Exploring Densities of Gaussian Quadratic Forms

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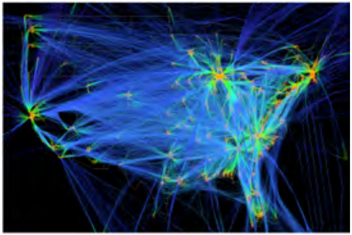


Presentation outline

1. Airport delay motivation
2. Moments and densities
3. Saddlepoint approximations
4. (An attempt at) Expansion approximations

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1. **Airport delay motivation**
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Spatial distribution of airport delays

- Imagine two scenarios, both with a total delay of 180 minutes:

- Some disruption, or off-nominal event caused the delays ...
- ... but one scenario is expected given historical correlations, while the other is unexpected.
- Operationally, the two scenarios are very different
  - What traffic management initiatives to deploy?
  - Airline recovery strategies?

Spatial distribution of airport delays (real example)

February 3, 2014

Total delay: **2.718×10^4 min**

August 8, 2016

Total delay: **2.715×10^4 min**

Delay network visualization courtesy of Karthik Gopalakrishnan

Airport delays as graph-supported signals

- For our purposes, graph signals live on vertices $\mathcal{V}$
  - Formally, a graph signal is a map $f : \mathcal{V} \to \mathbb{R}$
- Given N vertices (airports), at time t, the graph signal vector $\boldsymbol{x}_t$ is of the form:

$$\boldsymbol{x}_t = \begin{pmatrix} x_{1,t} \\ \vdots \\ x_{N,t} \end{pmatrix} \in \mathbb{R}_{\geq 0}^{N \times 1}.$$

- $x_{i,t}$ is the delay at airport i at time t

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- $x_{i,t}$ is the delay at airport i at time t
- $\boxed{\text{Let us consider } \boldsymbol{x} \text{ drawn from } \mathcal{N}(\mu, \Sigma)}$

Definition: Total variation (TV) of a graph signal

- Given an adjacency matrix $A = \left[a_{ij}\right]$ and the corresponding degree matrix $D = \text{diag}\left(\sum_j a_{1j}, \ldots, \sum_j a_{ij}\right)$, compute the (combinatorial) graph Laplacian $D - A = \mathcal{L} \in \mathbb{R}^{N \times N}$.
- Given $\mathcal{L}$ and a graph signal vector $\boldsymbol{x}_t \in \mathbb{R}^{N \times 1}$, the total variation (TV) of $\boldsymbol{x}_t$ on the graph is given by:

$$\boldsymbol{x}_t^\top \mathcal{L} \boldsymbol{x}_t = \frac{1}{2} \sum_{i \neq j} a_{ij} \left(x_{i,t} - x_{j,t}\right)^2 .$$

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- With $\boldsymbol{x}$ as m.v. Gaussian, call $\boxed{Q(\boldsymbol{x}) = \boldsymbol{x}^\top \mathcal{L} \boldsymbol{x}}$ a Gaussian quadratic form.

TV as a metric

February 3, 2014

Total delay: **2.718 × 10^4 min**
Total variation: **2.07 × 10^8 min^2**

August 8, 2016

Total delay: **2.715 × 10^4 min**
Total variation: **0.89 × 10^8 min^2**

Delay network visualization courtesy of Karthik Gopalakrishnan

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Moments of $Q(\boldsymbol{x}) = \boldsymbol{x}^\top \mathcal{L} \boldsymbol{x}$

Theorem (Theorem 3.2b.2 of Mathai & Provost (1992))

For $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$ *with valid* $m \times m$ *covariance matrix* Σ*, denote by* $Q(\boldsymbol{x}) = \boldsymbol{x}^\top A \boldsymbol{x}$ *where* A *is a* $m \times m$ *symmetric, real matrix. The* r^{th} *moment of* $Q(\boldsymbol{x})$ *is given by*

$$\mathbb{E}\left[Q(\boldsymbol{x})^r\right] = \sum_{r_1=0}^{r-1} \binom{r-1}{r_1} g(r-1-r_1) \sum_{r_2=0}^{r_1-1} \binom{r_1-1}{r_2} g(r_1-1-r_2) \cdots$$

where $g(k) = 2^k k! \left(\mathrm{tr}(A\Sigma)^{k+1} + (k+1)\boldsymbol{\mu}^\top (A\Sigma)^k A\boldsymbol{\mu}\right)$ *for* $k \in \mathbb{N}_{\geq 0}$.

Moments of $Q(x) = x^\top \mathcal{L} x$

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Of practical interest: Mean and variance

$$\mathbb{E}\left[Q(\mathbf{x})\right] = \mathrm{tr}(A\Sigma) + \boldsymbol{\mu}^\top A\boldsymbol{\mu},$$
$$\mathrm{Var}\left[Q(\mathbf{x})\right] = 2\,\mathrm{tr}(A\Sigma)^2 + 4\boldsymbol{\mu}^\top A\Sigma A\boldsymbol{\mu}.$$

Yay! But what about the density for $Q(\mathbf{x})$?

$Q(x)$'s messy density

- Only series expansions, unfortunately. No general closed form ...
- *Expansions:* Power series; Laguerre series; Central χ^2 densities; Confluent Hypergeometric functions; Zonal polynomials; Densities of Gamma variates

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- (Generalized) Laguerre polynomials $L_k^{(\alpha)}(x)$, Rodrigues formula:

$$L_k^{(\alpha)}(x) = \frac{1}{x!} e^x x^{-\alpha} \left(\frac{d^k}{dx^k} e^{-x} x^{k+a} \right)$$

with $\alpha > -1$ and $k = 0, 1, \ldots$

- And the density of $Q(x)$ is ...

$Q(x)$'s messy density

... not very fun to look at, or easy to poke around:

$$f_{Q(x)}(\boldsymbol{\lambda}; \mathbf{b}; q) = \sum_{k=0}^{\infty} c_k^{\boldsymbol{\lambda}, \mathbf{b}} \frac{k!}{2\beta\Gamma\left(\frac{m}{2} + k\right)} \left(\frac{q}{2\beta}\right)^{\frac{m}{2}-1} e^{-\frac{q}{2\beta}} L_k^{\left(\frac{m}{2}-1\right)}\left(\frac{q}{2\beta}\right),$$

for $q \in (0, \infty)$.

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$$f_{Q(x)}(\boldsymbol{\lambda}; \mathbf{b}; q) = \sum_{k=0}^{\infty} c_k^{\boldsymbol{\lambda},\mathbf{b}} \frac{k!}{2\beta\Gamma\left(\frac{m}{2}+k\right)} \left(\frac{q}{2\beta}\right)^{\frac{m}{2}-1} e^{-\frac{q}{2\beta}} L_k^{\left(\frac{m}{2}-1\right)}\left(\frac{q}{2\beta}\right),$$

for $q \in (0, \infty)$.

- β is an arbitrary positive constant
- $c_k^{\boldsymbol{\lambda},\mathbf{b}}$ are power series expansion coefficients with $c_0 = 1$, dependent on $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_m)$ and $\mathbf{b} = (b_1, \ldots, b_m)$
- $\mathrm{diag}(\boldsymbol{\lambda}) = P^\top \left(\Sigma^{1/2} A \Sigma^{1/2}\right) P$ for an orthogonal P
- Centrality parameter $\mathbf{b}^\top = P^\top \Sigma^{-1/2} \boldsymbol{\mu}$

Presentation outline

Saddlepoint approximations to the rescue (?)

- Unknown (univariate) density $f_X(x)$, known moment and cumulant generating functions $M_X(s), K_X(s) = \ln M_X(s)$

- Saddlepoint approximation (Daniels, 1954) provide extremely accurate, closed-form approximation to $f_X(x)$, has advantages over:
  - Enumerating exact probabilities ($\Rightarrow$ intractability issues)
  - Normal density approximation ($\Rightarrow$ may be inaccurate)
  - Brute force simulation with kernel density estimation ($\Rightarrow$ time consuming, KDE may be inaccurate)

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- The saddlepoint equation $\widehat{f}_X(x)$ approximates $f_X(x)$ on its support $\mathcal{X}$, given the saddlepoint $\hat{s} \triangleq \hat{s}(x)$ associated with $x \in \mathcal{X}$, where $\hat{s}$ is the solution to $dK(\hat{s})/ds = x$.

$$\widehat{f}_X(x) = \frac{1}{\sqrt{2\pi \frac{d^2}{ds^2} K_X(\hat{s})}} \exp\left(K(\hat{s}) - \hat{s}x\right).$$

The MGF for $Q(x)$

Theorem (Theorems 3.2a.1, 3.2a.2, and Corollary 3.2a.1 of Mathai & Provost (1992))

Let A be a real, symmetric $m \times m$ matrix, and $\mathbf{x} \in \mathbb{R}^{m\times 1}$ with $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$. The MGF $M_{Q(\mathbf{x})}(s)$ of $Q(\mathbf{x}) = \mathbf{x}^\top A\mathbf{x}$ can be written in a scalar form involving the eigenvalues of $\Sigma^{1/2}A\Sigma^{1/2}$ and constants that depend on the mean $\boldsymbol{\mu}$.

Specifically, let $\lambda_1, \ldots, \lambda_m$ be eigenvalues of $\Sigma^{1/2}A\Sigma^{1/2}$, and define the vector of constants $\mathrm{b} = (b_1, \ldots, b_m)^\top = P^\top \Sigma^{-1/2}\boldsymbol{\mu}$, where P is any $m \times m$ orthogonal matrix that diagonalizes $\Sigma^{1/2}A\Sigma^{1/2}$. Then, $M_{Q(\mathbf{x})}(s)$ can be rewritten as follows:

$$M_{Q(\mathbf{x})}(s) = \begin{cases} \exp\left(s\sum_{j=1}^{m} \frac{b_j^2\lambda_j}{1-2s\lambda_j}\right)\prod_{j=1}^{m}(1-2s\lambda_j)^{-\frac{1}{2}}, & \text{if } \boldsymbol{\mu} \neq 0, \\ \prod_{j=1}^{m}(1-2s\lambda_j)^{-\frac{1}{2}}, & \text{if } \boldsymbol{\mu} = 0. \end{cases}$$

Saddlepoint approximation ingredients

Start with central case $\boldsymbol{\mu} = 0$, we have:

$$K_Q(s) = \sum_{j=1}^{m} \ln\left((1-2s\lambda_j)^{-\frac{1}{2}}\right),$$

$$\frac{d}{ds}K_Q(s) = \sum_{j=1}^{m} \frac{\lambda_j}{1-2s\lambda_j},$$

$$\frac{d^2}{ds^2}K_Q(s) = \sum_{j=1}^{m} \frac{2\lambda_j^2}{(1-2s\lambda_j)^2}.$$

Problem: $m = 1$ and $m = 2$ are fine, $m = 3$ gets sketchy, $m \geq 4$ untenable ...

The problem is solving for the saddlepoint $\frac{d}{ds}K(\hat{s}) = x$.

⇒ Possibly tenable (visually) in `Maple` via implicit function evaluation (Butler, 2007)

Saddlepoint approximation ingredients

Non-central case is even worse in terms of solving for the saddlepoint.
First derive the ingredients:

$$
\begin{aligned}
K_Q(s) &= s\sum_{j=1}^{m}\frac{b_j^2\lambda_j}{1-2s\lambda_j}+\sum_{j=1}^{m}\ln\left((1-2s\lambda_j)^{-1/2}\right),\\
\frac{d}{ds}K_Q(s) &= \sum_{j=1}^{m}\frac{\lambda_j\left(1+b_j^2-2s\lambda_j\right)}{(1-2s\lambda_j)^2},\\
\frac{d^2}{ds^2}K_Q(s) &= 2\sum_{j=1}^{m}\frac{\lambda_j^2\left(-1-2b_j^2+2s\lambda_j\right)}{(-1+2s\lambda_j)^2}.
\end{aligned}
$$

Problem: $m = 1$ is “fine”, $m \geq 2$ untenable ...

Let's look back at the central case.

(Central case) Saddlepoints for $m = 1, 2$

Recall that $\lambda_1, \ldots, \lambda_m$ are eigenvalues of $\Sigma^{1/2} A \Sigma^{1/2}$ (known)

- For $m = 1$, the saddlepoint is

$$\hat{s} = \frac{1}{2}\left(\frac{1}{\lambda_1} - \frac{1}{x}\right)$$

- For $m = 2$, the saddlepoint(s) is

$$\hat{s} = \frac{1}{4\lambda_1\lambda_2 x}\left(\pm\sqrt{\lambda_1^2 x^2 - 2\lambda_1\lambda_2 x^2 + \lambda_2^2\left(4\lambda_1^2 + x^2\right)} + \lambda_2 x + \lambda_1\left(x - 2\lambda_2\right)\right)$$

- For $m = 3$ ...

(Central case) Saddlepoint for $m = 3$

$\hat{s} =$

$$
\begin{aligned}
&\frac{1}{12\, x\, \lambda_1 \lambda_2 \lambda_3} \Big(2\,(x\,\lambda_1 \lambda_2 - 3\,\lambda_1 \lambda_2 \lambda_3 + x\,(\lambda_1 + \lambda_2)\,\lambda_3) + \\
&\quad \left(2 \times 2^{1/3}\left(9\,\lambda_1^2 \lambda_2^2 \lambda_3^2 + x^2 \left(\lambda_2^2 \lambda_3^2 - \lambda_1 \lambda_2 \lambda_3\,(\lambda_2 + \lambda_3) + \lambda_1^2\left(\lambda_2^2 - \lambda_2 \lambda_3 + \lambda_3^2\right)\right)\right)\right) \Big/ \\
&\quad \Big(2\,x^3 \lambda_2^3 \lambda_3^3 - 3\,x^3 \lambda_1 \lambda_2^2 \lambda_3^2\,(\lambda_2 + \lambda_3) - 3\,x^3 \lambda_1^2 \lambda_2 \lambda_3 \left(\lambda_2^2 - 4\,\lambda_2 \lambda_3 + \lambda_3^2\right) + \\
&\qquad \lambda_1^3\left(-54\,\lambda_2^3 \lambda_3^3 + x^3\,(\lambda_2 - 2\,\lambda_3)\,(2\,\lambda_2 - \lambda_3)\,(\lambda_2 + \lambda_3)\right) + \\
&\qquad \frac{1}{64}\sqrt{\Big(4096\left(-54\,\lambda_1^3 \lambda_2^3 \lambda_3^3 + x^3\,(\lambda_1\,(\lambda_2 - 2\,\lambda_3) + \lambda_2 \lambda_3)\,(2\,\lambda_1 \lambda_2 - (\lambda_1 + \lambda_2)\,\lambda_3)\,(-2\,\lambda_2 \lambda_3 + \lambda_1\,(\lambda_2 + \lambda_3))\right)^2 + 4\left(-16\,(x\,\lambda_1 \lambda_2 - 3\,\lambda_1 \lambda_2 \lambda_3 + x\,(\lambda_1 + \lambda_2)\,\lambda_3)^2 + 48\,x\,\lambda_1 \lambda_2 \lambda_3\,(x\,(\lambda_1 + \lambda_2 + \lambda_3) - 2\,(\lambda_2 \lambda_3 + \lambda_1\,(\lambda_2 + \lambda_3)))\right)^3\Big)}\ \Big)^{1/3} + \\
&\quad 2^{2/3}\Big(2\,x^3 \lambda_2^3 \lambda_3^3 - 3\,x^3 \lambda_1 \lambda_2^2 \lambda_3^2\,(\lambda_2 + \lambda_3) - 3\,x^3 \lambda_1^2 \lambda_2 \lambda_3 \left(\lambda_2^2 - 4\,\lambda_2 \lambda_3 + \lambda_3^2\right) + \\
&\qquad \lambda_1^3\left(-54\,\lambda_2^3 \lambda_3^3 + x^3\,(\lambda_2 - 2\,\lambda_3)\,(2\,\lambda_2 - \lambda_3)\,(\lambda_2 + \lambda_3)\right) + \\
&\qquad \frac{1}{64}\sqrt{\Big(4096\left(-54\,\lambda_1^3 \lambda_2^3 \lambda_3^3 + x^3\,(\lambda_1\,(\lambda_2 - 2\,\lambda_3) + \lambda_2 \lambda_3)\,(2\,\lambda_1 \lambda_2 - (\lambda_1 + \lambda_2)\,\lambda_3)\,(-2\,\lambda_2 \lambda_3 + \lambda_1\,(\lambda_2 + \lambda_3))\right)^2 + 4\left(-16\,(x\,\lambda_1 \lambda_2 - 3\,\lambda_1 \lambda_2 \lambda_3 + x\,(\lambda_1 + \lambda_2)\,\lambda_3)^2 + 48\,x\,\lambda_1 \lambda_2 \lambda_3\,(x\,(\lambda_1 + \lambda_2 + \lambda_3) - 2\,(\lambda_2 \lambda_3 + \lambda_1\,(\lambda_2 + \lambda_3)))\right)^3\Big)}\ \Big)^{1/3}\Big)
\end{aligned}
$$

$$\texttt{Reduce}\left[\sum_{j=1}^{3} \frac{\lambda_j}{1-2s\lambda_j} \texttt{ == x, t, Cubics} \rightarrow \texttt{True}\right]$$

(Non-central case) Saddlepoint for $m = 1$

Recall that $\lambda_1, \ldots, \lambda_m$ are eigenvalues of $\Sigma^{1/2} A \Sigma^{1/2}$ and $b_1, \ldots, b_m$ elements of row vector $\Sigma^{-1/2}\mu$ (both known),

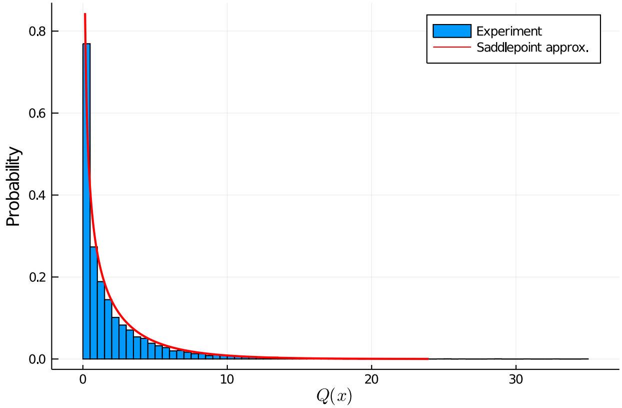
- For $m = 1$, the saddlepoint is

$$\hat{s} = \frac{\pm\sqrt{4b_1^2\lambda_1^3 x + \lambda_1^4} - \lambda_1^2 + 2\lambda_1 x}{4\lambda_1^2 x}$$

- For $m = 2$, the saddlepoint(s) does not fit my screen
- For $m = 3$, no thanks.

Saddlepoint approximation ($m = 2$)

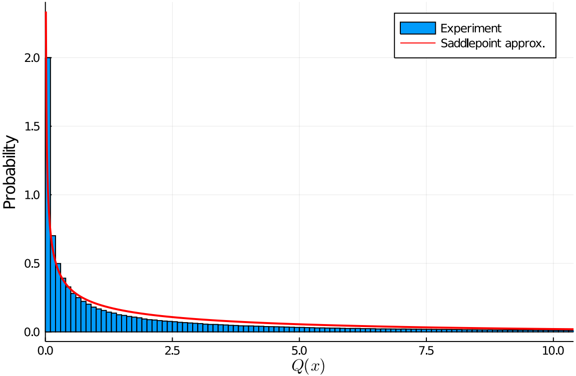
Implemented in `Julia`
2 node, central, with $\Sigma = I_{2\times 2}$



Approximation also decent for random $\Sigma =$ `randn(2, 2)`, then $\Sigma = \Sigma^\top \Sigma$.

Saddlepoint approximation ($m = 2$), "*randomized*"

2 node, central, with Σ = `randn(2, 2)`, then $\Sigma = \Sigma^\top \Sigma$
Repeat T times (including drawing $Q(x)$ samples), take *average* eigenvalues of $\Sigma^{1/2}\mathcal{L}\Sigma^{1/2}$, fit one saddlepoint approx. to entire histogram over T trials ...



(T = 1000 trials)

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Numerical attempt at other expansions

- *Expansions:* Power series; **Laguerre series**; **Central χ^2 densities**; Confluent Hypergeometric functions; Zonal polynomials; Densities of Gamma variates

Density:
$$f_{Q(x)}(\boldsymbol{\lambda}; \mathbf{b}; q) = \sum_{k=0}^{\infty} \frac{c_k^{\boldsymbol{\lambda},\mathbf{b}}}{\beta} \underbrace{f_{\chi^2}\left(m + 2k; \frac{q}{\beta}\right)}_{\chi^2 \text{ density}}$$

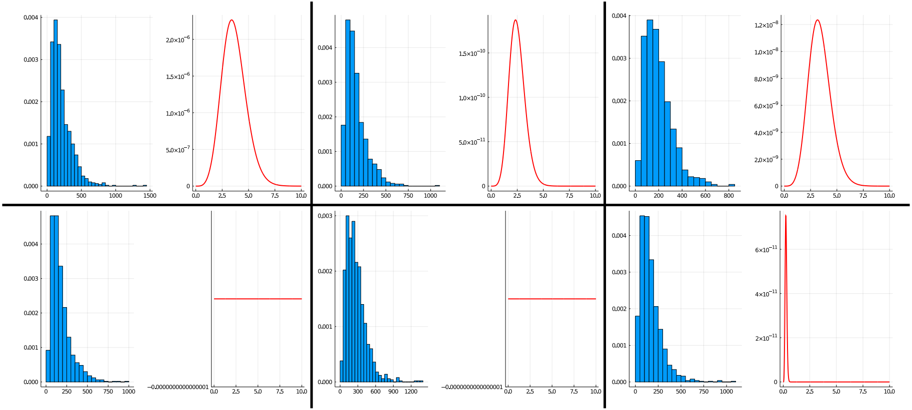
Expansion constant $c_k^{\boldsymbol{\lambda},\mathbf{b}}$ computed from:

$$c_k^{\boldsymbol{\lambda},\mathbf{b}} = \begin{cases} \exp\left(-\frac{1}{2}\sum_{j=1}^{m} b_j^2\right) \prod_{j=1}^{m} \left(\frac{\beta}{\lambda_j}\right)^{1/2}, & \text{if } k = 0, \\ \frac{1}{2k} \sum_{r=0}^{k-1} d_{k-r} c_r, & \text{if } k = 1, 2, \ldots \end{cases}$$

$$d_{k-r} = \sum_{j=1}^{m} \left(1 - \frac{\beta}{\lambda_j}\right)^{k-r} + \beta(k-r) \sum_{j=1}^{m} \left(\frac{b_j^2}{\lambda_j}\right)\left(1 - \frac{\beta}{\lambda_j}\right)^{k-r-1}$$

χ^2 density expansion

$m = 10$ node case (cycle), non-central ($\mu = \texttt{randn(m)}$), $\Sigma = \texttt{randn(m, m)}$, then $\Sigma = \Sigma^\top \Sigma$, expansion $k = 10$, take $\beta = \min_{j=1,\ldots,m} \lambda_i + \epsilon$



For smaller m, seems to do … "better", but the scaling is usually off on the value $Q(x)$. Numerical issue? My abilities at coding? Jury is still out!

Numerical attempt at other expansions

- *Expansions:* Power series; **Laguerre series**; **Central χ^2 densities**; Confluent Hypergeometric functions; Zonal polynomials; Densities of Gamma variates

$$f_{Q(x)}(\boldsymbol{\lambda}; \mathbf{b}; q) = \sum_{k=0}^{\infty} c_k^{\boldsymbol{\lambda},\mathbf{b}} \frac{k!}{2\beta\Gamma\left(\frac{m}{2}+k\right)} \left(\frac{q}{2\beta}\right)^{\frac{m}{2}-1} e^{-\frac{q}{2\beta}} L_k^{\left(\frac{m}{2}-1\right)}\left(\frac{q}{2\beta}\right)$$

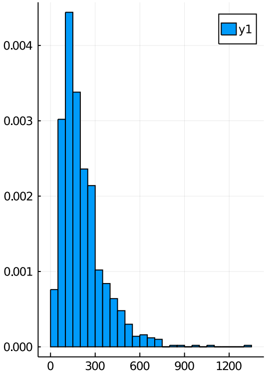
Expansion constant $c_k^{\boldsymbol{\lambda},\mathbf{b}}$ (slightly different from χ^2 expansion) computed from:

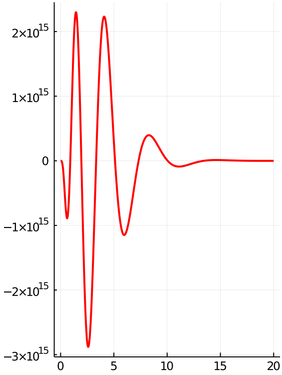
$$c_k^{\boldsymbol{\lambda},\mathbf{b}} = \begin{cases} \exp\left(-\frac{1}{2}\sum_{j=1}^{m} b_j^2\right) \prod_{j=1}^{m} (2\lambda_j)^{-1/2}, & \text{if } k = 0, \\ \frac{1}{k}\sum_{r=0}^{k-1} d_{k-r} c_r, & \text{if } k = 1, 2, \ldots \end{cases}$$

$$d_{k-r} = \frac{1}{2}\sum_{j=1}^{m}\left(1-\frac{\lambda_j}{\beta}\right)^{k-r} - \frac{k}{2\beta}\sum_{j=1}^{m}\lambda_j b_j^2\left(1-\frac{\lambda_j}{\beta}\right)^{k-r-1}.$$

Laguerre series expansion

$m = 10$ node case (cycle), non-central ($\mu = \texttt{randn}(m)$), $\Sigma = \texttt{randn}(m, m)$, then $\Sigma = \Sigma^\top \Sigma$, expansion $k = 10$, take $\beta = \min_{j=1,\dots,m} \lambda_i + \epsilon$





A little disappointing, but the debugging continues ...

Thank you for a great semester!