

Computation of equilibrium measures

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Abstract We present a new way of computing equilibrium measures, 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.

Keywords Equilibrium measure, orthogonal polynomials, random matrices, Riemann–Hilbert problems.

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1. Introduction

Equilibrium measures are essentially the distribution of charges on a conductor under the influence of an external field [10]. They have a wide field of applications, from the distribution of eigenvalues of large random matrices to the zeros of orthogonal polynomials [2].

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 definition of the equilibrium measure is the unique Borel measure $d\mu = \psi(x) dx$ such that

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

is minimal, cf. [10]. We will assume in this paper that $V \in \mathbb{C}^\infty(-\infty, \infty)$, though this condition can be relaxed.

There is an existing numerical method for computing equilibrium measures based on Leja points [7, 5, 10]. Leja points are a sequence of points which cover the support of the equilibrium measure. However, convergence is necessarily very slow, since 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 [6], 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 Riemann–Hilbert formulation:

Theorem 1.1 [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*

$$\phi^+(x) + \phi^-(x) = V'(x) \quad \text{for } x \in \text{supp } \mu \quad \text{and} \quad \phi(z) \underset{z \rightarrow \infty}{\sim} \frac{1}{z}.$$

Then

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

This formulation has been used to determine ψ *analytically* for weights where $V(x)$ 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 1.1 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

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

using the fast cosine transform [9], as reviewed in Section 2. There are, in fact, a family of solutions, depending on a parameter ξ . We refer to this as the inverse Cauchy transform, which we denote $\phi = \mathcal{P}_{\Sigma, \xi} f$.

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 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 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. First, a new approach for solving (1.2) when Σ consists of multiple intervals is derived. A Newton–Raphson iteration is then set-up, much like in the univariate 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, confirming the theory of [6].

2. Computation of the inverse Cauchy transform

Define the Joukowski map as

$$T(z) = \frac{1}{2} \left(z + \frac{1}{z} \right),$$

which maps the lower and upper half of the unit circle to the unit interval, and the interior and exterior of the unit circle to the complex plane off the unit interval $\mathbb{C} \setminus [-1, 1]$. We define four inverses:

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

The inverses T_\pm^{-1} have branch cuts along $[-1, 1]$ whilst T_\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:

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

While solving $\phi^+ + \phi^- = f$ over $[-1, 1]$ appears to be nontrivial, solving it over the unit circle is a trivial application of Laurent series/FFT: for $g(z) = \sum_{k=-\infty}^{\infty} \hat{g}_k z^k$, the function

$$\tilde{\phi} = \begin{cases} \sum_{k=0}^{\infty} \check{g}_k z^k & \text{for } |z| < 1 \\ \sum_{k=-1}^{-\infty} \check{g}_k z^k & \text{for } |z| > 1 \end{cases}$$

satisfies $\tilde{\phi}^+ + \tilde{\phi}^- = g$ on the unit circle, with $\tilde{\phi}(\infty) = 0$. We denote the map from g to $\tilde{\phi}$ as \mathcal{P} .

Now we use the Joukowski map to map the unit interval to the unit circle. Let $\tilde{\phi} = \mathcal{P}g$ for $g(z) = f(T(z))$. Then $\phi(z) = \frac{1}{2} [\tilde{\phi}(T_+^{-1}(z)) + \tilde{\phi}(T_-^{-1}(z))]$ satisfies the jump condition

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

Unfortunately,

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

However, consider the function

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

which is analytic off $[-1, 1]$. Note that κ is asymptotic to z^{-1} and satisfies

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

Thus we obtain:

Theorem 2.1 [9] *Suppose f is $\mathcal{C}^1[-1, 1]$ and its first derivative has bounded variation. Let $g(z) = f(T(z))$ and $\Phi = \mathcal{P}g$. For any constant $\xi \in \mathbb{C}$,*

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

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

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

We can express this in terms of Chebyshev coefficients. Suppose

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

Then

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

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. Let

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

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

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

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

$$\begin{aligned}\mathcal{P}_{\Sigma,\xi} f(z) &= \mathcal{P}_{(-1,1),\xi} \tilde{f}(M_{\Sigma}(z)) \\ &= \frac{1}{2} \sum_{k=0}^{\infty} \check{f}_{\Sigma,k} T_+^{-1}(M_{\Sigma}(z))^k - \frac{\check{f}_{\Sigma,0}}{2} M_{\Sigma}(z) \kappa_{\Sigma}(z) + \xi \kappa_{\Sigma}(z)\end{aligned}\tag{2.1}$$

where $\check{f}_{\Sigma,k}$ are the Chebyshev coefficients of f over the interval Σ , or equivalently, the Chebyshev coefficients of \tilde{f} over $(-1, 1)$, and

$$\kappa_{\Sigma}(z) = \kappa(M_{\Sigma}(z)).$$

3. Constructing the Newton–Raphson iteration

Over an arbitrary interval Σ , Theorem 2.1 implies that the computed $\mathcal{P}_{\Sigma,\xi} f$ function satisfies the following properties, where \check{f}_k are the Chebyshev coefficients of \tilde{f} :

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

Now we know for $\Sigma = \text{supp } \mu$ that ϕ is bounded and is asymptotic to $\frac{1}{x}$. 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 $J = (F_a(\Sigma), F_b(\Sigma))$ for

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

Numerical implementation is now straightforward. Define the n mapped Chebyshev points as $\mathbf{x}_{\Sigma} = M_{\Sigma}^{-1}(\mathbf{x})$, where \mathbf{x} are the n Chebyshev points of the second kind

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

We can approximate the Chebyshev coefficients $\check{f}_0, \dots, \check{f}_{n-1}$ using the fast discrete cosine transform (DCT) by sampling V' at \mathbf{x}_{Σ} . We denote this by the operator \mathcal{F} , so that, for a vector $\mathbf{f} = f(\mathbf{x})$ of samples at the points \mathbf{x} ,

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

is the polynomial which interpolates f at the points \mathbf{x} . It follows, for $\mathbf{f}_{\Sigma} = f(\mathbf{x}_{\Sigma})$, that

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

interpolates f at the points \mathbf{x}_{Σ} . Therefore,

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

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

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

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

Let D denote the Chebyshev differentiation matrix, so that $D\mathbf{f}$ is the values of the derivative of the interpolating polynomial at the points \mathbf{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 $\mathcal{O}(n \log n)$ time.

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 $\mathbf{a}\mathbf{b} = \text{diag}(\mathbf{a})\mathbf{b}$):

$$\begin{aligned} \mathbf{x}_{\Sigma,a} &= \partial_a M_\Sigma^{-1}(\mathbf{x}) = \frac{1}{2} - \frac{\mathbf{x}}{2}, & \mathbf{x}_{\Sigma,b} &= \partial_b M_\Sigma^{-1}(\mathbf{x}) = \frac{1}{2} + \frac{\mathbf{x}}{2}, \\ \partial_a \mathbf{f}_\Sigma &= \mathbf{x}_{\Sigma,a} f'(\mathbf{x}_\Sigma) \approx \mathbf{f}_{\Sigma,a} = \mathbf{x}_{\Sigma,a} D_\Sigma \mathbf{f}_\Sigma, \\ \partial_b \mathbf{f}_\Sigma &\approx \mathbf{f}_{\Sigma,b} = \mathbf{x}_{\Sigma,b} D_\Sigma \mathbf{f}_\Sigma, \\ F_a(\Sigma) &\approx \begin{pmatrix} \mathbf{e}_1^\top \mathcal{F} \mathbf{x}_{\Sigma,a} D_\Sigma \mathbf{f}_\Sigma \\ (b-a) \mathbf{e}_2^\top \mathcal{F} \mathbf{x}_{\Sigma,a} D_\Sigma \mathbf{f}_\Sigma - \mathbf{e}_2^\top \mathcal{F} \mathbf{f}_\Sigma \end{pmatrix}, \\ F_b(\Sigma) &\approx \begin{pmatrix} \mathbf{e}_1^\top \mathcal{F} \mathbf{x}_{\Sigma,b} D_\Sigma \mathbf{f}_\Sigma \\ (b-a) \mathbf{e}_2^\top \mathcal{F} \mathbf{x}_{\Sigma,b} D_\Sigma \mathbf{f}_\Sigma + \mathbf{e}_2^\top \mathcal{F} \mathbf{f}_\Sigma \end{pmatrix}. \end{aligned}$$

We can now construct the Newton–Raphson iteration, with an initial guess interval Σ^0 . As we run the iteration we obtain approximations $\Sigma^1, \Sigma^2, \dots$, which should hopefully converge to $\Sigma^\infty = \text{supp } \mu$. Indeed, convergence is guaranteed when V is convex, cf. Theorem 4.1.

We thus obtain the approximation to ϕ :

$$\phi(z) = \frac{1}{2} \sum_{k=1}^{\infty} \check{f}_k T_+^{-1}(M_{\text{supp } \mu}(z))^k \approx \phi_{n,m}(z) = \boldsymbol{\phi}_{\Sigma^m}(z) \mathcal{F} \mathbf{f}_{\Sigma^m},$$

for

$$\boldsymbol{\phi}_\Sigma(z) = \frac{1}{2} \left(1, T_+^{-1}(M_\Sigma(z)), \dots, T_+^{-1}(M_\Sigma(z))^{n-1} \right).$$

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

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

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

We know that $\frac{1}{2}(T_\downarrow^{-1}(x)^k + T_\uparrow^{-1}(x)^k)$ is precisely the Chebyshev polynomial of the first kind $T_k(x)$. But we also know that $\frac{i}{2}(T_\downarrow^{-1}(x)^k - T_\uparrow^{-1}(x)^k) = U_{k-1}(x)\sqrt{1-x^2}$ where U_k is the

Chebyshev polynomial of the second kind (via the substitution $x = \cos \theta$ [8]). In other words, for

$$\begin{aligned}\phi_{\Sigma}^{+}(z) &= \frac{1}{2} \left(1, T_{\downarrow}^{-1}(M_{\Sigma}(x)), \dots, T_{\downarrow}^{-1}(M_{\Sigma}(x))^{n-1} \right) \quad \text{and} \\ \phi_{\Sigma}^{-}(z) &= \frac{1}{2} \left(1, T_{\uparrow}^{-1}(M_{\Sigma}(x)), \dots, T_{\uparrow}^{-1}(M_{\Sigma}(x))^{n-1} \right),\end{aligned}$$

we have, for $x \in \Sigma$,

$$\begin{aligned}\phi_{\Sigma}^{+}(x) + \phi_{\Sigma}^{-}(x) &= (1, \dots, T_{n-1}(M_{\Sigma}(x))) \quad \text{and} \\ \phi_{\Sigma}^{+}(x) - \phi_{\Sigma}^{-}(x) &= -2i\sqrt{1 - M_{\Sigma}(x)^2}(0, 1, \dots, U_{n-2}(M_{\Sigma}(x))).\end{aligned}$$

Thus we obtain the rather nice expression:

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

4. Proof of uniqueness

The goal of this section is to demonstrate that, for convex V , F has a unique root. Combined with Theorem 1.1, finding the zero of F thus does indeed enable the computation of $d\mu$. In particular, it follows that

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

Theorem 4.1 *If V is smooth and convex, then F has a unique root.*

Proof:

Existence follows from Theorem 1.1, and the fact the the support of the equilibrium measure is a single interval when V is convex [2].

Because V'' is strictly positive and $V'(\pm\infty) = \pm\infty$, we know $V'(\chi) = 0$ for a unique point χ . Suppose $a < \chi$ is given. Since V' is negative, if $F(a, b) = 0$ it follows that $b > \chi$, otherwise we would have $F^1(a, \chi) < 0$ (where F^1 denotes the first term of F and F^2 the second term). 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 $b(a)$ 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 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

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

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

Q.E.D.

5. Examples

The canonical example of equilibrium measures from random matrix theory and orthogonal polynomials is the Gaussian distribution/Hermite weight, which corresponds to

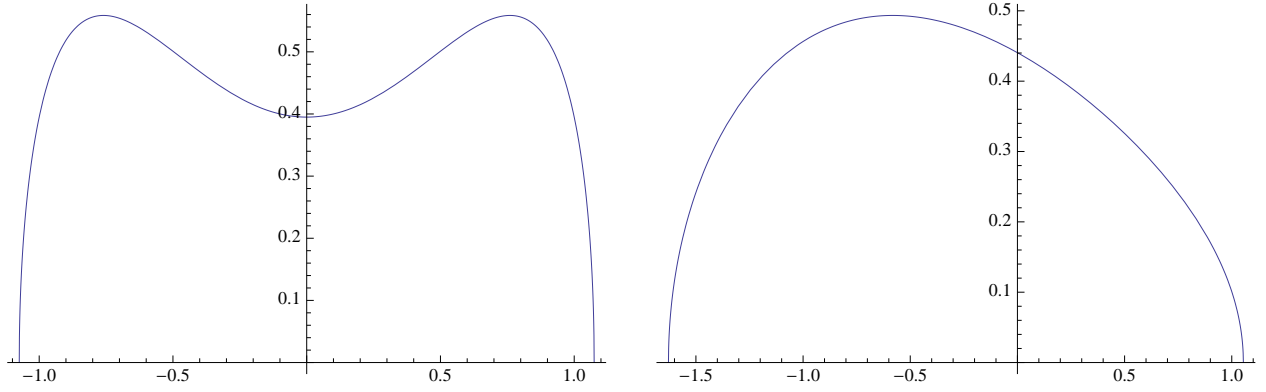


Figure 1: The equilibrium measure for $V(x) = x^4$ (left) and $V(x) = x^2 + \sin x$ (right).

$V(x) = x^2$. 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, (2.1) is exact, thus we obtain the semicircle distribution to machine precision (in a fraction of a second).

Another example is $V(x) = x^4$. We know 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 Figure 1.

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

6. Computing the inverse Cauchy transform over multiple intervals

The expression (2.1) is only valid 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

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

Let us express the 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 Hölder-continuous functions on Γ to Hölder-continuous functions on Ω by

$$\mathcal{P}_\Gamma(\Omega)g(x) = \mathcal{P}_\Gamma g(x) \quad \text{for} \quad x \in \Omega.$$

We thus want to satisfy

$$\begin{pmatrix} I & 2\mathcal{P}_{\Sigma_2}(\Sigma_1) & \dots & 2\mathcal{P}_{\Sigma_N}(\Sigma_1) \\ 2\mathcal{P}_{\Sigma_1}(\Sigma_2) & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \ddots & I & 2\mathcal{P}_{\Sigma_N}(\Sigma_{N-1}) \\ 2\mathcal{P}_{\Sigma_1}(\Sigma_N) & \ddots & 2\mathcal{P}_{\Sigma_{N-1}}(\Sigma_N) & I \end{pmatrix} \begin{pmatrix} g_1 \\ \vdots \\ g_N \end{pmatrix} = \begin{pmatrix} f_1 \\ \vdots \\ f_N \end{pmatrix}, \quad (6.1)$$

where f_i is the restriction of f to Σ_i .

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

$$\mathbf{f}_\Sigma = \begin{pmatrix} \mathbf{f}_{\Sigma_1} \\ \vdots \\ \mathbf{f}_{\Sigma_N} \end{pmatrix},$$

where the length of the vectors are $n_{\Sigma_1}, \dots, n_{\Sigma_N}$. Now let

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

where we define the $n_\Omega \times n_\Gamma$ matrix

$$P_\Gamma(\Omega) = \left[\phi_\Gamma(\mathbf{x}_\Omega) - \frac{1}{2}(M_\Gamma(\mathbf{x}_\Omega)\kappa_\Gamma(\mathbf{x}_\Omega), \mathbf{0}, \dots, \mathbf{0}) \right] \mathcal{F}.$$

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

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

we have

$$\mathcal{P}_\Sigma f \approx \sum_{j=1}^N \left[\phi_{\Sigma_j}(z) - \frac{1}{2}(M_{\Sigma_j}(z))\kappa_{\Sigma_j}(z), 0, \dots, 0 \right] \mathcal{F} I_j R_\Sigma^{-1} \mathbf{f}_\Sigma.$$

This is only a single solution to (1.2), though there in fact exists an N dimensional space of solutions. Define

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

For $x \in \Sigma_i$, we have

$$\kappa_\Sigma^+(x) + \kappa_\Sigma^-(x) = \prod_{k \neq i} \kappa_{\Sigma_k} \left(\kappa_{\Sigma_i}^+ + \kappa_{\Sigma_i}^- \right) = 0.$$

Moreover $\kappa_\Sigma(z) = \mathcal{O}(z^{-N})$, and hence we have

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

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

From the definition (2.1), it is clear that $\mathcal{P}_\Gamma(\Omega)$ is a bounded operator, and classical RH theory guarantees that the solution to (1.2) is unique [11], as long as the constants ξ_1, \dots, ξ_N are fixed. Convergence of this approximation as $n_{\Sigma_1}, \dots, n_{\Sigma_N} \rightarrow \infty$ is thus 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]).

7. Indefinite integral of the inverse Cauchy transform

In the Newton–Raphson iteration to be set-up, we have $2N$ unknowns: the left and right endpoints of Σ_i . Thus we expect to construct a function $F(\Sigma)$ with $2N$ components. The function ϕ must still be bounded at all endpoints of Σ ; hence, we require that the zeroth Chebyshev coefficients of the functions g_1, \dots, g_N vanish:

$$0 = \check{g}_{1,0} = \dots = \check{g}_{N,0}.$$

Now the asymptotic behaviour at infinity is the sum of each contribution, which depends on the first Chebyshev coefficients:

$$\mathcal{P}_\Sigma f(z) \sim \left[\frac{b_1 - a_1}{8} \check{g}_{1,1} + \dots + \frac{b_N - a_N}{8} \check{g}_{N,1} \right] \frac{1}{z}.$$

Thus we impose a condition that the sum in brackets is precisely one.

However, we still need $N - 1$ more conditions. Let $\Phi = \int \phi \, dz$ be an indefinite integral of $\phi = \mathcal{P}_\Sigma f$. Now, since $\phi^+ + \phi^- = V'$ on Σ_i , it follows that $\Phi^+ + \Phi^- = V + \ell_i$ on Σ_i . The missing conditions are that all of these constants of integration must be equal: $\ell_1 = \dots = \ell_N$ [6].

Since ϕ is a sum of $\mathcal{P}_{\Sigma_i} f$, we need to find the indefinite integral of \mathcal{P} over a single interval. Thus we return to the case where $\Sigma = (a, b)$. Note that

$$\int^z T_+^{-1}(M_\Sigma(z))^k \, dz = \frac{b-a}{4} \int^{T_+^{-1}(M_\Sigma(z))} (z^k - z^{k-2}) \, dx.$$

Therefore, we find that

$$\begin{aligned}
\int \kappa_{\Sigma}(z) dz &= \frac{b-a}{2} \log T_+^{-1}(M_{\Sigma}(z)), \\
\int M_{\Sigma}(z) \kappa_{\Sigma}(z) dz &= \frac{b-a}{2} [M_{\Sigma}(z) - T_+^{-1}(M_{\Sigma}(z))], \\
\int T_+^{-1}(M_{\Sigma}(z)) dx &= \frac{b-a}{4} \left[\frac{1}{2} T_+^{-1}(M_{\Sigma}(z))^2 - \log T_+^{-1}(M_{\Sigma}(z)) \right], \\
\int T_+^{-1}(M_{\Sigma}(z))^k dx &= \frac{b-a}{4} \left[\frac{1}{k+1} T_+^{-1}(M_{\Sigma}(z))^{k+1} - \frac{1}{k-1} T_+^{-1}(M_{\Sigma}(z))^{k-1} \right].
\end{aligned}$$

Define the $n \times n$ banded matrix

$$A = \begin{pmatrix} 0 & & & & & & \\ 2 & 0 & -1 & & & & \\ & \frac{1}{2} & & -\frac{1}{2} & & & \\ & & \frac{1}{3} & & -\frac{1}{3} & & \\ & & & \ddots & & \ddots & \\ & & & & \frac{1}{n-2} & & -\frac{1}{n-2} \\ & & & & & \frac{1}{n-1} & \end{pmatrix}.$$

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

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

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)

$$\Phi^{\pm}(x) \approx \frac{b-a}{8} [2\phi_{\Sigma}^{\pm}(x)A - \log T_{\downarrow}^{-1}(M_{\Sigma}(x))\mathbf{e}_2^{\top}] \mathcal{F}\mathbf{f}_{\Sigma},$$

and for $z < a$ we have

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

If Σ consists of multiple intervals, we sum the contributions

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

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:

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

where the first N conditions are that the zeroth Chebyshev coefficient of each g_i must vanish,

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

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

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

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

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

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 [6] 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 equal to a_i or b_i . We first note that the only term of \mathbf{f}_Σ depending on η_i is precisely \mathbf{f}_{Σ_i} , therefore we define

$$\mathbf{f}_{\Sigma, \eta_1} = \begin{pmatrix} \mathbf{f}_{\Sigma_1, \eta_1} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{pmatrix}, \mathbf{f}_{\Sigma, \eta_2} = \begin{pmatrix} \mathbf{0} \\ \mathbf{f}_{\Sigma_2, \eta_2} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{pmatrix}, \dots, \mathbf{f}_{\Sigma, \eta_N} = \begin{pmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{f}_{\Sigma_N, \eta_N} \end{pmatrix}.$$

Now for $\Gamma = \Sigma_i$ and $\eta = \eta_i$ we have

$$\phi_{\Gamma, \eta}(x) = \partial_\eta \phi_\Gamma(x) = \frac{M_{\Gamma, \eta}(x)[T_+^{-1}]'(M_\Gamma(x))}{2} (0, 1, \dots, (n-1)T_+^{-1}(M_\Gamma(x))^{n-2})$$

and

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

Therefore,

$$\partial_\eta P_\Gamma(\Omega) = \left[\frac{M_{\Gamma, \eta}(\mathbf{x}_\Omega)}{2(M_\Gamma(\mathbf{x}_\Omega) + 1)^{3/2}(M_\Gamma(\mathbf{x}_\Omega) - 1)^{3/2}} \mathbf{e}_1^\top + \phi_{\Gamma, \eta}(\mathbf{x}_\Omega) \right] \mathcal{F}.$$

On the other hand, if β is the left or right endpoint of Ω , we have

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

Thus we can evaluate the derivatives of R_Σ with respect to η equal to a_i, 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: given a value for N and initial guess intervals $\Sigma^0 = \Sigma_1^0 \cup \dots \cup \Sigma_N^0$, we can use F and its Jacobian to find approximations $\Sigma^m =$

$\Sigma_1^m \cup \dots \cup \Sigma_N^m$ for $m = 1, 2, \dots$. Then we have the approximation (where $\mathbf{n} = n_{\Sigma_1}, \dots, n_{\Sigma_N}$ are the number of Chebyshev points in each interval)

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

and

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

We hope that when N is chosen correctly that

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

Generic nonsingularity of the Jacobian [6] should imply that the method will converge to the true equilibrium measure whenever the initial guess is accurate enough. Moreover, we do know that the root of F is indeed the support of the equilibrium measure if the resulting Φ satisfies

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

where ℓ is the constant such that

$$\Phi^+(x) + \Phi^-(x) - V(x) = \ell \quad \text{for } x \in \Sigma. \quad [6]$$

Thus, in practice, if the Newton–Raphson iteration converges, we can determine whether the calculated domain Σ_m does indeed approximate the true support of the equilibrium measure by constructing

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

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

We must also ensure that the computed equilibrium measure is nonnegative. This can be determined by converting the mapped polynomial

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

to a mapped Chebyshev polynomial of the first kind using the formula

$$T_k(x) = \frac{1}{2} (U_k(x) - U_{k-2}(x)), \quad [8]$$

differentiating using the Chebyshev derivative matrix D and finding all roots of the resulting polynomial (and hence minima and maxima of (8.2)) using a colleague matrix method [4].

9. Examples

We consider the function

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

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

From [6], 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 Figure 3. At this point, the interval must be split and we thus switch to the multiple interval iteration with two interval. 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 [6].

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. Thus without an accurate initial guess, the two interval iteration can sometimes attempt to converge to this single interval solution (though it does not actually converge, as the two interval iteration cannot handle overlapping intervals reliably). Because 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 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 .

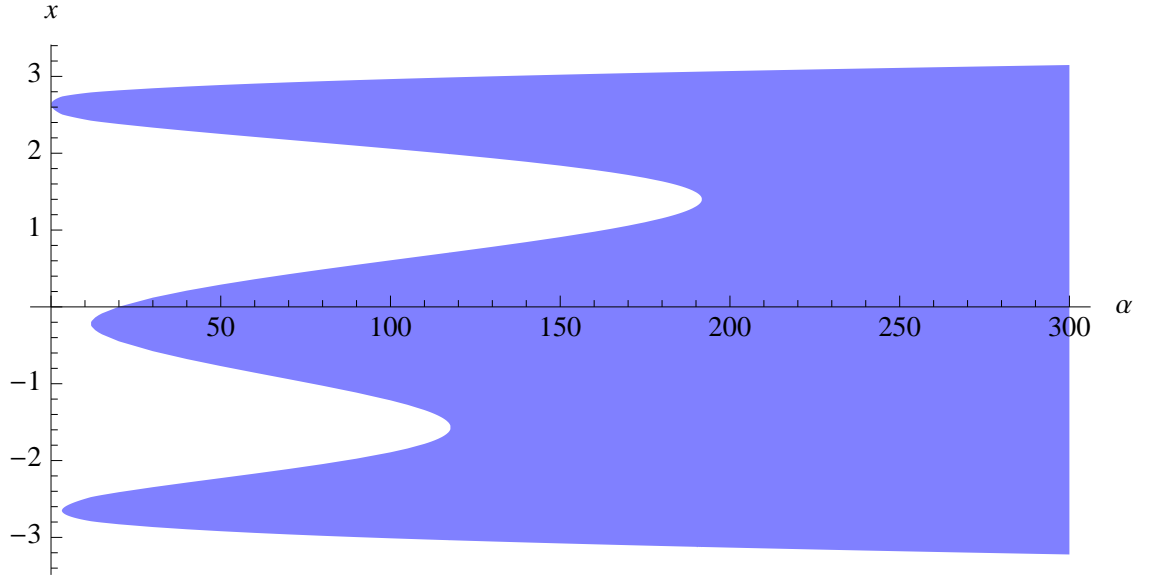


Figure 2: The support of the equilibrium measure for V_α over a range of α .

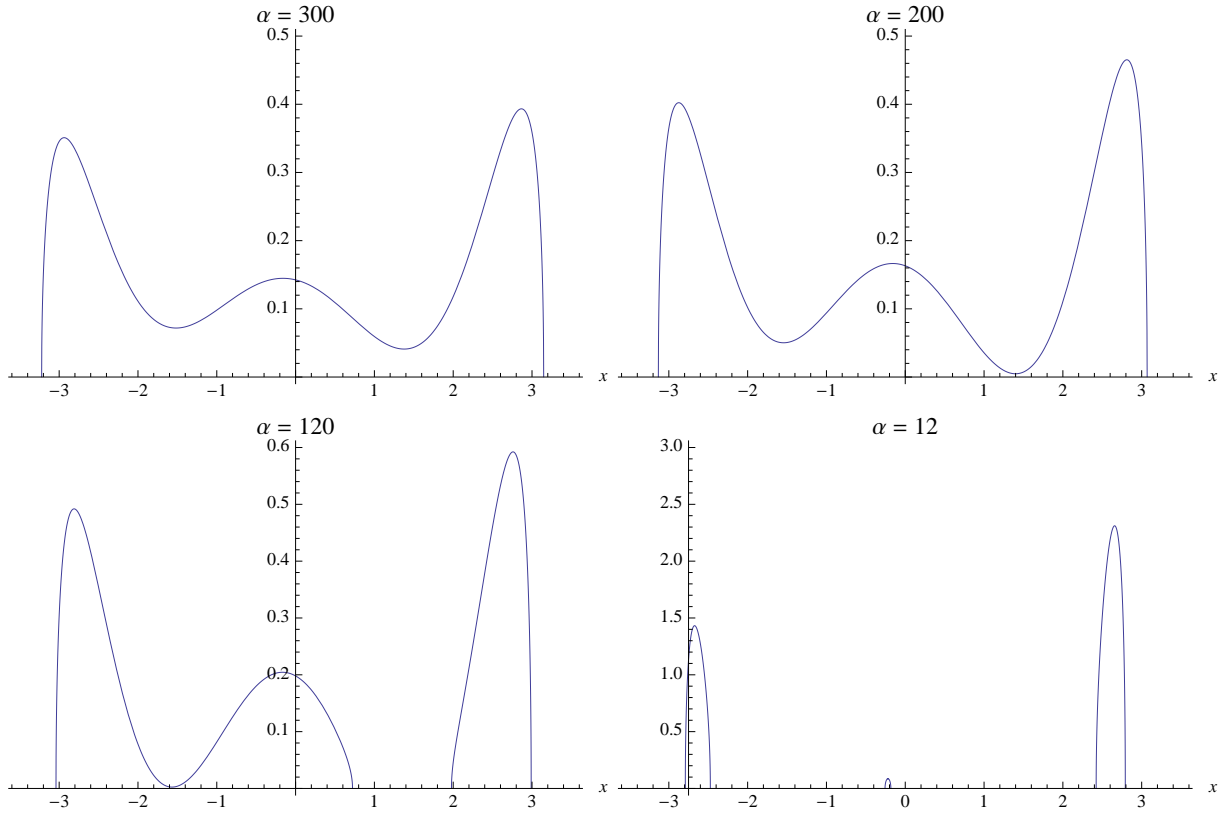


Figure 3: The equilibrium measure for V_α for $\alpha = 300, 200, 120$ and 12 .

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

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

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,

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

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

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

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, we know that $W_i(z) \sim z^{N-1}$ and $T_+(M_{\Omega}(z))^N \sim \left(\frac{b-a}{8}\right)^N z^{-N}$, 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 [8]. Using this expression, the full asymptotic series of each κ_j are determinable, by multiplying the series. Furthermore,

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

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 [8]. 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 can define

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

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.

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 $P_{\Gamma}(\Omega)$, which we transform:

$$\check{P}_{\Gamma}(\Omega) = \mathcal{F} P_{\Gamma}(\Omega) \mathcal{F}^{-1}.$$

In other words, while $P_{\Gamma}(\Omega)$ maps function values in Γ to function values in Ω , $\check{P}_{\Gamma}(\Omega)$ maps Chebyshev coefficients in Γ to Chebyshev coefficients in Ω . In particular, except for the first column, $\check{P}_{\Gamma}(\Omega)$ consists of the Chebyshev coefficients of ϕ_{Γ} .

Now we know ϕ_{Γ} is analytic in Ω , therefore the Chebyshev coefficients decay spectrally fast. Moreover, we know the closest singularity, hence the rate of decay. In detail, we first map Ω to the unit interval, and ϕ_{Γ} becomes $\phi_{\Gamma}(M_{\Omega}^{-1}(z))$, which has a branch cut along $M_{\Omega}^{-1}(\Gamma)$. The closest singularity is the closest endpoint of the mapped domain, hence define $\alpha = \min |M_{\Omega}^{-1}(M_{\Gamma}(\pm 1))|$. 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, $\phi_{\Gamma}(M_{\Omega}^{-1}(z))$ is analytic everywhere off its branch cut, including at infinity. Therefore it takes its maximum along the branch cut. Since T_{+}^{-1} maps the unit interval to the unit circle, we have $|\phi_{\Gamma}(M_{\Omega}(z))| \leq 1$ for all z . Thus we obtain that the k th Chebyshev coefficient is bounded by $2\rho^{-k}$ [12]. In other words, only the first

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

rows of $\check{P}_\Gamma(\Omega)$ are greater than ϵ .

Furthermore, we know, since Γ and Ω are disjoint that $|T_+(M_\Gamma(z))|$ is strictly less than one. Moreover, it is strictly monotonic on the real line. Therefore the k th column of ϕ_Γ , $T_+(M_\Gamma(z))^k$, decays in Ω exponentially fast as k increases, and all values in Ω are less than $T_+(M_\Gamma(M_\Omega^{-1}(\pm 1)))^k$. Thus only the first

$$\ell = \frac{\log \epsilon}{\log |T_+(M_\Omega^{-1}(\pm 1))|}$$

columns are greater than ϵ . Therefore $\check{P}_\Gamma(\Omega)$ can be expressed as a sparse matrix with only an $m \times \ell$ nonzero block. The size of this block is independent of n_i , and hence $R_\Omega \mathbf{b} = \mathbf{c}$ can be solved in $\mathcal{O}(\sum n_i)$ time.

There is another important use for this formulation: we can use it to determine how large each n_i need 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 $j = i \pm 1$).

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References

- [1] Atkinson, K.E., *The Numerical Solution of Integral Equations of the Second Kind*, Cambridge University Press, 1997.
- [2] Deift, P., *Orthogonal Polynomials and Random Matrices: a Riemann-Hilbert Approach*, American Mathematical Society, 2000.
- [3] Deift, P., Kriecherbauer, T. and McLaughlin, K.T.R., New results on the equilibrium measure for logarithmic potentials in the presence of an external field, *J Approximation Theory* **95** (1998), 388–475.
- [4] Good, I.J., The colleague matrix, a Chebyshev analogue of the companion matrix, *The Quarterly Journal of Mathematics* **12** (1961), 61.

- [5] Górski, J., Méthode des points extrémaux de résolution du problème de Dirichlet dans l'espace, *Ann. Math. Polon.* **1** (1950), 418–529.
- [6] Kuijlaars, A. B. J. and McLaughlin, K. T. R., 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. Maths* **53** (2000), 736–785.
- [7] Leja, F., Une méthode élémentaire de résolution du problème de Dirichlet dans le plan, *Ann. Soc. Math. Polon.* **23** (1950), 13–28.
- [8] Olver, F.W.J., Lozier, D.W., Boisvert, R.F. and Clarke, C.W., *NIST Handbook of Mathematical Functions*, Cambridge University Press, 2010.
- [9] Olver, S., Computing the Hilbert transform and its inverse, *Maths Comp.*, to appear.
- [10] Saff, E.B. and Totik, V., *Logarithmic Potentials with External Fields*, Springer, 1997.
- [11] Muskhelishvili, N.I., *Singular Integral Equations*, Groningen: Noordhoff (based on the second Russian edition published in 1946), 1953.
- [12] Trefethen, L.N., Is Gauss quadrature better than Clenshaw-Curtis?, *SIAM Review* **50** (2008), 67–87.