Evaluating theta functions in uniform quasi-linear time in any dimension

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Joint work with Noam D. Elkies

Plan of the talk

1. Introduction: evaluating theta functions
2. The “naive” algorithm
3. The duplication formula
4. The final algorithm

The Riemann theta function

Parameters:

- $g \geq 1$: the dimension (sometimes called genus)
- $\tau \in \mathcal{H}_g$, the Siegel upper half-space: this means $\tau \in \mathrm{Mat}_{g\times g}(\mathbb{C})$ is symmetric and $\mathrm{Im}(\tau)$ is positive definite ($y^T \,\mathrm{Im}(\tau) y > 0$ for all nonzero $y \in \mathbb{R}^g$).
- $z \in \mathbb{C}^g$.

Define the Riemann theta function:

$$\theta(z,\tau) = \sum_{n\in\mathbb{Z}^g} E(n^T \tau n + 2n^T z).$$

where $E(x) := \exp(\pi i x)$. This sum converges quickly (terms get small as $n \to \infty$).

If $g = 1$, this is the Jacobi theta function

$$\theta(z,\tau) = \sum_{n\in\mathbb{Z}} E(\tau n^2 + 2nz).$$

Theta functions with characteristics

More generally, for all theta characteristics $a, b \in \{0,1\}^g$, define:

$$\theta_{a,b}(z,\tau) = \sum_{n \in \mathbb{Z}^g + \frac{a}{2}} E\big(n^T \tau n + 2n^T(z + \tfrac{b}{2})\big).$$

Before, we had $a = b = 0$.

Remark

Up to an exponential factor, $\theta_{a,b}(z,\tau)$ is simply $\theta_{0,0}(z + \tau\frac{a}{2} + \frac{b}{2}, \tau)$. The reason for this notation will become clear on the next slide.

Why theta functions?

Theta functions are closely connected to elliptic curves and abelian varieties over $\mathbb{C}$.

1. If τ is fixed and z varies, then $\theta(\cdot, \tau)$ is (roughly) periodic with respect to the lattice $L = \mathbb{Z}^g + \tau\mathbb{Z}^g \subset \mathbb{C}^g$.

   The quotient $A = \mathbb{C}^g / L$ is an abelian variety of dimension g, and theta functions with characteristics are coordinate functions on A. For instance, take A to be the Jacobian of any algebraic curve.
2. Fixing $z = 0$ and letting τ vary, the theta constants $\theta_{a,b}(0, \cdot)$ are modular forms. They can be used as invariants to identify an abelian variety, a curve, etc.

These properties (periodicity, modular forms) are also generally helpful when manipulating theta functions, as we will see.

Evaluating theta functions

Algorithmic problem

Given $(z, \tau) \in \mathbb{C}^g \times \mathcal{H}_g$, and a precision $N \geq 0$, compute the complex numbers $\theta_{a,b}(z, \tau)$ for all $a, b \in \{0, 1\}^g$ at precision N up to an error of at most 2^{-N}.

In applications, N can be in the millions.

Typical use case

Consider an elliptic curve in the form $E = \mathbb{C}/\Lambda$, where $\Lambda \subset \mathbb{C}$ is a rank 2 lattice. Say E is defined over $\mathbb{Q}$. Weierstrass equation ?

1. Write $\Lambda = \mathbb{Z} + \tau\mathbb{Z}$.
2. Evaluate $\theta_{a,b}(0, \tau)$ for $a, b \in \{0, 1\}$ (4 values). The j-invariant $j(E) \in \mathbb{C}$ has an expression in terms of theta: compute it.
3. Recognize $j(E) \in \mathbb{Q}$ provided N is big enough, can then write an equation for E.

Main result

Theorem (in progress, joint with Noam D. Elkies)

There exists an algorithm which, given $g \geq 1$, $N \geq 0$, and given $\tau \in \mathcal{H}_g$ and $z \in \mathbb{C}^g$ that are suitably reduced, evaluates $\theta_{a,b}(z,\tau)$ to precision N in quasi-linear time $O(2^{O(g)}\mathcal{M}(N)\log N)$ uniformly in τ and z.

Based on the duplication formula. Implemented in FLINT 3.1.

Brief history of previous work

- The naive algorithm (see Deconinck et al., 2002) consists in summing up enough terms in the theta series

$$\theta_{a,b}(z,\tau) = \sum_{n\in\mathbb{Z}^g+\frac{a}{2}} E\big(n^T\tau n + 2n^T(z+\tfrac{b}{2})\big).$$

  Useful at low precisions, but not quasi-linear. Optimized in the $g=1$ case by Enge–Hart–Johansson (2018).
- Dupont (2006), Labrande–Thomé (2010): quasi-linear algorithm based on a clever use of Newton's method. Heuristic, mainly tested for $g \leq 2$. Does not beat the naive algorithm for $g=1$ in the feasible range.
- In some cases ($g \leq 2$) one can prove that the Newton approach works and yields a uniform algorithm (JK, 2022). Still not known to work for all τ as soon as $g \geq 3$.

Brief list of available implementations

Implementations based on the naive algorithm:

- Theta.jl by Agostini–Chua (2020), low precision only.
- Magma's Theta, arbitrary g and precisions, extremely slow.
- RiemannTheta, Sage package by Nils Bruin, arbitrary g and precisions, less slow.
- acb_modular (FLINT) by Enge–Hart–Johansson (2018). $g = 1$ only, uses interval arithmetic, fast.

Often also support theta functions with characteristics, derivatives.

Implementations based on Newton's method exist, but are not easily accessible.

New implementation: acb_theta in FLINT 3.1. Any g, fast, quasi-linear, uniform, uses interval arithmetic, supports characteristics and derivatives, extensively tested.

Use that one!

The “naive” algorithm

Convergence of the theta series

Recall:

$$\theta_{0,0}(z,\tau) = \sum_{n\in\mathbb{Z}^g} E(n^T\tau n + 2n^T z).$$

Write $Y = \mathrm{Im}(\tau)$ and $y = \mathrm{Im}(z)$. Then:

$$\begin{aligned}\left|E(n^T\tau n + 2n^T z)\right| &= \exp(-\pi n^T Y n - 2\pi n^T y)\\ &= C\exp(-\|n - x_0\|_\tau^2)\end{aligned}$$

where $\|\cdot\|_\tau$ is the Euclidean norm attached to πY, and C, x_0 depend only on τ and z.

Useful consequence

For each $N \geq 0$, the lattice points $n \in \mathbb{Z}^g$ indexing terms whose absolute value is $\geq 2^{-N}$ are exactly the points in an ellipsoid $\|n - x_0\|_\tau \leq R$ with $R = O(\sqrt{N})$.

The tail of the series

Proposition

Let $\tau \in \mathcal{H}_g$, let C be the Cholesky matrix attached to $\pi \operatorname{Im}(\tau)$ (meaning: C is upper-triangular and $\pi \operatorname{Im}(\tau) = C^T C$), and let $\gamma_1, \ldots, \gamma_g$ be the diagonal coefficients of C. For each $R \geq 4$, we have:

$$\sum_{n \in \mathbb{Z}^g,\, \|n - x_0\|_\tau > R} \exp(-\|n - x_0\|_\tau^2) \leq 2^{g+1} R^{g-1} \exp(-R^2) \prod_{i=1}^{g} \Big(1 + \frac{2}{\gamma_i}\Big).$$

$\to$ taking $R = O(\sqrt{N})$, the tail of the series is bounded by 2^{-N}.

A first step when evaluating is to obtain nicer ellipsoids (i.e. larger γ_i) by reducing the arguments τ and z.

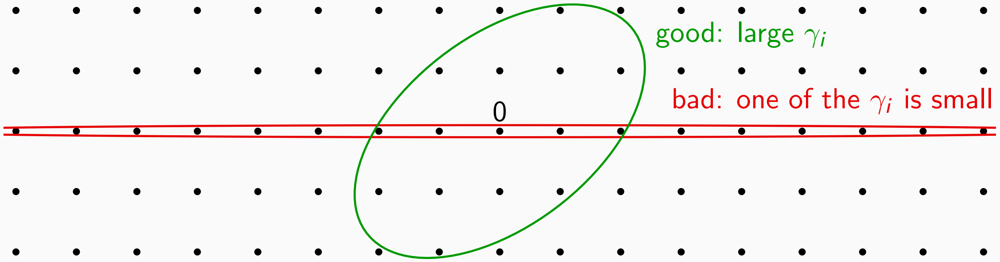
Argument reduction

Easy reductions using periodicity:

- reduce τ such that $|\mathrm{Re}(\tau)| \leq \frac{1}{2}$ (changes nothing)
- reduce z such that $z = u + \tau v$ with $u, v \in \mathbb{R}^g$ and $|u|, |v| \leq \frac{1}{2}$

  $\rightarrow$ the center of the ellipsoid is not far away from 0.

We also want to reduce $\mathrm{Im}(\tau)$. This changes the shape of the ellipsoids.



The symplectic group

The symplectic group $\mathrm{Sp}_{2g}(\mathbb{Z})$ consists of products of matrices of the form

$$\begin{pmatrix} I_g & S \\ 0 & I_g \end{pmatrix}, \qquad S \in \mathrm{Mat}_{g\times g}(\mathbb{Z}) \text{ symmetric}$$

$$\begin{pmatrix} U & 0 \\ 0 & U^{-T} \end{pmatrix}, \qquad U \in \mathrm{GL}_g(\mathbb{Z})$$

$$J_g := \begin{pmatrix} 0 & I_g \\ -I_g & 0 \end{pmatrix}.$$

Equivalently, all matrices M such that $M^T J_g M = J_g$.

The group $\mathrm{Sp}_{2g}(\mathbb{Z})$ acts on $\mathbb{C}^g \times \mathcal{H}_g$:

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \cdot (z,\tau) = \Big((\gamma\tau+\delta)^{-T} z,\ (\alpha\tau+\beta)(\gamma\tau+\delta)^{-1} \Big).$$

Theta as a modular form

Theorem (Mumford, Igusa)

Let $M = \left(\begin{smallmatrix} \alpha & \beta \\ \gamma & \delta \end{smallmatrix}\right) \in \mathrm{Sp}_{2g}(\mathbb{Z})$. Fix theta characteristics a, b. For every $(z, \tau) \in \mathbb{C}^g \times \mathcal{H}_g$:

$$\theta_{a,b}(M \cdot (z, \tau)) = \exp(\cdots) \cdot \zeta \cdot \sqrt{\det(\gamma\tau + \delta)} \cdot \theta_{a',b'}(z, \tau)$$

where:

- a', b' are other characteristics given by an explicit formula in terms of a, b, M,
- ζ is an 8th root of unity independent of z, τ,
- we must make a fixed choice of holomorphic sqrt of $\tau \mapsto \det(\gamma\tau + \delta)$ on $\mathcal{H}_g$.

Sort out the details $\to$ can act by $\mathrm{Sp}_{2g}(\mathbb{Z})$ before computing theta functions.

A nicer imaginary part

We have

$$\mathrm{Im}\big((\alpha\tau+\beta)(\gamma\tau+\delta)^{-1}\big) = (\gamma\tau+\delta)^{-T}\,\mathrm{Im}(\tau)(\gamma\tau+\delta)^{-1}.$$

Therefore:

- Can use lattice reduction (LLL) by taking $M = \begin{pmatrix} U & 0 \\ 0 & U^{-T} \end{pmatrix}$.
- Can increase $\det \mathrm{Im}(\tau)$ whenever $|\det(\gamma\tau+\delta)| < 1$. In particular, use the usual reduction for the action of $\mathrm{SL}_2(\mathbb{Z})$ on $\mathcal{H}_1$ on each diagonal coefficient.

Consequence

We can assume that $\mathrm{Im}(\tau)$ is LLL-reduced and its diagonal coefficients are $\geq \sqrt{3}/2$.

The ellipsoids we get in the naive algorithm are uniformly nice and round.

Naive algorithm: complexity

Result

Given reduced $(z, \tau) \in \mathbb{C}^g \times \mathcal{H}_g$ and $N \geq 1$, one can compute $\theta_{a,b}(z, \tau)$ for each individual characteristic (a, b) to N bits of precision using the naive algorithm in $O_g(N^{g/2}\mathcal{M}(N))$ binary operations, uniformly in τ and z.

Important optimizations in practice (but not really new):

- Compute exponentials only once, get subsequent terms by multiplying/squaring.
- Compute smaller terms (far from the center of the ellipsoid) at smaller precisions.
- Use existing functions when possible: `acb_modular_theta` ($g = 1$), `acb_dot`.

In FLINT, we implement ellipsoids as a recursive type to make all this easier to write.

Towards a quasi-linear algorithm

The naive algorithm is not quasi-linear... except when $\mathrm{Im}(\tau)$ is large!

If τ is reduced and each diagonal coefficient of $\mathrm{Im}(\tau)$ is $\Omega(N)$, then the ellipsoid to sum on contains $O(1)$ points $\to$ complexity $O_g(\mathcal{M}(N)\log N)$.

The duplication formula relates theta values at τ and 2τ.

Main idea

Use the duplication formula $k \simeq \log_2 N$ times starting from theta values at $2^k\tau$, computed in quasi-linear time with the naive algorithm.

The duplication formula

A typical duplication formula

The duplication formula is also used in the Newton approach to computing theta functions (Dupont, Labrande–Thomé).

We identify $\{0,1\}^g$ and $(\mathbb{Z}/2\mathbb{Z})^g$ (addition is xor).

Duplication formula

$$\theta_{a,b}(0,2\tau)^2 = \frac{1}{2^g} \sum_{b' \in (\mathbb{Z}/2\mathbb{Z})^g} (-1)^{a^T b'} \theta_{0,b'}(0,\tau)\, \theta_{0,b+b'}(0,\tau).$$

Note the particular role of $\theta_{0,b}$ compared to more general $\theta_{a,b}$.

For us, this goes in the wrong direction: we need to express theta values at τ in terms of theta values at 2τ.

A better formula

Cf. Koizumi, or Romain Cosset's thesis, or apply J_g to the previous formula:

Better duplication formula

$$\theta_{a,b}(0,\tau)^2 = \sum_{a' \in (\mathbb{Z}/2\mathbb{Z})^g} (-1)^{a'^T b} \theta_{a',0}(0,2\tau)\,\theta_{a+a',0}(0,2\tau).$$

This time, the 2^g "fundamental" theta values are the $\theta_{a,0}(0,\tau)$. For now, we focus on computing those and put $z = 0, b = 0$.

To apply the duplication formula, we need to:

1. Make the 2^g sums on the right (one for each $a \in \{0,1\}^g$, with $b = 0$). Do this in $O(2^g)$ operations with Hadamard transformations.
2. Extract square roots: get $\theta_{a,b}(0,\tau)$ from $\theta_{a,0}(0,\tau)^2$.

The root problem

Problems when extracting square roots:

1. We need to know what the correct sign is $\rightarrow$ need a low-precision approximation of $\theta_{a,0}(0,\tau)$. Can compute it using the naive algorithm.
2. Taking square roots brings a precision loss, perhaps as much as half of the current precision since $\sqrt{2^{-N}} = 2^{-N/2}$.

Both problems get worse the closer $\theta_{a,0}(0,\tau)$ gets to zero.

Dream scenario

There exists $\varepsilon > 0$ such that for all $k \geq 0$ and $a \in \{0,1\}^g$, we have $\left|\theta_{a,0}(0,2^k\tau)\right| \geq \varepsilon$.

This is however just false, since $\theta_{a,0}(0,2^k\tau) \underset{k\to\infty}{\longrightarrow} 0$ as soon as $a \neq 0$.

Need to quantify this to show that we're not killed by the naive algorithm and/or precision losses.

The absolute value of theta

Recall our previous analysis: the term corresponding to $n \in \mathbb{Z}^g + \frac{a}{2}$ in the series defining $\theta_{a,0}(0,\tau)$ has absolute value $\exp(-\|n\|_\tau^2)$.

Dream scenario 2

There exists $\varepsilon > 0$ such that for each $k \geq 0$, we have

$$\left|\theta_{a,0}(0, 2^k\tau)\right| \geq \varepsilon \exp\left(-2^k \operatorname{Dist}_\tau(0, \mathbb{Z}^g + \tfrac{a}{2})\right)$$

Here Dist_τ denotes the distance (between point and set) attached to the norm $\|\cdot\|_\tau$.

In other words $|\theta_{a,0}(\tau)|$ is comparable to the absolute value of the largest term appearing in the sum – no crazy cancellation occurs.

We expect this to be true (with a reasonable ε) for almost every τ.

The dream world

Assume Dream Scenario 2. Then each time we apply the duplication formula:

- Computing an approximation of $\theta_{a,0}(0,\tau)$ with the naive algorithm costs $O(1)$.
- We lose $O(1)$ bits of precision in square roots, provided that we think in terms of shifted absolute precision.

Convention

By "computing $\theta_{a,0}(0,2^k\tau)$ to shifted absolute precision N", we mean computing it to absolute precision $N + \left\lceil 2^k \operatorname{Dist}_\tau(0, \mathbb{Z}^g + \frac{a}{2}) / \log(2) \right\rceil$.

This accounts for the fact that $\left|\theta_{a,0}(0,2^k\tau)\right|$ is known to be small. In Dream Scenario 2, this is the same as relative precision.

- Small miracle: when summing in the duplication formula, we also lose only $O(1)$ bits of shifted absolute precision (parallelogram identity!)
- To initialize at $2^k = O(N)$, we use the naive algorithm and win.

The final algorithm

What? We're not done yet?

- For some special τ's, we might have unexpected vanishings of $\theta_{a,0}(0, 2^k\tau)$. Then the previous algorithm does not work.
- We also want to compute $\theta_{a,0}(z,\tau)$ for nonzero z.

Observation

Let $t \in \mathbb{R}^g$ be any vector. If, at each step, we compute $\theta_{a,0}(2^k v, 2^k\tau)$ for all $a \in \{0,1\}^g$ and all $v \in \{0, t, 2t, z, z+t, z+2t\}$, then we can bootstrap using variants of the duplication formula.

This requires us to take square roots of $\theta_{a,0}(2^k v, 2^k\tau)^2$ for $v \in \{t, 2t, z+t, z+2t\}$, but not $v = 0$ and $v = z$ (get those by division).

Introducing the real vector t changes nothing to ellipsoids and distances, but can prevent unexpected cancellations. In practice, a random t does the trick.

Theoretical result

Proposition (writeup in progress)

Fix $g \geq 1$ and $m \geq 0$. Then there exists $\varepsilon > 0$ such that for a proportion at least $1/2$ of vectors $t \in [0,1]^g$, the following holds:

For each reduced $(z, \tau) \in \mathbb{C}^g \times \mathcal{H}_g$, for each $a \in \{0,1\}^g$, for each $0 \leq k \leq m$, and for each $v \in \{t, 2t\}$, we have

$$\left|\theta_{a,0}(2^k v, 2^k \tau)\right| \geq \varepsilon \exp\left(-2^k \operatorname{Dist}_\tau(0, \mathbb{Z}^g + \tfrac{a}{2})\right),$$
$$\left|\theta_{a,0}(2^k (z+v), 2^k \tau)\right| \geq \varepsilon \exp\left(-2^k \operatorname{Dist}_\tau(x_0, \mathbb{Z}^g + \tfrac{a}{2})\right)$$

where x_0 denotes the center of the ellipsoid attached to z.

We can take ε to be (only) exponentially small in m and g.

Choosing t at random, the precision losses are mild with a probability $\geq 1/2$. ✓

Further comments

- If one of the diagonal coefficients γ_i is very large, the ellipsoids for $\|\cdot\|_\tau$ are thick in some directions while being very thin in other directions. We can leverage this by writing $\theta_{a,0}(z,\tau)$ as a (short) sum of theta values in smaller dimensions.

  This is more efficient than using the duplication formula in dimension g, and ensures that all the absolute precisions we consider are in $O(N)$.
  (This helps with the Hadamard method to apply the duplication formula.)
- This algorithm overcomes FLINT's implementation of the naive algorithm for $g = 1$ between 10 000 and 50 000 bits of precision.
- We compute derivatives of theta functions in quasi-linear time using finite differences.

Thank you!

https://flintlib.org/doc/acb_theta.html