

# Inverse Numerator Relationship Matrix

Peter von Rohr

2023-11-10

## Structure of $A^{-1}$

- ▶ Look at a simple example of  $A$  and  $A^{-1}$

Table 1: Pedigree Used To Compute Inverse Numerator Relationship Matrix

Calf	Sire	Dam
1	NA	NA
2	NA	NA
3	NA	NA
4	1	2
5	3	2

## Numerator Relationship Matrix $A$

$$A = \begin{bmatrix} 1.0000 & 0.0000 & 0.0000 & 0.5000 & 0.0000 \\ 0.0000 & 1.0000 & 0.0000 & 0.5000 & 0.5000 \\ 0.0000 & 0.0000 & 1.0000 & 0.0000 & 0.5000 \\ 0.5000 & 0.5000 & 0.0000 & 1.0000 & 0.2500 \\ 0.0000 & 0.5000 & 0.5000 & 0.2500 & 1.0000 \end{bmatrix}$$

## Inverse Numerator Relationship Matrix $A^{-1}$

$$A^{-1} = \begin{bmatrix} 1.5000 & 0.5000 & 0.0000 & -1.0000 & 0.0000 \\ 0.5000 & 2.0000 & 0.5000 & -1.0000 & -1.0000 \\ 0.0000 & 0.5000 & 1.5000 & 0.0000 & -1.0000 \\ -1.0000 & -1.0000 & 0.0000 & 2.0000 & 0.0000 \\ 0.0000 & -1.0000 & -1.0000 & 0.0000 & 2.0000 \end{bmatrix}$$

# Conclusions

- ▶  $A^{-1}$  has simpler structure than  $A$  itself
- ▶ Non-zero elements only at positions of parent-progeny and parent-mate positions
- ▶ Parent-mate positions are positive, parent-progeny are negative

# Henderson's Rules

- ▶ Based on LDL-decomposition of  $A$

$$A = L * D * L^T$$

where  $L$  Lower triangular matrix  
 $D$  Diagonal matrix

- ▶ Why?
  - ▶ matrices  $L$  and  $D$  can be inverted directly, we 'll see how ...
  - ▶ construct  $A^{-1} = (L^T)^{-1} * D^{-1} * L^{-1}$

## Example

$$L = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ 0.5 & 0.5 & 0.0 & 1.0 & 0.0 \\ 0.0 & 0.5 & 0.5 & 0.0 & 1.0 \end{bmatrix}$$

$$D = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.5 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.5 \end{bmatrix}$$

→ Verify that  $A = L * D * L^T$

# Decomposition of True Breeding Value

- ▶ True breeding value ( $u_i$ ) of animal  $i$

$$u_i = \frac{1}{2}u_s + \frac{1}{2}u_d + m_i$$

- ▶ Do that for all animals in pedigree

## Decomposition for Example

$$u_1 = m_1$$

$$u_2 = m_2$$

$$u_3 = m_3$$

$$u_4 = \frac{1}{2}u_1 + \frac{1}{2}u_2 + m_4$$

$$u_5 = \frac{1}{2}u_3 + \frac{1}{2}u_2 + m_5$$

## Matrix Vector Notation

- ▶ Define vectors  $u$  and  $m$  as
- ▶ Coefficients of  $u_s$  and  $u_d$  into matrix  $P$

$$u = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix}, m = \begin{bmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \\ m_5 \end{bmatrix}, P = \begin{bmatrix} 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.5 & 0.5 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.5 & 0.5 & 0.0 & 0.0 \end{bmatrix}$$

- ▶ Result: Decomposition of true breeding values

$$u = P \cdot u + m$$

# Recursive Decomposition

- ▶ True breeding values of  $s$  and  $d$  can be decomposed into

$$u_s = \frac{1}{2}u_{ss} + \frac{1}{2}u_{ds} + m_s$$
$$u_d = \frac{1}{2}u_{sd} + \frac{1}{2}u_{dd} + m_d$$

where

$ss$	sire of $s$
$ds$	dam of $s$
$sd$	sire of $d$
$dd$	dam of $d$

## Example

- ▶ Add animal 6 with parents 4 and 5 to our example pedigree

Calf	Sire	Dam
1	NA	NA
2	NA	NA
3	NA	NA
4	1	2
5	3	2
6	4	5

## First Step Of Decomposition

$$u_1 = m_1$$

$$u_2 = m_2$$

$$u_3 = m_3$$

$$u_4 = \frac{1}{2}u_1 + \frac{1}{2}u_2 + m_4$$

$$u_5 = \frac{1}{2}u_3 + \frac{1}{2}u_2 + m_5$$

$$u_6 = \frac{1}{2}u_4 + \frac{1}{2}u_5 + m_6$$

## Decompose Parents

$$u_1 = m_1$$

$$u_2 = m_2$$

$$u_3 = m_3$$

$$u_4 = \frac{1}{2}m_1 + \frac{1}{2}m_2 + m_4$$

$$u_5 = \frac{1}{2}m_3 + \frac{1}{2}m_2 + m_5$$

$$\begin{aligned} u_6 &= \frac{1}{2} \left( \frac{1}{2}(u_1 + u_2) + m_4 \right) + \frac{1}{2} \left( \frac{1}{2}(u_3 + u_2) + m_5 \right) + m_6 \\ &= \frac{1}{4}(u_1 + u_2) + \frac{1}{2}m_4 + \frac{1}{4}(u_3 + u_2) + \frac{1}{2}m_5 + m_6 \end{aligned}$$

## Decompose Grand Parents

- ▶ Only animal 6 has true breeding values for grand parents

$$\begin{aligned}u_6 &= \frac{1}{4}(u_1 + u_2) + \frac{1}{2}m_4 + \frac{1}{4}(u_3 + u_2) + \frac{1}{2}m_5 + m_6 \\ &= \frac{1}{4}m_1 + \frac{1}{4}m_2 + \frac{1}{4}m_3 + \frac{1}{4}m_2 + \frac{1}{2}m_4 + \frac{1}{2}m_5 + m_6 \\ &= \frac{1}{4}m_1 + \frac{1}{2}m_2 + \frac{1}{4}m_3 + \frac{1}{2}m_4 + \frac{1}{2}m_5 + m_6\end{aligned}$$

# Summary

$$u_1 = m_1$$

$$u_2 = m_2$$

$$u_3 = m_3$$

$$u_4 = \frac{1}{2}m_1 + \frac{1}{2}m_2 + m_4$$

$$u_5 = \frac{1}{2}m_3 + \frac{1}{2}m_2 + m_5$$

$$u_6 = \frac{1}{4}m_1 + \frac{1}{2}m_2 + \frac{1}{4}m_3 + \frac{1}{2}m_4 + \frac{1}{2}m_5 + m_6$$

# Matrix-Vector Notation

- ▶ Use vectors  $u$  and  $m$  again

$$u = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{bmatrix}, m = \begin{bmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \\ m_5 \\ m_6 \end{bmatrix}, L = \begin{bmatrix} 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 \\ 0.50 & 0.50 & 0.00 & 1.00 & 0.00 & 0.00 \\ 0.00 & 0.50 & 0.50 & 0.00 & 1.00 & 0.00 \\ 0.25 & 0.50 & 0.25 & 0.50 & 0.50 & 1.00 \end{bmatrix}$$

- ▶ Result of recursive decomposition of  $u_i$

$$u = L \cdot m$$

## Property of $L$

- ▶ Meaning of Element  $(L)_{ij}$  of Matrix  $L$ :

$$U = L * m$$
$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{bmatrix} = \begin{bmatrix} 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 \\ 0.50 & 0.50 & 0.00 & 1.00 & 0.00 & 0.00 \\ 0.00 & 0.50 & 0.50 & 0.00 & 1.00 & 0.00 \\ 0.25 & 0.50 & 0.25 & 0.50 & 0.50 & 1.00 \end{bmatrix} * \begin{bmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \\ m_5 \\ m_6 \end{bmatrix}$$

## Property of $L$ II

- ▶ Element  $(L)_{ij}$  ( $i > j$ ) is the proportion of  $m_j$  in  $u_i$
- ▶ Given:  $i$  has parents  $s$  and  $d$
- ▶  $m_j$  can only come from  $u_s$  and  $u_d$ , because  
 $u_i = 1/2u_s + 1/2u_d + m_i$
- ▶ The proportion of  $m_j$  in  $u_i$  is half the proportion of  $m_j$  in  $u_s$  and half the proportion of  $m_j$  in  $u_d$

$$\rightarrow L_{ij} = \frac{1}{2}L_{sj} + \frac{1}{2}L_{dj}$$

# Example

►  $L_{41}$ ,  $L_{62}$

$L_{41}$

$L_{62}$

Calf	Sire	Dam
1	NA	NA
2	NA	NA
3	NA	NA
4	1	2
5	3	2
6	4	5

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{bmatrix} = \begin{bmatrix} 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 \\ 0.50 & 0.50 & 0.00 & 1.00 & 0.00 & 0.00 \\ 0.00 & 0.50 & 0.50 & 0.00 & 1.00 & 0.00 \\ 0.25 & 0.50 & 0.25 & 0.50 & 0.50 & 1.00 \end{bmatrix} * \begin{bmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \\ m_5 \\ m_6 \end{bmatrix}$$

## Variance From Recursive Decomposition

$$\begin{aligned} \text{var}(u) &= \text{var}(L \cdot m) \\ &= L \cdot \text{var}(m) \cdot L^T \end{aligned}$$

where  $\text{var}(m)$  is the variance-covariance matrix of all components in vector  $m$ .

- ▶ covariances of components  $m_i$ ,  $\text{cov}(m_i, m_j) = 0$  for  $i \neq j$
- ▶  $\text{var}(m_i)$  computed as shown below

## What is the Variance $var(m_i)$

- ▶ Decomposition of  $var(u_i)$  using  $u_i = 1/2u_s + 1/2u_d + m_i$

$$\begin{aligned}var(u_i) &= var(1/2u_s + 1/2u_d + m_i) \\&= var(1/2u_s) + var(1/2u_d) + \frac{1}{2} * cov(u_s, u_d) + var(m_i) \\&= 1/4var(u_s) + 1/4var(u_d) + \frac{1}{2} * cov(u_s, u_d) + var(m_i)\end{aligned}$$

- ▶ From the definition of  $A$

$$\begin{aligned}var(u_i) &= (1 + F_i)\sigma_u^2 \\var(u_s) &= (1 + F_s)\sigma_u^2 \\var(u_d) &= (1 + F_d)\sigma_u^2 \\cov(u_s, u_d) &= (A)_{sd}\sigma_u^2 = 2F_i\sigma_u^2\end{aligned}$$

## Variance of Mendelian Sampling Terms

- ▶ What is  $var(m_i)$ ?
- ▶ Solve equation for  $var(u_i)$  for  $var(m_i)$

$$var(m_i) = var(u_i) - 1/4var(u_s) - 1/4var(u_d) - 2 * cov(u_s, u_d)$$

- ▶ Insert definitions from A

$$\begin{aligned} var(m_i) &= (1 + F_i)\sigma_u^2 - 1/4(1 + F_s)\sigma_u^2 - 1/4(1 + F_d)\sigma_u^2 - \frac{1}{2} * 2 * F_i\sigma_u^2 \\ &= \left( \frac{1}{2} - \frac{1}{4}(F_s + F_d) \right) \sigma_u^2 \end{aligned}$$

- ▶ True, for both parents  $s$  and  $d$  of animal  $i$  are known

## Unknown Parents

- ▶ Only parent  $s$  of animal  $i$  is known

$$\begin{aligned}u_i &= \frac{1}{2}u_s + m_i \\ \text{var}(m_i) &= \left(1 - \frac{1}{4}(1 + F_s)\right) \sigma_u^2 \\ &= \left(\frac{3}{4} - \frac{1}{4}F_s\right) \sigma_u^2\end{aligned}$$

- ▶ Both parents are unknown

$$\begin{aligned}u_i &= m_i \\ \text{var}(m_i) &= \sigma_u^2\end{aligned}$$

## Result

- ▶ variance-covariance matrix  $\text{var}(m)$  can be written as  $D * \sigma_u^2$  where  $D$  is diagonal

$$\begin{aligned}\rightarrow \text{var}(u) &= L \cdot \text{var}(m) \cdot L^T \\ &= L \cdot D * \sigma_u^2 \cdot L^T \\ &= L \cdot D \cdot L^T * \sigma_u^2 \\ &= A \sigma_u^2\end{aligned}$$

$$\rightarrow A = L \cdot D \cdot L^T$$

## Inverse of $A$ Based on $L$ and $D$

- ▶ Matrix  $A$  was decomposed into  $A = L \cdot D \cdot L^T$
- ▶ Get  $A^{-1}$  as  $A^{-1} = (L^T)^{-1} D^{-1} L^{-1}$
- ▶  $D^{-1}$  is diagonal again with elements

$$(D^{-1})_{ii} = 1/(D)_{ii}$$

## Inverse of $L$

- ▶ Compute  $m$  based on the two decompositions of  $u$

$$u = P \cdot u + m \quad \text{and} \quad u = L \cdot m$$

- ▶ Solve both for  $m$  and set them equal

$$m = u - P \cdot u = (I - P) \cdot u \quad \text{and} \quad m = L^{-1} \cdot u$$

$$(I - P) \cdot u = L^{-1} \cdot u$$

and

$$L^{-1} = I - P$$

## Example

Calf	Sire	Dam
1	NA	NA
2	NA	NA
3	NA	NA
4	1	2
5	3	2

## Matrix $D^{-1}$

- ▶ Because  $D$  is diagonal

$$D = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.5 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.5 \end{bmatrix}$$

- ▶ We get  $D^{-1}$  as

$$D^{-1} = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 2.0 \end{bmatrix}$$

## Matrix $L^{-1}$

- ▶ Use  $L^{-1} = I - P$
- ▶ Matrix  $P$  from simple decomposition

$$P = \begin{bmatrix} 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.5 & 0.5 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.5 & 0.5 & 0.0 & 0.0 \end{bmatrix}$$

- ▶ Therefore

$$L^{-1} = I - P = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ -0.5 & -0.5 & 0.0 & 1.0 & 0.0 \\ 0.0 & -0.5 & -0.5 & 0.0 & 1.0 \end{bmatrix}$$

## Decomposition of $A^{-1}$ I

$$A^{-1} = (L^{-1})^T \cdot D^{-1} \cdot L^{-1}$$

$$(L^{-1})^T \cdot D^{-1}$$

$$\begin{bmatrix} 1.0 & 0.0 & 0.0 & -0.5 & 0.0 \\ 0.0 & 1.0 & 0.0 & -0.5 & -0.5 \\ 0.0 & 0.0 & 1.0 & 0.0 & -0.5 \\ 0.0 & 0.0 & 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{bmatrix} \cdot \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 2.0 \end{bmatrix}$$

$$= \begin{bmatrix} 1.0 & 0.0 & 0.0 & -1.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & -1.0 & -1.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 2.0 \end{bmatrix}$$

## Decomposition of $A^{-1}$ II

$$A^{-1} = (L^{-1})^T \cdot D^{-1} \cdot L^{-1}$$

$$\begin{bmatrix} 1.0 & 0.0 & 0.0 & -1.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & -1.0 & -1.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 2.0 \end{bmatrix} \cdot \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ -0.5 & -0.5 & 0.0 & 1.0 & 0.0 \\ 0.0 & -0.5 & -0.5 & 0.0 & 1.0 \end{bmatrix}$$
$$= \begin{bmatrix} 1.5 & 0.5 & 0.0 & -1.0 & 0.0 \\ 0.5 & 2.0 & 0.5 & -1.0 & -1.0 \\ 0.0 & 0.5 & 1.5 & 0.0 & -1.0 \\ -1.0 & -1.0 & 0.0 & 2.0 & 0.0 \\ 0.0 & -1.0 & -1.0 & 0.0 & 2.0 \end{bmatrix}$$

# Decomposition of $A^{-1}$ III

$$\begin{array}{ccc} & D^{-1} & L^{-1} \\ \hline & \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 2.0 \end{bmatrix} & \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ -0.5 & -0.5 & 0.0 & 1.0 & 0.0 \\ 0.0 & -0.5 & -0.5 & 0.0 & 1.0 \end{bmatrix} \\ \hline \begin{bmatrix} 1.0 & 0.0 & 0.0 & -0.5 & 0.0 \\ 0.0 & 1.0 & 0.0 & -0.5 & -0.5 \\ 0.0 & 0.0 & 1.0 & 0.0 & -0.5 \\ 0.0 & 0.0 & 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{bmatrix} & \begin{bmatrix} 1.0 & 0.0 & 0.0 & -1.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & -1.0 & -1.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & -1.0 \\ 0.0 & 0.0 & 0.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 2.0 \end{bmatrix} & \begin{bmatrix} 1.5 & 0.5 & 0.0 & -1.0 & 0.0 \\ 0.5 & 2.0 & 0.5 & -1.0 & -1.0 \\ 0.0 & 0.5 & 1.5 & 0.0 & -1.0 \\ -1.0 & -1.0 & 0.0 & 2.0 & 0.0 \\ 0.0 & -1.0 & -1.0 & 0.0 & 2.0 \end{bmatrix} \\ (L^{-1})^T & (L^{-1})^T \cdot D^{-1} & A^{-1} \end{array}$$

# Henderson's Rules

- ▶ Both Parents Known
  - ▶ add 2 to the diagonal-element  $(i, i)$
  - ▶ add  $-1$  to off-diagonal elements  $(s, i)$ ,  $(i, s)$ ,  $(d, i)$  and  $(i, d)$
  - ▶ add  $\frac{1}{2}$  to elements  $(s, s)$ ,  $(d, d)$ ,  $(s, d)$ ,  $(d, s)$
- ▶ Only One Parent Known
  - ▶ add  $\frac{4}{3}$  to diagonal-element  $(i, i)$
  - ▶ add  $-\frac{2}{3}$  to off-diagonal elements  $(s, i)$ ,  $(i, s)$
  - ▶ add  $\frac{1}{3}$  to element  $(s, s)$
- ▶ Both Parents Unknown
  - ▶ add 1 to diagonal-element  $(i, i)$
- ▶ Valid without inbreeding