LDL^T and Cholesky Decompositions

L22

This amounts to an LU decomposition of a symmetric, positive-definite matrix that is twice as fast to compute!

Thm: A positive-definite, symmetric matrix S can be uniquely decomposed as

$$S = LDL^T \quad \text{and} \quad \boxed{S = L_1 L_1^T} \leftarrow \text{Cholesky}$$

where:

- D is diagonal with positive diagonal entries
- L is lower-unitriangular
- L_1 is lower-triangular with positive diagonal entries

See the supplement for a proof - it's basically Gram-Schmidt, with $x \cdot y$ replaced by $x^T S y$.

NB: L_1 has full column rank, so $S = L_1 L_1^T$ is necessarily positive-definite and symmetric! (L21)

NB: Let $U = DL^T$.

(scale the rows of L^T by the diagonal entries of D)

Then U is upper-triangular with positive diagonal entries, so U is in REF, so

$$S = L(DL^T) = LU \text{ is the LU decomposition.}$$

This tells us how to compute the LDL^T decomposition.

How to Compute $S = LDL^T$:

Let S be a symmetric matrix.

(1) Compute the LU decomposition $S = LU$.

→ If you have to do a row swap then stop: S is not positive-definite.

→ If the diagonal entries of U are not all positive then stop: S is not positive-definite.

(2) Let D = the matrix of diagonal entries of U. (Set the off-diagonal entries to zero.) Then $U = DL^T$ (magic!) and $S = LDL^T$.

NB: This is the wrong procedure – it doesn't take advantage of the fact that S is symmetric. If you're more clever, you can compute $S = LDL^T$ in $1/3\, n^3$ time, as opposed to $2/3\, n^3$ for LU. See the supplement if you want to know how.

NB: This is still an LU decomposition, so it lets you solve $Sx = b$ in $O(n^2)$ time.

NB: $S = QDQ^T$ and $S = LDL^T$ are both "diagonalizations" in the sense of quadratic forms – more on the HW.

Eg: Find the $S = LDL^T$ decomposition of

$$S = \begin{pmatrix} 2 & 4 & -2 \\ 4 & 9 & -1 \\ -2 & -1 & 14 \end{pmatrix}$$

We use the 2-column method:

$$\begin{array}{ccc} & L & U \\ & \begin{pmatrix} & & \\ & & \\ & & \end{pmatrix} & \begin{pmatrix} 2 & 4 & -2 \\ 4 & 9 & -1 \\ -2 & -1 & 14 \end{pmatrix} \\ \xrightarrow[R_3 += R_1]{R_2 -= 2R_1} & \begin{pmatrix} & & \\ 2 & & \\ -1 & & \end{pmatrix} & \begin{pmatrix} 2 & 4 & -2 \\ 0 & 1 & 3 \\ 0 & 3 & 12 \end{pmatrix} \\ \xrightarrow{R_3 -= 3R_2} & \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 3 & 1 \end{pmatrix} & \begin{pmatrix} 2 & 4 & -2 \\ 0 & 1 & 3 \\ 0 & 0 & 3 \end{pmatrix} \end{array}$$

So $S = LDL^T$ for

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 3 & 1 \end{pmatrix} \qquad D = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix}$$

Check:

$$DL^T = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix} \begin{pmatrix} 1 & 2 & -1 \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 4 & -2 \\ 0 & 1 & 3 \\ 0 & 0 & 3 \end{pmatrix} \overset{\text{(magic!)}}{=} U$$

✓

Cholesky from LDL^T:

If S is positive definite then $S = LDL^T$ where D is diagonal with positive diagonal entries.

If $D = \begin{pmatrix} d_1 & & 0 \\ & \ddots & \\ 0 & & d_n \end{pmatrix}$ set $\sqrt{D} = \begin{pmatrix} \sqrt{d_1} & & 0 \\ & \ddots & \\ 0 & & \sqrt{d_n} \end{pmatrix}$

Then $\sqrt{D} \cdot \sqrt{D} = D$ and $\sqrt{D}^T = \sqrt{D}$, so

$$LDL^T = L\sqrt{D}\sqrt{D}L^T = (L\sqrt{D})(L\sqrt{D})^T$$

So just set

$$\boxed{L_1 = L\sqrt{D} \implies S = L_1 L_1^T}$$

Strang: "$S = A^TA$ is how a positive-definite symmetric matrix is put together.

$S = L_1 L_1^T$ is how you pull it apart."

Eg: $\begin{pmatrix} 2 & 4 & -2 \\ 4 & 9 & -1 \\ -2 & -1 & 14 \end{pmatrix} = L_1 L_1^T$ for

$$L_1 = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 3 & 1 \end{pmatrix} \begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & \sqrt{1} & 0 \\ 0 & 0 & \sqrt{3} \end{pmatrix} = \begin{pmatrix} \sqrt{2} & 0 & 0 \\ 2\sqrt{2} & 1 & 0 \\ -\sqrt{2} & 3 & \sqrt{3} \end{pmatrix}$$

Diagonalizing Quadratic Forms

In the PCA we will be interested in minimizing/maximizing the following kind of function.

Def: A quadratic form in n variables is a function

$$q(x_1, x_2, \dots, x_n) = \text{sum of terms of the form } a_{ij}x_ix_j.$$

Eg: $q(x_1, x_2) = \frac{1}{2}x_1^2 + \frac{1}{2}x_2^2 - 5x_1x_2$

Non-Eg: $q(x_1, x_2) = x_1^2 + x_2^2 + x_1 + x_2$ is not quadratic - x_1, x_2 are linear terms

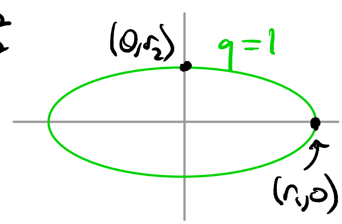
NB: Thinking of $x = (x_1, x_2, \dots, x_n)$ as a vector in $\mathbb{R}^n$, for any scalar c,

$$q(cx) = q(cx_1, \dots, cx_n) = \sum a_{ij}(cx_i)(cx_j)$$

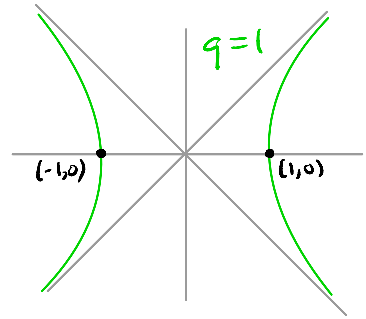
$$= c^2 \sum a_{ij}x_ix_j = c^2 q(x)$$

$$\boxed{q(cx) = c^2 q(x)}$$

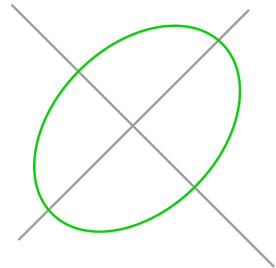
Eg: $q(x_1, x_2) = \left(\frac{x_1}{r_1}\right)^2 + \left(\frac{x_2}{r_2}\right)^2 = \frac{1}{r_1^2}x_1^2 + \frac{1}{r_2^2}x_2^2$ is a quadratic form and $q(x_1, x_2) = 1$ defines an ellipse centered at the origin with radii r_1 & r_2.



Eg: $q(x_1,x_2) = x_1^2 - x_2^2$ is a quadratic form and $q(x_1,x_2)=1$ defines a hyperbola. Indeed, you can factor $x_1^2 - x_2^2 = (x_1-x_2)(x_1+x_2) = 1$, so this is $xy=1$ for $x=x_1-x_2$, $y=x_1+x_2$ (change of variables)



Eg: $q(x_1,x_2) = \frac{5}{2}x_1^2 + \frac{5}{2}x_2^2 - x_1x_2 = 1$ also defines a conic section.
Is it an ellipse or a hyperbola?
What are the axes & radii?



This example is a lot harder because the quadratic form had a cross-term:

$$q(x_1,x_2) = \frac{5}{2}x_1^2 + \frac{5}{2}x_2^2 - x_1x_2$$

The quadratic forms with no cross-terms are the easiest to understand.

Def: A quadratic form is diagonal if it has no cross-terms. In other words, it has the form

$$q(x_1,\dots,x_n) = \lambda_1 x_1^2 + \lambda_2 x_2^2 + \cdots + \lambda_n x_n^2.$$

Eg: We can make a linear change of variables to eliminate the cross term in

$$q(x_1, x_2) = \frac{5}{2}x_1^2 + \frac{5}{2}x_2^2 - x_1x_2.$$

Set $x_1 = \frac{1}{\sqrt{2}}(y_1+y_2)$, $x_2 = \frac{1}{\sqrt{2}}(y_1-y_2)$. Then

$$\begin{aligned}
q(x_1, x_2) &= q\left(\tfrac{1}{\sqrt{2}}(y_1+y_2), \tfrac{1}{\sqrt{2}}(y_1-y_2)\right) \\
&= \frac{5}{2}\cdot\frac{1}{2}(y_1+y_2)^2 + \frac{5}{2}\cdot\frac{1}{2}(y_1-y_2)^2 - \frac{1}{2}(y_1+y_2)(y_1-y_2) \\
&= \frac{5}{4}(y_1^2+y_2^2+2y_1y_2) + \frac{5}{4}(y_1^2+y_2^2-2y_1y_2) - \frac{1}{2}(y_1^2-y_2^2) \\
&= \frac{5}{2}(y_1^2+y_2^2) - \frac{1}{2}(y_1^2-y_2^2) \\
&= 2y_1^2 + 3y_2^2
\end{aligned}$$

This is diagonal!

How did I know to change coordinates like this? Here's how to turn it into a question about symmetric matrices.

Fact: Every quadratic form can be written

$$q(x) = x^T S x$$

for a symmetric matrix S.

NB: $x^T S x = x \cdot (Sx)$ is a scalar.

Eg: $S = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 3 & 5 & 6 \end{pmatrix}$

$$x^T S x = (x_1 \; x_2 \; x_3) \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 3 & 5 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$= (x_1 \; x_2 \; x_3) \begin{pmatrix} 1x_1 + 2x_2 + 3x_3 \\ 2x_1 + 4x_2 + 5x_3 \\ 3x_1 + 5x_2 + 6x_3 \end{pmatrix}$$

$$\begin{aligned} = \; & 1x_1^2 + 2x_1x_2 + 3x_1x_3 \\ & + 2x_2x_1 + 4x_2^2 + 5x_2x_3 \\ & + 3x_3x_1 + 5x_3x_2 + 6x_3^2 \end{aligned}$$

$$= 1x_1^2 + 4x_2^2 + 6x_3^2 + 4x_1x_2 + 6x_1x_3 + 10x_2x_3$$

NB: The $(1,2)$ and $(2,1)$ entries both contribute to the x_1x_2 coefficient, but only the $(1,1)$ entry contributes to the x_1^2 coefficient.

How to get S from q?

The x_i^2 coefficients go on the diagonal, and half of the x_ix_j coefficient goes in each of the (i,j) and (j,i) entries:

$$\begin{aligned} q = \; & a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^2 \\ & + a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3 \end{aligned} \rightsquigarrow S = \begin{pmatrix} a_{11} & a_{12}/2 & a_{13}/2 \\ a_{12}/2 & a_{22} & a_{23}/2 \\ a_{13}/2 & a_{23}/2 & a_{33} \end{pmatrix}$$

NB: q is diagonal $\Longleftrightarrow$ S is diagonal: the a_{ij}'s are the coefficients of the cross terms. So:

$$x^T\begin{pmatrix}\lambda_1 & & 0\\ & \ddots & \\ 0 & & \lambda_n\end{pmatrix}x = \lambda_1 x_1^2 + \lambda_2 x_2^2 + \cdots + \lambda_n x_n^2$$

Key Idea: Let's orthogonally diagonalize S:

$$S = QDQ^T \qquad D = \begin{pmatrix}\lambda_1 & & 0\\ & \ddots & \\ 0 & & \lambda_n\end{pmatrix}$$

Let $x = Qy$: this is a linear change of variables. Then

$$q(x) = x^TSx = x^TQDQ^Tx \overset{x=Qy}{=} (Qy)^TQDQ^T(Qy)$$

$$= y^TQ^TQDQ^TQy \overset{Q^TQ=I_n}{=} y^TDy$$

$$= \lambda_1 y_1^2 + \lambda_2 y_2^2 + \cdots + \lambda_n y_n^2.$$

This is diagonal!

How to Diagonalize a Quadratic Form q:

(1) Write $q(x) = x^TSx$ for a symmetric matrix S

(hard part) (2) Orthogonally diagonalize $S = QDQ^T$

(3) Change variables $x = Qy$.

Then $q = \lambda_1 y_1^2 + \lambda_2 y_2^2 + \cdots + \lambda_n y_n^2$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of S.

Eg: $q(x_1,x_2) = \frac{5}{2}x_1^2 + \frac{5}{2}x_2^2 - x_1x_2$

(1) $q(x) = x^T S x$ for $S = \begin{pmatrix} 5/2 & -1/2 \\ -1/2 & 5/2 \end{pmatrix}$

(2) $S = QDQ^T$ for

$$Q = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad D = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}$$

(3) $x = Qy$: this means

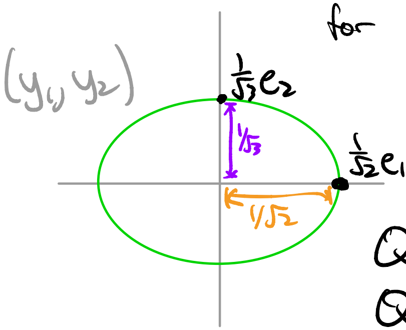
$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = Q\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}(y_1+y_2) \\ \frac{1}{\sqrt{2}}(y_1-y_2) \end{pmatrix}$$

$$\rightsquigarrow \quad q = 2y_1^2 + 3y_2^2$$

These explains where the formulas before came from! It also tells us how to draw the ellipse. This is easy in the (y_1, y_2)-coordinates:

$$q = 2y_1^2 + 3y_2^2 = \left(\frac{y_1}{r_1}\right)^2 + \left(\frac{y_2}{r_2}\right)^2$$

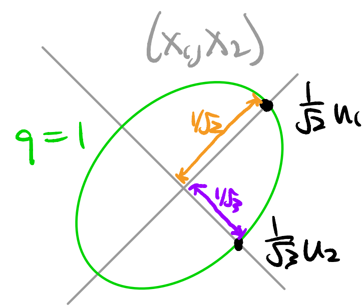
for $r_1 = \frac{1}{\sqrt{2}}$ $r_2 = \frac{1}{\sqrt{3}}$



$$\xrightarrow{\quad Q \quad}$$

$$Qe_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = u_1$$

$$Qe_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = u_2$$



So the axes are the lines thru u_1 & u_2 and the radii are $\frac{1}{\sqrt{2}}$ and $\frac{1}{\sqrt{3}}$. (NB $\|u_1\| = 1 = \|u_2\|$)

Diagonalization also tells us if $q(x)=1$ is an ellipse or a hyperbola:

- it's an ellipse if both eigenvalues are positive:

$$\lambda_1 y_1^2 + \lambda_2 y_2^2 = 1 \qquad \lambda_1, \lambda_2 > 0$$

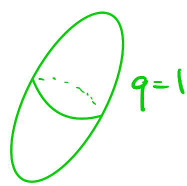
Since λ_1, λ_2 are the eigenvalues of S, this means S is positive-definite

- it's a hyperbola if $\lambda_1 > 0$ and $\lambda_2 < 0$ or vice-versa: this means S is indefinite.

Def: A quadratic form q is positive-definite if $q(x) > 0$ for all $x \neq 0$.

If $q(x) = x^T S x$, then q is positive-definite $\iff$ S is positive-definite by the positive-energy criterion.

In this case, $q=1$ defines an ellipsoid ("egg"), and orthogonally diagonalizing S computes its axes & radii.



How to Put an Ellipsoid in Standard Form:

Let q be a positive-definite quadratic form, so $q(x)=1$ defines an ellipsoid. Write $q(x)=x^T S x$.

Orthogonally diagonalize S:

$$S = QDQ^T \qquad Q=\begin{pmatrix} | & & | \\ u_1 & \cdots & u_n \\ | & & | \end{pmatrix} \qquad D=\begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}$$

The axes go thru $u_1, \ldots, u_n$, and the radii are $1/\sqrt{\lambda_1}, \ldots, 1/\sqrt{\lambda_n}$.

Eg: Let's diagonalize $q(x) = \frac{1}{5}(9x_1^2 + 6x_2^2 - 4x_1x_2)$

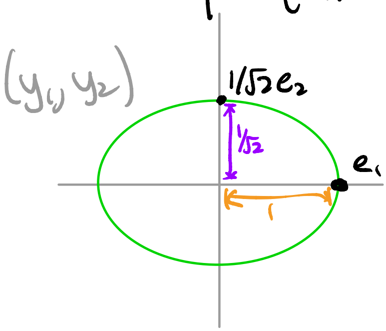
(1) $q(x) = x^T S x$ for $S = \frac{1}{5}\begin{pmatrix} 9 & -2 \\ -2 & 6 \end{pmatrix}$

(2) $S = QDQ^T$ for $Q = \frac{1}{\sqrt{5}}\begin{pmatrix} 1 & -2 \\ 2 & 1 \end{pmatrix} \quad D = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$

(3) $x = Qy \rightsquigarrow q = y_1^2 + 2y_2^2$

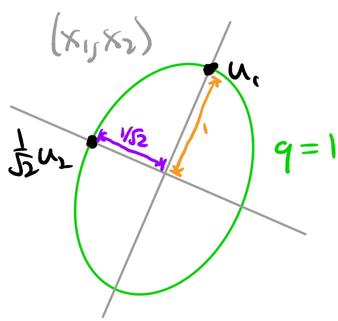
This means $q=1$ is an ellipse:

$$q = \left(\frac{y_1}{r_1}\right)^2 + \left(\frac{y_2}{r_2}\right)^2 = 1 \quad \text{for } r_1 = 1 \quad r_2 = \frac{1}{\sqrt{2}}$$



$$\xrightarrow{\quad Q \quad}$$

$$Qe_1 = \frac{1}{\sqrt{5}}\begin{pmatrix} 1 \\ 2 \end{pmatrix} = u_1$$
$$Qe_2 = \frac{1}{\sqrt{5}}\begin{pmatrix} -2 \\ 1 \end{pmatrix} = u_2$$



So the axes go thru u_1 & u_2, with radii 1 & $1/\sqrt{2}$.