An Approximate Solution to Consistency Equations

Zihao Hu
zihaohu@sjtu.edu.cn

Abstract

In this report, we propose a technique to approximate a fixed point of consistency mappings deriving from mean field inference. We convert these equations to linear systems by using a linear approximation to sigmoid function, then obtain a closed-form solution. This idea may also be used to solve an approximate solution for other energy functionals, like the Bethe free energy.

Technical Details

Let us consider a Gibbs distribution about $\mathbf{x} \in \{-1, 1\}^{n\times 1}$

$$p(\mathbf{x}) = \frac{1}{Z}\exp\{-\mathcal{E}(\mathbf{x})\}, \tag{1}$$

and its fully factorized mean field distribution

$$q(\mathbf{x}|\boldsymbol{\phi}) = \prod_i^n \phi_i^{(x_i+1)/2}(1-\phi_i)^{(1-x_i)/2}. \tag{2}$$

The KL-divergence between q and p is

$$\begin{aligned}\mathrm{KL}(q||p) = &\sum_i^n \phi_i \ln\phi_i + (1-\phi_i)\ln(1-\phi_i) \\ &+ \mathbb{E}_q[\mathcal{E}] + \ln Z.\end{aligned} \tag{3}$$

After letting the derivative of ϕ_i be zero, we obtain

$$\phi_i = \sigma(-\frac{\partial \mathbb{E}_q[\mathcal{E}]}{\partial \phi_i}). \tag{4}$$

For a binary random variable x which takes the value 1 with probability ϕ and the value -1 with probability $1-\phi$, $\mathbb{E}[x] = 1\times\phi + (-1)\times(1-\phi) = 2\phi - 1$. Since $\mathcal{E}$ is a polynomial of $\mathbf{x}$, Equation 4 usually has the form of

$$\boldsymbol{\phi} = \sigma(\mathbf{A}(2\boldsymbol{\phi}-1)+\mathbf{b}), \tag{5}$$

where $\mathbf{A}$ is a real symmetric matrix of $n\times n$ and $\mathbf{b}$ is a real vector. In addition, we wish to solve $\boldsymbol{\phi} \in [0,1]^{n\times 1}$ approximately.

We define $\lambda = \max(\sum_j^n |A_{ij}| + |b_i|)/c,\ i = 1, \cdots, n$, and solve the scaled problem

$$\boldsymbol{\phi} = \sigma(\lambda^{-1}(\mathbf{A}(2\boldsymbol{\phi}-\mathbf{1})+\mathbf{b})) \tag{6}$$

to ensure that each term inside the sigmoid is bounded by an interval $[-c, c]$, we compute a linear approximation for the sigmoid function: $\sigma(x) \approx c'x + c''$, where c' and c'' can be determined by minimizing the squared loss:

$$\min_{c_1,c_2}\int_{-c}^{c}(\sigma(x) - c'x - c'')^2 dx. \tag{7}$$

Since each term inside the sigmoid function in Equation 6 is a linear combination of $\boldsymbol{\phi}$, approximating these terms directly may cause considerable error. When $\mathbf{A}$ is invertible, we apply a linear transformation $\mathbf{v} = \lambda^{-1}\mathbf{A}(2\boldsymbol{\phi}-\mathbf{1})$, that is, $2\boldsymbol{\phi}-\mathbf{1} = \lambda\mathbf{A}^{-1}\mathbf{v}$, to make sure that each term inside the sigmoid function involves one variable in $\mathbf{v}$. After the approximation, Equation 6 turns out to be linear equations of $\mathbf{v}$ as

$$(\lambda\mathbf{A}^{-1} - 2c'\mathbf{I})\mathbf{v} = 2c'\lambda^{-1}\mathbf{b}, \tag{8}$$

where since $c'' \equiv 0.5$, it is eliminated automatically. When $\mathbf{A}$ is singular, we approximate (6) directly, and obtain

$$(\lambda\mathbf{I} - 2c'\mathbf{A})(2\boldsymbol{\phi} - \mathbf{1}) = 2c'\mathbf{b}. \tag{9}$$

We mainly discuss the case that $\mathbf{A}$ is invertible, while the case that $\mathbf{A}$ is singular can be solved similarly. In both cases, we have to inverse $(\lambda\mathbf{I} - 2c'\mathbf{A})$, so we use the following theorem to ensure its invertibility.

Theorem 1. *A sufficient condition for the invertibility of* $(\lambda\mathbf{I} - 2c'\mathbf{A})$ *is that* $2c' < 1/c$.

Proof. We denote the eigenvalue of $\mathbf{A}$ with the largest magnitude as λ_m. According to the Gershgorin circle theorem, recall that $\lambda = \max(\sum_j^n |A_{ij}| + |b_i|)/c, \quad i \in \{1, \cdots, n\}$, we have

$$|\lambda_m| \le \max(\sum_j^n |A_{ij}|) \le \lambda c, \quad i \in \{1, \cdots, n\}. \tag{10}$$

If $2c' < 1/c$, the eigenvalue of $2c'\mathbf{A}$ with the largest magnitude is less than λ, then $(\lambda\mathbf{I} - 2c'\mathbf{A})$ would be positive definite, which concludes the proof. $\square$

Since c' is determined by c, we can figure out that when $c < 2.5997$, the condition in Theorem 1 holds automatically.

Now according to whether $\mathbf{b} = \mathbf{0}$, (8) has two cases:

- For $\mathbf{b} \neq \mathbf{0}$, this problem has a closed-form solution

$$\mathbf{v} = 2c'\lambda^{-1}(\lambda\mathbf{A}^{-1} - 2c'\mathbf{I})^{-1}\mathbf{b}. \tag{11}$$

- For $\mathbf{b} = \mathbf{0}$, this linear system does not have non-zero solution, and we find the solution of

$$\min_{\mathbf{v}} \left\|(\lambda\mathbf{A}^{-1} - 2c'\mathbf{I})\mathbf{v}\right\|_2^2 \tag{12}$$

  instead. The solution of the problem is the eigenvector associated with the smallest eigenvalue of the matrix $(\lambda\mathbf{A}^{-1} - 2c'\mathbf{I})^T(\lambda\mathbf{A}^{-1} - 2c'\mathbf{I})$.

After solving $\mathbf{v}$, reminding that $\mathbf{v} + \lambda^{-1}\mathbf{b} \triangleq \mathbf{v}' \in [-c, c]$, we first re-normalize $\mathbf{v}'$ by

$$\mathbf{v}' = c\Big(2(\frac{\mathbf{v}' - \min(\mathbf{v}')}{\max(\mathbf{v}') - \min(\mathbf{v}')}) - 1\Big), \tag{13}$$

then use $\boldsymbol{\phi} = \sigma(\mathbf{v}')$ to obtain the final $\boldsymbol{\phi}$.

Actually, we can reduce the approximation error by scaling the original problem with $\lambda = \max(\sum_j^n |A_{ij}|)/c$, $i = 1, \cdots, n$. Now since each term inside the sigmoid is bounded by an interval $[b_i - c, b_i + c]$, we apply a linear approximation: $\sigma(x) \approx c_i x + d_i$, where c_i and d_i is determined by

$$\min_{c_i, d_i} \int_{b_i - c}^{b_i + c} (\sigma(x) - c_i x - d_i)^2 dx, \tag{14}$$

We denote $\mathbf{C}$ as a diagonal matrix with the i-th diagonal element as c_i, the largest one in $c_1, \cdots, c_n$ as c_m, and $\mathbf{d}$ as a column vector formed by d_i.

Using the approximation, Equation 6 is converted to be linear equations about $\mathbf{v}$

$$(\lambda\mathbf{A}^{-1} - 2\mathbf{C})\mathbf{v} = 2\lambda^{-1}\mathbf{C}\mathbf{b} + 2\mathbf{d} - \mathbf{1}, \tag{15}$$

which can be solved similarly as before.

We use the following theorem to guarantee the invertibility of $(\lambda\mathbf{I} - 2\mathbf{C}\mathbf{A})$.

Theorem 2. *A sufficient condition for the invertibility of* $(\lambda\mathbf{I} - 2\mathbf{C}\mathbf{A})$ *is that* $2|c_m| < 1/c$.

Proof. We denote the eigenvalue of $\mathbf{C}\mathbf{A}$ with the largest magnitude as λ_m^c. According to the Gershgorin circle theorem and $\lambda = \max(\sum_j^n |A_{ij}|)/c, \quad i \in \{1, \cdots, n\}$, we have

$$\begin{aligned} |\lambda_m^c| &\le \max(\sum_j^n |c_j A_{ij}|) \le |c_m| \max(\sum_j^n |A_{ij}|) \\ &\le \lambda |c_m| c, \quad i \in \{1, \cdots, n\}. \end{aligned} \tag{16}$$

If $2|c_m| < 1/c$, the eigenvalue of $2\mathbf{C}\mathbf{A}$ with the largest magnitude is less than λ, then $(\lambda\mathbf{I} - 2\mathbf{C}\mathbf{A})$ would be positive definite, which concludes the proof. $\square$

Actually, we can prove that $|c_m| \le c'$ always holds by showing that c_i in Equation 14 achieves maximum when $b_i = 0$. Therefore, the condition in Theorem 1 is also enough. We show the proof as follows.

After taking partial derivatives w.r.t c_i and d_i in Equation 14 and eliminating d_i, we reach

$$c_i \propto c(\ln(1+e^{b_i+c}) + \ln(1+e^{b_i-c})) + \mathrm{Li}_2(-e^{b_i+c}) - \mathrm{Li}_2(-e^{b_i-c}), \tag{17}$$

where $\mathrm{Li}_s(z)$ is the polylogarithm function. Its derivative with respect to b_i is

$$f(b_i) = c\sigma(b_i+c) + c\sigma(b_i-c) + \ln(1+e^{b_i-c}) - \ln(1+e^{b_i+c}). \tag{18}$$

We prove $f(b_i)$ is negative in $(0,\infty)$ and positive in $(-\infty,0)$, so c_i reaches maximum iff $b_i = 0$.

First, we derive $f(b_i)$'s derivative

$$f'(b_i) = \sigma(b_i+c)(c-1-c\sigma(b_i+c)) + \sigma(b_i-c)(c+1-c\sigma(b_i-c)). \tag{19}$$

It seems intractable to solve the zero set of the derivative, so we have to bypass the problem. Noticing that $f'(b_i)$ is a quadratic function of both $\sigma(b_i+c)$ and $\sigma(b_i-c)$, we convert the zero set of $f'(b_i)$ to the intersections of two curves

$$f'(b_i) = x(c-1-cx) + y(c+1-cy) \triangleq g(x,y) = 0 \tag{20}$$

and

$$\begin{cases} x = \sigma(b_i+c) \\ y = \sigma(b_i-c) \end{cases}. \tag{21}$$

The plot of $g(x,y)=0$ is, obviously, a circle. Although the second curve seems complex, we can eliminate the parameter b_i and obtain

$$x(1-y) = e^{2c}(1-x)y, \qquad 0 \le x \le 1, 0 \le y \le 1, \tag{22}$$

which is actually part of a hyperbola after inspecting its determinant.

Therefore, solving $f'(b)=0$ is equivalent to finding the intersections of

$$\begin{cases} (x-\frac{c-1}{2c})^2 + (y-\frac{c+1}{2c})^2 = \frac{c^2+1}{2c^2} \\ x(1-y) = e^{2c}(1-x)y \end{cases}, \quad 0 \le x \le 1, 0 \le y \le 1. \tag{23}$$

We can verify that the line $x+y=1$ is the common symmetry axis of both curves, so we can just discuss the intersections of two curves below the line and double the result. These two curves intersect $x+y=1$ with points $(\frac{c-1+\sqrt{c^2+1}}{2c}, \frac{c+1-\sqrt{c^2+1}}{2c})$ and $(\sigma(c), \sigma(-c))$, respectively. We can further find out that implicit relations of two curves can be converted to functions $h_1(x)$ and $h_2(x)$ in intervals $[0, \frac{c-1+\sqrt{c^2+1}}{2c}]$ and $[0, \sigma(c)]$, respectively. The point $(0,0)$ (corresponds to the case that $b \to -\infty$) can be easily verified to be an intersection point of two curves. We use the Bolzano's theorem to prove that there is an intersection point in the interval $(0, \frac{c-1+\sqrt{c^2+1}}{2c}]$. We shall show that $h_1'(0) = \frac{1-c}{1+c} < h_2'(0) = e^{-2c}$ and $h_1(\frac{c-1+\sqrt{c^2+1}}{2c}) = \frac{c+1-\sqrt{c^2+1}}{2c} > h_2(\sigma(c)) = \sigma(-c) > h_2(\frac{c-1+\sqrt{c^2+1}}{2c})$ hold for $\forall c > 0$ by converting these inequalities to equivalent but simpler propositions.

$$\begin{aligned} & e^{-2c} > \frac{1-c}{1+c} \\ \Leftrightarrow & e^{-2c}(1+c) > (1-c) \\ \Leftrightarrow & (1+c) > e^{-2c}(1-c) \\ \Leftrightarrow & e^{2c}(c-1) + (c+1) > 0. \end{aligned}$$

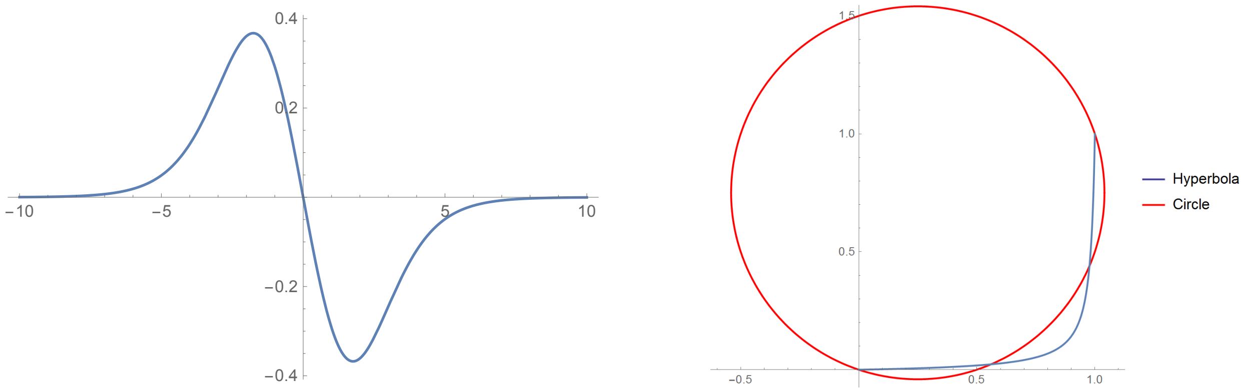
$$\begin{aligned} & \frac{c+1-\sqrt{c^2+1}}{2c} > \sigma(-c) \\ \Leftrightarrow & c+1+\sqrt{c^2+1} < 1+e^c \\ \Leftrightarrow & (e^c-c)^2 > c^2+1 \\ \Leftrightarrow & e^{2c} - 2ce^c - 1 > 0. \end{aligned}$$

We can easily verify that $e^{2c}(c-1)+(c+1) > 0$ and $e^{2c} - 2ce^c - 1 > 0$ hold for $\forall c > 0$. Since $h_1(0) = h_2(0)$ and $h_1'(0) < h_2'(0)$, we can say there exists $\epsilon > 0$ to make $h_1(\epsilon) < h_2(\epsilon)$. Then $h_1(\frac{c-1+\sqrt{c^2+1}}{2c}) > h_2(\frac{c-1+\sqrt{c^2+1}}{2c})$ yields that $h_1(x) = h_2(x)$ has a root in the interval $(\epsilon, \frac{c-1+\sqrt{c^2+1}}{2c})$. We denote the root as t.

These two curves possess at least four intersection points due to the symmetry, but a circle can intersect a hyperbola with at most four points, so the number of intersections is exactly four.

Now, we can reveal the monotonicity of $f(b_i)$ by inspecting relative positions of two curves. Recall that

$$f'(b_i) = x(c-1-cx) + y(c+1-cy). \tag{24}$$



(a) (b)

Figure 1: The plot of $f(b_i)$ and the intersections of two curves when $c = 2$.

If a point which lies on the hyperbola is inside the circle, we have $f'(b_i) > 0$, and vice versa. We draw plots of $f(b_i)$ and other two curves for the case $c = 2$ in Figure 1. Since in the interval $(0, t)$, $h_1(x) < h_2(x)$ and in $(t, \frac{c-1+\sqrt{c^2+1}}{2c}]$, $h_1(x) > h_2(x)$, we know that $f(b_i)$ increases in $(-\infty, \sigma^{-1}(t) - c)$ and $(\sigma^{-1}(1-t) + c, \infty)$, while decreases in $(\sigma^{-1}(t) - c, \sigma^{-1}(1-t) + c)$ using the relation that $x = \sigma(b_i + c)$. Combining the monotonicity with facts that $\lim_{b_i \to \pm\infty} f(b_i) = 0$ and $f(0) = 0$ concludes the proof.