$\pi(f) = \int_d f(x)\pi(x) = \int_d f(x)\pi(x) x Generic problem : estimation of an integral \pi(f)$

π

π

$\pi(f) by n^{-1} \sum_{i=1}^{n} f(X_i), where (X_i)_{i \geq 0} is a Markov chain associated with a Markov kernel P with invariant distribution \pi.$

π

Q

$X_0 \sim$

ν

$k \geq$

0

X_k

$Y_{k+1} \sim$

$Q(X_k, \cdot)$

$$X_{k+1} = \{ Y_{k+1} \text{ probability } \alpha(X_k, Y_{k+1}) \,, X_k \text{ probability } 1 - \alpha(X_k, Y_{k+1}) \,.$$

$$\alpha(x, y) = 1 \wedge \frac{\pi(y)}{\pi(x)} \,.$$

P

$x \in^d$

$\in$

d

$\int 1 \wedge \frac{\pi(y)}{\pi(x)} Q(x, y) +_x$

$() \int_d 1 - 1 \wedge \frac{\pi(y)}{\pi(x)} Q(x, y).$

P

π

$\int x \, \pi(x) P(x,) =$

$\int x \, \pi(x) P(x,)$

Q

$\int x \int \pi(x) \wedge \pi(y) Q(x, y) =$

$\int x \int \pi(x) \wedge \pi(y) Q(x, y),$

$, \in$

d

q

Q

$q(x, y) =$

$q(y, x)$

$x, y \in^{2d}$

$$q(x, y) = q(x - y) = q(y - x), Y_{k+1} = X_k + Z_{k+1}.$$

$\delta_{\varphi(x)}(y)?$

φ

$\varphi \in$

$C^1(^d, ^d), \varphi \circ$

$\varphi =$

$, Jac_\varphi(x) =$

$1.$

φ

$\delta_{\varphi(x)}(y) \, \varphi \in C^1(^d, ^d), \, \varphi \circ \varphi =, \, Jac_\varphi(x) = 1.$

$y =$

$\varphi(x)$

$Jac_\varphi(x) =$

1

$\int x \int \pi(x) \wedge \pi(y) Q(x, y) =$

$\int \pi(x) \wedge$

$\pi(\varphi(x))(\varphi(x)) x$

$=$

$\int_d \{\pi(\varphi(\varphi(x))) \wedge$

$\pi(\varphi(x))\}(\varphi(x))(\varphi(\varphi(x))) x$

$=$

$\int_d \{\pi(\varphi(y)) \wedge$

$\pi(y)\}(y)(\varphi(y)) y$

$=$

$\int x \int \pi(x) \wedge \pi(y) Q(x, y).$

π

$\propto$

$-U$

$U :^d \rightarrow$

C^1

$\nabla \log \pi \nabla U.$

U

d

$^d \times ^d$

$2d$

$\tilde{\pi}(q, p) \propto$

$\exp(-H(q, p)).$

H

q

p

U

$p^2/2$

$(q(t), p(t))_{t \geq 0}$

$$\{ \dot{}(t) = \frac{\partial}{\partial}((t), (t)) \quad = (t), \dot{}(t) = -\frac{\partial}{\partial}((t), (t)) = -\nabla((t)).$$

$s))$

$_ode_I I starting from. \varphi_t :^{2d} \to ^{2d}$

$\mathrm{C}^1(^{2d}, ^{2d})$

$(\varphi_t)_{t \geq 0}$

$(\varphi_t)_{t \geq 0}$

$t \mapsto$

$(q(t), p(t))$

$\partial H \frac{}{\partial q (q(t), p(t)) \frac{q(t)}{t} + \frac{\partial H}{\partial p}(q(t), p(t)) \frac{p(t)}{t} = 0,}$

$nitial conditions \, t \geq$

0

$_0, p_0).$

$(\varphi_t)_{t \geq 0}$

$t \mapsto$

$(q(t), p(t))$

$s \mapsto$

$(q(-s), -p(-s))$

$_ode_I I on_-$

$(q_0, -p_0)$

$s \mapsto$

$(q(s), p(s))$

$_ode_I I on_+$

(q_0, p_0)

$t \geq$

0

$_ode_I I \varphi_t(q(-t), -p(-t)) = \varphi_t \varphi_{-t}(q_0, -p_0) = (q_0, -p_0), which implies that \varphi_t^{-1}(q_0, p_0) = (\varphi_t^{(1)}(q_0, -_0), -\varphi_t^{(2)}(_0, -_0)).$

$(\varphi_t)_{t \geq 0}$

$t \mapsto$

$(q(t), p(t))$

sym-
plec-
tic

$t \in_+$

$B_t^T J B_t =$

J

B_t

φ_t

$\begin{bmatrix} 0_d & _d \\ -_d & 0_d \end{bmatrix}.$

$\det(B_t) =$

1

$f :^{2d} \to$

$\int_{2d} f(\varphi_t(q, p)) qp =$

$\int_{2d} f(q, p) qp.$

$\tilde{\pi}(\varphi_t)_{t \geq 0} \propto$

$f :^{2d} \to$

$\exp(-(,)).$

$\int_{2d} f(\varphi_t(q, p)) \exp -H(q, p) qp$

$=$

$\int_{2d} f(q, p) \exp -H(\varphi_t^{-1}(q, p)) qp$

$=$

$\int_{2d} f(q, p) \exp -H(\varphi_{-t}(q, p)) qp$

$=$

$\int_{2d} f(q, p) \exp -H(q, p) qp.$

$\tilde{\pi}$

$(\varphi_t)_{t \geq 0}$

$(\varphi_t)_{t \geq 0}$

$_ode which preserve reversibility and symplectiness :$

$Symplectic integrators, like the leap\text{-}frog (or Störmer - Verlet) integrator.$

$h \in_+^*$

$T \in^*$

$(_0, _0) \in^d$

$\times^d$

$k =$

$0, \ldots, T$

$\{ \; _{k+1/2} =_k$

$-(h/2) \nabla(_k)$

$_{k+1} =_k$

$+ h_{k+1/2}$

$_{k+1} =_{k+1/2}$

$-(h/2) \nabla(_{k+1}).$

$(_k, _k)_{k \in \{0, \ldots, T\}}$

$_ode at times \{$

$\in$

$\{0, \ldots, T\}\}$

$(_0, _0)$

h

T

T

$_inte.pdf$