

Inverse Numerator Relationship Matrix

Peter von Rohr

2021-11-12

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

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

Decomposition of Variance

- ▶ Analogous decomposition of $\text{var}(u_i)$

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

- ▶ From the definition of A

$$\text{var}(u_i) = (1 + F_i)\sigma_u^2$$

$$\text{var}(u_s) = (1 + F_s)\sigma_u^2$$

$$\text{var}(u_d) = (1 + F_d)\sigma_u^2$$

$$\text{cov}(u_s, u_d) = (A)_{sd}\sigma_u^2 = 2F_i\sigma_u^2$$

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

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

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 before

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

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

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

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