



Full length article

Computation of equilibrium measures

Sheehan Olver

Oxford University Mathematical Institute, Numerical Analysis Group, 24–29 St Giles', Oxford, OX1 3LB, UK

Received 23 August 2010; received in revised form 9 March 2011; accepted 30 March 2011

Available online 15 April 2011

Communicated by Arno B J Kuijlaars

Abstract

We present a new way of computing equilibrium measures numerically, based on the Riemann–Hilbert formulation. For equilibrium measures whose support is a single interval, the simple algorithm consists of a Newton–Raphson iteration where each step only involves fast cosine transforms. The approach is then generalized for multiple intervals.

© 2011 Elsevier Inc. All rights reserved.

Keywords: Equilibrium measure; Orthogonal polynomials; Random matrices; Riemann–Hilbert problems

1. Introduction

Equilibrium measures are essentially the distribution of charges on a conductor under the influence of an external field [15]. They have a wide field of applications, from the distribution of eigenvalues of large random matrices to the zeros of orthogonal polynomials with respect to general weights of the form [2]

$$e^{-nV(x)} dx.$$

Moreover, such orthogonal polynomials themselves can be represented as a matrix-valued Riemann–Hilbert problem, which requires the equilibrium measure to be rephrased in a canonical form [2]. The resulting Riemann–Hilbert problem can be solved numerically [12,10], using a recent MATHEMATICA package, RHPackage [13]. By combining a numerical approach for computing the equilibrium measure with the matrix-valued Riemann–Hilbert solver, we

E-mail address: Sheehan.Olver@sjc.ox.ac.uk.

could efficiently calculate orthogonal polynomials of arbitrarily large degree: the degree of the polynomial is simply a parameter in the Riemann–Hilbert problem, and the construction is independent of the lower order orthogonal polynomials. This could in turn be used to calculate random matrix distributions, which, in general, are expressible as Fredholm determinants with a kernel defined in terms of orthogonal polynomials [2].

Definition 1.1. Suppose we are given an external field $V : \mathbb{R} \rightarrow \mathbb{R}$ which has sufficient growth at infinity: $\frac{V(x)}{\log|x|} \rightarrow +\infty$ as $|x| \rightarrow \infty$. The equilibrium measure is the unique probability Borel measure $d\mu = \psi(x) dx$ such that

$$\iint \log \frac{1}{|t - s|} d\mu(t) d\mu(s) + \int V(s) d\mu(s) \tag{1.1}$$

is minimal; cf. [15].

There is an existing numerical method for computing equilibrium measures based on Leja points [8,5,15]. Leja points are a sequence of points which cover the support of the equilibrium measure. However, convergence is necessarily slow, as it is approximating a continuous domain by isolated points. One could imagine a finite element-like numerical approach based on (1.1), though, since the equilibrium measure generically has square root singularities at its endpoints [7], any naïve scheme would also exhibit extremely slow convergence rates.

Instead of constructing a numerical method based on (1.1), we will use the following RH formulation:

Theorem 1.2 ([2]). *Suppose $\text{supp } \mu$ consists of a finite number of intervals. Let ϕ be a function bounded and analytic in $\mathbb{C} \setminus \text{supp } \mu$ which satisfies*

$$\phi^+(x) + \phi^-(x) = V'(x) \quad \text{for } x \in \text{supp } \mu$$

and

$$\phi(z) = \frac{1}{z} + \mathcal{O}\left(\frac{1}{z^2}\right) \text{ as } z \rightarrow \infty,$$

where ϕ^+ is the limit from above and ϕ^- is the limit from below:

$$\phi^\pm(x) = \lim_{\epsilon \rightarrow 0^+} \phi(x \pm i\epsilon).$$

Then

$$\phi(z) = \int \frac{d\mu(s)}{z - s},$$

and hence

$$d\mu = \frac{i}{2\pi} [\phi^+(x) - \phi^-(x)] dx.$$

This formulation has been used to determine μ analytically when $V(x)$ is a polynomial, by writing the solution of $\phi^+ + \phi^- = V'$ as a Cauchy transform [2]. This analytic derivation is not trivial and will not necessarily work for non-polynomial V .

In this paper, we utilize Theorem 1.2 in a numerical manner, beginning with the case that $\text{supp } \mu$ is a single interval. Given a fixed interval $\Sigma = (a, b)$, we can efficiently solve (using

$\phi(\infty)$ as shorthand for $\lim_{z \rightarrow \infty} \phi(z)$)

$$\phi^+(x) + \phi^-(x) = f(x) \quad \text{for } x \in \Sigma \quad \text{and} \quad \phi(\infty) = 0, \tag{1.2}$$

using the fast cosine transform [11], as reviewed in Section 2. There are, in fact, a family of solutions, depending on a parameter ξ . We refer to this family as the inverse Cauchy transform.

Generically, the solution of (1.2) is unbounded: by choosing ξ appropriately, it can be imposed that the solution is bounded at either the left or right endpoint of Σ , but not both. However, if the zeroth Chebyshev coefficient of V' vanishes, then the solution can be bounded at both endpoints, each (generically) having a square root singularity. Moreover, we can compute the asymptotic behaviour of ϕ from the first Chebyshev coefficient of V' . Thus we can establish a function $F(\Sigma) = F(a, b)$ for which $F(\text{supp } \mu) = 0$. Moreover, the Jacobian of F is also easily computed, hence solving $F(\Sigma) = 0$ is a trivial application of the Newton–Raphson method. If V is strictly convex, this approximation is guaranteed to converge to the true equilibrium measure, as proved in Theorem 4.1.

This approach is then generalized for $\text{supp } \mu$ consisting of multiple intervals. In Section 6, a new solution for (1.2) when Σ consists of multiple intervals is derived. In Section 8, a Newton–Raphson iteration is set up, much like in the one-interval case, but now with additional conditions which depend on the indefinite integral of the inverse Cauchy transform. Fortunately, this is also computable. Using this method, we compute the equilibrium measure of a potential depending on a parameter in Section 9, confirming the theory of [7]. Finally, in Section 10, we describe how the method can be further optimized.

2. Computation of the inverse Cauchy transform

While solving (1.2) appears to be nontrivial, it can be readily solved by mapping the problem to an equivalent problem on the unit circle. Finding a function φ which is analytic off the unit circle and satisfies

$$\varphi^+(\zeta) + \varphi^-(\zeta) = g(\zeta) \quad \text{for } |\zeta| = 1 \quad \text{and} \quad \varphi(\infty) = 0$$

is a trivial application of Laurent series/FFT; we find that $\varphi = \mathcal{P}g$, as defined below:

Definition 2.1. Suppose $g(\zeta) = \sum_{k=-\infty}^{\infty} \hat{g}_k \zeta^k$. For $|\zeta| \neq 1$, define

$$\mathcal{P}g(\zeta) = \begin{cases} \sum_{k=0}^{\infty} \hat{g}_k \zeta^k & \text{for } |\zeta| < 1 \\ \sum_{k=-1}^{-\infty} \hat{g}_k \zeta^k & \text{for } |\zeta| > 1. \end{cases}$$

Then, for $|\zeta| = 1$,

$$\mathcal{P}^+g(\zeta) = \sum_{k=0}^{\infty} \hat{g}_k \zeta^k \quad \text{and} \quad \mathcal{P}^-g(\zeta) = \sum_{k=-1}^{-\infty} \hat{g}_k \zeta^k.$$

Now define the Joukowski map as

$$J(\zeta) = \frac{1}{2} \left(\zeta + \frac{1}{\zeta} \right),$$

which maps the lower and the upper half of the unit circle to the unit interval, and the interior and exterior of the unit circle to the slit complex plane $\mathbb{C} \setminus [-1, 1]$. We will use this map to translate the jump condition on the unit interval to one on the unit circle. To do this, we need the following four inverses:

Definition 2.2.

Map from $\mathbb{C} \setminus [-1, 1]$ to the interior of the unit circle:	$J_+^{-1}(z) = z - \sqrt{z-1}\sqrt{z+1}$
Map from $\mathbb{C} \setminus [-1, 1]$ to the exterior of the unit circle:	$J_-^{-1}(z) = z + \sqrt{z-1}\sqrt{z+1}$
Map from $[-1, 1]$ to the upper half circle:	$J_\uparrow^{-1}(x) = x + i\sqrt{1-x}\sqrt{1+x}$
Map from $[-1, 1]$ to the lower half circle:	$J_\downarrow^{-1}(x) = x - i\sqrt{1-x}\sqrt{1+x}$

The inverses J_\pm^{-1} have branch cuts along $[-1, 1]$, whilst J_\uparrow^{-1} are analytic along $(-1, 1)$ and have branch cuts along $(-\infty, -1]$ and $[1, \infty)$. Using the definition of the (principal branch) square root function, we can relate these four inverses:

$$\begin{aligned} \lim_{\epsilon \rightarrow 0^+} J_+^{-1}(x + \epsilon i) &= J_\downarrow^{-1}(x), & \lim_{\epsilon \rightarrow 0^-} J_+^{-1}(x + \epsilon i) &= J_\uparrow^{-1}(x), \\ \lim_{\epsilon \rightarrow 0^+} J_-^{-1}(x + \epsilon i) &= J_\uparrow^{-1}(x), & \lim_{\epsilon \rightarrow 0^-} J_-^{-1}(x + \epsilon i) &= J_\downarrow^{-1}(x). \end{aligned}$$

Let $\varphi = \mathcal{P}g$ for $g(\zeta) = f(J(\zeta))$. Then $\phi(z) = \frac{1}{2} [\varphi(J_+^{-1}(z)) + \varphi(J_-^{-1}(z))]$ satisfies the jump condition

$$\begin{aligned} \phi^+(x) + \phi^-(x) &= \frac{1}{2} [\varphi^+(J_\downarrow^{-1}(x)) + \varphi^-(J_\uparrow^{-1}(x)) + \varphi^-(J_\uparrow^{-1}(x)) + \varphi^+(J_\downarrow^{-1}(x))] \\ &= \frac{1}{2} [f(J(J_\downarrow^{-1}(x))) + f(J(J_\uparrow^{-1}(x)))] = f(x). \end{aligned}$$

Unfortunately,

$$\phi(\infty) = \frac{1}{2} [\varphi(0) + \varphi(\infty)] = \frac{\hat{g}_0}{2}.$$

However, consider the following function, known as the *fundamental solution* [9]:

Definition 2.3. For $z \notin [-1, 1]$, define

$$\kappa(z) = \frac{1}{\sqrt{z+1}\sqrt{z-1}}.$$

Then, for $x \in (-1, 1)$,

$$\kappa^\pm(x) = \mp \frac{i}{\sqrt{x+1}\sqrt{1-x}}.$$

Note that $\kappa(z)$ is analytic off of $[-1, 1]$, is asymptotic to z^{-1} as $z \rightarrow \infty$ and satisfies

$$\kappa^+(x) + \kappa^-(x) = 0 \quad \text{for } x \in (-1, 1).$$

Thus we obtain the following theorem.

Theorem 2.4 ([11]). *Suppose f is $C^1[-1, 1]$ and its first derivative has bounded variation. Let $g(\zeta) = f(J(\zeta))$ and $\varphi = \mathcal{P}g$. For any constant $\xi \in \mathbb{C}$,*

$$\mathcal{P}_{(-1,1),\xi} f(z) = \frac{\varphi(J_+^{-1}(z)) + \varphi(J_-^{-1}(z))}{2} - \frac{\hat{g}_0}{2} z\kappa(z) + \xi\kappa(z)$$

satisfies

$$\mathcal{P}_{(-1,1),\xi}^+ f + \mathcal{P}_{(-1,1),\xi}^- f = f \quad \text{and} \quad \mathcal{P}_{(-1,1),\xi} f(\infty) = 0,$$

where, for $x \in (-1, 1)$,

$$\begin{aligned} \mathcal{P}_{(-1,1),\xi}^+ f(x) &= \frac{1}{2} \left[\varphi^+(J_\downarrow^{-1}(x)) + \varphi^-(J_\uparrow^{-1}(x)) + i \frac{\hat{g}_0 x + \xi}{2\sqrt{1-x^2}} \right], \\ \mathcal{P}_{(-1,1),\xi}^- f(x) &= \frac{1}{2} \left[\varphi^+(J_\uparrow^{-1}(x)) + \varphi^-(J_\downarrow^{-1}(x)) - i \frac{\hat{g}_0 x + \xi}{2\sqrt{1-x^2}} \right]. \end{aligned}$$

We can express this in terms of Chebyshev coefficients, using the fact that $T_k(J(z)) = \frac{1}{2} [z^k + z^{-k}]$, where T_k is the k th Chebyshev polynomial.

Corollary 2.5 ([11]). *Suppose f is $C^1[-1, 1]$ and its first derivative has bounded variation. If*

$$f(x) = \sum_{k=0}^{\infty} \check{f}_k T_k(x),$$

then, for $z \notin [-1, 1]$,

$$\mathcal{P}_{(-1,1),\xi} f(z) = \frac{1}{2} \sum_{k=0}^{\infty} \check{f}_k J_+^{-1}(z)^k - \frac{\check{f}_0}{2} z\kappa(z) + \xi\kappa(z).$$

For $x \in (-1, 1)$,

$$\begin{aligned} \mathcal{P}_{(-1,1),\xi}^+ f(x) &= \frac{1}{2} \sum_{k=0}^{\infty} \check{f}_k J_\downarrow^{-1}(x)^k - \frac{\check{f}_0}{2} z\kappa^+(x) + \xi\kappa^+(x) \quad \text{and} \\ \mathcal{P}_{(-1,1),\xi}^- f(x) &= \frac{1}{2} \sum_{k=0}^{\infty} \check{f}_k J_\uparrow^{-1}(x)^k - \frac{\check{f}_0}{2} z\kappa^-(x) + \xi\kappa^-(x). \end{aligned}$$

Remark. When \check{f}_0 vanishes (which will be the case below), we could have alternatively expressed this in terms of the following integral operator [2]:

$$\mathcal{P}_{(-1,1),0} f(z) = \frac{\sqrt{z^2-1}}{2\pi i} \int_{-1}^1 \frac{f(x)}{\sqrt{1-x^2} x-z} dx. \tag{2.1}$$

In fact, this integral operator is precisely the summation term in Corollary 2.5. However, the expression in terms of Chebyshev coefficients is preferable from a numerical standpoint: it converges uniformly for all $z \in \mathbb{C} \setminus [-1, 1]$, even as z approaches $[-1, 1]$, whereas attempting to compute (2.1) with quadrature requires dealing with the singularities in the kernel. There are

known methods to handle such singularities [6], however, they are not as efficient as the Chebyshev coefficient approach, break down as z approaches the endpoints of the interval, are prone to issues with round-off error and do not converge uniformly for all z in $\mathbb{C} \setminus [-1, 1]$.

Of course, we are not solving the equation over the interval $(-1, 1)$, but rather over $\Sigma = (a, b)$. This is handled by a conformal map.

Definition 2.6. Let

$$M_\Sigma(z) = \frac{2z - a - b}{b - a}$$

be the map from Σ to the unit interval, with inverse

$$M_\Sigma^{-1}(z) = \frac{a + b}{2} + \frac{b - a}{2}z.$$

Note that, for $\tilde{f}(x) = f(M_\Sigma^{-1}(x))$,

$$\phi(z) = \left[\mathcal{P}_{(-1,1),\xi} \tilde{f} \right] (M_\Sigma(z))$$

satisfies, for $x \in (a, b)$,

$$\phi^+(x) + \phi^-(x) = \left[\mathcal{P}_{(-1,1),\xi}^+ \tilde{f} \right] (M_\Sigma(x)) + \left[\mathcal{P}_{(-1,1),\xi}^- \tilde{f} \right] (M_\Sigma(x)) = \tilde{f}(M_\Sigma(x)) = f(x)$$

with $\phi(\infty) = 0$.

Thus, we have the following definition.

Definition 2.7. Suppose $f(x) = \sum_{k=0}^\infty \check{f}_{\Sigma,k} T_k(M_\Sigma(x))$; i.e., $\check{f}_{\Sigma,k}$ are the Chebyshev coefficients of $f(M_\Sigma^{-1}(x))$. For $z \notin (a, b)$, define

$$\mathcal{P}_{\Sigma,\xi} f(z) = \frac{1}{2} \sum_{k=0}^\infty \check{f}_{\Sigma,k} J_+^{-1}(M_\Sigma(z))^k - \frac{\check{f}_{\Sigma,0}}{2} M_\Sigma(z) \kappa_\Sigma(z) + \xi \kappa_\Sigma(z)$$

where

$$\kappa_\Sigma(z) = \kappa(M_\Sigma(z)) = \frac{b - a}{2\sqrt{z - b}\sqrt{z - a}}.$$

Then, for $x \in (a, b)$,

$$\mathcal{P}_{\Sigma,\xi}^+ f(x) = \frac{1}{2} \sum_{k=0}^\infty \check{f}_{\Sigma,k} J_\downarrow^{-1}(M_\Sigma(x))^k - \frac{\check{f}_{\Sigma,0}}{2} M_\Sigma(x) \kappa_\Sigma^+(x) + \xi \kappa_\Sigma^+(x) \quad \text{and}$$

$$\mathcal{P}_{\Sigma,\xi}^- f(x) = \frac{1}{2} \sum_{k=0}^\infty \check{f}_{\Sigma,k} J_\uparrow^{-1}(M_\Sigma(x))^k - \frac{\check{f}_{\Sigma,0}}{2} M_\Sigma(x) \kappa_\Sigma^-(x) + \xi \kappa_\Sigma^-(x).$$

We remark that in the numerical method that we will construct, the constant ξ will always be zero. Thus we will also use the following notation:

Definition 2.8.

$$\mathcal{P}_\Sigma = \mathcal{P}_{\Sigma,0}.$$

3. Constructing the Newton–Raphson iteration

Over an arbitrary interval $\Sigma = (a, b)$, **Theorem 2.4** implies that the computed $\mathcal{P}_{\Sigma, \xi} f$ function satisfies the following properties, where \check{f}_k are the Chebyshev coefficients of \check{f} :

- $\mathcal{P}_{\Sigma, \xi} f$ is bounded at a and b if and only if $\check{f}_{\Sigma, 0}$ and ξ are zero;
- $\mathcal{P}_{\Sigma, \xi} f(z) = \frac{(b-a)(4\xi + \check{f}_{\Sigma, 1})}{8z} + \mathcal{O}(z^{-2})$ as $z \rightarrow \infty$.

For $\Sigma = \text{supp } \mu$, ϕ is bounded and is asymptotic to $\frac{1}{z}$. The only way in which this is possible is if we fix $\xi = 0$, and choose Σ so that $\check{f}_{\Sigma, 0} = 0$ and $(b - a)\check{f}_{\Sigma, 1} = 8$, where $f = V'$. In other words, we want to find a root of the function

$$F(\Sigma) = \begin{pmatrix} \check{f}_{\Sigma, 0} \\ (b - a)\check{f}_{\Sigma, 1} - 8 \end{pmatrix} = \begin{pmatrix} \frac{1}{\pi} \int_{-1}^1 \frac{V'(M_{\Sigma}^{-1}(x))}{\sqrt{1 - x^2}} dx \\ 2 \frac{b - a}{\pi} \int_{-1}^1 \frac{V'(M_{\Sigma}^{-1}(x))x}{\sqrt{1 - x^2}} dx - 8 \end{pmatrix}.$$

This function is easily differentiated, hence we can express its Jacobian as $(F_a(\Sigma), F_b(\Sigma))$ for

$$\begin{aligned} F_a(\Sigma) &= \begin{pmatrix} \frac{1}{2\pi} \int_{-1}^1 \frac{(1 - x)V''(M_{\Sigma}^{-1}(x))}{\sqrt{1 - x^2}} dx \\ -\frac{2}{\pi} \int_{-1}^1 \frac{V'(M_{\Sigma}^{-1}(x))x}{\sqrt{1 - x^2}} dx + \frac{b - a}{\pi} \int_{-1}^1 \frac{(1 - x)V''(M_{\Sigma}^{-1}(x))x}{\sqrt{1 - x^2}} dx \end{pmatrix}, \\ F_b(\Sigma) &= \begin{pmatrix} \frac{1}{2\pi} \int_{-1}^1 \frac{(1 + x)V''(M_{\Sigma}^{-1}(x))}{\sqrt{1 - x^2}} dx \\ \frac{2}{\pi} \int_{-1}^1 \frac{V'(M_{\Sigma}^{-1}(x))x}{\sqrt{1 - x^2}} dx + \frac{b - a}{\pi} \int_{-1}^1 \frac{(1 + x)V''(M_{\Sigma}^{-1}(x))x}{\sqrt{1 - x^2}} dx \end{pmatrix}. \end{aligned} \tag{3.1}$$

Numerical implementation

Numerical implementation is now straightforward, using the fast discrete cosine transform (DCT).

Definition 3.1. The n mapped Chebyshev points are

$$\mathbf{x}_{\Sigma} = M_{\Sigma}^{-1}(\mathbf{x}),$$

where \mathbf{x} are the n Chebyshev points of the second kind

$$\mathbf{x} = \left(-1, \cos \pi \left(1 - \frac{1}{n - 1} \right), \dots, \cos \frac{\pi}{n - 1}, 1 \right).$$

We can approximate the Chebyshev coefficients $\check{f}_0, \dots, \check{f}_{n-1}$ using the DCT by sampling V' at \mathbf{x}_{Σ} . We denote this by the operator \mathcal{F} .

Definition 3.2. For a vector $f = f(\mathbf{x})$ of samples at the points \mathbf{x} , \mathcal{F} is the unique transform matrix such that

$$(T_0(x), \dots, T_{n-1}(x))\mathcal{F}f$$

is the polynomial which interpolates f at the points \mathbf{x} .

It follows, for $f_\Sigma = f(x_\Sigma)$, that

$$(T_0(M_\Sigma(x)), \dots, T_{n-1}(M_\Sigma(x)))\mathcal{F}f_\Sigma$$

interpolates f at the points x_Σ . Therefore,

$$\check{f}_{\Sigma,k} \approx \mathbf{e}_{k+1}^\top \mathcal{F}f_\Sigma.$$

The function we wish to find a root of is thus approximately

$$F(\Sigma) \approx \begin{pmatrix} \mathbf{e}_1^\top \mathcal{F}f_\Sigma \\ (b-a)\mathbf{e}_2^\top \mathcal{F}f_\Sigma - 8 \end{pmatrix}.$$

Note that $\mathbf{e}_j^\top \mathcal{F}$ can be computed in $\mathcal{O}(n)$ operations using the trapezium rule (after the transformation $x = \cos \theta$). The integrals in the Jacobian of F can also be computed using the trapezium rule. Instead, (and equivalently) we will proceed by differentiating the discretization of F .

Definition 3.3. Let D denote the Chebyshev differentiation matrix, so that Df are the values of the derivative of the interpolating polynomial at the points x . Then $D_\Sigma = \frac{2}{b-a}D$ is the derivative matrix for other intervals.

D (and hence D_Σ) can be applied to a vector in $\mathcal{O}(n \log n)$ operations using the DCT.

To compute the Jacobian, we differentiate each term in F by the endpoints of Σ : a and b . This is straightforward (here, for brevity, we define multiplication on the left by a column vector \mathbf{a} as $\mathbf{a}b = \text{diag}(\mathbf{a})b$):

$$\mathbf{x}_{\Sigma,a} = \partial_a M_\Sigma^{-1}(x) = \frac{1}{2} - \frac{x}{2}, \quad \mathbf{x}_{\Sigma,b} = \partial_b M_\Sigma^{-1}(x) = \frac{1}{2} + \frac{x}{2},$$

$$\partial_a f_\Sigma = \mathbf{x}_{\Sigma,a} f'(x_\Sigma) \approx f_{\Sigma,a} = \mathbf{x}_{\Sigma,a} D_\Sigma f_\Sigma,$$

$$\partial_b f_\Sigma \approx f_{\Sigma,b} = \mathbf{x}_{\Sigma,b} D_\Sigma f_\Sigma,$$

$$F_a(\Sigma) \approx \begin{pmatrix} \mathbf{e}_1^\top \mathcal{F} \mathbf{x}_{\Sigma,a} D_\Sigma f_\Sigma \\ (b-a)\mathbf{e}_2^\top \mathcal{F} \mathbf{x}_{\Sigma,a} D_\Sigma f_\Sigma - \mathbf{e}_2^\top \mathcal{F} f_\Sigma \end{pmatrix},$$

$$F_b(\Sigma) \approx \begin{pmatrix} \mathbf{e}_1^\top \mathcal{F} \mathbf{x}_{\Sigma,b} D_\Sigma f_\Sigma \\ (b-a)\mathbf{e}_2^\top \mathcal{F} \mathbf{x}_{\Sigma,b} D_\Sigma f_\Sigma + \mathbf{e}_2^\top \mathcal{F} f_\Sigma \end{pmatrix}.$$

We can now construct the Newton–Raphson iteration.

Definition 3.4. The interval Σ^m denotes the m th iterate of the Newton–Raphson method applied to F (whose Jacobian is (F_a, F_b)) with initial guess interval Σ^0 .

The sequence $\Sigma^1, \Sigma^2, \dots$ should hopefully converge to $\Sigma^\infty = \text{supp } \mu$. Indeed, convergence is guaranteed when V is strictly convex; cf. Theorem 4.1.

Constructing the equilibrium measure

Once the support of the equilibrium measure is calculated, we can compute the equilibrium measure itself, by calculating the associated $\phi = \mathcal{P}_{\text{supp } \mu} V'$.

Definition 3.5. For $z \notin \Sigma^m$, define

$$\phi_{n,m}(z) = \phi_{\Sigma^m}(z) \mathcal{F}f_{\Sigma^m},$$

where

$$\phi_{\Sigma}(z) = \frac{1}{2}(1, J_+^{-1}(M_{\Sigma}(z)), \dots, J_+^{-1}(M_{\Sigma}(z))^{n-1}).$$

Then, for $x \in \Sigma^m$,

$$\phi_{n,m}^{\pm}(x) = \phi_{\Sigma^m}^{\pm}(x) \mathcal{F}f_{\Sigma^m},$$

where

$$\phi_{\Sigma}^+(z) = \frac{1}{2}(1, J_{\downarrow}^{-1}(M_{\Sigma}(x)), \dots, J_{\downarrow}^{-1}(M_{\Sigma}(x))^{n-1}) \quad \text{and}$$

$$\phi_{\Sigma}^-(z) = \frac{1}{2}(1, J_{\uparrow}^{-1}(M_{\Sigma}(x)), \dots, J_{\uparrow}^{-1}(M_{\Sigma}(x))^{n-1}).$$

This is clearly an approximation to ϕ :

$$\phi(z) = \frac{1}{2} \sum_{k=1}^{\infty} \check{f}_k J_+^{-1}(M_{\text{supp } \mu}(z))^k \approx \phi_{n,m}(z).$$

Note that the term $M_{\Sigma}(z)\kappa_{\Sigma}(z)$ can be dropped as we assume that the zeroth Chebyshev coefficient vanishes.

From ϕ , we can find the equilibrium measure $d\mu = \psi(x) dx$:

$$-i\pi \psi(x) = \phi^+(x) - \phi^-(x) = \frac{1}{2} \sum_{k=1}^{\infty} \check{f}_k \left[J_{\downarrow}^{-1}(M_{\text{supp } \mu}(x))^k - J_{\uparrow}^{-1}(M_{\text{supp } \mu}(x))^k \right].$$

We know that $\frac{1}{2}(J_{\downarrow}^{-1}(x)^k + J_{\uparrow}^{-1}(x)^k)$ is precisely the Chebyshev polynomial of the first kind $T_k(x)$. But we also know that $\frac{1}{2}(J_{\downarrow}^{-1}(x)^k - J_{\uparrow}^{-1}(x)^k) = U_{k-1}(x)\sqrt{1-x^2}$ (via the substitution $x = \cos \theta$ [14]), where U_k is the Chebyshev polynomial of the second kind. In other words, we have, for $x \in \Sigma$,

$$\phi_{\Sigma}^+(x) + \phi_{\Sigma}^-(x) = (1, \dots, T_{n-1}(M_{\Sigma}(x))) \quad \text{and}$$

$$\phi_{\Sigma}^+(x) - \phi_{\Sigma}^-(x) = -2i\sqrt{1 - M_{\Sigma}(x)^2}(0, 1, \dots, U_{n-2}(M_{\Sigma}(x))).$$

Thus we obtain the rather nice approximation $\psi(x) \approx \psi_{n,m}(x)$, for the following definition.

Definition 3.6. For $x \in \Sigma^m$, define

$$\begin{aligned} \psi_{n,m}(x) &= \frac{i}{2\pi} [\phi_{\Sigma^m}^+(x) - \phi_{\Sigma^m}^-(x)] \mathcal{F}f_{\Sigma^m} \\ &= \frac{\sqrt{1 - M_{\Sigma^m}(x)^2}}{\pi}(0, 1, \dots, U_{n-2}(M_{\Sigma^m}(x))) \mathcal{F}f_{\Sigma^m}. \end{aligned}$$

4. Proof of uniqueness

The goal of this section is to demonstrate that, for strictly convex V , F has a unique root. Combined with [Theorem 1.2](#), finding the zero of F thus does indeed enable the computation of μ . In particular, it follows that

$$\psi(x) = \lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} \psi_{n,m}(x).$$

Theorem 4.1. *If $V \in C^2(-\infty, \infty)$ is strictly convex and $\frac{V(x)}{\log|x|} \rightarrow +\infty$ as $|x| \rightarrow \infty$, then F has a unique root.*

Proof. Existence follows from Theorem 1.2, and the fact that the support of the equilibrium measure is a single interval when V is strictly convex [2].

Note that, since $V(x)$ goes to $+\infty$ at both $\pm\infty$, we have $V'(-x) < 0 < V'(x)$ for x sufficiently large. Combining this with the fact that V'' is strictly positive, we know $V'(\chi) = 0$ for a unique point χ . Suppose $a < \chi$ is given. If $b < \chi$, then V' is negative in (a, b) , hence we would have $F^1(a, b) < 0$ (where F^1 denotes the first term of F and F^2 the second term). Since $0 < \epsilon < V'(x)$ for x sufficiently large, we can take $b > \chi$ large enough so that $F^1(a, b) > 0$. From (3.1) we have

$$\frac{\partial F^1}{\partial b} = \frac{1}{2\pi} \int_{-1}^1 \frac{(1+x)V''(M_{\Sigma}^{-1}(x))}{\sqrt{1-x^2}} dx > 0,$$

hence $F^1(a, b)$ as a function of b is monotonically increasing. Therefore, given a , there is a unique, smooth $b(a) > \chi$ such that $F^1(a, b(a)) = 0$.

We can differentiate this formula with respect to a , giving us

$$b'(a) = -\frac{\partial_a F^1(a, b(a))}{\partial_b F^1(a, b(a))}.$$

We have shown that the denominator is positive. Similar logic proves that the numerator is also positive, and we have $b'(a) < 0$.

We now show that $F^2(a, b(a))$ is monotonic with respect to a (I am grateful to Tom Claeys for suggesting this argument). Let $\eta(a) = -\frac{b'(a)+1}{b'(a)-1}$. Note that $\frac{d}{da} M_{(a,b(a))}^{-1}(x) = \frac{1+b'(a)}{2} + \frac{b'(a)-1}{2}x$. Then, using the fact that $F^1(a, b(a))$ vanishes,

$$\begin{aligned} \frac{d}{da} \int_{-1}^1 \frac{V'(M_{a,b(a)}^{-1}(x))x}{\sqrt{1-x^2}} dx &= \frac{d}{da} \int_{-1}^1 \frac{V'(M_{\Sigma}(x))(x-\eta(a))}{\sqrt{1-x^2}} dx \\ &= \int_{-1}^1 \frac{V''(M_{\Sigma}(x)) \left(\frac{1+b'(a)}{2} + \frac{b'(a)-1}{2}x \right) (x-\eta(a))}{\sqrt{1-x^2}} dx, \end{aligned}$$

where we use the fact that

$$\frac{1}{\pi} \int_{-1}^1 \frac{V'(M_{\Sigma}(x))\eta'(a)}{\sqrt{1-x^2}} dx = \eta'(a)F^1(a, b(a)) = 0.$$

Thus we have

$$\begin{aligned} \frac{\pi}{2} \frac{d}{da} F^2(a, b(a)) &= (b' - 1) \int_{-1}^1 \frac{V'(M_{\Sigma}^{-1}(x))x}{\sqrt{1-x^2}} dx \\ &\quad + (b - a) \int_{-1}^1 \frac{V''(M_{\Sigma}(x)) \left(\frac{1+b'}{2} + \frac{b'-1}{2}x \right) (x-\eta(a))}{\sqrt{1-x^2}} dx \\ &= (b' - 1) \int_{-1}^1 \frac{V'(M_{\Sigma}^{-1}(x))(x-\chi)}{\sqrt{1-x^2}} dx \\ &\quad + 2 \frac{b-a}{b'-1} \int_{-1}^1 \frac{V''(M_{\Sigma}(x)) \left(\frac{1+b'}{2} + \frac{b'-1}{2}x \right)^2}{\sqrt{1-x^2}} dx. \end{aligned}$$

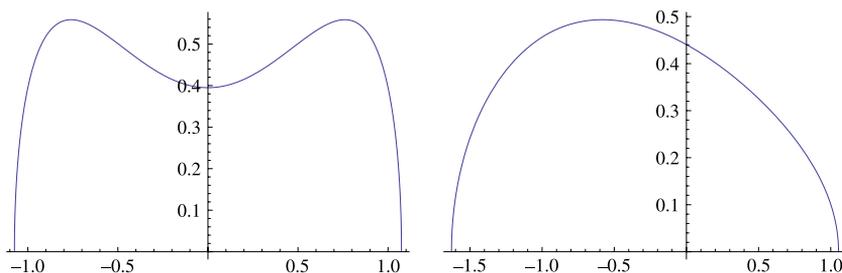


Fig. 1. The equilibrium measure for $V(x) = x^4$ (left) and $V(x) = x^2 + \sin x$ (right).

We have $b - a > 0$ and $b' < 0$, therefore each term above is strictly negative, and hence $F^2(a, b(a))$ is strictly monotone in a . Thus a and b which satisfy $F(a, b) = 0$ are unique. \square

5. Examples

The canonical example of an equilibrium measure from random matrix theory and orthogonal polynomials is the Gaussian distribution/Hermite weight, which corresponds to $V(x) = x^2$. The equilibrium measure is the well-known Wigner semicircle distribution, with support $[-\sqrt{2}, \sqrt{2}]$ and

$$\psi(x) = \frac{1}{\pi} \sqrt{2 - x^2}.$$

With the initial guess of $\Sigma^0 = [-1, 1]$, we converge to $[-\sqrt{2}, \sqrt{2}]$ within machine precision in 6 iterations. For a polynomial, Definition 2.7 is a finite sum, thus we obtain the semicircle distribution to machine precision (in a fraction of a second).

Another example is $V(x) = x^4$. The exact value of Σ is $(-\frac{\sqrt{2}}{3^{1/4}}, \frac{\sqrt{2}}{3^{1/4}})$ [2]. Our approach computes this to machine precision again in 6 iterations. We then obtain the equilibrium measure depicted in Fig. 1.

The approach works for non-polynomial distributions as well. In Fig. 1, we plot the computed equilibrium measure for $V(x) = x^2 + \sin x$.

6. Computing the inverse Cauchy transform over multiple intervals

Definition 2.7 is only applicable if Σ is a single interval. However, suppose $\Sigma = \Sigma_1 \cup \dots \cup \Sigma_N = (a_1, b_1) \cup \dots \cup (a_N, b_N)$, and we wish to find a ϕ such that

$$\phi^+ + \phi^- = f \quad \text{on } \Sigma \text{ with } \phi(\infty) = 0.$$

Let us express a solution as $\phi = \mathcal{P}_{\Sigma_1} g_1 + \dots + \mathcal{P}_{\Sigma_N} g_N$, for functions g_1, \dots, g_N to be determined, where the constant ξ in each operator is taken to be zero. Clearly, for any sufficiently smooth choice of g_i , ϕ decays at ∞ . We define a map from the space of functions which are $\mathcal{C}^1[\Sigma_j]$ with bounded variation to the space of analytic functions on Σ_j by

$$\mathcal{P}_{\Sigma_i}|_{\Sigma_j} g(x) = \mathcal{P}_{\Sigma_j} g(x) \quad \text{for } x \in \Sigma_i.$$

We thus want to find g_1, \dots, g_N which satisfy

$$\mathcal{R}_\Sigma \begin{pmatrix} g_1 \\ \vdots \\ g_N \end{pmatrix} = \begin{pmatrix} f_1 \\ \vdots \\ f_N \end{pmatrix}, \tag{6.1}$$

where f_i is the restriction of f to Σ_i and

$$\mathcal{R}_\Sigma = \begin{pmatrix} I & 2\mathcal{P}_{\Sigma_2|_{\Sigma_1}} & \cdots & 2\mathcal{P}_{\Sigma_N|_{\Sigma_1}} \\ 2\mathcal{P}_{\Sigma_1|_{\Sigma_2}} & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \ddots & I & 2\mathcal{P}_{\Sigma_N|_{\Sigma_{N-1}}} \\ 2\mathcal{P}_{\Sigma_1|_{\Sigma_N}} & \ddots & 2\mathcal{P}_{\Sigma_{N-1}|_{\Sigma_N}} & I \end{pmatrix}.$$

Theorem 6.1. Eq. (6.1) has a unique solution for g_i and f_i in $C^1[\Sigma_i]$ with bounded variation.

Proof. From (2.1), it is clear that $\mathcal{P}_{\Sigma_i|_{\Sigma_j}}$ is a compact operator, therefore \mathcal{R}_Σ is the identity operator plus a compact operator. The theorem will follow from the Fredholm alternative by showing that \mathcal{R}_Σ has trivial kernel.

If $(k_1, \dots, k_N)^\top$ is in the kernel of \mathcal{R}_Σ , then

$$\tilde{\kappa} = \mathcal{P}_{\Sigma_1}k_1 + \cdots + \mathcal{P}_{\Sigma_N}k_N$$

satisfies $\tilde{\kappa}^+ + \tilde{\kappa}^- = 0$ on Σ . Therefore, $\tilde{\kappa}$ can be expressed in terms of the *fundamental solution* [9], i.e.,

$$\tilde{\kappa}(z) = p(z)\kappa_\Sigma(z),$$

for

$$\kappa_\Sigma(z) = \kappa_{\Sigma_1}(z) \cdots \kappa_{\Sigma_N}(z)$$

and p an $(N - 1)$ th degree polynomial.

On Σ_i , we can write

$$\tilde{\kappa}(z) = \frac{\check{k}_{i,0}}{2} M_{\Sigma_i}(z)\kappa_{\Sigma_i}(z) + \text{bounded terms},$$

hence

$$\tilde{\kappa}(z) = -\frac{\check{k}_{i,0}}{2} \kappa_{\Sigma_i}(z) + \mathcal{O}(1) \quad \text{as } z \rightarrow a_i,$$

$$\tilde{\kappa}(z) = \frac{\check{k}_{i,0}}{2} \kappa_{\Sigma_i}(z) + \mathcal{O}(1) \quad \text{as } z \rightarrow b_i.$$

Thus we get $2N$ conditions on p , so that $p(z)\kappa_\Sigma(z) - \frac{\check{k}_{i,0}}{2} M_{\Sigma_i}(z)\kappa_{\Sigma_i}(z)$ is bounded at each endpoint:

$$p(a_1) = \check{k}_{1,0}\kappa_{\Sigma_2}(a_1) \cdots \kappa_{\Sigma_N}(a_1)$$

$$p(b_1) = -\check{k}_{1,0}\kappa_{\Sigma_2}(b_1) \cdots \kappa_{\Sigma_N}(b_1)$$

⋮

$$p(a_N) = \check{k}_{N,0} \kappa_{\Sigma_1}(a_N) \cdots \kappa_{\Sigma_{N-1}}(a_N)$$

$$p(b_N) = -\check{k}_{N,0} \kappa_{\Sigma_1}(b_N) \cdots \kappa_{\Sigma_{N-1}}(b_N)$$

Note that $\text{sign } \kappa_{\Sigma_i}(a_j) = \text{sign } \kappa_{\Sigma_i}(b_j)$ for $j \neq i$. It follows that p switches signs over each Σ_i , thence has N roots. Therefore, p is identically zero, and hence so are k_1, \dots, k_N . \square

We thus know that ϕ has the form of $\mathcal{P}_{\Sigma, \xi_1, \dots, \xi_N} f$, defined by

Definition 6.2.

$$\mathcal{P}_{\Sigma, \xi_1, \dots, \xi_N} f = \mathcal{P}_{\Sigma_1} g_1 + \cdots + \mathcal{P}_{\Sigma_N} g_N + \left(\xi_1 + \xi_2 z + \cdots + \xi_N z^{N-1} \right) \kappa_{\Sigma}(z),$$

where g_1, \dots, g_N satisfy (6.1) and $\kappa_{\Sigma}(z) = \kappa_{\Sigma_1}(z) \cdots \kappa_{\Sigma_N}(z)$.

The parameters can again be used to impose boundedness of the solution at N of the $2N$ endpoints. For our purposes, however, we take $\xi_1 = \cdots = \xi_N = 0$.

Numerical discretization

Our numerical approach is to discretize (6.1). We first define

$$f_{\Sigma} = \begin{pmatrix} f_1 \\ \vdots \\ f_N \end{pmatrix},$$

where the length of the vectors are n_1, \dots, n_N . Now let

$$R_{\Sigma} = \begin{pmatrix} I & 2P_{\Sigma_2|_{\Sigma_1}} & \cdots & 2P_{\Sigma_N|_{\Sigma_1}} \\ 2P_{\Sigma_1|_{\Sigma_2}} & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \ddots & I & 2P_{\Sigma_N|_{\Sigma_{N-1}}} \\ 2P_{\Sigma_1|_{\Sigma_N}} & \ddots & 2P_{\Sigma_{N-1}|_{\Sigma_N}} & I \end{pmatrix},$$

where we define the $n_j \times n_i$ matrix

$$P_{\Sigma_i|_{\Sigma_j}} = \left[\phi_{\Sigma_i}(x_{\Sigma_j}) - \frac{1}{2}(M_{\Sigma_i}(x_{\Sigma_j})\kappa_{\Sigma_i}(x_{\Sigma_j}), \mathbf{0}, \dots, \mathbf{0}) \right] \mathcal{F}.$$

(We leave the dimensions of the operator \mathcal{F} implicit; in this case, it is $n_i \times n_i$.) Then, for

$$I_1 = (I, \mathbf{0}, \dots, \mathbf{0}), \dots, I_N = (\mathbf{0}, \dots, \mathbf{0}, I), \quad (\text{so that } I_k f_{\Sigma} = f_k)$$

we have

$$\begin{aligned} \mathcal{P}_{\Sigma, \xi_1, \dots, \xi_N} f(z) \approx & \sum_{j=1}^N \left[\phi_{\Sigma_j}(z) - \frac{1}{2}(M_{\Sigma_j}(z)\kappa_{\Sigma_j}(z), \mathbf{0}, \dots, \mathbf{0}) \right] \mathcal{F} I_j R_{\Sigma}^{-1} f_{\Sigma} \\ & + \left(\xi_1 + \xi_2 z + \cdots + \xi_N z^{N-1} \right) \kappa_{\Sigma}(z). \end{aligned}$$

Since \mathcal{R}_{Σ} is the identity operator plus a compact operator, convergence of this approximation as $n_1, \dots, n_N \rightarrow \infty$ is guaranteed, and at the exact same rate as approximating g_1, \dots, g_N by Chebyshev polynomials, by standard collocation method theorems (cf., for example [1]).

Over a single interval $\Sigma = (a, b)$ we have

$$\Phi(z) \approx \frac{b-a}{8} \left[2\phi_{\Sigma}(z)A - \log J_+^{-1}(M_{\Sigma}(z))\mathbf{e}_2^{\top} \right] \mathcal{F}f_{\Sigma} + \xi \frac{b-a}{2} \log J_+^{-1}(M_{\Sigma}(z)).$$

Behaviour on the real line

In what follows, we assume $\xi = 0$. Note that Φ has a branch cut along $(-\infty, b)$, and below we will need to evaluate $\Phi^+ + \Phi^-$ along the branch cut. For $z \in (a, b)$ we have (relating $-$ with \uparrow and $+$ with \downarrow)

$$\Phi^{\pm}(x) \approx \frac{b-a}{8} \left[2\phi_{\Sigma}^{\pm}(x)A - \log J_{\mp}^{-1}(M_{\Sigma}(x))\mathbf{e}_2^{\top} \right] \mathcal{F}f_{\Sigma},$$

and for $z < a$ we have

$$\Phi^{\pm}(z) \approx \frac{b-a}{8} \left[2\phi_{\Sigma}(z)A - \left(\log \left| J_+^{-1}(M_{\Sigma}(z)) \right| \mp i\pi \right) \mathbf{e}_2^{\top} \right] \mathcal{F}f_{\Sigma}.$$

If Σ consists of multiple intervals, we sum the contributions

$$\Phi(z) \approx \sum_{j=1}^N \frac{b_j - a_j}{8} \left[2\phi_{\Sigma_j}(z)A - \log J_+^{-1}(M_{\Sigma_j}(z))\mathbf{e}_2^{\top} \right] \mathcal{F}I_j R_{\Sigma}^{-1} f_{\Sigma}.$$

This has a branch cut along $(-\infty, b_N)$. Using the above expressions, it is straightforward to determine $\Phi^+ + \Phi^-$. Our remaining $N - 1$ conditions are then

$$\begin{aligned} \Phi^+(b_1) + \Phi^-(b_1) - V(b_1) &= \Phi^+(a_2) + \Phi^-(a_2) - V(a_2), \\ &\vdots \\ \Phi^+(b_{N-1}) + \Phi^-(b_{N-1}) - V(b_{N-1}) &= \Phi^+(a_N) + \Phi^-(a_N) - V(a_N). \end{aligned}$$

8. Multiple interval Newton–Raphson iteration

We thus want to find the root of the following function:

$$F(\Sigma) = \begin{pmatrix} F_1(\Sigma) \\ \vdots \\ F_N(\Sigma) \\ G(\Sigma) \\ H_1(\Sigma) \\ \vdots \\ H_{N-1} \end{pmatrix}.$$

The first N conditions are that the zeroth Chebyshev coefficients of each g_i must vanish,

$$F_i(\Sigma) = \mathbf{e}_1^{\top} \mathcal{F}I_i R_{\Sigma}^{-1} f_{\Sigma}.$$

The next condition is that $\mathcal{P}_{\Sigma} f(z)$ must be asymptotic to $\frac{1}{z}$,

$$G(\Sigma) = \mathbf{e}_2^{\top} [(b_1 - a_1)\mathcal{F}I_1 + \dots + (b_N - a_N)\mathcal{F}I_N] R_{\Sigma}^{-1} f_{\Sigma} - 8.$$

The last $N - 1$ conditions ensure that the constants of integration must be the same,

$$\begin{aligned}
 H_i(\Sigma) = & \sum_{j=1}^{i-1} \frac{b_j - a_j}{4} \left[2\phi_{\Sigma_j}(b_i)A - \log J_+^{-1}(M_{\Sigma_j}(b_i))\mathbf{e}_2^\top \right] \mathcal{F}I_j R_{\Sigma}^{-1} \mathbf{f}_{\Sigma} \\
 & + \frac{b_i - a_i}{4} \mathbf{e}_{-1}^\top \mathcal{F}^{-1} A \mathcal{F}I_i R_{\Sigma}^{-1} \mathbf{f}_{\Sigma} \\
 & + \sum_{j=i+1}^N \frac{b_j - a_j}{4} \left[2\phi_{\Sigma_j}(b_i)A - \log \left| J_+^{-1}(M_{\Sigma_j}(b_i)) \right| \mathbf{e}_2^\top \right] \mathcal{F}I_j R_{\Sigma}^{-1} \mathbf{f}_{\Sigma} \\
 & - \sum_{j=1}^i \frac{b_j - a_j}{4} \left[2\phi_{\Sigma_j}(a_{i+1})A - \log J_+^{-1}(M_{\Sigma_j}(a_{i+1}))\mathbf{e}_2^\top \right] \mathcal{F}I_j R_{\Sigma}^{-1} \mathbf{f}_{\Sigma} \\
 & - \frac{b_{i+1} - a_{i+1}}{4} \mathbf{e}_1^\top \mathcal{F}^{-1} A \mathcal{F}I_{i+1} R_{\Sigma}^{-1} \mathbf{f}_{\Sigma} \\
 & - \sum_{j=i+2}^N \frac{b_j - a_j}{4} \left[2\phi_{\Sigma_j}(a_{i+1})A - \log \left| J_+^{-1}(M_{\Sigma_j}(a_{i+1})) \right| \mathbf{e}_2^\top \right] \mathcal{F}I_j R_{\Sigma}^{-1} \mathbf{f}_{\Sigma} \\
 & - V(b_i) + V(a_{i+1}).
 \end{aligned}$$

We have chosen to compare the constants at the endpoints b_i and a_{i+1} . Any two points in Σ_i and Σ_{i+1} would have worked equally well, however, choosing endpoints simplifies the Jacobian slightly.

Remark. A similar system of equations was set up in [7] to determine the continuity properties of the $\Sigma_1, \dots, \Sigma_N$ for potentials which depend on a parameter. Their system was in terms of standard moments and the expression (10.1). Though these two systems are mathematically equivalent, we touch on why our approach is more appropriate in a numerical context in Section 10.

Computing the Jacobian is now more complicated than in the single interval case. However, each component can be differentiated with respect to the endpoints of Σ . Let η_i denote either a_i or b_i . We first note that the only term of \mathbf{f}_{Σ} depending on η_i is precisely \mathbf{f}_i , therefore we have

$$\mathbf{f}_{\Sigma, \eta_1} = \begin{pmatrix} \mathbf{f}_{1, \eta_1} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{pmatrix}, \quad \mathbf{f}_{\Sigma, \eta_2} = \begin{pmatrix} \mathbf{0} \\ \mathbf{f}_{2, \eta_2} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{pmatrix}, \quad \dots, \quad \mathbf{f}_{\Sigma, \eta_N} = \begin{pmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{f}_{N, \eta_N} \end{pmatrix}.$$

Now we have

$$\begin{aligned}
 \phi_{\Sigma_i, \eta_i}(x) &= \partial_{\eta_i} \phi_{\Sigma_i}(x) \\
 &= \frac{M'_{\Sigma_i, \eta_i}(x)[J_+^{-1}]'(M_{\Sigma_i}(x))}{2} (0, 1, \dots, (n_i - 1)J_+^{-1}(M_{\Sigma_i}(x))^{n_i-2})
 \end{aligned}$$

and

$$\phi'_{\Sigma_i}(x) = \frac{M'_{\Sigma_i}(x)[J_+^{-1}]'(M_{\Sigma_i}(x))}{2} (0, 1, \dots, (n_i - 1)J_+^{-1}(M_{\Sigma_i}(x))^{n_i-2}).$$

Therefore,

$$\partial_{\eta_i} P_{\Sigma_i} |_{\Sigma_j} = \left[\frac{M_{\Sigma_i, \eta_i}(\mathbf{x}_{\Sigma_j})}{2(M_{\Sigma_i}(\mathbf{x}_{\Sigma_j}) + 1)^{3/2}(M_{\Sigma_i}(\mathbf{x}_{\Sigma_j}) - 1)^{3/2}} \mathbf{e}_1^\top + \boldsymbol{\phi}_{\Sigma_i, \eta_i}(\mathbf{x}_{\Sigma_j}) \right] \mathcal{F}.$$

On the other hand, we have

$$\partial_{\eta_j} P_{\Sigma_i} |_{\Sigma_j} = \mathbf{x}_{\Sigma_j, \eta_j} \left[\frac{M'_{\Sigma_i}(\mathbf{x}_{\Sigma_j})}{2(M_{\Sigma_i}(\mathbf{x}_{\Sigma_j}) + 1)^{3/2}(M_{\Sigma_i}(\mathbf{x}_{\Sigma_j}) - 1)^{3/2}} \mathbf{e}_1^\top + \boldsymbol{\phi}'_{\Sigma_i}(\mathbf{x}_{\Sigma_j}) \right] \mathcal{F}.$$

Thus we can evaluate the derivatives of R_Σ with respect to every a_i and b_i . Finally,

$$R_{\Sigma, \eta}^{-1} = \partial_\eta R_\Sigma^{-1} = -R_\Sigma^{-1} R_{\Sigma, \eta} R_\Sigma^{-1}.$$

By combining these formulæ, it is straightforward to compute the Jacobian of F .

We can thus set up a Newton–Raphson iteration.

Definition 8.1. $\Sigma^m = \Sigma_1^m \cup \dots \cup \Sigma_N^m$ denotes the m th iterate of the Newton–Raphson method applied to F with initial guess intervals $\Sigma^0 = \Sigma_1^0 \cup \dots \cup \Sigma_N^0$.

We can now construct the approximations (where $\mathbf{n} = n_1, \dots, n_N$ are the number of Chebyshev points in each interval) $\phi(z) \approx \phi_{\mathbf{n}, m}(z)$ and $d\mu = \psi(x) dx \approx \psi_{\mathbf{n}, m}(x) dx$, which are defined as in what follows.

Definition 8.2. For $z \notin \Sigma^m$, define

$$\phi_{\mathbf{n}, m}(z) = \sum_{j=1}^N \boldsymbol{\phi}_{\Sigma_j^m}(z) \mathcal{F} I_j R_{\Sigma^m}^{-1} \mathbf{f}_{\Sigma^m}.$$

For $x \in \Sigma_k^m$, define

$$\begin{aligned} \psi_{\mathbf{n}, m}(x) &= \frac{i}{2\pi} [\phi_{\mathbf{n}, m}^+(x) - \phi_{\mathbf{n}, m}^-(x)] \\ &= \frac{\sqrt{1 - M_{\Sigma_k^m}(x)^2}}{\pi} (0, 1, \dots, U_{n-2}(M_{\Sigma_k^m}(x))) \mathcal{F} I_k R_{\Sigma^m}^{-1} \mathbf{f}_{\Sigma^m}. \end{aligned}$$

We hope that when N is chosen correctly that

$$\psi(x) \stackrel{?}{=} \lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} \psi_{\mathbf{n}, m}(x).$$

Generic nonsingularity of the Jacobian [7] implies that the method will converge to the true equilibrium measure whenever the initial guess is sufficiently accurate.

Verification of solution

Though we cannot guarantee *a priori* that Σ^m will converge to the true equilibrium measure, we can still verify convergence numerically. We know (cf. [2]) that $\Sigma = \text{supp } \mu$ if the following conditions hold true:

- (1) $F(\Sigma) = 0$;
- (2) For $\phi = \mathcal{P}_\Sigma V'$, $\frac{i}{2\pi} [\phi^+ - \phi^-] \geq 0$ on Σ ;

(3) $\Phi = \int \phi \, dz$ satisfies

$$\Phi^+(x) + \Phi^-(x) - V(x) \leq \ell \quad \text{for } x \notin \Sigma, \tag{8.1}$$

where ℓ is the constant such that [7]

$$\Phi^+(x) + \Phi^-(x) - V(x) = \ell \quad \text{for } x \in \Sigma.$$

If the Newton–Raphson iteration converges, then the first condition is satisfied. The second condition (that the resulting measure is indeed nonnegative) can be verified by converting the mapped Chebyshev polynomial of the second kind

$$(0, 1, \dots, U_{n-2}(M_{\Sigma_k^m}(x))) \mathcal{F} I_k R_{\Sigma^m}^{-1} \mathbf{f}_{\Sigma^m} \tag{8.2}$$

to a mapped Chebyshev polynomial of the first kind, using the formula [14]

$$T_k(x) = \frac{1}{2} (U_k(x) - U_{k-2}(x)).$$

Differentiating with the Chebyshev derivative matrix D and finding all roots of the resulting polynomial using a colleague matrix method [4]; which are the minima and maxima of (8.2).

The third condition can be verified by constructing

$$\Phi_{n,m}(x) = \sum_{j=1}^N \frac{b_j - a_j}{8} \left[2\phi_{\Sigma_j^m}(z)A - \log J_+^{-1}(M_{\Sigma_j^m}(z))\mathbf{e}_2^\top \right] \mathcal{F} I_j R_{\Sigma^m}^{-1} \mathbf{f}_{\Sigma^m},$$

and testing (8.1) (using the formulæ from Section 7 for $\Phi_{n,m}^\pm$, which has a branch cut along $(-\infty, b_N)$). Since V grows at ∞ , we only need to test (8.1) for finite x .

9. Examples

We consider the function

$$V_\alpha(x) = \frac{(x - 3)(x - 2)(1 + x)(2 + x)(3 + x)(2x - 1)}{\alpha},$$

where α is a parameter. Fig. 2 plots the computed equilibrium measure support for a range of α .

From [7], we know that the support of the equilibrium measure is a single interval for α large, and so we use the single interval Newton–Raphson iteration to compute the equilibrium measure in this regime. As α approaches approximately 191.7, the computed equilibrium measure becomes negative, as seen in Fig. 3. At this point, the interval must be split and we thus switch to the multiple interval iteration with two intervals. At α approximately 117.7, the computed equilibrium measure again becomes negative, and must be split into three intervals. Then, at α approximately 11.7, the equilibrium measure disappears over one interval of support, and we return to the case of two intervals. Finally, at α approximately 3.1, another interval vanishes. The remaining single interval surrounds the global minimum of V_α , precisely as predicted by the theory in [7].

We remark that, in the multiple interval case, the initial guess for the Newton–Raphson iteration is crucial to ensure convergence to the true equilibrium measure. Indeed, the single interval iteration continues to converge even when the computed equilibrium measure becomes negative, and what is computed continues to satisfy all the required properties, other than positivity. Thus, without an accurate initial guess, the two-interval iteration can sometimes

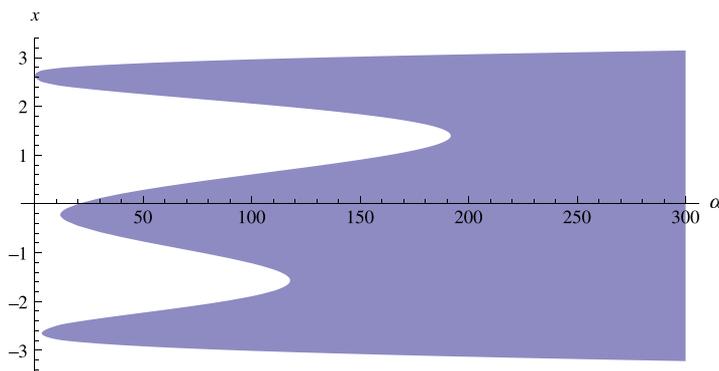


Fig. 2. The support of the equilibrium measure for V_α over a range of α .

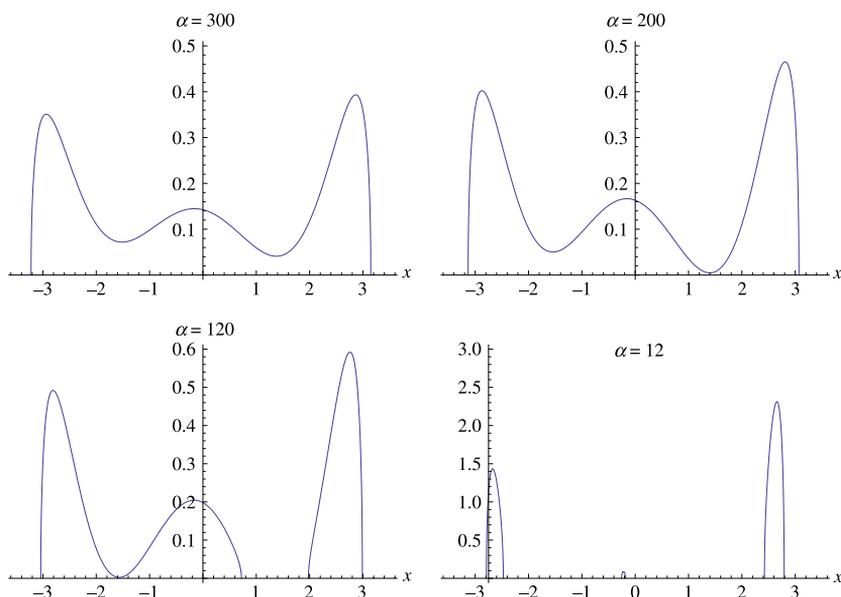


Fig. 3. The equilibrium measure for V_α for $\alpha = 300, 200, 120$ and 12 .

attempt to converge to this single interval solution (though it does not actually converge, as the two-interval iteration cannot handle overlapping intervals reliably). Since the equilibrium measure is continuous, we managed to ensure accurate initial guesses by using the computed support from previous values of α . Another approach that might work is to use some sort of constrained optimization in place of our simple Newton–Raphson iteration to ensure that the computed equilibrium measure remains positive, and that the intervals never overlap.

10. Speeding up the algorithm over multiple intervals

The algorithm we have constructed for computing \mathcal{P} over multiple intervals is significantly slower than the algorithm for single intervals: $\mathcal{O}([N \sum n_i]^3)$ versus $\mathcal{O}(n \log n)$. In this section,

we present two approaches to achieve $\mathcal{O}(\gamma(N)) + \mathcal{O}(\sum n_i \log n_i)$ accuracy, where $\gamma(N)$ is some function independent of n_i .

The first approach is based on Theorem 1.38 in [3], where an expression for $\mathcal{P}f$ over multiple intervals is given as a sum of Cauchy transforms, subject to conditions on f . We rederive this result in the context of the operator \mathcal{P} , i.e., without reduction to Cauchy transforms.

Define

$$\bar{\mathcal{P}}_{(a,b)} f(z) = \frac{1}{2} \sum_{k=0}^{\infty} \check{f}_k J_+(M_{(a,b)}(z))^k$$

and

$$w_{(a,b)}(z) = \sqrt{z-a}\sqrt{z-b} \quad \text{and} \quad W_i(z) = \prod_{k \neq i} w_{\Sigma_k}(z).$$

Now consider the function

$$\bar{\phi}(z) = W_1(z)\bar{\mathcal{P}}_{\Sigma_1} f(z) = w_{\Sigma_2}(z) \cdots w_{\Sigma_N}(z)\bar{\mathcal{P}}_{\Sigma_1} f(z).$$

For $x \in \Sigma_i$ and $i \neq 1$, $w_{\Sigma_i}^+ = -w_{\Sigma_i}^-$ whilst all other terms are analytic; therefore,

$$\bar{\phi}^+(x) + \bar{\phi}^-(x) = 0 \quad \text{for } x \in \Sigma_2 \cup \cdots \cup \Sigma_N.$$

On the other hand, for $x \in \Sigma_1$,

$$\bar{\phi}^+(x) + \bar{\phi}^-(x) = W_1(z) \left[\bar{\mathcal{P}}_{\Sigma_1}^+ f(x) + \bar{\mathcal{P}}_{\Sigma_1}^- f(x) \right] = W_1(x) f(x).$$

This motivates the definition

$$\bar{\mathcal{P}}_{\Sigma} f(z) = W_1(z)\bar{\mathcal{P}}_{\Sigma_1} \left[\frac{f}{W_1} \right] (z) + \cdots + W_N(z)\bar{\mathcal{P}}_{\Sigma_N} \left[\frac{f}{W_N} \right] (z), \tag{10.1}$$

So that $\bar{\mathcal{P}}_{\Sigma}^+ f + \bar{\mathcal{P}}_{\Sigma}^- f = f$ in Σ .

In general, $\bar{\mathcal{P}}_{\Sigma} f$ does not vanish at infinity. However, $W_i(z) \sim z^{N-1}$ and $J_+(M_{\Sigma_j}(z))^N \sim \left(\frac{b-a}{8}\right)^N z^{-N}$, therefore only the terms up to $N - 1$ in $\bar{\mathcal{P}}_{\Sigma_i}$ do not decay. Now consider the functions

$$\kappa_j(z) = z^j \kappa_{\Sigma}(z) = \frac{z^j}{w_1(z) \cdots w_N(z)},$$

satisfying $\kappa_j^+ + \kappa_j^- = 0$ and $\kappa_j(z) \sim z^{j-N}$. We can add a linear combination of these functions to $\bar{\mathcal{P}}_{\Sigma} f$ to ensure that it decays at infinity, while maintaining the jump condition along Σ . To do this, we first note that

$$\frac{1}{w_i} = \frac{1}{z} + \frac{a_i + b_i}{2z^2} + \cdots + \left(\frac{a_i + b_i}{2}\right)^{k-1} {}_2F_1\left(\frac{1-k}{2}, 1 - \frac{k}{2}; \frac{(a_i - b_i)^2}{a_i + b_i^2}\right) + \cdots.$$

This can be derived from the series of w_i around infinity and the series representation of the hypergeometric function [14]. Using this expression, the full asymptotic series of each κ_j are determinable, by multiplying the series. Furthermore,

$$J_{\uparrow}^{-1}(x) = \sum_{k=0}^{\infty} \frac{C_k}{2^{2k+1}} \frac{1}{z^{2k+1}}$$

where $C_k = \frac{1}{k+1} \binom{2k}{k}$ are the Catalan numbers. This expression follows from the generating function of the Catalan numbers [14]. Thus, we can also determine the full asymptotic series of $\bar{\mathcal{P}}$, again by multiplying series.

Though no simple expression is obtained, for small N we can write down the solution explicitly. In particular, if Σ consists of two intervals we obtain

$$\begin{aligned} \mathcal{P}_{\Sigma, \xi_1, \xi_2} f &= \bar{\mathcal{P}}_{\Sigma} f - \check{p}_{1,0} \left[\frac{\kappa_3}{2} - \kappa_2 \frac{a_1 + b_1 + 2a_2 + 2a_2}{4} \right] - \check{p}_{1,1} \kappa_2 \frac{b_1 - a_1}{8} \\ &\quad - \check{p}_{2,0} \left[\frac{\kappa_3}{2} - \kappa_2 \frac{2a_1 + 2b_1 + a_2 + a_2}{4} \right] - \check{p}_{2,1} \kappa_2 \frac{b_2 - a_2}{8} + \xi_1 \kappa_0 + \xi_2 \kappa_1, \end{aligned}$$

where $p_1 = \frac{f_1}{w_1}$ and $p_2 = \frac{f_2}{w_2}$ (and f_1 and f_2 are again the restrictions of f to Σ_1 and Σ_2 , respectively). While this approach works well for computing \mathcal{P} , at least for small N , the construction of the function F used in the Newton–Raphson iteration would be significantly more complicated. Moreover, it is not clear how to determine the indefinite integral of this expression for \mathcal{P}_{Σ} , and therefore we do not know how to construct all of the terms in F . Thus we will not pursue this approach further.

Sparsity of R_{Σ}

Instead, we return to the previous approach used. The calculation in the algorithm which takes $\mathcal{O}([N \sum n_i]^3)$ operations is inverting the matrix R_{Σ} . However, consider the term $P_{\Sigma_i} |_{\Sigma_j}$, which we transform:

$$\check{P}_{\Sigma_i} |_{\Sigma_j} = \mathcal{F} P_{\Sigma_i} |_{\Sigma_j} \mathcal{F}^{-1}.$$

In other words, while $P_{\Sigma_i} |_{\Sigma_j}$ maps function values in Σ_i to function values in Σ_j , $\check{P}_{\Sigma_i} |_{\Sigma_j}$ maps Chebyshev coefficients in Σ_i to Chebyshev coefficients in Σ_j . In particular, except for the first column, $\check{P}_{\Sigma_i} |_{\Sigma_j}$ consists of the Chebyshev coefficients of ϕ_{Σ_i} . We will show that the only entries of $\check{P}_{\Sigma_i} |_{\Sigma_j}$ which are greater than ϵ lie in an $m \times l$ block. The dimensions m and l will be independent of n_i , and hence $R_{\Sigma_j} \mathbf{b} = \mathbf{c}$ can be solved in $\mathcal{O}(\sum n_i \log n_i)$ time.

We first find the number of rows needed. We know that ϕ_{Σ_i} is analytic in Σ_j , therefore the Chebyshev coefficients decay spectrally fast. Moreover, we can find the closest singularity, and hence the rate of decay. Mapping Σ_j to the unit interval, ϕ_{Σ_i} becomes $\phi_{\Sigma_i}(M_{\Sigma_j}^{-1}(z))$, which has a branch cut along $M_{\Sigma_j}^{-1}(\Sigma_i)$. The closest singularity is the closest endpoint of the mapped domain $\alpha = \min |M_{\Sigma_j}^{-1}(M_{\Sigma_i}(\pm 1))|$. The ellipse with foci at ± 1 that runs through α has major and minor semiaxis lengths which sum to $\rho = \alpha + \sqrt{\alpha^2 - 1}$. Moreover, $\phi_{\Sigma_i}(M_{\Sigma_j}^{-1}(z))$ is analytic everywhere off its branch cut, including at infinity. Therefore, it takes its maximum along the branch cut. Since J_{+}^{-1} maps the unit interval to the unit circle, we have $|\phi_{\Sigma_i}(M_{\Sigma_j}(z))| \leq 1$ for all z . Thus the k th Chebyshev coefficient is bounded by $2\rho^{-k}$ [16]. In other words, only the first

$$m = -\frac{\log \epsilon - \log 2}{\log \rho}$$

rows of $\check{P}_{\Sigma_i} |_{\Sigma_j}$ are greater than ϵ .

We can now determine the number of columns needed. Since Σ_i and Σ_j are disjoint, $|J_{+}(M_{\Sigma_i}(z))|$ is strictly less than one. Moreover, it is strictly monotonic on the real line.

Therefore, the k th column of $\phi_{\Sigma_i}, J_+(M_{\Sigma_i}(z))^k$, decays in Σ_j exponentially fast as k increases, and all values in Σ_j are less than $J_+(M_{\Sigma_i}^{-1}(M_{\Sigma_j}^{-1}(\pm 1)))^k$. Thus only the first

$$l = \frac{\log \epsilon}{\log \left| J_+(M_{\Sigma_j}^{-1}(\pm 1)) \right|}$$

columns are greater than ϵ .

There is another important use for this formulation: we can use it to determine how large each n_i needs to be so that g_i are computed to sufficient accuracy. In the single interval case, n large enough to interpolate V' was sufficient; so if V was an m th degree polynomial, $n = m$ is sufficient. This is not true in the multiple interval case. Fortunately, we now know that only the low order Chebyshev coefficients are affected. Thus we take n_i to be the maximum of the number of terms needed to interpolate V' and the number of nonzero columns in each $\check{P}_{\Sigma_i}(\Sigma_j)$ for $j \neq i$ (which, clearly, will be maximized for $j = i \pm 1$).

11. Closing remarks

We have demonstrated that equilibrium measures can be computed numerically, whether they are supported on a single or multiple intervals. This approximation could be used to compute the asymptotics of general orthogonal polynomials and their roots, as well as global mean distribution of random matrix eigenvalues and other random matrix distributions.

Acknowledgements

I thank Arno Kuijlaars for pointing out [7], which facilitated the construction of the Newton–Raphson method for the multiple interval case. I also thank Tom Claeys, for helping me with the proof of [Theorem 4.1](#). Finally, I thank the anonymous referees for their helpful comments and suggestions.

References

- [1] K.E. Atkinson, *The Numerical Solution of Integral Equations of the Second Kind*, Cambridge University Press, 1997.
- [2] P. Deift, *Orthogonal Polynomials and Random Matrices: a Riemann–Hilbert Approach*, American Mathematical Society, 2000.
- [3] P. Deift, T. Kriecherbauer, K.T.R. McLaughlin, New results on the equilibrium measure for logarithmic potentials in the presence of an external field, *J. Approx. Theory* 95 (1998) 388–475.
- [4] I.J. Good, The colleague matrix, a Chebyshev analogue of the companion matrix, *Q. J. Math.* 12 (1961) 61–68.
- [5] J. Górski, Méthode des points extrémaux de résolution du problème de Dirichlet dans l'espace, *Ann. Polon. Math.* 1 (1955) 418–429.
- [6] F.W. King, *Hilbert Transforms: Volume 1*, Cambridge University Press, 2009.
- [7] A.B.J. Kuijlaars, K.T.R. McLaughlin, Generic behavior of the density of states in random matrix theory and equilibrium problems in the presence of real analytic external fields, *Comm. Pure Appl. Math.* 53 (2000) 736–785.
- [8] F. Leja, Une méthode élémentaire de résolution du problème de Dirichlet dans le plan, *Ann. Soc. Math. Polon.* 23 (1950) 13–28.
- [9] N.I. Muskhelishvili, *Singular Integral Equations*, Noordhoff, Groningen, 1953, based on the second Russian edition published in 1946.
- [10] S. Olver, *A general framework for solving Riemann–Hilbert problems numerically*, NA-10/05, Maths Institute, Oxford University, 2010.
- [11] S. Olver, Computing the Hilbert transform and its inverse, *Math. Comp.* 80 (2011) 1745–1767.

- [12] S. Olver, Numerical solution of Riemann–Hilbert problems: painlevé II, *Found. Comput. Math.* 11 (2011) 153–179.
- [13] S. Olver, RHPackage. <http://www.comlab.ox.ac.uk/people/Sheehan.Olver/projects/RHPackage.html>.
- [14] F.W.J. Olver, D.W. Lozier, R.F. Boisvert, C.W. Clarke, *NIST Handbook of Mathematical Functions*, Cambridge University Press, 2010.
- [15] E.B. Saff, V. Totik, *Logarithmic Potentials with External Fields*, Springer, 1997.
- [16] L.N. Trefethen, Is Gauss quadrature better than Clenshaw–Curtis? *SIAM Rev.* 50 (2008) 67–87.