Inverse Numerator Relationship Matrix

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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

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

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

$\rightarrow$ 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

$$
\begin{aligned}
u_1 &= m_1 \\
u_2 &= m_2 \\
u_3 &= m_3 \\
u_4 &= \frac{1}{2}u_1 + \frac{1}{2}u_2 + m_4 \\
u_5 &= \frac{1}{2}u_3 + \frac{1}{2}u_2 + m_5
\end{aligned}
$$

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 $var(u_i)$

based on the decomposition of u_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 $var(m_i)$

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

- Insert definitions from A

Diagonal Element of Matrix D for animal i

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

var(m_4) = (1/2 - 1/4(F_1 + F_2)) \sigma_u^2; obtain F_1 and F_2 from matrix A

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

Unknown Parents

- Only parent s of animal i is known

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

- Both parents are unknown

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

Recursive Decomposition

So far: Simple Decomposition: u = P * u + m

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

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

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

$$u_1 = m_1$$

$$u_2 = m_2$$

$$u_3 = m_3$$

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

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

new animal 6: $$u_6 = \frac{1}{2}u_4 + \frac{1}{2}u_5 + m_6$$

Decompose Parents

$$
\begin{aligned}
u_1 &= m_1 \\
u_2 &= m_2 \\
u_3 &= m_3 \\
u_4 &= \frac{1}{2}m_1 + \frac{1}{2}m_2 + m_4 \\
u_5 &= \frac{1}{2}m_3 + \frac{1}{2}m_2 + m_5 \\
u_6 &= \frac{1}{2}\left(\frac{1}{2}(u_1 + u_2) + m_4\right) + \frac{1}{2}\left(\frac{1}{2}(u_3 + u_2) + m_5\right) + m_6 \\
&= \frac{1}{4}(u_1 + u_2) + \frac{1}{2}m_4 + \frac{1}{4}(u_3 + u_2) + \frac{1}{2}m_5 + m_6
\end{aligned}
$$

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

Full recursive decomposition:
==> all breeding values are decomposed into sums of mendelian sampling terms

$$
\begin{aligned}
u_1 &= m_1 \\
u_2 &= m_2 \\
u_3 &= m_3 \\
u_4 &= \frac{1}{2} m_1 + \frac{1}{2} m_2 + m_4 \\
u_5 &= \frac{1}{2} m_3 + \frac{1}{2} m_2 + m_5 \\
u_6 &= \frac{1}{4} m_1 + \frac{1}{2} m_2 + \frac{1}{4} m_3 + \frac{1}{2} m_4 + \frac{1}{2} m_5 + m_6
\end{aligned}
$$

Matrix-Vector Notation

Matrix L is lower-triangular

- Use vectors u and m again

$$u = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{bmatrix}, \ m = \begin{bmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \\ m_5 \\ m_6 \end{bmatrix}, \ L = \begin{array}{r} 1 \\ 2 \\ 3 \\ \\ \\ \\ \end{array} \begin{bmatrix} 1.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 & 0.00 & 0.00 \\ 0.00 & 0.00 & 1.00 & 0.00 & 0.00 & 0.00 \\ 0.50 & 0.50 & 0.00 & 1.00 & 0.00 & 0.00 \\ 0.00 & 0.50 & 0.50 & 0.00 & 1.00 & 0.00 \\ 0.25 & 0.50 & 0.25 & 0.50 & 0.50 & 1.00 \end{bmatrix}$$

- Result of recursive decomposition of u_i

$$u = L \cdot m$$

Property of L

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

$$\mathbf{u} = \mathbf{L} * \mathbf{m}$$

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

Property of L II

lower triangle of L

- 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 $u_i = 1/2 u_s + 1/2 u_d + m_i$
- 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}

proportion of m_2 in the breeding value of u_6

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

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

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

- covariances of components m_i, $cov(m_i, m_j) = 0$ for $i \neq j$
- $var(m_i)$ computed as shown before

Result

Text

- variance-covariance matrix $var(m)$ can be written as $D * \sigma_u^2$ where D is diagnoal

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

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

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

simple decomposition **full recursive decomposition**

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

- 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

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

Matrix P is obtained from simple decomposition of u

Example

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

Matrix D^{-1}

(D)44 = (1/2 - 1/4(F_1 + F_2))
where F_1 is inbreeding coefficient
of animal 1 and F_2 is the inbreeding
coefficient of animal 2 and they are
obtained from the diagonal elements
of matrix A, as F_1 = (A)11 - 1 and
F_2 = (A)22 - 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

$$P = \begin{bmatrix} 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.5 & 0.5 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.5 & 0.5 & 0.0 & 0.0 \end{bmatrix} \begin{matrix} \\ \\ \\ 4 \\ 5 \end{matrix}$$

- 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

rule for animal 4

- 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)

Rule for animals 1, 2 and 3

- Valid without inbreeding

Apply Henderson's rules for our example pedigree:
Preparation step: Start with empty matrix A^{-1}, all elements are 0

Animal 1: both parents unknown ==> add to empty matrix +1 to diagonal element (1,1)
Animal 2: …
Animal 3: …
Animal 4: parents 1 and 2:
  add +2 to (4,4),
  subtract 1 from (1,4), (2,4), (4,1) and element (4,2)
  add 1/2 to (1,1), (2,2), (1,2) and (2,1)
Animal 5:
Animal 6:

Add up all the contributions:

(A)11: +1 + 1/2 = 1.5

In R: verify the computation of A inverse by the function getAInv()