Coin Sampling: Gradient-Based Bayesian Inference without Learning Rates

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Outline

Background

The Problem

Sampling Problem: Generate samples from a target probability distribution π on $\mathbb{R}^d$, given some information about π.

Two common scenarios:

(i) The target admits a density $\pi(x)$ w.r.t. the Lebesgue measure, which is known up to some intractable normalising constant. That is,

$$\pi(x) := \frac{e^{-U(x)}}{Z},$$

where the potential $U : \mathbb{R}^d \to \mathbb{R}$ is known, and the constant $Z = \int_{\mathbb{R}^d} e^{-U(x)} \mathrm{d}x$ is unknown.

(ii) We have access to samples from the target π: $x_1, \ldots, x_n \sim \pi$.

We will focus on the first setting.

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Motivation: Bayesian Inference

Bayesian Inference: learn the posterior distribution of a parameter $x \in \mathbb{R}^d$, given some observed data $\mathcal{D}$.

- Let $\mathcal{D} = (w_i, y_i)_{i=1}^p$ be a dataset of i.i.d. examples, with features w_i and labels y_i.
- Assume some underlying model for the data, parameterised by $x \in \mathbb{R}^d$, e.g.,

$$p(\mathcal{D}|x) = \prod_{i=1}^p p(y_i|w_i, x) \propto \exp\left(-\tfrac{1}{2}\sum_{i=1}^p ||y_i - f(w_i, x)||^2\right).$$

- Assume also some prior distribution $x \sim p_0$ for the parameter $x \in \mathbb{R}^d$, e.g.,

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- By Bayes' rule, the **posterior distribution** is then given by

$$p(x|\mathcal{D}) = \frac{p(\mathcal{D}|x)p_0(x)}{Z}, \quad Z = \int_{\mathbb{R}^d} p(\mathcal{D}|x)p_0(x)\mathrm{d}x.$$

- In particular, writing $\pi := p(\cdot|\mathcal{D})$ for the posterior over the parameter $x \in \mathbb{R}^d$, we have

$$\pi(x) = \frac{e^{-U(x)}}{Z}, \quad U(x) = \frac{1}{2}\sum_{i=1}^{p} ||y_i - f(w_i, x)||^2 + \frac{||x||^2}{2}.$$

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Sampling as Optimisation

Let's assume that $\pi \in \mathcal{P}_2(\mathbb{R}^d) := \{\mu : \int_{\mathbb{R}^d} ||x||^2 \mu(\mathrm{d}x) < \infty\}$.

We can then recast the sampling problem as an **optimisation problem**:

$$\pi = \underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\min}\ \mathcal{F}(\mu),$$

where $\mathcal{F} : \mathcal{P}(\mathbb{R}^d) \to \mathbb{R}$ is a **dissimilarity functional** which is uniquely minimised at π.

A general strategy for solving this problem is to simulate a **time-discretisation** of the **gradient flow** of $\mathcal{F}$ over $\mathcal{P}_2(\mathbb{R}^d)$.

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This framework has been fruitful in the design and analysis of many existing sampling algorithms. For example:

- **Langevin Monte Carlo** (LMC): forward-flow discretisation of the gradient flow of the KL divergence with respect to the quadratic Wasserstein metric [Wib18, DMM19].
- **Stein Variational Gradient Descent** (SVGD): explicit Euler discretisation of the gradient flow of the KL divergence with respect to a kernelised Wasserstein metric [LW16, DNS23].
- Lots of other examples, e.g., **kernel Stein discrepancy descent** [KPCAF+21], **Laplacian adjusted Wasserstein gradient descent** [CLL+20], etc.

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Learning Rates

One feature common to all of these approaches is the need to specify an appropriate **learning rate** or **step size** γ.

- It should be **sufficiently small** to ensure **convergence to the target measure**, or a close approximation thereof.
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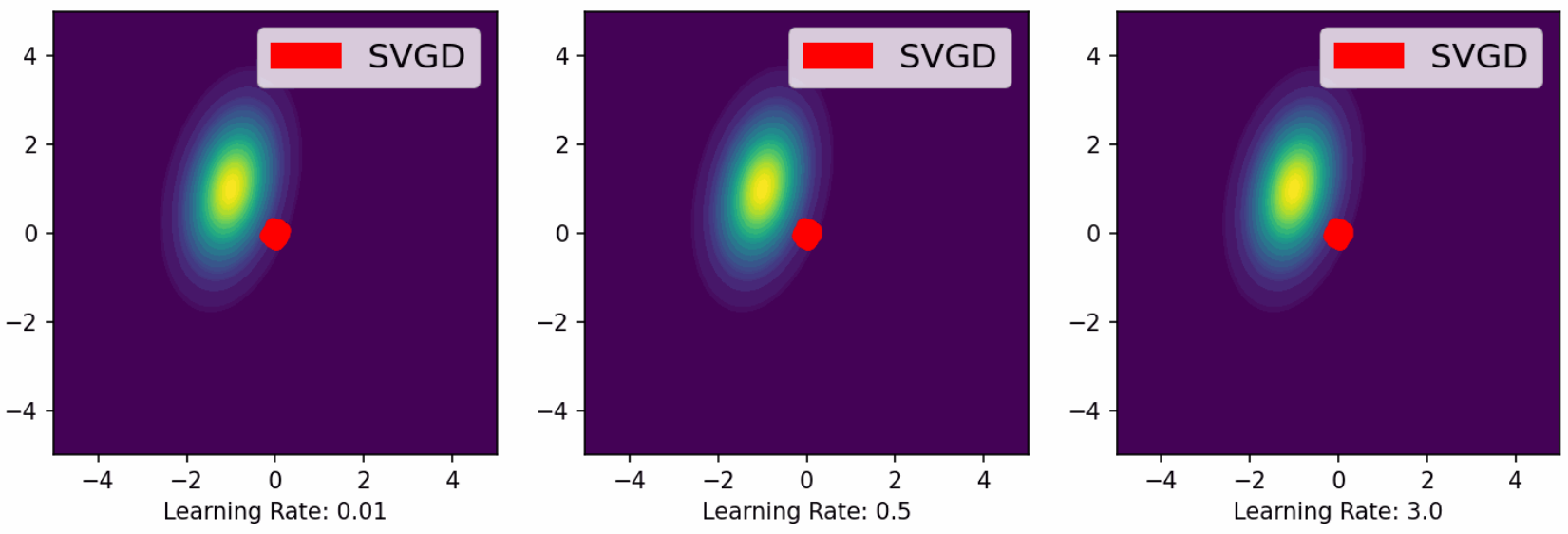

Learning Rates

In theory, existing **non-asymptotic convergence rates** for LMC [Dal17, DM17, DM19] and SVGD [KSA$^+$20, SSP22, SR22] allow us to derive **optimal learning rates** for these algorithms.

- In practice, the optimal learning rate is a **function of the unknown target measure**, and so it can't actually be computed.

No More Learning Rates?

There are various existing approaches to selecting learning rates, none of which are entirely satisfactory:

- Run the algorithm of choice for **multiple learning rates**, and select the learning rate which **minimises an appropriately chosen metric**.
- Use ideas from the optimisation literature to design effective **step size schedules** [CCG+16, LCCC16, KSL22].

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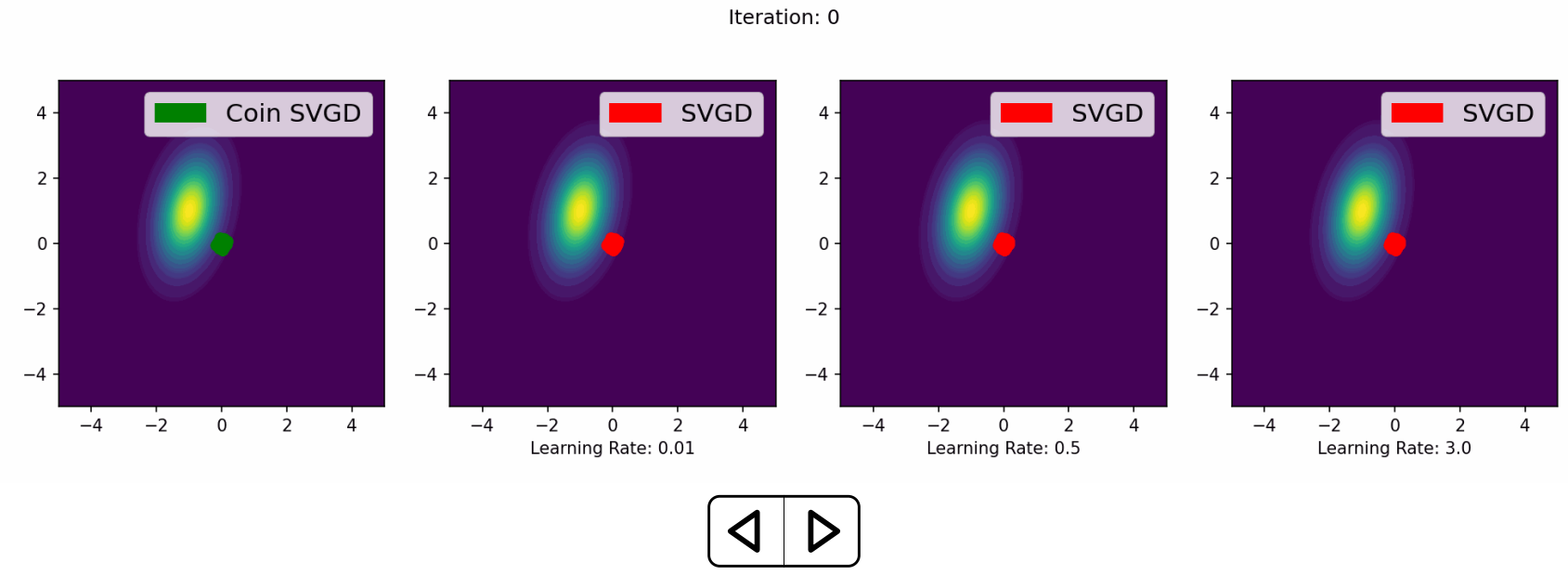

Optimisation in Euclidean Space

Preliminaries

Suppose that f is **convex**. We say that $g \in \mathbb{R}^d$ is a **subgradient** of f at x, and write $g \in \partial f(x)$ if, for any $z \in \mathbb{R}^d$,

$$f(z) - f(x) \geq \langle g, z - x \rangle$$

If f is **differentiable** at x, then the **differential set** $\partial f(x)$ contains only $\nabla f(x)$, the **gradient** of f at x.

We define the **convex conjugate** of f as the function $f^* : \mathbb{R}^d \to \mathbb{R}$ such that

$$f^*(u) = \sup_{x \in \mathcal{X}} [\langle u, x \rangle - f(x)]$$

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Gradient Flows in Euclidean Space

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex. Suppose we are interested in the following optimisation problem

$$x^* = \arg\min_{x \in \mathcal{X}} f(x).$$

We can solve this problem using the **gradient flow** of f, defined as the solution $x : [0, \infty) \to \mathbb{R}^d$ of the **differential inclusion**

$$\dot{x}_t \in -\partial f(x_t).$$

This inclusion admits a unique, absolutely continuous solution for almost all $t \geq 0$ [Bré73]. Moreover, the **function** $t \mapsto f(x_t)$ **is decreasing**, with $\lim_{t\to\infty} f(x_t) = \inf_{x\in\mathbb{R}^d} f(x)$ [PS10].

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Gradient Descent in Euclidean Space

In practice, it is necessary to use a time-discretisation of this gradient flow.

- The **backward Euler discretisation**, which results in the proximal point algorithm [Gül91, De 93]

$$x_{t+1} \in \arg\min_{x \in \mathbb{R}^d} \left[f(x) + \frac{1}{2\gamma} ||x - x_t||^2 \right].$$

- The **forward Euler discretisation**, which results in the subgradient descent algorithm [Sho85]

$$x_{t+1} = x_t - \gamma g_t \ , \quad g_t \in \partial f(x_t).$$

The properties of these algorithms depend, of course, on the choice of learning rate $\gamma > 0$.

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Optimal Learning Rates

Given an L-Lipschitz function, one can show that the iterates of the subgradient descent algorithm satisfy [Zin03]

$$f\left(\frac{1}{T}\sum_{t=1}^{T} x_t\right) - f(x^*) \leq \frac{1}{T}\left[\frac{||x_1 - x^*||^2}{2\gamma} + \frac{L^2 T\gamma}{2}\right].$$

This implies that the optimal learning rate is $\gamma_{\text{opt}} = \frac{||x_1 - x^*||}{L\sqrt{T}}$, which yields the optimal error bound

$$f(\bar{x}_T) - f(x^*) \leq \frac{L||x_1 - x^*||}{\sqrt{T}}.$$

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Consider a gambler who bets on the outcomes of a series of adversarial coin flips.

The gambler starts with an initial wealth $w_0 = \varepsilon > 0$. In the t^{th} round, the gambler **bets on the outcome of a coin flip** $c_t \in \{-1, 1\}$, where $+1$ denotes heads and -1 denotes tails.

We will encode the gambler's bets in the t^{th} round by $x_t \in \mathbb{R}$. In particular, $\operatorname{sign}(x_t) \in \{-1, 1\}$ will denote **whether the bet is on heads or tails**, and $|x_t| \in \mathbb{R}$ will denote the **size of the bet**.

Thus, in the t^{th} round, the gambler **wins** $|x_t c_t| = x_t c_t$ if $\operatorname{sign}(c_t) = \operatorname{sign}(x_t)$, and **loses** $|x_t c_t| = -x_t c_t$ otherwise.

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We will encode the gambler's bets in the t^{th} round by $x_t \in \mathbb{R}$. In particular, $\operatorname{sign}(x_t) \in \{-1, 1\}$ will denote **whether the bet is on heads or tails**, and $|x_t| \in \mathbb{R}$ will denote the **size of the bet**.

Thus, in the t^{th} round, the gambler **wins** $|x_t c_t| = x_t c_t$ if $\operatorname{sign}(c_t) = \operatorname{sign}(x_t)$, and **loses** $|x_t c_t| = -x_t c_t$ otherwise.

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Suppose that we write w_t for the wealth of the gambler at the end of the t^{th} round. Clearly, we then have that

$$w_t = \varepsilon + \sum_{i=1}^{t} c_i x_i.$$

We will impose the additional restriction that the gambler's bets satisfy $x_t = \beta_t w_{t-1}$, for some **betting fraction** $\beta_t \in [-1, 1]$. This is equivalent to the assumption that the gambler **cannot borrow any money**.

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How should we choose the betting fraction $\beta_t \in [-1, 1]$?

- If we **knew the probability of heads** p, then the optimal strategy is given by $\beta_t = \mathbb{E}[c_t] = 2p - 1$ [Kel56].
- If we **knew the future outcomes**, then the optimal **fixed fraction** is given by $\beta_t = T^{-1} \sum_{i=1}^{T} c_i$. This guarantees the wealth increases exponentially.
- If we **don't know the future outcomes**, then the **KT estimator** yields the betting strategy $\beta_t = t^{-1} \sum_{i=1}^{t-1} c_i$. This guarantees almost the same wealth that one would obtain knowing in advance the fraction of heads [KT81].

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Recalling our previous formula for the wealth, we see that this betting fraction yields the **sequence of bets**

$$x_t = \beta_t w_{t-1} = \frac{\sum_{i=1}^{t-1} c_i}{t} \left(\varepsilon + \sum_{i=1}^{t-1} c_i x_i \right).$$

One can show that this betting strategy guarantees that the wealth **grows exponentially** [OP16]

$$w_T \geq h\left(\sum_{t=1}^{T} c_t \right) := \frac{\varepsilon}{K\sqrt{T}} \exp\left(\frac{\left(\sum_{t=1}^{T} c_t \right)^2}{2T} \right).$$

In fact, this holds for **continuous outcomes** $c_t \in [-1, 1]$, and not just for $c_t \in \{-1, 1\}$.

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Coin Betting and Parameter Free Optimisation

What is the connection between **convex optimisation** and **coin betting**?

- Let $f : \mathbb{R} \to \mathbb{R}$ be a convex function, with $\nabla f(x) \in [-1, 1]$ for all $x \in \mathbb{R}$.
- Consider a betting game where, in the t^{th} round, we bet x_t on $c_t = -\nabla f(x_t) \in [-1, 1]$ according to our strategy from the last slide. Thus

$$x_t = -\frac{\sum_{i=1}^{t-1} \nabla f(x_i)}{t} \left(\varepsilon - \sum_{i=1}^{t-1} \nabla f(x_i) x_i \right).$$

- Remarkably, we can show that the **average of the bets converges to** $x^* = \arg\min_{x \in \mathbb{R}} f(x)$ at a rate governed by our betting strategy.

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The essential steps are as follows [OP16]

$$f\left(\frac{1}{T}\sum_{t=1}^{T} x_t\right) - f(x^*) \leq \frac{1}{T}\sum_{t=1}^{T}\left(f(x_t) - f(x^*)\right) \qquad \text{(Jensen's inequality)}$$

$$\leq \frac{1}{T}\left(\sum_{t=1}^{T} c_t x^* - \sum_{t=1}^{T} c_t x_t\right) \qquad \text{(convexity)}$$

$$\leq \frac{1}{T}\left(\left(\sum_{t=1}^{T} c_t\right) x^* - h\left(\sum_{t=1}^{T} c_t\right) + \varepsilon\right) \qquad \text{(bound on } w_T\text{)}$$

$$\leq \frac{1}{T}\left(\max_{v}\left[v x^* - h(v)\right] + \varepsilon\right) \qquad \text{(max over } v = \textstyle\sum_{t=1}^{T} c_t\text{)}$$

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Coin Betting and Parameter Free Optimisation

By substituting an appropriate bound for the convex conjugate h^*, this result yields the following **convergence rate** [OP16]

$$f(\bar{x}_T) - f(x^*) \leq K \frac{||x^*|| \sqrt{\log(1 + \frac{24T^2||x^*||^2}{\varepsilon^2}) + \varepsilon}}{\sqrt{T}}.$$

We can compare this with the convergence rate of subgradient descent with the **unknown optimal learning rate**:

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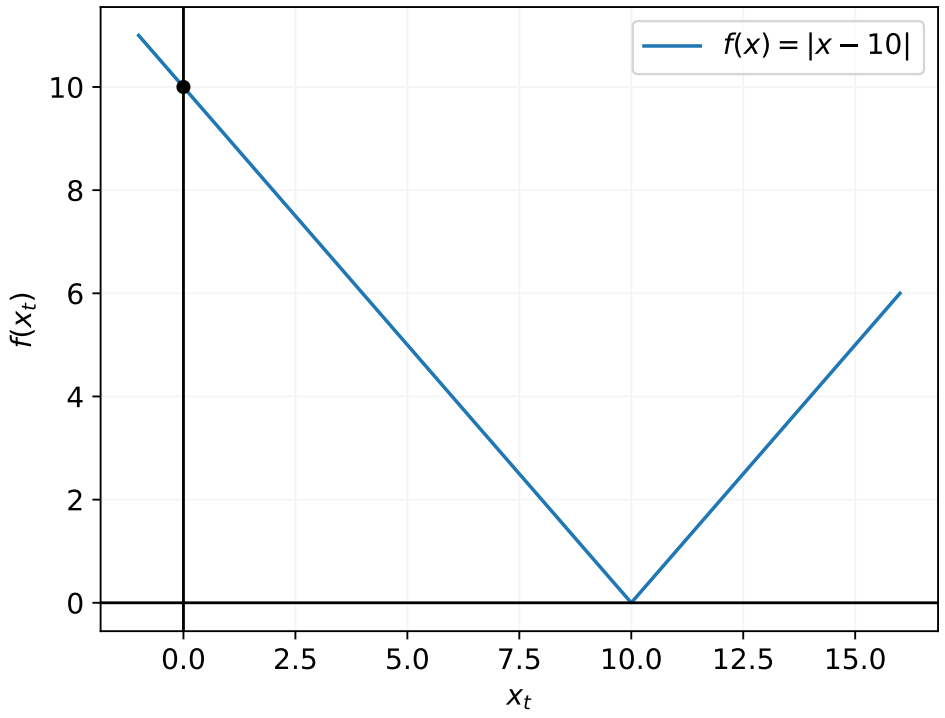


Initial wealth.

$w_0 = 1$

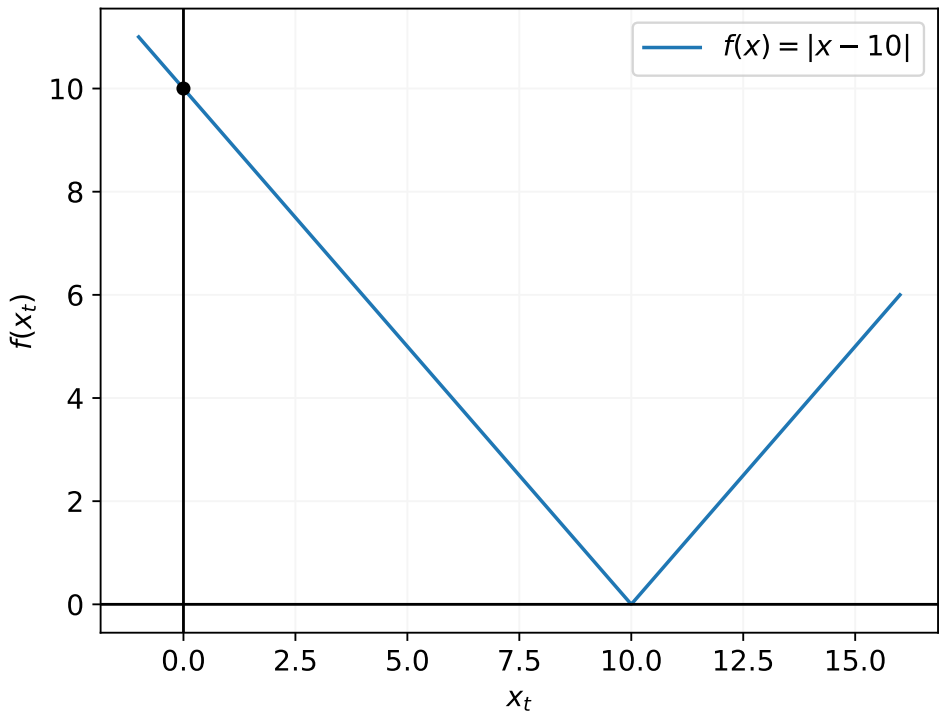
Betting fraction.

$$\beta_1 = \frac{\sum_{i=1}^{0} c_i}{1} = 0$$

Initial bet.

$x_1 = \beta_1 w_0 = 0.$

Coin Betting and Parameter Free Optimisation



Current wealth.

$w_0 = 1$

Current bet.

$x_1 = 0$

Outcome.

$c_1 = -\nabla f(x_1) = 1$

New wealth.

$w_1 = w_0 + c_1 x_1 = 1$

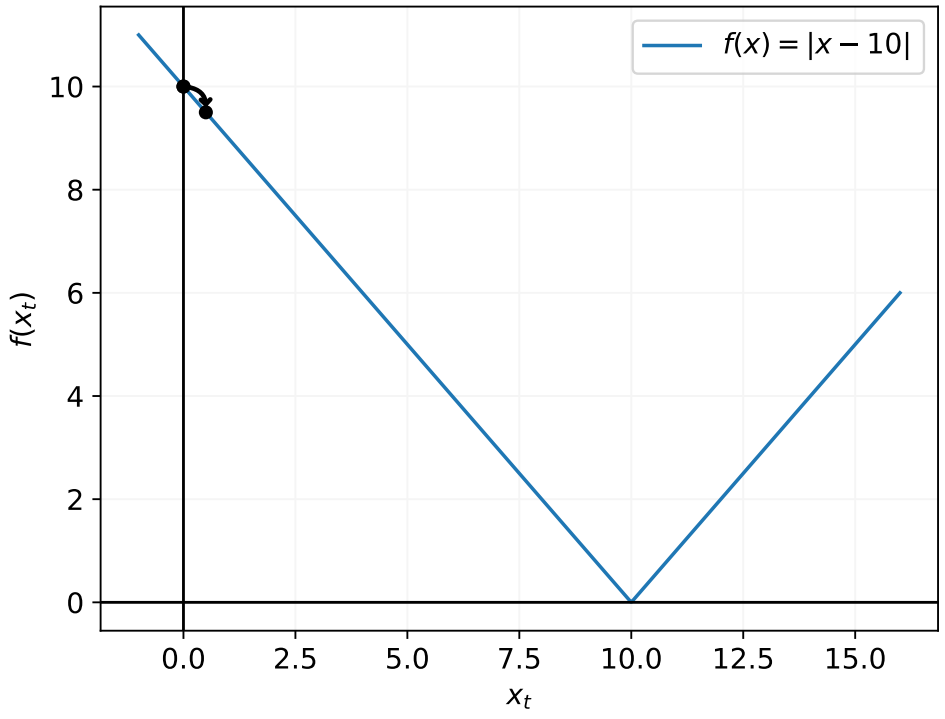
New betting fraction.

$$\beta_2 = \frac{\sum_{i=1}^{1} c_i}{2} = 0.5$$

New bet.

$x_2 = \beta_2 w_1 = 0.5.$

Coin Betting and Parameter Free Optimisation



Current wealth.

$w_0 = 1$

Current bet.

$x_1 = 0$

Outcome.

$c_1 = -\nabla f(x_1) = 1$

New wealth.

$w_1 = w_0 + c_1 x_1 = 1$

New betting fraction.

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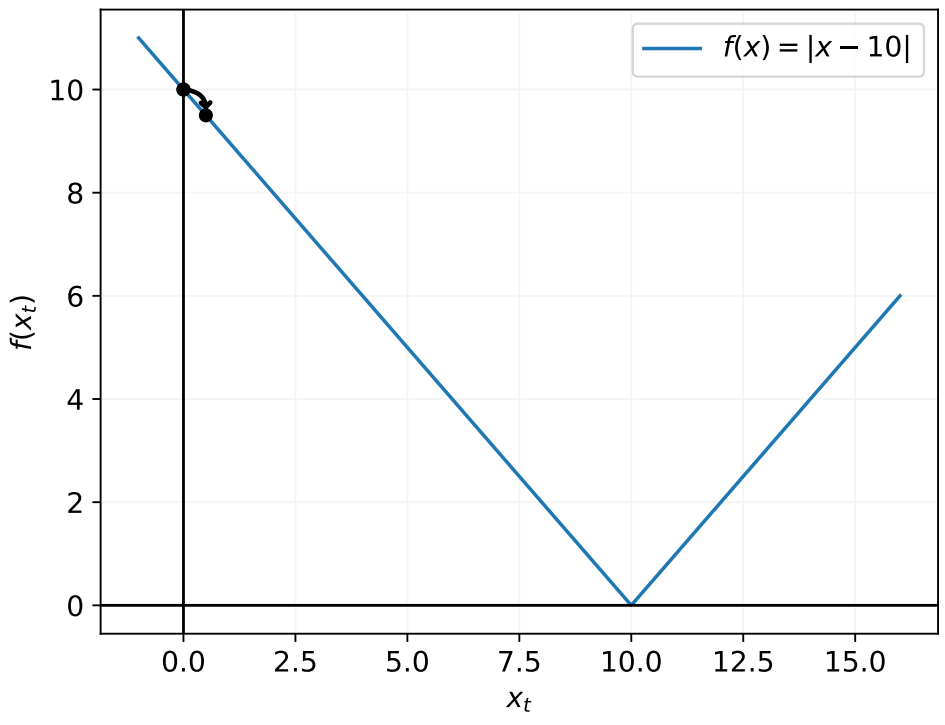
New bet.

$x_2 = \beta_2 w_1 = 0.5.$

Coin Betting and Parameter Free Optimisation



Current wealth.

$w_1 = 1$

Current bet.

$x_2 = 0.5$

Outcome.

$c_2 = -\nabla f(x_2) = 1$

New wealth.

$w_2 = w_1 + c_2 x_2 = 1.5$

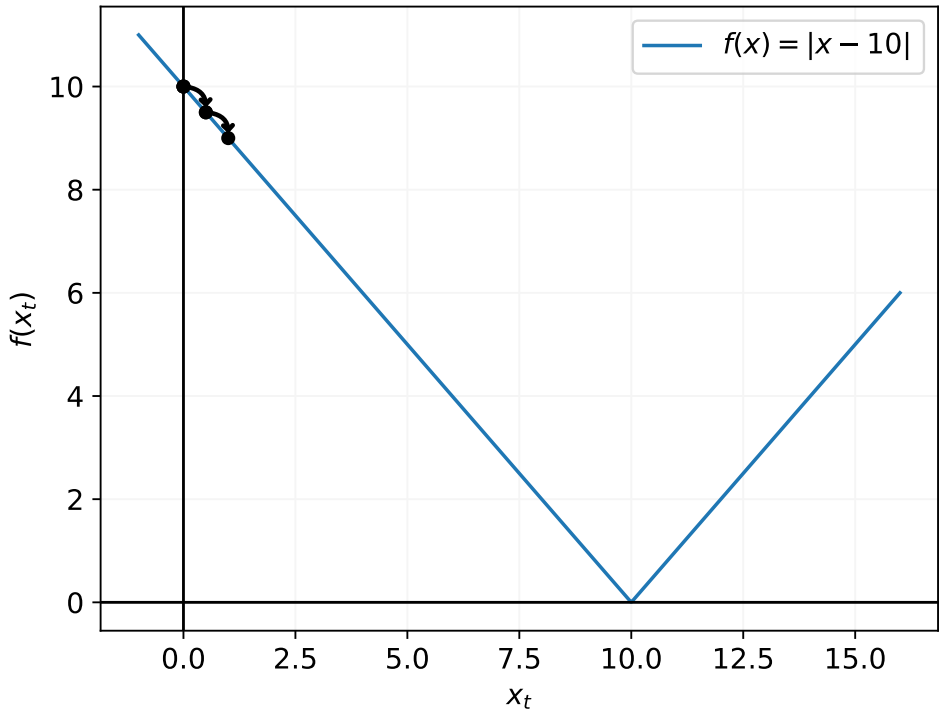
New betting fraction.

$$\beta_3 = \frac{\sum_{i=1}^{2} c_i}{3} = 0.\dot{6}$$

New bet.

$x_3 = \beta_3 w_2 = 1.$

Coin Betting and Parameter Free Optimisation



Current wealth.

$w_1 = 1$

Current bet.

$x_2 = 0.5$

Outcome.

$c_2 = -\nabla f(x_2) = 1$

New wealth.

$w_2 = w_1 + c_2 x_2 = 1.5$

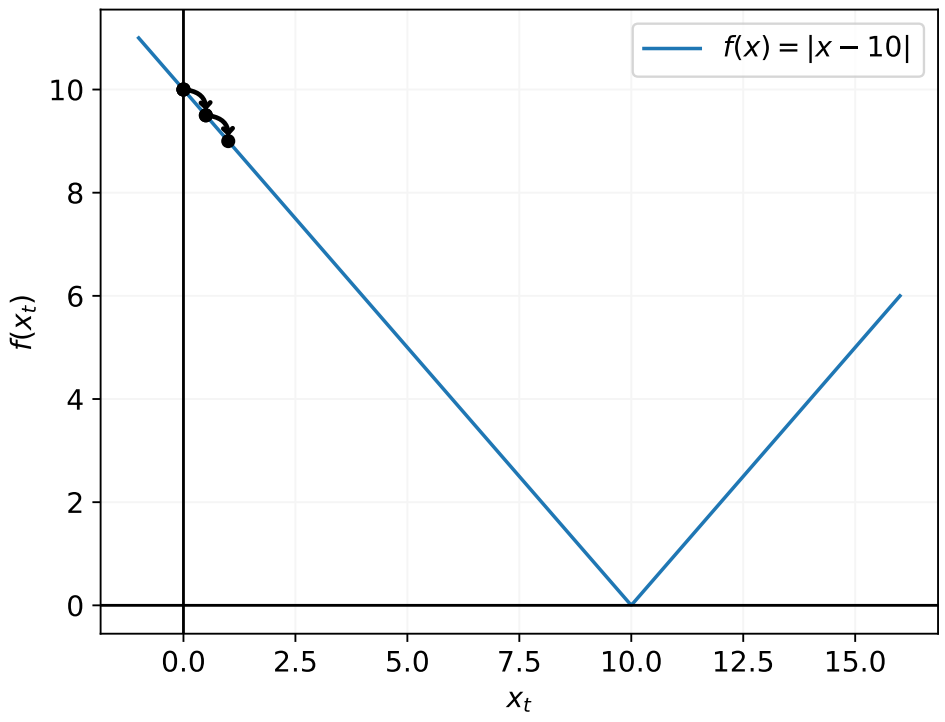
New betting fraction.

$$\beta_3 = \frac{\sum_{i=1}^{2} c_i}{3} = 0.\dot{6}$$

New bet.

$x_3 = \beta_3 w_2 = 1.$

Coin Betting and Parameter Free Optimisation



Current wealth.

$w_2 = 1.5$

Current bet.

$x_3 = 1$

Outcome.

$c_3 = -\nabla f(x_3) = 1$

New wealth.

$w_3 = w_2 + c_3 x_3 = 2.5$

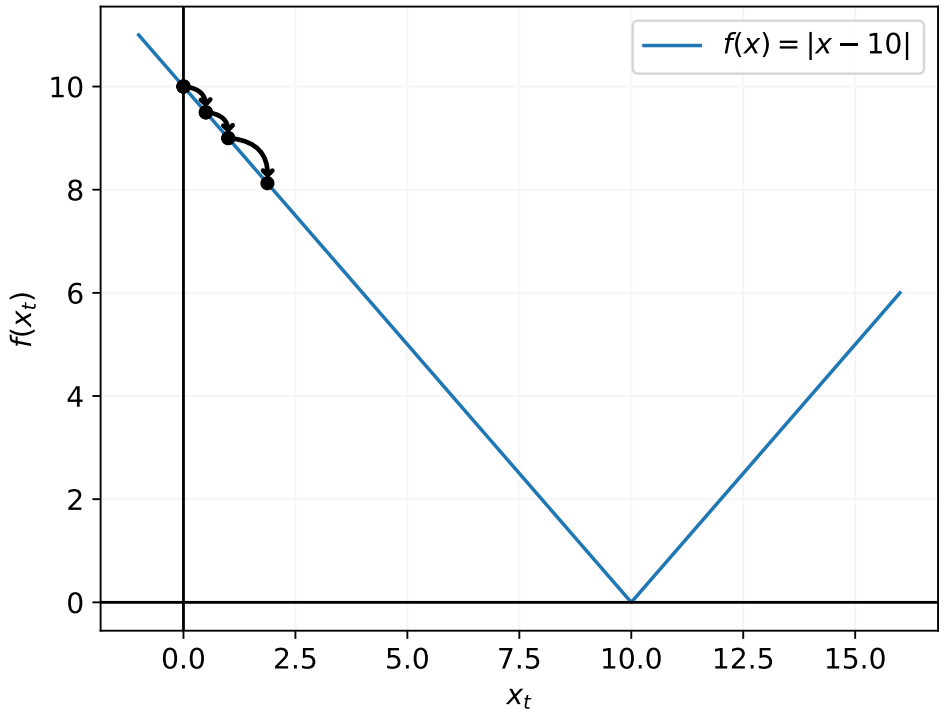
New betting fraction.

$$\beta_4 = \frac{\sum_{i=1}^{3} c_i}{4} = 0.75$$

New bet.

$x_4 = \beta_4 w_3 = 1.875$

Coin Betting and Parameter Free Optimisation



Current wealth.

$w_2 = 1.5$

Current bet.

$x_3 = 1$

Outcome.

$c_3 = -\nabla f(x_3) = 1$

New wealth.

$w_3 = w_2 + c_3 x_3 = 2.5$

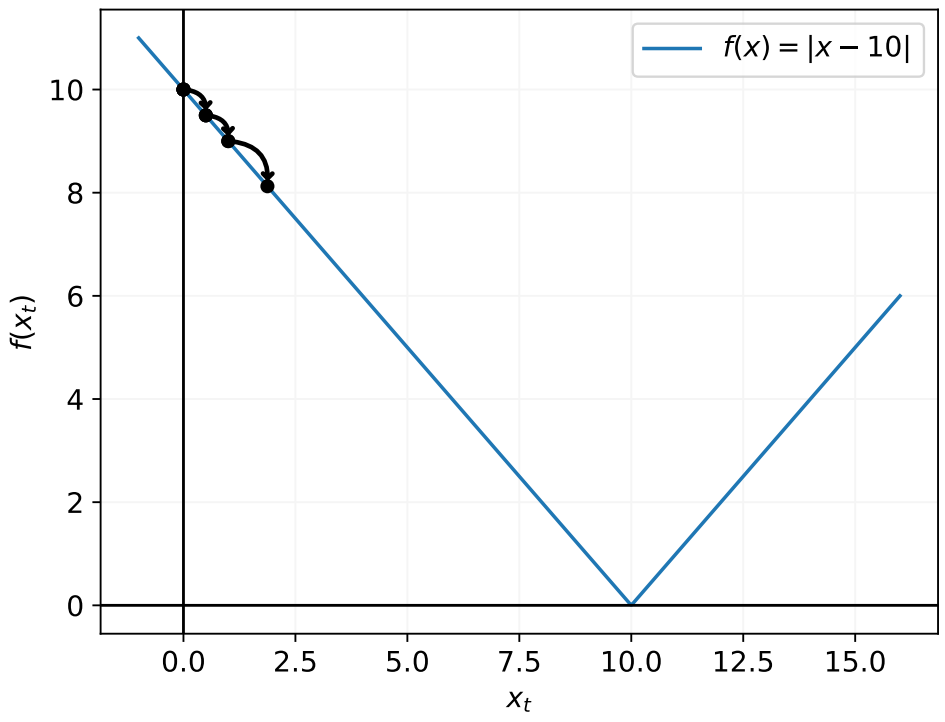
New betting fraction.

$$\beta_4 = \frac{\sum_{i=1}^{3} c_i}{4} = 0.75$$

New bet.

$x_4 = \beta_4 w_3 = 1.875$

Coin Betting and Parameter Free Optimisation



Current wealth.

$w_3 = 2.5$

Current bet.

$x_4 = 1.875$

Outcome.

$c_4 = -\nabla f(x_4) = 1$

New wealth.

$w_4 = w_3 + c_4 x_4 = 4.375$

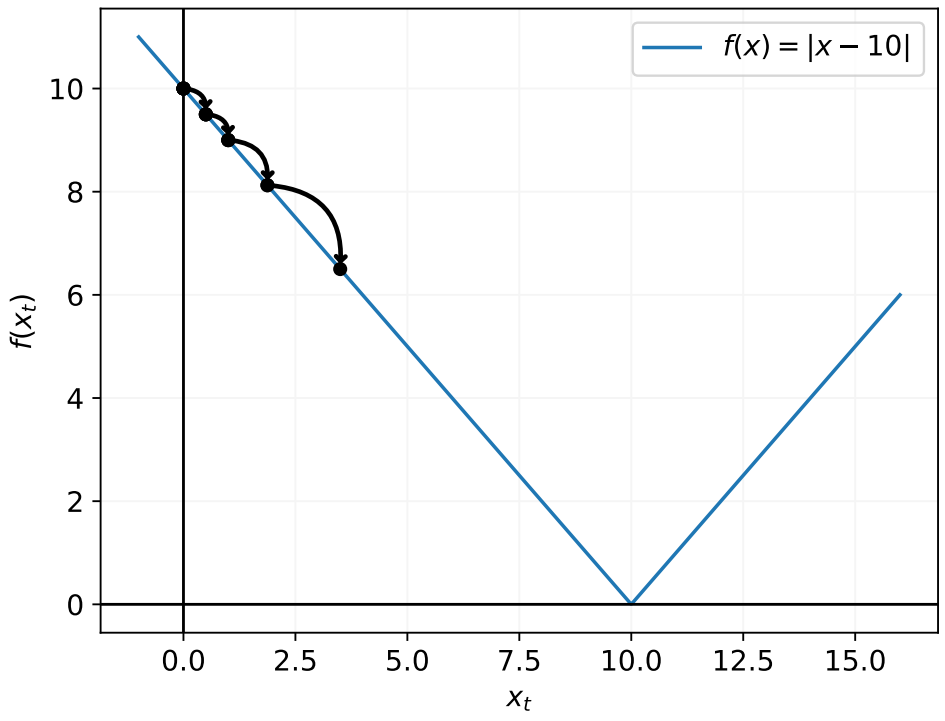
New betting fraction.

$$\beta_5 = \frac{\sum_{i=1}^{4} c_i}{5} = 0.8$$

New bet.

$x_5 = \beta_5 w_4 = 3.5$

Coin Betting and Parameter Free Optimisation



Current wealth.

$w_3 = 2.5$

Current bet.

$x_4 = 1.875$

Outcome.

$c_4 = -\nabla f(x_4) = 1$

New wealth.

$w_4 = w_3 + c_4 x_4 = 4.375$

New betting fraction.

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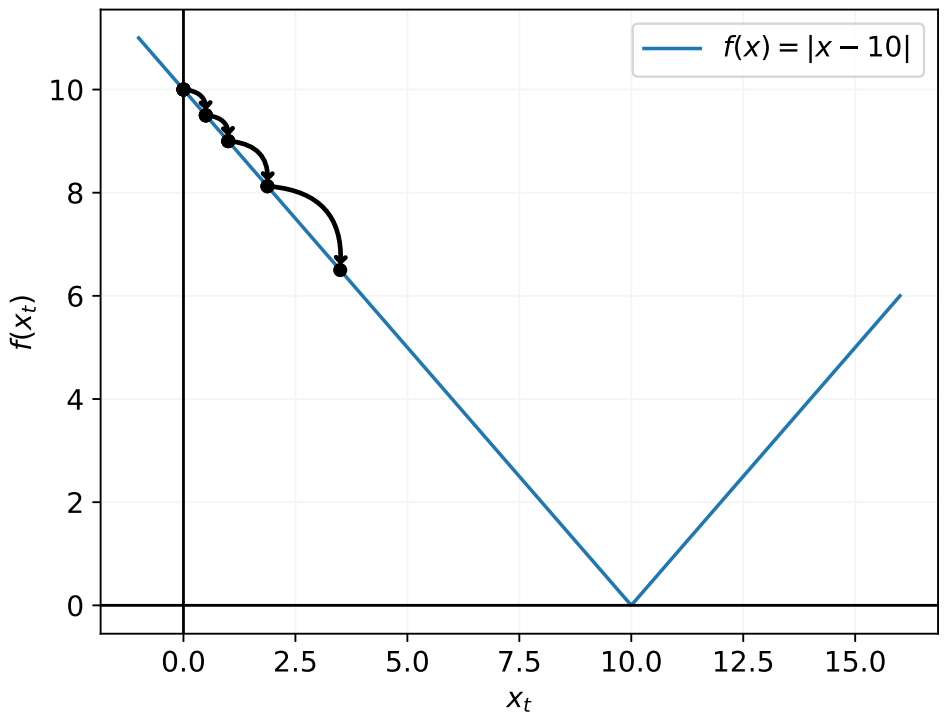
New bet.

$x_5 = \beta_5 w_4 = 3.5$

Coin Betting and Parameter Free Optimisation



Current wealth.

$w_4 = 4.375$

Current bet.

$x_5 = 3.5$

Outcome.

$c_5 = -\nabla f(x_5) = 1$

New wealth.

$w_5 = w_4 + c_5 x_5 = 7.875$

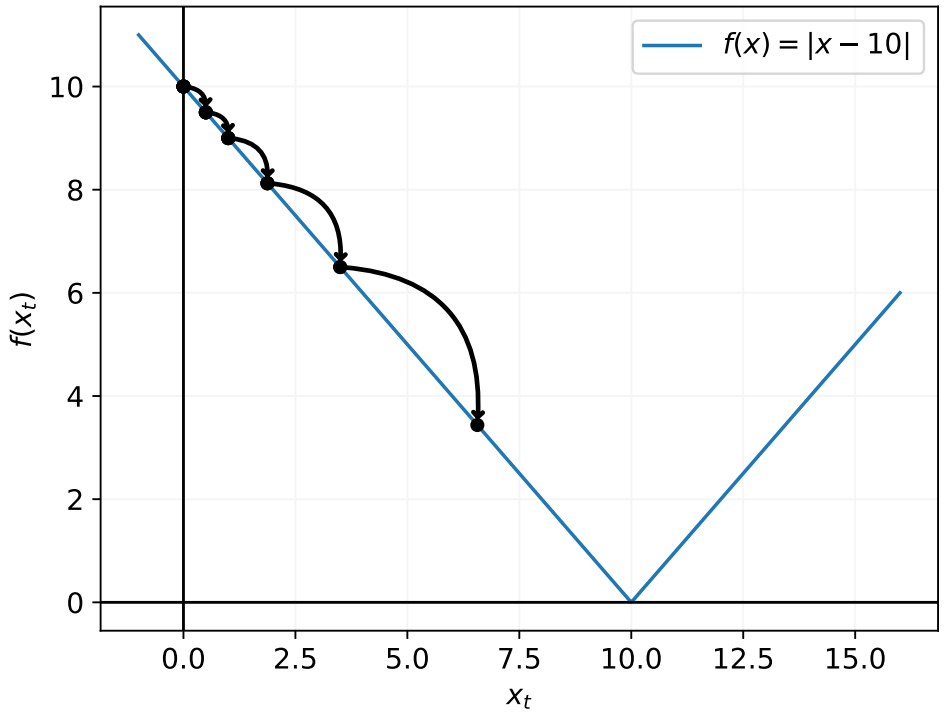
New betting fraction.

$$\beta_6 = \frac{\sum_{i=1}^{5} c_i}{6} = 0.8\dot{3}$$

New bet.

$x_6 = \beta_6 w_5 = 6.5625$

Coin Betting and Parameter Free Optimisation



Current wealth.

$w_4 = 4.375$

Current bet.

$x_5 = 3.5$

Outcome.

$c_5 = -\nabla f(x_5) = 1$

New wealth.

$w_5 = w_4 + c_5 x_5 = 7.875$

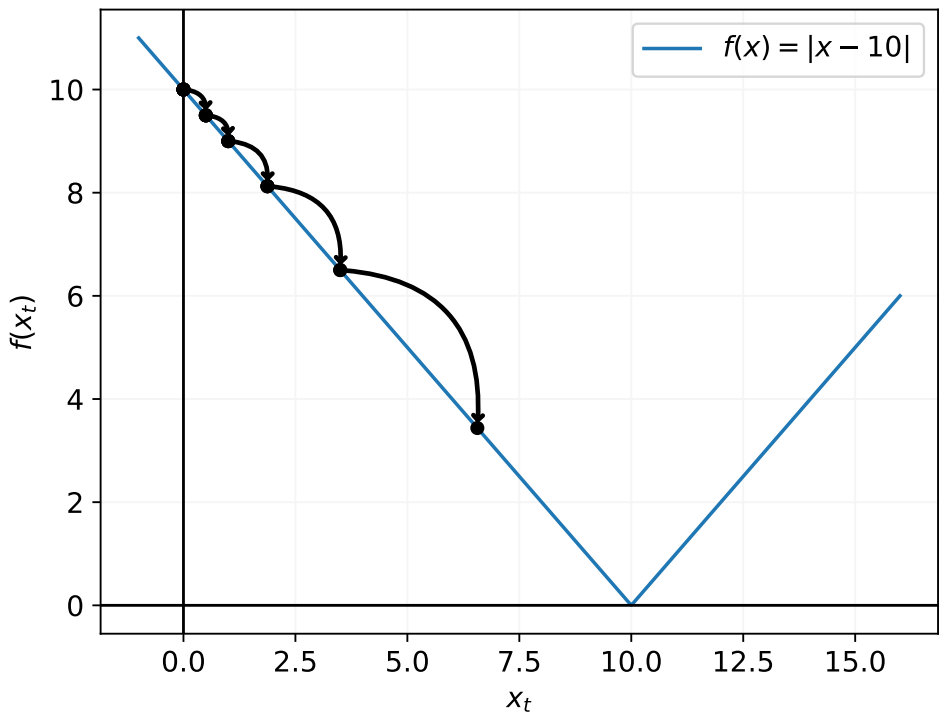
New betting fraction.

$$\beta_6 = \frac{\sum_{i=1}^{5} c_i}{6} = 0.8\dot{3}$$

New bet.

$x_6 = \beta_6 w_5 = 6.5625$

Coin Betting and Parameter Free Optimisation



Current wealth.

$w_5 = 7.875$

Current bet.

$x_6 = 6.5625$

Outcome.

$c_6 = -\nabla f(x_6) = 1$

New wealth.

$w_6 = w_5 + c_6 x_6 = 14.4375$

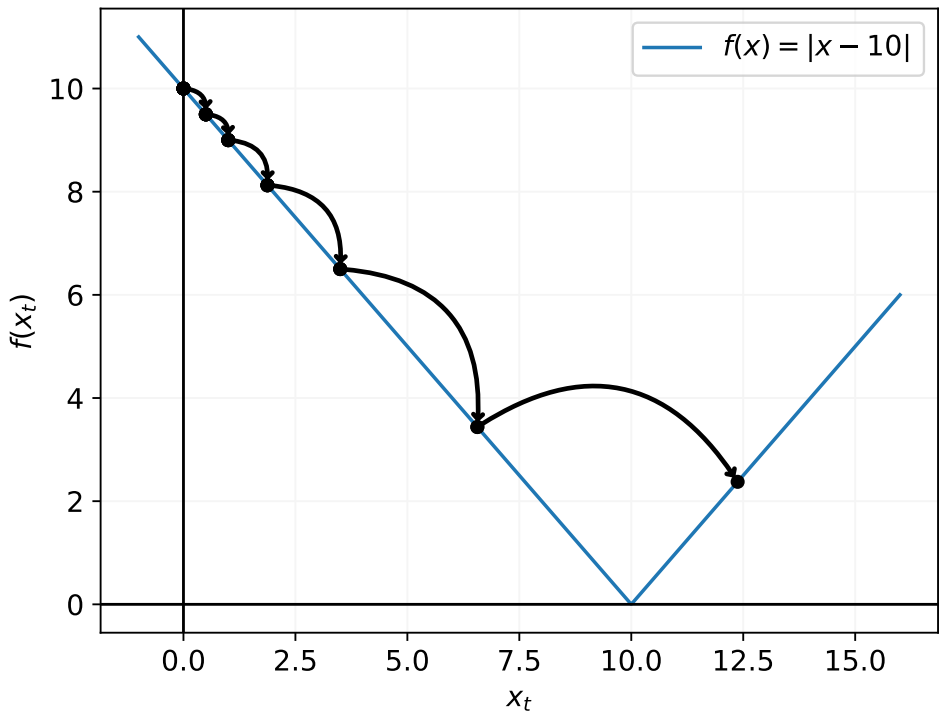
New betting fraction.

$$\beta_7 = \frac{\sum_{i=1}^{6} c_i}{7} = 0.\dot{8}57142\dot{}$$

New bet.

$x_7 = \beta_7 w_6 = 12.375$

Coin Betting and Parameter Free Optimisation



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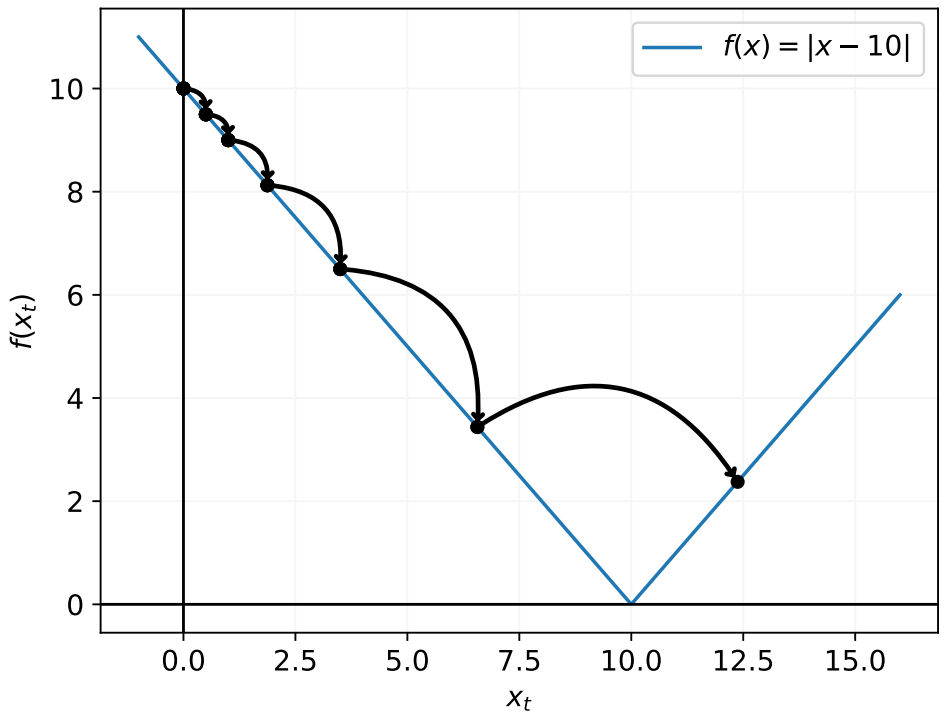


Current wealth.

$w_6 = 14.4375$

Current bet.

$x_7 = 12.375$

Outcome.

$c_7 = -\nabla f(x_7) = -1$

New wealth.

$w_7 = w_6 + c_7 x_7 = 2.0625$

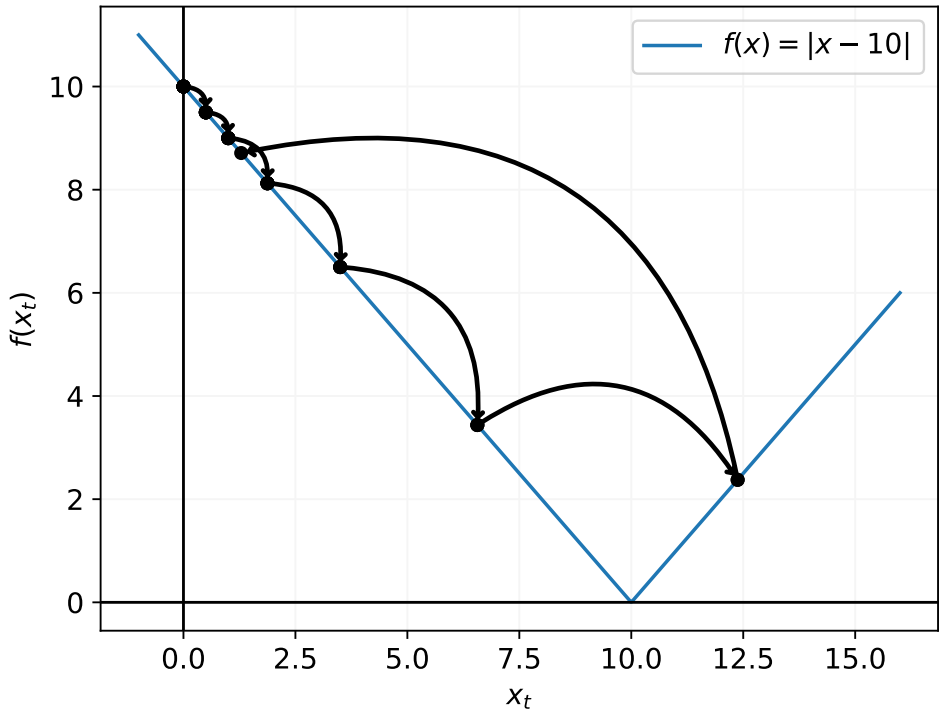
New betting fraction.

$$\beta_8 = \frac{\sum_{i=1}^{7} c_i}{8} = 0.625$$

New bet.

$x_8 = \beta_8 w_7 = 1.2890625$

Coin Betting and Parameter Free Optimisation



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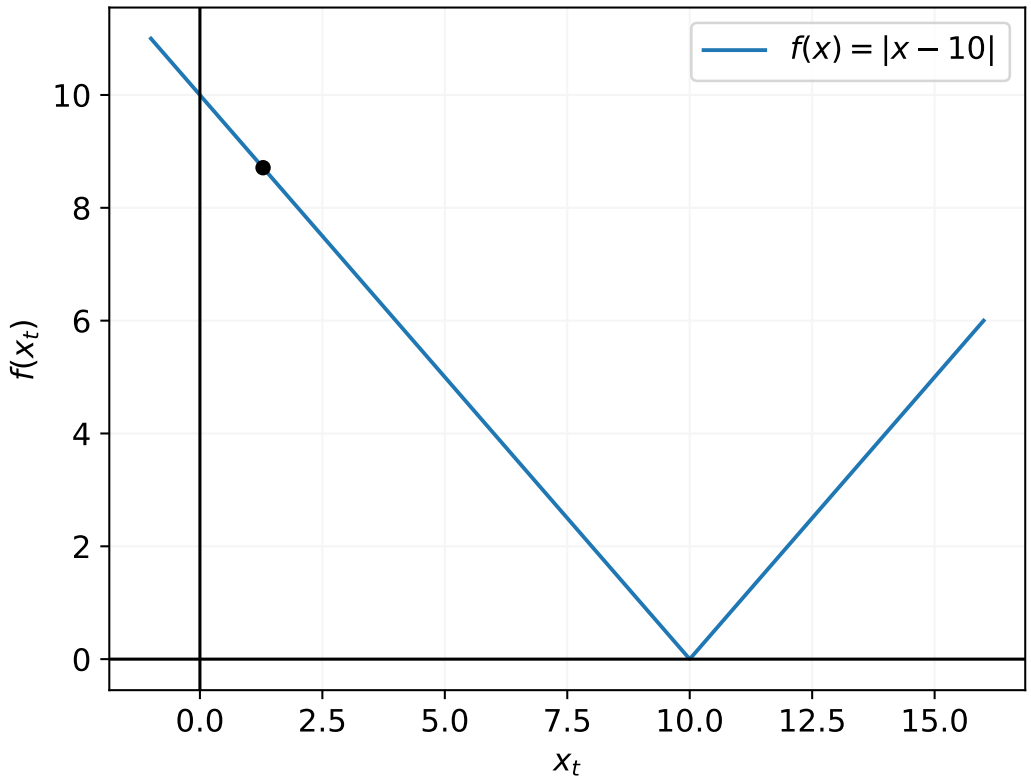

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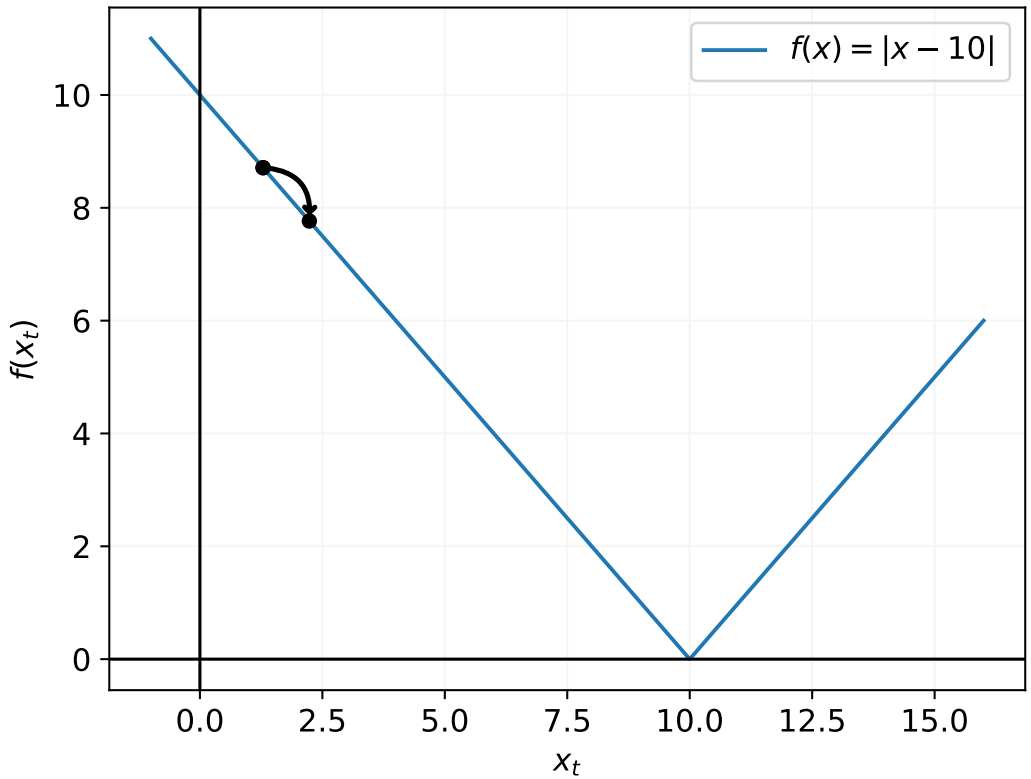

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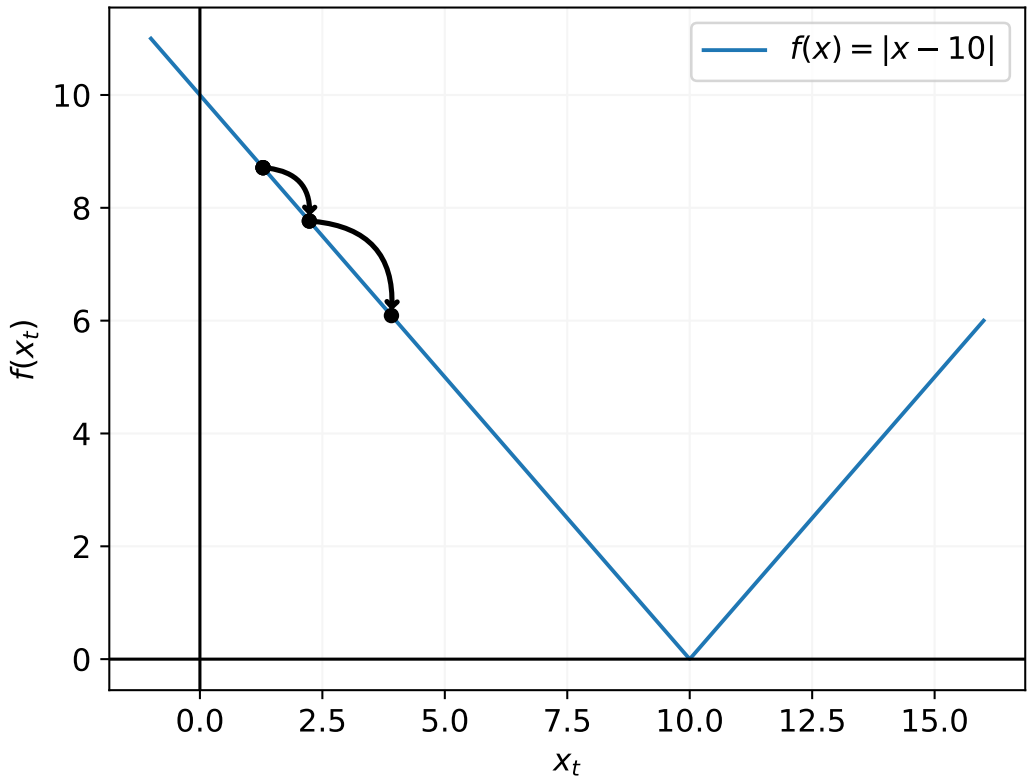

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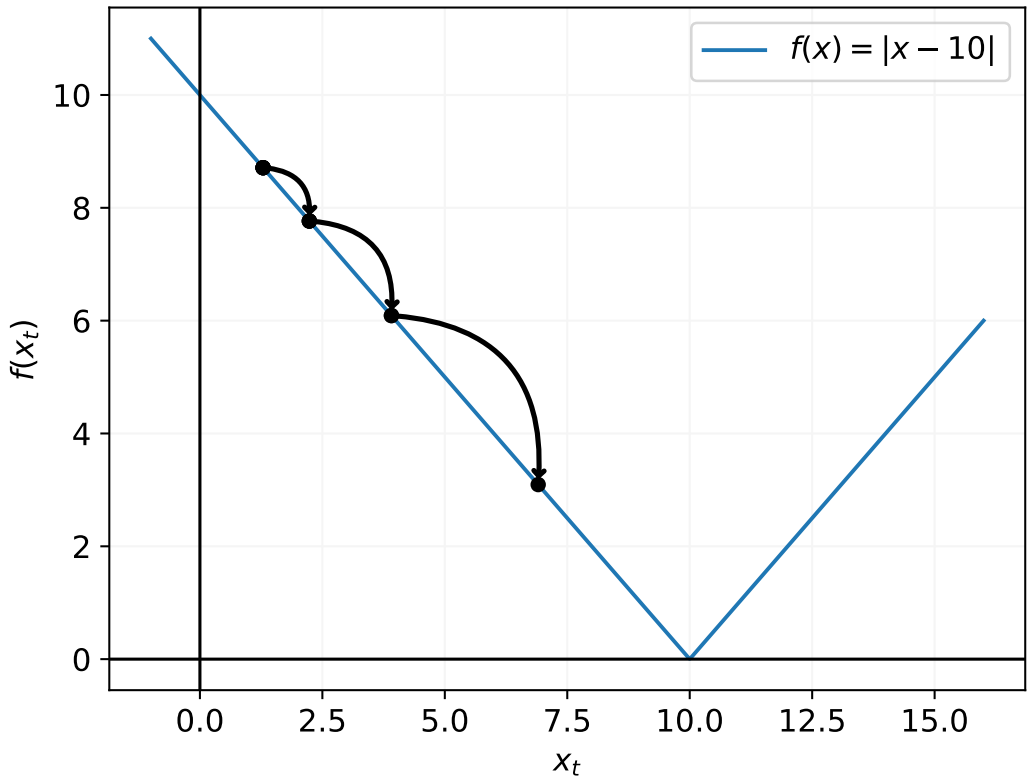

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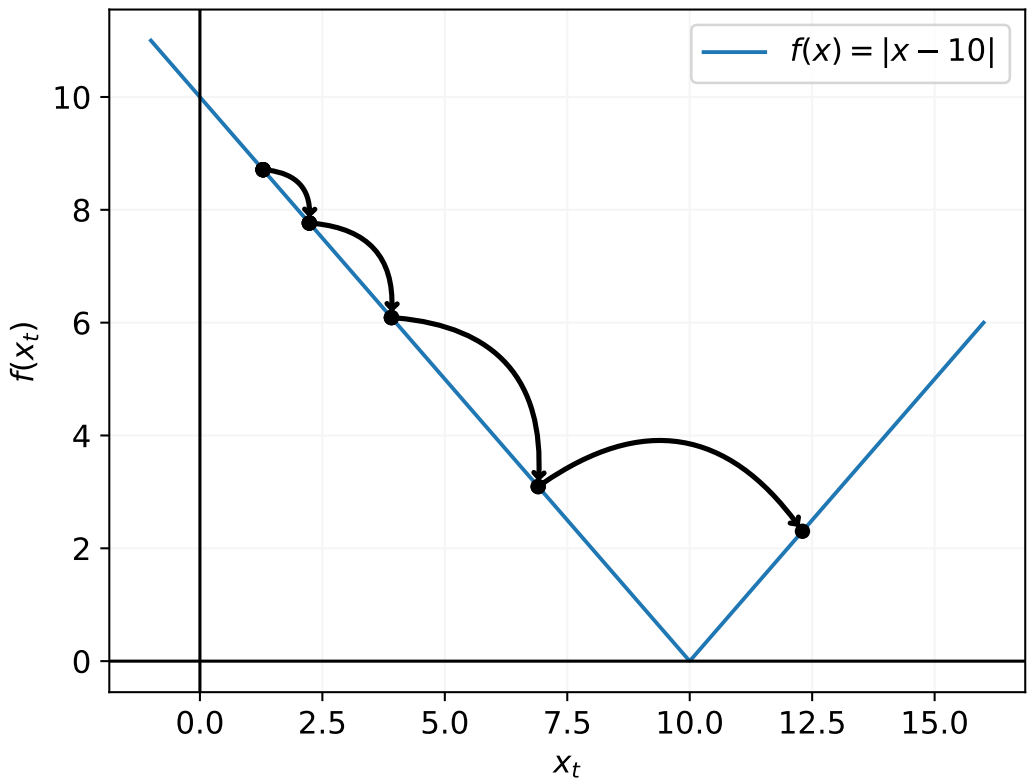

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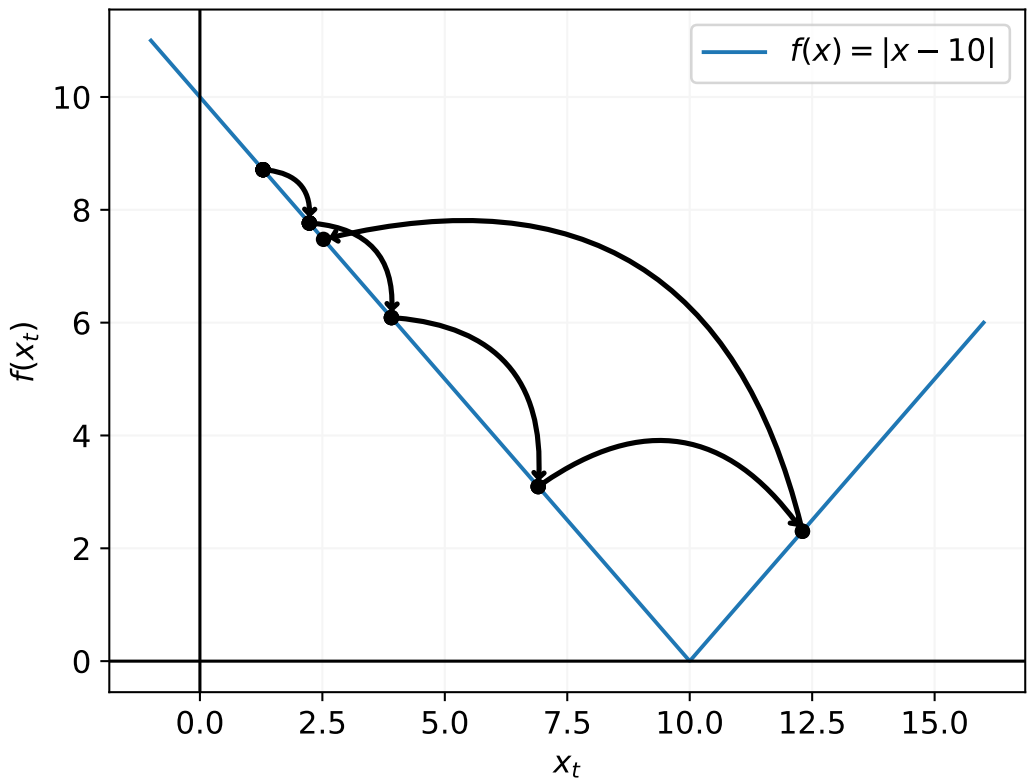

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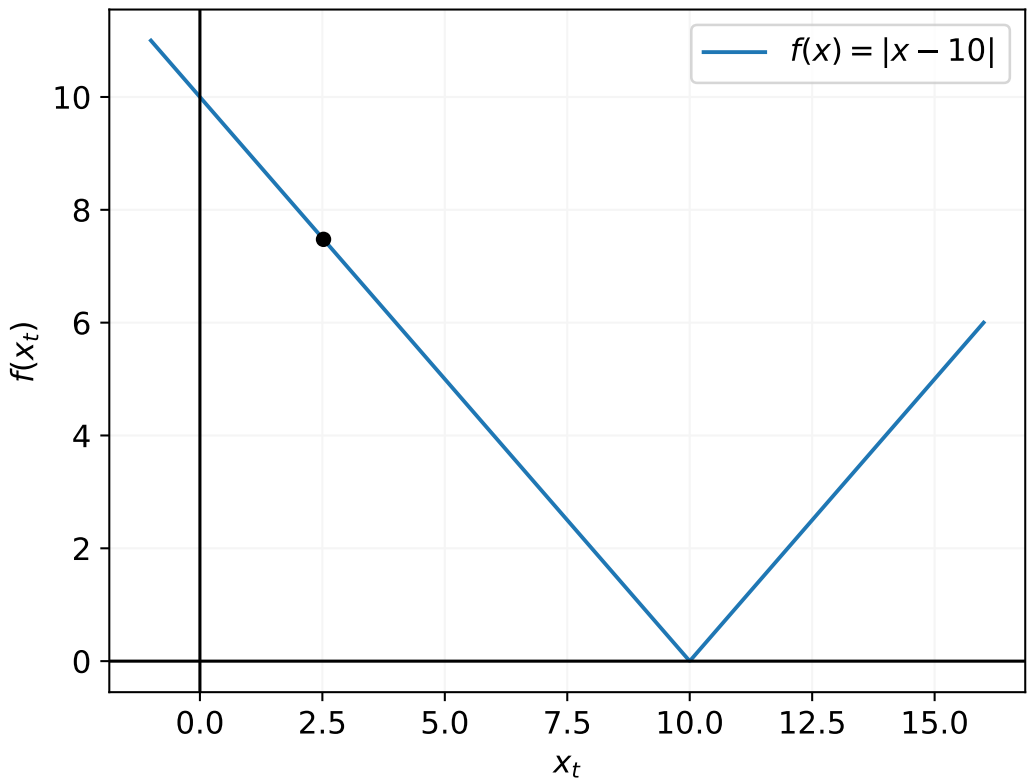

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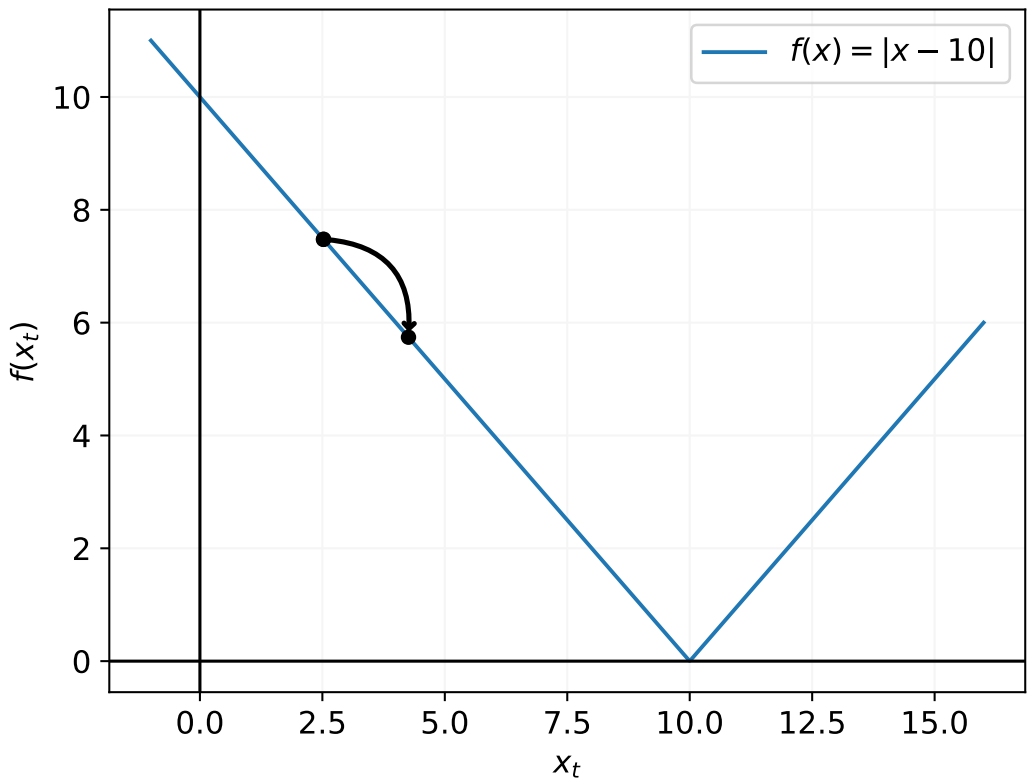

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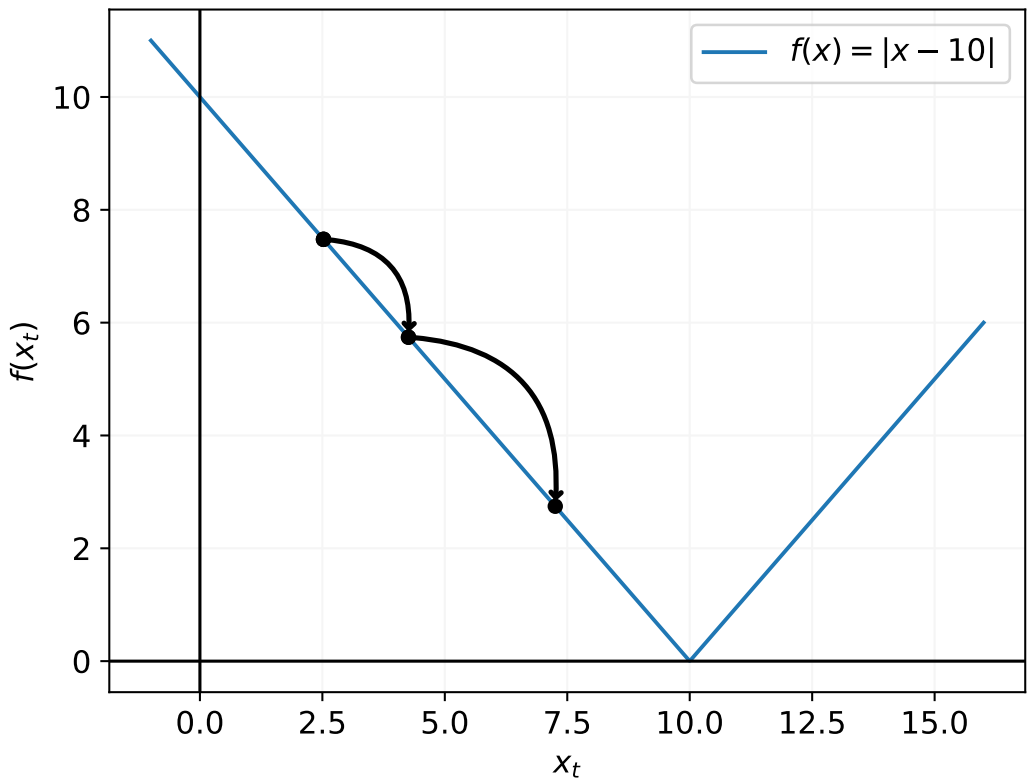

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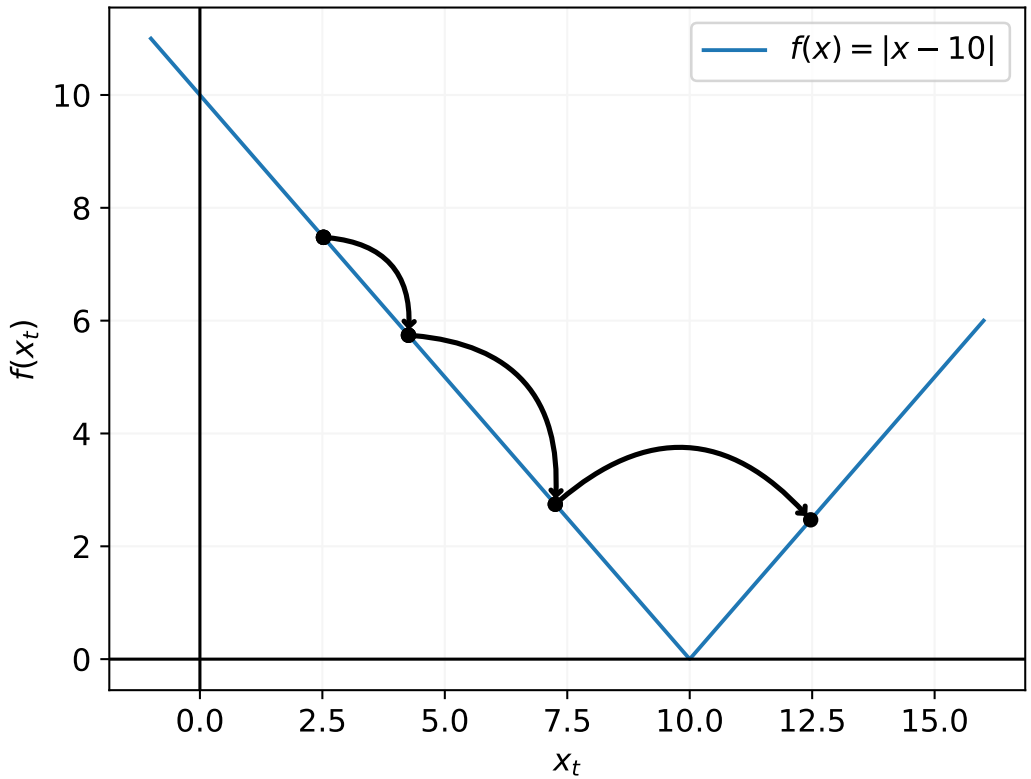

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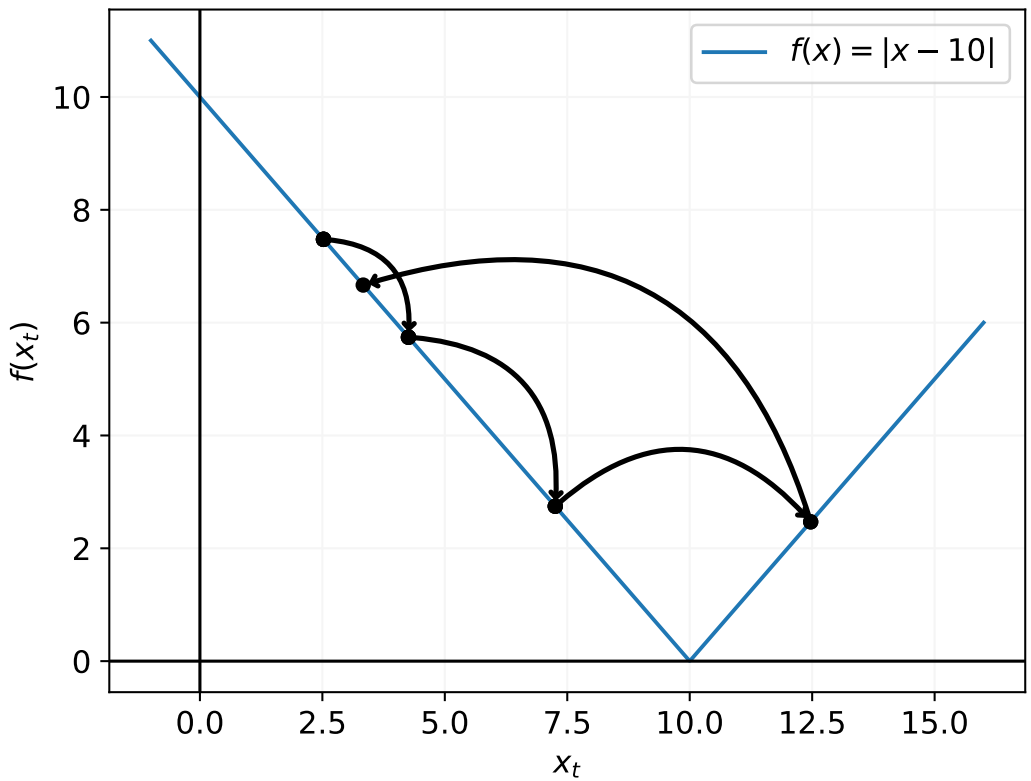

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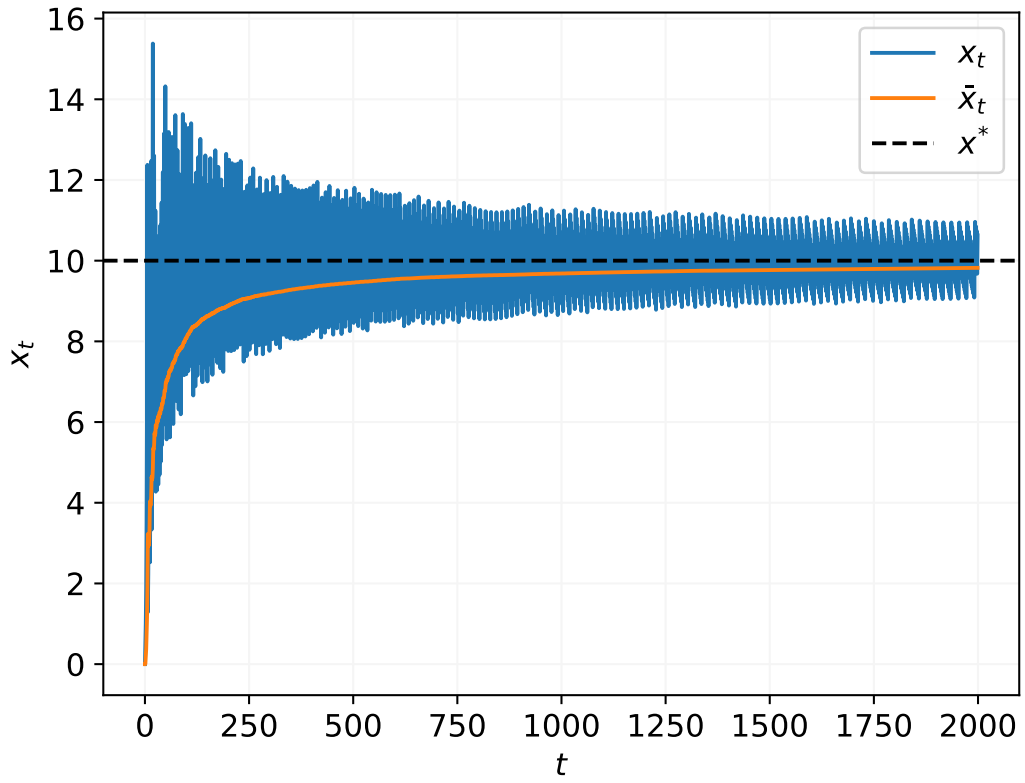

Going from $\mathbb{R}$ to $\mathbb{R}^d$

Thus far we have just just considered $f : \mathbb{R} \to \mathbb{R}$. What about the case where $f : \mathbb{R}^d \to \mathbb{R}$?

There are a few different approaches. The most straightforward are:

- **Inner products**.

$$x_t = -\frac{\sum_{i=1}^{t-1} \nabla f(x_i)}{t} \left(\varepsilon - \sum_{i=1}^{t-1} \langle \nabla f(x_i), x_i \rangle \right).$$

- **Coordinate-wise updates**. For $j = 1, \ldots, d$,

$$x_{t,j} = -\frac{\sum_{i=1}^{t-1} \partial_j f(x_i)}{t} \left(\varepsilon - \sum_{i=1}^{t-1} \partial_j f(x_i) x_{i,j} \right).$$

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Optimisation in Wasserstein Space

The Wasserstein Space

Let $\mathcal{P}_2(\mathbb{R}^d)$ denote the space of probability distributions on $\mathbb{R}^d$ with finite second moments:

$$\mathcal{P}_2(\mathbb{R}^d) = \left\{ \mu \in \mathcal{P}(\mathbb{R}^d) : \int_{\mathbb{R}^d} ||x||^2 \mu(\mathrm{d}x) < \infty \right\}.$$

Let W_2 denote the Wasserstein 2-distance between μ and ν, defined according to

$$W_2^2(\mu, \nu) = \inf_{\gamma \in \Gamma(\mu,\nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} ||x - y||^2 \gamma(\mathrm{d}x, \mathrm{d}y).$$

where $\Gamma(\mu, \nu)$ denotes the set of **couplings** between μ and ν (i.e., joint distributions on $\mathbb{R}^d \times \mathbb{R}^d$ with marginals μ and ν).

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Recall that we are interested in solving the following **optimisation problem**:

$$\pi = \underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\min}\ \mathcal{F}(\mu)$$

where $\mathcal{F} : \mathcal{P}(\mathbb{R}^d) \to \mathbb{R}$ is a **dissimilarity functional** which is uniquely minimised at π.

There are various possible choices for $\mathcal{F}$. A typical choice is the **Kullback-Leibler (KL) divergence**

$$\mathrm{KL}(\mu|\pi) = \begin{cases} \displaystyle\int_{\mathbb{R}^d} \log\left(\frac{\mathrm{d}\mu}{\mathrm{d}\pi}(x)\right)\mu(\mathrm{d}x) & , \quad \mu \ll \pi, \\ +\infty & , \quad \text{else.} \end{cases}$$

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To solve this optimisation problem, a natural approach would be to consider the **gradient flow** of $\mathcal{F}$ over the Wasserstein space.

First, we will need to define an appropriate notion of the gradient on $(\mathcal{P}_2(\mathbb{R}^d), W_2)$.

Definition

Let $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. Consider a **perturbation on the Wasserstein space** $(\mathrm{id} + \varepsilon h)_{\#}\mu$, for $h \in L^2(\mu)$. Then, if

$$\mathcal{F}\left((\mathrm{id} + \varepsilon h)_{\#}\mu\right) = \mathcal{F}(\mu) + \varepsilon \langle \nabla_{W_2}\mathcal{F}(\mu), h \rangle_{\mu} + o(\varepsilon)$$

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The Wasserstein gradient can be related to the **first variation** of $\mathcal{F}$ at μ, defined as follows.

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we say that $\mathcal{F}'(\mu) : \mathbb{R}^d \to \mathbb{R}$ is the **first variation** of $\mathcal{F}$ at μ.

In particular, in most cases of interest [AGG08, Theorem 10.4.13], we have that

$$\nabla_{W_2}\mathcal{F}(\mu) = \nabla\mathcal{F}'(\mu).$$

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$$\partial_t \mu_t + \nabla \cdot (v_t \mu_t) = 0 \ , \quad v_t = -\nabla_{W_2} \mathcal{F}(\mu_t).$$

How can we interpret this? Let $x = (x_t)_{t \geq 0}$ be the integral curve of the vector fields $(v_t)_{t \geq 0}$, viz

$$\dot{x}_t = -\nabla_{W_2} \mathcal{F}(\mu_t)(x_t) \ , \quad v_t = -\nabla_{W_2} \mathcal{F}(\mu_t),$$

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Wasserstein Gradient Flows: A Quick Example

Suppose we consider $\mathcal{F}(\mu) = \mathrm{KL}(\mu||\pi)$. In this case, the first variation is $\mathcal{F}'(\mu) = \log\left(\frac{\mu}{\pi}\right)$, and thus $\nabla_{W_2}\mathcal{F}(\mu) = \nabla \log\left(\frac{\mu}{\pi}\right)$.

The Wasserstein gradient flow can thus be written as

$$\frac{\partial \mu_t}{\partial t} = \nabla \cdot \left[\mu_t \nabla \log\left(\frac{\mu_t}{\pi}\right)\right] = \nabla \cdot (\mu_t \nabla U) + \Delta \mu_t.$$

This is nothing more than the Fokker-Planck equation of the **overdamped Langevin dynamics**

$$\mathrm{d}x_t = -\nabla U(x_t)\mathrm{d}t + \sqrt{2}\mathrm{d}w_t$$

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$$\frac{\partial \mu_t}{\partial t} = \nabla \cdot \left[\mu_t \nabla \log\left(\frac{\mu_t}{\pi}\right)\right] = \nabla \cdot (\mu_t \nabla U) + \Delta \mu_t.$$

This is nothing more than the Fokker-Planck equation of the **overdamped Langevin dynamics**

$$\mathrm{d}x_t = -\nabla U(x_t)\mathrm{d}t + \sqrt{2}\mathrm{d}w_t$$

where $w = (w_t)_{t\geq 0}$ is a standard $\mathbb{R}^d$-valued Brownian motion.

Wasserstein Gradient Descent

In practice, we we will need to **discretise** the Wasserstein gradient flow. Similar to the Euclidean case, we have several options:

- The **backward Euler discretisation**, which results in the JKO scheme [JKO98]

$$\mu_{t+1} \in \underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\min} \left[\mathcal{F}(\mu) + \frac{1}{2\gamma} \mathbb{W}_2^2(\mu, \mu_t) \right],$$

- The **forward Euler discretisation**, which results in the **Wasserstein gradient descent** algorithm [GHLR22]

$$\mu_{t+1} = (\mathbf{id} - \gamma \xi_t)_{\#} \mu_t \ , \quad \xi_t = \nabla_{W_2} \mathcal{F}(\mu_t),$$

In $\mathbb{R}^d$, writing $\mu_t = \mathrm{Law}(x_t)$, this corresponds to

$$x_{t+1} = x_t - \gamma \nabla_{W_2} \mathcal{F}(\mu_t)(x_t) \ , \quad x_0 \sim \mu_0.$$

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For different choices of $\mathcal{F}$, the forward Euler discretisation yields several existing sampling algorithms.

- **Maximum mean discrepancy descent** (MMDD) [AKSG19].
- **Kernel Stein discrepancy descent** (KSDD) [KPCAF+21].

If, in addition, we replace the Wasserstein gradient $\nabla\mathcal{F}(\mu)$ by a kernelised approximation (more on this later), we also have

- **Stein variational gradient descent** (SVGD) [LW16].
- **Laplacian adjusted Wasserstein gradient descent** (LAWGD)[CLL+20].

However, similar to before, the convergence properties of all of these methods depend on the choice of **step size** γ.

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For example, assuming the Wasserstein (sub) gradients satisfy $||\xi_t(x)|| \leq L$ for all $x \in \mathbb{R}^d$, Wasserstein (sub) gradient descent satisfies [GHLR22]

$$\mathcal{F}\left(\frac{1}{T}\sum_{t=1}^{T}\mu_t\right) - \mathcal{F}(\pi) \leq \frac{1}{T}\left[\frac{W_2^2(\mu_1,\pi)}{2\gamma} + \frac{L^2 T\gamma}{2}\right].$$

This implies that the **optimal** worst case learning rate is given by $\gamma_{\text{opt}} = \frac{W_2(\mu_1,\pi)}{L\sqrt{T}}$, and thus the **optimal error bound** is

$$\mathcal{F}\left(\frac{1}{T}\sum_{t=1}^{T}\mu_t\right) - \mathcal{F}(\pi) \leq \frac{LW_2(\mu_1,\pi)}{\sqrt{T}}.$$

Once again, this rate cannot be achieved in practice, since γ_{opt} depends on the **unknown** Wasserstein distance $W_2(\mu_1,\pi)$.

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We will obtain a **learning-rate free** sampling algorithm by extending the coin-betting approach to $\mathcal{P}_2(\mathbb{R}^d)$. The setup is similar to before.

- Consider a gambler with **initial wealth** w_0, for some $w_0 > 0$.
- We suppose that the **gambler** bets $(x_t - x_0)_{t=1}^T$ on a series of outcomes $(c_t)_{t=1}^T$, for some baseline $x_0 \in \mathbb{R}^d$.
- The **wealth** of the gambler thus accumulates as

$$w_t = w_0 + \sum_{s=1}^{t} \langle c_s, x_s - x_0 \rangle.$$

- We once again assume the bets satisfy $x_t - x_0 = \beta_t w_{t-1}$, and that $\beta_t = \frac{1}{t} \sum_{s=1}^{t-1} c_s$.
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We will now need a few additional definitions in order to define our algorithm.

- Let $x_0 \sim \mu_0$, for some initial distribution $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$
- Let $\varphi_t : \mathbb{R}^d \to \mathbb{R}^d$ denote the function which maps $x_0 \mapsto x_t$.
- Let $\mu_t \in \mathcal{P}_2(\mathbb{R}^d)$ be the **push-forward** of μ_0 under the function $\varphi_t : \mathbb{R}^d \to \mathbb{R}^d$:

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This definition means that, given $x_0 \sim \mu_0$, the random variable $x_t := \varphi_t(x_0)$ is **distributed according to** μ_t.

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How do we go from this **betting game** to a **sampling algorithm**?

- Consider a **hypothetical betting game** where $x_0 \sim \mu_0$, and we bet $x_t - x_0$ on $c_t = -\nabla_{W_2}\mathcal{F}(\mu_t)(x_t)$.

- The **sequence of bets** and **betting measures** associated with this betting game are then given by

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- In the paper, we obtain a sufficient condition under which $\bar{\mu}_T$ **converges to** $\pi = \arg\min_{\mu\in\mathcal{P}_2(\mathbb{R}^d)}\mathcal{F}(\mu)$ at a rate determined by the betting strategy.

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Coin Wasserstein Gradient Descent

Suppose that $\mathcal{F} : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ is a **geodesically convex** functional, and that $||\nabla_{W_2}\mathcal{F}(\mu_t)(x_t)|| \leq L$ for $t \in [1, T]$.

Then, under this sufficient condition, we can show that

$$\mathcal{F}\left(\frac{1}{T}\sum_{t=1}^{T}\mu_t\right) - \mathcal{F}(\pi) \leq \frac{L}{T}\left[w_0 + \int_{\mathbb{R}^d} ||x|| \sqrt{T \ln\left(1 + \frac{96K^2T^2||x||^2}{w_0^2}\right)}\pi(\mathrm{d}x) + \int_{\mathbb{R}^d} ||x|| \sqrt{T \ln\left(1 + \frac{96T^2||x||^2}{w_0^2}\right)}\mu_0(\mathrm{d}x)\right].$$

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Coin Wasserstein Gradient Descent

In a very simple case, where $\mu_0 \sim \mathcal{N}(m_0, \Sigma)$ and $\pi \sim \mathcal{N}(m_\pi, \Sigma)$, we can improve this bound to

$$\mathcal{F}\left(\frac{1}{T}\sum_{t=1}^{T}\mu_t\right) - \mathcal{F}(\pi) \leq \frac{L}{T}\left[w_0 + ||m_\pi - m_0||\sqrt{T \ln\left(1 + \frac{24\,T^2\,||m_\pi - m_0||^2}{w_0^2}\right)}\right].$$

Particle-Based Coin Wasserstein Gradient Descent

Recall our update equation from before:

$$x_t = x_0 - \frac{\sum_{s=1}^{t-1} \nabla_{W_2} \mathcal{F}(\mu_s)(x_s)}{t} \left(w_0 - \sum_{s=1}^{t-1} \langle \nabla_{W_2} \mathcal{F}(\mu_s)(x_s), x_s - x_0 \rangle \right).$$

Problem. The updates depend on the **unknown** μ_s, the density of x_s at time s.

Solution. Replace this quantity by the **empirical measure** of n **interacting particles**. Let $x_0^1, \ldots, x_0^N \sim \mu_0$. Then, for $i \in [N]$, writing $\hat{\mu}_t^N = \frac{1}{N} \sum_{i=1}^N \delta_{x_t^i}$, update

$$x_t^i = x_0^i - \frac{\sum_{s=1}^{t-1} \nabla_{W_2} \mathcal{F}(\hat{\mu}_s^N)(x_s^i)}{t} \left(w_0 - \sum_{s=1}^{t-1} \langle \nabla_{W_2} \mathcal{F}(\hat{\mu}_s^N)(x_s^i), x_s^i - x_0^i \rangle \right).$$

Particle-Based Coin Wasserstein Gradient Descent

Recall our update equation from before:

$$x_t = x_0 - \frac{\sum_{s=1}^{t-1} \nabla_{W_2} \mathcal{F}(\mu_s)(x_s)}{t} \left(w_0 - \sum_{s=1}^{t-1} \langle \nabla_{W_2} \mathcal{F}(\mu_s)(x_s), x_s - x_0 \rangle \right).$$

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Coin Stein Variational Gradient Descent

Our update equation now reads

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Problem. If $\mathcal{F}(\mu) = \mathrm{KL}(\mu|\pi)$, then $\nabla_{W_2}\mathcal{F}(\mu) = \nabla \ln \frac{\mu}{\pi}$ is ill defined when $\mu = \hat{\mu}^N$ is a discrete measure.

Solution. Replace $\nabla_{W_2}\mathcal{F}(\mu)$ by $P_\mu \nabla_{W_2}\mathcal{F}(\mu)$, its image under the integral operator $P_\mu f(x) = \int_{\mathbb{R}^d} k(x,y) f(y) \mu(y) \mathrm{d}y$. We thus update

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Coin Stein Variational Gradient Descent

Key Point. Using integration by parts, we have that

$$\begin{aligned} P_\mu \nabla \log \frac{\mu}{\pi}(x) &= \int k(x,y) \nabla \log \left(\frac{\mu}{\pi}\right)(y) \mu(\mathrm{d}y) \\ &= \int -k(x,y) \nabla \log \pi(y) \mu(\mathrm{d}y) + \int k(x,y) \nabla \mu(\mathrm{d}y) \\ &= \int_{\mathbb{R}^d} \left[k(x,y) \nabla U(y) - \nabla_y k(x,y)\right] \mu(\mathrm{d}y). \end{aligned}$$

Thus, in particular,

$$P_{\hat{\mu}_s^N} \nabla \log \left(\frac{\hat{\mu}_s^N}{\pi}\right)(x_s^i) = \frac{1}{N} \sum_{j=1}^{N} \left[k(x_s^i, x_s^j) \nabla U(x_s^j) - \nabla_2 k(x_s^i, x_s^j)\right].$$

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Coin SVGD vs SVGD

SVGD is a particle approximation of **Wasserstein gradient descent** for $\mathcal{F}(\mu) = \mathrm{KL}(\mu||\pi)$, with $\nabla_{W_2}\mathcal{F}(\mu)$ replaced by $P_{\hat{\mu}^N}\nabla_{W_2}\mathcal{F}(\hat{\mu}^N)$. This gives

$$x_t^i = x_{t-1}^i - \gamma P_{\hat{\mu}_{t-1}^N} \nabla \log\left(\frac{\hat{\mu}_{t-1}^N}{\pi}\right)(x_{t-1}^i).$$

Coin SVGD is a particle approximation of **coin Wasserstein gradient descent** for $\mathcal{F}(\mu) = \mathrm{KL}(\mu||\pi)$, with $\nabla_{W_2}\mathcal{F}(\mu)$ replaced by $P_{\hat{\mu}^N}\nabla_{W_2}\mathcal{F}(\hat{\mu}^N)$. This gives

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Coin KSDD and Coin LAWGD

By varying the **choice of** $\mathcal{F}$, or using different **approximations for** $\nabla_{W_2}\mathcal{F}(\mu)$, we can obtain coin analogues of other particle-based sampling algorithms.

In the paper [SN23], we also consider

- Coin kernel Stein discrepancy descent (KSDD) [KPCAF+21].
- Coin Laplacian adjusted Wasserstein gradient descent (LAWGD) [CLL+20].

Coin KSDD and Coin LAWGD

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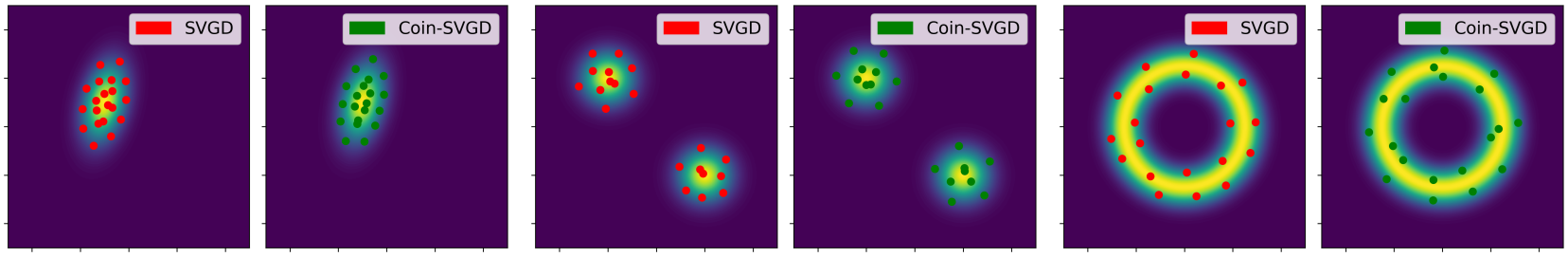
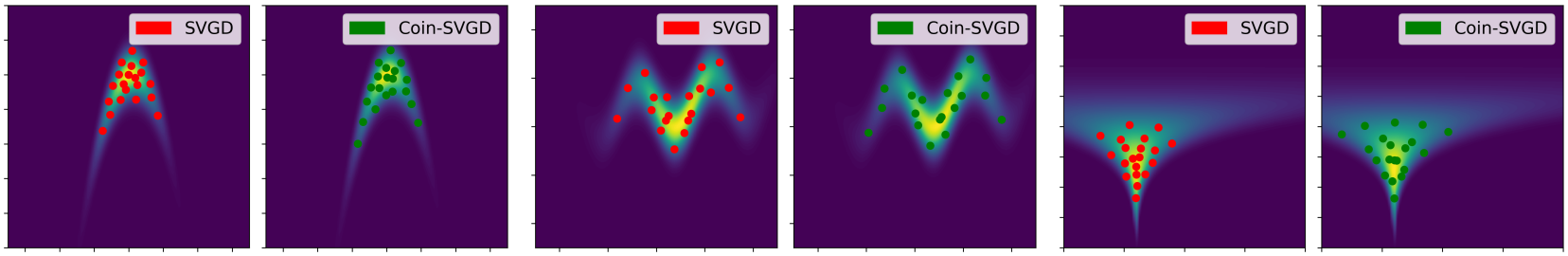
Numerical Results

Toy Examples



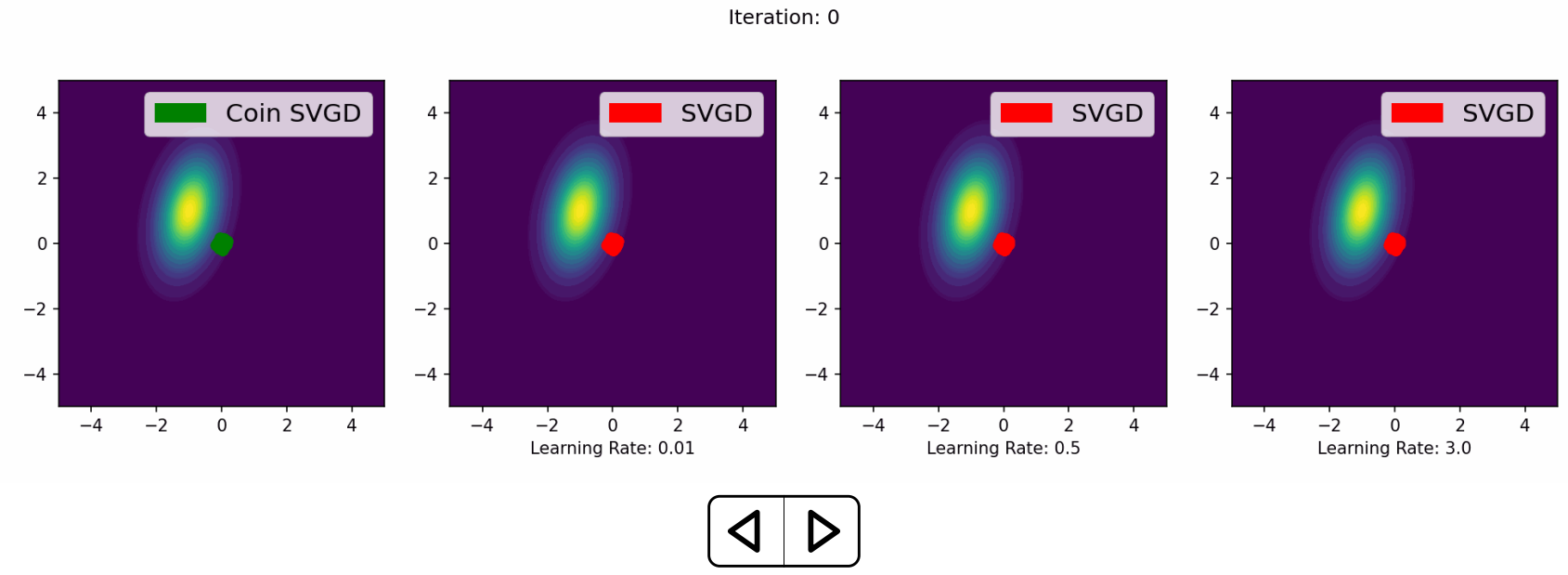
(a) Gaussian. (b) Mixture of Gaussians. (c) 'Donut'.



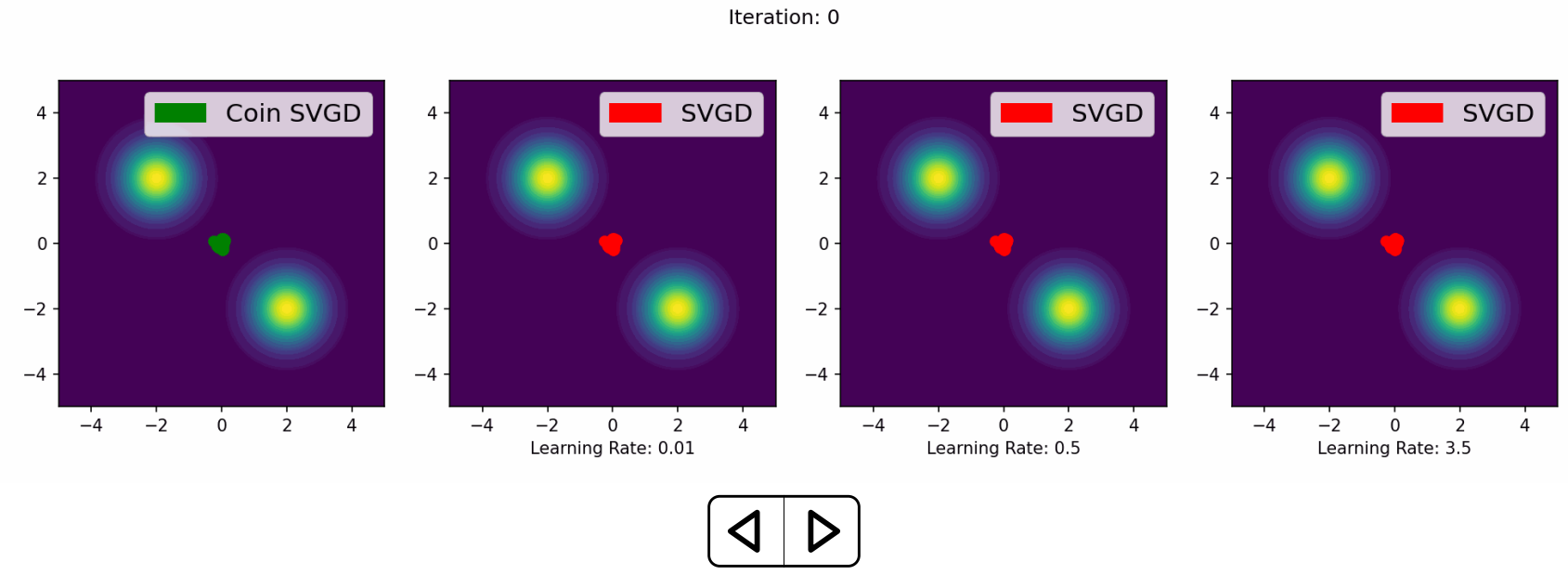
(d) Rosenbrock. (e) 'Squiggle'. (f) 'Funnel'.

Figure: **A comparison between SVGD [LW16] and its learning-rate free analogue, Coin SVGD**.

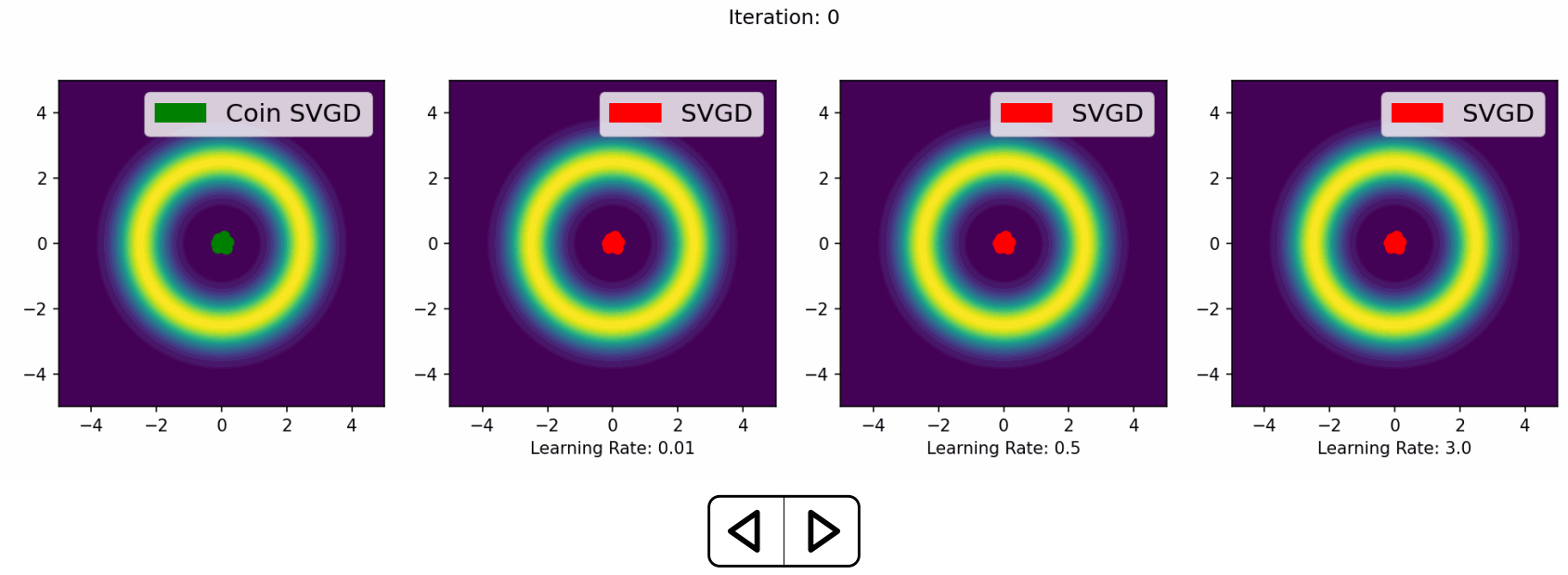
Toy Examples



Toy Examples



Toy Examples



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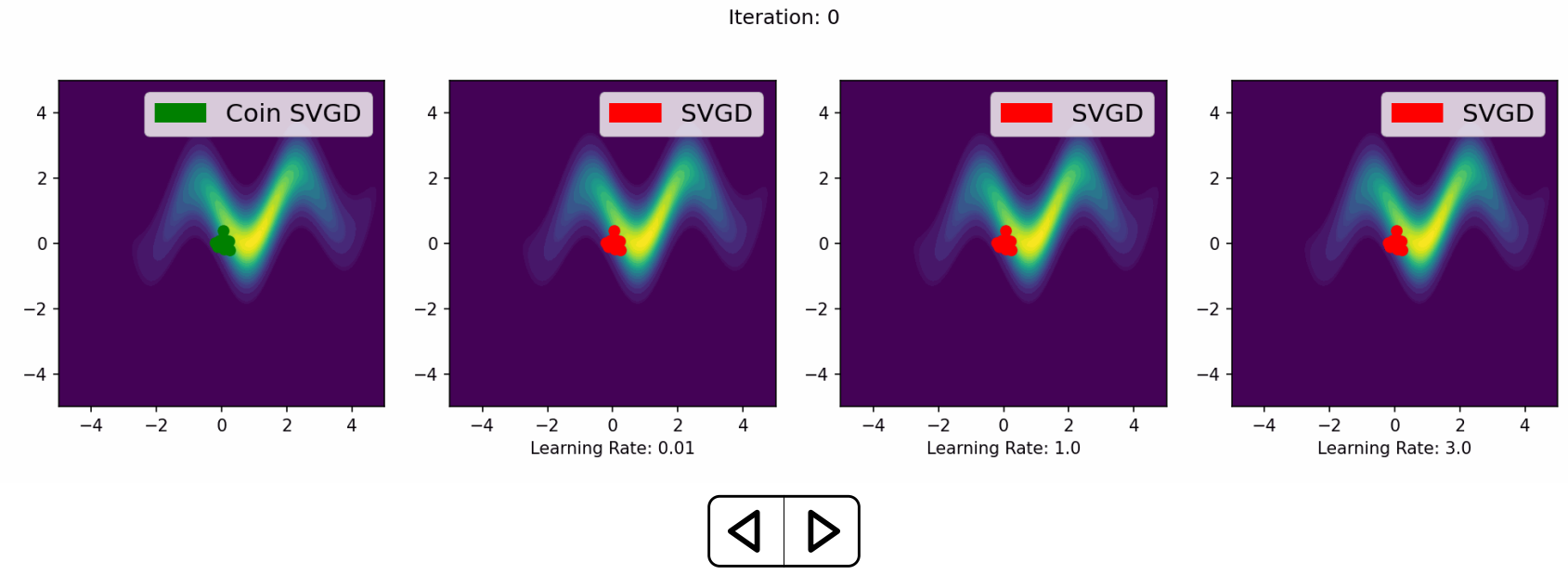

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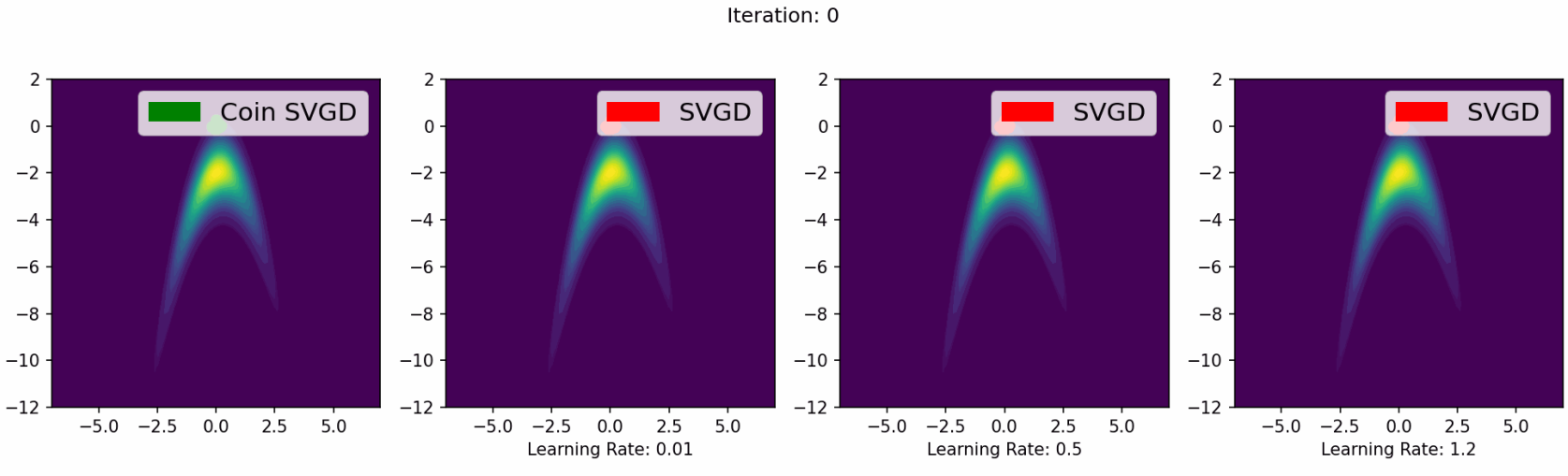

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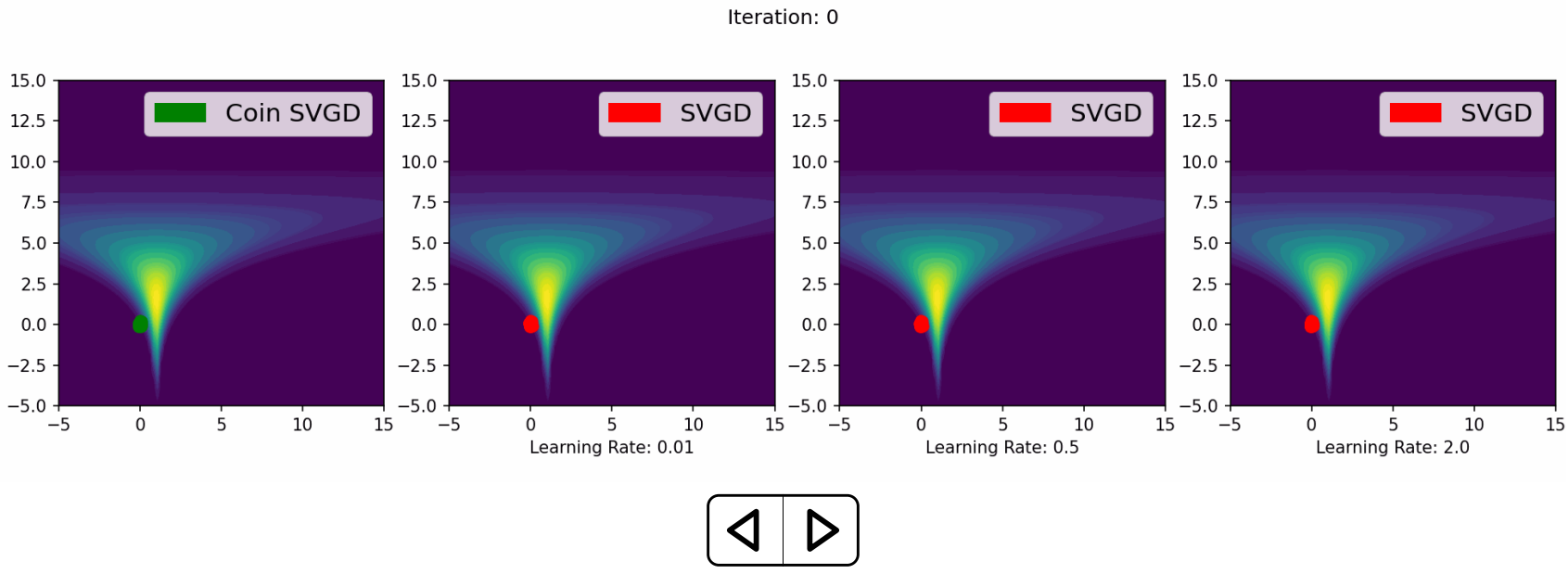
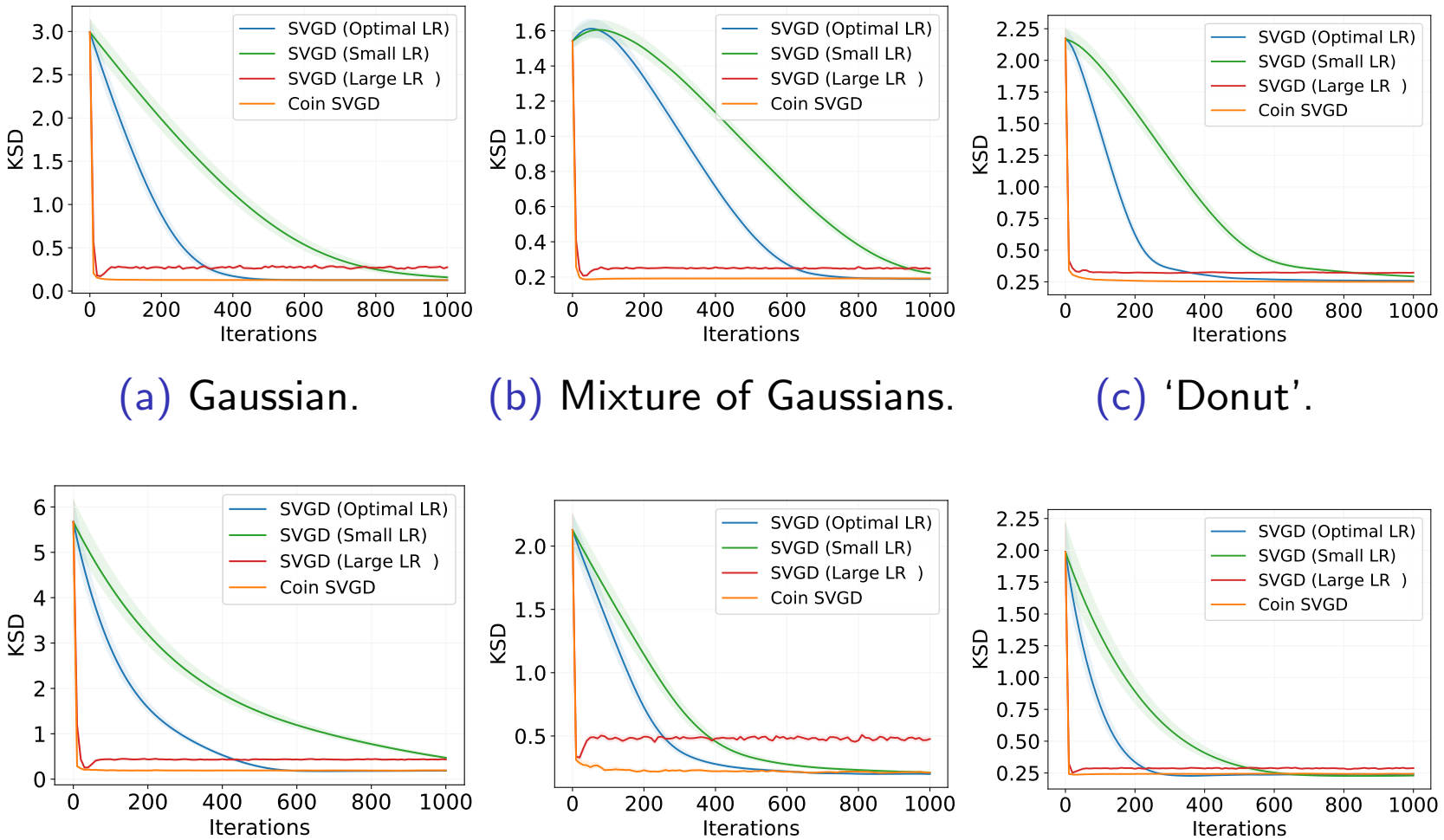


Toy Examples



(a) Gaussian. (b) Mixture of Gaussians. (c) 'Donut'.

(d) Rosenbrock. (e) 'Squiggle'. (f) 'Funnel'.

Figure: **Kernel Stein Discrepancy (KSD) vs Iterations (T).**

Toy Examples

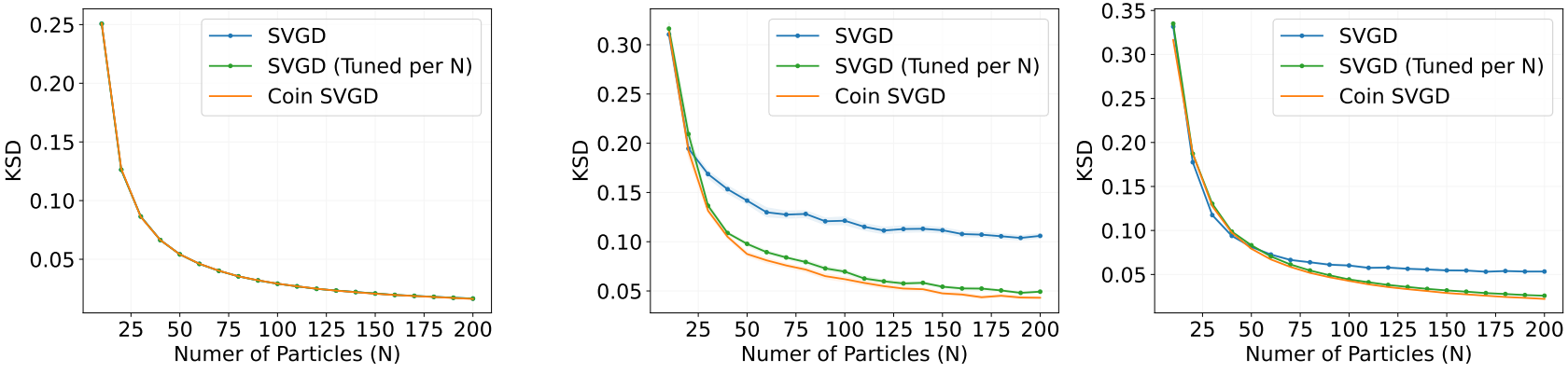


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Figure: **Kernel Stein Discrepancy (KSD) vs Number of Particles (N).**

Independent Component Analysis

Suppose we observe $\boldsymbol{x} \in \mathbb{R}^p$. The task of ICA is to infer the **unmixing matrix** $\mathbf{W} \in \mathbb{R}^{p \times p}$ such that $\boldsymbol{x} = \mathbf{W}^{-1}\boldsymbol{s}$, where $\boldsymbol{s} \in \mathbb{R}^p$ denote latent independent sources.

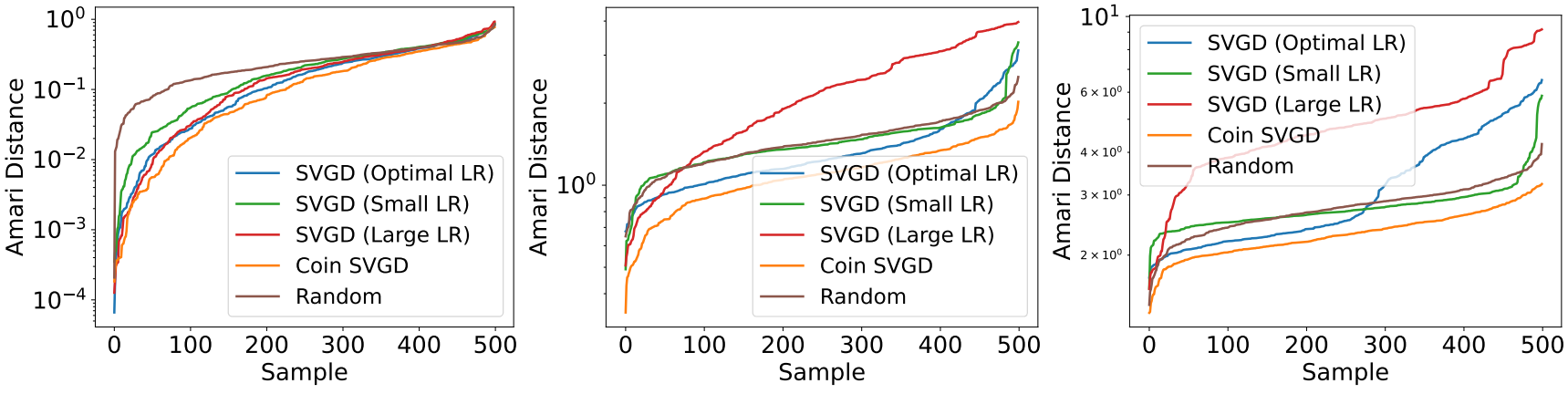
We assume each component s_i has the same density: $s_i \sim p_s$. The log-likelihood is then $\log p(\boldsymbol{x}|\mathbf{W}) = \log|\mathbf{W}| + \sum_{i=1}^{p} p_s([\mathbf{W}\boldsymbol{x}]_i)$.

For the prior, we assume that the entries of $\mathbf{W}$ are i.i.d., with law $\mathcal{N}(0,1)$. The posterior is then $p(\mathbf{W}|\boldsymbol{x}) \propto p(\boldsymbol{x}|\mathbf{W})p(\mathbf{W})$, with

$$\nabla_{\mathbf{W}} \log p(\mathbf{W}|\boldsymbol{x}) = (\mathbf{W}^{-1})^T - \frac{p_s'(\mathbf{W}\boldsymbol{x})}{p_s(\mathbf{W}\boldsymbol{x})}\boldsymbol{x}^T - \mathbf{W}$$

where p_s is chosen such that $\frac{p_s'(\cdot)}{p_s(\cdot)} = \tanh(\cdot)$ (see [KPCAF+21]).

Independent Component Analysis



(a) $p = 2$ (b) $p = 4$ (c) $p = 8$

Figure: **Results for the Bayesian ICA model**: Amari distances between the true unmixing matrix and the estimated unmixing matrices output by SVGD and Coin SVGD (lower is better).

Bayesian Logistic Regression

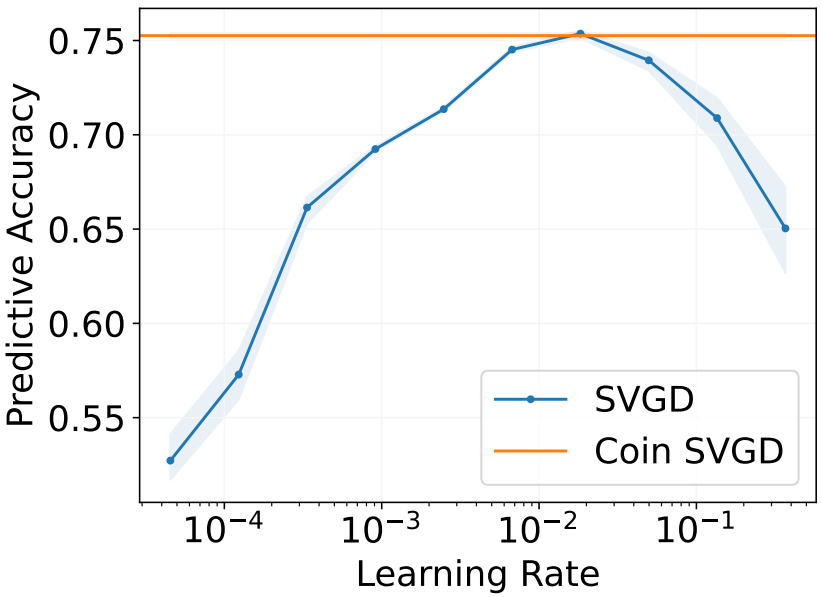
Let $\mathcal{D} = \{\boldsymbol{x}_i, y_i\}_{i=1}^N$ be a dataset with feature vectors $\boldsymbol{x}_i \in \mathbb{R}^p$, and binary labels $y_i \in \{-1, 1\}$.

We assume that $p(y_i = 1|\boldsymbol{x}_i, \boldsymbol{w}) = (1 + \exp(-\boldsymbol{w}^T \boldsymbol{x}_i))^{-1}$, for some $\boldsymbol{w} \in \mathbb{R}^p$.

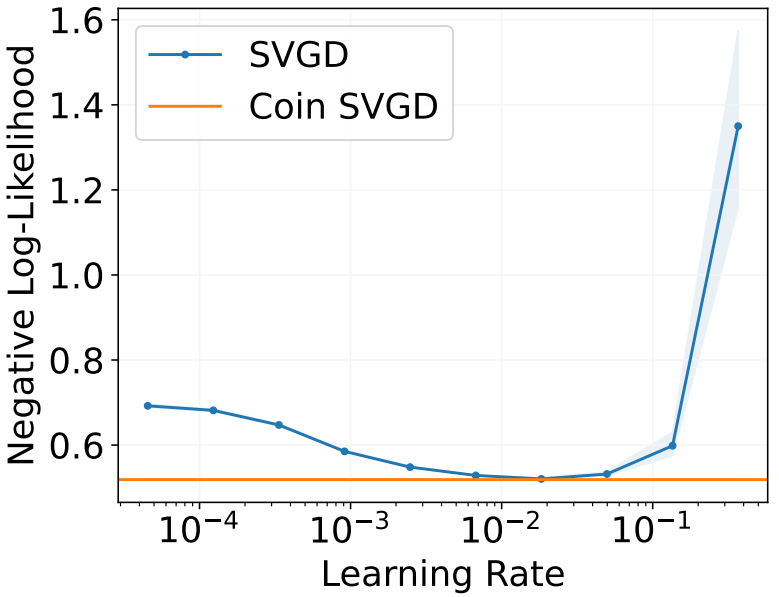
We put a **Gaussian prior** $p(\boldsymbol{w}|\alpha) = \mathcal{N}(\boldsymbol{w}|0, \alpha^{-1})$ on the weights $\boldsymbol{w}$, and a **Gamma prior** $p(\alpha) = \mathrm{Gamma}(\alpha|1, 0.01)$ on the precision $\alpha \in \mathbb{R}_+$.

We test our algorithm using the **Covertype dataset**, which consists of 581,012 data points and 54 features.

Bayesian Logistic Regression



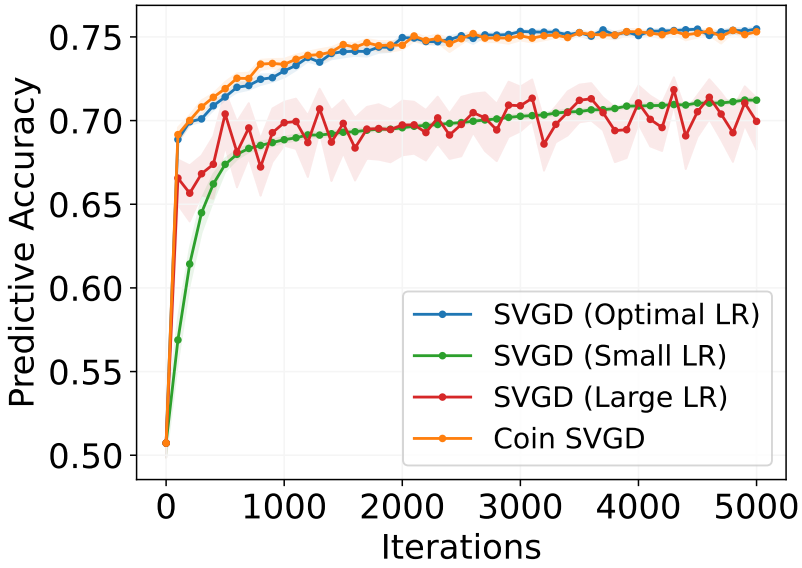
(a) Test Accuracy



(b) Negative Log-Likelihood

Figure: **Results for the Bayesian logistic regression model**: test-accuracy and the log-likelihood for SVGD and Coin SVGD.

Bayesian Logistic Regression



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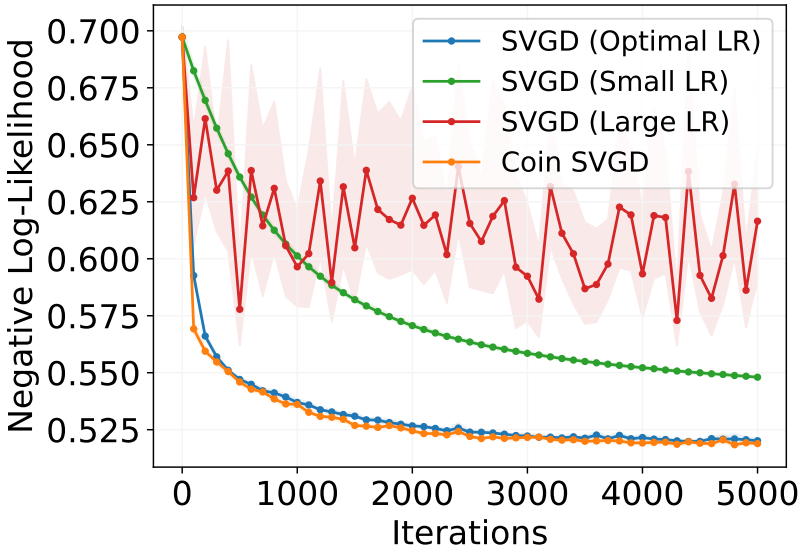


(b) Negative Log-Likelihood

Figure: **Results for the Bayesian logistic regression model**: test-accuracy and the log-likelihood for SVGD (three learning rates) and Coin SVGD as a function of the number of iterations.

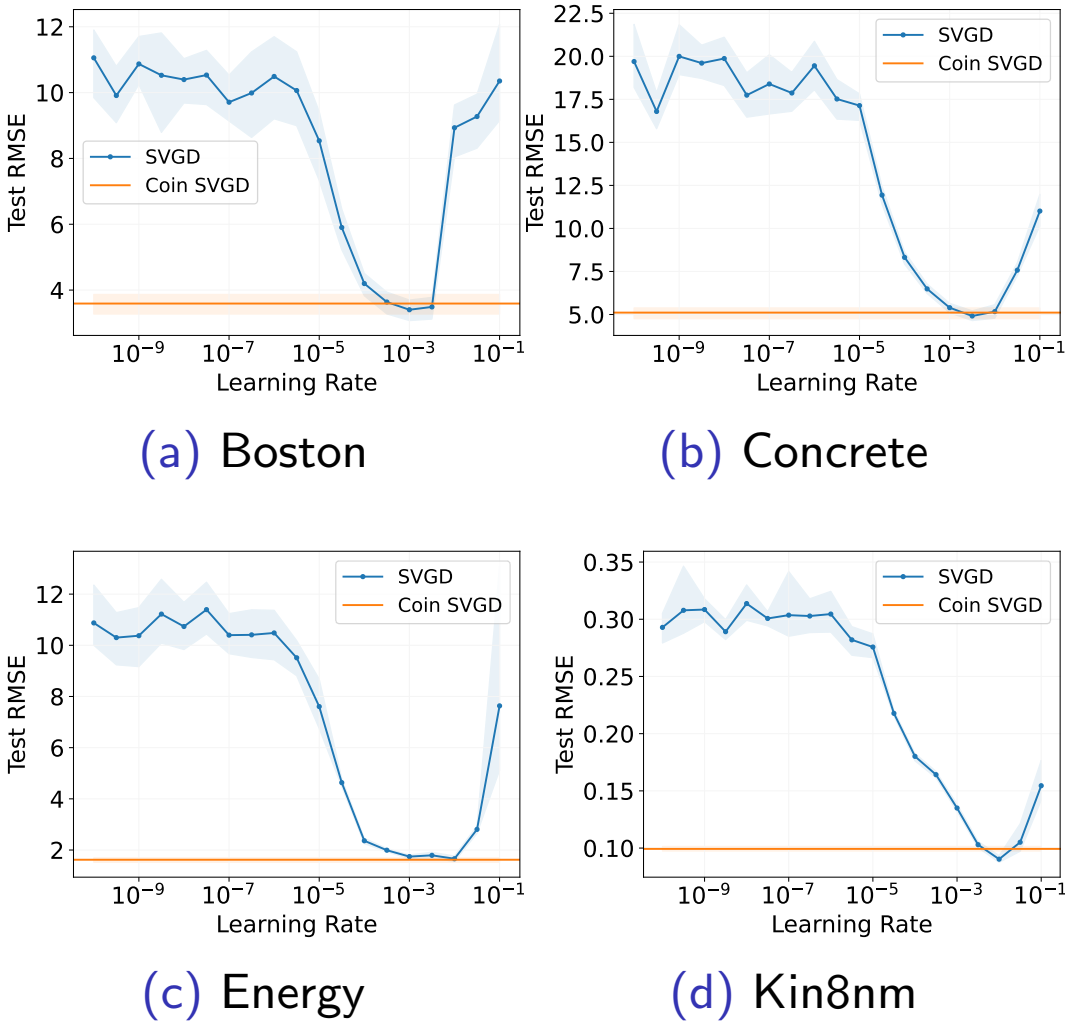
Bayesian Neural Network

We use a **two-layer neural network** with 50 hidden units with $\mathrm{RELU}(x) = \max(0, x)$ as the activation function (see also [LW16]).

We assume the output is **normal**, and place a $\mathrm{Gamma}(1, 0.1)$ prior on the **inverse covariance**. Meanwhile, we assign an **isotropic Gaussian prior** to the **neural network weights**.

We test the performance of our algorithm on several benchmark **UCI datasets**.

Bayesian Neural Network



(a) Boston (b) Concrete

(c) Energy (d) Kin8nm

Figure: **Results for the Bayesian neural network**: test RMSE for SVGD and Coin SVGD after $T = 2000$ iterations for four UCI benchmark datasets.

Probabilistic Matrix Factorisation

Let $\mathbf{R} \in \mathbb{R}^{N \times M}$ be a matrix of ratings for N users and M movies, where R_{ij} is the rating user i gave to movie j.

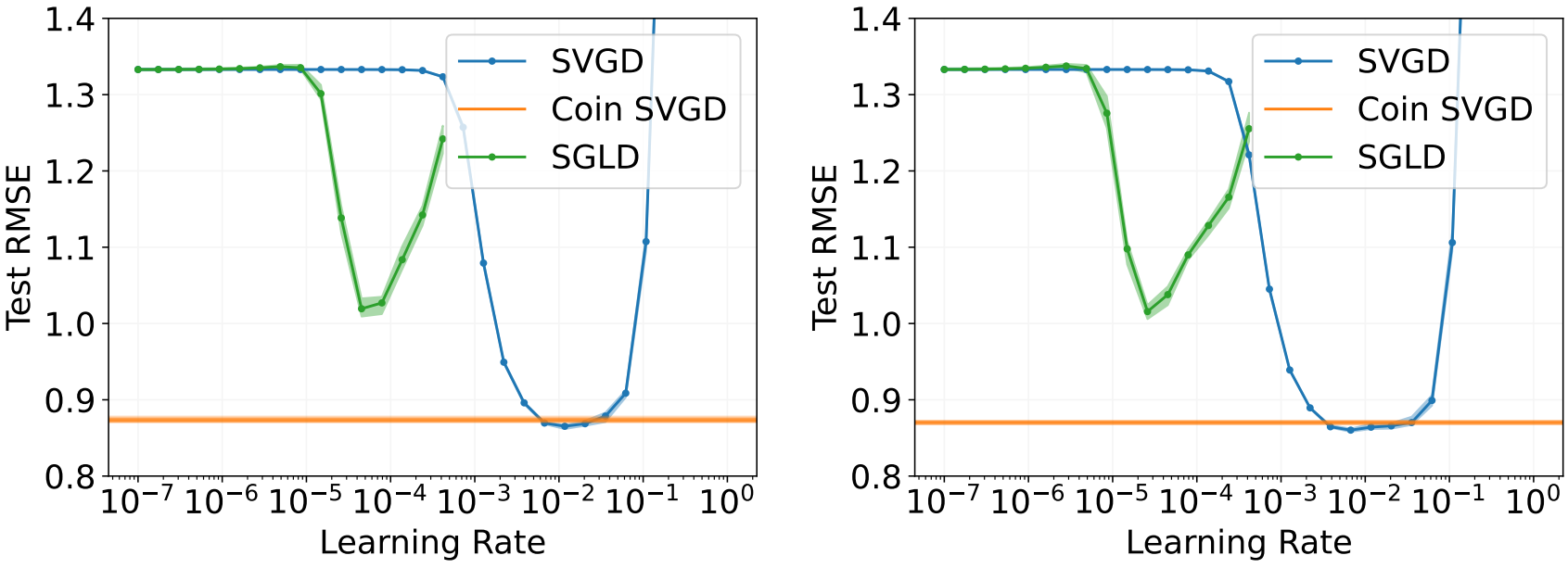
Define matrices $\mathbf{U}$ and $\mathbf{V}$ for users and movies, respectively, where $\mathbf{U}_i \in \mathbb{R}^d$ and $\mathbf{V}_j \in \mathbb{R}^d$ are latent feature vectors for user i and movie j. The **likelihood for the rating matrix** is given by

$$p(\mathbf{R}|\mathbf{U}, \mathbf{V}, \alpha) = \prod_{i=1}^{N} \prod_{j=1}^{M} \left[\mathcal{N}(R_{ij}|\mathbf{U}_i^T \mathbf{V}_j, \alpha^{-1}) \right]^{I_{ij}}$$

where I_{ij} denotes an indicator variable which equals 1 if users i gave a rating for movie j. See paper for further details of the setup.

We test our algorithm on the **MovieLens dataset** [HK15], which consists of 100,000 ratings, taking values $\{1,2,3,4,5\}$, for 1,682 movies from 943 users.

Probabilistic Matrix Factorisation



(a) $T = 1000$. (b) $T = 2000$.

Figure: **Results for the Bayesian probabilistic matrix factorisation model**: RMSE for SGLD, SVGD, and Coin SVGD.

Conclusions

Summary

The efficiency of many sampling algorithms is dependent on the **learning rate**.

By leveraging ideas from convex optimisation, namely **coin betting**, we can obtain **learning-rate free analogues** of many existing particle-based algorithms (e.g., SVGD, KSDD, etc.)

Coin sampling algorithms are **easy to implement**, and offer **performance comparable to the optimal performance** of existing particle-based algorithms.

Extensions

Recently we have extended this work in a couple of different directions:

- Learning-rate free Bayesian inference in **constrained domains** [SMN23].
- Learning-rate free **marginal maximum likelihood training** of **latent variable models** [SDN23].

In both cases, the key idea is to reformulate the problem as an **optimisation problem on the space of probability measures**, before applying our techniques.

Future Work

There are a few interesting directions for future work:

- Which other particle-based sampling algorithms can be **'coinified'**?
- Is there a learning-rate free analogue of LMC based on coin betting?
- Can we improve the convergence rate using other **betting strategies**?
- Is it possible to establish convergence under more **standard assumptions** (e.g., LSI)?
- Can we use similar ideas to develop learning-rate free algorithms for sampling in **constrained domains**?

Some References

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Any Questions?

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