



Fundamentals of Genomic Prediction and Data-Driven Crop Breeding (November 24-28, 2025)

Understanding Regression and Ordinary Least Squares

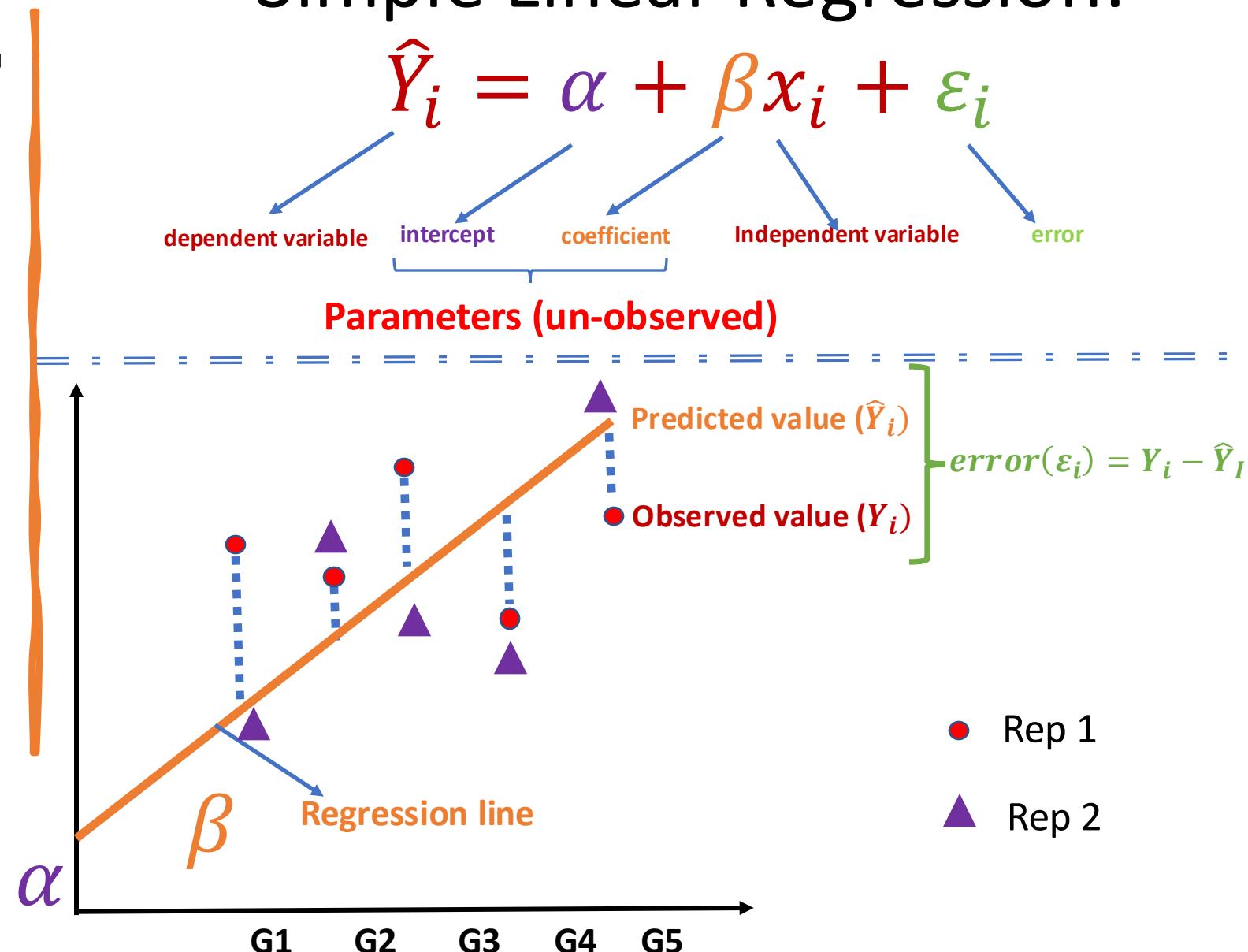
Module 2
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Ordinary Least squares (OLS)

The aim is to estimate α and β (fixed) parameters by minimizing the squared errors

Simple Linear Regression:



OLS Extended to Markers

Simple marker regression model

$$Y_n = \mu_m + X_m \beta_n + \varepsilon$$

↓
 y_1
 y_2
 y_3
 y_4
.
 y_n

μ_m is mean of nth marker

↓
 y_{11} 0 0
 y_{21} 2 2
 y_{31} 2 2
 y_{41} 0 0
 y_{51} 0 0
.
 y_{m1} 2 2

β_n is the additive effect of nth marker

↓
error for marker assumed $\varepsilon \sim N(0, \sigma_e^2)$, with mean 0 and marker variance σ_e^2

X_m is a vector or design matrix containing alleles (0, 2 or 1) and connecting it to phenotypic values.

Y_n are the phenotypic values of nth plants/individuals

Aim is to minimize residual squares

$$\operatorname{argmin}(\varepsilon^\top \varepsilon) = \operatorname{argmin}(y - X\beta)^\top (y - X\beta)$$

$$\beta = \dots (X^\top X)^{-1} X^\top Y$$

Determines β such that residual squares are minimal called as **Least Squares**

$$V_\beta = (X^\top X)^{-1} \sigma_e^2$$

$$\text{where, } \sigma_e^2 = \frac{1}{n-1} \sum (y_i - \beta_i)^2$$

variance-covariance estimate for the sample estimates

Numeric Conversion is Key for Regression

Nucleotide Format

	SNP1	SNP2	SNP3	SNP4	SNP5	SNPm
Allele	A/G	C/T	G/A	T/C	A/G	C/T	A/G
Genotype 1	AA	CC	GA	TT	GG	CC	AA
Genotype 2	AA	TT	AA	TT	GG	TT	AA
Genotype 3	AG	TT	GG	TT	GG	TT	AG
Genotype 4	GG	CC	AA	TC	AA	CC	NA
Genotype n	AG	TT	AA	TC	AG	TT	GG

Numeric Format

	SNP1	SNP2	SNP3	SNP4	SNP5	SNPm
Reference Allele	A/G	C/T	G/A	T/C	A/G	C/T	A/G
Genotype 1	2	2	1	2	0	2	2
Genotype 2	2	0	0	2	0	0	2
Genotype 3	1	0	2	2	0	0	2
Genotype 4	0	2	0	1	2	2	NA
Genotype n	1	0	0	1	1	0	0

General Linear Model

$$y = X\beta + \varepsilon$$

where,

y = vector of dependent values (observed)

X = Design matrix for observations

β =unknow parameter to estimate

ε =residuals (deviations) and are equal to $y - X\beta$

Ordinary Least Square (OLS)

$$\varepsilon \sim MNV(0, \sigma_\varepsilon^2 I)$$

$$\beta = (\hat{X}X)^{-1} \hat{X}Y$$

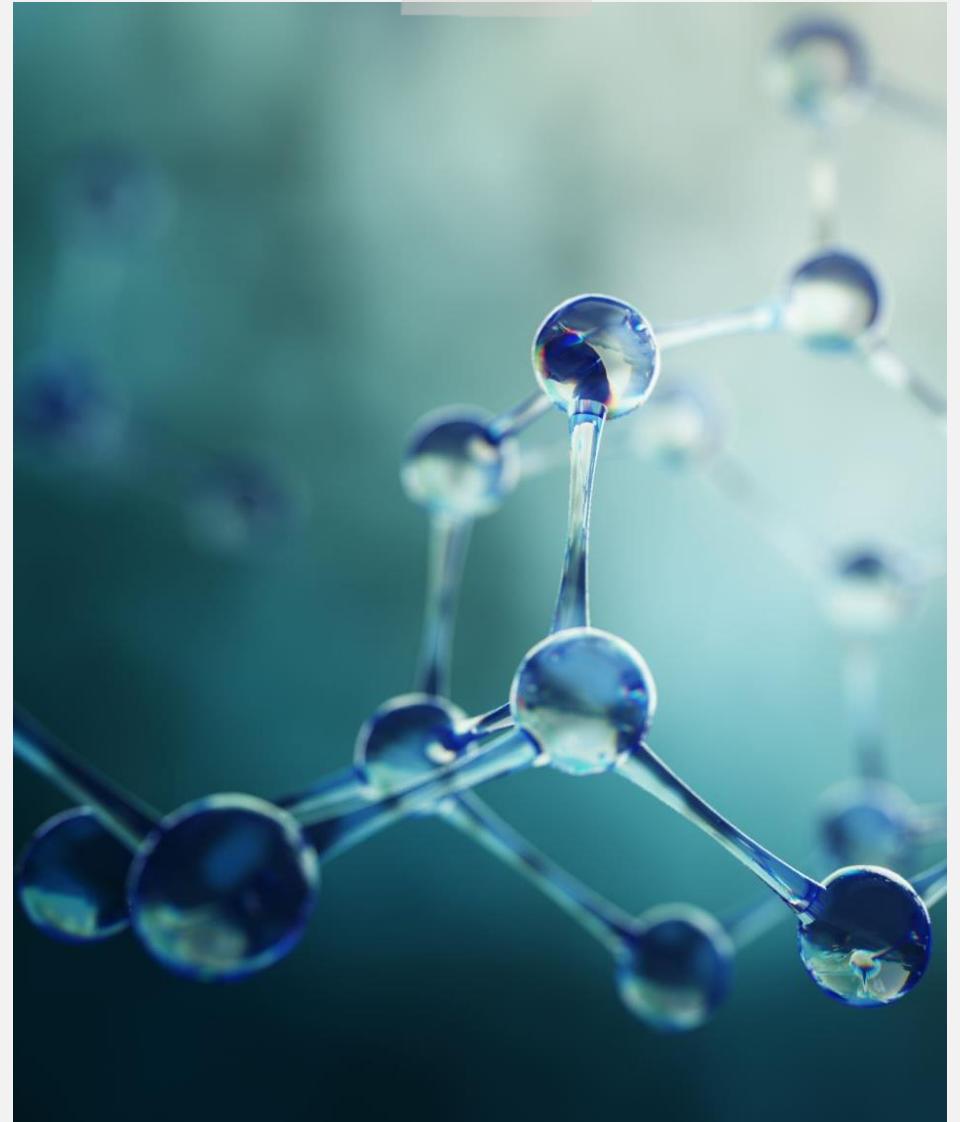
Residuals are homoscedastic and uncorrelated

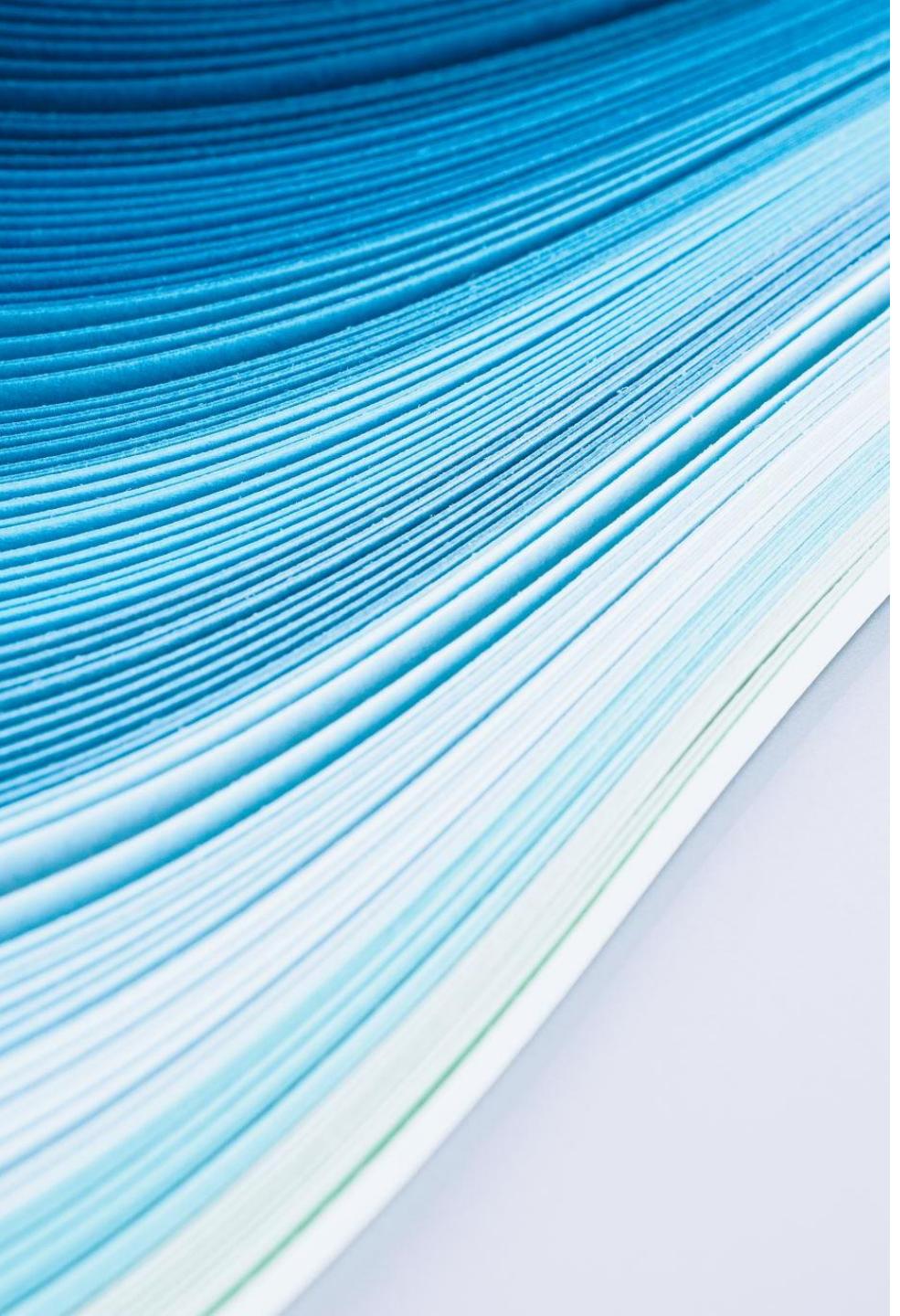
Generalized Least Square (GLS)

$$\varepsilon \sim MNV(0, V)$$

$$\beta = (\hat{X}V^{-1}X)^{-1} \hat{X}V^{-1}Y$$

Residuals are heteroscedastic and/or dependent,





OLS is BLUE?

Expected value:

$$\begin{aligned} E(\widehat{\beta}) &= (\widehat{X}\widehat{X})^{-1} \widehat{X} \widehat{E}(Y) \\ &= (\widehat{X}\widehat{X})^{-1} \widehat{X} \widehat{(\beta)} \\ E(\widehat{\beta}) &= \beta \end{aligned}$$

estimation is true β , and when this condition is met, it is called *unbiased*

When Gauss Markov Theorem is met

1. $E(\varepsilon) = 0$ (*expectation of error is 0*)
2. $\text{variance } = I\sigma^2$ (*errors are uncorrelated*)
3. Homoscedasticity of errors

Then, **OLS → BLUE**

Baseline Model of GS

$$y = \mu + \sum_k x_k \beta_k + \varepsilon$$



How the marker effects (β) are distributed

Solution

- Markers are fitted as random
- We constrain these markers (penalty).
- What distribution are these markers sampled from (Optimization of the constraints)