Score matching and nonparametric estimators of drift functions for stochastic differential equations

Manfred Opper

joint work with Philip Batz, Andreas Ruttor,

April 13, 2016
Let $q_\theta(\cdot)$ be a family of probability densities. Try to estimate $p(x)$ by finding 'best' $\theta$. Using samples $x_i \sim p(x)$ for $i = 1, \ldots, n$. 
Let $q_\theta(\cdot)$ be a family of probability densities. Try to estimate $p(x)$ by finding 'best' $\theta$. using samples $x_i \sim p(x)$ for $i = 1, \ldots, n$.

Maximum likelihood (and Bayes) estimation often suffers from normalisation problem $q_\theta(x) = \frac{\tilde{q}_\theta(x)}{Z_\theta}$ with intractable $Z_\theta$. 

Score matching: the basic identity (Hyvärinen, 2005)

$$
J(p \| q_\theta) = \frac{1}{2} \int p(x) \| \nabla \ln p(x) - \nabla \ln q_\theta(x) \|^2 = \int p(x) \left\{ \frac{1}{2} \| \nabla \ln q_\theta(x) \|^2 + \nabla^2 \ln q_\theta(x) \right\} + \text{const}
$$
Let $q_\theta(\cdot)$ be a family of probability densities. Try to estimate $p(x)$ by finding 'best' $\theta$. using samples $x_i \sim p(x)$ for $i = 1, \ldots, n$.

Maximum likelihood (and Bayes) estimation often suffers from **normalisation** problem $q_\theta(x) = \frac{\hat{q}_\theta(x)}{Z_\theta}$ with intractable $Z_\theta$.

Score matching: the basic identity (Hyvärinen, 2005)

\[
J(p\|q_\theta) = \frac{1}{2} \int p(x) \|\nabla \ln p(x) - \nabla \ln q_\theta(x)\|^2 \\
= \int p(x) \left\{ \frac{1}{2} \|\nabla \ln q_\theta(x)\|^2 + \nabla^2 \ln q_\theta(x) \right\} + \text{const}
\]
Use minimisation of empirical loss

\[ \sum_{i=1}^{n} \left\{ \frac{1}{2} \| \nabla \ln q_\theta(x_i) \|^2 + \nabla^2 \ln q_\theta(x_i) \right\} \]

independent of \( Z_\theta \)!
Use minimisation of empirical loss

\[
\sum_{i=1}^{n} \left\{ \frac{1}{2} \| \nabla \ln q_\theta(x_i) \|^2 + \nabla^2 \ln q_\theta(x_i) \right\}
\]

independent of \( Z_\theta \)!

Nonparametric extension (Sriperumbudur, Fukumizu, Kumar, Gretton and Hyvärinen, 2014). Set \( \psi(x) \doteq \ln \tilde{q}(x) \)

\[
\sum_{i=1}^{n} \left\{ \frac{1}{2} \| \nabla \psi(x_i) \|^2 + \nabla^2 \psi(x_i) \right\} + \frac{1}{2} \| \psi(\cdot) \|^2_{\text{RKHS}}
\]
Use minimisation of empirical loss

\[ \sum_{i=1}^{n} \left\{ \frac{1}{2} \| \nabla \ln q_{\theta}(x_i) \|^2 + \nabla^2 \ln q_{\theta}(x_i) \right\} \]

independent of \( Z_{\theta} \) !

Nonparametric extension (Sriperumbudur, Fukumizu, Kumar, Gretton and Hyvärinen, 2014). Set \( \psi(x) = \ln \tilde{q}(x) \)

\[ \sum_{i=1}^{n} \left\{ \frac{1}{2} \| \nabla \psi(x_i) \|^2 + \nabla^2 \psi(x_i) \right\} + \frac{1}{2} \| \psi(\cdot) \|^2_{\text{RKHS}} \]

yields estimate of \( \nabla \ln p(x) \) !
Some applications of score matching

- Learning structure of graphical models
- Finding modes of probability densities
- Gradient free Hamiltonian Monte Carlo
- Sequential importance sampling
- ...

Manfred Opper joint work with Philip Batz, Andreas Ruttor (AI group, TU Berlin)
Problem of learning drift functions for stochastic differential equations
Nonparametric estimates using a generalisation of score matching
Applications to Langevin models
Relation to Maximum likelihood and Bayes
Kullback–Leibler divergence, control and a normalizer
Future work and open problems
Stochastic differential equations

• Dynamics defined by SDEs for $Z \in \mathbb{R}^d$.

\[ dZ_t = g(Z_t)\, dt + \sigma(Z_t) \times dW_t \]

- Drift
- Diffusion
- Wiener process

• Limit of discrete time process

\[ Z_{t+\Delta} - Z_t = g(Z_t)\Delta + \sigma(Z_t)\sqrt{\Delta} \, \epsilon_t . \]

with $\epsilon_t$ i.i.d. Gaussian for $\Delta \to 0$. 

Manfred Opper joint work with Philip Batz, Andreas Ruttor (AI group, TU Berlin)
Dynamics defined by SDEs for $Z \in \mathbb{R}^d$.

\[ dZ_t = g(Z_t)\,dt + \sigma(Z_t) \times dW_t \]

- Drift
- Diffusion
- Wiener process

Limit of discrete time process

\[ Z_{t+\Delta} - Z_t = g(Z_t)\Delta + \sigma(Z_t)\sqrt{\Delta} \epsilon_t. \]

with $\epsilon_t$ i.i.d. Gaussian for $\Delta \to 0$.

Learn the function $g(\cdot)$ from a set of (noise free) observations $z(t_1), z(t_2), \ldots, z(t_n)$. 
Nonparametric (Gaussian process) approach

Use a Gaussian Process prior $g(\cdot) \sim \mathcal{GP}(0, K(z, z'))$ over drift functions. (Papaspiliopoulos, Pokern, Roberts and Stuart 2012).

![Graph showing nonparametric estimation of drift](image-url)
In Euler discretization the SDE looks like
\[ Z_{t+\Delta t} - Z_t = g(Z_t)\Delta + \sqrt{\Delta} \epsilon_t, \text{ for } \Delta \to 0. \]
Likelihood for densely observed path

- In Euler discretization the SDE looks like
  \[ Z_{t+\Delta t} - Z_t = g(Z_t)\Delta + \sqrt{\Delta} \epsilon_t, \text{ for } \Delta \to 0. \]
- Hence the likelihood for the drift is
  \[
  p(Z_0:T|g) \propto \exp \left[ -\frac{1}{2\Delta} \sum_t ||Z_{t+\Delta} - Z_t||^2 \right] \times 
  \exp \left[ -\frac{1}{2} \sum_t ||g(Z_t)||^2 \Delta + \sum_t g(Z_t) \cdot (Z_{t+\Delta} - Z_t) \right].
  \]
  allows for simple GP based estimation of the function \( g(\cdot) \).
Likelihood for densely observed path

- In Euler discretization the SDE looks like
  \[ Z_{t+\Delta t} - Z_t = g(Z_t)\Delta + \sqrt{\Delta} \epsilon_t, \text{ for } \Delta \to 0. \]
- Hence the likelihood for the drift is
  \[
p(Z_0:T|g) \propto \exp \left[ -\frac{1}{2\Delta} \sum_t ||Z_{t+\Delta} - Z_t||^2 \right] \times \]
  \[ \exp \left[ -\frac{1}{2} \sum_t ||g(Z_t)||^2 \Delta + \sum_t g(Z_t) \cdot (Z_{t+\Delta} - Z_t) \right]. \]

  allows for simple GP based estimation of the function \( g(\cdot) \).
- This essentially leads to the estimate
  \[ g(z) \approx E \left[ \frac{Z_{t+\Delta} - Z_t}{\Delta} | Z_t = z \right]. \text{ Works well for } \Delta \to 0. \]
For not so small $\Delta$ it does not work well! Data from
\[ dz = (z - z^3)dt + dW. \]

Estimation from sparse observations in time not trivial! Approximation
using imputation of hidden process possible (Ruttor, Batz and Opper, 2013).
Drift estimation from empirical density only

- Given stationary density $p(z)$ of the process. Determine the drift $g$? Assume that $\sigma(\cdot)$ is known and $g(z) = r(z) + f(z)$, with $r(z)$ known.
Given stationary density $p(z)$ of the process. Determine the drift $g$?

Assume that $\sigma(\cdot)$ is known and $g(z) = r(z) + f(z)$, with $r(z)$ known.

Partial answer:

'minimal' solution minimising a quadratic functional

$$\frac{1}{2} \int p(z) f(z) \cdot A^{-1}(z)f(z) \, dz$$
Drift estimation from empirical density only

- Given stationary density $p(z)$ of the process. Determine the drift $g$?
  Assume that $\sigma(\cdot)$ is known and $g(z) = r(z) + f(z)$, with $r(z)$ known.

- Partial answer:
  'minimal' solution minimising a quadratic functional
  \[
  \frac{1}{2} \int p(z) f(z) \cdot A^{-1}(z)f(z) \, dz
  \]

- Lagrange–functional
  \[
  \frac{1}{2} \int f(z) \cdot A^{-1}(z)f(z) \, dz - \int \psi(z) \{\mathcal{L}p(z) - \nabla \cdot (f(z)p(z))\} \, dz
  \]
  with Fokker–Planck operator corresponding to $r(z)$
  \[
  \mathcal{L}p(z) = -\nabla \cdot (r(z)p(z)) + \frac{1}{2} \text{tr} \left[ \nabla \nabla^\top (D(z)p(z)) \right]
  \]
  with $D(z) \doteq \sigma(z)\sigma(z)^\top$. 
Variation yields \( f(z) = A(z)\nabla\psi(z) \). Inserting back into Lagrangean yields dual functional

\[
\varepsilon[\psi] = \int \left\{ \frac{1}{2} \nabla\psi(z) \cdot A(z) \nabla\psi(z) + \mathcal{L}^*\psi(z) \right\} p(z)dz
\]

with \( \mathcal{L}^* \) adjoint operator which fulfils \( \int \psi(z)\mathcal{L}p(z)dz = \int p(z)\mathcal{L}^*\psi(z)dz \) and is given by

\[
\mathcal{L}^*\psi(z) = r(z) \cdot \nabla\psi(z) + \frac{1}{2} \text{tr} \left[ D(z)\nabla\nabla^\top\psi(z) \right]
\]

For ’thermal equilibrium’ \( A = I \) and \( D = 2I \) and \( r = 0 \) this corresponds to score matching! Stationary density \( p(z) \propto e^{2\psi(z)} \) and \( f(z) = \nabla\psi(x) \)
Regularized empirical loss

- Given ergodic sample \( \{z_i\}_{i=1}^n \) replace

\[
p(z) \rightarrow \hat{p}(z) = \frac{1}{n} \sum_{i=1}^{n} \delta(z - z_i)
\]

- Results in empirical functional

\[
C \sum_{i=1}^{n} \left\{ \frac{1}{2} \nabla \psi(z_i) \cdot A(z_i) \nabla \psi(z_i) + \mathcal{L}^* \psi(z_i) \right\}
\]
Regularized empirical loss

- Given ergodic sample \( \{z_i\}_{i=1}^n \) replace

\[
p(z) \rightarrow \hat{p}(z) = \frac{1}{n} \sum_{i=1}^n \delta(z - z_i)
\]

- Results in empirical functional

\[
C \sum_{i=1}^n \left\{ \frac{1}{2} \nabla \psi(z_i) \cdot A(z_i) \nabla \psi(z_i) + \mathcal{L}^* \psi(z_i) \right\} + \frac{1}{2} \int \int \psi(z) K^{-1}(z, z') \psi(z') \, dzdz'
\]

regularised by kernel \( K \).
Variation wrt $\psi$ yields

$$
\psi(z) + C \sum_{j=1}^{n} \mathcal{L}^{*}_{z'}[\psi] \ K(z, z')_{z'=z_j} = 0
$$
Variation wrt $\psi$ yields

$$\psi(z) + C \sum_{j=1}^{n} L_{z'}^*[\psi] K(z, z')_{z'=z_j} = 0$$

regularised version of equation (valid for any function $h(\cdot)$)

$$\int p(z') L_{z'}^*[\psi] h(z') dz' = \int h(z') L_{z'}^*[\psi] p(z') dz' = 0$$

applied to $p \to \hat{p}$ and $h_z(z') = K(z, z')$. 
Variation wrt $\psi$ yields

$$\psi(z) + C \sum_{j=1}^{n} \mathcal{L}^*_z \psi \, K(z, z')_{z'=z_j} = 0$$

regularised version of equation (valid for any function $h(\cdot)$)

$$\int p(z') \mathcal{L}^*_z \psi h(z') \, dz' = \int h(z') \mathcal{L}^*_z \psi p(z') \, dz' = 0$$

applied to $p \rightarrow \hat{p}$ and $h_z(z') = K(z, z')$.

If $\nabla \psi(z)$ known at all sample points $z = z_i$, get $\psi(z)$ for all $z$.

Take gradient

$$\nabla \psi(z_i) + C \sum_{j=1}^{n} \mathcal{L}^*_z \psi \nabla_z K(z, z')_{z=z_i, z'=z_j} = 0$$
Langevin dynamics

Classical mechanics in terms of (generalized) coordinates and velocities $X, V \in \mathbb{R}^d$

\[
dX_t = V_t dt, \quad dV_t = g_v(X_t, V_t)dt + \sigma_v(X_t, V_t)dW_t.
\]
Langevin dynamics

- Classical mechanics in terms of (generalized) coordinates and velocities $X, V \in \mathbb{R}^d$

$$dX_t = V_t dt, \quad dV_t = g_V(X_t, V_t) dt + \sigma_V(X_t, V_t) dW_t.$$

- If drift is of the form $g_V(x, v) = r_v(x, y) + \nabla_v \psi(x, v)$ use functional for estimation

$$\varepsilon[\psi] = \int p(x, v) \left\{ L^* \psi(x, v) + \frac{1}{2}(\nabla_v \psi(x, v))^2 \right\} \, dx \, dv$$

where

$$L^* \psi(x, v) = \left( v \cdot \nabla_x + r_v(x, v) \cdot \nabla_v + \frac{1}{2} \text{tr} (D_v(x, v) \nabla_v \nabla_v) \right) \psi(x, v).$$
Condition $f_v(x, v) = \nabla_v \phi(x, v)$ restricts the velocity dependency!
Condition \( f_v(x, v) = \nabla_v \phi(x, v) \) restricts the velocity dependency!

Possible choice

\[
 f_v(x, v) = f(x) - \Lambda v = \nabla_v \left\{ v \cdot f(x) - \frac{1}{2} v \cdot \Lambda v \right\},
\]
Condition \( f_v(x, \nu) = \nabla_v \phi(x, \nu) \) restricts the velocity dependency!

Possible choice

\[
f_v(x, \nu) = f(x) - \Lambda \nu = \nabla_v \left\{ \nu \cdot f(x) - \frac{1}{2} \nu \cdot \Lambda \nu \right\},
\]

Note: If \( r_v = -\Lambda \nu \) then \( \mathcal{L}^* \psi(x, \nu) = \mathcal{L}^*(\nu \cdot f(x)) \) is independent of the diffusion term \( D_v(x, \nu) \):

\( \rightarrow \) Estimate \( f(x) \) without knowing the diffusion.
Example: Double well

\[ f(x, v) = 4(x - x^3) - \lambda v \]
Example: Nonconservative force

\[ f^{(1)}(x) = x^{(1)}(1 - (x^{(1)})^2 - (x^{(2)})^2) - x^{(2)} \]
\[ f^{(2)}(x) = x^{(2)}(1 - (x^{(1)})^2 - (x^{(2)})^2) - x^{(1)} \]

Polynomial kernel with \( p = 4 \) and \( n = 2000 \)
Cart and Pole model

\[ f(x) = a \sin x \] and \[ r(v) = -\lambda v \] and diffusion \[ D_v = (\sigma \cos(x))^2. \]
Kernel density estimators as alternative?

Explicit solutions to drift for Langevin models

\[ f^{(i)}(x) = \sum_{j=1}^{d} \frac{\partial E[v^{(i)}v^{(j)}|x]}{\partial x(j)} + \sum_{j=1}^{d} E[v^{(i)}v^{(j)}|x] \frac{\partial \ln p(x)}{\partial x(j)} - E[r^{(i)}|x], \]
Explicit solutions to drift for Langevin models

\[ f^{(i)}(x) = \sum_{j=1}^{d} \frac{\partial E[v^{(i)}v^{(j)}|x]}{\partial x(j)} + \sum_{j=1}^{d} E[v^{(i)}v^{(j)}|x] \frac{\partial \ln p(x)}{\partial x(j)} - E[r^{(i)}|x], \]

Simplifies only for 'thermal equilibrium' \( f(x) = \nabla \phi \) and \( D_v \propto \Sigma \), \( r = -\Lambda v \) where \( \Lambda \) and \( \Sigma \) are diagonal with \( \frac{2\lambda_i}{\sigma_i^2} = \beta \). One has then

\[ E[v^{(i)}v^{(j)}|x] = \frac{1}{2\beta} \delta_{ij} \] and \( E[r^{(i)}|x] = 0. \)
Extension: Other evolution equations

- Replace white noise $\sigma_v(X, V)dW \rightarrow U(t)dt$ where $U(t)$ Markovian.
- Include noise in state variable $Z = (X, V, U)$
- Example: $U(t) = \pm 1$ random telegraph process and $x, v, u \in \mathbb{R}$ with drift $g_v(x, v) = -\lambda v + f(x)$
Extension: Other evolution equations

- Replace white noise $\sigma_v(X, V)dW \rightarrow U(t)dt$ where $U(t)$ Markovian.
- Include noise in state variable $Z = (X, V, U)$
- Example: $U(t) = \pm 1$ random telegraph process and $x, v, u \in R$ with drift $g_v(x, v) = -\lambda v + f(x)$
- Fokker Planck $\rightarrow$ Master equation

$$0 = -\partial_x (vp(x, v, u) - \partial_v [(f(x) - \lambda v + u)p(x, v, u)])$$

$$+ \gamma (p(x, v, -u) - p(x, v, u))$$
Extension: Other evolution equations

- Replace white noise $\sigma_v(X, V)dW \to U(t)dt$ where $U(t)$ Markovian.
- Include noise in state variable $Z = (X, V, U)$
- Example: $U(t) = \pm 1$ random telegraph process and $x, v, u \in \mathbb{R}$ with drift $g_v(x, v) = -\lambda v + f(x)$
- Fokker Planck $\to$ Master equation

$$0 = -\partial_x (vp(x, v, u) - \partial_v [(f(x) - \lambda v + u)p(x, v, u)]) + \gamma (p(x, v, -u) - p(x, v, u))$$

- Adjoint operator

$$\mathcal{L}^* \psi = \{v \partial_x + (u - \lambda v) \partial_v\} \psi + \gamma (\psi(x, v, -1) - \psi(x, v, 1))$$
Extension: Other evolution equations

- Replace white noise $\sigma_v(X, V)dW \rightarrow U(t)dt$ where $U(t)$ Markovian.
- Include noise in state variable $Z = (X, V, U)$
- Example: $U(t) = \pm 1$ random telegraph process and $x, v, u \in R$ with drift $g_v(x, v) = -\lambda v + f(x)$
- Fokker Planck $\rightarrow$ Master equation

\[
0 = -\partial_x (v p(x, v, u) - \partial_v [(f(x) - \lambda v + u)p(x, v, u)]) + \gamma (p(x, v, -u) - p(x, v, u))
\]

- Adjoint operator

\[
\mathcal{L}^* \psi = \{ v \partial_x + (u - \lambda v) \partial_v \} \psi + \gamma (\psi(x, v, -1) - \psi(x, v, 1))
\]

- Parametrisation $\psi(x, v) = vf(x)$ leads to functional

\[
\varepsilon[f] = \frac{1}{2} \sum_{u=\pm 1} \int p(x, v, u) \left\{ f^2(x) + 2f'(x)v^2 + 2f(x)(u - \lambda v) \right\} dx dv
\]
The case $A = D$: Likelihood for densely observed path

\[-\ln p(Z_0: T \mid g) = \frac{1}{2} \sum_t \left\{ \|g(Z_t)\|^2 \Delta t - 2\langle g(Z_t), (Z_{t+\Delta t} - Z_t)\rangle \right\} + \text{const}\]

with $\langle u, v \rangle \doteq u^\top D^{-1} v$. 
The case $A = D$: Likelihood for densely observed path

\[- \ln p(Z_0:T | g) = \frac{1}{2} \sum_t \{||g(Z_t)||^2 \Delta t - 2\langle g(Z_t), (Z_{t+\Delta t} - Z_t) \rangle \} + \text{const}\]

with $\langle u, v \rangle = u^\top D^{-1} v$. Assume $g = r + D\nabla \psi$ take $\Delta t \to 0$ and apply Ito formula

\[= \text{const} + \frac{1}{2} \int_0^T \{ \nabla \psi \cdot D \nabla \psi \ dt + 2r \cdot \nabla \psi \ dt - 2\nabla \psi \cdot dZ_t \} \]
The case \( A = D \): Likelihood for densely observed path

\[
- \ln p(Z_0:T|g) = \frac{1}{2} \sum_t \left\{ \| g(Z_t) \|^2 \Delta t - 2 \langle g(Z_t), (Z_{t+\Delta t} - Z_t) \rangle \right\} + \text{const}
\]

with \( \langle u, v \rangle \doteq u^\top D^{-1} v \). Assume \( g = r + D \nabla \psi \) take \( \Delta t \to 0 \) and apply Itô formula

\[
= \text{const} + \frac{1}{2} \int_0^T \left\{ \nabla \psi \cdot D \nabla \psi \, dt + 2r \cdot \nabla \psi \, dt - 2 \nabla \psi \cdot dZ_t \right\}
\]

\[
= \frac{1}{2} \int_0^T \left\{ \nabla \psi \cdot D \nabla \psi + 2r \cdot \nabla \psi + \text{tr}(D \nabla \nabla^\top \psi) \right\} \, dt - \psi(Z_T) + \psi(Z_0)
\]
The case $A = D$: Likelihood for densely observed path

$$- \ln p(Z_0:T | g) = \frac{1}{2} \sum_{t} \left\{ \|g(Z_t)\|^2 \Delta t - 2 \langle g(Z_t), (Z_{t+\Delta t} - Z_t) \rangle \right\} + \text{const}$$

with $\langle u, v \rangle = u^\top D^{-1} v$. Assume $g = r + D \nabla \psi$ take $\Delta t \to 0$ and apply Ito formula

$$= \text{const} + \frac{1}{2} \int_0^T \left\{ \nabla \psi \cdot D \nabla \psi \, dt + 2r \cdot \nabla \psi \, dt - 2 \nabla \psi \cdot dZ_t \right\}$$

$$= \frac{1}{2} \int_0^T \left\{ \nabla \psi \cdot D \nabla \psi + 2 r \cdot \nabla \psi + \text{tr}(D \nabla \nabla^\top \psi) \right\} \, dt - \psi(Z_T) + \psi(Z_0)$$

$$\approx \frac{T}{2} \int \left\{ \nabla \psi \cdot D \nabla \psi + 2 r \cdot \nabla \psi + \text{tr}(D \nabla \nabla^\top \psi) \right\} p(z) \, dz$$
Back to the optimisation problem

We considered minimisation of

$$\frac{1}{2} \int p(z) f(z) \cdot A^{-1}(z)f(z) \, dz$$

under the linear constraint that

$$-\nabla \cdot (r(z)p(z)) + \frac{1}{2} \text{tr} \left[ \nabla \nabla^\top (D(z)p(z)) \right] = 0$$
The case \( A = D\): Kullback-Leibler divergence

- Kullback-Leibler (KL) divergence between the path probabilities for diffusion processes with drifts \( g(z) = r(z) + f(z) \) and \( r(z) \):

\[
D(p(Z_0: T | r + f) || p(Z_0: T | r)) = \frac{1}{2} \int_0^T dt \int p_t(z) f(z) \cdot D^{-1}(z) f(z) dz
\]

assuming equal diffusions \( D(z) \).
The case $A = D$: Kullback Leibler divergence

- Kullback-Leibler (KL) divergence between the path probabilities for diffusion processes with drifts $g(z) = r(z) + f(z)$ and $r(z)$:

$$D(p(Z_0:T|r+f)||p(Z_0:T|r)) = \frac{1}{2} \int_0^T dt \int p_t(z)f(z) \cdot D^{-1}(z)f(z)dz$$

assuming equal diffusions $D(z)$.

- For $T \to \infty$ the relative entropy rate is

$$\lim_{T \to \infty} \frac{1}{T} D(p(Z_{r+f}0:T)||p_r(Z_0:T|r) = \frac{1}{2} \int p(z)f(z) \cdot D^{-1}(z)f(z)dz.$$ 

Hence, the choice $A = D$ may be understood as a generalized as minimum relative entropy solution where the stationary density is given as a constraint.
Find extra drift (control) \( f(\cdot) \) such that the cost rate

\[
C[f] \equiv \lim_{T \to \infty} \frac{1}{T} D(p_{r+f}(Z_0:T) \| p_{r}(Z_0:T)) + \int p_{r+f}(z) U(z) dz
\]

is minimized! \( U(z) \) are state costs.
KL control problem and normalizer

- Find extra drift (control) $f(\cdot)$ such that the cost rate

$$C[f] \doteq \lim_{T \to \infty} \frac{1}{T} D(p_{r+f}(Z_0:T) \| p_r(Z_0:T)) + \int p_{r+f}(z) U(z) \, dz$$

is minimized! $U(z)$ are state costs.

- Note that for the finite $T$ problem the controlled path probabilities satisfies

$$p_{r+f}(Z_0:T) = \frac{1}{\zeta_T} p_r(Z_0:T) e^{-\int_0^T U(Z_t) \, dt}$$

where the normaliser is given by

$$\zeta_T = E_r \left[ e^{-\int_0^T U(Z_t) \, dt} \right]$$  \hspace{1cm} (1)
If the stationary controlled density $p$ is known (or we can sample from it) we can compute

- the log–normalizer in the limit via

$$
- \lim_{T \to \infty} \frac{1}{T} \ln \zeta_T = \int p(z) U(z) dz - \min_{\psi} \int \left\{ \frac{1}{2} \nabla \psi(z) \cdot A(z) \nabla \psi(z) + \mathcal{L}^* \psi(z) \right\} p(z) dz
$$
If the stationary controlled density $p$ is known (or we can sample from it) we can compute

- the log–normalizer in the limit via

$$\lim_{T \to \infty} \frac{1}{T} \ln \zeta_T = \int p(z) U(z) dz - \min_{\psi} \int \left\{ \frac{1}{2} \nabla \psi(z) \cdot A(z) \nabla \psi(z) + L^* \psi(z) \right\} p(z) dz$$

- and the control via

$$f(z) = D(z) \nabla \ln \psi(z)$$
Could this be helpful to solve the control problem?

- Sampling from the 'smoothing density' $p(z)$ is not easy.
- Sampling from the 'filtering density' $p_{filt}^t(z) = p(z|U(Z_\tau), \tau \leq t)$ is possible using particle filters.
- In certain cases estimates of $\nabla \ln p_{filt}^t(z)$ can be related to $\nabla \ln p(z)$. 
Analytically solvable example: Uncontrolled drift $r(z) = 4z(1 - z^2)$ and path costs $U(z) = \beta r(z)$.

\[ \beta = 0.2 \]

\[ \beta = 0.5 \]
$\beta = 1.0$

$\beta = 2.0$
Future work and open problems

- Generalisation to dynamics
- Other Markov processes
- Relation to Bayes and hyper parameter selection
- Convergence rates for non i.i.d. data
- Inclusion of noise in data?
- Unobserved variables?
- Inclusion of information from time order of data?