Adaptive Gradient Langevin Algorithms for Stochastic Optimization and Bayesian Inference

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PhD thesis publicly defended on September 11th, 2023

Outline

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1. Introduction
   - Optimization
   - Stochastic gradient descent algorithm
   - Langevin equation and algorithms
   - Objectives and Contributions

Optimization problem

Let $V : \mathbb{R}^d \to \mathbb{R}$,

Objective: $\underset{x \in \mathbb{R}^d}{\text{Minimize}} \quad V(x).$

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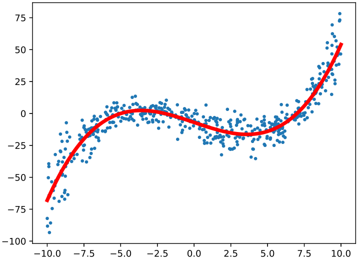
Examples:

1. Determining optimal allocation of resources to minimize production output while minimizing costs.
2. Maximize the gains along a controlled time process with respect to the strategy.
3. Minimize the error of a model to the true data for prediction and regression tasks.

Example: Regression and Neural Networks

- Data $(u_i, v_i) \in \mathbb{R}^{d_{\text{in}}} \times \mathbb{R}^{d_{\text{out}}}$ (inputs and outputs) for $1 \leq i \leq N$ with $N \gg 1$.



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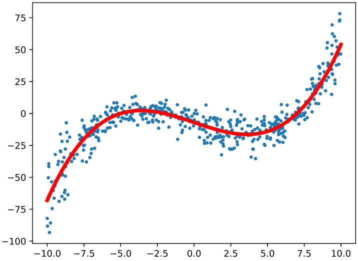
$$\text{Find } \Phi : \mathbb{R}^{d_{\text{in}}} \to \mathbb{R}^{d_{\text{out}}}$$
$$\text{such that: } \forall i,\ \Phi(u_i) \approx v_i.$$



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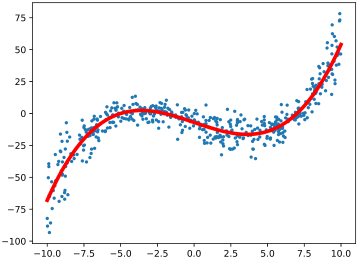

• We parametrize Φ with a finite number of parameters: $\{\Phi_x : x \in \mathbb{R}^d\}$. For example, affine parametrization:

$$\Phi_{x_1,x_2}(u) = x_1 \cdot u + x_2, \quad x_1 \text{ matrix, } x_2 \text{ vector.}$$

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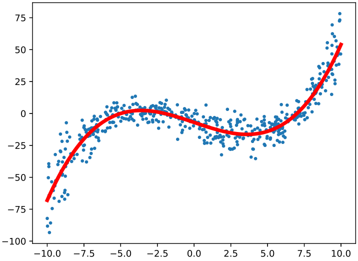

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• **Objective as an optimization problem:** minimize the MSE:

$$\min_{x \in \mathbb{R}^d} \frac{1}{N} \sum_{i=1}^{N} |\Phi_x(u_i) - v_i|^2 =: \min_{x \in \mathbb{R}^d} V(x).$$

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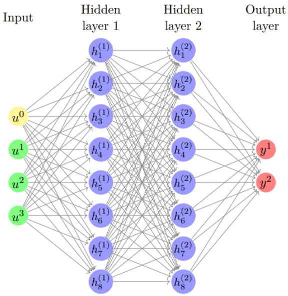
- **Neural Networks** are families of parametrized functions that can approximate many functions in practice (Cybenko, 1989), (AlexNet 2012).



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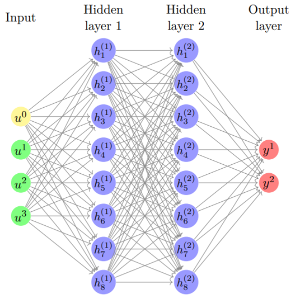
Input: $h_0 = u$,

$h_k = \varphi(\alpha_k \cdot h_{k-1} + \beta_k) \in \mathbb{R}^{d_k},\ 1 \leq k \leq K-1,$

Output: $h_K = \alpha_K \cdot h_{K-1} + \beta_K =: \Phi_{(\alpha_k,\beta_k)_{0\leq k\leq K}}(u)$



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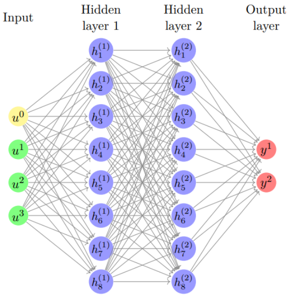
where

- φ is a non-linear function applied coordinate-wise,
- (d_k) is a sequence of dimensions,
- $(\alpha_k)_k$ are matrices and $(\beta_k)_k$ are vectors parametrizing the neural network.

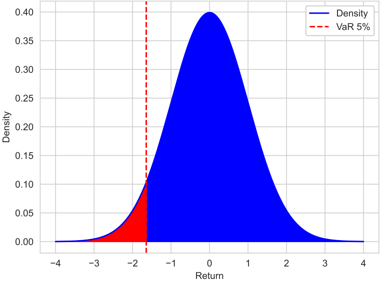


Example: Computation of quantiles and VaR

For Z some random variable, the quantile of order $\alpha \in [0,1]$ is

$$q_\alpha := \inf\{u \in \mathbb{R} : \mathbb{P}(Z \leq u) \geq \alpha\}.$$

In finance, q_α is called **Value at Risk** and is widely used for risk management (Jorion, 1996).



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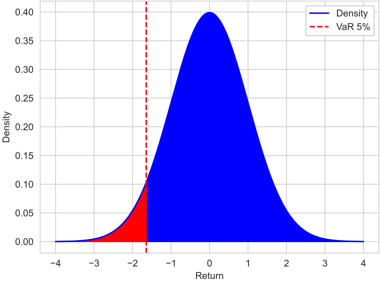
Following (Uryasev and Rockafellar, 2001) we have the characterization:

$$q_\alpha = \underset{x\in\mathbb{R}}{\text{argmin}} \ \mathbb{E}\left[x + \frac{1}{1-\alpha}(Z-x)_+\right],$$

where $(\cdot)_+$ denotes the positive part.



Example: Stochastic control

- Dynamical stochastic system Y_t depending on some control u_t with Brownian motion W_t:
$$dY_t^u = b(Y_t^u, u_t)dt + \sigma(Y_t^u, u_t)dW_t, \ \ t \in [0, T].$$

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- We can parametrize u by some neural network with parameter x:

$$u_t = u_x(t, Y_t)$$

and obtain an optimization problem on x with $V(x) = J(u_x)$.

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Gradient Descent Algorithm (GD)

Gradient descent algorithm: Assuming that $V \in \mathcal{C}^1$, for each iteration compute the gradient and "go down" the gradient with non-increasing positive step sequence (γ_k):

Gradient Descent Algorithm

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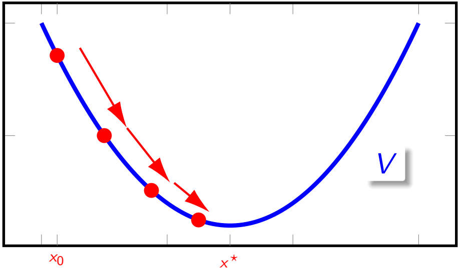

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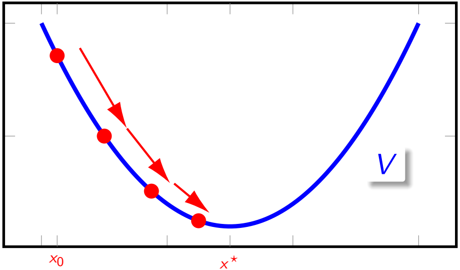

$\Longrightarrow$ Greedy algorithm: focus on local improvements around the current position at each iteration.

Example of Gradient Descent

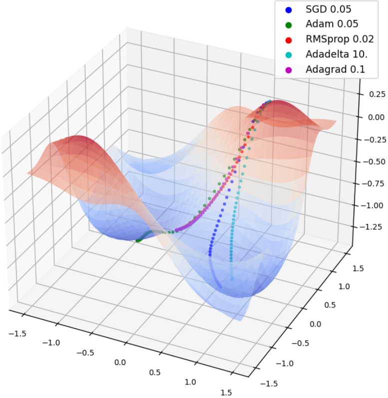

Figure: Example of different variants of gradient descent algorithms with $V(x, y) = -\sin(x^2)\cos(3y^2)e^{-x^2y^2} - e^{-(x+y)^2}$.

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3. Remark: in the 1st case we can also write:

$$V(x) = \mathbb{E}_Z[v(x, Z)], \quad Z \in \{1, \dots, N\}, \quad v(x, Z) = V_Z(x).$$

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Stochastic Gradient Descent Algorithm, Mini-Batch version

With initialization $x_0 \in \mathbb{R}^d$ and step sequence (γ_k):

$$x_{n+1} = x_n - \gamma_{n+1} \frac{1}{M} \sum_{i=1}^{M} \nabla v(x_n, Z_{n+1}^i),$$
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Introduced in (Robbins and Monro, 1951); Robbins-Siegmund Lemma of convergence (Robbins and Siegmund, 1971).

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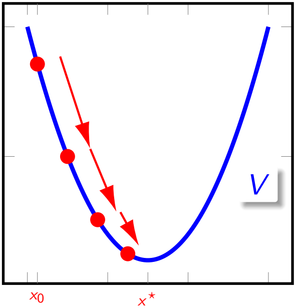
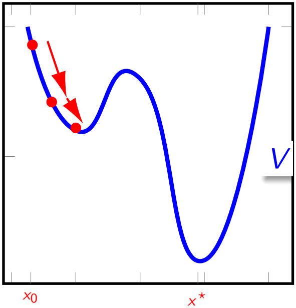
Problem: traps for gradient descent

The gradient descent x_n can be trapped in a local (but not global) minimum (e.g. if V is not convex):





Langevin Equation

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Stochastic Gradient Langevin Dynamics (SGLD), (Welling and Teh, 2011)

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- The continuous version becomes:

Langevin equation

$$dX_s = -\nabla V(X_s) ds + \sigma dW_s$$

where (W_s) is a Brownian motion.

- Its invariant measure is the **Gibbs measure**

$$\nu_\sigma(x) dx \propto e^{-2V(x)/\sigma^2} dx.$$

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- For small σ, ν_σ is concentrated around argmin(V):
Solve the Langevin equation $\implies$ approximation of ν_σ $\implies$ approximation of argmin(V).

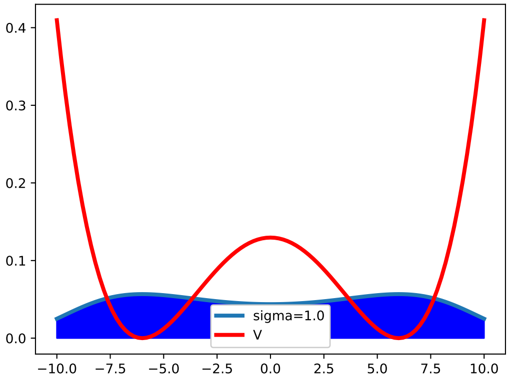
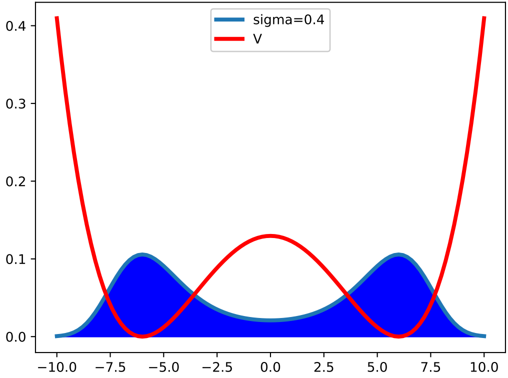


Figure: Concentration of Gibbs measure



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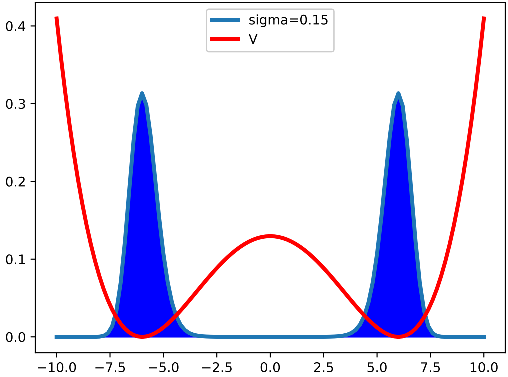

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Bayesian inference and sampling from distribution

Stochastic algorithms are also used for sampling from a probability measure.

- Given data $u_1, \dots, u_N$ with $N \gg 1$, we consider a family of probability distributions $\{p(u|x)du : \; x \in \mathbb{R}^d\}$ and a prior densities $p_0(x)dx$. Then the posterior distribution on x, $p(x|u_1, \dots, u_N)$, has density proportional to

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$$V(x) := -\log(p_0(x)) - \log(p(u_1|x)) - \cdots - \log(p(u_N|x)),$$

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$$\bar{X}_{n+1} = \bar{X}_n + \gamma_{n+1} b(\bar{X}_n) + \sqrt{\gamma_{n+1}}\sigma(\bar{X}_n)U_{n+1}, \quad U_n \sim \mathcal{N}(0, I_d) \text{ i.i.d.},$$
$$\nu_n := \frac{1}{\Gamma_n}\sum_{k=1}^{n} \gamma_k \delta_{\bar{X}_k}, \quad \Gamma_n = \gamma_1 + \ldots + \gamma_n.$$

- (Durmus and Moulines, 2017, 2019; Brosse et al., 2019) focus on the Langevin equation.

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$$x_{n+1} = x_n - \gamma_{n+1} \nabla V(x_n) + a(\gamma_1 + \cdots + \gamma_{n+1}) \sigma \sqrt{\gamma_{n+1}} \xi_{n+1}, \quad \xi_{n+1} \sim \mathcal{N}(0, I_d),$$

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- The 'instantaneous' invariant measure $\nu_{a(t)\sigma}(dx) \propto \exp\left(-2V(x)/(a^2(t)\sigma^2)\right)$ converges itself to argmin(V)

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- The 'instantaneous' invariant measure $\nu_{a(t)\sigma}(dx) \propto \exp\left(-2V(x)/(a^2(t)\sigma^2)\right)$ converges itself to $\mathrm{argmin}(V)$
- Schedule $a(t) = A\log^{-1/2}(t)$ then $X_t \underset{t\to\infty}{\longrightarrow} \mathrm{argmin}(V)$ in law (Chiang et al., 1987; Miclo, 1992), (Monmarché, Fournier, and Tardif, 2021)

Langevin Simulated Annealing

- Another possibility : make $\sigma \to 0$ while iterating the algorithm:

$$x_{n+1} = x_n - \gamma_{n+1}\nabla V(x_n) + a(\gamma_1 + \cdots + \gamma_{n+1})\sigma\sqrt{\gamma_{n+1}}\xi_{n+1}, \quad \xi_{n+1} \sim \mathcal{N}(0, I_d),$$

where $a(t)$ is decreasing and $a(t) \underset{t\to\infty}{\longrightarrow} 0$.
The continuous version becomes :

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- (Gelfand and Mitter, 1991): the convergence of the algorithm (x_n) .

Multiplicative noise and Adaptive algorithms

- Noise $\sigma > 0 \implies$ isotropic, homogeneous noise $\implies$ not adapted to V.

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$$dY_t = -(\sigma\sigma^\top \nabla V)(Y_t)dt + a(t)\sigma(Y_t)dW_t + \underbrace{\left(a^2(t) \left[\sum_{j=1}^{d} \partial_i(\sigma\sigma^\top)(Y_t)_{ij} \right]_{1 \le i \le d} \right)}_{\text{correction term} \quad \Upsilon(Y_t)} dt$$

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• Correction term so that $\nu_{a(t)} \propto \exp\left(-2V(x)/a^2(t)\right)$ is still the "instantaneous" invariant measure (Li et al., 2016; Pagès and Panloup, 2023).

Outline

1. Introduction
   - Optimization
   - Stochastic gradient descent algorithm
   - Langevin equation and algorithms
   - Objectives and Contributions

Part I: Convergence of Langevin algorithms

- Convergence of the Langevin equation Y_t with multiplicative noise to $\text{argmin}(V)$ as well as the discretized scheme $\bar{Y}_t$.
- Weak convergence for Wasserstein-1 and Total Variation.
- For $\mathcal{D} = \mathcal{W}_1$ or d_{TV} and $\nu^\star$ being the target measure, we have

$$\mathcal{D}(Y_t, \nu^\star) \leq \mathcal{D}(Y_t, \nu_{a(t)}) + \mathcal{D}(\nu_{a(t)}, \nu^\star)$$

$\implies$ Investigate the rate of $\mathcal{D}(\nu_a, \nu^\star)$ as $a \to 0$, including cases where $\nabla^2 V(x)$ is not positive definite for some $x \in \text{argmin}(V)$.

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Contributions:

1. Pierre Bras and Gilles Pagès. *Convergence of Langevin-Simulated Annealing algorithms with multiplicative noise*. *Mathematics of Computation*, 2023, and presented to the conference *MCM23*.
2. Pierre Bras and Gilles Pagès. *Convergence of Langevin-Simulated Annealing algorithms with multiplicative noise II: Total Variation*. *Monte Carlo Methods and Applications*, 29(3):203–219, 2023.
3. Pierre Bras. *Convergence rates of Gibbs measures with degenerate minimum*. *Bernoulli*, 28(4):2431 – 2458, 2022.

Part II: Adaptive Langevin algorithms for deep neural networks

- Implement Langevin algorithms for different choices of σ (Adam, RMSprop, Adadelta etc) and compare with their corresponding non-Langevin counterpart.
- Investigate the benefits of Langevin algorithms on very deep learning: image classification, deep stochastic control.
- (on-going) Introduce deep pathwise variance reduction for SDEs with reinforcement learning approaches.

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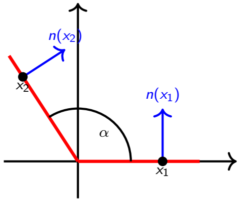
Contributions:

1. Pierre Bras. *Langevin algorithms for very deep Neural Networks with application to image classification*. *Procedia Computer Science*, 222:303 – 310, 2023, and presented at a workshop of IJCNN23.
2. Pierre Bras and Gilles Pagès. *Langevin algorithms for Markovian Neural Networks and Deep Stochastic control*. *IJCNN23 Proceedings*, 2023.
3. Pierre Bras and Gilles Pagès. *Policy Gradient Optimal Correlation Search for Variance Reduction in Monte Carlo simulation and Maximum Optimal Transport*. *arXiv e-prints*, page arXiv:2307.12703, 2023.

Part III: Numerical Simulation of Stochastic processes

• For Part I, we need bounds for d_{TV} between a stochastic process and its Euler scheme **in small time**. We use a multi-level Richardson-Romberg method.



• We study weak error rates of numerical schemes for (regular) stochastic Volterra equations, having in mind the rough case:

$$X_t = X_0 + \int_0^t K_1(t,s)b(X_s)ds + \int_0^t K_2(t,s)\sigma(X_s)dW_s.$$

• We study the Brownian motion in $\mathbb{R}^2$ which is stopped or reflected on a wedge; we give density formulas as well as simulation algorithms.

Contributions:

1. Pierre Bras, Gilles Pagès, and Fabien Panloup. *Total variation distance between two diffusions in small time with unbounded drift: application to the Euler-Maruyama scheme.*. *Electron. J. Probab.*, 27:1–19, 2022.
2. Pierre Bras and Masaaki Fukasawa. *Weak error rates for numerical schemes of non-singular Stochastic Volterra equations with application to option pricing under path-dependent volatility*. *In review*.
3. Pierre Bras and Arturo Kohatsu-Higa. *Simulation of reflected Brownian motion on two dimensional wedges. Stochastic Process. Appl.*, 156:349–378, 2023.

Outline

2 Convergence of adaptive Langevin-Simulated Annealing algorithms
- Convergence of Langevin-Simulated Annealing algorithms for $\mathcal{W}_1$ and d_{TV}
- Convergence rates of Gibbs measures with degenerate minimum

Outline

2. Convergence of adaptive Langevin-Simulated Annealing algorithms
   - Convergence of Langevin-Simulated Annealing algorithms for $\mathcal{W}_1$ and d_{TV}
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Objectives and assumptions

$$dY_t = -(\sigma\sigma^\top \nabla V)(Y_t)dt + a(t)\sigma(Y_t)dW_t + \underbrace{\left(a^2(t)\left[\sum_{j=1}^{d} \partial_i(\sigma\sigma^\top)(Y_t)_{ij}\right]_{1\leq i\leq d}\right)}_{\text{correction term} \quad \Upsilon(Y_t)} dt$$

$a(t) = A/\sqrt{\log(t)}$,

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Prove the convergence of Y_t to $\nu^\star$ for $\mathcal{W}_1$ and d_{TV}:

$$\mathcal{W}_1(X,Y) = \sup\left\{\left|\mathbb{E}[f(X)] - \mathbb{E}[f(Y)]\right| : [f]_{\text{Lip}} = 1\right\},$$

$$d_{TV}(X,Y) = \sup\left\{\left|\mathbb{E}[f(X)] - \mathbb{E}[f(Y)]\right| : \sup_{\mathbb{R}^d} f = 1\right\}.$$

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Important assumptions (Pagès and Panloup, 2023):

1. V is strongly convex outside some compact set, ∇V is Lipschitz.
2. σ is bounded and elliptic: $\sigma\sigma^\top \ge \sigma_0 I_d$, $\sigma_0 > 0$.

Domino strategy

- *Domino strategy:* (Pagès and Panloup, 2023) for f 1-Lipschitz, P^1, P^2 kernels of processes X, Y, (γ_n) step sequence and $\Gamma_n := \gamma_1 + \cdots + \gamma_n$, we have:

$$\begin{aligned}
\mathcal{W}_1(Y_{\Gamma_n}, X_{\Gamma_n}) &\leq |\mathbb{E}f(Y_{\Gamma_n}) - \mathbb{E}f(X_{\Gamma_n})| \\
&= |P^2_{\gamma_1} \circ \cdots \circ P^2_{\gamma_n} f(x) - P^2_{\Gamma_n} f(x)| \\
&= \left| \sum_{k=1}^{n} P^2_{\gamma_1} \circ \cdots \circ P^2_{\gamma_{k-1}} \circ (P^2_{\gamma_k} - P^1_{\gamma_k}) \circ P^1_{\Gamma_n - \Gamma_k} f(x) \right| \\
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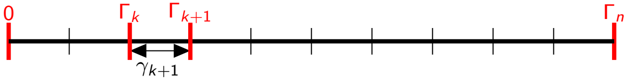

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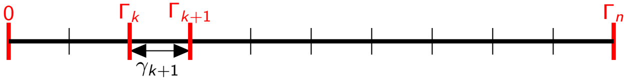

In the sum we bound two types of terms:

1. For large k $\implies$ Error in small time $\implies$ use bounds for $\|X^x_t - Y^x_t\|_p$
2. For small k $\implies$ Ergodic properties (Eberle, 2016; Wang, 2020).

Plan of the proof

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$$a_n = A\log^{-1/2}(T_n),$$

and obtain ergodic bounds for $\mathcal{W}_1(X_{T_{n+1}}, \nu_{a_{n+1}})$; then

$$\mathcal{W}_1(X_{T_n}, \nu^\star) \leq \mathcal{W}_1(X_{T_n}, \nu_{a_n}) + \mathcal{W}_1(\nu_{a_n}, \nu^\star) \to 0.$$

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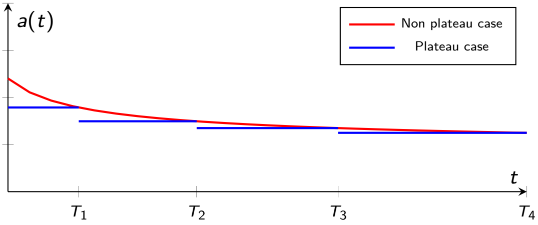
- We then use the *domino strategy* to give bounds on $\mathcal{W}_1(X_{T_n}, Y_{T_n})$:

$$\mathcal{W}_1(Y_{T_n}, \nu^\star) \leq \mathcal{W}_1(Y_{T_n}, X_{T_n}) + \mathcal{W}_1(X_{T_n}, \nu^\star) \to 0.$$


a(t)
Non plateau case
Plateau case
t
T1
T2
T3
T4

Convergence of the Euler scheme with decreasing steps

Euler-Maruyama scheme

$$\bar{Y}^{x_0}_{\Gamma_{n+1}} = \bar{Y}_{\Gamma_n} + \gamma_{n+1}\left(b_{a(\Gamma_n)}(\bar{Y}^{x_0}_{\Gamma_n}) + \zeta_{n+1}(\bar{Y}^{x_0}_{\Gamma_n})\right) + a(\Gamma_n)\sigma(\bar{Y}^{x_0}_{\Gamma_n})(W_{\Gamma_{n+1}} - W_{\Gamma_n})$$

γ_{n+1} decreasing to 0, $\sum_n \gamma_n = \infty$, $\sum_n \gamma_n^2 < \infty$, $\Gamma_n = \gamma_1 + \cdots + \gamma_n$,

$\forall x,\ \mathbb{E}[\zeta_n(x)] = 0$ (mini-batch noise).

$\Longrightarrow$ Same strategy of proof.

Total variation case

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$$\begin{aligned} |f(X_t) - f(Y_t)| &\leq [f]_{\mathrm{Lip}} |X_t - Y_t| && \text{if } f \text{ is Lipschitz.} \\ |f(X_t) - f(Y_t)| &\leq ??? && \text{if } f \text{ is bounded.} \end{aligned}$$

- We investigate d_{TV} bounds in short time for general SDEs:

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- We investigate d_{TV} bounds in short time for general SDEs:

For $\quad dX_t = b_1(X_t)dt + \sigma_1(X_t)dW_t, \quad dY_t = b_2(Y_t)dt + \sigma_2(Y_t)dW_t,$
$\quad X_0 = Y_0, \quad \sigma_1(X_0) = \sigma_2(Y_0),$

then

$$\mathrm{d}_{\mathrm{TV}}(X_t, Y_t) \le Ct^{1/2}e^{c\sqrt{\log(1/t)}}.$$

These results uses:

Theorem

Let Z_1 and Z_2 be two random vectors admitting densities p_1 and p_2. Then

$$\mathrm{d}_{\mathrm{TV}}(Z_1, Z_2) \leq C_{d,r} \mathcal{W}_1(Z_1, Z_2)^{2r/(2r+1)} \left(\int_{\mathbb{R}^d} \left(\|\nabla^{2r} p_1(\xi)\| + \|\nabla^{2r} p_2(\xi)\| \right) d\xi \right)^{1/(2r+1)}.$$

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We use a **weighted multi-level Richardson-Romberg extrapolation** (Giles, 2008; Lemaire and Pagès, 2017):

- $f_\varepsilon(x) := \mathbb{E}[f(x + \varepsilon^{1/2}\zeta)]$ is Lipschitz, $\quad \zeta \sim \mathcal{N}(0, I_d)$,
- Taylor expansion of $y \mapsto \mathbb{E}[f(Z_1 + y)]$,
- $$|\mathbb{E}f(Z_1) - \mathbb{E}f(Z_2)| \le \left| \mathbb{E}f(Z_1) - \sum_{i=1}^r w_i \mathbb{E}f_{\varepsilon/n_i}(Z_1) \right| + \left| \sum_{i=1}^r w_i \mathbb{E}f_{\varepsilon/n_i}(Z_1) - \sum_{i=1}^r w_i \mathbb{E}f_{\varepsilon/n_i}(Z_2) \right| + \left| \sum_{i=1}^r w_i \mathbb{E}f_{\varepsilon/n_i}(Z_2) - \mathbb{E}f(Z_2) \right|,$$
- We choose w_i and n_i to cancel all the terms up to $i = r - 1$.

Outline

2. Convergence of adaptive Langevin-Simulated Annealing algorithms
   - Convergence of Langevin-Simulated Annealing algorithms for $\mathcal{W}_1$ and d_{TV}
   - Convergence rates of Gibbs measures with degenerate minimum

- To get the convergence of Langevin algorithms, we need the convergence of

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$$\nu_a(x) \propto \exp\left(-2V(x)/a^2\right),$$
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- It is known to be of order a if $\mathrm{argmin}(V)$ is finite and $\nabla^2 V(x_i^\star) > 0$ for all $x_i^\star \in \mathrm{argmin}(V)$ (Hwang, 1980, 1981). Then

$$\nu^\star = \left(\sum_i \det(\nabla^2 V(x_i^\star))^{-1/2}\right)^{-1} \sum_i \det(\nabla^2 V(x_i^\star))^{-1/2} \delta_{x_i^\star}.$$

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- We investigate the case where $\text{argmin}(V)$ is finite with **degenerate minimum**.
- This happens in practice when training over-parametrized neural networks (Sagun, Bottou, and LeCun, 2016):

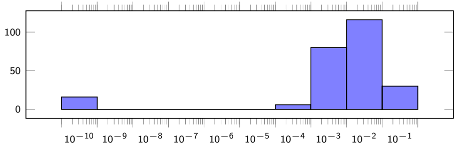

Figure: Distribution of the eigenvalues of the Hessian matrix at the end of training of a neural network on the MNIST dataset.

Considering recursively the spaces of cancellation of $\nabla^{2k}V$, we obtain:

Theorem

Assume that $\text{argmin}(V) = \{x^\star\}$. Define (F_k) recursively as

$$F_0 = \mathbb{R}^d,\ F_k = \{h \in F_{k-1} :\ \forall h' \in F_{k-1},\ \nabla^{2k}V(x^\star)\cdot h \otimes h'^{\otimes 2k-1} = 0\}$$

and E_k the orthogonal complement of F_k in F_{k-1}. Let B a basis adapted to $\mathbb{R}^d = E_1 \oplus \cdots \oplus E_p$ and $\alpha_i = 1/(2j)$ on the subspace E_j, then if $X \sim \nu_a$:

$$\left(\frac{1}{a^{2\alpha_1}}, \dots, \frac{1}{a^{2\alpha_d}}\right) * (B^{-1}\cdot(X_{a^2} - x^\star)) \to X \ \text{ as } a \to 0,\ \text{in law},$$

where X has a density proportional to $e^{-g(x)}$ with

$$g(x) = \sum_{k=2}^{2p}\frac{1}{k!}\sum_{\substack{i_1,\dots,i_p\in\{0,\dots,k\}\\ i_1+\cdots+i_p=k\\ \frac{i_1}{2}+\cdots+\frac{i_p}{2p}=1}}\binom{k}{i_1,\dots,i_p}\nabla^k V(x^\star)\cdot p_{E_1}(B\cdot x)^{\otimes i_1}\otimes\cdots\otimes p_{E_p}(B\cdot x)^{\otimes i_p}.$$

(Extension of (Athreya and Hwang, 2010)).

Outline

3. Adaptive Langevin algorithms for Neural Networks
   - Langevin versus non-Langevin for very deep learning
   - Langevin algorithms for Markovian Neural Networks and Deep Stochastic control
   - Policy Gradient Optimal Correlation Search for Variance Reduction in Monte Carlo simulation and Maximum Optimal Transport

Outline

3 Adaptive Langevin algorithms for Neural Networks

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Preconditioned Langevin Gradient Descent

Preconditioned Langevin Gradient Descent (Li et al., 2016)

For some preconditioner rule P_{n+1} depending on the previous updates of the gradient ($g_n \simeq \nabla V(\theta_n)$) and $\sigma > 0$:

$$\begin{aligned} \text{Preconditioned Gradient Descent:} \quad & \theta_{n+1} = \theta_n - \gamma_{n+1} P_{n+1} \cdot g_{n+1}, \\ \text{Preconditioned Langevin:} \quad & \theta_{n+1} = \theta_n - \gamma_{n+1} P_{n+1} \cdot g_{n+1} + \sigma \sqrt{\gamma_{n+1}} \mathcal{N}(0, \boldsymbol{P_{n+1}}) \end{aligned}$$

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For some preconditioner rule P_{n+1} depending on the previous updates of the gradient ($g_n \simeq \nabla V(\theta_n)$) and $\sigma > 0$:

$$\text{Preconditioned Gradient Descent:} \quad \theta_{n+1} = \theta_n - \gamma_{n+1} P_{n+1} \cdot g_{n+1},$$

$$\text{Preconditioned Langevin:} \quad \theta_{n+1} = \theta_n - \gamma_{n+1} P_{n+1} \cdot g_{n+1} + \sigma\sqrt{\gamma_{n+1}}\mathcal{N}(0, \boldsymbol{P_{n+1}})$$

- Per-dimension adaptive step size.
- Adding noise is known to improve the learning in some cases. (Neelakantan et al., 2015; Anirudh Bhardwaj, 2019; Gulcehre et al., 2016)

Examples of gradient algorithms

Algorithm Adam (Kingma and Ba, 2015)

Parameters: $\beta_1, \beta_2, \lambda > 0$
$M_{n+1} = \beta_1 M_n + (1 - \beta_1) g_{n+1}$
$\mathrm{MS}_{n+1} = \beta_2 \,\mathrm{MS}_n + (1 - \beta_2) g_{n+1} \odot g_{n+1}$
$\widehat{M}_{n+1} = M_{n+1}/(1 - \beta_1^{n+1})$
$\widehat{\mathrm{MS}}_{n+1} = \mathrm{MS}_{n+1}/(1 - \beta_2^{n+1})$
$P_{n+1} = \mathrm{diag}\left(\mathbb{1} \oslash \left(\lambda \mathbb{1} + \sqrt{\widehat{\mathrm{MS}}_{n+1}}\right)\right)$
$\theta_{n+1} = \theta_n - \gamma_{n+1} P_{n+1} \cdot \widehat{M}_{n+1}.$

Algorithm RMSprop (Tieleman and Hinton, 2012)

Parameters: $\alpha, \lambda > 0$
$\mathrm{MS}_{n+1} = \alpha \,\mathrm{MS}_n + (1 - \alpha) g_{n+1} \odot g_{n+1}$
$P_{n+1} = \mathrm{diag}\left(\mathbb{1} \oslash \left(\lambda \mathbb{1} + \sqrt{\mathrm{MS}_{n+1}}\right)\right)$
$\theta_{n+1} = \theta_n - \gamma_{n+1} P_{n+1} \cdot g_{n+1}$

Algorithm Adadelta (Zeiler, 2012)

Parameters: $\beta_1, \beta_2, \lambda > 0$
$\mathrm{MS}_{n+1} = \beta_1 \,\mathrm{MS}_n + (1 - \beta_1) g_{n+1} \odot g_{n+1}$
$P_{n+1} = \mathrm{diag}\left((\lambda \mathbb{1} + \widehat{\mathrm{MS}}_n) \oslash \left(\lambda \mathbb{1} + \sqrt{\widehat{\mathrm{MS}}_n}\right)\right)$
$\theta_{n+1} = \theta_n - \gamma_{n+1} P_{n+1} \cdot g_{n+1}.$
$\widehat{\mathrm{MS}}_{n+1} = \beta_2 \,\mathrm{MS}_n + (1 - \beta_2)(\theta_{n+1} - \theta_n) \odot (\theta_{n+1} - \theta_n).$

Training very deep Neural Networks

- Very deep neural networks are crucial, in particular in image classification (He et al., 2016).
- However much more difficult to train: much more "non-linear", local traps, vanishing gradients (Dauphin et al., 2014).
- (Neelakantan et al., 2015): hints that noisy optimizers bring more improvements.

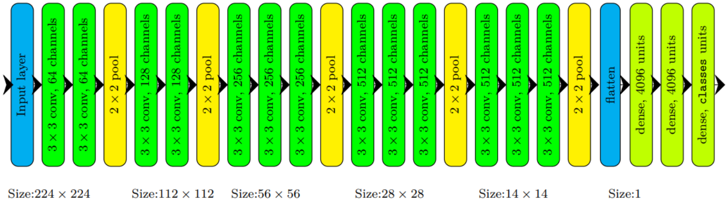

Figure: Architecture of the VGG-16 network for an input image of size 224 × 224.

We compare Preconditioned Langevin optimizers with their non-Langevin counterparts while increasing the depth of the networkon the MNIST, CIFAR-10 and CIFAR-100 datasets.

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We implement the package `langevin_optimizers` for ready-to-use `TensorFlow` optimizers using the method `_resource_apply_dense` from the base class `tf.keras.optimizers.Optimizer`.

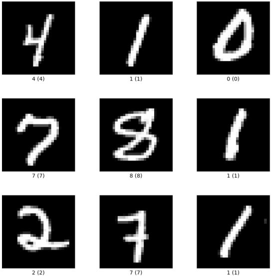


Figure: MNIST image dataset

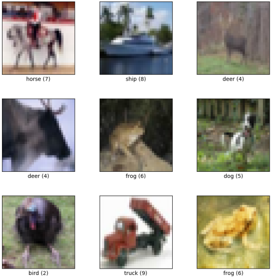


Figure: CIFAR-10 image dataset

Results for dense (fully connected) networks

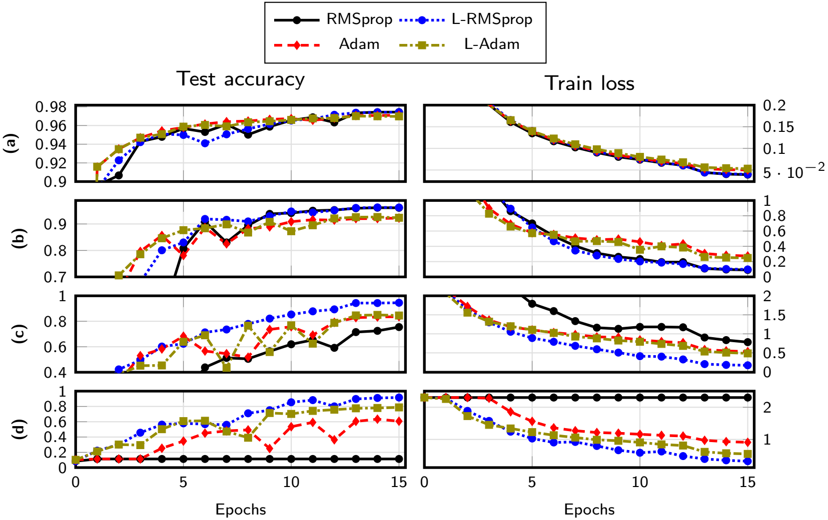


Figure: Training of neural networks of various depths on the MNIST dataset using Langevin algorithms compared with their non-langevin counterparts. (a): 3 hidden layers, (b): 20 hidden layers, (c): 30 hidden layers, (d): 40 hidden layers.

Layer Langevin Algorithm

Idea: The deepest layers of the network bear the most non-linearities $\implies$ are more subject to Langevin optimization

Layer Langevin Algorithm

$$\theta_{n+1}^{(i)} = \theta_n^{(i)} - \gamma_{n+1}[P_{n+1} \cdot g_{n+1}]^{(i)} + \mathbb{1}_{i \in \mathcal{J}} \sigma \sqrt{\gamma_{n+1}} \left[\mathcal{N}(0, P_{n+1})\right]^{(i)},$$

where $\mathcal{J}$: subset of weight indices; P_n: preconditioner.

We choose $\mathcal{J}$ to be the first k layers.

An example of Layer Langevin optimization

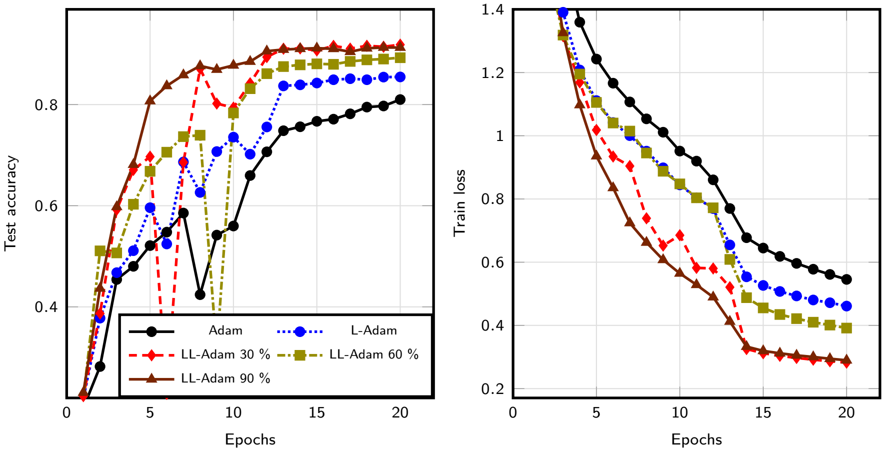


Figure: Layer Langevin comparison on a dense neural network with 30 hidden layers on the MNIST dataset.

Application to deep architectures for image classification

- Typical architecture in image recognition: Succession of convolutional layers with non-linearities (ReLU) (Simonyan and Zisserman, 2015)
- Residual connections: each layer behaves in part like the identity layer to pass the information through the successive layers (He et al., 2016; Huang et al., 2017).

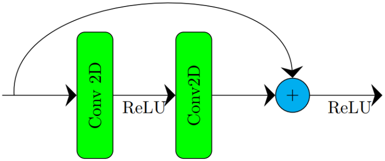
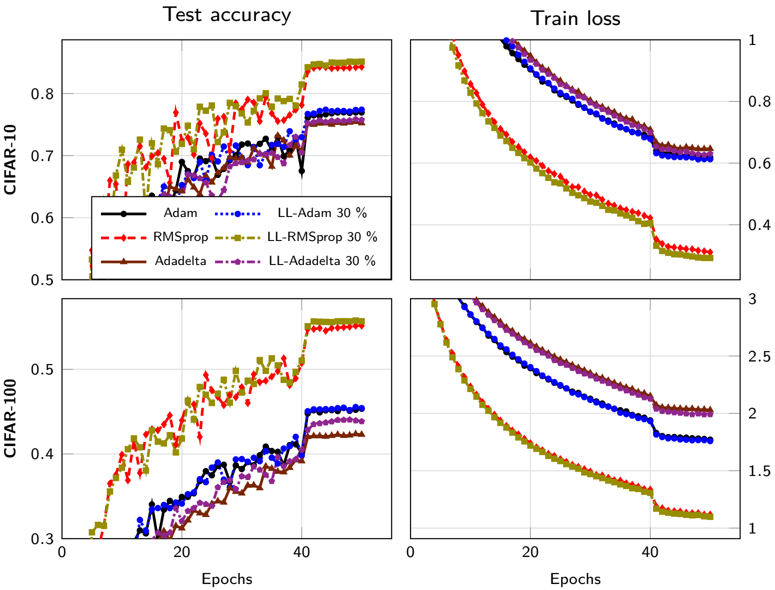


Figure: ResNet elementary block

Layer Langevin for training of ResNet-20



Outline

3 Adaptive Langevin algorithms for Neural Networks
- Langevin versus non-Langevin for very deep learning
- Langevin algorithms for Markovian Neural Networks and Deep Stochastic control
- Policy Gradient Optimal Correlation Search for Variance Reduction in Monte Carlo simulation and Maximum Optimal Transport

Stochastic control

$$\min_u J(u) := \mathbb{E}\left[\int_0^T G(Y_t)dt + F(Y_T)\right],$$
$$dY_t = b(Y_t, u_t)dt + \sigma(Y_t, u_t)dW_t, \ \ t \in [0, T],$$

G: path-dependent return, F: final return, u_t: control, Y_t: trajectory.

Discretization and numerical scheme

Euler-Maruyama scheme

$$\min_{\theta} \bar{J}(\bar{u}_\theta) := \mathbb{E}\Big[\sum_{k=0}^{N-1}(t_{k+1}-t_k)G(\bar{Y}^\theta_{t_{k+1}}) + F(\bar{Y}^\theta_{t_N})\Big],$$

$$\bar{Y}^\theta_{t_{k+1}} = \bar{Y}^\theta_{t_k} + (t_{k+1}-t_k)b\big(\bar{Y}^\theta_{t_k}, \bar{u}_{k,\theta}(\bar{Y}^\theta_{t_k})\big) + \sqrt{t_{k+1}-t_k}\,\sigma\big(\bar{Y}^\theta_{t_k}, \bar{u}_{k,\theta}(\bar{Y}^\theta_{t_k})\big)\xi_{k+1},$$

$\xi_k \sim \mathcal{N}(0, I_{d_2})$ i.i.d.

- **Time discretization** of $[0, T]$: $t_k := kT/N,\ k \in \{0, \dots, N\}, \quad h := T/N.$
- **Control** u with **parameter** θ using either one time-dependant neural network either N distinct neural networks: $u_{t_k} = \bar{u}_\theta(t_k, Y_{t_k})$ or $u_{t_k} = \bar{u}_{\theta^k}(Y_{t_k})$

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- We refer to (Gobet and Munos, 2005; Han and E, 2016).
- The gradient is computed by recursively tracking the dependency of along the trajectory (Giles and Glasserman, 2005; Giles, 2007).

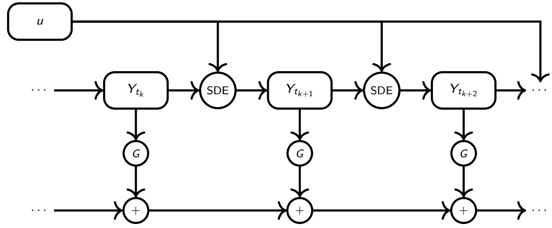

Figure: Markovian Neural Network with one control.

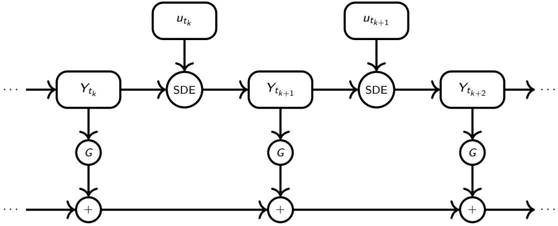

Figure: Markovian neural network with one control for every time step. Layer Langevin algorithms can be used in this case.

Fishing quotas, (Laurière, Pagès, and Pironneau, 2023)

Fish biomass $Y_t \in \mathbb{R}^{d_1}$ with:

- Inter-species interaction κY_t
- Fishing following imposed quotas u_t
- Objective: keep Y_t close to an ideal state $\mathcal{Y}_t$.

Figure: Source: Unsplash

$$dY_t = Y_t * ((r - u_t - \kappa Y_t)dt + \eta dW_t)$$
$$J(u) = \mathbb{E}\left[\int_0^T (|Y_t - \mathcal{Y}_t|^2 - \langle \alpha, u_t \rangle)dt + \beta[u]^{0,T}\right]$$

Deep Financial Hedging, (Buehler, Gonon, Teichmann, and Wood, 2019)

We aim to replicate some payoff Z defined on some portfolio S_t by trading some of the assets with transaction costs; the control u_t is the amount of held assets. The objective is

Figure: Source: Unsplash

$$J(u) = \nu\left(-Z + \sum_{k=0}^{N-1}\langle u_{t_k}, S_{t_{k+1}} - S_{t_k}\rangle - \sum_{k=0}^{N}\langle c_{tr}, S_{t_k} * |u_{t_k} - u_{t_{k-1}}|\rangle\right)$$

where ν is a convex risk measure. We consider the assets S_t to be follow a Heston model and are tradable along with variance swap options.

Results for Deep Hedging

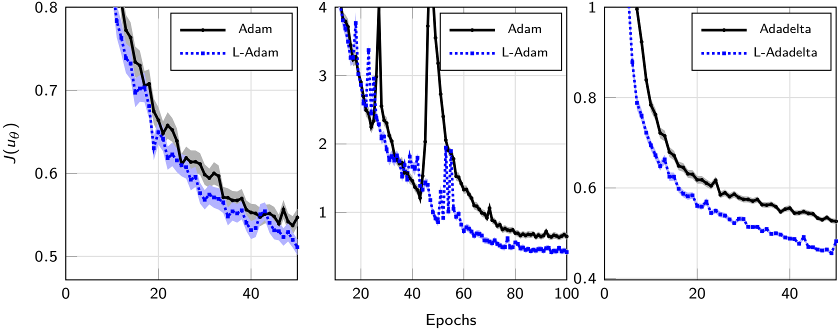

Figure: Comparison of algorithms with $N = 30, 50, 50$ respectively

Table: Best performance

	Adam, $N = 30$	Adam, $N = 50$	Adadelta, $N = 50$
Vanilla	0.4448	0.6355	0.4671
Langevin	0.4306	0.4182	0.3773

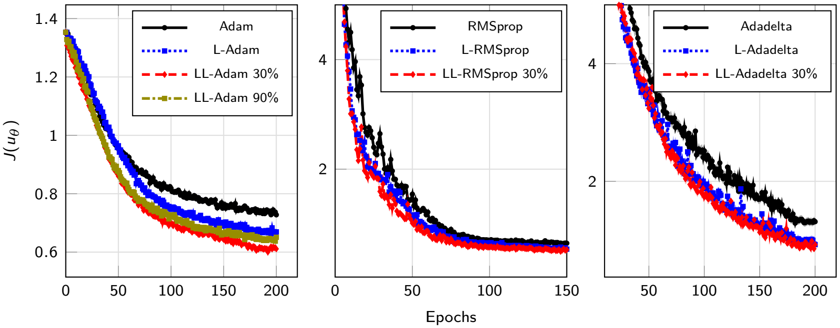

Figure: Training of the deep hedging problem with multiple controls with $N = 10$

Table: Best performance

	Adam	RMSprop	Adadelta
Vanilla	0.7278	0.5618	1.2900
Langevin	0.6626	0.4441	0.9250
Layer Langevin 30%	0.6004	0.4102	0.8554
Layer Langevin 90%	0.6377	–	–

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For the process:

$$Y_0 \in \mathbb{R}^d, \quad dY_t = b(Y_t)dt + \sigma(Y_t)dW_t,$$

and $f : \mathbb{R}^d \to \mathbb{R}$, we are looking for an **estimator of** $\mathbb{E}[f(Y_T)]$ with reduced variance.
We propose the **unbiased** estimator:

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Correlation estimator

$$\text{Estimator: } \left(f(Y_T^1) + f(Y_T^2)\right)/2,$$
$$dY_t^1 = b(Y_t^1)dt + \sigma(Y_t^1)dW_t^1,$$
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$$d\langle W_t^1, W_t^2\rangle = \rho_t dt.$$

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$$d\langle W_t^1, W_t^2\rangle = \rho_t dt.$$

- For $\rho_t \equiv -I_d$, this gives the **antithetic method** (Hammersley and Morton, 1956).

Optimal correlation search

- We look to minimize the variance of the estimator through the choice of $\rho_t = \rho(t, Y_t^1, Y_t^2)$ as a neural network.
- We write the correlation search as stochastic control:

$$\text{Minimize } \ \mathbb{E}\big[f(Y_T^1)f(Y_T^2)\big].$$

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$$\text{Minimize} \quad \mathbb{E}\left[f(Y_T^1)f(Y_T^2)\right].$$

- We solve using gradient descent and **Reinforcement Learning** approaches.
- Package `relocor`: *REinforcement Learning Optimal CORrelation search*, using `OpenAI Gym`.

Simulations

- We test variance reduction for option pricing with multi-basket Black-Scholes and Heston models.
- We give examples where we achieve better than trivial correlations (antithetic, minus-plus etc).

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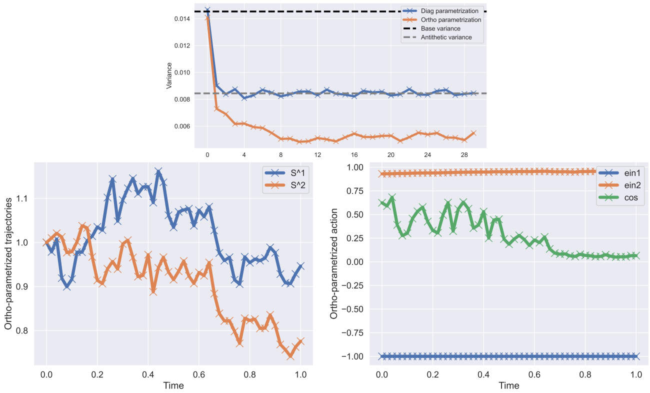

Figure: Black-Scholes variance reduction with $d = 2$. Left: trajectories of the assets; Right: coefficients of the diagonal matrix and cosine of the rotation matrix.

Link with maximal optimal transport

- We look to correlate two random variables Y_T^1 and Y_T^2 with fixed marginal law and the variance reduction can be written as:

$$\max_{\rho} \mathbb{E}\left|f(Y_T^1) - f(Y_T^2)\right|^2.$$

- Any coupling between Y_T^1 and Y_T^2 can be written as coupling W^1 and W^2 with ρ.
- $\Longrightarrow$ Our reduction variance is in fact a L^2-optimal **maximal** transport.

Outline

4 Conclusion and perspectives

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- We give theoretical founding including degenerate minimum cases.
- We prove the interest of Langevin or Layer Langevin algorithms for various problems, involving very deep learning.
- Langevin algorithms have returned to the forefront of research: latent diffusion generative models (Rombach et al., 2021).

Figure: Théâtre d'Opéra Spatial

Thank you for your attention !

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