Statistical Estimation

Suppose we use the following model for our measurements:

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}_0 + \boldsymbol{e},$$

where $\boldsymbol{y} \in \mathbb{R}^M$, \boldsymbol{A} is an $M \times N$ matrix, $\boldsymbol{x}_0 \in \mathbb{R}^N$ is what we are interested in estimating, and $\boldsymbol{e} \in \mathbb{R}^M$ is a **random error**.

We will assume that each entry of \boldsymbol{e} has zero mean:

$$E[e[m]] = 0, m = 1, ..., M, E[e] = 0.$$

We will characterize e through its **covariance matrix**

$$R[\ell, m] = \mathbb{E}[e[\ell]e[m]],$$

or more compactly

$$\boldsymbol{R} = \mathrm{E}[\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}].$$

The diagonal of \mathbf{R} contains the variances of the entries of \mathbf{e} , while the off diagonal terms capture the correlations (which is the same as covariance, since all of the e[m] are zero mean).

For example, if two measurement errors have

$$var(e[1]) = E[e[1]^2] = 3, \quad var(e[2]) = E[e[2]^2] = 2,$$

and $cov(e[1], e[2]) = E[e[1]e[2]] = -1,$

then

$$\mathbf{R} = \begin{bmatrix} 3 & -1 \\ -1 & 2 \end{bmatrix}.$$

It is always true that covariance matrices are symmetric and positive semi-definite (so their eigenvalues are ≥ 0).

A handy fact that we will use repeatedly below is that if e has covariance matrix \mathbf{R} , then for any matrix \mathbf{M} , the covariance of $\mathbf{M}e$ is \mathbf{I}

$$\mathrm{E}[\boldsymbol{M}\boldsymbol{e}(\boldsymbol{M}\boldsymbol{e})^{\mathrm{T}}] = \mathrm{E}[\boldsymbol{M}\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}\boldsymbol{M}^{\mathrm{T}}] = \boldsymbol{M}\,\mathrm{E}[\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}]\boldsymbol{M}^{\mathrm{T}} = \boldsymbol{M}\boldsymbol{R}\boldsymbol{M}^{\mathrm{T}}.$$

Questions:

1. Suppose that the entries of \boldsymbol{e} have variances $\nu_m^2 = \mathrm{E}[e[m]^2]$. Calculate

$$E[\|e\|_2^2] =$$
______.

(the expected energy of e).

Answer:

$$E[\|e\|_{2}^{2}] = \sum_{m=1}^{M} E[e[m]^{2}]$$
$$= \sum_{m=1}^{M} \nu_{m}^{2}.$$

$$Q[i,j] = (\boldsymbol{M}\boldsymbol{e})[i](\boldsymbol{M}\boldsymbol{e})[j] = \langle \boldsymbol{e}, \boldsymbol{m}_i \rangle \langle \boldsymbol{m}_j, \boldsymbol{e} \rangle = \sum_{\ell} \sum_{k} M[i,\ell] M[j,k] e[\ell] e[k],$$

and

$$\mathrm{E}[Q[i,j]] = \sum_{\ell} \sum_{k} M[i,\ell] M[j,k] R[\ell,k] = (\boldsymbol{M} \boldsymbol{R} \boldsymbol{M}^{\mathrm{T}})[i,j],$$

so $E[Q] = MRM^{T}$.

If you want to see why that second-to-last step is true more explicitly, set $Q = Mee^{T}M^{T}$. Then if m_i is the ith row of M,

2. Now let \boldsymbol{D} be a diagonal matrix

$$oldsymbol{D} = egin{bmatrix} d_1 & & & & \ & d_2 & & \ & & \ddots & \ & & & d_M \end{bmatrix}.$$

Calculate

$$\mathbb{E}[\|\boldsymbol{D}\boldsymbol{e}\|_2^2] = \underline{\qquad}.$$

Answer:

$$\mathrm{E}[\|oldsymbol{D}oldsymbol{e}\|_2^2] = \sum_{m=1}^M \mathrm{E}[d_m^2 e[m]^2] \ = \sum_{m=1}^M d_m^2
u_m^2.$$

3. Suppose $e \in \mathbb{R}^M$ has covariance matrix R. Let L be an $N \times M$ matrix. Calculate

$$\mathbb{E}[\|\boldsymbol{L}\boldsymbol{e}\|_2^2] = \underline{\hspace{1cm}}.$$

Answer: We use two facts which are easily verified (do this at home). First, the inner product of two vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^N$ is equal to the trace of their outer product:

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle = \operatorname{trace}(\boldsymbol{u} \boldsymbol{v}^{\mathrm{T}}).$$

Second, if \boldsymbol{Q} is a square matrix whose entries are random variables, then

$$E[trace(\boldsymbol{Q})] = trace(E[\boldsymbol{Q}]).$$

Then

$$E[\|\boldsymbol{L}\boldsymbol{e}\|_{2}^{2}] = E[\langle \boldsymbol{L}\boldsymbol{e}, \boldsymbol{L}\boldsymbol{e} \rangle]$$

$$= E[\operatorname{trace}(\boldsymbol{L}\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}\boldsymbol{L}^{\mathrm{T}})]$$

$$= \operatorname{trace}\left(E[\boldsymbol{L}\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}\boldsymbol{L}^{\mathrm{T}}]\right)$$

$$= \operatorname{trace}\left(\boldsymbol{L}E[\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}]\boldsymbol{L}^{\mathrm{T}}\right)$$

$$= \operatorname{trace}(\boldsymbol{L}\boldsymbol{R}\boldsymbol{L}^{\mathrm{T}}).$$

Uncorrelated errors

Suppose that the random errors are uncorrelated, so that the covariance matrix is diagonal

$$oldsymbol{R} = \mathrm{E}[oldsymbol{e}oldsymbol{e}^{\mathrm{T}}] = egin{bmatrix}
u_1^2 & 0 & 0 & \cdots & \\
0 &
u_2^2 & 0 & \cdots & \\
\vdots & & \ddots & & \\
& & &
u_M^2 \end{bmatrix}$$

If ν_m is large, it means that we do not have much confidence in our measurement y_m . On the other hand, if ν_m is small, it means that our measurement y_m is most likely very close to the true value of $(\mathbf{A}\mathbf{x}_0)[m]$

We will see this rigorously below, but in this case, the "correct" weighting for each component is simply the inverse of the standard deviation; the weighting matrix \boldsymbol{W} should be diagonal with

$$W[m,m] = rac{1}{
u_m}, \qquad (m{W} = m{R}^{-1/2}).$$

Then the weighted least-squares estimate is given by

$$\hat{\boldsymbol{x}}_{ ext{wls}} = (\boldsymbol{A}^{ ext{T}} \boldsymbol{W}^{ ext{T}} \boldsymbol{W} \boldsymbol{A})^{-1} \boldsymbol{A}^{ ext{T}} \boldsymbol{W}^{ ext{T}} \boldsymbol{W} \boldsymbol{y}$$

$$= (\boldsymbol{A}^{ ext{T}} \boldsymbol{R}^{-1} \boldsymbol{A})^{-1} \boldsymbol{A}^{ ext{T}} \boldsymbol{R}^{-1} \boldsymbol{y}.$$

The reconstruction error of this estimate is

$$egin{aligned} m{x}_0 - \hat{m{x}}_{ ext{wls}} &= m{x}_0 - (m{A}^{ ext{T}}m{R}^{-1}m{A})^{-1}m{A}^{ ext{T}}m{R}^{-1}(m{A}m{x}_0 + m{e}) \ &= -(m{A}^{ ext{T}}m{R}^{-1}m{A})^{-1}m{A}^{ ext{T}}m{R}^{-1}m{e} \end{aligned}$$

The **mean-square error** (MSE) of the error for this estimate is calculated using the result of Question 3 above:

$$E[\|\boldsymbol{x}_{0} - \hat{\boldsymbol{x}}_{wls}\|_{2}^{2}] = \operatorname{trace}\left((\boldsymbol{A}^{T}\boldsymbol{R}^{-1}\boldsymbol{A})^{-1}\boldsymbol{A}^{T}\boldsymbol{R}^{-1}\boldsymbol{R}\boldsymbol{R}^{-1}\boldsymbol{A}(\boldsymbol{A}^{T}\boldsymbol{R}^{-1}\boldsymbol{A})^{-1}\right)$$

$$= \operatorname{trace}\left((\boldsymbol{A}^{T}\boldsymbol{R}^{-1}\boldsymbol{A})^{-1}\boldsymbol{A}^{T}\boldsymbol{R}^{-1}\boldsymbol{A}(\boldsymbol{A}^{T}\boldsymbol{R}^{-1}\boldsymbol{A})^{-1}\right)$$

$$= \operatorname{trace}\left((\boldsymbol{A}^{T}\boldsymbol{R}^{-1}\boldsymbol{A})^{-1}\right)$$

Example. We take M readings of a patient's pulse, each has an error of ν^2 . In this case, the underlying quantity (the pulse) x_0 is a scalar. The optimal estimate (no matter what ν is) is

$$\hat{x} = \frac{1}{M} (y[1] + y[2] + \dots + y[M]).$$

What is the mean-square error for this estimate?

Answer: The mean-square error is

$$E[|x_0 - \hat{x}|^2] = E\left[\left|x_0 - \frac{1}{M}\sum_{m=1}^{M}(x_0 + e[m])\right|^2\right]$$

$$= E\left[\left|\frac{1}{M}\sum_{m=1}^{M}e[m]\right|^2\right]$$

$$= \frac{1}{M^2}E[\langle \boldsymbol{e}, \boldsymbol{e} \rangle]$$

$$= \frac{1}{M^2}E[\operatorname{trace}(\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}})]$$

$$= \frac{1}{M^2}\operatorname{trace}(E[\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}])$$

$$= \frac{\nu^2}{M},$$

where the last step follows from the fact that the covariance matrix of the errors e is diagonal.

Now suppose that the variance for each of the M measurements is different; $\nu_1^2, \nu_2^2, \dots, \nu_M^2$.

Now what is the best estimate \hat{x} ?

What is the MSE of this estimate?

Answers: We have

$$m{A} = egin{bmatrix} 1 \ 1 \ dots \ 1 \end{bmatrix}, \qquad m{R}^{-1} = egin{bmatrix} 1/
u_1^2 & & & \ & 1/
u_2^2 & & \ & & \ddots & \ & & 1/
u_M^2 \end{bmatrix},$$

and

$$(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{R}^{-1}\boldsymbol{A})^{-1} = \left(\sum_{m=1}^{M} 1/\nu_m^2\right)^{-1},$$

and so

$$\hat{x} = \frac{\sum_{m=1}^{M} y[m] / \nu_m^2}{\sum_{m=1}^{M} 1 / \nu_m^2}.$$

The MSE is

trace
$$((\mathbf{A}\mathbf{R}^{-1}\mathbf{A})^{-1}) = \left(\sum_{m=1}^{M} 1/\nu_m^2\right)^{-1}$$
.

Best Linear Unbiased Estimator (BLUE)

We now return to the general estimation problem: we observe

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}_0 + \boldsymbol{e},$$

where $\boldsymbol{e} \in \mathbb{R}^M$ is random with

$$E[e] = 0, \quad E[ee^{T}] = R.$$

Since e is random, the observations y are also random. We can now ask what is the best statistical estimate of x_0 . We will restrict ourselves to estimators that have the following properties:

1. **Linearity**. That is, our estimate can be computed by applying a fixed matrix to \boldsymbol{y} ,

$$\hat{\boldsymbol{x}} = \boldsymbol{L}\boldsymbol{y},$$

for some $N \times M$ matrix \boldsymbol{L} .

2. **Unbiased**. Since the estimate \hat{x} is a function of random variables, it is itself a random variable. Our estimator is unbiased if

$$E[\hat{\boldsymbol{x}}] = \boldsymbol{x}_0,$$

which means the expectation of the estimation error is zero,

$$E[\hat{\boldsymbol{x}} - \boldsymbol{x}_0] = \boldsymbol{0}.$$

We will search for the best such estimator; the best linear unbiased estimator (BLUE).

Let's make it clear what we mean by "best". We mean that the MSE of the estimation error, $E[\|\hat{\boldsymbol{x}} - \boldsymbol{x}_0\|_2^2]$ is minimized.

The estimator is linear, so we can write

$$\hat{\boldsymbol{x}} = \boldsymbol{L}\boldsymbol{y} = \boldsymbol{L}(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{e}) = \boldsymbol{L}\boldsymbol{A}\boldsymbol{x} + \boldsymbol{L}\boldsymbol{e},$$

for some matrix \boldsymbol{L} which we will optimize. We want the estimator to be unbiased, so

$$egin{array}{lll} {f 0} &=& {
m E}[{m x}_0 - \hat{m x}] = {
m E}[{m x}_0 - {m L}{m A}{m x} - {m L}{m e}] \ &= {m x}_0 - {m L}{m A}{m x}_0 - {
m E}[{m L}{m e}] \ &= {m x}_0 - {m L}{m A}{m x}_0, \end{array}$$

where the last step comes from the fact that E[Le] = 0, since E[e] = 0. Thus we need L to obey

$$LAx_0 = x_0.$$

That is, we want L to be a **left inverse** of A, meaning LA = I.

With these two properties in hand, the variance of our estimate for a qualifying \boldsymbol{L} is

$$E[\|\boldsymbol{x}_0 - \hat{\boldsymbol{x}}\|_2^2] = E[\|\boldsymbol{x}_0 - \boldsymbol{L}\boldsymbol{A}\boldsymbol{x}_0 - \boldsymbol{L}\boldsymbol{e}\|_2^2]$$

$$= E[\|\boldsymbol{L}\boldsymbol{e}\|_2^2]$$

$$= E[\operatorname{trace}(\boldsymbol{L}\boldsymbol{R}\boldsymbol{L}^{\mathrm{T}})].$$

So we would like to find the matrix which minimizes

$$\underset{\boldsymbol{L} \in \mathbb{R}^{N \times M}}{\text{minimize}} \ \ \text{trace}(\boldsymbol{L}\boldsymbol{R}\boldsymbol{L}^{\mathrm{T}}) \ \ \ \text{subject to} \ \ \boldsymbol{L}\boldsymbol{A} = \mathbf{I}.$$

I propose that the solution to the above is

$$L_0 = (A^{\mathrm{T}}R^{-1}A)^{-1}A^{\mathrm{T}}R^{-1}.$$

Let's check this. Clearly $L_0 A = I$, so L_0 is a left inverse. It remains to show that for any other left inverse L,

$$\operatorname{trace}(\boldsymbol{L}\boldsymbol{R}\boldsymbol{L}^{\mathrm{T}}) \geq \operatorname{trace}(\boldsymbol{L}_{0}\boldsymbol{R}\boldsymbol{L}_{0}^{\mathrm{T}}).$$

Write a candidate \boldsymbol{L} as

$$\boldsymbol{L} = \boldsymbol{L}_0 + (\boldsymbol{L} - \boldsymbol{L}_0).$$

Then

$$trace(\boldsymbol{L}\boldsymbol{R}\boldsymbol{L}^{T}) = trace(\boldsymbol{L}_{0}\boldsymbol{R}\boldsymbol{L}_{0}^{T}) + trace(\boldsymbol{L}_{0}\boldsymbol{R}(\boldsymbol{L} - \boldsymbol{L}_{0})^{T}) + trace((\boldsymbol{L} - \boldsymbol{L}_{0})\boldsymbol{R}\boldsymbol{L}_{0}^{T}) + trace((\boldsymbol{L} - \boldsymbol{L}_{0})\boldsymbol{R}(\boldsymbol{L} - \boldsymbol{L}_{0})^{T}).$$

Note that

$$RL_0^{\mathrm{T}} = RR^{-1}A(A^{\mathrm{T}}R^{-1}A)^{-1} = A(A^{\mathrm{T}}R^{-1}A)^{-1}.$$

Thus

$$(m{L} - m{L}_0) m{R} m{L}_0^{
m T} = (m{L} - m{L}_0) m{A} (m{A}^{
m T} m{R}^{-1} m{A})^{-1} = m{0}$$

since both LA = I and $L_0A = I$. We are left with

$$trace(\boldsymbol{L}\boldsymbol{R}\boldsymbol{L}^{T}) = trace(\boldsymbol{L}_{0}\boldsymbol{R}\boldsymbol{L}_{0}^{T}) + trace((\boldsymbol{L} - \boldsymbol{L}_{0})\boldsymbol{R}(\boldsymbol{L} - \boldsymbol{L}_{0})^{T}).$$

Since $(\boldsymbol{L} - \boldsymbol{L}_0)\boldsymbol{R}(\boldsymbol{L} - \boldsymbol{L}_0)^{\mathrm{T}}$ is symmetric and postive semi-definite, the term on the right is ≥ 0 . So we conclude

 $\operatorname{trace}(\boldsymbol{L}\boldsymbol{R}\boldsymbol{L}^{\mathrm{T}}) \geq \operatorname{trace}(\boldsymbol{L}_{0}\boldsymbol{R}\boldsymbol{L}_{0}^{\mathrm{T}})$ for all left inverses \boldsymbol{L} .

Best Linear Unbiased Estimator (BLUE):

From observations,

$$y = Ax_0 + e,$$
 $E[ee^T] = R,$

the BLUE is

$$\hat{\boldsymbol{x}}_{\text{blue}} = (\boldsymbol{A}^{\text{T}}\boldsymbol{R}^{-1}\boldsymbol{A})^{-1}\boldsymbol{A}^{\text{T}}\boldsymbol{R}^{-1}\boldsymbol{y}.$$

A quick calculation shows

$$\boldsymbol{L}_0 \boldsymbol{R} \boldsymbol{L}_0^{\mathrm{T}} = (\boldsymbol{A}^{\mathrm{T}} \boldsymbol{R}^{-1} \boldsymbol{A})^{-1},$$

and so the MSE of the BLUE is

$$E[\|\boldsymbol{x}_0 - \hat{\boldsymbol{x}}_{\text{blue}}\|_2^2] = \text{trace}((\boldsymbol{A}^{\text{T}}\boldsymbol{R}^{-1}\boldsymbol{A})^{-1})$$

$$= \text{sum of eigenvalues of } (\boldsymbol{A}^{\text{T}}\boldsymbol{R}^{-1}\boldsymbol{A})^{-1}.$$

 $(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{R}^{-1}\boldsymbol{A})^{-1}$ is sometimes called the **information matrix**.

Exercise: We measure

$$y = Ax + e$$

with

$$\boldsymbol{A} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \boldsymbol{y} = \begin{bmatrix} 0 \\ 5 \end{bmatrix}, \quad \mathrm{E}[\boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}] = \boldsymbol{R} = \begin{bmatrix} 3 & -1 \\ -1 & 2 \end{bmatrix}.$$

1. Find the best linear unbiased estimate. Hint:

$$\boldsymbol{R}^{-1} = \frac{1}{5} \begin{bmatrix} 2 & 1 \\ 1 & 3 \end{bmatrix}.$$

2. Calculate $E[\|\boldsymbol{x}_0 - \hat{\boldsymbol{x}}_{\text{blue}}\|_2^2]$.