Inverse Numerator Relationship Matrix

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Recap: 2022-11-18

- * Introduction into numerator relationship matrix A
- * Computation of elements of A
- * MME require A^{-1}, the inverse of A

* For our examples in the course, A^{-1} by pedigreemm::getAinv(), only possible for small datasets.

==> Find a strategy to efficiently construct A^{-1} directly from the pedigree, without first constructing A.

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
$\sqrt{1}$	NA	NA
2	NA	NA
3	NA	NA
4	1	2
5	3	2

Founder animals = Animals without known parents

Numerator Relationship Matrix A

	1.0000	0.0000	0.0000	0.5000	0.0000]
	0.0000	1.0000	0.0000	0.5000	0.5000
A =	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	0.0000 0.5000 0.5000 0.2500 1.0000

In R: pedigreemm:getA()

Inverse Numerator Relationship Matrix A^{-1}

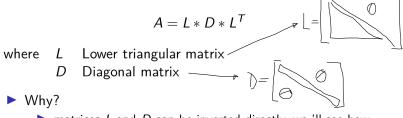
$$A^{-1} = \begin{bmatrix} 1.5000 & 0.5000 & 0.0000 & -1.0000 & 0.0000 \\ 0.5000 & 2.0000 & 0.5000 & -1.0000 & -1.0000 \\ 0.0000 & 0.5000 & 1.5000 & 0.0000 & -1.0000 \\ -1.0000 & -1.0000 & 0.0000 & 2.0000 & 0.0000 \\ 0.0000 & -1.0000 & -1.0000 & 0.0000 & 2.0000 \end{bmatrix}$$

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



• matrices L and D can be inverted directly, we 'll see how ...

• construct $A^{-1} = (L^T)^{-1} * D^{-1} * L^{-1}$

Given A can be decomposed into the product:

A = L * D * L^{T}, then this can be used to construct the inverse A^{-1},

namely, it follows that

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

this is important, because, inverses L^{-1} and D^{-1} are simpler to compute

Why is $A^{-1} = (L^T)^{-1} * D^{-1} * L^{-1}$?

Because A^{-1} is defined as the matrix that satisfies A^{-1}*A = I

Check: ((L^T)^{-1} * D^{-1} * L^{-1})*L * D * L^{T} = (L^T)^{-1} * D^{-1} * I * D * L^{T} = (L^T)^{-1} * D^{-1} * D * L^{T}=(L^T)^{-1} * L^{T} = I

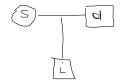
Example

$$L = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ 0.5 & 0.5 & 0.0 & 1.0 & 0.0 \\ 0.0 & 0.5 & 0.5 & 0.0 & 1.0 \end{bmatrix} \rightarrow \text{lower triangular}$$

$$D = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.5 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.5 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.5 & 5 \end{bmatrix}$$

$$\rightarrow \text{Verify that } A = L * D * \begin{bmatrix} T \\ T \end{bmatrix} \xrightarrow{} \text{upper triangular}$$

Decomposition of True Breeding Value



• True breeding value (u_i) of animal *i*

$$u_i = \frac{1}{2}u_s + \frac{1}{2}u_d + \underline{m}_i$$

Mendelian sampling deviation

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Do that for all animals in pedigree

$$(U_i \neq U_j =) \quad \begin{array}{c} U_i = \dots \\ U_i = M_j \\ W_i \neq M_j \\ + M_j \end{array} \quad \begin{array}{c} U_i = M_j \\ U_i =$$

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

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

Result: Decomposition of true breeding values

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

Recursive Decomposition

Decomposition so far was for the true breeding value of animal i into breeding values of parents s and d. Continuing this decomposition with breeding values of parents s and d, leads to the following

True breeding values of s and d can be decomposed into

sire of s 🕀 dam of s $--- u_s = \boxed{\frac{1}{2}u_{ss} + \frac{1}{2}u_{ds}} + m_s$ $u_d = \boxed{\frac{1}{2}u_{sd} + \frac{1}{2}u_{dd}} + m_d$ where ss sire of s grand parents of i ds dam of s sd sire of d dd dam of d

Example

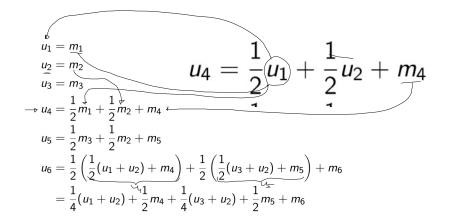
Add animal 6 with parents 4 and 5 to our example pedigree

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

First Step Of Decomposition

-

Decompose Parents

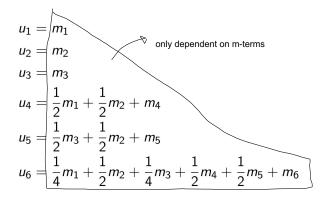


Decompose Grand Parents

Only animal 6 has true breeding values for grand parents

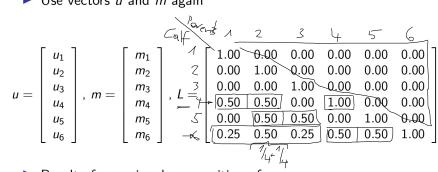
$$u_{6} = \frac{1}{4} \begin{pmatrix} u_{1} + u_{2} \end{pmatrix} + \frac{1}{2}m_{4} + \frac{1}{4}(u_{3} + u_{2}) + \frac{1}{2}m_{5} + m_{6} \\ = \frac{1}{4}m_{1} + \frac{1}{4}m_{2} + \frac{1}{4}m_{3} + \frac{1}{4}m_{2} + \frac{1}{2}m_{4} + \frac{1}{2}m_{5} + m_{6} \\ = \frac{1}{4}m_{1} + \frac{1}{2}m_{2} + \frac{1}{4}m_{3} + \frac{1}{2}m_{4} + \frac{1}{2}m_{5} + m_{6} \end{pmatrix}$$

Summary



Matrix-Vector Notation

Use vectors u and m again

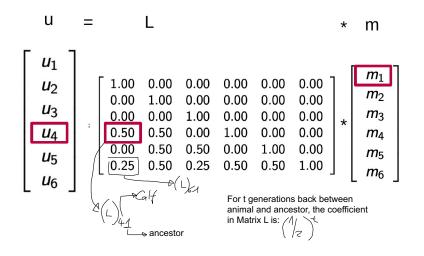


 \triangleright Result of recursive decomposition of u_i

$$u = L \cdot m$$

Property of L

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



Property of *L* II

Mendelian Sampling term of ancestor j of animal i

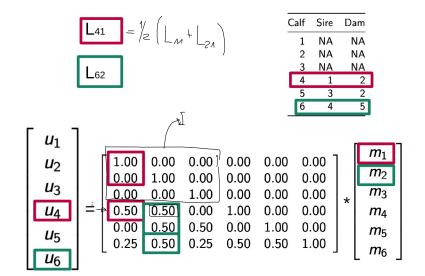
- Element $(L)_{ij}$ (i > j) is the proportion of m_j in u_i
- Given: i has parents s and d
- m_j can only come from u_s and u_d , because $u_i = 1/2u_s + 1/2u_d + m_i$
- The proportion of m_j in u_i is half the proportion of m_j in u_s and half the proportion of m_j in u_d

$$ightarrow L_{ij} = rac{1}{2}L_{sj} + rac{1}{2}L_{dj}$$

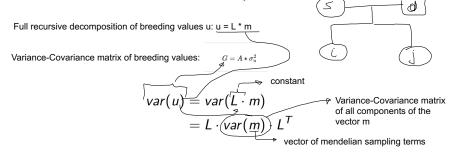
If animals i and j are not related, that means, if j is not an ancestor of i ==> $L_{ij} = 0$, (L) {51} = 0

Example

► *L*₄₁, *L*₆₂



Variance From Recursive Decomposition



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 below

==> var(m) is a diagonal matrix. On the diagonal of var(m), we can find the variance (var(m_i)) for the mendelian sampling component (m_i) of animal i.

What is the Variance $var(m_i)$

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

scalar (just a number)
simple decomposition

$$var(u_i) = var(1/2u_s + 1/2u_d + m_i)$$

$$= var(1/2u_s) + var(1/2u_d) + \frac{1}{2} * cov(u_s, u_d) + var(m_i)$$

$$= 1/4var(u_s) + 1/4var(u_d) + \frac{1}{2} * cov(u_s, u_d) + var(m_i)$$
From the definition of $G = A * \sigma_u^2$
i-th diagonal element of A
element of G

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

$$var(u_d) = (1 + F_s)\sigma_u^2$$

$$var(u_d) = (1 + F_s)\sigma_u^2$$

$$F_i = \frac{1}{2} * (A)_{sd}$$

Variance of Mendelian Sampling Terms

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

$$var(m_i) = \underbrace{var(u_i)}_{Var(u_i)} - \frac{1}{4}var(u_s) - \frac{1}{4}var(u_d) - 2 * cov(u_s, u_d)$$

$$linsert definitions from XG$$

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

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

Unknown Parents

Only parent s of animal i is known

s of animal *i* is known

$$u_{i} = \frac{1}{2}u_{s} + \underline{m_{i}}$$

$$var(m_{i}) = \left(1 - \frac{1}{4}(1 + F_{s})\right)\sigma_{u}^{2}$$

$$= \left(\frac{3}{4} - \frac{1}{4}F_{s}\right)\overline{\sigma_{u}^{2}}$$

L Ŝ

Both parents are unknown

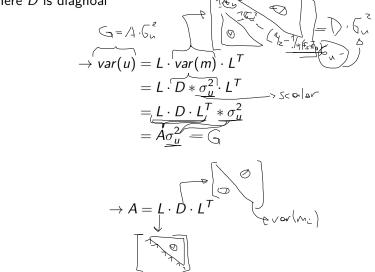
founder

$$u_{i} = m_{i}$$

$$var(m_{i}) = \int \sigma_{u}^{2}$$
Using var(m_{i}) to build up the diagonal matrix: var(m)
$$(var(m_{i}) = \int \sigma_{u}^{2} + \int \sigma_{u}^{2}$$

Result

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

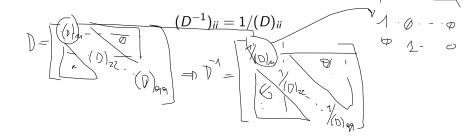


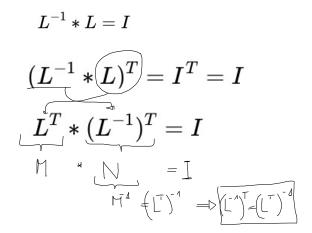
Inverse of A Based on L and D

$$A^{-1} = \underbrace{(\underline{L}^T)^{-1}}_{\left(\lfloor \underline{-}^{\prime} \rfloor \right)^T} * D^{-1} * L^{-1} = \underbrace{(L^{-1})^T * D^{-1} * L^{-1}}_{\mathcal{F}}$$

Matrix A was decomposed into A = L · D · L^T
 Get A⁻¹ as A⁻¹ = (L^T)⁻¹D⁻¹L⁻¹

• D^{-1} is diagonal again with elements

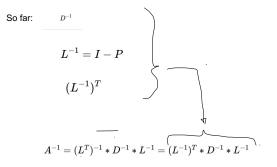




Inverse of
$$L \rightarrow L^{-1} Z$$

Compute m based on the two decompositions of u $\underbrace{u = \underbrace{P \cdot u}_{(-1)} + \underline{m}}_{\text{substance}} \text{ and } \underbrace{u = L \cdot \underline{m}}_{(-1)}$ full- recorsive pre-malty h v. [Solve both for *m* and set them equal L^{-1} = L^{-1} Lm $m = u - P \cdot u = (I - P) \cdot u$ and $m = L^{-1} \cdot u$ $\underbrace{(I-P)}_{\Box} \cdot \underline{u} = \underbrace{L^{-1}}_{\Box} \cdot \underline{u}$ and

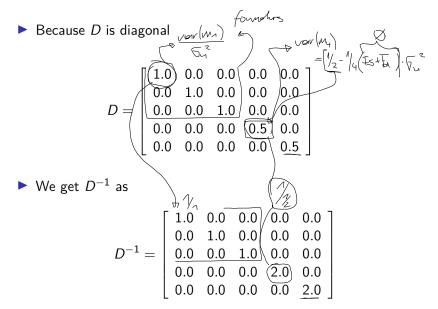
$$L^{-1} = I - \underbrace{P}_{P}$$



Example

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

Matrix D^{-1}



Matrix L^{-1}

► Use
$$L^{-1} = I - P$$

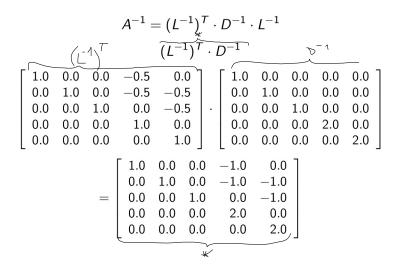
Matrix P from simple decomposition

$$P = \begin{bmatrix} 7 & 7 & 7 & 7 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.5 & 0.5 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.5 & 0.5 & 0.0 & 0.0 \end{bmatrix}$$

► 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



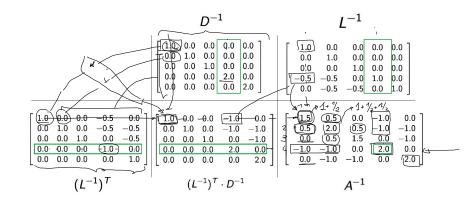
Decomposition of A^{-1} II

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

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

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

Decomposition of A^{-1} III



Henderson's Rules

 $\rightarrow Var(M_{L}) = (1/2 - 1/4(F_{s} + F_{or}))^{2}$

- 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

For a general pedigree with inbreeding, we have to know the inbreeding coefficients of all animals. Inbreeding coefficients can be obtained from the diagonal elements of A. But for large pedigree, we cannot compute all diagonal elements of A.