Optimizing Probability Distributions for Learning: Sampling meets Optimization

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May 2, 2019

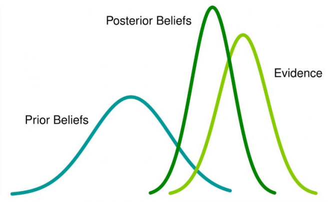
Sampling Problems

Bayesian inference

Compute $P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$.

Write the density of $P(\theta|D)$ as

$$\frac{\exp(-U(\theta))}{\int \exp(-U(\theta))\, d\theta}.$$



www.analyticsvidhya.com

Langevin diffusion

Simulate a stochastic differential equation:

$$dx_t = -\nabla U(x_t)\, dt + \sqrt{2}\, dB_t.$$

Stationary distribution has density $p^*(\theta) \propto \exp(-U(\theta))$.

Sampling Problems

Prediction as a repeated game

- Player chooses action $a_t \in \mathcal{A}$,
- Adversary chooses outcome y_t,
- Player incurs loss $\ell(a_t, y_t)$.

Aim to minimize **regret**:
$\sum_t \ell(a_t, y_t) - \min_a \sum_t \ell(a, y_t)$.

Exponential weights strategy

$$p_t(a) \propto \exp\left(-U(a)\right),$$

$$\text{with} \quad U(a) := \eta \sum_{s=1}^{t-1} \ell(a, y_s).$$

Langevin diffusion

Simulate a stochastic differential equation:

$$dx_t = -\nabla U(x_t)\, dt + \sqrt{2}\, dB_t.$$

Stationary distribution has density $p^*(a) \propto \exp(-U(a))$.

Sampling Algorithms

Langevin diffusion

$$\text{SDE:} \qquad dx_t = -\nabla U(x_t)\, dt + \sqrt{2}\, dB_t.$$

Stationary distribution has density $p^*(\cdot) \propto \exp(-U(\cdot))$.

Discrete Time: Langevin MCMC Sampler (Euler-Maruyama)

$$x_{k+1} = x_k - \eta \nabla U(x_k) + \sqrt{2\eta}\xi_k, \qquad \xi_k \sim \mathcal{N}(0, I).$$

- How close to the desired p^* is p_k (the density of x_k)?
- How rapidly does it converge?

Viewpoint

Sampling as optimization over the space of probability distributions.

Sampling Algorithms for Optimization

Parameter optimization in deep neural networks

- Use training data $(x_1, y_1), \ldots, (x_n, y_n) \in \mathcal{X} \times \mathcal{Y}$ to choose parameters θ of a deep neural network $f_\theta : \mathcal{X} \to \mathcal{Y}$.
- Aim to minimize loss $U(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f_\theta(x_i))$.
- Gradient: $\theta_{k+1} = \theta_k - \eta_k \nabla U(\theta_k)$
- Stochastic gradient: Random θ_0, $\qquad \theta_{k+1} = \theta_k - \eta_k \nabla \hat{U}_{\xi_k}(\theta_k)$
- ... with minibatch gradient estimates, $\hat{U}_{\xi_k}(\theta) = \frac{1}{\xi_k} \sum_{i \in \xi_k} \ell(y_i, f_\theta(x_i))$
- ... and decreasing stepsizes η_k.

- What is the distribution of θ_k?
- View stochastic gradient methods as sampling algorithms.

Outline

- The Langevin diffusion
- Optimization theory for sampling methods
  - Convergence of Langevin MCMC in KL-divergence
  - Nesterov acceleration in sampling
  - The nonconvex case
- Sampling methods for optimization
  - Stochastic gradient methods as SDEs

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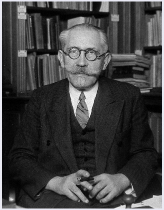
Langevin Diffusion

Langevin diffusion

Stochastic differential equation:

$$dx_t = \underbrace{-\nabla U(x_t)\, dt}_{\text{drift}} + \sqrt{2}\, dB_t,$$

where $x_t \in \mathbb{R}^d$, $U : \mathbb{R}^d \to \mathbb{R}$, dB_t is standard Brownian motion on $\mathbb{R}^d$.



Paul Langevin
wikipedia.org

Define p_t as the density of x_t.

Under mild regularity assumptions, $p_t \to p^*$; $\quad p^*(x) \propto \exp(-U(x))$.

Discretization of the Langevin Diffusion

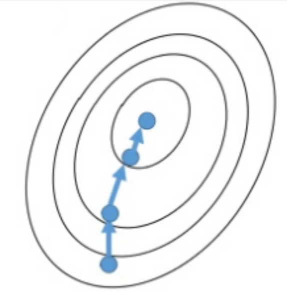
Langevin Markov Chain

Choose step-size η and simulate the Markov chain:

$$x_{k+1} = x_k - \eta \nabla U(x_k) + \sqrt{2\eta}\xi_k, \qquad \xi_k \overset{iid}{\sim} \mathcal{N}(0, I_d).$$

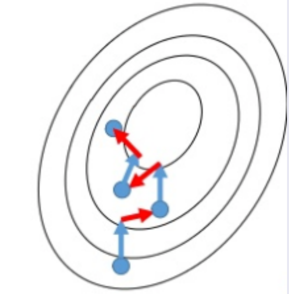
Gradient descent

$$x_{k+1} = x_k - \eta \nabla U(x_k)$$



Langevin Markov Chain

$$x_{k+1} = x_k - \eta \nabla U(x_k) + \sqrt{2\eta}\xi_k$$



Langevin Markov Chain

$$x_{k+1} = x_k - \eta \nabla U(x_k) + \sqrt{2\eta}\xi_k, \qquad \xi_k \overset{iid}{\sim} \mathcal{N}(0, I_d).$$

How does the density p_k of x_k evolve?

Asymptotic results

Under regularity conditions, for shrinking step-size η_k, $\|p_k - p^*\|_{TV} \to 0$.

e.g., (Gelfand and Mitter, 1991), (Roberts and Tweedie, 1996)

Arnak Dalalyan mediamax.am

Quantitative results

For suitably small (fixed) η and $k = \tilde{\Omega}\left(\frac{d}{\epsilon^2}\right)$,

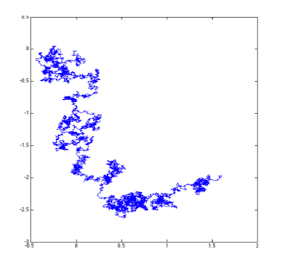
$\|p_k - p^*\|_{TV} \leq \epsilon.$ (Dalalyan, 2014)

$W_2(p_k, p^*) \leq \epsilon.$ (Durmus and Moullines, 2016)

Langevin Diffusion as Gradient Flow

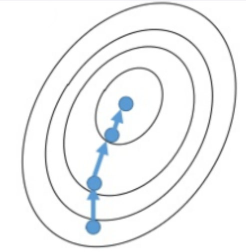
Langevin Diffusion in $\mathbb{R}^d$

$$dx_t = -\nabla U(x_t)\,dt + \sqrt{2}\,dB_t.$$



Gradient flow in $\mathcal{P}(\mathbb{R}^d)$

p_t minimizes $\frac{d}{dt}\mathcal{H}(\mathbf{p}_t) + \frac{1}{2}|\mathbf{p}_t'|^2$.



(Jordan, Kinderlehrer and Otto, 1998), (Ambrosio, Gigli and Savaré, 2005)

Richard Jordan

David Kinderlehrer

Felix Otto

Luigi Ambrosio

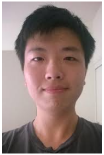
Nicola Gigli

Giuseppe Savaré

$W_2(\mathbf{p}_t, \mathbf{p}_{t+h})$

Sampling as Optimization

- Sampling algorithms can be viewed as deterministic optimization procedures over a space of probability distributions.
- Can we apply tools and techniques from optimization to sampling?



Xiang Cheng

An Optimization Analysis in $\mathcal{P}(\mathbb{R}^d)$

Convergence of Langevin MCMC in KL-divergence.
Xiang Cheng and PB.
arXiv:1705.09048[stat.ML]; ALT 2018.

Langevin MCMC

$$x_{k+1} = x_k - \eta \nabla U(x_k) + \sqrt{2\eta}\xi_k, \qquad \xi_k \overset{iid}{\sim} \mathcal{N}(0, I_d).$$

How does the density p_k of x_k evolve?

Theorem

For smooth, strongly convex U, that is, $\forall x, mI \preceq \nabla^2 U(x) \preceq LI$,

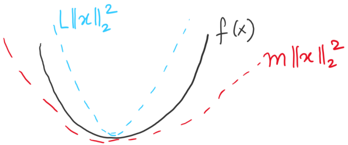
suitably small η and $k = \tilde{\Omega}\left(\frac{d}{\epsilon}\right)$ ensure that $\mathcal{KL}\left(\mathbf{p}^k \| \mathbf{p}^*\right) \leq \epsilon$.

Implies older bounds for TV and W_2:

For suitably small η and $k = \tilde{\Omega}\left(\frac{d}{\epsilon^2}\right)$,

$\|p_k - p^*\|_{TV} \leq \epsilon$. (Dalalyan, 2014)

$W_2(p_k, p^*) \leq \epsilon$. (Durmus and Moullines, 2016)



Analog with gradient flow over $\mathbb{R}^d$

Minimization over $\mathbb{R}^d$

Minimize $f : \mathbb{R}^d \to \mathbb{R}$ using gradient flow $y_t : \mathbb{R}^+ \to \mathbb{R}^d$ wrt Euclidean norm:

$$\min \quad \left(\frac{d}{dt} f(y_t) + \frac{1}{2} \left\| \frac{d}{dt} y_t \right\|^2 \right)$$

$$\frac{d}{dt} f(y_t) = \left\langle \nabla f(y_t), \frac{d}{dt} y_t \right\rangle$$

$$\frac{d}{dt} f(y_t^*) = -\|\nabla f(y_t^*)\|_2^2$$

Minimization over $\mathcal{P}(\mathbb{R}^d)$

Minimize $\mathcal{H}(\mathbf{p}) = \mathcal{KL}\left(\mathbf{p} \| \mathbf{p}^*\right)$ using gradient flow $\mathbf{p}_t : \mathbb{R}^+ \to \mathcal{P}(\mathbb{R}^d)$ wrt W_2:

$$\min \quad \left(\frac{d}{dt} \mathcal{H}(\mathbf{p}_t) + \frac{1}{2} \left| \mathbf{p}_t' \right|^2 \right)$$

$$\frac{d}{dt} \mathcal{H}(\mathbf{p}_t) = \mathbb{E}_{x \sim \mathbf{p}_t} \left[\left\langle \nabla_x \frac{\partial \mathcal{H}}{\partial \mathbf{p}}(\mathbf{p}_t)(x), v_t(x) \right\rangle \right]$$

$$\frac{d}{dt} \mathcal{H}(\mathbf{p}_t^*) = -\mathbb{E}_{x \sim \mathbf{p}_t^*} \left[\left\| \nabla \frac{\partial \mathcal{H}}{\partial \mathbf{p}}(\mathbf{p}_t^*)(x) \right\|_2^2 \right]$$

Notation

- $\mathcal{P}(\mathbb{R}^d)$: set of densities over $\mathbb{R}^d$.
- $\mathcal{H}(\mathbf{p}) = \mathcal{KL}\left(\mathbf{p} \| \mathbf{p}^*\right) = \int \log \frac{p(x)}{p^*(x)} p(x)\, dx.$
- $W_2^2(p,q) = \inf_{\gamma \in \Gamma(p,q)} \mathbb{E}_{(x,y)\sim\gamma} \|x-y\|_2^2$, with
  $\Gamma(p,q)$: all joint distributions on $\mathbb{R}^d \times \mathbb{R}^d$ with marginals p and q.
- For a curve $\mathbf{p}_t : \mathbb{R}^+ \to \mathcal{P}(\mathbb{R}^d)$, the metric derivative is

  $$|\mathbf{p}_t'| = \lim_{h\to 0} \frac{W_2(\mathbf{p}_t, \mathbf{p}_{t+h})}{h}.$$
- If v_t is tangent to $\mathbf{p}_t$, then $|\mathbf{p}_t'|^2 = \mathbb{E}_{x\sim\mathbf{p}_t}\left[\|v_t(x)\|_2^2\right]$.
- Fréchet derivative: $\frac{\partial\mathcal{H}}{\partial\mathbf{p}_t}(\mathbf{p}_t) = 1 + \log\left(\frac{\mathbf{p}_t}{\mathbf{p}^*}\right)$.
- $\frac{d}{dt}\mathcal{H}(\mathbf{p}_t) = \mathbb{E}_{x\sim\mathbf{p}_t}\left[\left\langle \nabla_x \frac{\partial\mathcal{H}}{\partial\mathbf{p}_t}(\mathbf{p}_t)(x), v_t(x)\right\rangle\right]$

Analog with gradient flow over $\mathbb{R}^d$

Minimization over $\mathbb{R}^d$

m-strong convexity of f implies $f(y) - f(y^*) \leq \frac{1}{m}\|\nabla f(y)\|_2^2$.

Hence $\dfrac{d}{dt}\left(f(y_t) - f(y^*)\right) \leq -m(f(y_t) - f(y^*))$.

Minimization over $\mathcal{P}(\mathbb{R}^d)$

m-strong convexity of U implies m-geodesic-convexity of $\mathcal{H}(\mathbf{p})$ in W_2,

which implies $\mathcal{H}(\mathbf{p}) - \mathcal{H}(\mathbf{p}^*) \leq \frac{1}{m}\mathbb{E}_{x\sim\mathbf{p}}\left[\left\|\nabla \frac{\partial \mathcal{H}}{\partial \mathbf{p}}(\mathbf{p})(x)\right\|_2^2\right]$.

Hence $\dfrac{d}{dt}\left(\mathcal{H}(\mathbf{p}_t) - \mathcal{H}(\mathbf{p}^*)\right) \leq -m(\mathcal{H}(\mathbf{p}_t) - \mathcal{H}(\mathbf{p}^*))$.

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Xiang Cheng

Niladri Chatterji

Mike Jordan

Nesterov acceleration in $\mathcal{P}(\mathbb{R}^d)$

Underdamped Langevin MCMC: A non-asymptotic analysis.
Xiang Cheng, Niladri Chatterji, PB and Mike Jordan.
arXiv:1707.03663 [stat.ML]; COLT18.

Nesterov acceleration in sampling

Kramers' Equation (1940)

Stochastic differential equation:

$$\begin{aligned} dx_t &= v_t\, dt, \\ dv_t &= \underbrace{-v_t\, dt}_{\text{friction}} - \underbrace{\nabla U(x_t)\, dt}_{\text{acceleration}} + \sqrt{2}\, dB_t, \end{aligned}$$

where $x_t, v_t \in \mathbb{R}^d$, $U : \mathbb{R}^d \to \mathbb{R}$, dB_t is standard Brownian motion on $\mathbb{R}^d$.

Hendrick A. Kramers
wikipedia.org

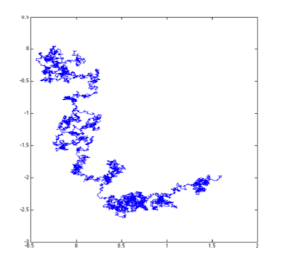
Define p_t as the density of (x_t, v_t).
Under mild regularity assumptions, $p_t \to p^*$:

$$p^*(x) \propto \exp\left(-U(x) - \frac{1}{2}\|v\|_2^2\right).$$

Nesterov acceleration in sampling

(Overdamped) Langevin Diffusion

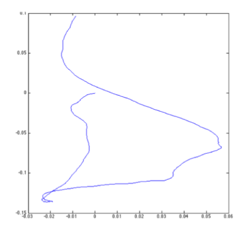
$$dx_t = -\nabla U(x_t)\,dt + \sqrt{2}\,dB_t.$$



Underdamped Langevin Diffusion

$$dx_t = v_t\,dt,$$

$$dv_t = -v_t\,dt - \nabla U(x_t)\,dt + \sqrt{2}\,dB_t.$$



Nesterov acceleration in sampling

Underdamped Langevin Markov Chain

Choose step-size η and simulate the SDE:

$$\begin{aligned} d\tilde{x}_t &= \tilde{v}_t\,dt \\ d\tilde{v}_t &= -\tilde{v}_t\,dt - \nabla U(\tilde{x}_{k\eta})\,dt + \sqrt{2}\,dB_t \end{aligned}$$

for $k\eta \le t < (k+1)\eta$.

(Not the standard Euler-Maruyama discretization.)

- A version of Hamiltonian Monte Carlo

  (Duane, Kennedy, Pendleton and Roweth, 1987), (Neal, 2011)

- How does the density p_k of $(\tilde{x}_{k\eta}, \tilde{v}_{k\eta})$ evolve?

Nesterov acceleration in sampling

Theorem

For smooth, strongly convex U, suitably small η and $k = \tilde{\Omega}\left(\frac{\sqrt{d}}{\epsilon}\right)$, underdamped Langevin MCMC gives $W_2(p_k, p^*) \leq \epsilon$.

Idea of proof: uses tools from (Eberle, Guillin and Zimmer, 2017)

Synchronous coupling (shared Brownian motion); strong convexity.

Significantly faster than overdamped Langevin:

For suitably small η and $k = \tilde{\Omega}\left(\frac{d}{\epsilon^2}\right)$, $W_2(p_k, p^*) \leq \epsilon$.

(Durmus and Moullines, 2016)

Related work

HMC (Lee and Vempala, 2017)

With separability assumption (Mangoubi and Smith, 2017), (Mangoubi and Vishnoi, 2018).

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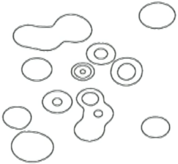
Nonconvex potentials

- Multi-modal p (nonconvex U)?



Xiang Cheng

Niladri Chatterji

Yasin Abbasi-Yadkori

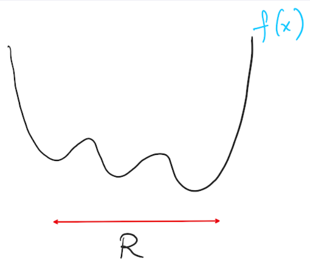
Mike Jordan

Sharp convergence rates for Langevin dynamics in the nonconvex setting.
Xiang Cheng, Niladri Chatterji, Yasin Abbasi-Yadkori, PB and Mike Jordan.
arXiv:1805.01648 [stat.ML].

Nonconvex potentials

Assumptions

- Smooth everywhere: $\nabla^2 U \preceq LI$.
- Strongly convex outside a ball:
  $\forall x, y,\ \|x - y\|_2 \geq R \Rightarrow U(x) \geq U(y) + \langle U(y), x - y\rangle + \frac{m}{2}\|x - y\|_2^2$.



Nonconvex potentials

Theorem

Suppose U is L-smooth and strongly convex outside a ball of radius R and η is suitably small.

1. If $k = \tilde{\Omega}\left(\frac{d}{\epsilon^2}\exp(LR^2)\right)$,
   then overdamped Langevin MCMC has $W_1(p_k, p^*) \leq \epsilon$.
2. If $k = \tilde{\Omega}\left(\frac{\sqrt{d}}{\epsilon}\exp(LR^2)\right)$,
   then underdamped Langevin MCMC has $W_1(p_k, p^*) \leq \epsilon$.

- We can think of LR^2 is a measure of non-convexity of U.
- The improvement from overdamped to underdamped is the same as in the convex case.

Nonconvex potentials

Idea of proof

- Synchronous coupling when far away; exploits strong convexity.
- Eberle's (2016) reflection coupling (1-D Brownian motion along the line between) when close: this 1-D random walk couples.
- Since it is in 1-D, the rate is not exponential in dimension.

Related work

- Weaker assumptions; exponential in dimension. (Raginsky, Rakhlin and Telgarsky, 2017)
- Stronger assumptions: mixtures of Gaussians. (Ge, Lee and Risteski, 2017)
- Metropolis-Hastings version. (Bou-Rabee, Eberle and Zimmer, 2018)

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Sampling Algorithms for Optimization

Xiang Cheng

Mike Jordan

Quantitative central limit theorems for discrete stochastic processes.
Xiang Cheng, PB and Mike Jordan.
arXiv:1902.00832 [math.ST].

Sampling Algorithms for Optimization

Parameter optimization in deep neural networks

- Use training data $(x_1, y_1), \ldots, (x_n, y_n) \in \mathcal{X} \times \mathcal{Y}$ to choose parameters θ of a deep neural network $f_\theta : \mathcal{X} \to \mathcal{Y}$.
- Aim to minimize loss $U(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f_\theta(x_i))$.
- Stochastic gradient: Random θ_0, $\qquad \theta_{k+1} = \theta_k - \eta \nabla \hat{U}_{\xi_k}(\theta_k)$,
- ... with minibatch gradient estimates, $\hat{U}_{\xi_k}(\theta) = \frac{1}{\xi_k} \sum_{i \in \xi_k} \ell(y_i, f_\theta(x_i))$

Sampling Algorithms for Optimization

- This has the form:

$$\begin{aligned} x_{k+1} &= x_k - \eta \nabla \hat{U}_{\xi_k}(x_k) \\ &= x_k - \eta \nabla U(x_k) + \sqrt{\eta}\, T_{\xi_k}(x_k), \end{aligned}$$

- ... which is suggestive of a Langevin diffusion but ...
- The noise $T_{\xi_k}(x) = \sqrt{\eta}\left(\nabla U(x) - \nabla \hat{U}_{\xi_k}(x)\right)$ is not Gaussian, and depends on x.
- What is the stationary distribution of x_k?
- How rapidly is it approached?

Sampling Algorithms for Optimization

Definitions

- $x_{k+1} = x_k - \eta \nabla U(x_k) + \sqrt{\eta} T_{\xi_k}(x_k)$, with $\xi_k \overset{iid}{\sim} q$.
- Define the covariance of the noise: $\sigma_x^2 := \mathbb{E}_\xi \left[T_\xi(x) T_\xi(x)^\top \right]$.
- Consider the SDE: $dx_t = -\nabla U(x_t)\, dt + \sqrt{2}\sigma_{x_t}\, dB_t$.
- Let p^* denote its stationary distribution.

Theorem

For U smooth, strongly convex, bounded third derivative, σ_x^2 uniformly bounded, $T_\xi(\cdot)$ smooth, bounded third derivatives, $\log p^*$ with bounded third derivatives,

If η is sufficiently small, $W_2(\hat{p}, p^*) \le \epsilon$, $(x_\infty \sim \hat{p})$

and for $k = \tilde{\Omega}\left(\frac{d^7}{\epsilon^2}\right)$, $W_2(p_k, p^*) \le \epsilon$. $(x_k \sim p_k)$

The classical CLT (with U quadratic) shows that the $1/\sqrt{k}$ rate is optimal.

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Further Work

- Optimization theory for sampling methods
  - Large scale problems: stochastic gradient estimates
  - Variance reduction with stochastic gradient estimates
  - Convergence in KL for underdamped Langevin, nonconvex
  - With constraints
  - Lower bounds
- Sampling methods for optimization
  - Stochastic gradient with momentum?
  - Nonconvex loss U?
  - Role of noise covariance in behavior of stochastic gradient method?

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