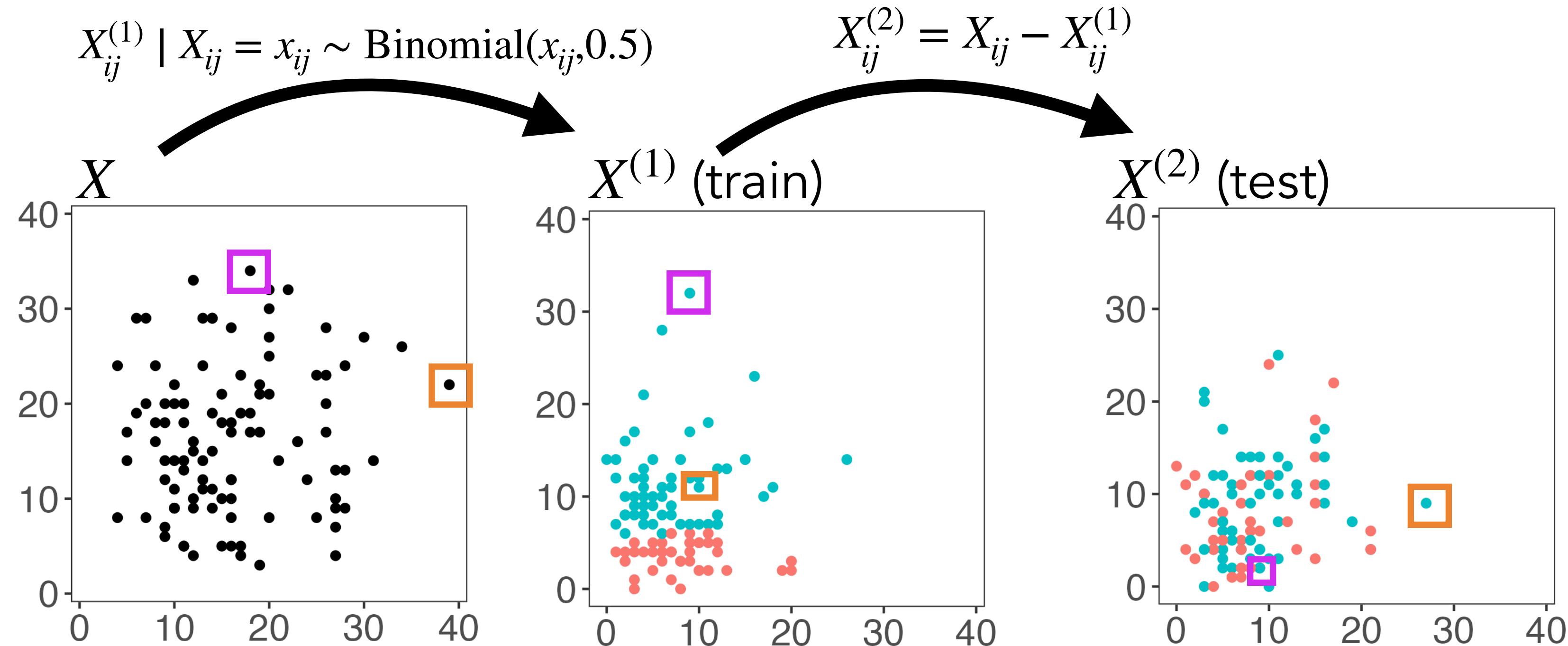
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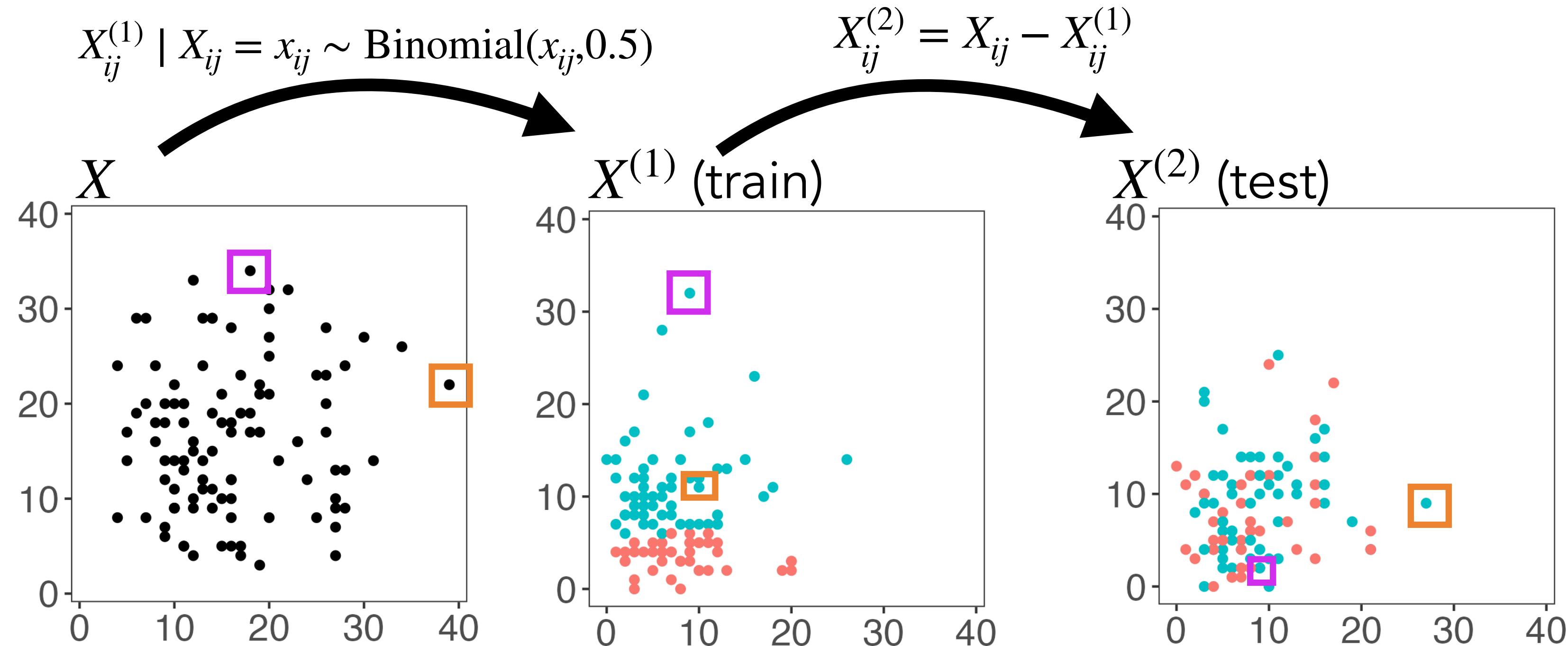
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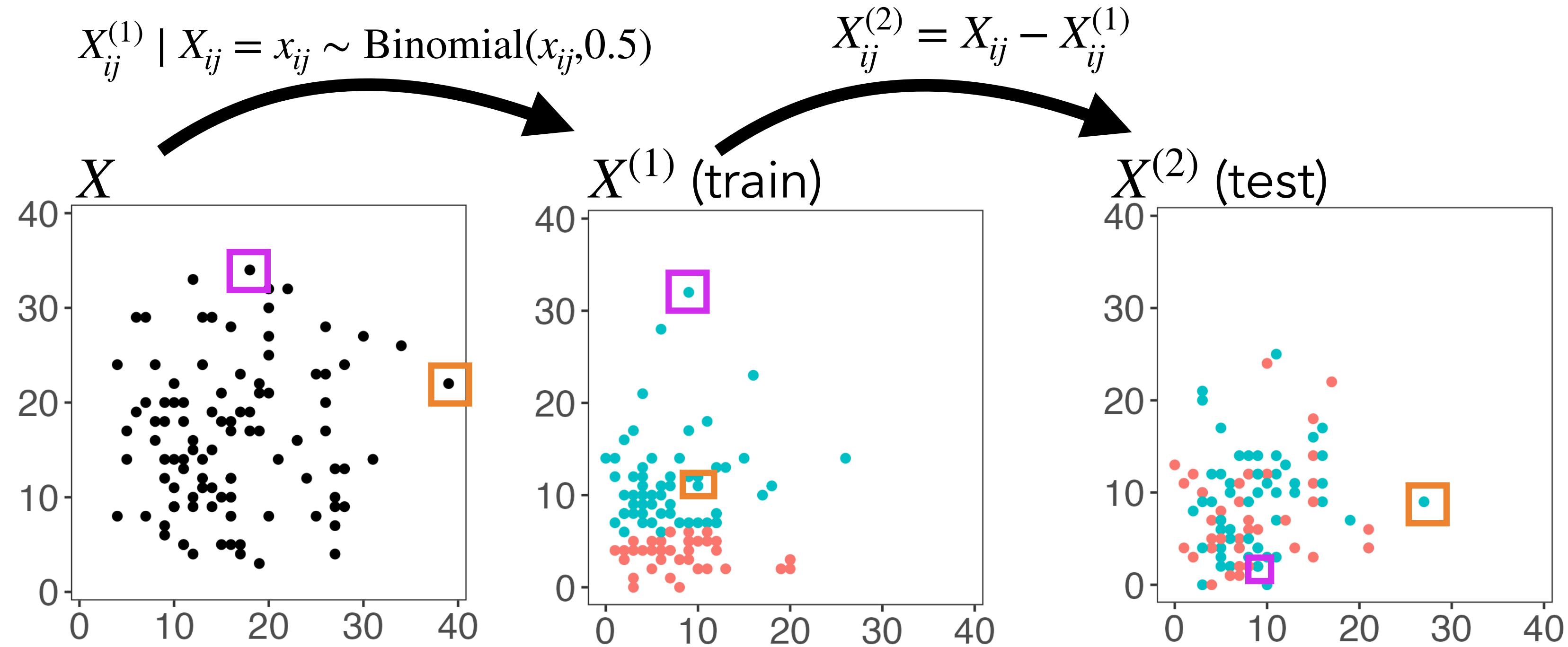


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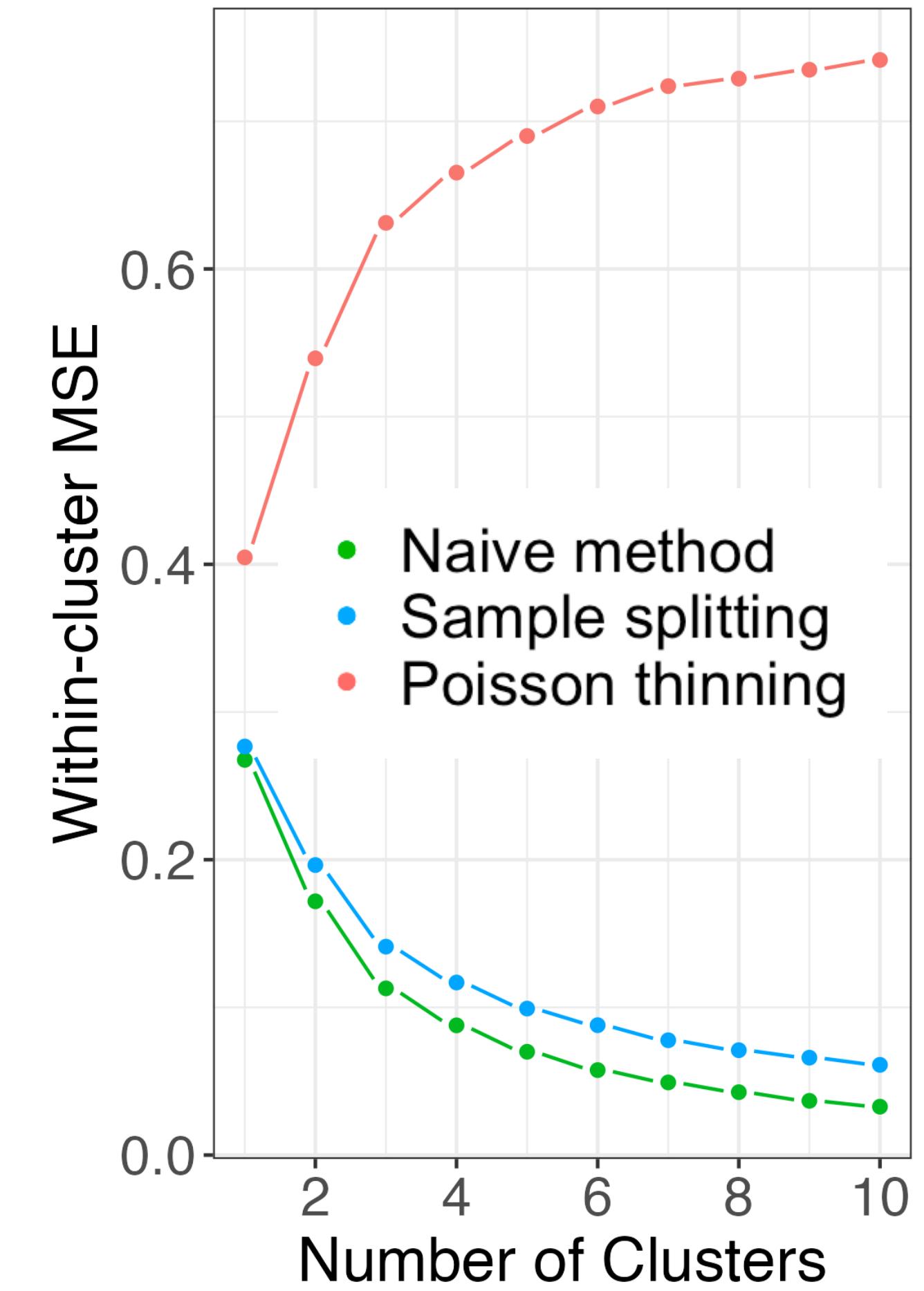
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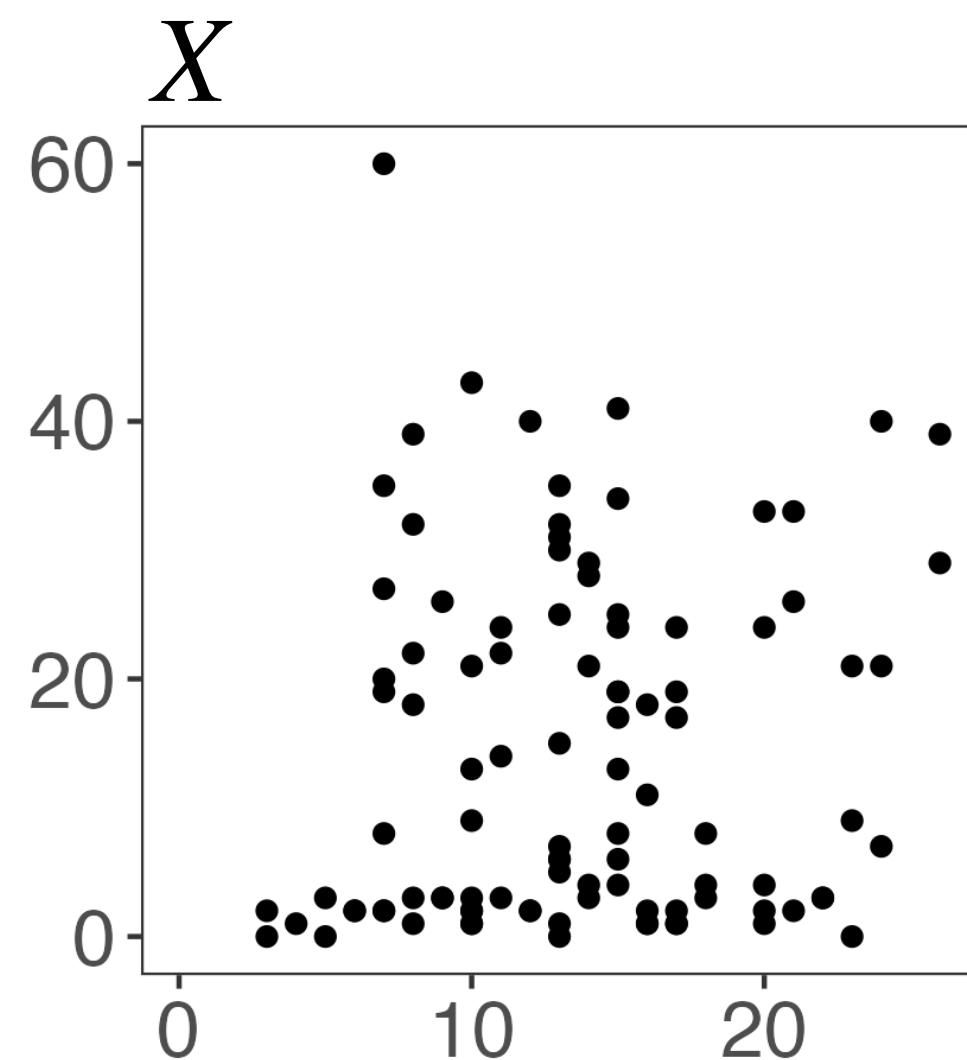
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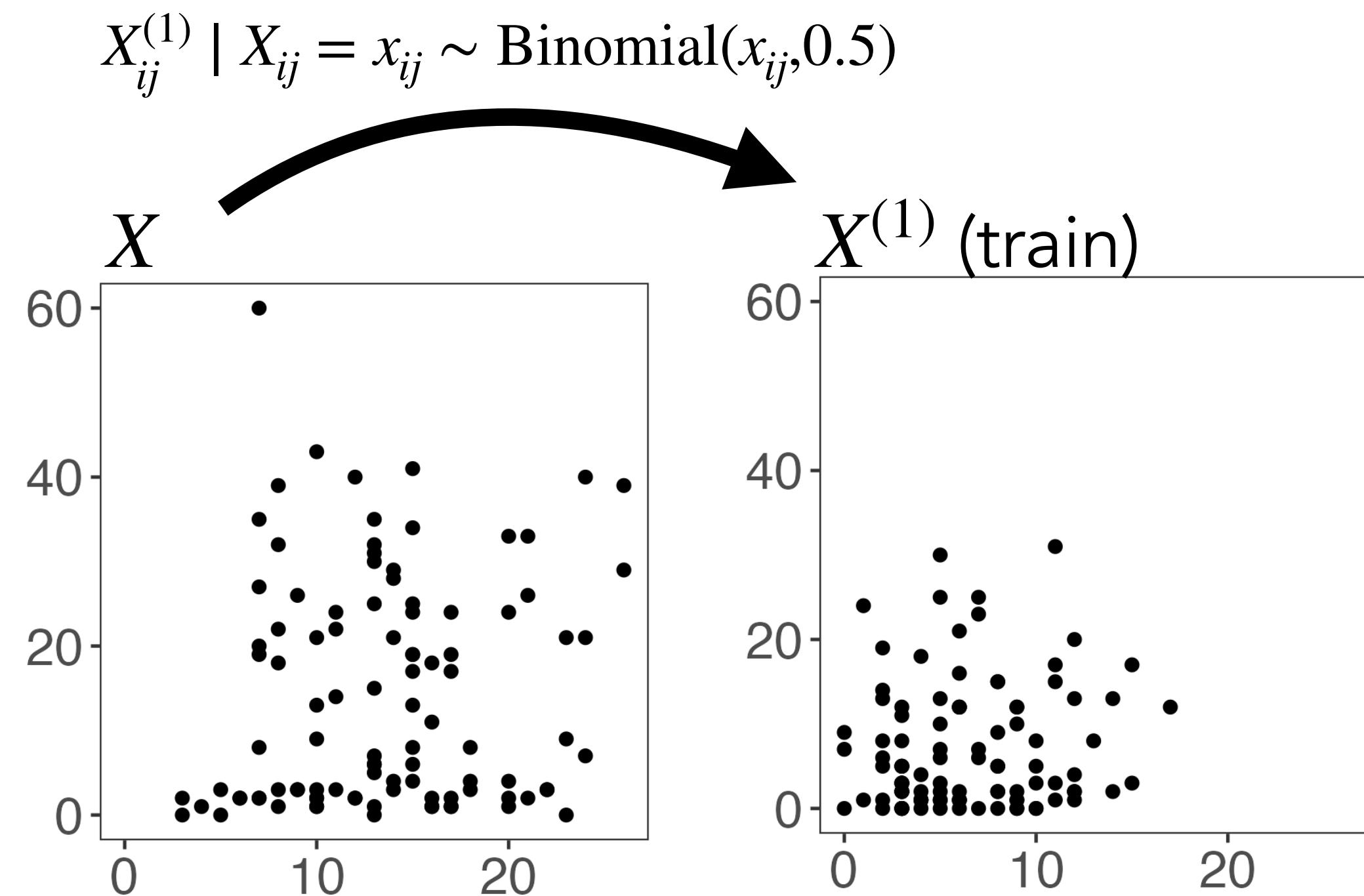


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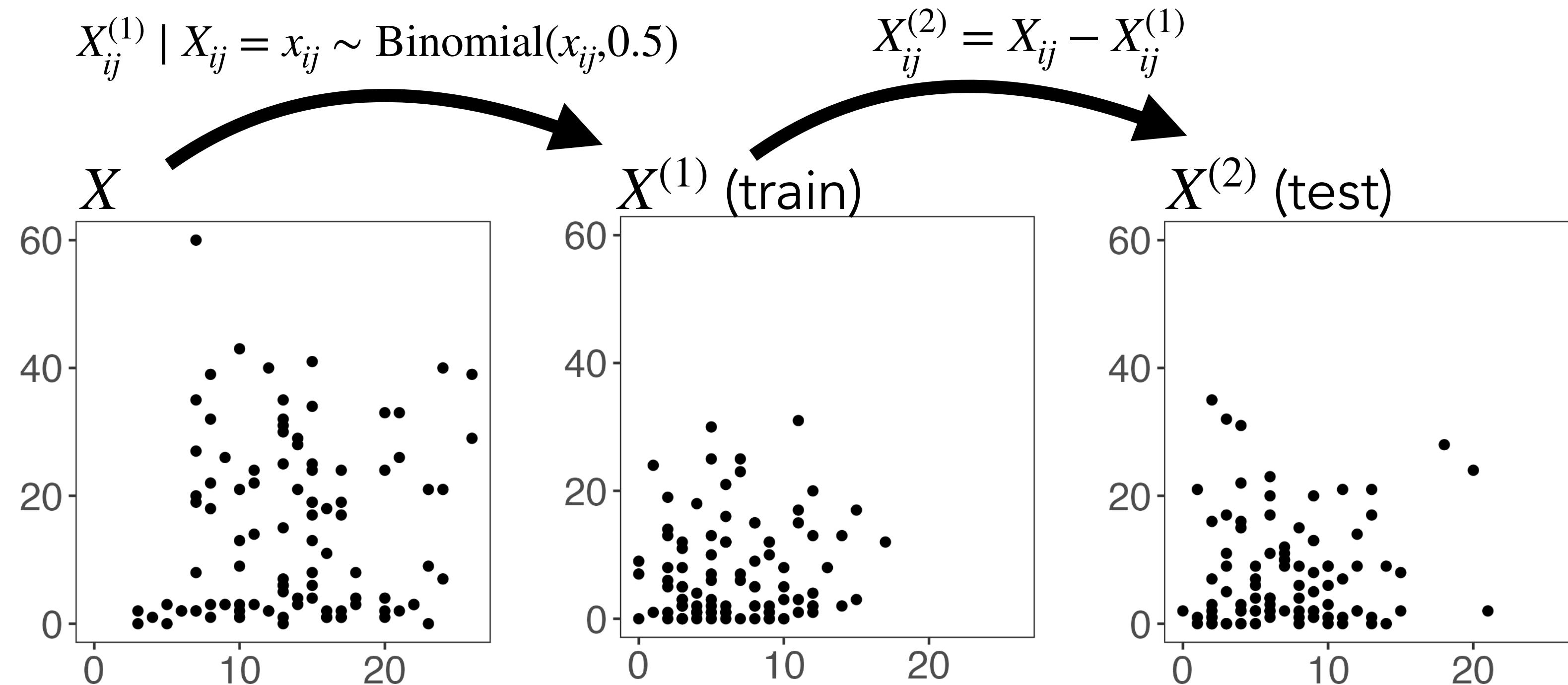
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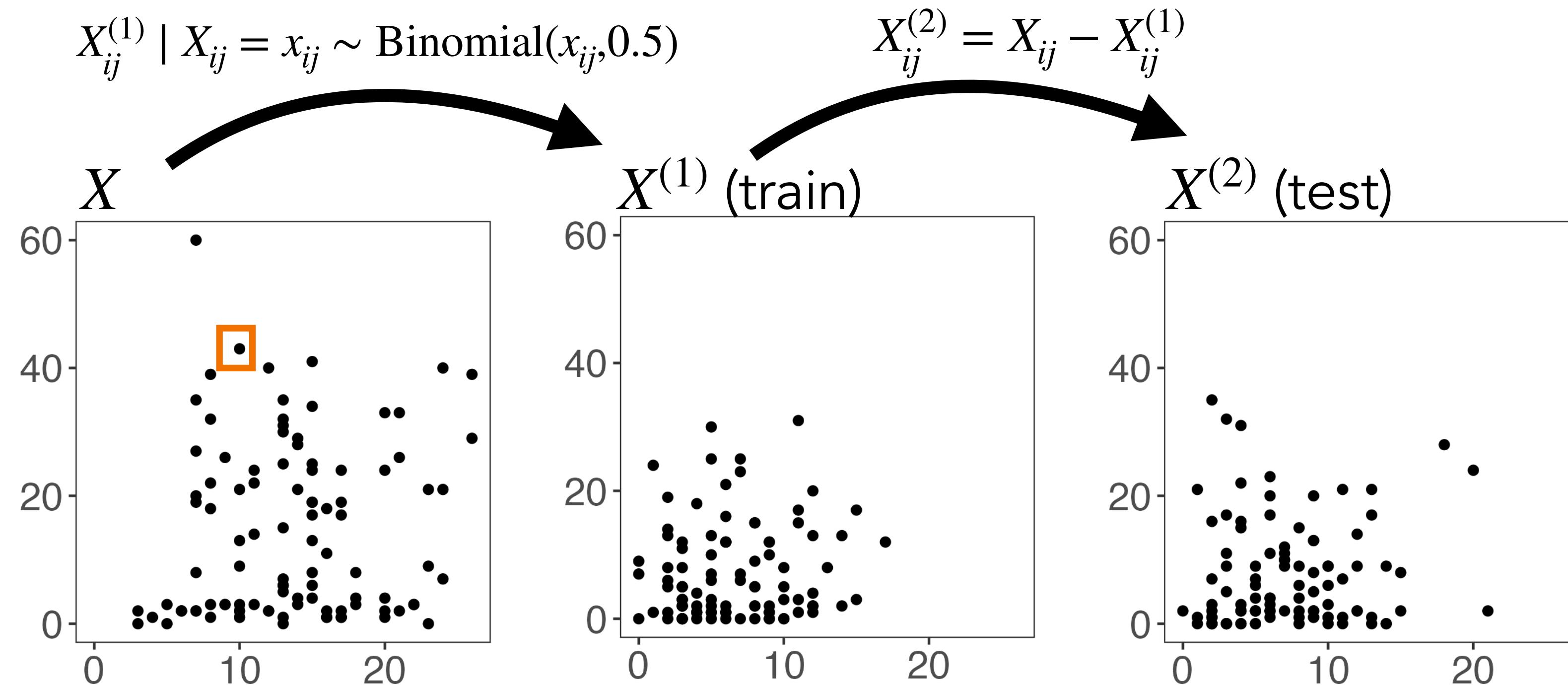
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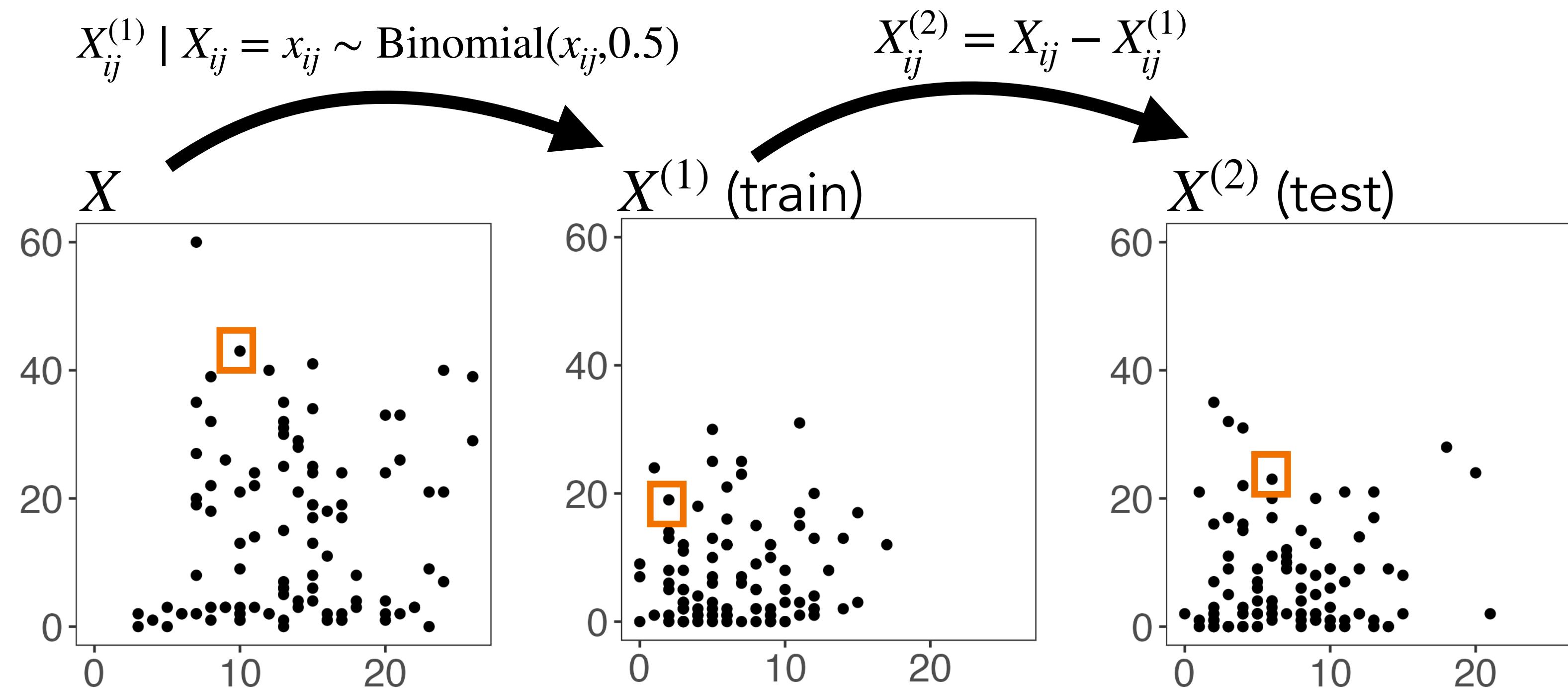
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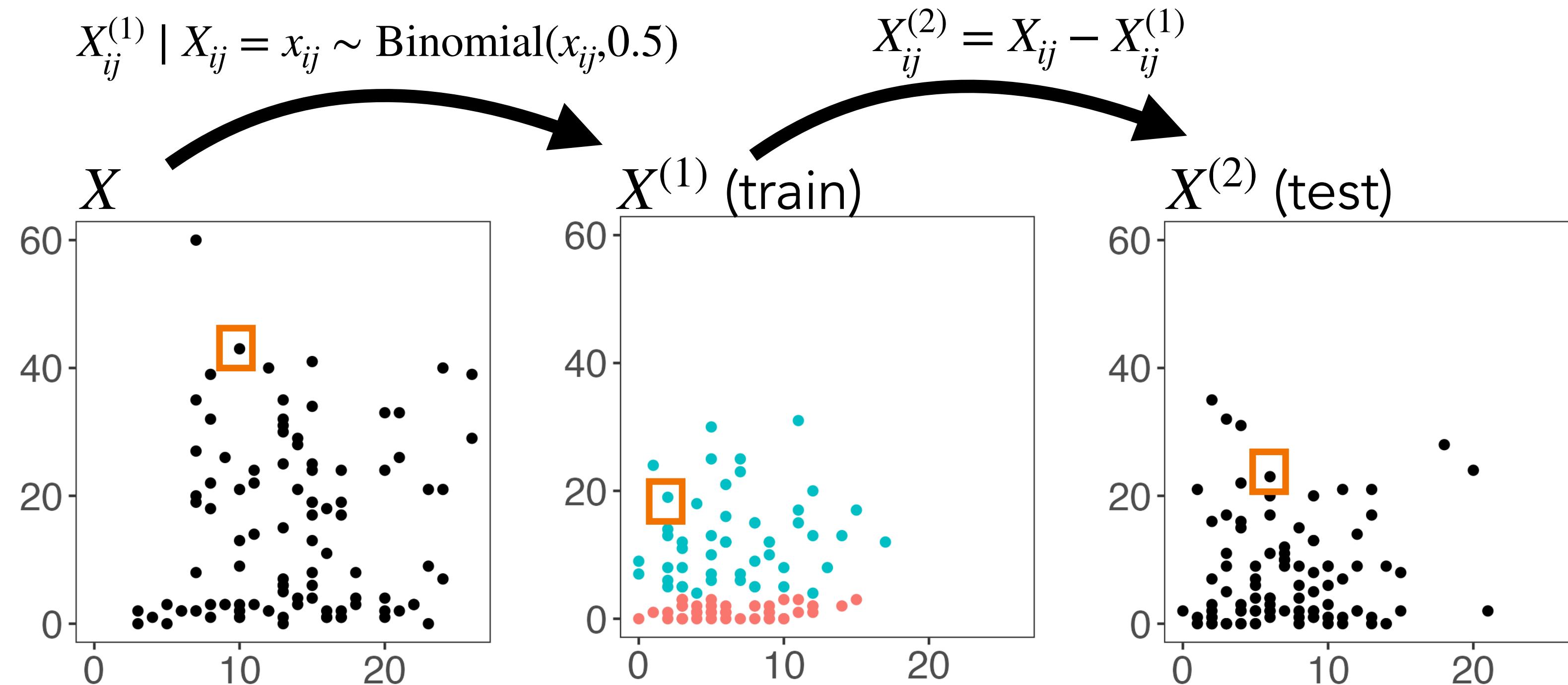
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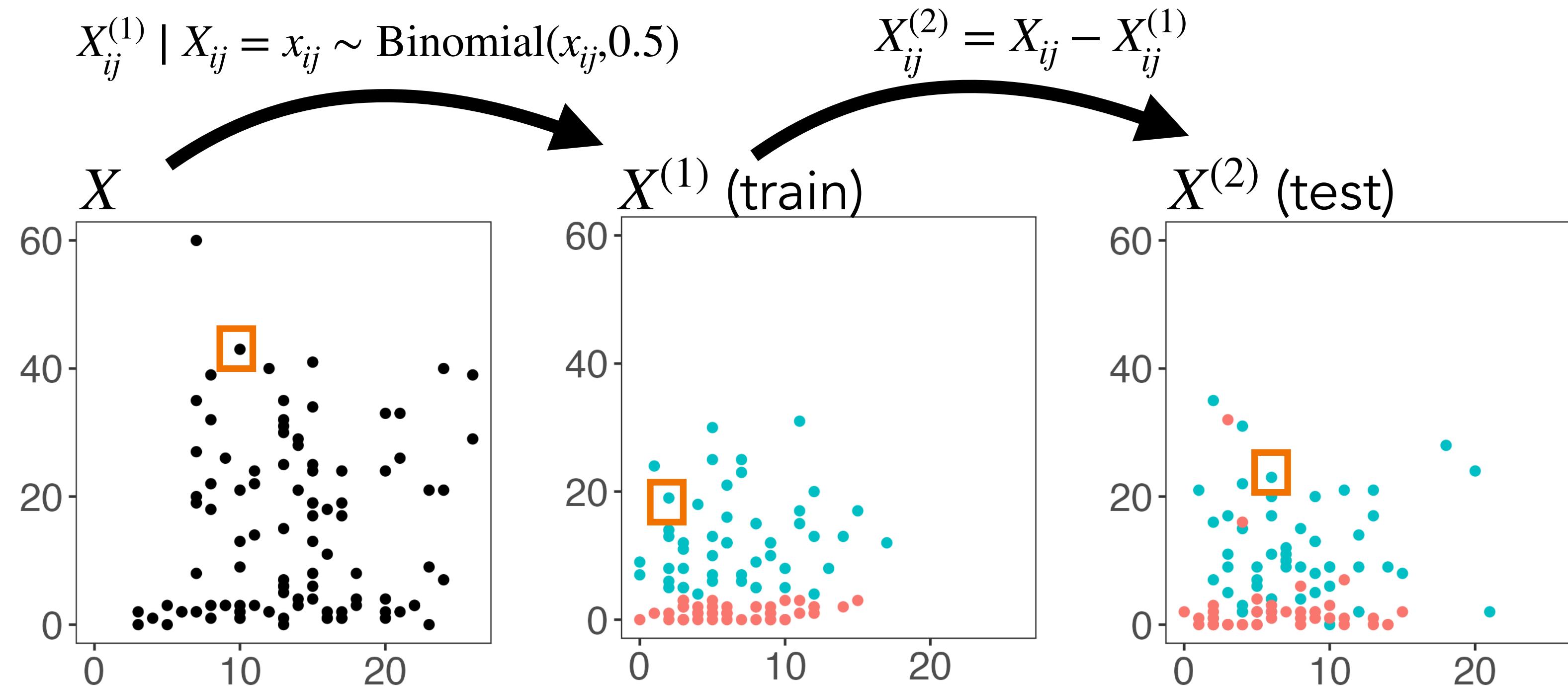
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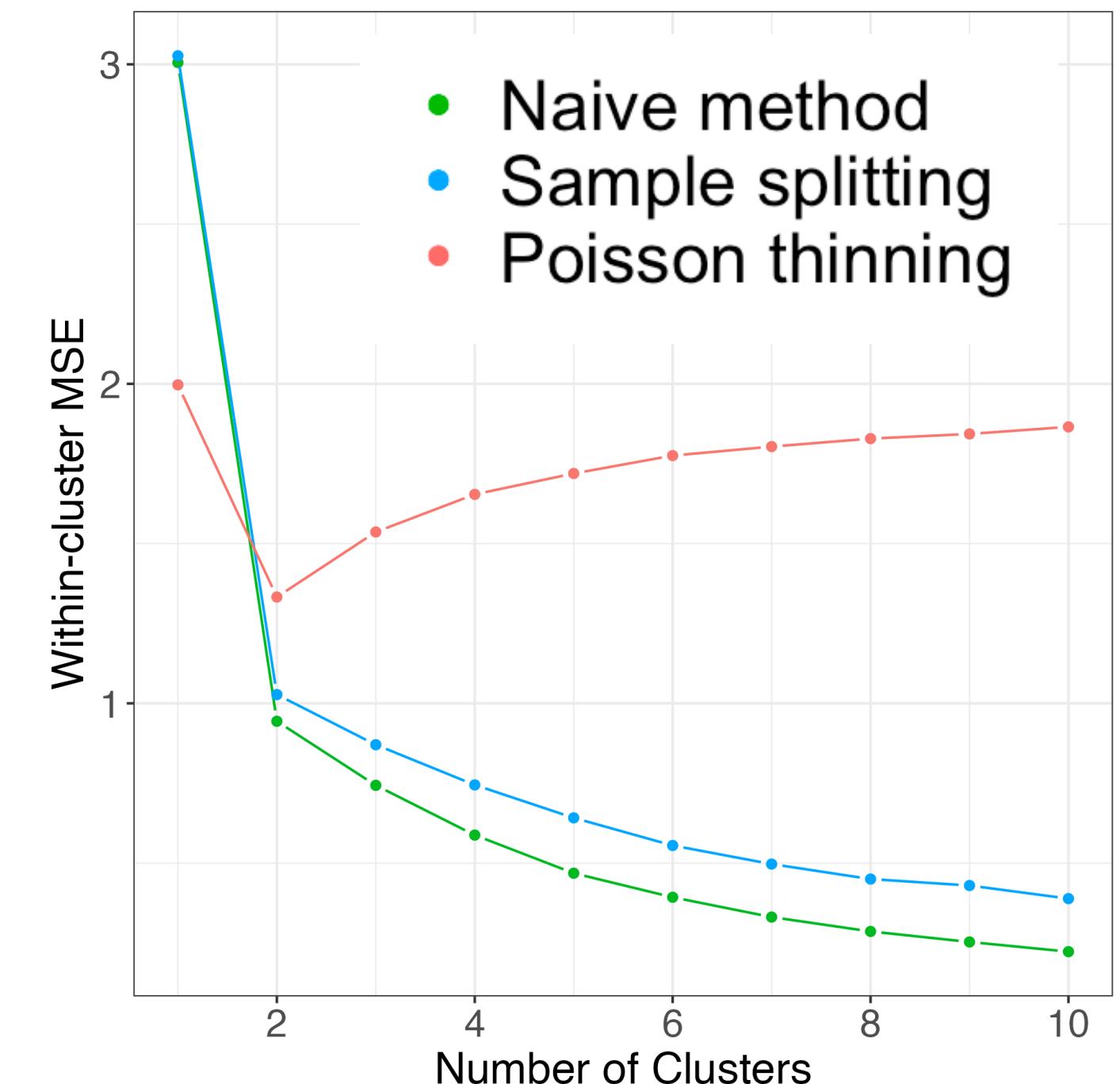
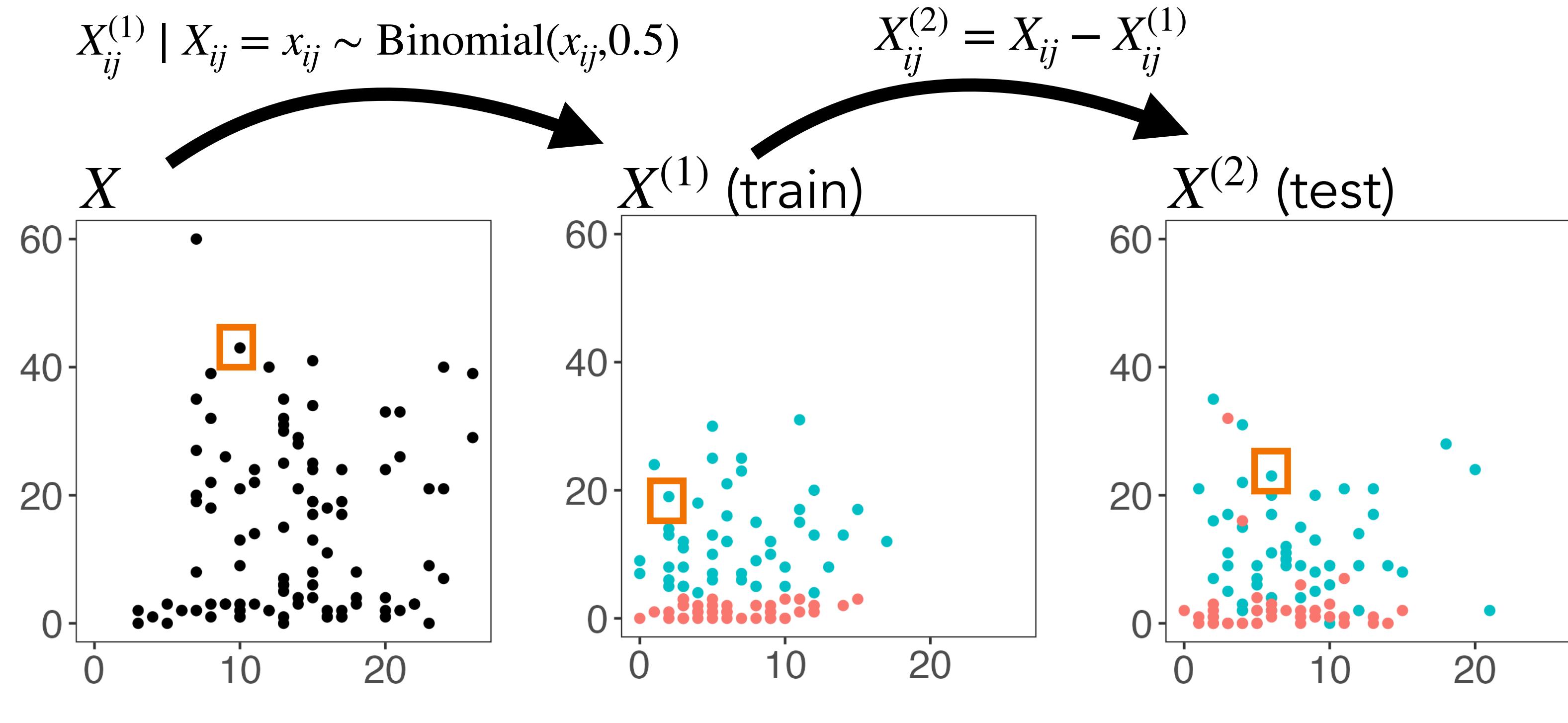
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2. Poisson thinning
3. **Data thinning**
4. Application to changepoint detection
5. Generalized data thinning

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

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

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**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
$X \sim N(\mu, \sigma^2)$	(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
$X \sim N_k(\mu, \Sigma)$.	(μ, Σ) .
$X \sim \text{Multinomial}_k(r, p)$	r , if p is fixed
$X \sim \text{Wishart}_p(n, \Sigma)$	n , if p and Σ are fixed.

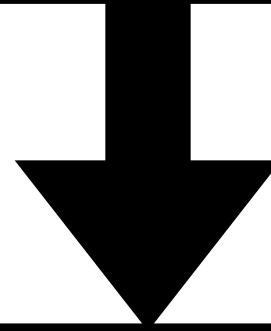
Data thinning for convolution-closed distributions

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

Data thinning for convolution-closed distributions

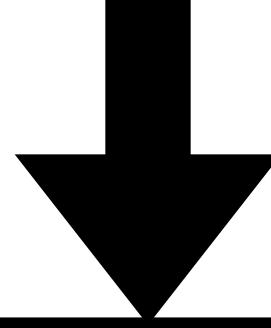
We know x could have arisen as $x' + x''$, where
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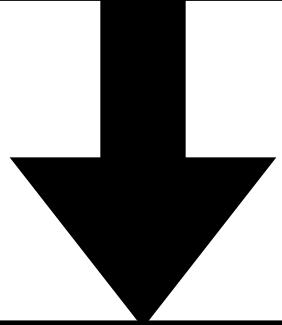


If we had observed x' and x'' , we would have satisfied our goal of data thinning!

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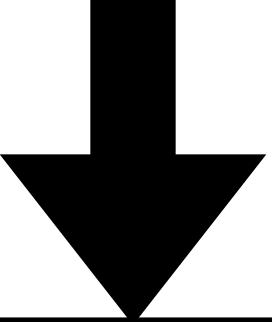
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Can we work backwards to recover x' and x'' ?

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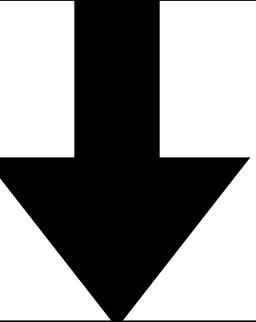
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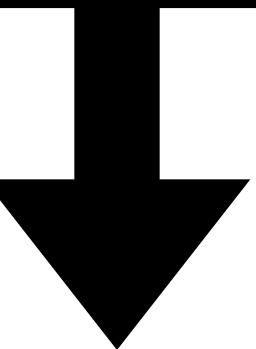
Let $G_{\epsilon,x}$ be the conditional distribution of $X' | X = x$.

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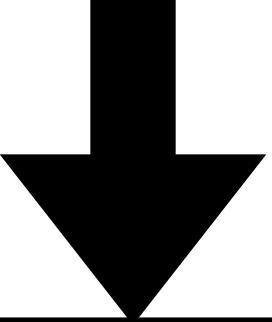
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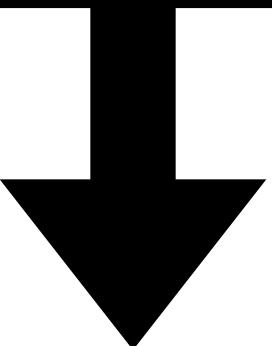
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If we had observed x' and x'' , we would have satisfied our goal of data thinning!

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

Theorem:

$X^{(1)} \sim F_{\epsilon\lambda}$, $X^{(2)} \sim F_{(1-\epsilon)\lambda}$, $X^{(1)} \perp\!\!\!\perp X^{(2)}$.

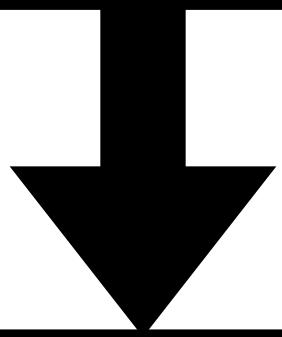
Data thinning for the Poisson distribution

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

Data thinning for the Poisson distribution

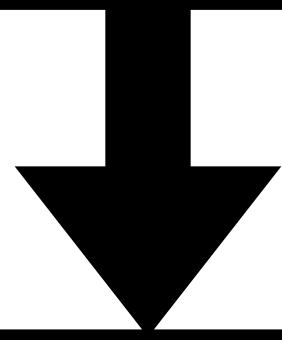
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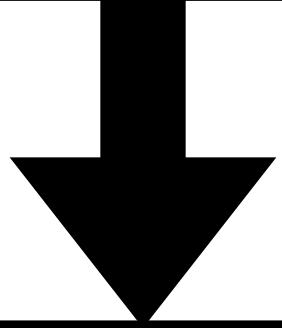


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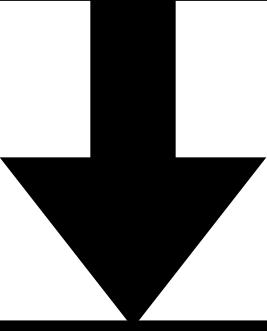
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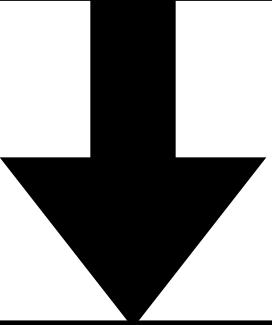
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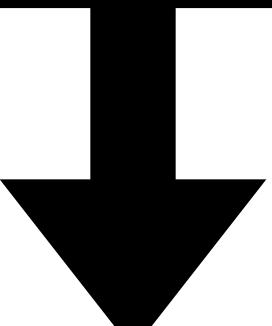
The conditional distribution of $X' | X = x$ is Binomial(x, ϵ).

Data thinning for the Poisson distribution

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



Draw $X^{(1)}$ from $\text{Binomial}(x, \epsilon)$. Let $X^{(2)} := X - X^{(1)}$.

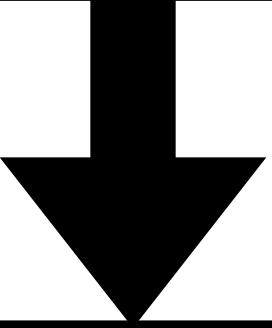
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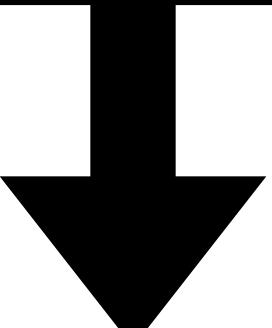
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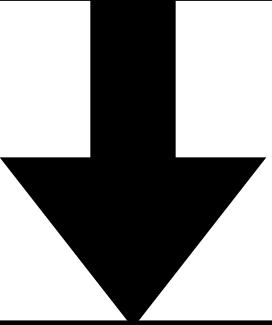
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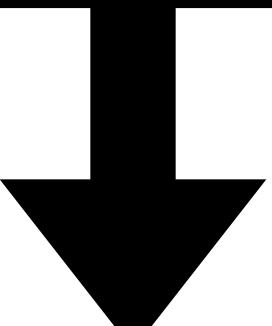
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If we had observed x' and x'' , we would have satisfied our goal of data thinning!

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

The conditional distribution of $X' | X = x$ is $\text{Binomial}(x, \epsilon)$.

We have recovered Poisson thinning!

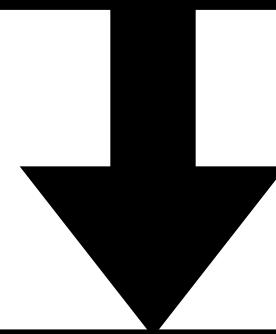
Data thinning recipe for the negative binomial distribution

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

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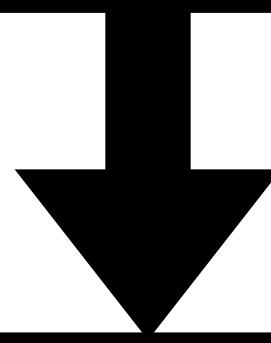
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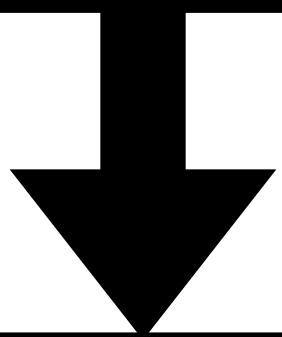


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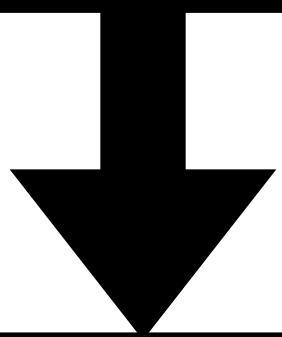
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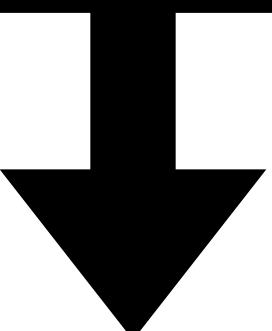
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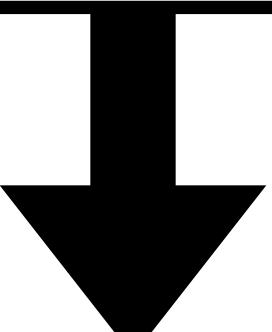
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Draw $X^{(1)}$ from BetaBinomial($x, \epsilon b, (1 - \epsilon)b$).
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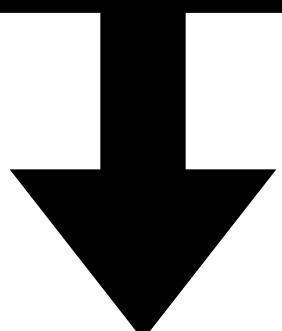
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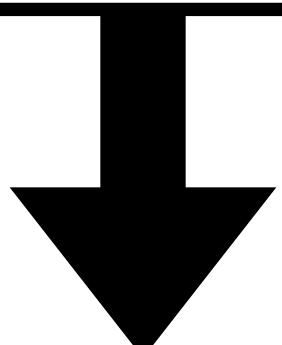
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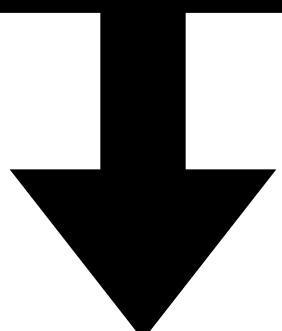
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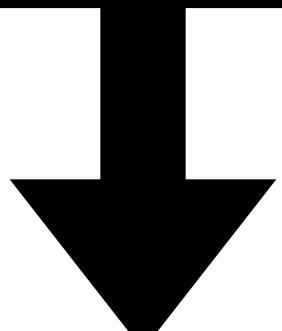
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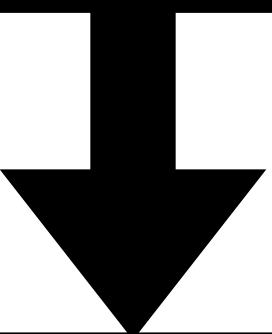
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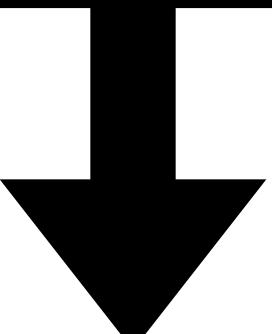
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We observe realization x from $X \sim \text{NB}(\mu, b)$.



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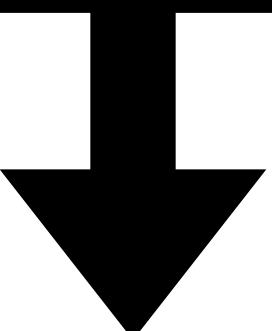
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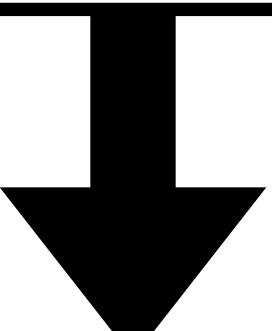
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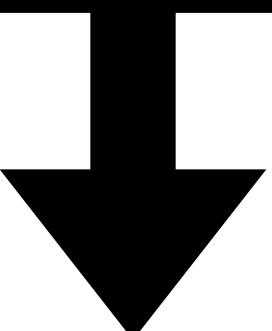
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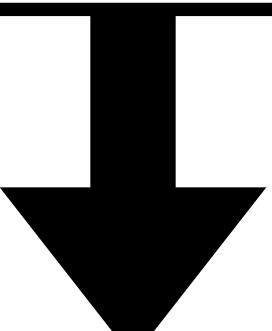
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Can we work backwards to recover x' and x'' ?

The conditional distribution of $X' | X = x$ is BetaBinomial($x, \epsilon b, (1 - \epsilon) b$).

$$\text{Cov}(X^{(1)}, X^{(2)}) = \epsilon(1 - \epsilon) \frac{\mu^2}{b} \left(1 - \frac{b + 1}{\tilde{b} + 1}\right).$$

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:

Poisson(λ)

Binomial(x, ϵ)

Distribution of $X^{(1)}$:

Poisson($\epsilon\lambda$)

Distribution of $X^{(2)}$,

where $X^{(2)} = X - X^{(1)}$:

Poisson($(1 - \epsilon)\lambda$)

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

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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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 $X^{(2)} = X - X^{(1)}$:
Poisson(λ)	Binomial(x, ϵ)	Poisson($\epsilon\lambda$)	Poisson($(1 - \epsilon)\lambda$)
$N(\mu, \sigma^2)$	$N(\epsilon x, \epsilon(1 - \epsilon)\sigma^2)$	$N(\epsilon\mu, \epsilon\sigma^2)$	$N((1 - \epsilon)\mu, (1 - \epsilon)\sigma^2)$

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

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Related work on Gaussian thinning:

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

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Gamma(α, β)	$x \cdot \text{Beta}(\epsilon\alpha, (1 - \epsilon)\alpha)$.	Gamma($\epsilon\alpha, \beta$)	Gamma($(1 - \epsilon)\alpha, \beta$)
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$N(\mu, \sigma^2)$	$N_M(\epsilon\mu, \sigma^2 \text{diag}(\epsilon) - \sigma^2 \epsilon \epsilon^T)$.	$N(\epsilon_m \mu, \epsilon_m \sigma^2)$
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Outline

1. Motivation: sample splitting doesn't always work
2. Poisson thinning
3. Data thinning
- 4. Application to changepoint detection**
5. Generalized data thinning

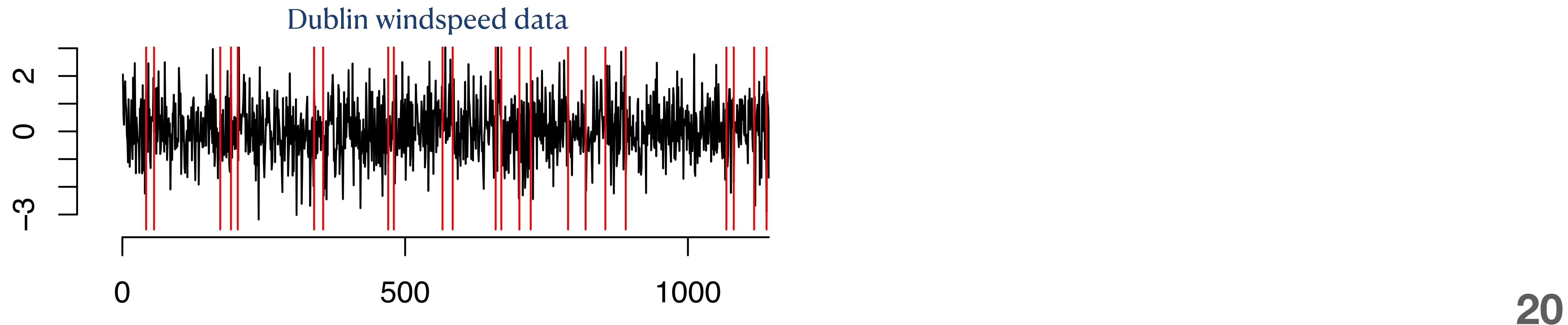
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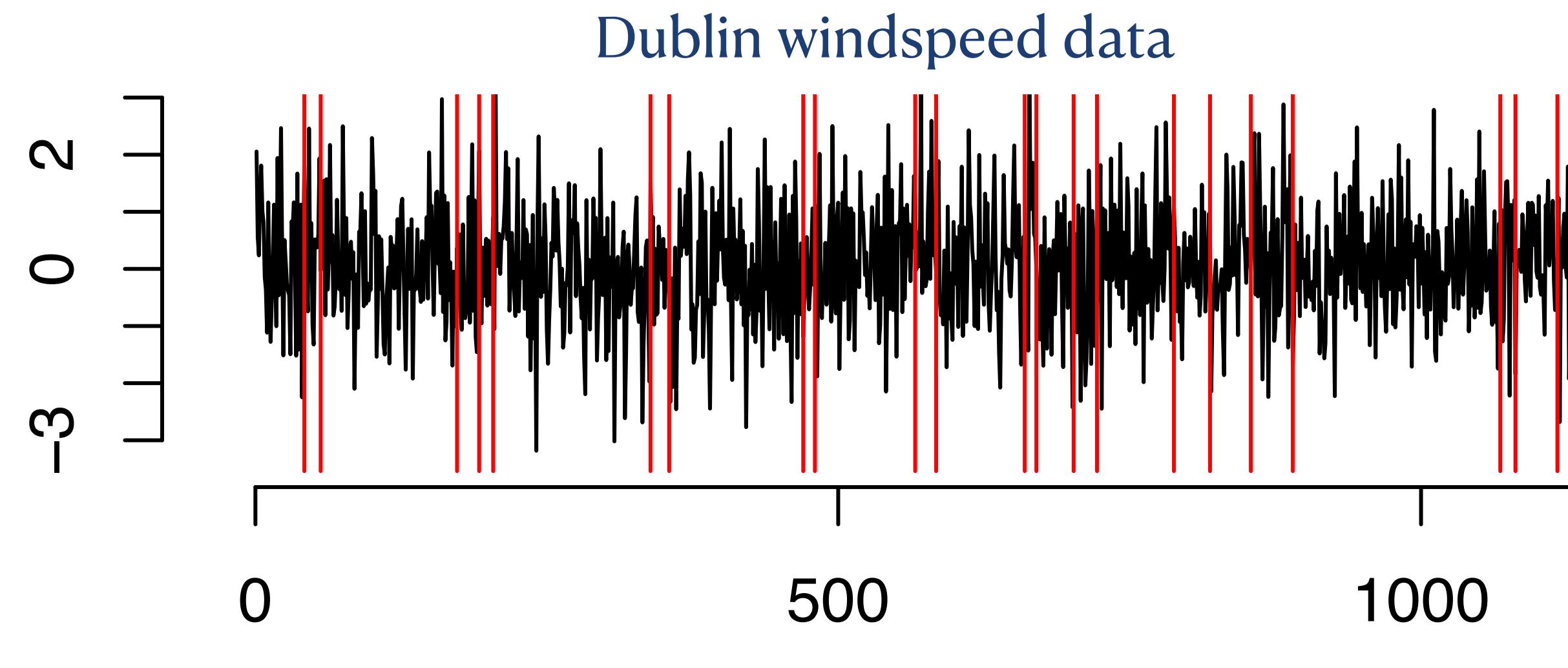
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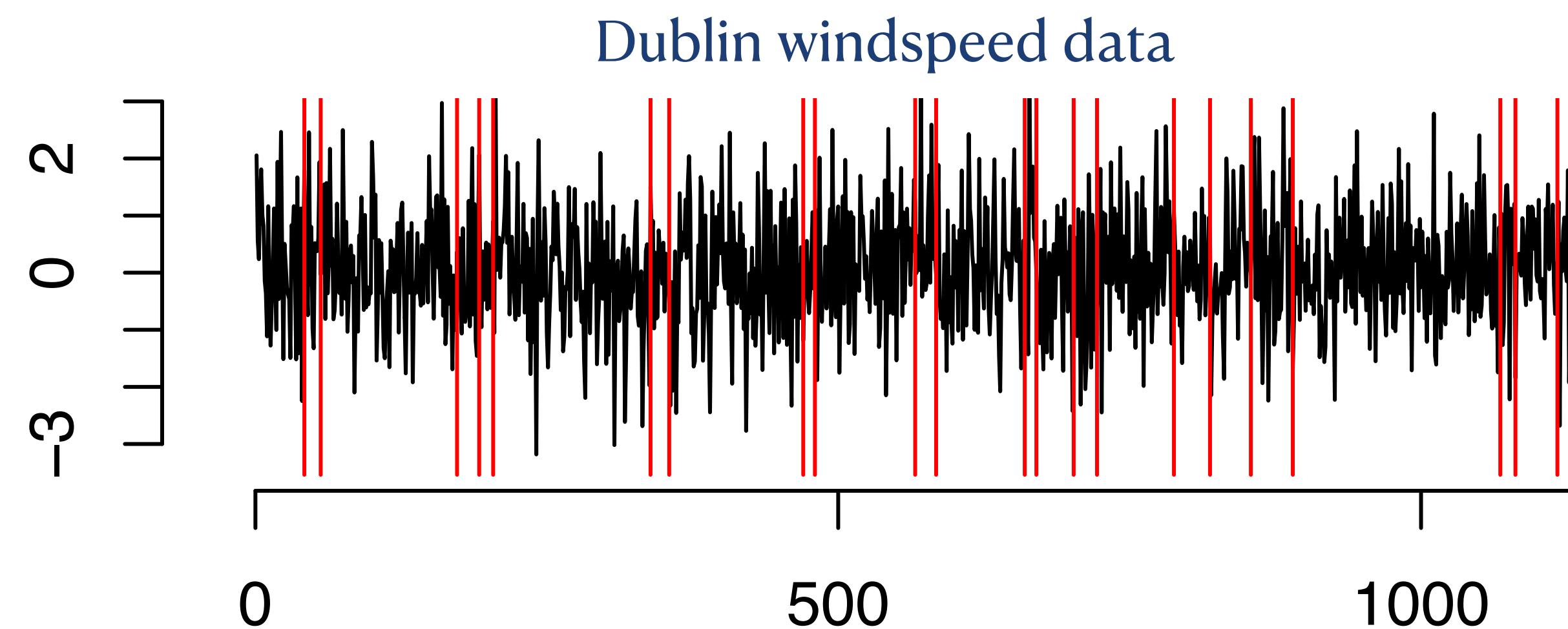
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Idea: thin the data, such that we can estimate changepoints on training set and evaluate significance on test set.

We do not know how to thin a Gaussian with unknown variance

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

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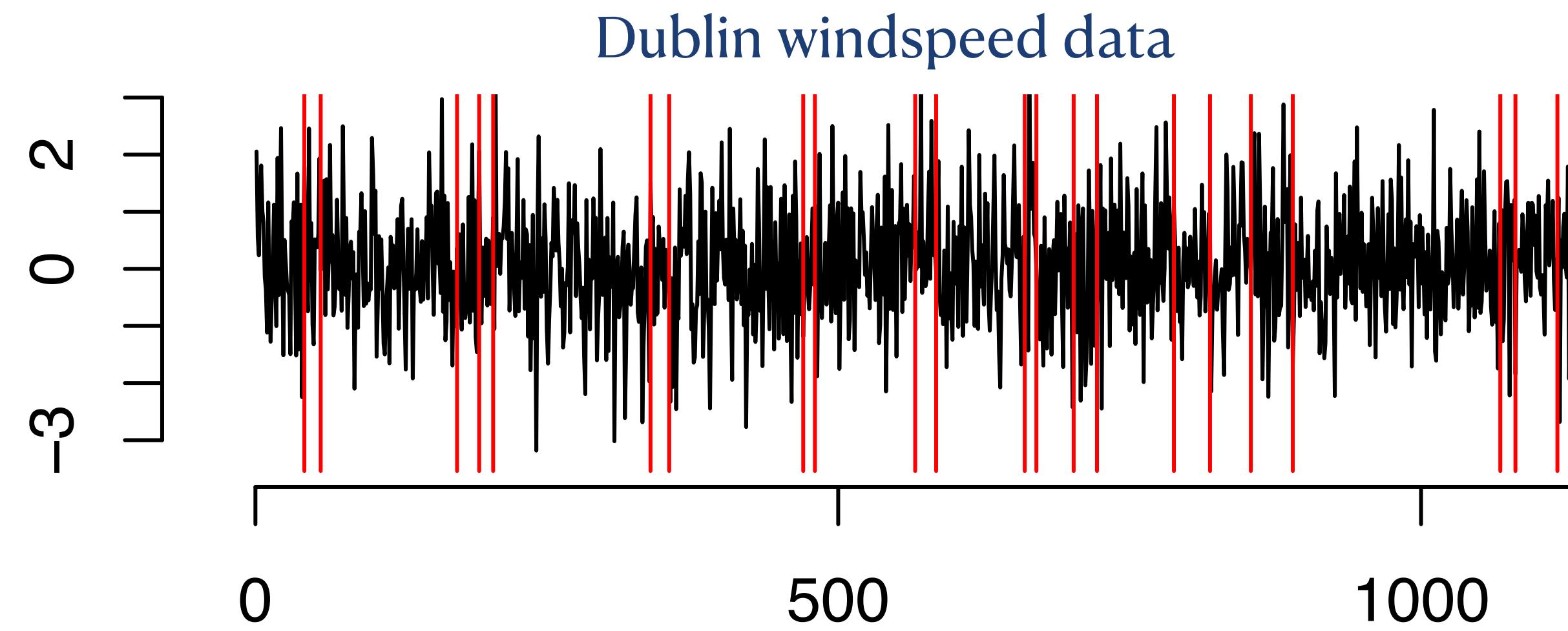
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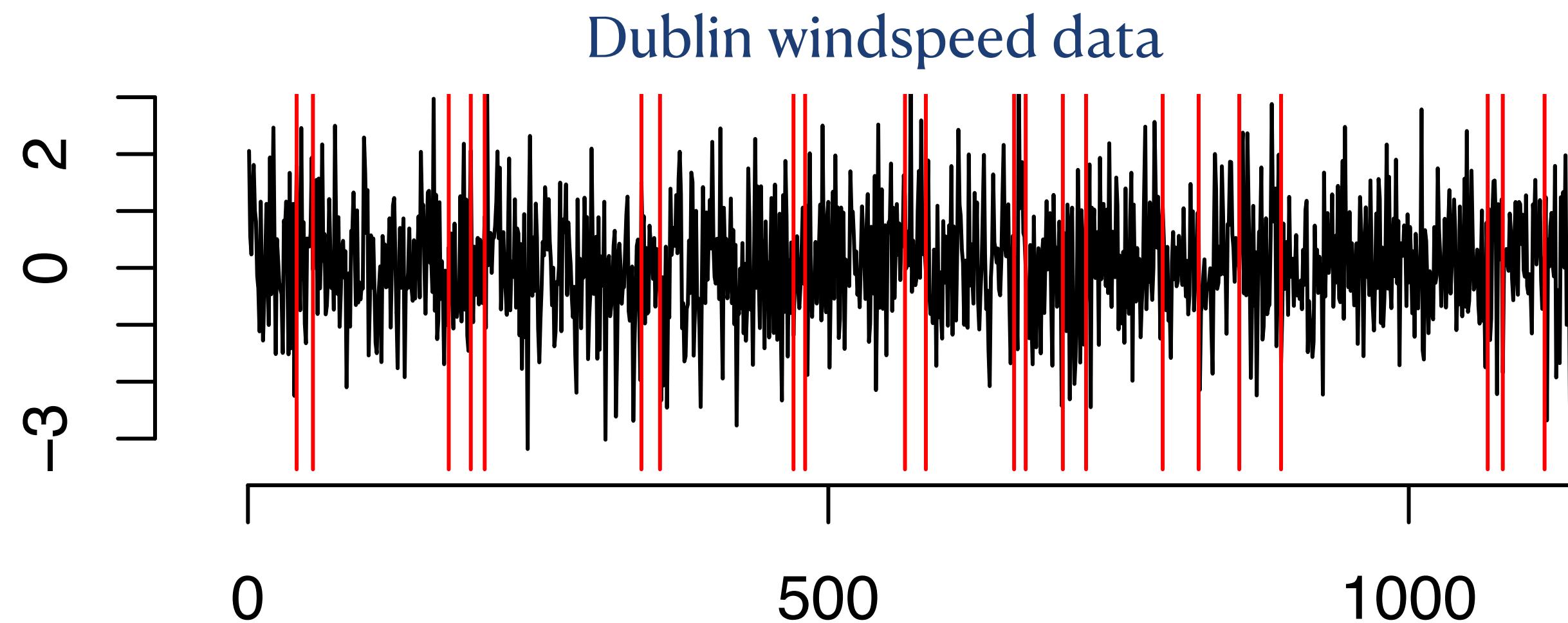
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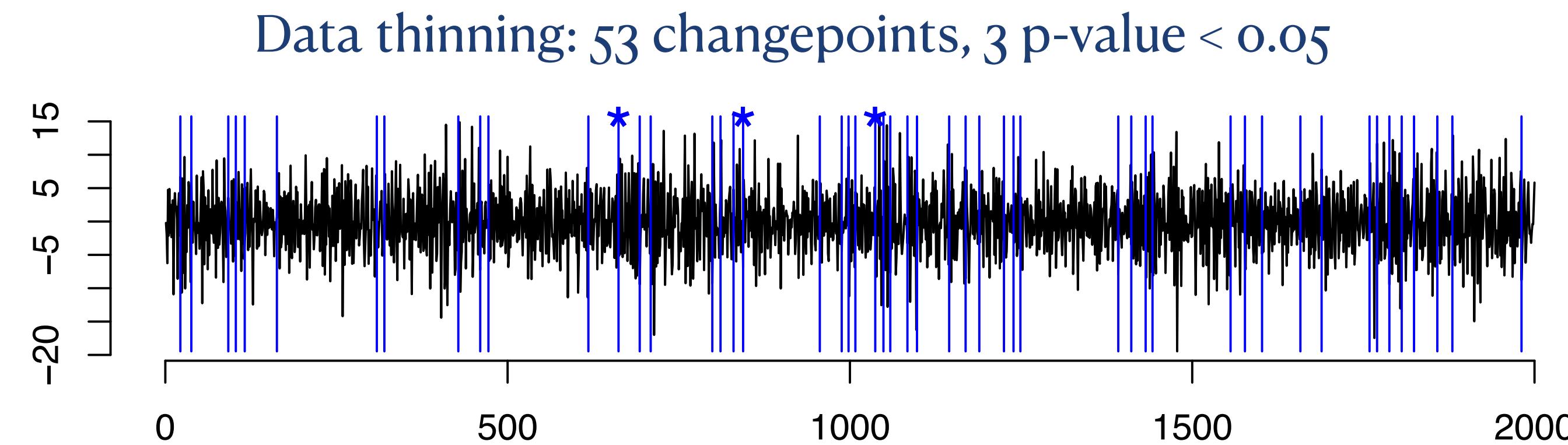
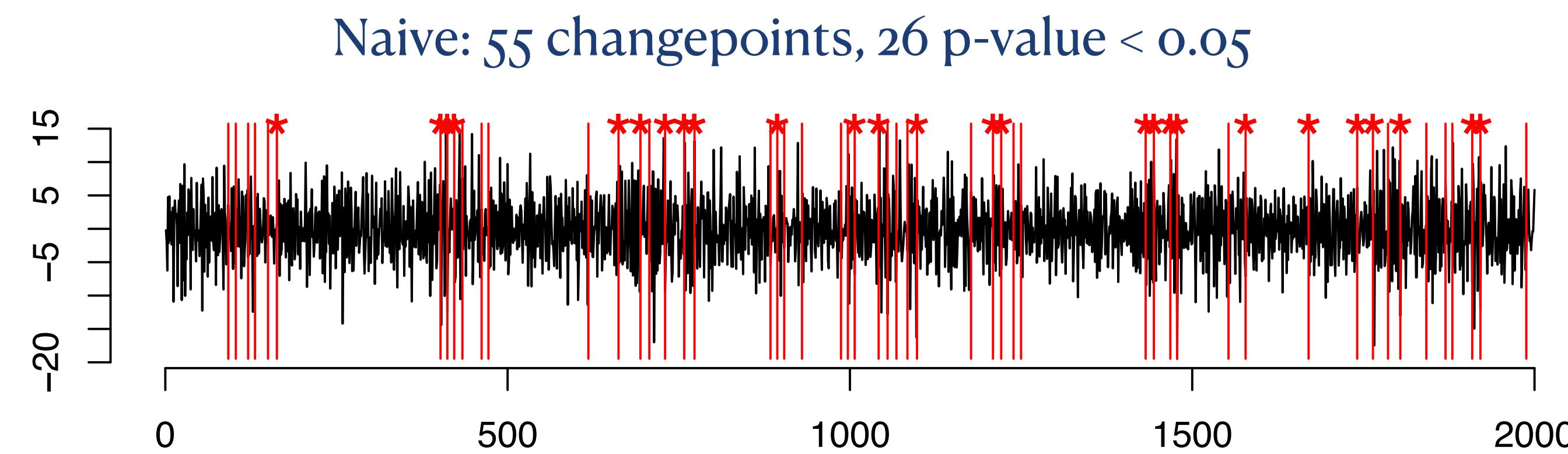
Define $Z_i := X_i^2$. Note that $Z_i \sim \text{Gamma}(0.5, 0.5/\theta_i^2)$.

Naive method: Estimate and test changepoints on Z_i .

Thinning: Thin Z_i into $Z_i^{(1)} \sim \text{Gamma}(0.25, 0.5/\theta_i^2)$ and $Z_i^{(2)} \sim \text{Gamma}(0.25, 0.5/\theta_i^2)$.

Identify changepoints using $Z^{(1)}$, and test using $Z^{(2)}$.

Dublin wind speed data



Outline

1. Motivation: sample splitting doesn't always work
2. Poisson thinning
3. Data thinning
4. Application to changepoint detection
5. **Generalized data thinning**

Revisiting the goals of data thinning

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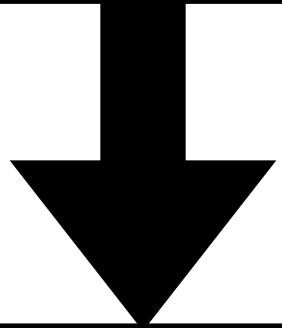
Generalized thinning with non-additive decompositions

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

Generalized thinning with non-additive decompositions

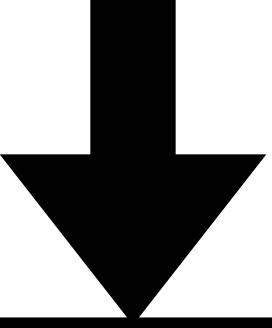
We know x could have arisen as $T(x', x'')$, where
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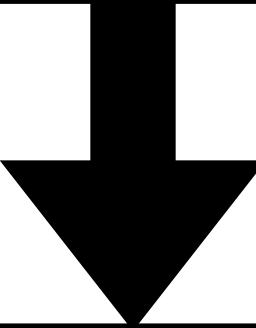


Can we work backwards to recover
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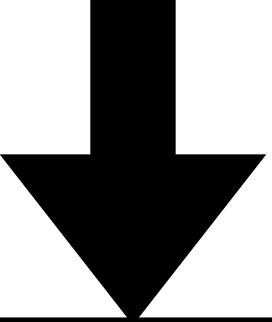
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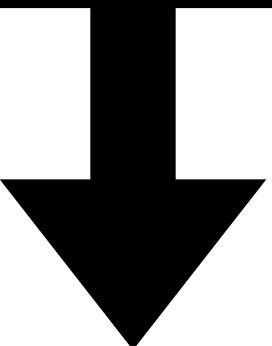
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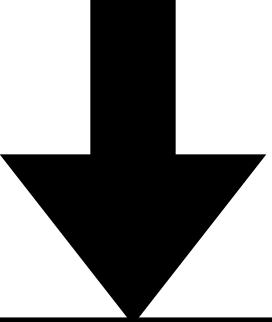
Draw $(X^{(1)}, X^{(2)})$ from $G_{x,\theta}$.

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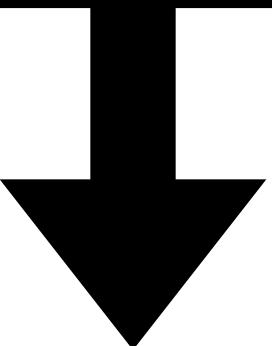
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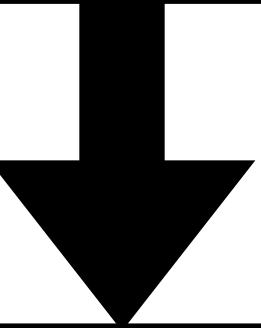
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Theorem:

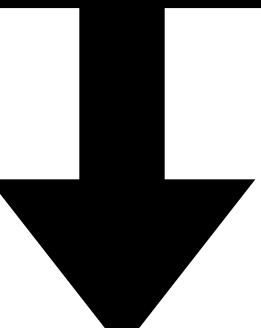
$$X^{(1)} \sim Q_\theta^1, \quad X^{(2)} \sim Q_\theta^2, \quad X^{(1)} \perp\!\!\!\perp X^{(2)}.$$

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

Let $G_{x,\theta}$ 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 $G_{x,\theta}$ 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 $X^{(k)} \stackrel{ind.}{\sim} Q_\theta^{(k)}$.	Sufficient statistic T (sufficient for θ)
Natural exponential family (in parameter θ)	$N(\theta, \sigma^2)$	$N(\epsilon_k \theta, \epsilon_k \sigma^2)$	
	Poisson(θ)	Poisson($\epsilon_k \theta$)	
	NegBin(r, θ)	NegBin($\epsilon_k r, \theta$)	
	Binomial(r, θ)	Binomial($\epsilon_k r, \theta$)	$\sum_{k=1}^K X^{(k)}$
	Gamma(α, θ)	Gamma($\epsilon_k \alpha, \theta$)	
	$N_p(\boldsymbol{\theta}, \Sigma)$	$N_p(\epsilon_k \boldsymbol{\theta}, \epsilon_k \Sigma)$	
	Multinomial $_p(r, \boldsymbol{\theta})$	Multinomial $_p(\epsilon_k r, \boldsymbol{\theta})$	
General exponential family (in parameter θ)	Gamma($K/2, \theta$)	$N(0, \frac{1}{2\theta})$	$\sum_{k=1}^K (X^{(k)})^2$
	Gamma(K, θ)	Weibull($\theta^{-\frac{1}{\nu}}, \nu$)	$\sum_{k=1}^K (X^{(k)})^\nu$
	Beta(θ, β)	Beta($\frac{1}{K}\theta + \frac{k-1}{K}, \frac{1}{K}\beta$)	$(\prod_{k=1}^K X^{(k)})^{1/K}$
	Beta(α, θ)	Beta($\frac{1}{K}\alpha, \frac{1}{K}\theta + \frac{k-1}{K}$)	$(\prod_{k=1}^K (1 - X^{(k)}))^{1/K}$
	Gamma(θ, β)	Gamma($\frac{1}{K}\theta + \frac{k-1}{K}, \frac{1}{K}\beta$)	$(\prod_{k=1}^K X^{(k)})^{1/K}$
	Weibull(θ, ν)	Gamma($\frac{1}{K}, \theta^{-\nu}$)	$(\sum_{k=1}^K X^{(k)})^{1/\nu}$
	Pareto(ν, θ)	Gamma($\frac{1}{K}, \theta$)	$\nu \times \text{Exp}(\sum_{k=1}^K X^{(k)})$
	$N(0, \theta)$	Gamma($\frac{1}{2K}, \frac{1}{2\theta}$)	$X^2 = \sum_{k=1}^K X^{(k)}$
Truncated support family	$N_K(\theta_1 \mathbf{1}_K, \theta_2 I_K)$	$N(\theta_1, \theta_2)$	sample mean and variance
	Unif($0, \theta$)	$\theta \cdot \text{Beta}(\frac{1}{K}, 1)$	$\max(X^{(1)}, \dots, X^{(K)})$
	$\theta \cdot \text{Beta}(\alpha, 1)$	$\theta \cdot \text{Beta}(\frac{\alpha}{K}, 1)$	
Non-parametric	F^n	F^{n_k}	$\text{sort}(X^{(1)}, \dots, X^{(K)})$

References

The image shows two side-by-side screenshots of arXiv preprint pages. Both pages have a red header bar with the arXiv logo, a search bar, and a 'Help | Advanced' link.

Left Preprint:

- Path: arXiv > stat > arXiv:2301.07276
- Category: Statistics > Methodology
- Submitted: 18 Jan 2023
- Title: Data thinning for convolution-closed distributions
- Authors: Anna Neufeld, Ameer Dharamshi, Lucy L. Gao, Daniela Witten
- Abstract: 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.

Right Preprint:

- Path: Statistics > Methodology
- Submitted: 22 Mar 2023
- Title: Generalized Data Thinning Using Sufficient Statistics
- Authors: Ameer Dharamshi, Anna Neufeld, Keshav Motwani, Lucy L. Gao, Daniela Witten, Jacob Bien

Acknowledgements



Daniela Witten
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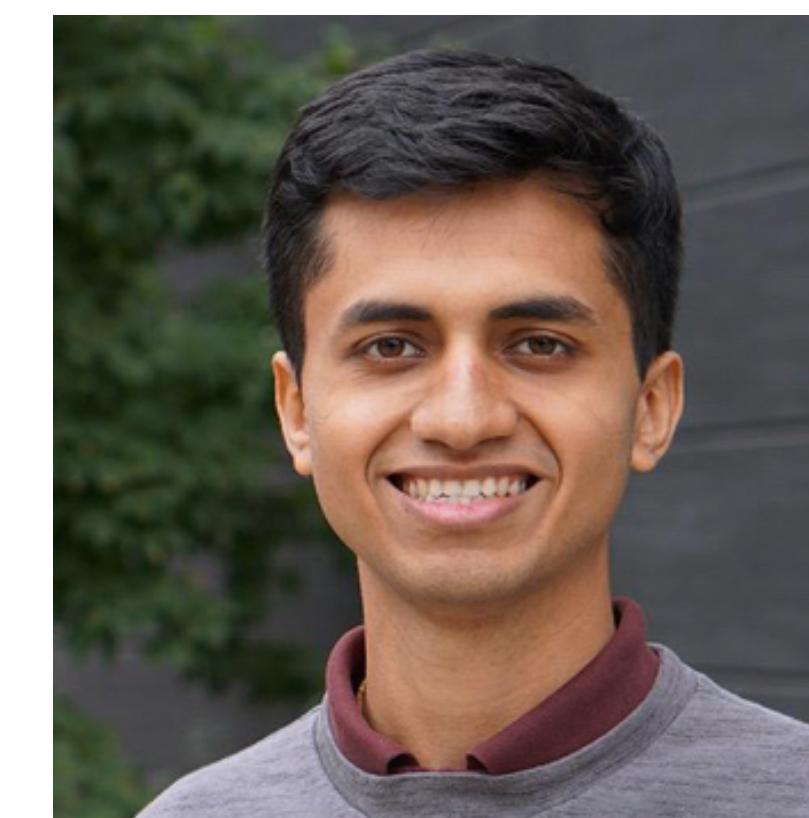
Lucy Gao
University of British Columbia



Ameer Dharamshi
University of Washington



Jacob Bien
University of Southern California

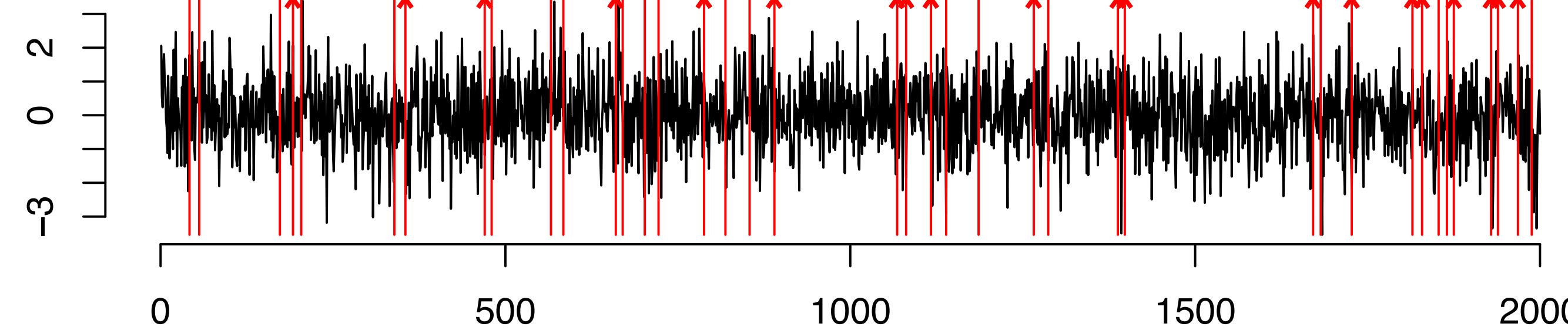


Keshav Motwani
University of Washington

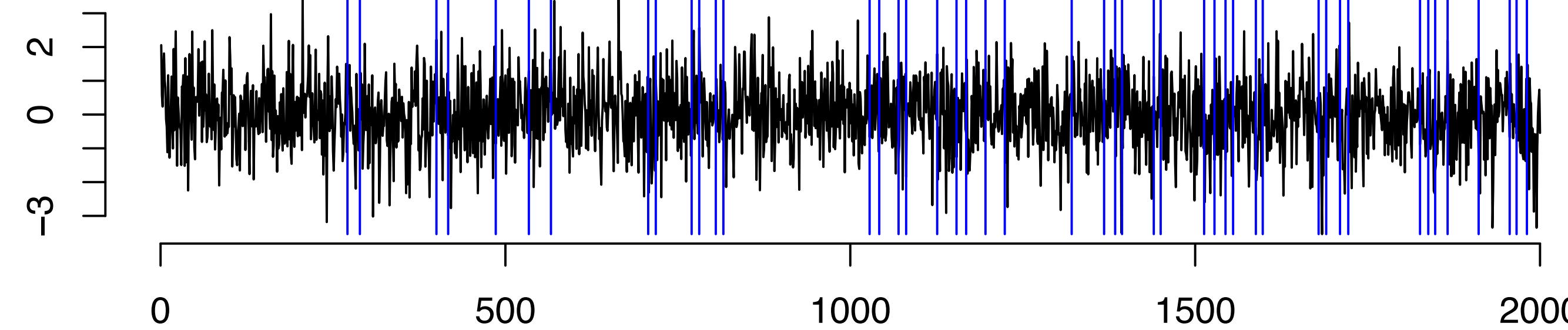
Questions?

Simulated data with no changepoints

Naive: 42 changepoints, 20 with p-value < 0.05

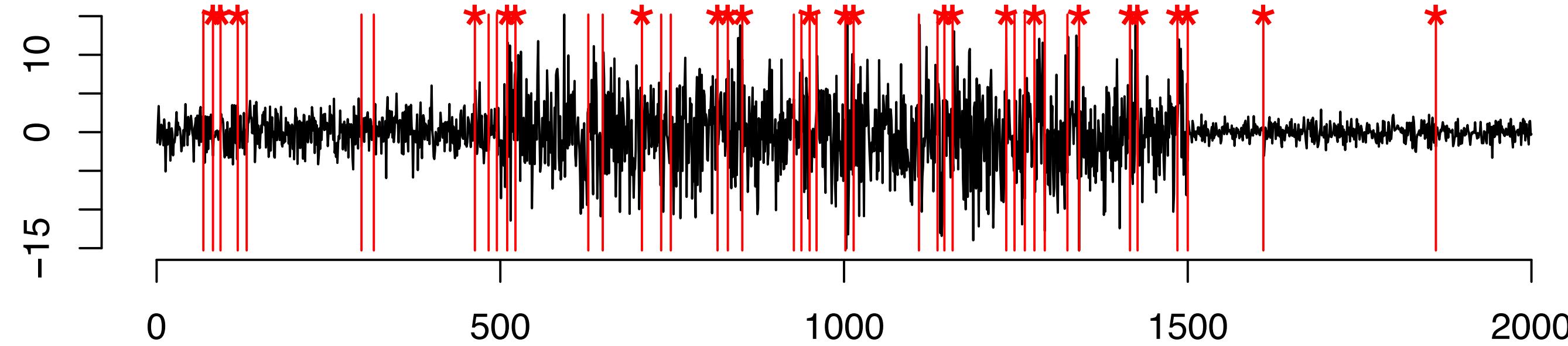


Data thinning: 48 changepoints, o with p-value < 0.05

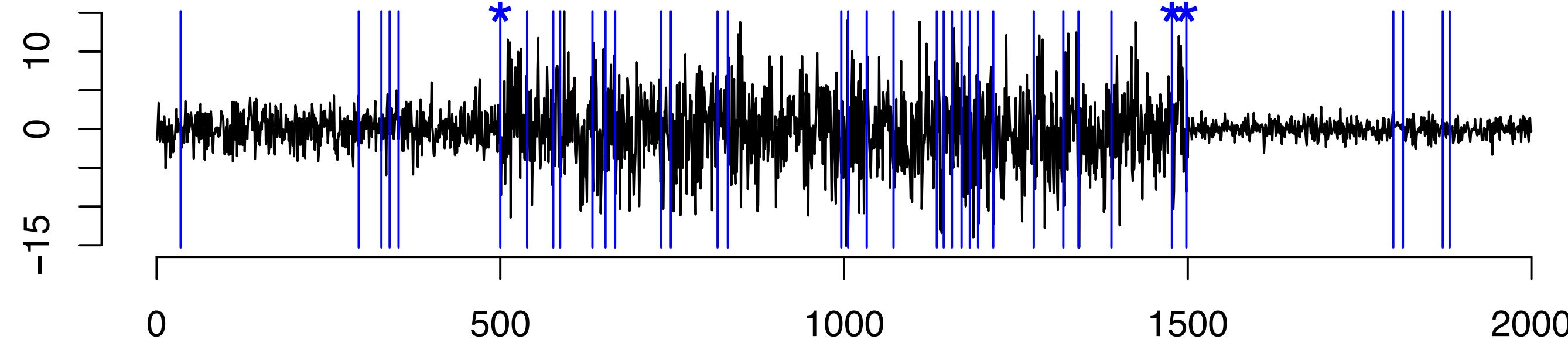


Simulated data with two true changepoints

Naive: 45 changepoints, 24 with p-value < 0.05

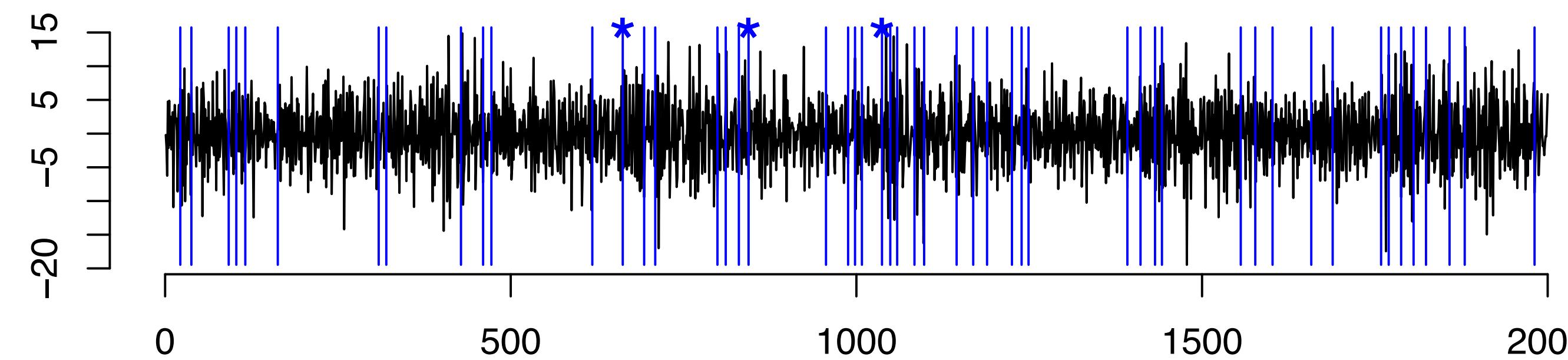


Data thinning: 39 changepoints, 3 with p-value < 0.05

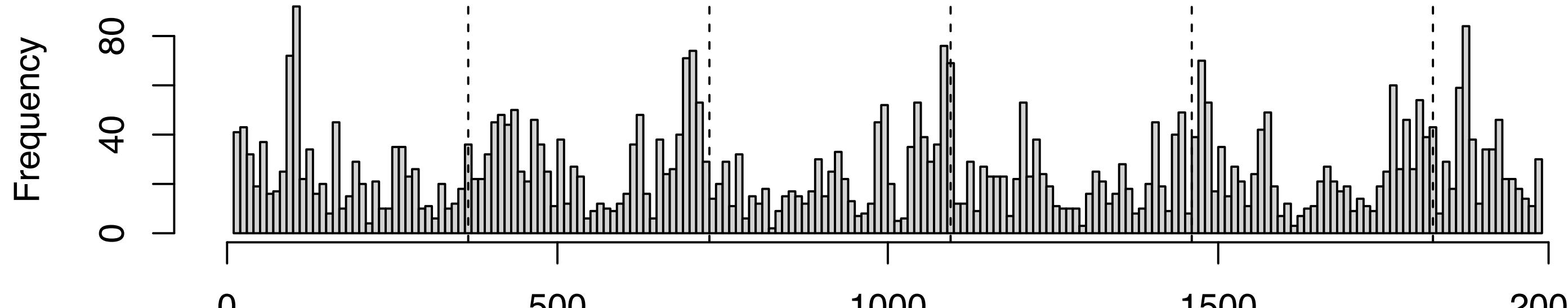


Are the results of our data analysis stable?

Data thinning: 53 changepoints, 3 p-value < 0.05



Number of data thinning replicates with changepoint



Number of data thinning replicates with p-value < 0.05

