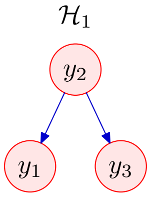
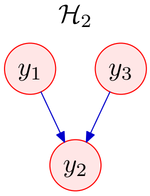
Gaussian Quiz



1. Assuming that the variables y_1, y_2, y_3 in this belief network have a joint Gaussian distribution, which of the following matrices *could be* the covariance matrix?

$$
\begin{array}{cccc}
\text{A} & \text{B} & \text{C} & \text{D} \\
\begin{bmatrix} 9 & 3 & 1 \\ 3 & 9 & 3 \\ 1 & 3 & 9 \end{bmatrix} &
\begin{bmatrix} 8 & -3 & 1 \\ -3 & 9 & -3 \\ 1 & -3 & 8 \end{bmatrix} &
\begin{bmatrix} 9 & 3 & 0 \\ 3 & 9 & 3 \\ 0 & 3 & 9 \end{bmatrix} &
\begin{bmatrix} 9 & -3 & 0 \\ -3 & 10 & -3 \\ 0 & -3 & 9 \end{bmatrix}
\end{array}
$$

2. Which of the matrices could be the *inverse* covariance matrix?



3. Which of the matrices could be the covariance matrix of the second graphical model?

4. Which of the matrices could be the inverse covariance matrix of the second graphical model?

5. Let three variables y_1, y_2, y_3 have covariance matrix $\mathbf{K}_{(3)}$, and inverse covariance matrix $\mathbf{K}^{-1}_{(3)}$.

$$
\mathbf{K}_{(3)} = \begin{bmatrix} 1 & .5 & 0 \\ .5 & 1 & .5 \\ 0 & .5 & 1 \end{bmatrix} \qquad
\mathbf{K}^{-1}_{(3)} = \begin{bmatrix} 1.5 & -1 & .5 \\ -1 & 2 & -1 \\ .5 & -1 & 1.5 \end{bmatrix}
$$

Now focus on the variables y_1 and y_2. Which statements about *their* covariance matrix $\mathbf{K}_{(2)}$ and inverse covariance matrix $\mathbf{K}^{-1}_{(2)}$ are true?

$$
\overset{\text{(A)}}{\mathbf{K}_{(2)} = \begin{bmatrix} 1 & .5 \\ .5 & 1 \end{bmatrix}} \qquad
\overset{\text{(B)}}{\mathbf{K}^{-1}_{(2)} = \begin{bmatrix} 1.5 & -1 \\ -1 & 2 \end{bmatrix}}
$$

The Humble Gaussian Distribution

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Abstract

These are elementary notes on Gaussian distributions, aimed at people who are about to learn about Gaussian processes. I emphasize the following points.

What happens to a covariance matrix and inverse covariance matrix when we omit a variable.

What it means to have zeros in a covariance matrix.

What it means to have zeros in an inverse covariance matrix.

How probabilistic models expressed in terms of ‘energies’ relate to Gaussians.

Why eigenvectors and eigenvalues don't have any fundamental status.

1 Introduction

Let's chat about a Gaussian distribution with zero mean, such as

$$P(\mathbf{y}) = \frac{1}{Z} e^{-\frac{1}{2}\mathbf{y}^{\mathsf{T}}\mathbf{A}\mathbf{y}}, \tag{1}$$

where $\mathbf{A} = \mathbf{K}^{-1}$ is the inverse of the covariance matrix, $\mathbf{K}$, and $Z = [\det 2\pi\mathbf{K}]^{1/2}$. I'm going to emphasize dimensions throughout this note, because I think dimension-consciousness enhances understanding.[1] I'll write

$$\mathbf{K} = \begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{12} & K_{22} & K_{23} \\ K_{13} & K_{23} & K_{33} \end{bmatrix} \tag{4}$$

[1] It's conventional to write the diagonal elements in $\mathbf{K}$ as σ_i^2 and the offdiagonal elements as σ_{ij}. For example

$$\mathbf{K} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_2^2 & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_3^2 \end{bmatrix} \tag{2}$$

A confusing convention, since it implies that σ_{ij} has different dimensions from σ_i, even if all axes i, j have the same dimensions!

Another way of writing an off-diagonal coefficient is

$$K_{ij} = \rho_{ij}\sigma_i\sigma_j, \tag{3}$$

where ρ is the correlation coefficient between i and j. This is a better notation since it's dimensionally consistent in the way it uses the letter σ. But I will stick with the notation K_{ij}.

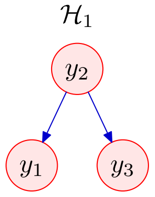
The definition of the covariance matrix is

$$K_{ij} = \langle y_i y_j \rangle \tag{5}$$

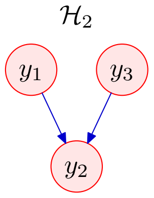
so the dimensions of the element K_{ij} are (dimensions of y_i) times (dimensions of y_j).

1.1 Examples

Let's work through a few graphical models.



EXAMPLE 1



EXAMPLE 2

1.1.1 Example 1

Maybe y_2 is the temperature outside some buildings (or rather, the deviation of the outside temperature from its mean), and y_1 is the temperature deviation inside building 1, and y_3 is the temperature inside building 3. This graphical model says that if you know the outside temperature y_2 then y_1 and y_3 are independent.

Let's consider this generative model:

$$\begin{aligned} y_2 &= \nu_2 && (6)\\ y_1 &= w_1 y_2 + \nu_1 && (7)\\ y_3 &= w_3 y_2 + \nu_3, && (8) \end{aligned}$$

where $\{\nu_i\}$ are independent normal variables with variances $\{\sigma_i^2\}$.

Then we can write down the entries in the covariance matrix, starting with the diagonal entries

$$K_{11} = \langle y_1 y_1 \rangle = \langle (w_1\nu_2 + \nu_1)(w_1\nu_2 + \nu_1) \rangle = w_1^2 \langle {\nu_2}^2 \rangle + 2w_1 \langle \nu_1 \nu_2 \rangle + \langle {\nu_1}^2 \rangle = w_1^2\sigma_2^2 + \sigma_1^2 \tag{9}$$

$$K_{22} = \sigma_2^2 \tag{10}$$

$$K_{33} = w_3^2\sigma_2^2 + \sigma_3^2 \tag{11}$$

So we can fill in this much:

$$\mathbf{K} = \begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{12} & K_{22} & K_{23} \\ K_{13} & K_{23} & K_{33} \end{bmatrix} = \begin{bmatrix} w_1^2\sigma_2^2 + \sigma_1^2 & & \\ & \sigma_2^2 & \\ & & w_3^2\sigma_2^2 + \sigma_3^2 \end{bmatrix} \tag{12}$$

The off diagonal terms are

$$K_{12} = \langle y_1 y_2 \rangle = \langle (w_1\nu_2 + \nu_1)(\nu_2) \rangle = w_1\sigma_2^2 \tag{13}$$

(and similarly for K_{23}) and

$$K_{13} = \langle y_1 y_3 \rangle = \langle (w_1\nu_2 + \nu_1)(w_3\nu_2 + \nu_3) \rangle = w_1 w_3 \sigma_2^2 \tag{14}$$

So the covariance matrix is:

$$\mathbf{K} = \begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{12} & K_{22} & K_{23} \\ K_{13} & K_{23} & K_{33} \end{bmatrix} = \begin{bmatrix} w_1^2\sigma_2^2 + \sigma_1^2 & w_1\sigma_2^2 & w_1 w_3 \sigma_2^2 \\ & \sigma_2^2 & w_3\sigma_2^2 \\ & & w_3^2\sigma_2^2 + \sigma_3^2 \end{bmatrix} \tag{15}$$

(where the remaining blank elements can be filled in by symmetry).

Now let's think about the inverse covariance matrix.

One way to get to it is to write down the joint distribution.

$$\begin{aligned} P(y_1, y_2, y_3 \,|\, \mathcal{H}_1) &= P(y_2)P(y_1 \,|\, y_2)P(y_3 \,|\, y_2) & (16) \\ &= \frac{1}{Z_2}\exp\left(-\frac{y_2^2}{2\sigma_2^2}\right)\frac{1}{Z_1}\exp\left(-\frac{(y_1 - w_1 y_2)^2}{2\sigma_1^2}\right)\frac{1}{Z_3}\exp\left(-\frac{(y_3 - w_3 y_2)^2}{2\sigma_3^2}\right) & (17) \end{aligned}$$

We can now collect all the terms in $y_i y_j$.

$$\begin{aligned} P(y_1, y_2, y_3) &= \frac{1}{Z'}\exp\left(-\frac{y_2^2}{2\sigma_2^2} - \frac{(y_1 - w_1 y_2)^2}{2\sigma_1^2} - \frac{(y_3 - w_3 y_2)^2}{2\sigma_3^2}\right) \\ &= \frac{1}{Z'}\exp\left(-y_2^2\left[\frac{1}{2\sigma_2^2} + \frac{w_1^2}{2\sigma_1^2} + \frac{w_3^2}{2\sigma_3^2}\right] - y_1^2\frac{1}{2\sigma_1^2} + 2y_1y_2\frac{w_1}{2\sigma_1^2} - y_3^2\frac{1}{2\sigma_3^2} + 2y_3y_2\frac{w_3}{2\sigma_3^2}\right) \\ &= \frac{1}{Z'}\exp\left(-\frac{1}{2}\begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix}\begin{bmatrix} \frac{1}{\sigma_1^2} & -\frac{w_1}{\sigma_1^2} & \mathbf{0} \\ -\frac{w_1}{\sigma_1^2} & \left[\frac{1}{\sigma_2^2} + \frac{w_1^2}{\sigma_1^2} + \frac{w_3^2}{\sigma_3^2}\right] & -\frac{w_3}{\sigma_3^2} \\ \mathbf{0} & -\frac{w_3}{\sigma_3^2} & \frac{1}{\sigma_3^2} \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}\right) \end{aligned}$$

So the inverse covariance matrix is

$$\mathbf{K}^{-1} = \begin{bmatrix} \frac{1}{\sigma_1^2} & -\frac{w_1}{\sigma_1^2} & \mathbf{0} \\ -\frac{w_1}{\sigma_1^2} & \left[\frac{1}{\sigma_2^2} + \frac{w_1^2}{\sigma_1^2} + \frac{w_3^2}{\sigma_3^2}\right] & -\frac{w_3}{\sigma_3^2} \\ \mathbf{0} & -\frac{w_3}{\sigma_3^2} & \frac{1}{\sigma_3^2} \end{bmatrix}$$

The first thing I'd like you to notice here is the zeroes. $[\mathbf{K}^{-1}]_{13} = \mathbf{0}$.

The meaning of a zero in an inverse covariance matrix (at location i, j) is *conditional on all the other variables, these two variables i and j are independent.*

Next, notice that whereas y_1 and y_2 were positively correlated (assuming $w_1 > 0$), the coefficient $[\mathbf{K}^{-1}]_{12}$ is negative. It's common that a covariance matrix $\mathbf{K}$ in which all the elements are non-negative has an inverse that includes some negative elements. So positive off-diagonal terms in the covariance matrix always describe positive correlation; but the off-diagonal terms in the inverse covariance matrix can't be interpreted that way. The sign of an element (i, j) in the inverse covariance matrix does *not* tell you about the correlation between those two variables. For example, remember: there is a zero at $[\mathbf{K}^{-1}]_{13}$. But that doesn't mean that variables y_1 and y_3 are uncorrelated. Thanks to their parent y_2, they are correlated, with covariance $w_1 w_3 \sigma_2^2$.

The off-diagonal entry $[\mathbf{K}^{-1}]_{ij}$ in an inverse covariance matrix indicates *how y_i and y_j are correlated if we condition on all the other variables apart from those two:* if $[\mathbf{K}^{-1}]_{ij} < 0$, they are *positively* correlated, conditioned on the others; if $[\mathbf{K}^{-1}]_{ij} > 0$, they are *negatively* correlated.

The inverse covariance matrix is great for reading out properties of conditional distributions in which we condition on *all the variables except one.*

For example, look at $\left[\mathbf{K}^{-1}\right]_{11} = \frac{1}{\sigma_1^2}$; if we know y_2 and y_3, then the probability distribution of y_1 is Gaussian with variance $1/\left[\mathbf{K}^{-1}\right]_{11}$. That one was easy.

Look at $\left[\mathbf{K}^{-1}\right]_{22} = \left[\frac{1}{\sigma_2^2} + \frac{w_1^2}{\sigma_1^2} + \frac{w_3^2}{\sigma_3^2}\right]$. if we know y_1 and y_3, then the probability distribution of y_2 is Gaussian with variance

$$\frac{1}{\left[\mathbf{K}^{-1}\right]_{22}} = \frac{1}{\frac{1}{\sigma_2^2} + \frac{w_1^2}{\sigma_1^2} + \frac{w_3^2}{\sigma_3^2}}. \tag{18}$$

That's not so obvious, but it's familiar if you've applied Bayes theorem to Gaussians – when we do inference of a parent like y_2 given its children, the inverse-variances of the prior and the likelihoods add. Here, the parent variable's inverse variance (also known as its precision) is the sum of the precision contributed by the prior $\frac{1}{\sigma_2^2}$, the precision contributed by the measurement of y_1, $\frac{w_1^2}{\sigma_1^2}$, and the precision contributed by the measurement of y_3, $\frac{w_3^2}{\sigma_3^2}$.

The off-diagonal entries in $\mathbf{K}$ tell us how the *mean* of [the conditional distribution of one variable given the others] depends on [the others].

Let's take variable y_3 conditioned on the other two, for example.

$$\begin{aligned} P(y_3 \,|\, y_1, y_2, \mathcal{H}_1) &\propto P(y_1, y_2, y_3 \,|\, \mathcal{H}_1) \\ &\propto \frac{1}{Z'} \exp\left(-\frac{1}{2} \begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix} \begin{bmatrix} \frac{1}{\sigma_1^2} & -\frac{w_1}{\sigma_1^2} & 0 \\ -\frac{w_1}{\sigma_1^2} & \left[\frac{1}{\sigma_2^2} + \frac{w_1^2}{\sigma_1^2} + \frac{w_3^2}{\sigma_3^2}\right] & -\frac{w_3}{\sigma_3^2} \\ 0 & -\frac{w_3}{\sigma_3^2} & \frac{1}{\sigma_3^2} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \right) \end{aligned}$$

Let's highlight in Blue the terms y_1, y_2 that are fixed and known and uninteresting, and highlight in Green everything that is multiplying the interesting term y_3.

$$\begin{aligned} P(y_3 \,|\, y_1, y_2, \mathcal{H}_1) &\propto P(y_1, y_2, y_3 \,|\, \mathcal{H}_1) \\ &\propto \frac{1}{Z'} \exp\left(-\frac{1}{2} \begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix} \begin{bmatrix} \frac{1}{\sigma_1^2} & -\frac{w_1}{\sigma_1^2} & 0 \\ -\frac{w_1}{\sigma_1^2} & \left[\frac{1}{\sigma_2^2} + \frac{w_1^2}{\sigma_1^2} + \frac{w_3^2}{\sigma_3^2}\right] & -\frac{w_3}{\sigma_3^2} \\ 0 & -\frac{w_3}{\sigma_3^2} & \frac{1}{\sigma_3^2} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \right) \end{aligned}$$

All those blue multipliers in the central matrix aren't achieving anything. We can just ignore them (and redefine the constant of proportionality). For the benefit of anyone with a colour-blind printer, here it is again:

$$P(y_3 \,|\, y_1, y_2, \mathcal{H}_1) \;\propto\; \exp\left(-\frac{1}{2} \begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{w_3}{\sigma_3^2} \\ 0 & -\frac{w_3}{\sigma_3^2} & \frac{1}{\sigma_3^2} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \right)$$

$$P(y_3\,|\,y_1,y_2,\mathcal{H}_1) \;\propto\; \exp\left(-\frac{1}{2}\frac{1}{\sigma_3^2}\left[y_3\right]^2 - \left[y_3\right]\left[0\times y_1 - \frac{w_3}{\sigma_3^2}\times y_2\right]\right)$$

We obtain the mean by completing the square. [2]

$$P(y_3\,|\,y_1,y_2,\mathcal{H}_1) \;\propto\; \exp\left(-\frac{1}{2}\frac{1}{\sigma_3^2}\left[y_3 - \frac{\left[0\times y_1 + \frac{w_3}{\sigma_3^2}\times y_2\right]}{\frac{1}{\sigma_3^2}}\right]^2\right)$$

In this case, this all collapses down, of course, to

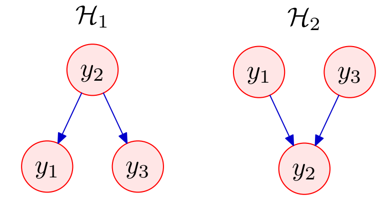
$$P(y_3\,|\,y_1,y_2,\mathcal{H}_1) \;\propto\; \exp\left(-\frac{1}{2}\frac{1}{\sigma_3^2}\left[y_3 - w_3 y_2\right]^2\right), \tag{19}$$

as defined in the original generative model (8).

In general, the offdiagonal coefficients K^{-1} tell us the sensitivity of [the mean of the conditional distribution] to the other variables.

$$\mu_{y_3\,|\,y_1,y_2} = \frac{-K^{-1}_{13}y_1 - K^{-1}_{23}y_2}{K^{-1}_{33}} \tag{20}$$

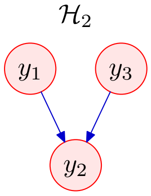
So the conditional mean of y_3 is a linear function of the known variables, and the offdiagonal entries in $\mathbf{K}^{-1}$ tell us the *coefficients* in that linear function.



Example 1 Example 2

1.2 Example 2

Here's another example, where two parents have one child. For example, the price of electricity y_2 from a power station might depend on the price of gas, y_1, and the price of carbon emission rights, y_3.



Example 2

[2] 'Completing the square' is $\frac{1}{2}ay^2 - by = \frac{1}{2}a(y-b/a)^2 + \text{constant}$.

$$y_2 = w_1 y_1 + w_3 y_3 + \nu_2 \tag{21}$$

Note that the units in which gas price, electricity price, and carbon price are measured are all different (pounds per cubic metre, pennies per kWh, and euros per tonne, for example). So y_1, y_3, and y_3 have different dimensions from each other. Most people who do data modelling treat their data as 'just numbers', but I think it is a useful discipline to keep track of dimensions and to carry out only dimensionally valid operations. [Dimensionally valid operations satisfy the two rules of dimensions: (1) only add, subtract and compare quantities that have like dimensions; (2) arguments of all functions like exp, log, sin must be dimensionless. Rule 2 is really just a special case of rule 1, since $\exp(x) = 1 + x + x^2 + \ldots$, so to satisfy rule 1, the dimensions of x must be the same as the dimensions of 1.]

What is the covariance matrix?

Here we assume that the parent variables y_1 and y_3 are uncorrelated.

The covariance matrix is

$$\mathbf{K} = \begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{12} & K_{22} & K_{23} \\ K_{13} & K_{23} & K_{33} \end{bmatrix} = \begin{bmatrix} \sigma_1^2 & w_1\sigma_1^2 & 0 \\ & \sigma_2^2 + w_1^2\sigma_1^2 + w_3^2\sigma_3^2 & w_3\sigma_3^2 \\ & & \sigma_3^2 \end{bmatrix} \tag{22}$$

Notice the zero correlation between the uncorrelated variables $(1, 3)$.

What do you think the $(1, 3)$ entry in the inverse covariance matrix will be? Let's work it out in the same way as before. The joint distribution is

$$\begin{aligned} P(y_1, y_2, y_3 \,|\, \mathcal{H}_2) &= P(y_1)P(y_3)P(y_2 \,|\, y_1, y_3) & (23) \\ &= \frac{1}{Z_1}\exp\left(-\frac{y_1^2}{2\sigma_1^2}\right)\frac{1}{Z_3}\exp\left(-\frac{y_3^2}{2\sigma_3^2}\right)\frac{1}{Z_2}\exp\left(-\frac{(y_2 - w_1y_1 - w_3y_3)^2}{2\sigma_2^2}\right) & (24) \end{aligned}$$

We collect all the terms in $y_i y_j$.

$$\begin{aligned} P(y_1, y_2, y_3) &= \frac{1}{Z'}\exp\left(-\frac{y_1^2}{2\sigma_1^2} - \frac{y_3^2}{2\sigma_3^2} - \frac{(y_2 - w_1y_1 - w_3y_3)^2}{2\sigma_2^2}\right) \\ &= \frac{1}{Z'}\exp\left(-y_1^2\left[\frac{1}{2\sigma_1^2} + \frac{w_1^2}{2\sigma_2^2}\right] - y_2^2\frac{1}{2\sigma_2^2} + 2y_1y_2\frac{w_1}{2\sigma_1^2}\right. \\ &\qquad\qquad \left. -y_3^2\left[\frac{1}{2\sigma_3^2} + \frac{w_3^2}{2\sigma_2^2}\right] + 2y_3y_2\frac{w_3}{2\sigma_2^2} - 2y_3y_1\frac{w_1w_3}{2\sigma_2^2}\right) \\ &= \frac{1}{Z'}\exp\left(-\frac{1}{2}\begin{bmatrix} y_1 & y_2 & y_3 \end{bmatrix}\begin{bmatrix} \left[\frac{1}{2\sigma_1^2} + \frac{w_1^2}{\sigma_2^2}\right] & -\frac{w_1}{\sigma_2^2} & +\frac{w_1w_3}{\sigma_2^2} \\ -\frac{w_1}{\sigma_2^2} & \frac{1}{\sigma_2^2} & -\frac{w_3}{\sigma_2^2} \\ +\frac{w_1w_3}{\sigma_2^2} & -\frac{w_3}{\sigma_2^2} & \left[\frac{1}{2\sigma_3^2} + \frac{w_3^2}{\sigma_2^2}\right] \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}\right) \end{aligned}$$

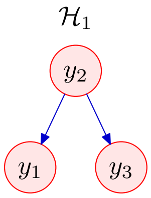
So the inverse covariance matrix is

$$\mathbf{K}^{-1} = \begin{bmatrix} \left[\frac{1}{2\sigma_1^2} + \frac{w_1^2}{\sigma_2^2}\right] & -\frac{w_1}{\sigma_2^2} & +\frac{w_1w_3}{\sigma_2^2} \\ -\frac{w_1}{\sigma_2^2} & \frac{1}{\sigma_2^2} & -\frac{w_3}{\sigma_2^2} \\ +\frac{w_1w_3}{\sigma_2^2} & -\frac{w_3}{\sigma_2^2} & \left[\frac{1}{2\sigma_3^2} + \frac{w_3^2}{\sigma_2^2}\right] \end{bmatrix} \tag{25}$$

Notice (assuming $w_1 > 0$ and $w_3 > 0$) that the offdiagonal term connecting a parent and a child $[\mathbf{K}^{-1}]_{12}$ is negative and the offdiagonal term connecting the two parents $[\mathbf{K}^{-1}]_{13}$ is positive. This positive term indicates that, conditional on all the other variables (*i.e.*, y_2), the two parents y_1 and y_3 are anticorrelated. That's 'explaining away'. Once you know the price of electricity was average, for example, you can deduce that if gas was more expensive than normal, carbon probably was less expensive than normal.

2 Omission of one variable

Consider example 1.



EXAMPLE 1

The covariance matrix of all three variables is:

$$\mathbf{K} = \begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{12} & K_{22} & K_{23} \\ K_{13} & K_{23} & K_{33} \end{bmatrix} = \begin{bmatrix} w_1^2\sigma_2^2 + \sigma_1^2 & w_1\sigma_2^2 & w_1 w_3 \sigma_2^2 \\ & \sigma_2^2 & w_3\sigma_2^2 \\ & & w_3^2\sigma_2^2 + \sigma_3^2 \end{bmatrix} \tag{26}$$

If we decide we want to talk about the joint distribution of just y_1 and y_2, the covariance matrix is simply the sub-matrix:

$$\mathbf{K}_2 = \begin{bmatrix} K_{11} & K_{12} \\ K_{12} & K_{22} \end{bmatrix} = \begin{bmatrix} w_1^2\sigma_2^2 + \sigma_1^2 & w_1\sigma_2^2 \\ & \sigma_2^2 \end{bmatrix} \tag{27}$$

This follows from the definition of the covariance,

$$K_{ij} = \langle y_i y_j \rangle. \tag{28}$$

The inverse covariance matrix, on the other hand, does not change in such a simple way. The 3×3 inverse covariance matrix was:

$$\mathbf{K}^{-1} = \begin{bmatrix} \frac{1}{\sigma_1^2} & -\frac{w_1}{\sigma_1^2} & \mathbf{0} \\ -\frac{w_1}{\sigma_1^2} & \left[\frac{1}{\sigma_2^2} + \frac{w_1^2}{\sigma_1^2} + \frac{w_3^2}{\sigma_3^2}\right] & -\frac{w_3}{\sigma_3^2} \\ \mathbf{0} & -\frac{w_3}{\sigma_3^2} & \frac{1}{\sigma_3^2} \end{bmatrix}$$

When we work out the 2×2 inverse covariance matrix, all the Blue terms that originated from the child y_3 are lost. So we have

$$\mathbf{K}_2^{-1} = \begin{bmatrix} \frac{1}{\sigma_1^2} & -\frac{w_1}{\sigma_1^2} \\ -\frac{w_1}{\sigma_1^2} & \left[\frac{1}{\sigma_2^2} + \frac{w_1^2}{\sigma_1^2}\right] \end{bmatrix}$$

Specifically, notice that $\left[\mathbf{K}_2^{-1}\right]_{22}$ is *different* from the $(2,2)$ entry in the three by three $\mathbf{K}^{-1}$.

We conclude: *Leaving out a variable leaves* $\mathbf{K}$ *unchanged but changes* $\mathbf{K}^{-1}$*.*

This conclusion is important for understanding the answer to the question, *'When working with Gaussian processes, why not parameterize the* inverse *covariance instead of the covariance function?'*

The answer is: you can't write down the inverse covariance associated with two points! The inverse covariance depends capriciously on *what the other variables are.*

3 Energy models

Sometimes people express probabilistic models in terms of energy functions that are minimized in the most probable configuration. For example, in regression with cubic splines, a regularizer is defined which describes the energy that a steel ruler would have if bent into the shape of the curve.

Such models usually have the form:

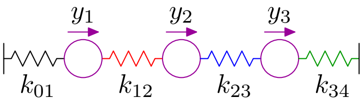
$$P(\mathbf{y}) = \frac{1}{Z} e^{-\dfrac{E(\mathbf{y})}{T}}, \tag{29}$$

and in simple cases, the energy $E(\mathbf{y})$ may be a quadratic function of $\mathbf{y}$, such as

$$E(\mathbf{y}) = -\sum_{i<j} J_{ij} y_i y_j + \sum_i a_i y_i^2 \tag{30}$$

If so, then the distribution is a Gaussian (just like (1)), and the 'couplings' J_{ij} are minus the coefficients in the *inverse* covariance matrix.

As a simple example, consider a set of three masses coupled by springs, and subjected to thermal perturbations.



THREE MASSES, FOUR SPRINGS

The equlibrium positions are $(y_1, y_2, y_3, y_4) = (0, 0, 0, 0)$, and the spring constants are k_{ij}. The extension of the second spring is $y_2 - y_1$. The energy of this system is

$$\begin{aligned} E(\mathbf{y}) &= \frac{1}{2}k_{01}y_1^2 + \frac{1}{2}k_{12}(y_2-y_1)^2 + \frac{1}{2}k_{23}(y_3-y_2)^2 + \frac{1}{2}k_{34}y_3^2 \\ &= \frac{1}{2}\left[\begin{array}{ccc} y_1 & y_2 & y_3 \end{array}\right]\left[\begin{array}{ccc} k_{01}+k_{12} & -k_{12} & 0 \\ -k_{12} & k_{12}+k_{23} & -k_{23} \\ 0 & -k_{23} & k_{23}+k_{34} \end{array}\right]\left[\begin{array}{c} y_1 \\ y_2 \\ y_3 \end{array}\right] \end{aligned}$$

So at temperature T, the probability distribution of the displacements is Gaussian with inverse covariance matrix

$$\frac{1}{T}\left[\begin{array}{ccc} k_{01}+k_{12} & -k_{12} & 0 \\ -k_{12} & k_{12}+k_{23} & -k_{23} \\ 0 & -k_{23} & k_{23}+k_{34} \end{array}\right] \tag{31}$$

Notice that there are 0 entries between displacements y_1 and y_3, the two masses that are not directly coupled by a spring.

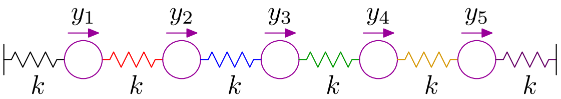


Figure 1. FIVE MASSES, SIX SPRINGS

So inverse covariance matrices are sometimes very sparse. If we have five masses in a row connected by identical springs k for example, then

$$\mathbf{K}^{-1} = \frac{k}{T}\begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}. \tag{32}$$

But this sparsity doesn't carry over to the covariance matrix, which is

$$\mathbf{K} = \frac{T}{k}\begin{bmatrix} 0.83 & 0.67 & 0.50 & 0.33 & 0.17 \\ 0.67 & 1.33 & 1.00 & 0.67 & 0.33 \\ 0.50 & 1.00 & 1.50 & 1.00 & 0.50 \\ 0.33 & 0.67 & 1.00 & 1.33 & 0.67 \\ 0.17 & 0.33 & 0.50 & 0.67 & 0.83 \end{bmatrix}. \tag{33}$$

4 Eigenvectors and eigenvalues are meaningless

There seems to be a knee-jerk reaction when people see a square matrix: 'what are its eigenvectors?' But here, where we are discussing quadratic forms, eigenvectors and eigenvalues have no fundamental status. They are dimensionally invalid objects. Any algorithm that features eigenvectors either didn't need to do so, or shouldn't have done so. (I think the whole idea of principal component analysis is misguided, for example.)

Hang on, you say, what about the three masses example? Don't those three masses have meaningful normal modes? Yes, they do, but those modes are *not* the eigenvectors of the spring matrix (31). Remember, I didn't tell you what the masses of the masses were!

I'm not saying that eigenvectors are never meaningful. What I'm saying is, in the context of quadratic forms

$$\frac{1}{2}\mathbf{y}^{\mathsf{T}}\mathbf{A}\mathbf{y}, \tag{34}$$

eigenvectors are meaningless and arbitrary.

Consider a covariance matrix describing the correlation between something's mass y_1 and its length y_2.

$$\mathbf{K} = \begin{bmatrix} K_{11} & K_{12} \\ K_{12} & K_{22} \end{bmatrix} \tag{35}$$

The dimensions of K_{11} are mass-squared. K_{11} might be measured in kg^2, for example. The dimensions of $K_{12} \equiv \langle y_1 y_2 \rangle$ are mass times length. K_{12} might be measured in kg m, for example.

Here's an example, which might describe the correlation between weight and height of some animals in a survey.

$$\mathbf{K} = \begin{bmatrix} K_{11} & K_{12} \\ K_{12} & K_{22} \end{bmatrix} = \begin{bmatrix} 10000\,\mathrm{kg}^2 & 70\,\mathrm{kg}\,\mathbf{m} \\ 70\,\mathrm{kg}\,\mathbf{m} & 1\,\mathbf{m}^2 \end{bmatrix} \tag{36}$$

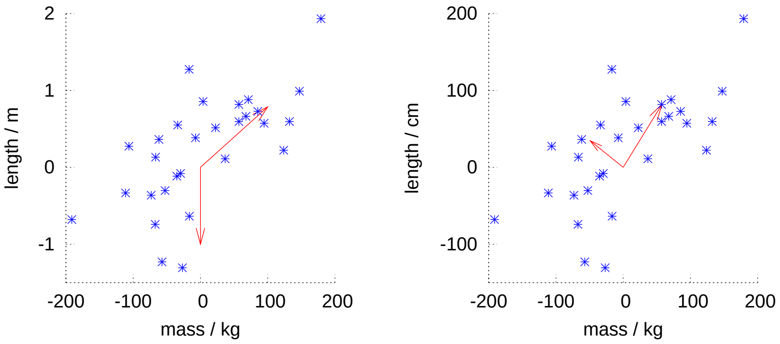


Figure 2. DATASET WITH ITS ‘EIGENVECTORS’. As the text explains, the eigenvectors of covariance matrices are meaningless and arbitrary.

The knee-jerk reaction is “let’s find the principal components of our data”, which means “ignore those silly dimensional units, and just find the eigenvectors of $\begin{bmatrix} 10000 & 70 \\ 70 & 1 \end{bmatrix}$. But let’s consider what this means. An eigenvector is a vector satisfying

$$\begin{bmatrix} 10000\,\mathrm{kg}^2 & 70\,\mathrm{kg}\,\mathbf{m} \\ 70\,\mathrm{kg}\,\mathbf{m} & 1\,\mathbf{m}^2 \end{bmatrix} \mathbf{e} = \lambda \mathbf{e}. \tag{37}$$

By asking for an eigenvector, we are imagining that two equations are true – first, the top row:

$$10000\,\mathrm{kg}^2\,\mathrm{e}_1 + 70\,\mathrm{kg}\,\mathbf{m}\,\mathrm{e}_2 = \lambda \mathrm{e}_1, \tag{38}$$

and, second, the bottom row:

$$70\,\mathrm{kg}\,\mathbf{m}\,\mathrm{e}_1 + 1\,\mathbf{m}^2\,\mathrm{e}_2 = \lambda \mathrm{e}_2. \tag{39}$$

These expressions violate the rules of dimensions. Try all you like, but you won’t be able to find dimensions for e_1, e_2, and λ such that rule 1 is satisfied.

No, no, the matlab lover says, I leave out the dimensions, and I get:

```
>  [e,v] = eig(s)
e =   0.0070002  -0.9999755           v = 5.0998e-01   0.0000e+00
     -0.9999755  -0.0070002               0.0000e+00   1.0000e+04
```

I notice that the eigenvectors $(0.007, -0.9999)$, and $(0.9999, 0.007)$, which are almost aligned with the coordinate axes. Very interesting! I also notice that the eigenvalues are 10^4 and 0.5. What an interestingly large eigenvalue ratio! Wow, that means that there is one very big principal component, and the second one is much smaller. Ooh, how interesting.

But this is nonsense. If we change the units in which we measure length from **m** to cm then the covariance matrix can be written:

$$\mathbf{K} = \begin{bmatrix} K_{11} & K_{12} \\ K_{12} & K_{22} \end{bmatrix} = \begin{bmatrix} 10000\,\mathrm{kg}^2 & 7000\,\mathrm{kg\,cm} \\ 7000\,\mathrm{kg\,cm} & 10000\,\mathrm{cm}^2 \end{bmatrix} \tag{40}$$

This is exactly the same covariance matrix of exactly the same data. But the eigenvectors and eigenvalues are now:

```
e =  -0.70711   0.70711      v =  3000       0
      0.70711   0.70711              0   17000
```

Figure 2 illustrates this situation.

On the left, a data set of masses and lengths measured in metres. The arrows show the ‘eigenvectors’. (The arrows don’t look ‘orthogonal’ in this plot because a step of one unit on the x-axis happens to cover less paper than a step of one unit on the y-axis.) On the right, exactly the same data set but with lengths measured in centimetres. The arrows show the ‘eigenvectors’.

In conclusion, eigenvectors of the matrix in a quadratic form are not fundamentally meaningful. [Properties of that matrix that *are* meaningful include its determinant.]

4.1 Aside

This complaint about eigenvectors comes hand in hand with another complaint, about ‘steepest descent’. A steepest descent algorithm is dimensionally invalid. A *step* in a parameter space does not have the same dimensions as a *gradient*. To turn a gradient into a sensible step direction, you need a *metric*. The metric defines how ‘big’ a step is (in rather the same way that when gnuplot plotted the data above, it chose a vertical scale and a horizontal scale). Once you know how big alternative steps are, it becomes meaningful to take the step that is ‘steepest’ (that is, it’s the direction with the biggest change in function value per unit ‘distance’ moved).

Without a metric, steepest descents algorithms are not *covariant*. That is, the algorithm would behave differently if you just changed the units in which one parameter is measured.

Appendix: Answers to quiz

For the first four, you can quickly guess the answers based on whether the $(1, 3)$ entries are zero or not. For a careful answer you should also check that the matrices really are positive definite (they are) and that they are realisable by the respective graphical models (which isn’t guaranteed by the preceding constraints).

1. A and B

2. C and D

3. C and D

4. A and B

5. A is true, B is false.