

Use R to generate random positive definite matrix with zero constraints

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How to use R to generate a random symmetric positive definite matrix with zero constraints?



For example, I would like to generate a 4 by 4 random symmetric positive definite matrix $\Omega\in\mathbb{R}^{4 imes4}$, and we know $\Omega_{1,2}=\Omega_{2,1}=\Omega_{1,3}=\Omega_{3,1}=0$. How can I do that in R?



What I had in mind is something like Cholesky decomposition $LL^T=\Omega$, where row L_i and row L_i are orthogonal if $\Omega_{ij}=0$. Possibly solve by the Lagrangian multiplier. But I am not really sure how to implement this. Or if this is possible at all.



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edited yesterday





3 — I haven't thought about it deeply, but what I have in my mind is that you cannot randomly generate a PD matrix with an equal probability. Think that any positive constant times the identity matrix is positive definite and we cannot even randomly choose a positive number from positive real numbers unless you employ a proper distribution on the range. – Stati yesterday 🖍



@Stati Thanks. I am looking for a general way to generate PD with zero constraints. Of course, cIsatisfies the zeros, but it is not general. Also, I understand that some zero structures are simply less "likely", or are hard, to generate a PD random matrix. - Tan yesterday



Yes, cI is an extreme case. However, if you cannot generate it even in a restrictive situation, it would be much harder to do that in general. – Stati yesterday 🖍



Generate the non-zero elements in the subdiagonal part of the matrix, eg from an Exponential distribution, complete by symmetry and check for definite positivity. If not, repeat, &tc. - Xi'an yesterday 🧪

3 Answers

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I'm not sure if this is what you want, but for the specific example you gave (this doesn't necessarily generalize easily to arbitrary zero constraints, as the algebra can get messy!)

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ullet if L is a lower-triangular matrix with positive values on the diagonal then $\Omega=LL^{ op}$ is positive definite (requiring the diagonal to be positive is not necessary for positive

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definiteness, but makes the decomposition unique: see Pinheiro and Bates 1996 "Unconstrained parametrizations for variance-covariance matrices").

- $\Omega_{12}=L_{11}L_{21}$ and $\Omega_{13}=L_{11}L_{31}$. Thus, I *think* that without any further loss of generality, a lower-triangular matrix with a positive diagonal and $L_{21}=L_{31}=0$ will give you the constraint pattern you want. (Setting $L_{11}=0$ would give you a singular matrix.)
- "random" is pretty vague. (You didn't say "uniform" ...) We could for example pick $\theta_{ii}\sim U(0,20)$, $\theta_{ij}\sim U(-10,10)$ (for $i\neq j$ and $\{i,j\}$ not equal to $\{2,1\}$ or $\{3,1\}$).

```
set.seed(101)
m \leftarrow matrix(0, 4, 4)
diag(m) <- runif(4, max=20)</pre>
m[lower.tri(m)] <- runif(6, min=-10, max=10)</pre>
m[2,1] \leftarrow m[3,1] \leftarrow 0
S <- m %*% t(m)
         [,1]
                     [,2]
                                 [,3]
                                             [,4]
[1,] 55.41265 0.0000000
                           0.000000 12.634888
[2,] 0.00000 0.7682458 -2.919309
[3,] 0.00000 -2.9193087 212.553839
                                       4.881917
[4,] 12.63489 2.1388607
                            4.881917 182.698471
eigen(S)$values
[1] 213.387898 183.174454 54.170033 0.700823
```

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edited 21 hours ago

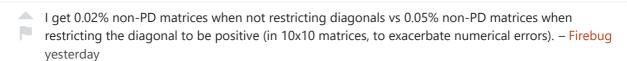
answered yesterday

Ben Bolker

32.9k

90 121

A Is positive diagonal in L even required for $\Sigma = LL^T$ to be PD? – Firebug yesterday ho



1 See edits – Ben Bolker yesterday

Great! I always searched for that reference as well, was needing it for a project actually, so thank you! – Firebug yesterday



Every d imes d symmetric positive (semi)definite matrix Σ can be factored as



$$\Sigma = \Lambda'\,Q'\,Q\,\Lambda$$



where Q is an orthonormal matrix and Λ is a diagonal matrix with non-negative(positive) entries $\lambda_1, \ldots, \lambda_d$. (Σ is always the covariance matrix of *some* d-variate distribution and QQ' will be its correlation matrix; the λ_i are the standard deviations of the marginal distributions.)

Let's interpret this formula. The (i,j) entry $\Sigma_{i,j}$ is the dot product of columns i and j of Q, multiplied by $\lambda_i \lambda_j$. Thus, the zero-constraints on Σ are orthogonality constraints on the dot products of the columns of Q.

(Notice that all diagonal entries of a positive-definite matrix must be nonzero, so I assume the zero-constraints are all off the diagonal. I also extend any constraint on the (i,j) entry to a constraint on the (j,i) entry, to assure symmetry of the result.)

One (completely general) way to impose such constraints is to generate the columns of Q sequentially. Use any method you please to create a $d \times d$ matrix of initial values. At step $i=1,2,\ldots,d$, alter column i regressing it on all the columns $1,2,\ldots,i-1$ of Q that need to be orthogonal to it and retaining the residuals. Normalize those results so their dot product (sum of squares) is unity. That is column i of Q.

Having created an instance of Q, randomly generate the diagonal of Λ any way you please (as discussed in the closely related answer at https://stats.stackexchange.com/a/215647/919).

The following R function $r_{\mathbb{Q}}$ uses iid standard Normal variates for the initial values by default. I have tested it extensively with dimensions d=1 through 200, checking systematically that the intended constraints hold. I also tested it with Poisson(0.1) variates, which--because they are likely to be zero--generate highly problematic initial solutions.

The principal input to ro is a logical matrix indicating where the zero-constraints are to be applied. Here is an example with the constraints specified in the question.

As a convenience, you may pass the diagonal of Λ as the second argument to rQ. Its third argument, f, must be a random number generator (or any other function for which f(n) returns a numeric vector of length n).

```
R <- R %*% diag(Lambda)
crossprod(R)
```

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First, generate the random symmetric matrix. Second, apply ledoit wolf regularization to make it SPD.

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answered yesterday



81 166



Does ledoit wolf regularization keeps sparsity? - Tan yesterday