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A numerical solution of the constrained energy problem[☆]

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Abstract

An algorithm is proposed to solve the constrained energy problem from potential theory. Numerical examples are presented, showing the accuracy of the algorithm. The algorithm is also compared with another numerical method for the same problem.

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1. Introduction

In logarithmic potential theory the properties of (super-)harmonic functions in the complex plane are studied. With relatively few ingredients, a deep theory is built. The constrained energy problem (CEP) is an important problem in this logarithmic potential theory. So knowledge of its solution is certainly of theoretical interest.

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Logarithmic potential theory also has a lot of applications. The CEP can be applied in a number of apparently unrelated domains. It can be used to study weak limits of zeros of orthogonal polynomials [8,11,15,16]. It can also be used in the theory of integrable systems [7,11].

The authors got interested in the CEP by another application, namely convergence theory of Krylov subspace methods [1–5,10,12]. The connection with logarithmic potential theory is excellently described in the review papers [9,13]. The CEP can be used in this context to obtain accurate information on the convergence of the Arnoldi method for computing eigenvalues [10,12].

However, the CEP is not easy to solve explicitly. Only for some cases an explicit solution is known, and for other cases some properties can be derived without being able to obtain an explicit solution. Hence it would be interesting to obtain an approximate numerical solution.

In [6] a numerical method to solve the CEP is devised based on constrained Leja points. In a way, this is a natural approach. However, we feel that the method developed here gives better results. The numerical algorithm presented here is closely related to a theoretical algorithm called the iterated balayage algorithm [14].

The paper is organized as follows. In the next section some elements of potential theory are introduced and Section 3 explains how the algorithm works. The numerical experiments are presented in Section 4, followed by the conclusions.

2. Potential theory

In this section some definitions and properties of logarithmic potential theory will appear. For a more detailed treatment, the reader is referred to [17,18].

The logarithmic potential of a measure μ is defined as

$$U^\mu(z) = \int \log \frac{1}{|z - z'|} d\mu(z') \quad (1)$$

and its logarithmic energy is given by

$$I(\mu) = \iint \log \frac{1}{|z - z'|} d\mu(z') d\mu(z). \quad (2)$$

An important problem in logarithmic potential theory is the *energy problem*. Let $K \subset \mathbb{C}$ be a compact set:

Energy problem:

Minimize $I(\mu)$ among all Borel probability measures μ supported on K .

If there exists a probability measure on K with finite energy, the solution to this problem is unique and is called the *equilibrium measure of K* . It is denoted by μ_K . It can also be characterized in terms of its potential:

Property 2.1. Let μ_K be the solution of the energy problem. Then the potential U^{μ_K} is constant almost everywhere on K (with respect to μ_K) and smaller everywhere else. Moreover it is the only probability measure with that property.

A related problem is the *constrained energy problem* (CEP). Let σ be a Borel probability measure in the complex plane with compact support K and finite logarithmic energy $I(\sigma)$, and let $t \in (0, 1)$.

Constrained energy problem:

Minimize $I(\mu)$ among all Borel probability measures μ that satisfy $0 \leq t\mu \leq \sigma$.

Note that it is still asked that the support of the measure is contained in a fixed compact set K . We will suppose that the constraint σ is fixed and we will not indicate it in the notation; the solution of this CEP will be denoted by μ_t .

It is clear that if $t\mu_K \leq \sigma$, then the equilibrium measure also solves the CEP: $\mu_t = \mu_K$. As for the equilibrium measure, there is also a characterizing property in terms of the potential.

Property 2.2. Assume U^σ is continuous and real-valued and let μ_t be the solution of the CEP. Then U^{μ_t} is equal to a constant C_t on $\text{supp}(\sigma - t\mu_t)$ and smaller than or equal to C_t everywhere else. Moreover, the only probability measure μ that satisfies $0 \leq t\mu \leq \sigma$ and whose potential U^μ is constant on $\text{supp}(\sigma - t\mu)$ and smaller everywhere else, is μ_t .

So here also the potential is constant on a certain set and smaller everywhere else. Since $0 \leq t\mu_t \leq \sigma$, this set $\text{supp}(\sigma - t\mu_t)$ is just the set where $t\mu < \sigma$ (in the sense of densities). The algorithm will use the characterization from this property to obtain the solution. For conciseness, we give the equivalent formulation:

Constrained energy problem: (equivalent formulation)

Find a Borel probability measure μ that satisfies $0 \leq t\mu \leq \sigma$ so that its potential U^μ is constant on $\text{supp}(\sigma - t\mu)$ and smaller everywhere else.

A very useful property can be obtained if we drop the condition $0 \leq t\mu \leq \sigma$. The following lemma can be deduced from [8, Theorem 2.8] and from [14, Lemma 3]. We use the notation v^+ for the positive part of a signed measure v .

Lemma 2.3. Suppose μ is a probability measure (not necessarily with $t\mu \leq \sigma$) whose potential is constant on $\text{supp}(\sigma - t\mu)$. Then $\text{supp}(\sigma - t\mu_t)$ is a subset of $\text{supp}((\sigma - t\mu)^+)$.

So if there is a probability measure μ whose potential U^μ is constant on $\text{supp}(\sigma - t\mu)$, then on the region where $t\mu \geq \sigma$, we know that $t\mu_t = \sigma$.

3. The algorithm

From now on we will only be concerned with constraints σ living on the real line, so that all integrals will be over \mathbb{R} . First the main idea of the algorithm will be introduced. Then we will treat the necessary discretization. Finally some refinement ideas will be discussed, followed by an operation count.

3.1. Main loop

Using Lemma 2.3, we devise an algorithmic approach to solve the CEP. First we look for a Borel probability measure $\mu^{(1)}$ with support K whose potential is constant on K . This means $\mu^{(1)}$ is the equilibrium measure μ_K of the set K . Then on the region where $t\mu^{(1)} \geq \sigma$, we know that $t\mu_t = \sigma$, so we put $\mu^{(2)} = \sigma/t$ there, and on the other region we ask $U^{\mu^{(2)}}$ to be constant. This process will be repeated until at a certain point $\mu^{(k)} \leq \sigma/t$. Then the solution μ_t will be equal to $\mu^{(k)}$. However, this theoretical version of the algorithm will only terminate for very special input. For most sets of input it will run infinitely. Since this is only the case for the theoretical version, and not for the discrete version of the algorithm, this is not a problem.

In a high level language, this algorithm would look like

```

I := supp(σ)
J := ∅
while μ ⋈ σ/t
    μ|J := 1/t σ|J
    solve { U^μ|I = C - U^μ|J
           ||μ|I|| = 1 - ||μ|J||
    }
    I := {“ tμ < σ” }
    J := {“ tμ ≥ σ” }
μ_t := μ
    
```

The set I is the region where μ is not known yet, J is the set where μ is already known to be equal to σ/t . The potential of μ needs to be constant on I , so we solve $U^\mu = U^{\mu|I} + U^{\mu|J} = C$ (where C is an unknown constant), keeping in mind that μ has to be a probability measure: $\|\mu\| = \|\mu|I\| + \|\mu|J\| = 1$.

The output of this algorithm is a probability measure μ_t that satisfies $0 \leq t\mu_t \leq \sigma$ and whose potential U^{μ_t} is constant on $\text{supp}(\sigma - t\mu_t)$. If the potential is also smaller than this constant outside of $\text{supp}(\sigma - t\mu)$, Property 2.2 tells us that μ_t is the solution of the CEP. This will be proven in the next lemma. After step k of the algorithm, the intermediate solution will be called $\mu^{(k)}$, $C^{(k)}$ will be the constant value of its potential and $S_k := \text{supp}(\sigma - t\mu^{(k)})$.

Lemma 3.1. *For every k , the potential $U^{\mu^{(k)}}$ is smaller than the constant $C^{(k)}$ outside S_k .*

Proof. The proof will use induction on k .

The first intermediate solution $\mu^{(1)}$ is the equilibrium measure of K . Its potential $U^{\mu^{(1)}}$ is harmonic in $\mathbb{C} \setminus K$, on K it has the value $C^{(1)}$ and at ∞ it is $-\infty$. The maximum principle for harmonic functions [17,18] then assures that $U^{\mu^{(1)}}$ is smaller than $C^{(1)}$ outside of K .

Now suppose that $U^{\mu^{(k-1)}}$ is smaller than $C^{(k-1)}$ outside S_{k-1} . By construction, $S_k \subset S_{k-1}$, so it is sufficient to prove that

$$U^{\mu^{(k)}} - C^{(k)} \leq U^{\mu^{(k-1)}} - C^{(k-1)}. \tag{3}$$

On S_k , the relation

$$U^{\mu_k - \mu_{k-1}} = C^{(k)} - C^{(k-1)} \tag{4}$$

holds. Outside of S_k , $\mu_k - \mu_{k-1}$ is a negative measure, so from

$$U^{\mu_k - \mu_{k-1}} = U^{(\mu_k - \mu_{k-1})|_{S_k}} + U^{(\mu_k - \mu_{k-1})|_{S_k^c}}, \tag{5}$$

we learn that $U^{\mu_k - \mu_{k-1}}$ is subharmonic outside of S_k , since the first term is harmonic outside of S_k and the second term is subharmonic being the potential of a negative measure. Using the fact that a subharmonic function reaches its maximum on the boundary, (4) proves (3). \square

3.2. Discretization

Lemma 3.1 tells us that if the theoretical algorithm of the previous subsection converges, the output solves the CEP. In this subsection, we will suppose that we have a discretization $\{x_1, x_2, \dots, x_N\}$ of $\text{supp}(\sigma)$ and translate the algorithm to the discretization. The next subsection will explain how to choose a suitable discretization.

A measure μ will be represented by a vector v containing the values μ_j of the density $d\mu/dx$ in the discretization points x_j . We will ask the (in)equalities of the CEP to hold only in the discretization points.

In order to be able to compute the mass of a measure μ represented in this way, we will consider it to be piecewise linear with respect to the Lebesgue measure:

$$d\mu(x) = (a_j x + b_j) dx \quad \text{for } x \in [x_{j-1}, x_j]. \tag{6}$$

The mass of the piecewise linear measure is given by

$$\frac{1}{2} \sum_{j=2}^N (\mu_{j-1} + \mu_j)(x_j - x_{j-1}).$$

This expression is linear in the μ_j 's, so we can create a row vector m , that depends only on the discretization points x_j , such that the equality $mv = \|\mu\|$ holds for every piecewise linear measure μ with discretization $v = [\mu_1 \mu_2 \dots \mu_N]^t$.

We also need to compute the potential of a piecewise linear measure. Using integration by parts, we find that a primitive function of $x \mapsto \log 1/|x - y|$ is

$$f(x, y) := \begin{cases} (x - y)(\log |x - y| - 1) & \text{if } x \neq y, \\ 0 & \text{if } x = y \end{cases} \tag{7a}$$

and one of $x \mapsto x \log 1/|x - y|$ is

$$g(x, y) := \begin{cases} \frac{1}{2} \log |x - y|(x^2 - y^2) + \frac{1}{4}(x + y)^2 & \text{if } x \neq y, \\ x^2 & \text{if } x = y. \end{cases} \tag{7b}$$

Thus

$$\begin{aligned}
 U^\mu(y) &= \int \log \frac{1}{|x - y|} d\mu(x) \\
 &= \sum_{j=2}^N \int_{x_{j-1}}^{x_j} \log \frac{1}{|x - y|} (a_j x + b_j) dx \\
 &= \sum_{j=2}^N a_j (g(x_j, y) - g(x_{j-1}, y)) + b_j (f(x_j, y) - f(x_{j-1}, y)).
 \end{aligned} \tag{8}$$

Using (6), we can compute the a_j 's and the b_j 's in terms of the μ_j 's:

$$\begin{cases} \mu_{j-1} = a_j x_{j-1} + b_j, \\ \mu_j = a_j x_j + b_j, \end{cases} \Rightarrow \begin{cases} a_j = \frac{\mu_j - \mu_{j-1}}{x_j - x_{j-1}}, \\ b_j = \mu_j - a_j x_j = \frac{x_j \mu_{j-1} - x_{j-1} \mu_j}{x_j - x_{j-1}}. \end{cases}$$

Plugging this into Eq. (8), we see that the potential, evaluated at the discretization points x_j is linear in the μ_j 's. Hence there is a matrix P , depending only on the discretization points x_j , so that for every piecewise linear measure μ with discretization v ,

$$U^\mu(x_j) = (Pv)_j.$$

Now we can write down the discretized version of the CEP, the one we will solve. Suppose we have a set of discretization points $\{x_1, x_2, \dots, x_N\}$ with corresponding vector m and matrix P . Let s be the discretization of the constraint σ .

Constrained energy problem: (discretized version)

Find a vector v satisfying $m \cdot v = 1$ and $0 \leq tv \leq s$ (element-wise), so that Pv is constant on the components where $tv < s$, and smaller everywhere else.

So we limit our search space to the set of piecewise linear measures (represented by vectors) and we also weaken the demands on the measure: the constraint is only felt in the discretization points.

Finally, we write down the discretized version of the algorithm.

$$\begin{aligned}
 I &:= \{1, 2, \dots, N\} \\
 J &:= \emptyset \\
 \text{while } v \not\leq s/t & \\
 \quad v(J) &:= \frac{1}{t} s(J) \\
 \quad \text{solve } \begin{cases} P(I, I) \cdot v(I) = C - P(I, J) \cdot v(J) \\ m(I) \cdot v(I) = 1 - m(J) \cdot v(J) \end{cases} & \\
 \quad I &:= \{“tv < s”\} \\
 \quad J &:= \{“tv \geq s”\} \\
 v_t &:= v
 \end{aligned}$$

Here I is the set of indices where v is not known yet and $J = \{1, 2, \dots, N\} \setminus I$ is the set of indices where v is already known to be equal to s/t . The vector $v(J)$ is the vector consisting of the components of v with indices in J and the matrix $P(I, J)$ is the matrix consisting of the rows and columns of P with row indices in I and column indices in J . So we solve the system $P(I, *)v = C$ under the constraint that $mv = 1$, and write everything that is known to the right-hand side.

As mentioned in the previous subsection, the theoretical algorithm usually does not terminate in finite time. It should be noted that the discretized algorithm will terminate, since in every step at least one discretization point is added to J . (When no discretisation point is added, the stopping criterion is fulfilled.)

3.3. Refinement

If we compare the output of the algorithm sketched above with theoretical solutions of the CEP (in cases where these theoretical solutions are known), the error is rather small (see Section 4). However, in the endpoints of $\text{supp}(\sigma - t\mu)$ (i.e. the transition between $t\mu = \sigma$ and $t\mu < \sigma$) it is much bigger than away from those endpoints. This is not a big surprise. Theoretically, in typical cases, the density of μ_t should have a vertical tangent in those points. The exact solution is not well approximated by a piecewise linear measure in those points.

There are some possible solutions to this problem. One could put extra parameters in the model for the measure, trying to make it possible for the measure to ‘go vertically’ there. This solution implies a bigger system of equations to solve in each step. This makes the computation much slower, but even more important is the memory usage of the algorithm, which is also greatly increased.

Another approach is restarting the algorithm with a different set of discretization points. In the neighborhood of these ‘bad points’, we add some discretization points, to get a better approximation there. This can be done repetitively. This last idea turned out to be the most effective. One should take care about the accuracy, however; for the construction of the matrix P differences between consecutive discretization points appear in denominators. Not only does this lead to a loss of correct digits in the formation of the elements of P . This also causes the condition number of P to increase; the condition number is more or less proportional to the inverse of the minimal node spacing.

3.4. Time complexity

If N is the number of discretization points, creating the potential matrix P will take $\mathcal{O}(N^2)$ operations and solving a system with it takes $\mathcal{O}(N^3)$ (if we use a direct method). We cannot actually prove a bound for the number of iterations, but even for a large number of discretization points, the algorithm converges after some 10–20 iteration steps. This gives a total number of $\mathcal{O}(N^3)$ iterations.

We implemented the algorithm in MATLAB.¹ If we use 1000 discretization points for the examples treated in the next section, the algorithm takes less than 30 s to complete on a 1.5 GHz Pentium 4-processor with 512 MB of memory.

4. Numerical examples

In this section, we will study the solution given by our algorithm for different sets of input. First we will examine cases in which the support of the constraint consists of one interval and where the solution is explicitly known. We will compare our solution with the theoretical one. We will also compare this with the results from [6]. After that we will look at some cases where the support of the constraint consists of several intervals. No explicit solution is known in these cases.

4.1. One interval

4.1.1. Rakhmanov’s example

Suppose $d\sigma = \frac{1}{2} dx|_{[-1,1]}$. In [16] the solution to the CEP with constraint σ is given:

$$t \frac{d\mu_t}{dx}(x) = \begin{cases} \frac{1}{2} & \text{if } x \in [-1, -r] \cup [r, 1], \\ \frac{1}{\pi} \arctan\left(\frac{t}{1-t^2-x^2}\right) & \text{if } x \in [-r, r], \end{cases} \tag{9}$$

where $r = \sqrt{1-t^2}$. For $t = 0.5$, σ and $t\mu_t$ are plotted in Fig. 1(a).

For 500 equidistant discretization points for $[-1, 1]$, the error of the computed solution is plotted in Fig. 1(b). The maximal deviation of the theoretical solution is 2.8×10^{-3} and the condition number of the matrix P is 7.1×10^3 . Refining the discretization as described in Section 3.3, we can get the maximal deviation down to 3.1×10^{-5} . The minimal node spacing is 6.1×10^{-7} and the condition number is 5.4×10^7 . The error is plotted in Fig. 1(c).

4.1.2. Ullman distribution

Now take the case where $d\sigma = (2/\pi)\sqrt{1-x^2}$ on $[-1, 1]$. In [8] the solution is given:

$$t \frac{d\mu_t}{dx}(x) = \begin{cases} \frac{2}{\pi} \sqrt{1-x^2} & \text{if } x \in [-1, -r] \cup [r, 1], \\ \frac{2}{\pi} \left(\sqrt{1-x^2} - \sqrt{1-t-x^2} \right) & \text{if } x \in [-r, r], \end{cases} \tag{10}$$

¹ MATLAB is a registered trademark of The Mathworks, inc.

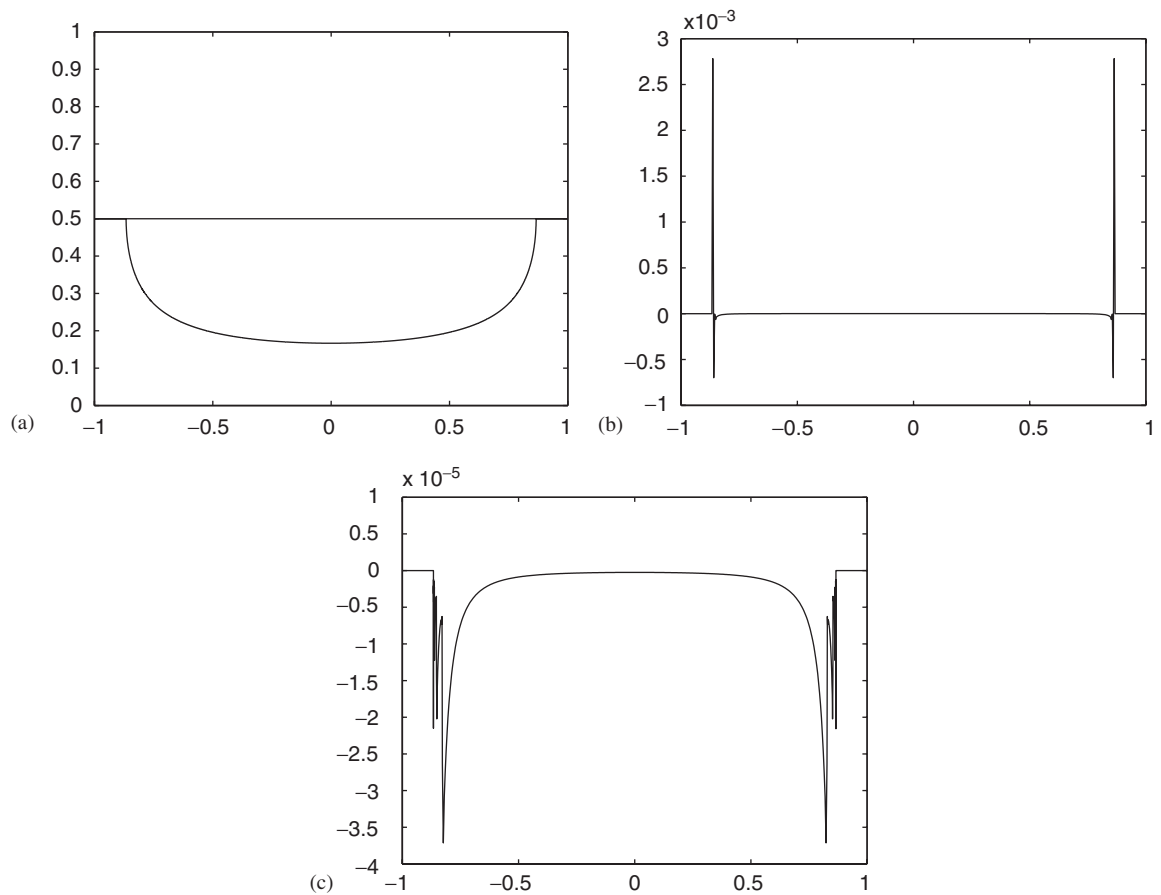


Fig. 1. Example 4.1.1: (a) constraint σ and theoretical solution $t\mu_t$; (b) error of the computed solution with 500 equidistant discretization points; and (c) error of the computed solution after the refinement.

where $r = \sqrt{1-t}$. In Fig. 2(a), σ and $t\mu_t$ are shown for $t = 0.4$. In Fig. 2(b) the errors of the computed solution are plotted for 500 equidistant discretization points. The maximal deviation is 1.9×10^{-4} . Using the refinement technique, this error could not be made significantly smaller.

4.1.3. Comparison with the constrained Leja point algorithm

In [6], the CEP is solved numerically using Leja points. Only plots are given there, which only allows for a qualitative comparison. However, looking at the difference between the theoretical solution and the computed one, one has to conclude that the results we get are far more accurate (even without any refinement). No operation count or timing is given, so a speed comparison is impossible.

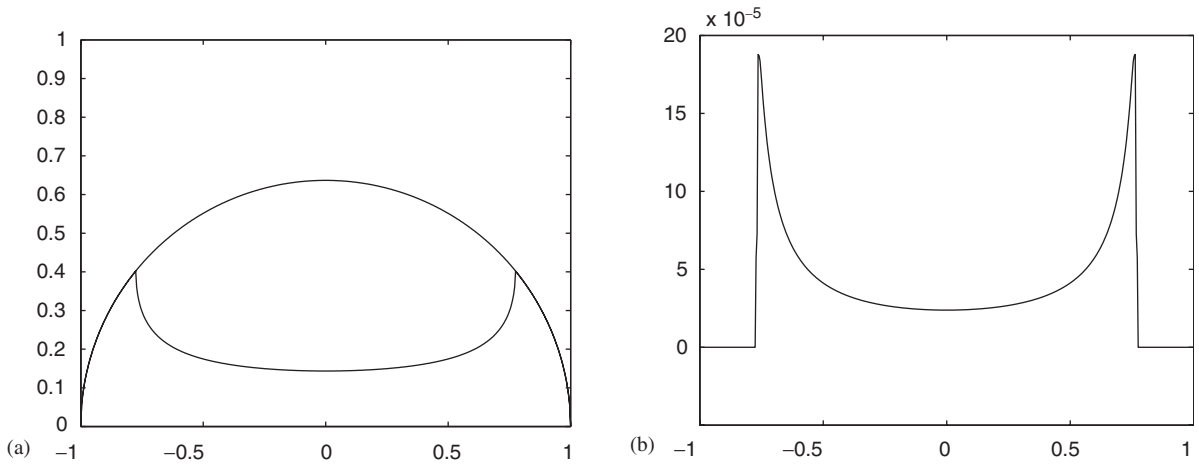


Fig. 2. Example 4.1.2: (a) constraint σ and theoretical solution $t\mu_t$; and (b) error of the computed solution with 500 equidistant discretization points.

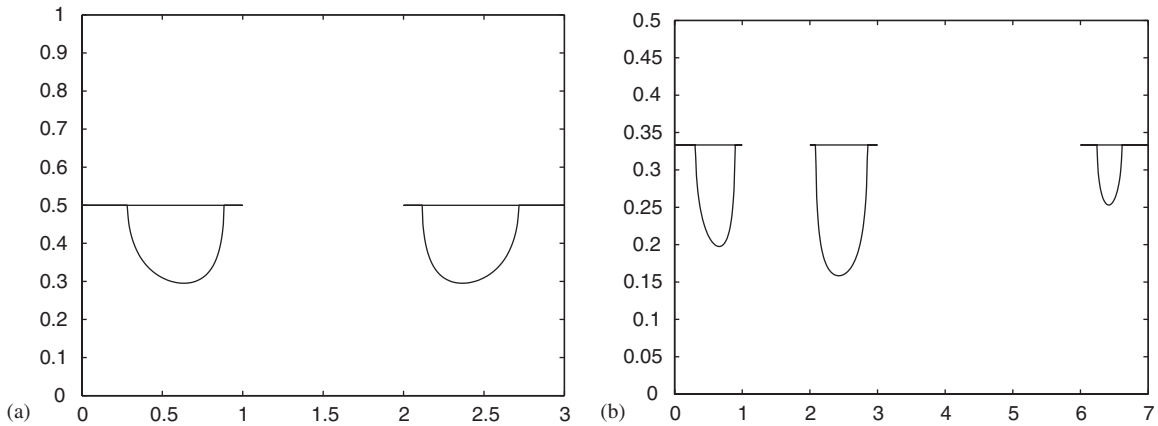


Fig. 3. Numerical results for multiple intervals: (a) a constant constraint on $[0, 1] \cup [2, 3]$, $t = 0.8$; and (b) a constant constraint on $[0, 1] \cup [2, 3] \cup [6, 7]$, $t = 0.8$.

4.2. More intervals

For the multiple interval case, we look at the constant constraint on $[0, 1] \cup [2, 3]$ and on $[0, 1] \cup [2, 3] \cup [6, 7]$, with $t = 0.8$. To the best of our knowledge, no explicit solution is known. The numerical results can be found in Fig. 3.

5. Conclusion

We have devised an algorithm for solving the constrained energy problem which appears in logarithmic potential theory. The algorithm is based on Property 2.2, which allows for an equivalent formulation of the CEP, only using the logarithmic potential. This is important since the logarithmic potential is a linear functional of the measure, so that a discretization gives a system of linear equations.

In [6], the constrained Leja point algorithm is proposed to solve the CEP. That approach seems natural, but the results we obtain are better.

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