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Chapter 2

Quadratic Forms of Random Variables

2.1 Quadratic Forms

For a $k \times k$ symmetric matrix $\mathbf{A} = \{a_{ij}\}$ the quadratic function of k variables $\mathbf{x} = (x_1, \dots, x_n)'$ defined by

$$Q(\boldsymbol{x}) = \boldsymbol{x}' \boldsymbol{A} \boldsymbol{x} = \sum_{i=1}^{k} \sum_{j=1}^{k} a_{i,j} x_i x_j$$

is called the *quadratic form* with matrix A.

If A is not symmetric, we can have an equivalent expression/quadratic form replacing A by (A + A')/2.

Definition 1. $Q(\mathbf{x})$ and the matrix \mathbf{A} are called positive definite if

$$Q(\boldsymbol{x}) = \boldsymbol{x}' \boldsymbol{A} \boldsymbol{x} > 0, \quad \forall \, \boldsymbol{x} \in \mathbb{R}^k, \; \boldsymbol{x} \neq \boldsymbol{0}$$

and positive semi-definite if

$$Q(\boldsymbol{x}) \geq \forall \, \boldsymbol{x} \in \mathbb{R}^k$$

For negative definite and negative semi-definite, replace the > and \geq in the above definitions by < and \leq , respectively.

Theorem 1. A symmetric matrix \mathbf{A} is positive definite if and only if it has a Cholesky decomposition $\mathbf{A} = \mathbf{R}'\mathbf{R}$ with strictly positive diagonal elements in \mathbf{R} , so that \mathbf{R}^{-1} exists. (In practice this means that none of the diagonal elements of \mathbf{R} are very close to zero.)

Proof. The "if" part is proven by construction. The Cholesky decomposition, \mathbf{R} , is constructed a row at a time and the diagonal elements are evaluated as the square roots of expressions calculated from the current row of \mathbf{A} and previous rows of \mathbf{R} . If the expression whose square root is to be calculated is not positive then you can determine a non-zero $\mathbf{x} \in \mathbb{R}^k$ for which $\mathbf{x}' \mathbf{A} \mathbf{x} \leq 0$.

Suppose that A = R'R with R invertible. Then

$$x'Ax = x'R'Rx = ||Rx||^2 \ge 0$$

with equality only if $\mathbf{R}\mathbf{x} = \mathbf{0}$. But if \mathbf{R}^{-1} exists then $\mathbf{x} = \mathbf{R}^{-1}\mathbf{0}$ must also be zero.

Transformation of Quadratic Forms:

Theorem 2. Suppose that B is a $k \times k$ nonsingular matrix. Then the quadratic form $Q^*(y) = y'B'ABy$ is positive definite if and only if Q(x) = x'Ax is positive definite. Similar results hold for positive semi-definite, negative definite and negative semi-definite.

Proof.

$$Q^*(\boldsymbol{y}) = \boldsymbol{y}' \boldsymbol{B}' \boldsymbol{A} \boldsymbol{B} \boldsymbol{y} = \boldsymbol{x}' \boldsymbol{A} \boldsymbol{x} > 0$$

where $x = By \neq 0$ because $y \neq 0$ and B is nonsingular.

Theorem 3. For any $k \times k$ symmetric matrix A the quadratic form defined by A can be written using its spectral decomposition as

$$Q(\boldsymbol{x}) = \boldsymbol{x}' \boldsymbol{A} \boldsymbol{x} = \sum_{i=1}^k \lambda_i \| \boldsymbol{q}'_i \boldsymbol{x} \|^2$$

where the eigendecomposition of \mathbf{A} is $\mathbf{Q}' \mathbf{\Lambda} \mathbf{Q}$ with $\mathbf{\Lambda}$ diagonal with diagonal elements λ_i , $i = 1, \ldots, k$, \mathbf{Q} is the orthogonal matrix with the eigenvectors, \mathbf{q}_i , $i = 1, \ldots, k$ as its columns. (Be careful to distinguish the bold face \mathbf{Q} , which is a matrix, from the unbolded $Q(\mathbf{x})$, which is the quadratic form.)

Proof. For any $\boldsymbol{x} \in \mathbb{R}^k$ let $\boldsymbol{y} = \boldsymbol{Q}' \boldsymbol{x} = \boldsymbol{Q}^{-1} \boldsymbol{x}$. Then

$$Q(\boldsymbol{x}) = \operatorname{tr}(\boldsymbol{x}'\boldsymbol{A}\boldsymbol{x}) = \operatorname{tr}(\boldsymbol{x}'\boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}'\boldsymbol{x}) = \operatorname{tr}(\boldsymbol{y}'\boldsymbol{\Lambda}\boldsymbol{y}) = \operatorname{tr}(\boldsymbol{\Lambda}\boldsymbol{y}\boldsymbol{y}') = \sum_{i=1}^{k} \lambda_{i}y_{i}^{2} = \sum_{i=1}^{k} \lambda_{i}\|\boldsymbol{q}_{i}'\boldsymbol{x}\|^{2}$$

This proof uses a common "trick" of expressing the scalar $Q(\mathbf{x})$ as the trace of a 1×1 matrix so we can reverse the order of some matrix multiplications.

Corollary 1. A symmetric matrix **A** is positive definite if and only if its eigenvalues are all positive, negative definite if and only if its eigenvalues are all negative, and positive semi-definite if all its eigenvalues are non-negative.

Corollary 2. rank(A) = rank(Λ) hence rank(A) equals the number of non-zero eigenvalues of A

2.2 Idempotent Matrices

Definition 2 (Idempotent). The $k \times k$ matrix A, is idempotent if $A^2 = A A = A$.

Definition 3 (Projection matrices). A symmetric, idempotent matrix A is a projection matrix. The effect of the mapping $x \to Ax$ is orthogonal projection of x onto col(A).

Theorem 4. All the eigenvalues of an idempotent matrix are either zero or one.

Proof. Suppose that λ is an eigenvalue of the idempotent matrix A. Then there exists a non-zero x such that $Ax = \lambda x$. But Ax = AAx because A is idempotent. Thus

$$\lambda \boldsymbol{x} = \boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}(\lambda \boldsymbol{x}) = \lambda(\boldsymbol{A}\boldsymbol{x}) = \lambda^2 \boldsymbol{x}$$

and

$$\mathbf{0} = \lambda^2 \boldsymbol{x} - \lambda \boldsymbol{x} = \lambda (\lambda - 1) \boldsymbol{x}$$

for some non-zero \boldsymbol{x} , which implies that $\lambda = 0$ or $\lambda = 1$.

Corollary 3. The $k \times k$ symmetric matrix A is idempotent of rank(A) = r iff A has r eigenvalues equal to 1 and k - r eigenvalues equal to 0

Proof. A matrix A with r eigenvalues of 1 and k - r eigenvalues of zero has r non-zero eigenvalues and hence rank(A) = r. Because A is symmetric its eigendecomposition is $A = Q\Lambda Q'$ for an orthogonal Q and a diagonal Λ . Because the eigenvalues of Λ are the same as those of A, they must be all zeros or ones. That is all the diagonal elements of Λ are zero or one. Hence Λ is idempotent, $\Lambda \Lambda = \Lambda$, and

$$AA = Q\Lambda Q'Q\Lambda Q' = Q\Lambda Q' = A$$

is also idempotent.

Corollary 4. For a symmetric idempotent matrix A, we have tr(A) = rank(A), which is the dimension of col(A), the space into which A projects.

2.3 Expected Values and Covariance Matrices of Random Vectors

An k-dimensional vector-valued random variable (or, more simply, a random vector), \mathcal{X} , is a k-vector composed of k scalar random variables

$$\mathcal{X} = (\mathcal{X}_1, \ldots, \mathcal{X}_k)'$$

If the expected values of the component random variables are $\mu_i = E(\mathcal{X}_i), i = 1, \dots, k$ then

$$E(\mathcal{X}) = \boldsymbol{\mu}_{\mathcal{X}} = (\mu_1, \dots, \mu_k)'$$

Suppose that $\mathcal{Y} = (\mathcal{Y}_1, \dots, \mathcal{Y}_m)'$ is an *m*-dimensional random vector, then the *covariance* of \mathcal{X} and \mathcal{Y} , written $\text{Cov}(\mathcal{X}, \mathcal{Y})$ is

$$\Sigma_{XY} = \operatorname{Cov}(\mathcal{X}, \mathcal{Y}) = E[(\mathcal{X} - \boldsymbol{\mu}_{\mathcal{X}})(\mathcal{Y} - \boldsymbol{\mu}_{\mathcal{Y}})']$$

The variance-covariance matrix of \mathcal{X} is

$$\operatorname{Var}(\mathcal{X}) = \boldsymbol{\Sigma}_{XX} = E[(\mathcal{X} - \boldsymbol{\mu}_{\mathcal{X}})(\mathcal{X} - \boldsymbol{\mu}_{\S})]$$

Suppose that c is a constant m-vector, A is a constant $m \times k$ matrix and $\mathcal{Z} = Z\mathcal{X} + c$ is a linear transformation of \mathcal{X} . Then

$$E(\mathcal{Z}) = \mathbf{A}E(\mathcal{X}) + \mathbf{c}$$

 \square

and

$$\operatorname{Var}(\mathcal{Z}) = \boldsymbol{A} \operatorname{Var}(\mathcal{X}) \boldsymbol{A}'$$

If we let $\mathcal{W} = B\mathcal{Y} + d$ be a linear transformation of \mathcal{Y} for suitably sized B and d then

$$\operatorname{Cov}(\mathcal{Z}, \mathcal{W}) = \boldsymbol{A} \operatorname{Cov}(\mathcal{X}, \mathcal{Y}) \boldsymbol{B}'$$

Theorem 5. The variance-covariance matrix $\Sigma_{\mathcal{X},\mathcal{X}}$ of \mathcal{X} is a symmetric and positive semi-definite matrix

Proof. The result follows from the property that the variance of a scalar random variable is non-negative. Suppose that \boldsymbol{b} is any nonzero, constant k-vector. Then

$$0 \leq \operatorname{Var}(\boldsymbol{b}'\mathcal{X}) = \boldsymbol{b}'\boldsymbol{\Sigma}_{\mathcal{X}\mathcal{X}}\boldsymbol{b}$$

which is the positive, semi-definite condition.

2.4 Mean and Variance of Quadratic Forms

Theorem 6. Let \mathcal{X} be a k-dimensional random vector and \mathbf{A} be a constant $k \times k$ symmetric matrix. If $E(\mathcal{X}) = \boldsymbol{\mu}$ and $\operatorname{Var}(\mathcal{X}) = \boldsymbol{\Sigma}$, then

$$E(\mathcal{X}' A \mathcal{X}) = \operatorname{tr}(A \Sigma) + \mu' A \mu$$

Proof.

$$E(\mathcal{X}' \mathbf{A} \mathcal{X}) = \operatorname{tr}(E(\mathcal{X}' \mathbf{A} \mathcal{X}))$$

= $E[\operatorname{tr}(\mathcal{X}' \mathbf{A} \mathcal{X})]$
= $E[\operatorname{tr}(\mathbf{A} \mathcal{X} \mathcal{X}')]$
= $\operatorname{tr}(\mathbf{A} E[\mathcal{X} \mathcal{X}'])$
= $tr(\mathbf{A} (\operatorname{Cov}(\mathcal{X}) + \boldsymbol{\mu} \boldsymbol{\mu}'))$
= $tr(\mathbf{A} \boldsymbol{\Sigma}_{\mathcal{X} \mathcal{X}}) + \operatorname{tr}(\mathbf{A} \boldsymbol{\mu} \boldsymbol{\mu}')$
= $tr(\mathbf{A} \boldsymbol{\Sigma}_{\mathcal{X} \mathcal{X}}) + \boldsymbol{\mu}' \mathbf{A} \boldsymbol{\mu}$

2.5 Distribution of Quadratic Forms in Normal Random Variables

Definition 4 (Non-Central χ^2). If \mathcal{X} is a (scalar) normal random variable with $E(\mathcal{X}) = \mu$ and $\operatorname{Var}(\mathcal{X}) = 1$, then the random variable $\mathcal{V} = \mathcal{X}^2$ is distributed as $\chi_1^2(\lambda^2)$, which is called the noncentral χ^2 distribution with 1 degree of freedom and non-centrality parameter $\lambda^2 = \mu^2$. The mean and variance of \mathcal{V} are

$$E[\mathcal{V}] = 1 + \lambda^2 \text{ and } \operatorname{Var}[\mathcal{V}] = 2 + 4\lambda^2$$

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As described in the previous chapter, we are particularly interested in random *n*-vectors, \mathbf{Y} , that have a *spherical normal distribution*.

Theorem 7. Let $\mathcal{Y} \sim \mathcal{N}(\boldsymbol{\mu}, \sigma^2 \boldsymbol{I}_n)$ be an n-vector with a spherical normal distribution and \boldsymbol{A} be an $n \times n$ symmetric matrix. Then the ratio $\mathcal{Y}' \boldsymbol{A} \mathcal{Y} / \sigma^2$ will have a $\chi_r^2(\lambda^2)$ distribution with $\lambda^2 = \boldsymbol{\mu}' \boldsymbol{A} \boldsymbol{\mu} / \sigma^2$ if and only if \boldsymbol{A} is idempotent with rank $(\boldsymbol{A}) = r$

Proof. Suppose that A is idempotent (which, in combination with being symmetric, means that it is a projection matrix) and has rank(A) = r. Its eigendecomposition, $A = V\Lambda V'$, is such that V is orthogonal and Λ is $n \times n$ diagonal with exactly r = rank(A) ones and n - r zeros on the diagonal. Without loss of generality we can (and do) arrange the eigenvalues in decreasing order so that $\lambda_j = 1, j = 1, \ldots, r$ and $\lambda_j = 0, j = r + 1, \ldots, n$ Let $\mathcal{X} = V'\mathcal{Y}$

$$\frac{\mathcal{Y}' A \mathcal{Y}}{\sigma^2} = \frac{\mathcal{Y}' V \Lambda V' \mathcal{Y}}{\sigma^2}$$
$$= \frac{\mathcal{X}' \Lambda \mathcal{X}}{\sigma^2}$$
$$= \sum_{j=1}^n \lambda_j \frac{\mathcal{X}_j^2}{\sigma^2}$$
$$= \sum_{j=1}^r \frac{\mathcal{X}_j^2}{\sigma^2}$$

(Notice that the last sum is to j = r, not j = n.) However, $\frac{\chi_j}{\sigma} \sim \mathcal{N}(\boldsymbol{v}_j'\boldsymbol{\mu}/\sigma, 1)$ so $\frac{\chi_j^2}{\sigma^2} \sim \chi_1^2((\boldsymbol{v}_j'\boldsymbol{\mu}/\sigma)^2)$. Therefore

$$\sum_{j=1}^{r} \frac{\chi_j^2}{\sigma^2} \sim \chi_{(r)}^2(\lambda^2) \text{ where } \lambda^2 = \frac{\mu' V \Lambda V' \mu}{\sigma^2} = \frac{\mu' A \mu}{\sigma^2}$$

Corollary 5. For A a projection of rank r, $(\mathcal{Y}'A\mathcal{Y})/\sigma^2$ has a central χ^2 distribution if and only if $A\mu = 0$

Proof. The χ_r^2 distribution will be central if and only if

$$0 = \mu' A \mu = \mu' A A \mu = \mu' A' A \mu = ||A\mu||^2$$

Corollary 6. In the full-rank Gaussian linear model, $\mathbf{Y} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}_n)$, the residual sum of squares, $\|\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}\|^2$ has a central $\sigma^2 \chi^2_{n-r}$ distribution.

Proof. In the full rank model with the QR decomposition of X given by

$$oldsymbol{X} = egin{bmatrix} oldsymbol{Q}_1 & oldsymbol{Q}_2 \end{bmatrix} egin{bmatrix} oldsymbol{R} \ oldsymbol{0} \end{bmatrix}$$

and \mathbf{R} invertible, the fitted values are $Q_1 Q'_1 \mathcal{Y}$ and the residuals are $Q_2 Q_2 Q_2 \mathbf{y}$ so the residual sum of squares is the quadratic form $\mathcal{Y}' Q_2 Q'_2 \mathcal{Y}$. The matrix defining the quadratic form, $Q_2 Q'_2$, is a projection matrix. It is obviously symmetric and it is idempotent because $Q_2 Q'_2 Q_2 Q'_2 = Q_2 Q'_2$. As

$$oldsymbol{Q}_2'oldsymbol{\mu}=oldsymbol{Q}_2'oldsymbol{X}oldsymbol{eta}_0=oldsymbol{Q}_2'oldsymbol{Q}_1oldsymbol{R}oldsymbol{eta}_0=oldsymbol{0}_{(n-p) imes n}oldsymbol{R}oldsymbol{eta}_0=oldsymbol{0}_{(n-p) imes p}oldsymbol{eta}_0=oldsymbol{0}_{n-p}$$

the ratio

$$\frac{\mathcal{Y}' \boldsymbol{Q}_2 \boldsymbol{Q}_2' \mathcal{Y}}{\sigma^2} \sim \chi_{n-p}^2$$

and the RSS has a central $\sigma^2 \chi^2_{n-p}$ distribution.

R Exercises: Let's check some of these results by simulation. First we claim that if $\mathcal{X} \sim \mathcal{N}(\mu, 1)$ then $\mathcal{X}^2 \sim \chi^2(\lambda^2)$ where $\lambda^2 = \mu^2$. First simulate from a standard normal distribution

[1] 1.992403

The mean and variance of the simulated values agree quite well with the theoretical values of 1 and 2, respectively.

To check the form of the distribution we could plot an empirical density function but this distribution has its maximum density at 0 and is zero to the left of 0 so an empirical density is a poor indication of the actual shape of the density. Instead, in Fig. 2.1, we present the quantilequantile plot for this sample versus the (theoretical) quantiles of the χ_1^2 distribution.

Now simulate a non-central χ^2 with non-centrality parameter $\lambda^2 = 4$

```
> V1 <- rnorm(100000, mean=2)^2
> zapsmall(summary(V1))
Min. 1st Qu. Median Mean 3rd Qu. Max.
0.000 1.773 3.994 5.003 7.144 39.050
> var(V1)
```

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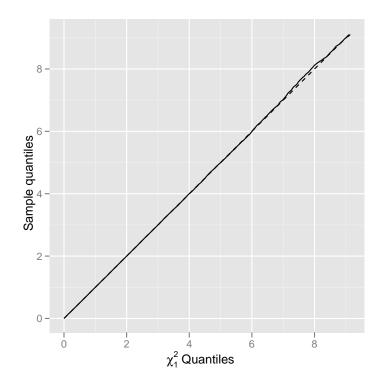


Figure 2.1: A quantile-quantile plot of the squares of simulated $\mathcal{N}(0,1)$ random variables versus the quantiles of the χ_1^2 distribution. The dashed line is a reference line through the origin with a slope of 1.

[1] 17.95924

The sample mean is close to the theoretical value of $5 = 1 + \lambda^2$ and the sample variance is close to the theoretical value of $2 + 4\lambda^2$ although perhaps not as close as one would hope in a sample of size 100,000.

A quantile-quantile plot versus the non-central distribution, $\chi_1^2(4)$, (Fig. 2.2) and versus the central distribution, χ_1^2 , shows that the sample does follow the claimed distribution $\chi_1^2(4)$ and is stochastically larger than the χ_1^2 distribution.

More interesting, perhaps is the distribution of the residual sum of squares from a regression model. We simulate from our previously fitted model lm1

```
> lm1 <- lm(optden ~ carb, Formaldehyde)
> str(Ymat <- data.matrix(unname(simulate(lm1, 10000))))
num [1:6, 1:10000] 0.088 0.258 0.444 0.521 0.619 ...
- attr(*, "dimnames")=List of 2
...$ : chr [1:6] "1" "2" "3" "4" ...
...$ : NULL</pre>
```

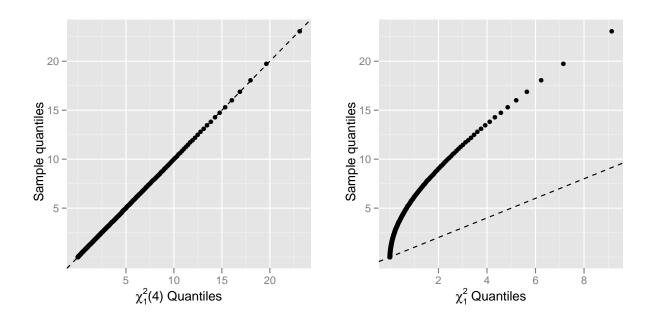


Figure 2.2: Quantile-quantile plots of a sample of squares of $\mathcal{N}(2,1)$ random variables versus the quantiles of a $\chi_1^2(4)$ non-central distribution (left panel) and a χ_1^2 central distribution (right panel)

```
> str(RSS <- deviance(fits <- lm(Ymat ~ carb, Formaldehyde)))
num [1:10000] 0.000104 0.000547 0.00055 0.000429 0.000228 ...
> fits[["df.residual"]]
[1] 4
```

Here the Ymat matrix is 10,000 simulated response vectors from model 1m1 using the estimated parameters as the true values of β and σ^2 . Notice that we can fit the model to all 10,000 response vectors in a single call to the 1m() function.

The deviance() function applied to a model fit by lm() returns the residual sum of square, which is not technically the deviance but is often the quantity of interest.

These simulated residual sums of squares should have a $\sigma^2 \chi_4^2$ distribution where σ^2 is the residual sum of squares in model 1m1 divided by 4.

```
> (sigsq <- deviance(lm1)/4)</pre>
```

```
[1] 7.48e-05
```

> summary(RSS)

Min. 1st Qu. Median Mean 3rd Qu. Max. 6.997e-07 1.461e-04 2.537e-04 3.026e-04 4.114e-04 1.675e-03

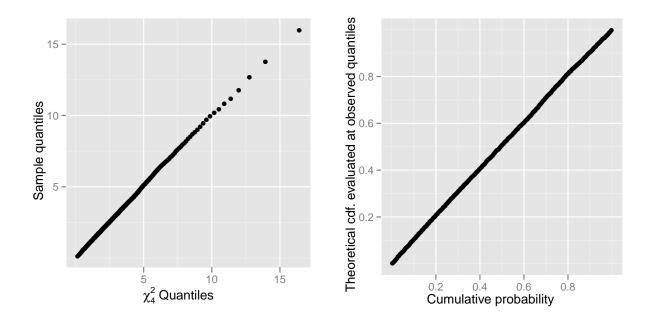


Figure 2.3: Quantile-quantile plot of the scaled residual sum of squares, RSSsq, from simulated responses versus the quantiles of a χ_4^2 distribution (left panel) and the corresponding probability-probability plot on the right panel.

We expect a mean of $4\sigma^2$ and a variance of $2 \cdot 4(\sigma^2)^2$. It is easier to see this if we divide these values by σ^2

```
> summary(RSSsc <- RSS/sigsq)
Min. 1st Qu. Median Mean 3rd Qu. Max.
0.009354 1.953000 3.392000 4.045000 5.500000 22.390000</pre>
```

```
> var(RSSsc)
```

[1] 8.000057

A quantile-quantile plot with respect to the χ_4^2 distribution (Fig. 2.3) shows very good agreement between the empirical and theoretical quantiles. Also shown in Fig. 2.3 is the probability-probability plot. Instead of plotting the sample quantiles versus the theoretical quantiles we take equally spaced values on the probability scale (function ppoints()), evaluate the sample quantiles and then apply the theoretical cdf to the empirical quantiles. This should also produce a straight line. It has the advantage that the points are equally spaced on the x-axis.

We could also plot the empirical density of these simulated values and overlay it with the theoretical density (Fig. 2.4).

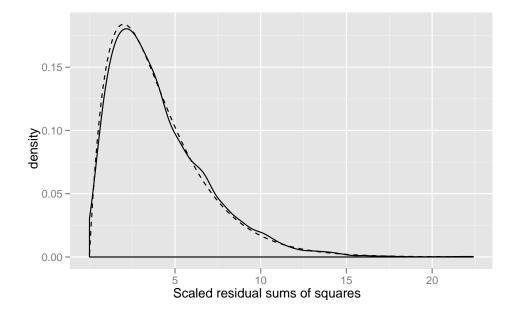


Figure 2.4: Empirical density plot of the scaled residual sums of squares, RSSsq, from simulated responses. The overlaid dashed line is the density of a χ_4^2 random variable. The peak of the empirical density gets shifted a bit to the right because of the way the empirical density if calculated. It uses a symmetric kernel which is not a good choice for a skewed density like this.