A Hamilton-Jacobi-based Proximal Operator

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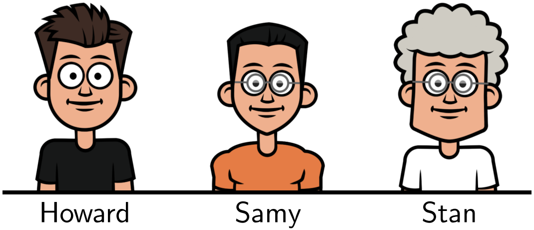
Scope: Optimization with proximals when we do not have exact formulas

Problem: For a continuous and weakly convex function $f : \mathbb{R}^n \to \mathbb{R}$ and $t > 0$, estimate

$$\mathrm{prox}_{tf}(x) = \underset{y}{\mathrm{argmin}}\, f(y) + \frac{1}{2t}\|y - x\|^2,$$

only *using evaluations of f.*



Key Ingredients

- Moreau Envelope
- Hamilton-Jacobi PDEs
- Cole-Hopf Transformation
- Monte Carlo Sampling

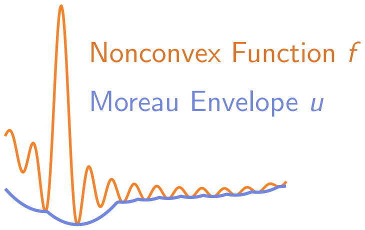
Given a function $f : \mathbb{R}^n \to \mathbb{R}$ and time $t > 0$, the Moreau envelope u is

$$u(x,t) \triangleq \min_y f(y) + \frac{1}{2t}\|y - x\|^2.$$

When it exists, the gradient is

$$\nabla u(x,t) = \frac{1}{t}(x - \mathrm{prox}_{tf}(x))$$

$$\implies \quad \mathrm{prox}_{tf}(x) = x - t\nabla u(x,t).$$



Hamilton-Jacobi PDEs

The envelope u solves

$$\begin{cases} u_t + \frac{1}{2}\|\nabla u\|^2 = 0 & \text{in } \mathbb{R}^n \times (0, \infty) \\ u = f & \text{on } \mathbb{R}^n \times \{t = 0\}. \end{cases}$$

For small $\delta > 0$, we can approximate u using the viscous PDE

$$\begin{cases} u_t^\delta + \frac{1}{2}\|\nabla u^\delta\|^2 = \frac{\delta}{2}\Delta u^\delta & \text{in } \mathbb{R}^n \times (0, \infty) \\ u^\delta = f & \text{on } \mathbb{R}^n \times \{t = 0\}. \end{cases}$$

Cole-Hopf Transformation

Using an idea from Cole and Hopf, we use the change of variables

$$v^\delta = \exp(-u^\delta/\delta),$$

for which v^δ solves the heat equation

$$\begin{cases} v_t^\delta - \frac{\delta}{2}\Delta v^\delta = 0 & \text{in } \mathbb{R}^n \times (0,\infty) \\ v^\delta = \exp(-f/\delta) & \text{on } \mathbb{R}^n \times \{t=0\}. \end{cases}$$

Monte Carlo Sampling

For a heat kernel $\Phi_{\delta t}$, the heat equation solution v^δ can be written as

$$v^\delta(x,t) = \Big(\Phi_{\delta t} * \exp(-f/\delta)\Big)(x) = \mathbb{E}_{y\sim\mathcal{N}(x,\delta t)}\left[\exp\left(-f(y)/\delta\right)\right],$$

with the expectation over a normal distribution with variance δt and mean x. Then

$$\nabla v^\delta(x,t) = -\frac{1}{\delta t}\cdot\mathbb{E}_{y\sim\mathcal{N}(x,\delta t)}\left[(x-y)\exp\left(-f(y)/\delta\right)\right],$$

which implies

$$\nabla u^\delta(x,t) = \frac{1}{t}\cdot\left(x - \frac{\mathbb{E}_{y\sim\mathcal{N}(x,\delta t)}\left[y\cdot\exp\left(-f(y)/\delta\right)\right]}{\mathbb{E}_{y\sim\mathcal{N}(x,\delta t)}\left[\exp\left(-f(y)/\delta\right)\right]}\right).$$

Using the gradient of the Moreau envelope and our approximation,

$$\begin{aligned} \mathrm{prox}_{tf}(x) &= x - t\nabla u(x,t) \\ &\approx x - t\nabla u^{\delta}(x,t) \\ &= \frac{\mathbb{E}_{y\sim\mathcal{N}(x,\delta t)}\left[y \cdot \exp\left(-f(y)/\delta\right)\right]}{\mathbb{E}_{y\sim\mathcal{N}(x,\delta t)}\left[\exp\left(-f(y)/\delta\right)\right]}. \end{aligned}$$

(Informal) Theorem: If t is sufficiently small and $u(x,t) \geq 0$, then

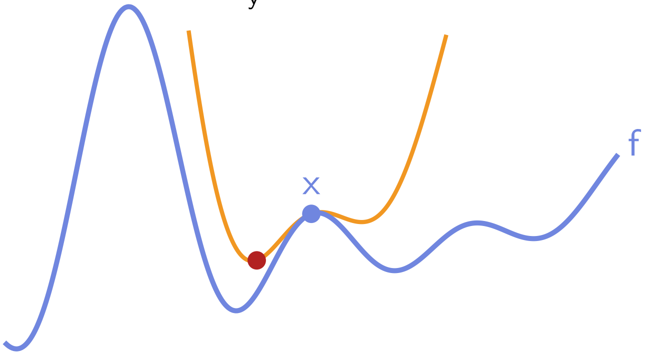
$$\lim_{\delta\to 0^+} \frac{\mathbb{E}_{y\sim\mathcal{N}(x,\delta t)}\left[y \cdot \exp\left(-f(y)/\delta\right)\right]}{\mathbb{E}_{y\sim\mathcal{N}(x,\delta t)}\left[\exp\left(-f(y)/\delta\right)\right]} = \mathrm{prox}_{tf}(x).$$

Algorithm 1 HJ-Prox – Approximation of Proximal Operator

```
HJ-Prox(x, t; f, δ, N, α, ε) :
    for i ∈ [N]:
        Sample y^i ~ 𝒩(x, δt/α)
        z_i ← f(y^i)
    if exp(−αz_i/δ) ≤ ε for large proportion of samples:
        return HJ-Prox(x, t; f, δ, N, α/2, ε)
    prox ← softmax(−αz/δ)^⊤ [y^1 ··· y^N]
    return prox
```

Proximal Computation Example

$$\text{prox}_{tf}(x) = \underset{y}{\text{argmin}}\; f(y) + \frac{1}{2t}\|y - x\|^2$$



Proximal Computation Example

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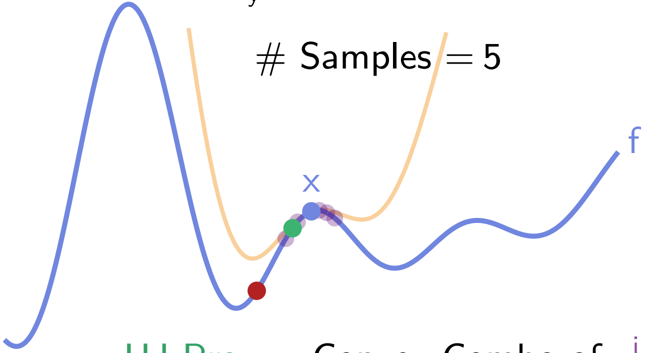

HJ-Prox = Convex Combo of y^i

y^i weight = $\mathrm{softmax}(-f(y)/\delta)$

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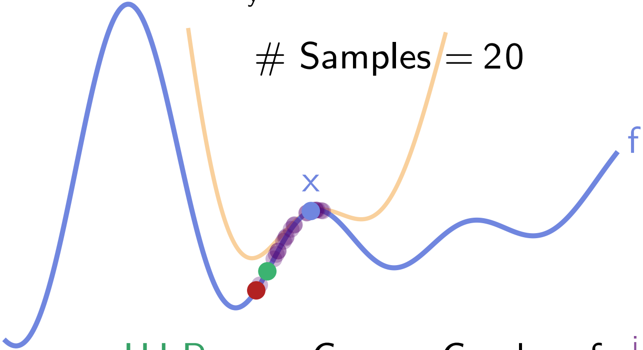

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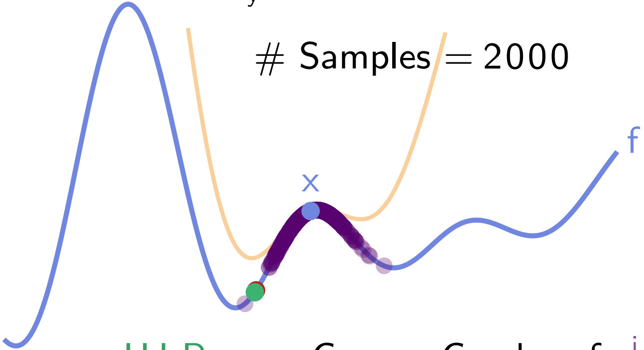
$\#$ Samples $= 2000$



HJ-Prox = Convex Combo of y^i

y^i weight $= \text{softmax}(-f(y)/\delta)$

Consider a constrained minimization problem where objective values f can only be accessed via a noisy oracle $\mathcal{O}$, *i.e.*

$$\min_{x \in \mathbb{R}^{1000}} \mathbb{E}[\mathcal{O}(x)] \quad \text{s.t.} \quad Ax = b,$$

where the expectation is over the noise. We assume A is large and under-determined. Using HJ-Prox, we solve with the linearized method of multipliers via updates

$$x^{k+1} = \text{prox}_{t\mathcal{O}}\left(x^k - tA^\top(u^k + \lambda(Ax^k - b))\right)$$

$$u^{k+1} = u^k + \lambda(Ax^{k+1} - b).$$

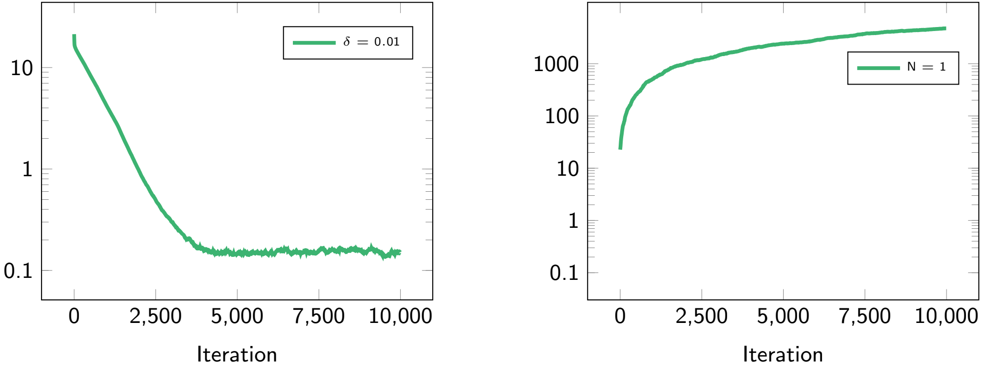


Figure 1: Plots of linearized method of multipliers using HJ-Prox estimates for each proximal. Gradient descent on constraint violation is provided for reference and does not use the oracle $\mathcal{O}$.

Relative Error Plots with HJ-Prox

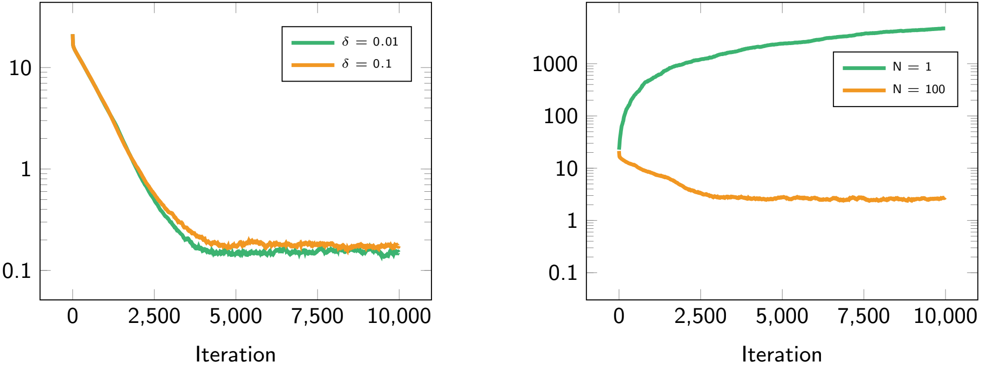


Figure 2: Plots of linearized method of multipliers using HJ-Prox estimates for each proximal. Gradient descent on constraint violation is provided for reference and does not use the oracle $\mathcal{O}$.

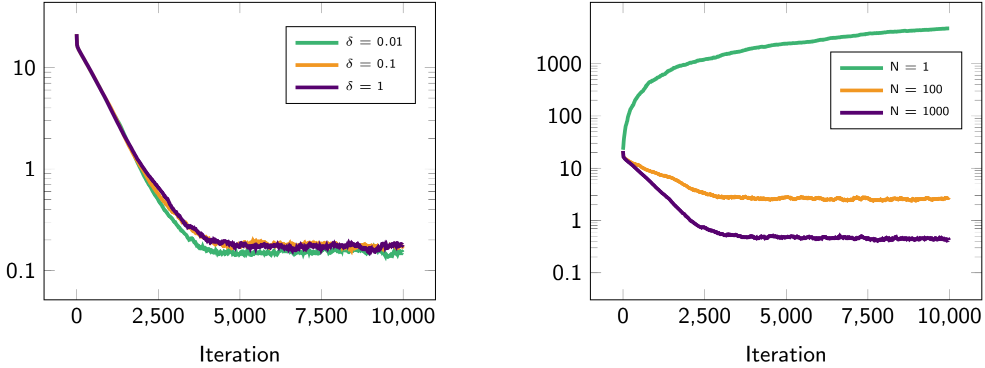


Figure 3: Plots of linearized method of multipliers using HJ-Prox estimates for each proximal. Gradient descent on constraint violation is provided for reference and does not use the oracle $\mathcal{O}$.

Relative Error Plots with HJ-Prox

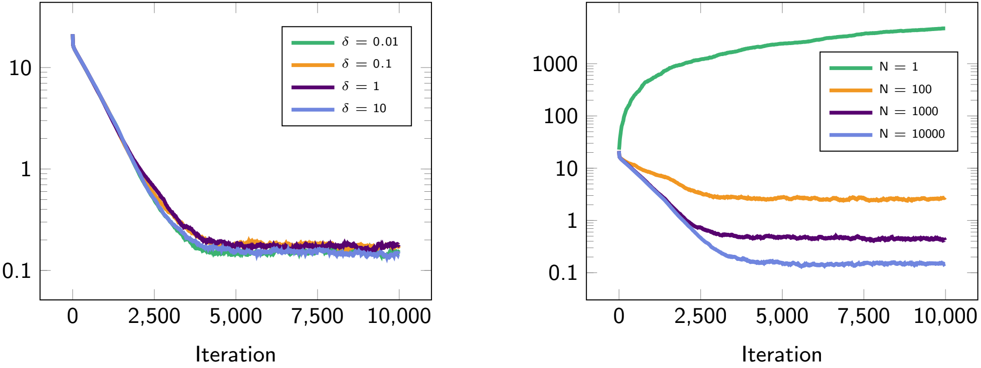


Figure 4: Plots of linearized method of multipliers using HJ-Prox estimates for each proximal. Gradient descent on constraint violation is provided for reference and does not use the oracle $\mathcal{O}$.

Relative Error Plots with HJ-Prox

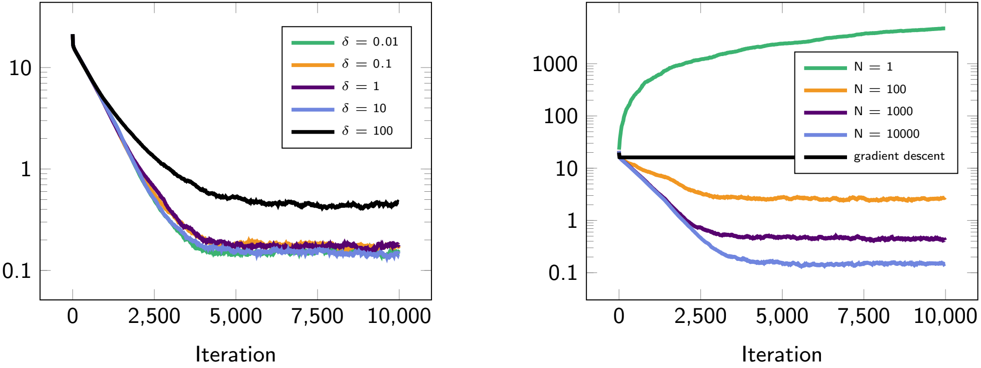


Figure 5: Plots of linearized method of multipliers using HJ-Prox estimates for each proximal. Gradient descent on constraint violation is provided for reference and does not use the oracle $\mathcal{O}$.

Summary

- HJ-Prox gives a simple zeroth-order approximation to proximals
- The parameter δ smooths approximations (potentially helpful for denoising)
- HJ-Prox can be embedded inside optimization algorithms

  (*e.g.* proximal gradient, Douglas Rachford, ADMM, PDHG)

Preprint: arxiv.org/abs/2211.12997

Reprint: https://www.pnas.org/doi/10.1073/pnas.2220469120