Mathematical notes for the Lefschetz–thimble plotter

1 Problem class

We consider one–dimensional complex integrals of the form

$$I(\kappa) \;=\; \int_\Gamma \exp\!\big(-\kappa\, W(z)\big)\, \mathrm{d}z, \tag{1}$$

where $W\colon \mathbb{C} \to \mathbb{C}$ is holomorphic, $\kappa \in \mathbb{C}$ is a (typically large) parameter, and Γ is an integration contour in the complex plane.

The steepest–descent (Picard–Lefschetz) geometry is controlled by:

- the critical points ("saddles") z_σ of W, defined by $W'(z_\sigma) = 0$;
- the phase of κ (a non–zero argument rotates the constant–phase condition).

In the code in this repository we take $\kappa = 1$ by default. This loses no geometric information when $\kappa \in \mathbb{R}_{>0}$ (it merely rescales the flow time), and it is straightforward to reinsert κ if required.

2 Saddles and non–degeneracy

A saddle is any $z_\sigma \in \mathbb{C}$ satisfying

$$W'(z_\sigma) = 0. \tag{2}$$

For the standard local picture we assume the saddle is non–degenerate,

$$W''(z_\sigma) \neq 0. \tag{3}$$

In particular, near such a saddle one has the quadratic approximation

$$W(z) = W(z_\sigma) + \tfrac{1}{2} W''(z_\sigma)(z - z_\sigma)^2 + \mathcal{O}\big((z - z_\sigma)^3\big). \tag{4}$$

3 Holomorphic gradient flow

Write $z(u) = x(u) + \mathrm{i}y(u)$. The holomorphic gradient flow associated with the weight $\exp(-\kappa W)$ is

$$\frac{\mathrm{d}z}{\mathrm{d}u} = \pm\, \overline{\kappa\, W'(z)}. \tag{5}$$

The choice of sign corresponds to increasing or decreasing $\mathrm{Re}(\kappa W)$ along the flow.

A one–line computation explains why this flow is natural. Along any solution of (5),

$$\frac{\mathrm{d}}{\mathrm{d}u}\big(\kappa W(z(u))\big) = \kappa W'(z(u))\, \frac{\mathrm{d}z}{\mathrm{d}u} = \pm\, \kappa W'(z)\, \overline{\kappa W'(z)} = \pm\, |\kappa W'(z)|^2 \in \mathbb{R}_{\geq 0}. \tag{6}$$

Consequently,

$$\frac{\mathrm{d}}{\mathrm{d}u}\, \mathrm{Im}(\kappa W(z(u))) = 0, \qquad \frac{\mathrm{d}}{\mathrm{d}u}\, \mathrm{Re}(\kappa W(z(u))) = \pm |\kappa W'(z(u))|^2. \tag{7}$$

Thus each flow line is a constant–phase curve (constant $\mathrm{Im}(\kappa W)$), and $\mathrm{Re}(\kappa W)$ varies monotonically along it.

4 Thimbles and dual thimbles (one variable)

Fix the *upward* sign convention in (5),

$$\frac{\mathrm{d}z}{\mathrm{d}u} = +\kappa\overline{W'(z)}. \tag{8}$$

Then:

- the *thimble* $\mathcal{J}_\sigma$ is the unstable manifold of (8) at z_σ, i.e. the set of points whose backward flow approaches the saddle:

$$\mathcal{J}_\sigma = \{z(0) : z(u) \text{ solves (8) and } \lim_{u\to-\infty} z(u) = z_\sigma\}; \tag{9}$$

- the *dual thimble* $\mathcal{K}_\sigma$ is the stable manifold of (8) at z_σ, i.e. points whose forward flow approaches the saddle:

$$\mathcal{K}_\sigma = \{z(0) : z(u) \text{ solves (8) and } \lim_{u\to+\infty} z(u) = z_\sigma\}. \tag{10}$$

In one complex dimension, $\mathcal{J}_\sigma$ and $\mathcal{K}_\sigma$ are real one–dimensional curves through z_σ. In the full Picard–Lefschetz story, intersection numbers between Γ and $\mathcal{K}_\sigma$ determine which thimbles contribute to the original integral.

5 Local direction and the two "arms"

Because the saddle is a fixed point of the flow, one cannot initialise the ODE exactly at z_σ; the numerical solver would simply remain there. Instead, we start a small distance away, in the correct tangent directions.

Let $\lambda = \kappa W''(z_\sigma)$. Near z_σ we have

$$\kappa W(z) = \kappa W(z_\sigma) + \tfrac{1}{2}\lambda(z - z_\sigma)^2 + \cdots . \tag{11}$$

Imposing the constant–phase condition $\mathrm{Im}(\kappa W(z)) = \mathrm{Im}(\kappa W(z_\sigma))$ at quadratic order gives

$$\mathrm{Im}\big(\lambda(z - z_\sigma)^2\big) = 0, \qquad \text{i.e.} \qquad \lambda(z - z_\sigma)^2 \in \mathbb{R}. \tag{12}$$

Writing $z - z_\sigma = r\,\mathrm{e}^{\mathrm{i}\theta}$ and $\lambda = |\lambda|\mathrm{e}^{\mathrm{i}\phi}$, this becomes $\sin(\phi + 2\theta) = 0$, hence

$$\theta = -\tfrac{\phi}{2} + \frac{k\pi}{2}, \qquad k \in \mathbb{Z}. \tag{13}$$

A convenient unit vector in the thimble direction is therefore

$$v = \exp\!\big(-\tfrac{\mathrm{i}}{2}\,\mathrm{Arg}(\lambda)\big). \tag{14}$$

The dual direction is rotated by $\pi/2$. In the implementation this is encoded by an additional phase shift.

Finally, each manifold has two local branches through the saddle, so we take two opposite initial points

$$z_{0,\pm} = z_\sigma \pm \varepsilon\, v, \tag{15}$$

and integrate the flow from both to draw the full curve.

6 Speed normalisation for high–degree potentials

For high–degree polynomials, the raw flow speed can grow very rapidly because $|W'(z)|$ grows like a high power of $|z|$. For plotting, it is often useful to bound the speed while keeping the same geometric trajectories.

If $f(z)$ is a vector field and $g(z) > 0$ is any positive real function, then the ODEs

$$\frac{\mathrm{d}z}{\mathrm{d}u} = f(z), \qquad \frac{\mathrm{d}z}{\mathrm{d}s} = g(z)\, f(z) \tag{16}$$

have the *same integral curves* in the complex plane (only the parametrisation changes). This is the mechanism behind the "speed–normalised" option in the code:

$$\frac{\mathrm{d}z}{\mathrm{d}u} = \pm \frac{\overline{W'(z)}}{1 + |\overline{W'(z)}|}. \tag{17}$$

The denominator is positive and bounded away from zero, so the geometry is unchanged, but the numerical solver is far less likely to run away.

7 Mapping to the repository code

With $\kappa = 1$, the code implements the upward flow

$$\frac{\mathrm{d}z}{\mathrm{d}u} = \pm\overline{W'(z)} \tag{18}$$

by evolving $x(u), y(u)$ with

$$x'(u) = \pm\,\mathrm{Re}\,\overline{W'(x + \mathrm{i}y)}, \qquad y'(u) = \pm\,\mathrm{Im}\,\overline{W'(x + \mathrm{i}y)}. \tag{19}$$

The local direction v is chosen using (14), and the two initial points are $z_{0,\pm} = z_\sigma \pm \varepsilon v$. The plotting window `box` is used as a stop condition (we halt integration once the curve leaves the visible region).

Practical note. For a general complex phase of κ, replace $W'(z)$ by $\kappa W'(z)$ everywhere in the flow and in the definition $\lambda = \kappa W''(z_\sigma)$. This rotates the thimble/dual directions exactly as expected.