The complex multivariate Gaussian distribution

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Abstract

Here I introduce **cmvnorm**, a complex generalization of the **mvtnorm** package. A complex generalization of the Gaussian process is suggested and numerical results presented using the package. An application in the context of approximating the Weierstrass sigma function using a complex Gaussian process is given.

Keywords: Complex multivariate Gaussian distribution, Gaussian process, Weierstrass sigma function, emulator.

1. Introduction

Complex-valued random variables find applications in many areas of science such as signal processing (Kay 1989), radio engineering (Ozarow 1994), and atmospheric physics (Mandic, Javidi, Goh, Kuh, and Aihara 2009). In this short paper I introduce **cmvnorm**, a package for investigating one commonly encountered complex-valued probability distribution, the complex Gaussian.

The real multivariate Gaussian distribution is well supported in R (R Core Team 2014; Genz, Bretz, Miwa, Mi, Leisch, Scheipl, and Hothorn 2014), having density function

$$f(\mathbf{x}; \boldsymbol{\mu}, \Sigma) = \frac{e^{-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1}(\mathbf{x} - \boldsymbol{\mu})}}{\sqrt{|2\pi\Sigma|}} \qquad \mathbf{x} \in \mathbb{R}^n,$$
(1)

where |M| denotes the determinant of matrix M. Here, $\boldsymbol{\mu} = \mathbb{E}\left[\mathbf{X}\right] \in \mathbb{R}^n$ is the mean vector and $\Sigma = \mathbb{E}\left[\left(\mathbf{X} - \boldsymbol{\mu}\right) \left(\mathbf{X} - \boldsymbol{\mu}\right)^T\right]$ the covariance of random vector \mathbf{X} ; we write $\mathbf{X} \sim \mathcal{N}_n\left(\boldsymbol{\mu}, \Sigma\right)$. One natural generalization would be to consider $\mathbf{Z} \sim \mathcal{NC}_n\left(\boldsymbol{\mu}, \Gamma\right)$, the complex multivariate Gaussian, with density function

$$f(\mathbf{z}; \boldsymbol{\mu}, \Gamma) = \frac{e^{-(\mathbf{z}-\boldsymbol{\mu})^*\Gamma^{-1}(\mathbf{z}-\boldsymbol{\mu})}}{|\pi\Gamma|} \qquad \mathbf{z} \in \mathbb{C}^n$$
 (2)

where \mathbf{z}^* denotes the Hermitian transpose of complex vector \mathbf{z} . Now $\boldsymbol{\mu} \in \mathbb{C}^n$ is the complex mean and $\Gamma = \mathbb{E}\left[(\mathbf{Z} - \boldsymbol{\mu}) (\mathbf{Z} - \boldsymbol{\mu})^* \right]$ is the complex variance; Γ is a Hermitian positive definite matrix. Note the simpler form of (2), essentially due to Gauss's integral operating more cleanly over the complex plane than the real line:

$$\int_{\mathbb{C}} e^{-z^*z} dz = \int_{x \in \mathbb{R}} \int_{y \in \mathbb{R}} e^{-\left(x^2 + y^2\right)} dx dy = \int_{\theta = 0}^{2\pi} \int_{r=0}^{\infty} e^{-r^2} r dr d\theta = \pi.$$

A zero mean complex random vector \mathbf{Z} is said to be *circularly symmetric* (Goodman 1963) if $\mathbb{E}\left[\mathbf{Z}\mathbf{Z}^{T}\right]=0$, or equivalently \mathbf{Z} and $e^{i\alpha}\mathbf{Z}$ have identical distributions for any $\alpha\in\mathbb{R}$. Equation (2) clearly has this property.

Most results from real multivariate analysis have a direct generalization to the complex case, as long as "transpose" is replaced by "Hermitian transpose". For example, $\mathbf{X} \sim \mathcal{N}_n(\mathbf{0}, \Sigma)$ implies $B\mathbf{X} \sim \mathcal{N}_n(\mathbf{0}, B^T \Sigma B)$ for any constant matrix $B \in \mathbb{R}^{m \times n}$, and analogously $\mathbf{Z} \sim \mathcal{NC}_n(\mathbf{0}, \Gamma)$ implies $B\mathbf{Z} \sim \mathcal{NC}_n(\mathbf{0}, B^* \Gamma B)$, $B \in \mathbb{C}^{m \times n}$. Similar generalizations operate for Schur complement methods on partitioned matrices.

Also, linear regression generalizes similarly. Specifically, consider $\mathbf{y} \in \mathbb{R}^n$. If $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$ where X is a $n \times p$ design matrix, $\boldsymbol{\beta} \in \mathbb{R}^p$ a vector of regression coefficients and $\boldsymbol{\epsilon} \sim \mathcal{N}_n(\mathbf{0}, \Sigma)$ is a vector of errors, then $\hat{\boldsymbol{\beta}} = \left(X^T \Sigma^{-1} X\right)^{-1} X^T \Sigma^{-1} \mathbf{y}$ is the maximum likelihood estimator for $\boldsymbol{\beta}$. The complex generalization is to write $\mathbf{z} = Z\boldsymbol{\beta} + \boldsymbol{\epsilon}$, $Z \in \mathbb{C}^{n \times p}$, $\boldsymbol{\beta} \in \mathbb{C}^p$, $\boldsymbol{\epsilon} \sim \mathcal{N}\mathcal{C}_n(\mathbf{0}, \Gamma)$ which gives $\hat{\boldsymbol{\beta}} = \left(Z^* \Gamma^{-1} Z\right)^{-1} Z^* \Gamma^{-1} \mathbf{z}$. Such considerations suggest a natural complex generalization of the Gaussian process.

This short vignette introduces the **cmvnorm** package which furnishes some functionality for the complex multivariate Gaussian distribution, and applies it in the context of a complex generalization of the **emulator** package.

2. The package in use

Random complex vectors are generated using the rcmvnorm() function, analogous to rmvnorm():

```
> set.seed(1)

> library("cmvnorm",quietly=TRUE)

> cm <- c(1,1i)

> cv <- matrix(c(2,1i,-1i,2),2,2)

> (z <- rcmvnorm(6, mean=cm, sigma=cv))

[,1] [,2]

[1,] 0.9680986+0.5525419i 0.0165969+2.9770976i

[2,] 0.2044744-1.4994889i 1.8320765+0.8271259i

[3,] 1.0739973+0.2279914i -0.7967020+0.1736071i

[4,] 1.3171073-0.9843313i 0.9257146+0.5524913i

[5,] 1.3537303-0.8086236i -0.0571337+0.3935375i

[6,] 2.9751506-0.1729231i 0.3958585+3.3128439i
```

Function dcmvnorm() returns the density according to (2):

> dcmvnorm(z,cm,cv)

```
[1] 5.103754e-04 1.809636e-05 2.981718e-03 1.172242e-03 4.466836e-03 [6] 6.803356e-07
```

So it is possible to determine a maximum likelihood for the mean using direct numerical optimization

- > helper <- function(x) $\{c(x[1]+1i*x[2], x[3]+1i*x[4])\}$
- > objective <- function(x,cv){-sum(dcmvnorm(z,mean=helper(x),sigma=cv,log=TRUE))}
- > helper(optim(c(1,0,1,0),objective,cv=cv)\$par)

[1] 1.315409-0.447863i 0.385704+1.372762i

(helper functions are needed because optim() optimizes over \mathbb{R}^n as opposed to \mathbb{C}^n). This shows reasonable agreement with the true value of the mean and indeed the analytic value of the MLE, specifically

> colMeans(z)

[1] 1.315426-0.447472i 0.386068+1.372784i

3. The Gaussian process

In the context of the emulator, a (real) Gaussian process is usually defined in terms of a random function $\eta: \mathbb{R}^p \longrightarrow \mathbb{R}$ which, for any set of points $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ in its domain \mathcal{D} the random vector $\{\eta(\mathbf{x}_1), \dots, \eta(\mathbf{x}_n)\}$ is multivariate Gaussian.

It is convenient to specify $\mathbb{E}\left[\eta\left(\mathbf{x}\right)|\boldsymbol{\beta}\right] = h\left(\mathbf{x}\right)\boldsymbol{\beta}$, that is, the expectation of the process at point $\mathbf{x} \in \mathcal{D}$ conditional on the (unknown) vector of coefficients $\boldsymbol{\beta}$. Here $h \colon \mathbb{R}^p \longrightarrow \mathbb{R}^q$ specifies the q known regressor functions of $\mathbf{x} = (x_1, \dots, x_p)^T$; a common choice is $h\left(\mathbf{x}\right) = (1, x_1, \dots, x_p)^T$ [giving q = p + 1], but one is in principle free to choose any function of \mathbf{x} . One writes $H^T = (h\left(\mathbf{x}_1\right), \dots, h\left(\mathbf{x}_n\right))$ when considering the entire design matrix X; the R idiom is regressor.multi().

The covariance is typically given by

$$\mathsf{COV}\left(\eta(\mathbf{x}), \eta(\mathbf{x}')\right) = V\left(\mathbf{x} - \mathbf{x}'\right)$$

where $V: \mathbb{R}^n \longrightarrow \mathbb{R}$ must be chosen so that the variance matrix of any finite set of observations is always positive-definite. Bochner's theorem (Feller 1971, chapter XIX) shows that $V(\cdot)$ must be proportional to the characteristic function (CF) of a symmetric probability Borel measure.

Oakley (1999) uses techniques which have clear complex analogues to show that the posterior mean of $\eta(\mathbf{x})$ is given by

$$h(\mathbf{x})^{T} \boldsymbol{\beta} + (\mathsf{COV}(\mathbf{x}, \mathbf{x}_{1}), \dots, \mathsf{COV}(\mathbf{x}, \mathbf{x}_{n}))^{T} A^{-1} (\mathbf{y} - H\hat{\boldsymbol{\beta}})$$
 (3)

Here A is an $n \times n$ matrix of correlations between the observations, $\sigma^2 A_{ij} = \text{COV}(\eta(\mathbf{x}_i), \eta(\mathbf{x}_j))$ where σ^2 is an overall variance term; and $\hat{\boldsymbol{\beta}} = (X^T A^{-1} X)^{-1} X^T A^{-1} \mathbf{y}$ is the maximum likelihood estimator for $\boldsymbol{\beta}$.

Equation (3) furnishes a cheap approximation to $\eta(\mathbf{x})$ and is known as the 'emulator'.

3.1. Complex Gaussian processes

The complex case is directly analogous, with $\eta \colon \mathbb{C}^p \longrightarrow \mathbb{C}$ and $\beta \in \mathbb{C}^q$. Writing $\mathsf{COV}(\eta(\mathbf{z}_1), \ldots, \eta(\mathbf{z}_n)) = \Omega$, so that element (i, j) of matrix Ω is $\mathsf{COV}(\eta(\mathbf{z}_i), \eta(\mathbf{z}_j))$, we may relax the requirement that Ω be symmetric positive definite to requiring only Hermitian positive definiteness. This allows one to use the characteristic function of any, possibly non-symmetric, random variable Ψ with density function $f \colon \mathbb{R}^p \longrightarrow \mathbb{R}$ and characteristic function ϕ :

$$\Omega_{ij} = \mathsf{COV}\left(\eta\left(\mathbf{z}_{i}\right), \eta\left(\mathbf{z}_{j}\right)\right) = \phi\left(\mathbf{z}_{i} - \mathbf{z}_{j}\right) \tag{4}$$

That Ω remains Hermitian positive definite may be shown by evaluating a quadratic form with it and arbitrary $\mathbf{w} \in \mathbb{C}^n$ and establishing that it is real and non-negative:

$$\begin{split} \mathbf{w}^*\Omega\mathbf{w} &= \sum_{i,j} \overline{\mathbf{w}_i} \mathsf{COV} \left(\eta \left(\mathbf{z}_i \right), \eta \left(\mathbf{z}_j \right) \right) \mathbf{w}_j & \text{definition of quadratic form} \\ &= \sum_{i,j} \overline{\mathbf{w}_i} \phi \left(\mathbf{z}_i - \mathbf{z}_j \right) \mathbf{w}_j & \text{covariance function is the CF of } \Psi \\ &= \sum_{i,j} \overline{\mathbf{w}_i} \left[\int_{\mathbf{t} \in \mathbb{C}^n} e^{\mathrm{i} \operatorname{Re} \, \mathbf{t}^* (\mathbf{z}_i - \mathbf{z}_j)} f \left(\mathbf{t} \right) \, d\mathbf{t} \right] \mathbf{w}_j & \text{definition of CF of } \Psi \\ &= \int_{\mathbf{t} \in \mathbb{C}^n} \left[\sum_{i,j} \overline{\mathbf{w}_i} e^{\mathrm{i} \operatorname{Re} \, (\mathbf{t}^* \mathbf{z}_i)} \overline{\mathbf{w}_j} e^{\mathrm{i} \operatorname{Re} \left(\mathbf{t}^* \mathbf{z}_j \right)} f \left(\mathbf{t} \right) \right] \, d\mathbf{t} & \text{integration and summation commute} \\ &= \int_{\mathbf{t} \in \mathbb{C}^n} \left[\sum_{i,j} \overline{\mathbf{w}_i} e^{\mathrm{i} \operatorname{Re} \left(\mathbf{t}^* \mathbf{z}_i \right)} \overline{\overline{\mathbf{w}_j} e^{\mathrm{i} \operatorname{Re} \left(\mathbf{t}^* \mathbf{z}_j \right)}} f \left(\mathbf{t} \right) \right] \, d\mathbf{t} & \text{expand and rearrange} \\ &= \int_{\mathbf{t} \in \mathbb{C}^n} \left| \sum_i \overline{\mathbf{w}_i} e^{\mathrm{i} \operatorname{Re} \left(\mathbf{t}^* \mathbf{z}_i \right)} \right|^2 f \left(\mathbf{t} \right) \, d\mathbf{t} & \text{algebra} \\ &\geqslant 0. & \text{integral of sum of real positive functions} \end{split}$$

(This motivates the definition of the characteristic function of a complex multivariate random variable **Z** as $\mathbb{E}\left[e^{i\operatorname{Re}(\mathbf{t}^*\mathbf{Z})}\right]$). Thus the covariance matrix is Hermitian positive definite: although its entries are not necessarily real, its eigenvalues are all nonnegative.

In the real case one typically chooses Ψ to be a zero-mean Gaussian distribution; in the complex case one can use the complex multivariate distribution given in equation (2) which has characteristic function

$$\exp\left(i\operatorname{Re}\left(\mathbf{t}^{*}\boldsymbol{\mu}\right) - \frac{1}{4}\mathbf{t}^{*}\Gamma\mathbf{t}\right) \tag{5}$$

and following Hankin (2012) in writing $\mathfrak{B} = \Gamma/4$, we can write the variance matrix as a product of a (real) scalar σ^2 term and

$$c(\mathbf{t}) = \exp\left(i\operatorname{Re}\left(\mathbf{t}^*\boldsymbol{\mu}\right) - \mathbf{t}^*\mathfrak{B}\mathbf{t}\right). \tag{6}$$

Thus the covariance matrix Ω is given by

$$\Omega_{ij} = \mathsf{COV}\left(\eta\left(\mathbf{z}_{i}\right), \eta\left(\mathbf{z}_{j}\right)\right) = \sigma^{2} c\left(\mathbf{z}_{i} - \mathbf{z}_{j}\right). \tag{7}$$

In (6), \mathfrak{B} has the same meaning as in conventional emulator techniques and controls the modulus of the covariance between $\eta(\mathbf{z})$ and $\eta(\mathbf{z}')$; $\boldsymbol{\mu}$ governs the phase.

Given the above, it seems to be reasonable to follow Oakley (1999) and admit only diagonal \mathfrak{B} ; but now distributions with nonzero mean can be considered. Such a parametrization gives 3p (real) hyperparameters; compare 2p if \mathbb{C}^p is identified with \mathbb{R}^{2p} .

4. Functions of several complex variables

Analytic functions of several complex variables are an important and interesting class of objects; Krantz (1987) motivates and discusses the discipline. Formally, consider $f: \mathbb{C}^n \longrightarrow \mathbb{C}$, $n \geq 2$ and write $f(z_1, \ldots, z_n)$. Function f is analytic if it satisfies the Cauchy-Riemann conditions in each variable separately, that is $\partial f/\partial \bar{z}_j = 0$, $1 \leq j \leq n$.

Such an f is continuous (due to a "non-trivial theorem of Hartogs") and continuously differentiable to arbitrarily high order. Krantz goes on to state some results which are startling if one's exposure to complex analysis is restricted to functions of a single variable: for example, any isolated singularity is removable.

5. Numerical illustration of these ideas

The natural definition of complex Gaussian process above, together with the features of analytic functions of several complex variables, suggests that a complex emulation of analytic functions of several complex variables might be a useful technique.

The ideas presented above, and the **cmvnorm** package, can now be used to sample directly from an appropriate complex gaussian distribution and estimate the roughness parameters:

```
> val <- latin.hypercube(40,2,names=c('a','b'),complex = TRUE)
> head(val)
```

```
a b
[1,] 0.7375+0.2375i 0.2375+0.7125i
[2,] 0.6875+0.5875i 0.1375+0.3375i
[3,] 0.4625+0.5375i 0.9875+0.5875i
[4,] 0.7875+0.0625i 0.0625+0.7875i
[5,] 0.3875+0.0375i 0.5875+0.7625i
[6,] 0.2125+0.5625i 0.7625+0.9625i
```

(function latin.hypercube() is used to generate a random complex design matrix). We may now specify a variance matrix using simple values for the roughness hyperparameters $\mathfrak{B} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$ and $\boldsymbol{\mu} = (1, i)^T$:

```
> true_scales <- c(1,2)
> true_means <- c(1,1i)</pre>
```

```
> A <- corr_complex(val, means=true_means, scales=true_scales)
> round(A[1:4,1:4],2)
```

```
[,1] [,2] [,3] [,4] [1,] 1.00+0.00i 0.59-0.27i 0.25-0.10i 0.89+0.11i [2,] 0.59+0.27i 1.00+0.00i 0.20+0.00i 0.42+0.26i [3,] 0.25+0.10i 0.20+0.00i 1.00+0.00i 0.10+0.06i [4,] 0.89-0.11i 0.42-0.26i 0.10-0.06i 1.00+0.00i
```

Function corr_complex() is a complex generalization of corr(); matrix A is Hermitian positive-definite:

```
> all(eigen(A)$values > 0)
```

[1] TRUE

It is now possible to make a single multivariate observation d of this process, using $\beta = (1, 1+i, 1-2i)^T$:

```
> true_beta <- c(1,1+1i,1-2i)
> d <- drop(rcmvnorm(n=1,mean=regressor.multi(val) %*% true_beta,sigma=A))
> head(d)
```

```
[1] 3.212719+1.594901i 1.874278+0.345517i 3.008503-0.767618i 3.766526+2.071882i [5] 3.712913+0.800983i 3.944167+0.924833i
```

thus d is a single observation from a complex multivariate Gaussian distribution. Most of the functions of the **emulator** package operate without modification. Thus **betahat.fun()**, which calculates the maximum likelihood estimate $\hat{\boldsymbol{\beta}} = \left(H^*A^{-1}H\right)^{-1}H^TA^{-1}\mathbf{y}$ takes complex values directly:

> betahat.fun(val,solve(A),d)

```
const a b 0.593632-0.0128655i 0.843608+1.0920437i 1.140372-2.5053751i
```

However, because the likelihood function is different, the interpolant() functionality is implemented in the cmvnorm package by interpolant.quick.complex(), named in analogy to interpolant.quick() of package emulator.

For example, it is possible to evaluate the posterior distribution of the process at (0.5, 0.3 + 0.1i), a point at which no observation has been made:

```
> interpolant.quick.complex(rbind(c(0.5,0.3+0.1i)),d,
+ val,solve(A),scales=true_scales,means=true_means,give.Z=TRUE)
```

```
$mstar.star
[1] 1.706402-1.008601i

$Z
[1] 0.203295

$prior
[1] 1.608085-0.104419i
```

Thus the posterior distribution for the process is complex Gaussian at this point with a mean of about 1.71 - 1.01i and a variance of about 0.2.

5.1. Analytic functions

These techniques are now used to emulate an analytic function of several complex variables. A complex function's being analytic is a very strong restriction; Needham (2004) uses 'rigidity' to describe the severe constraint that analyticity represents.

Here the Weierstrass σ -function (Chandrasekharan 1985) is chosen as an example, on the grounds that Littlewood and Offord (1948) consider it to be a typical entire function in a well-defined sense. The elliptic package (Hankin 2006) is used for numerical evaluation. The σ -function takes a primary argument z and two invariants g_1, g_2 , so a three-column complex design matrix is required:

```
> library("elliptic")
> valsigma <-
+    2+1i + round(latin.hypercube(30,3,names=c("z","g1","g2"),complex=TRUE)/4,2)
> head(valsigma)

    z    g1    g2
[1,] 2.17+1.15i 2.09+1.22i 2.21+1.09i
[2,] 2.11+1.01i 2.04+1.03i 2.25+1.15i
```

```
[3,] 2.10+1.04i 2.15+1.00i 2.22+1.20i
[4,] 2.13+1.10i 2.24+1.21i 2.01+1.16i
[5,] 2.20+1.00i 2.20+1.06i 2.08+1.08i
```

[6,] 2.05+1.10i 2.19+1.04i 2.11+1.03i

(an offset is needed because $\sigma(z, g_1, g_2) = z + \mathcal{O}(z^5)$). The σ -function can now be evaluated at the points on the design matrix:

```
> dsigma <- apply(valsigma,1,function(u){sigma(u[1],g=u[2:3])})</pre>
```

One way of estimating the roughness parameters is to use maximum likelihood. The likelihood for any set of roughness parameters is given by Oakley (1999) as $(\sigma^2)^{-\frac{n-q}{2}} |A|^{-1/2} |H^T A^{-1} H|^{-1/2}$ with complex generalization $(\sigma^2)^{-(n-q)} |A|^{-1} |H^* A^{-1} H|^{-1}$ which is calculated in the package by function scales.likelihood.complex(); this can be used to return the log-likelihood for a specific set of roughness parameters:

Numerical methods can then be used to find the maximum likelihood estimate. Because function optim() optimizes over \mathbb{R}^n , helper functions are again needed which translate from the optimand to scales and means:

```
> scales <- function(x)\{\exp(x[c(1,2,2)])\}
> means <- function(x)\{x[c(3,4,4)] + 1i*x[c(5,6,6)]\}
```

Because the diagonal elements of \mathfrak{B} are strictly positive, their *logarithms* are optimized, following Hankin (2005); it is implicitly assumed that the scales and means associated with g_1 and g_2 are equal.

Function corr_complex() may now be used to calculate the covariance of the observations:

```
> Asigma <- corr_complex(z1=valsigma,scales=scales(u),means=means(u))
```

So now we can compare the emulator against the "true" value:

```
> interpolant.quick.complex(rbind(c(2+1i,2+1i,2+1i)), zold=valsigma,
+ d=dsigma,Ainv=solve(Asigma),scales=scales(u),means=means(u))
```

```
[1] 3.078956+1.259993i
```

```
> sigma(2+1i,g=c(2+1i,2+1i))
```

[1] 3.078255+1.257819i

showing reasonable agreement. It is also possible to test the hypothesis $H_{\mathbb{R}}$: $\mu \in \mathbb{R}^2$ (that is, the variance matrix A is real), by calculating the likelihood ratio of the unconstrained model (6) to that obtained by $H_{\mathbb{R}}$. This may be achieved by constraining the optimization to satisfy $\mu \in \mathbb{R}^2$:

Observing that D is in the tail region of its asymptotic distribution, χ_3^2 , the hypothesis $H_{\mathbb{R}}$ may be rejected.

6. Conclusions

The **cmvnorm** package for the complex multivariate Gaussian distribution has been introduced and motivated. The Gaussian process has been generalized to the complex case, and a complex generalization of the emulator technique has been applied to an analytic function of several complex variables. The complex variance matrix was specified using a novel parameterization which accommodated non-real covariances in the context of circulary symmetric random variables. Further work might include numerical support for the complex multivariate Student t distribution.

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