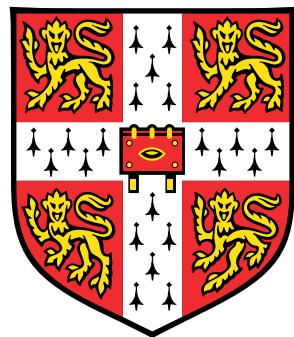


# **Optimal Importance Sampling in Quantum Monte Carlo for Lattice Models**



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This dissertation is submitted for the degree of  
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St. John's College

May 2021



I would like to dedicate this thesis to ...



## **Declaration**

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification in this, or any other university. This dissertation is my own work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and Acknowledgements. This dissertation contains fewer than 15,000 words including appendices, figure legends, and tables.

Blaž Stojanovič  
May 2021



## **Acknowledgements**

And I would like to acknowledge ...

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## **Abstract**

This is where you write your abstract ...



# Table of contents

|   |             |
|---|-------------|
| <b>List of figures</b>  | <b>xiii</b> |
| <b>List of tables</b>   | <b>xv</b>   |
| <b>Nomenclature</b>   | <b>xvii</b> |
| <b>1 Introduction</b>   | <b>1</b>    |
| 1.1 Thesis Contributions . . . . .  | 1           |
| 1.2 Thesis Structure . . . . .  | 1           |
| <b>2 Background</b>   | <b>3</b>    |
| 2.1 Lattice models . . . . .  | 3           |
| 2.1.1 Historical introduction . . . . .                                   | 3           |
| 2.1.2 The Schrödinger equation and the Feynman path integral . . . . .    | 3           |
| 2.1.3 Examples of lattice models . . . . .                                | 4           |
| 2.2 The Feynman-Kac formula . . . . .                                     | 5           |
| 2.2.1 Stochastic processes . . . . .                                      | 5           |
| 2.2.2 Feynman-Kac formula . . . . .                                       | 5           |
| 2.2.3 Stoquastic Hamiltonians and Lattice-model representations . . . . . | 7           |
| 2.3 Quantum Monte Carlo . . . . .   | 8           |
| 2.3.1 Overview . . . . .  | 8           |
| 2.4 Machine Learning . . . . .  | 9           |
| 2.4.1 Convolutional Neural Networks . . . . .                             | 9           |
| 2.4.2 Overview of ML approaches to the Quantum many-body problem          | 9           |
| <b>3 Methodology</b>  | <b>13</b>   |
| 3.1 Numerical Methods . . . . .   | 13          |
| 3.1.1 Discretizing the Feynman-Kac formula . . . . .                      | 13          |
| 3.1.2 Automatic differentiation . . . . .                                 | 13          |

|   |  |           |
|---|--|-----------|
| 3.1.3                                       | Gradient based optimisation . . . . .  | 13        |
| 3.2   | <i>Optimal sampling</i> . . . . .      | 13        |
| <b>4</b>                                    | <b>Results</b>                         | <b>15</b> |
| 4.1   | Transverse Field Ising model . . . . . | 15        |
| 4.2   | Heisenberg model . . . . .             | 15        |
| 4.3   | Bose-Hubbard model . . . . .           | 15        |
| <b>5</b>                                    | <b>Conclusion</b>                      | <b>17</b> |
| 5.1   | Direction for future work . . . . .    | 17        |
| 5.2   | Remarks . . . . .                      | 17        |
| <b>References</b>                           |  | <b>19</b> |
| <b>Appendix A Jax ecosystem</b>             |  | <b>21</b> |
| <b>Appendix B Gradient estimation</b>       |  | <b>23</b> |
| <b>Appendix C Probability distributions</b> |  | <b>27</b> |

# List of figures

|     |  |    |
|-----|--|----|
| 2.1 | Feynman-Kac for a 1D free particle . . . . . | 10 |
| B.1 | The reparametrization trick . . . . .        | 24 |



## **List of tables**



# Nomenclature

## **Acronyms / Abbreviations**

CNN Convolutional Neural Network

DL Deep Learning

DMC Diffusion Quantum Monte Carlo

GAN General Adversarial Network

ML Machine Learning

NN Neural Network

QMC Quantum Monte Carlo

VAE Variational Autoencoder

VMC Variational Quantum Monte Carlo



# **Chapter 1**

## **Introduction**

### **1.1 Thesis Contributions**

### **1.2 Thesis Structure**



# Chapter 2

## Background

### 2.1 Lattice models

#### 2.1.1 Historical introduction

I think starting from the magnetism point of view might be the best way to go, slowly lead into the field of condensed matter theory and lattice models.

#### 2.1.2 The Schrödinger equation and the Feynman path integral

The wavefunction

$$\Psi(r_1, \dots, r_N) \quad (2.1)$$

the Schrödinger equation

$$i \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \hat{H} \psi(\mathbf{r}, t) \quad (2.2)$$

for a single particle in an external potential  $\hat{V}(\mathbf{r})$  the Hamiltonian is

$$\hat{H} \phi(\mathbf{r}) = -\frac{1}{2} \nabla^2 \phi(\mathbf{r}) + \hat{V}(\mathbf{r}) \phi(\mathbf{r}). \quad (2.3)$$

Alternatively to the Schrödinger equation one can use an integral Green's function representation to express the wavefunction  $\psi$  at some future time  $t_2$  given initial condition  $\psi(\mathbf{r}, t_1)$  as

$$\psi(\mathbf{r}_2, t_2) = \int \mathcal{K}(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) \psi(\mathbf{r}_1, t_1) d\mathbf{r}_1. \quad (2.4)$$

The solution to equation

$$\left( i \frac{\partial}{\partial t_2} - H_{\mathbf{r}_2} \right) \mathcal{K}(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) = i\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2) \quad (2.5)$$

and the *propagator*  $\mathcal{K}(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1)$  is expressed using the Feynman path integral

$$\mathcal{K}(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) = \int_{\substack{\mathbf{r}(t_1)=\mathbf{r}_1 \\ \mathbf{r}(t_2)=\mathbf{r}_2}} D\mathbf{r}(t) \exp \left( i \int_{t_1}^{t_2} \mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}) dt \right), \quad (2.6)$$

where  $\mathcal{L}$  is the classical Lagrangian function of the system

$$\mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}) = \frac{1}{2} \dot{\mathbf{r}}^2 - \hat{V}(\mathbf{r}), \quad (2.7)$$

and the integral is over all paths that satisfy the endpoint conditions.

### 2.1.3 Examples of lattice models

$$\hat{\sigma}_i^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_i \quad \hat{\sigma}_i^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_i \quad \hat{\sigma}_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_i \quad (2.8)$$

#### Transverse Field Ising model

$$\hat{H}_{\text{Ising}} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - h \sum_i \sigma_i^x \quad (2.9)$$

#### Heisenberg model

$$\hat{H}_{\text{Heisenberg}} = -\frac{1}{2} \sum_{j=1}^N [J_x \hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + J_y \hat{\sigma}_j^y \hat{\sigma}_{j+1}^y + J_z \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z + h \hat{\sigma}_j^z] \quad (2.10)$$

#### Bose-Hubbard model

$$\hat{H}_{\text{BH}} = -t \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i \quad (2.11)$$

## 2.2 Feynman-Kac: connecting Quantum Mechanics and Stochastic Processes

### 2.2.1 Stochastic processes

Introduce minimal necessary basics to understand the following section/discussions. This includes

- Random variables
- Markov chains
- Transition matrices
- Brownian walk, measures on the Brownian walk.



Golden ratio

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### 2.2.2 Feynman-Kac formula

The Feynman path integral formulation (2.6) was extensively used by physicists for decades, even in the absence of a formal mathematical formulation which is hard to define because of the difficulties with defining an appropriate measure on the path space. Kac [2] provided a rigorous formulation of the *real-valued* case of the Feynman path integral, and the resulting *Feynman-Kac* formula provides a bridge between *parabolic* partial differential equations and stochastic processes.

To illustrate the Feynman-Kac formula let us consider a single particle with Hamiltonian

$$\hat{H} = -\frac{d^2}{dx^2} + V(x) \quad (2.12)$$

and the Schrödinger equation in *imaginary time*, which is of the elliptic type,

$$\partial_t |\psi_t\rangle = -\hat{H} |\psi_t\rangle. \quad (2.13)$$

Its formal solution, the time propagation of an initial wave function  $|\phi_0\rangle$  at  $t = 0$ , is written as

$$|\psi_t\rangle = e^{-\hat{H}t} |\phi_0\rangle. \quad (2.14)$$

From the spectral decomposition of the operator  $e^{-\hat{H}t}$  in terms of eigenstates  $|\phi_n\rangle$  and eigen-energies  $E_n$  of the Hamiltonian  $\hat{H}$

$$e^{-\hat{H}t} = \sum_n e^{-E_n t} |\phi_n\rangle \langle \phi_n|, \quad (2.15)$$

it follows that the term corresponding to the ground state of the system  $|\phi_0\rangle$  decays the slowest. Thus starting in some initial state and propagating for a long imaginary time *it* leads into the ground state with the decay rate giving the ground state energy as

$$\lim_{t \rightarrow \infty} |\psi_t\rangle \propto e^{-E_0 t} |\phi_0\rangle, \quad (2.16)$$

where  $E_0$  is the ground state energy and  $|\phi_0\rangle$  is the corresponding state. Kac noticed that the kinetic term of the Lagrangian in (2.6) could be interpreted as a measure on Brownian walks, and a solution to the imaginary time Schrödinger equation can be written as

$$\psi(x, t) = \mathbb{E}_{X \sim \text{Brownian with } X_t=x} \left[ \exp \left( - \int_0^t V(X_\tau, \tau) d\tau \right) \psi(X_0, 0) \right], \quad (2.17)$$

where only the **endpoint** at time  $t$  of the Brownian process fixed, whereas the starting point at time  $t = 0$  is not,  $\psi(x, 0)$  encodes the initial condition into this representation. When there is no external potential  $V(x) = 0$ , the Schrödinger equation in imaginary time is the diffusion equation and the Feynman-Kac solution is simply

$$\begin{aligned} \psi(x, t) &= \mathbb{E}_{X \sim \text{Brownian with } X_t=x} [\psi(X_0, 0)] \\ &= \frac{1}{\sqrt{2\pi t}} \int e^{-(x-x')^2/2t} \psi_0(x') dx' \end{aligned} \quad (2.18)$$

An illustration of the Feynman-Kac approach to the problem with no external potential  $V(x)$  in 1D is depicted in figure 2.1

### **2.2.3 Stoquastic Hamiltonians and Lattice-model representations**

general Stochquastic hamiltonian -> Feynman kac for general process

**Quantum Ising model**

**Heisenberg model**

**Bose-Hubbard model**

## 2.3 Quantum Monte Carlo

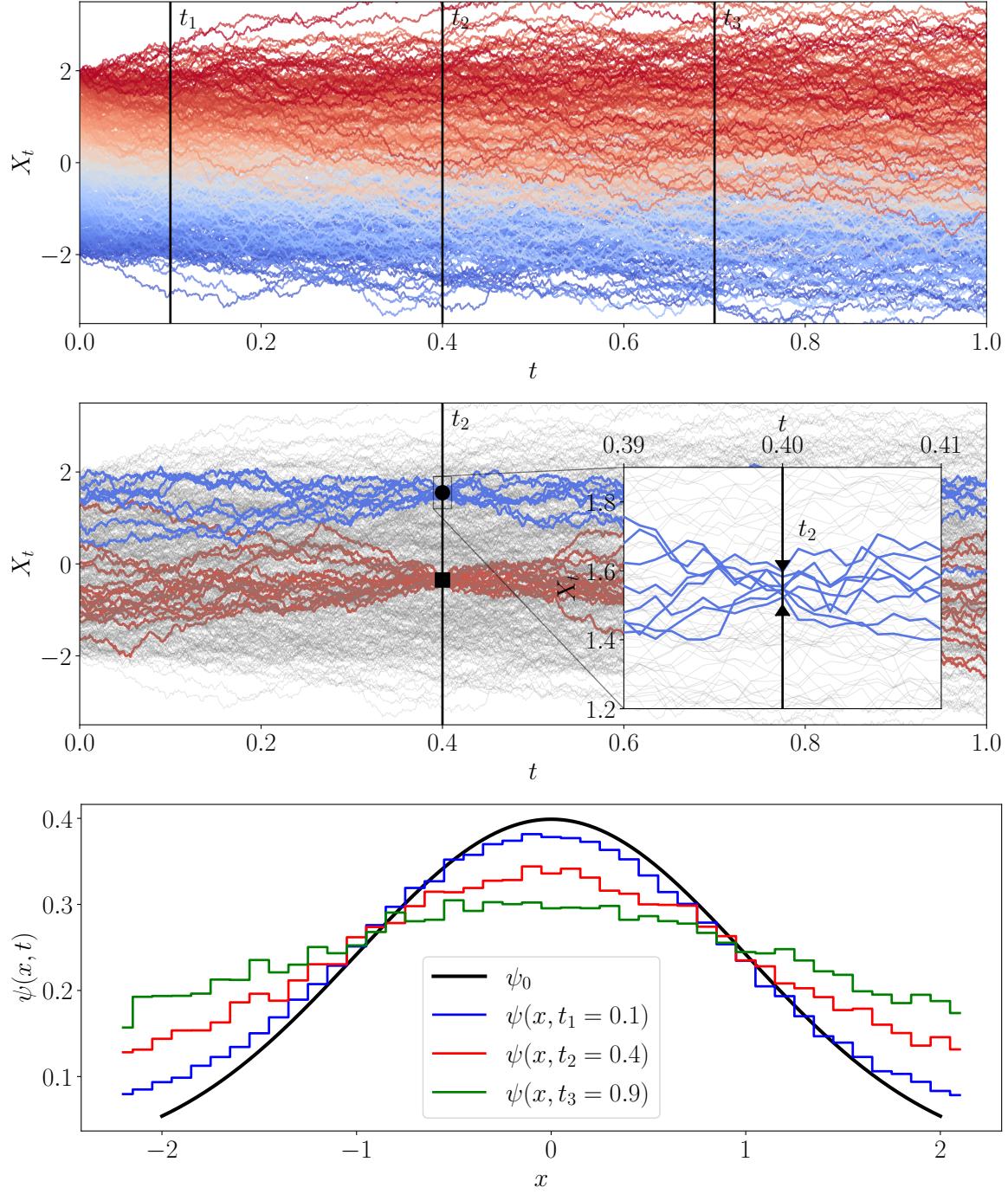
Nekje povej, kaksen complexity imajo QMC problemi za fermione in bozone.

### 2.3.1 Overview

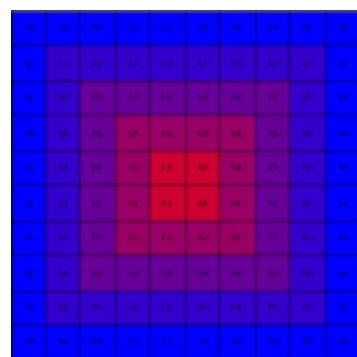
## 2.4 Machine Learning

### 2.4.1 Convolutional Neural Networks

### 2.4.2 Overview of ML approaches to the Quantum many-body problem



**Fig. 2.1 Feynman-Kac for a 1D free particle.** **top:**  $N = 400$  Brownian walks starting from different  $x_0$ , the color signifies initial position. In order to evaluate  $\psi$  between  $x - \frac{\delta x}{2}$  and  $x + \frac{\delta x}{2}$  at some time  $t$  we must first find Brownian paths that end there. **middle:** The paths that pass through at  $x \in (1.5, 1.6)$  (blue) and through  $x \in (-0.4, -0.3)$  (red) are colored, others are left in grey. **bottom:** Time evolution of the initial condition  $\psi_0 = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$ , by estimating  $\mathbb{E}[\psi(X_0, 0)]$  from the filtered paths at each timestep.





# **Chapter 3**

## **Methodology**

### **3.1 Numerical Methods**

**3.1.1 Discretizing the Feynman-Kac formula**

**3.1.2 Automatic differentiation**

**3.1.3 Gradient based optimisation**

### **3.2 *Optimal sampling*: optimal sampling in lattice models**



# **Chapter 4**

## **Results**

**4.1 Transverse Field Ising model**

**4.2 Heisenberg model**

**4.3 Bose-Hubbard model**



# **Chapter 5**

## **Conclusion**

### **5.1 Direction for future work**

### **5.2 Remarks**



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## **Appendix A**

### **Jax ecosystem**



# Appendix B

## Gradient estimation

In order to perform gradient descent on the ELBO objective, we need to be able to evaluate its gradients with respect to parameters  $\theta$  and  $\phi$ . Taking the gradient w.r.t generative parameters  $\theta$  is straightforward, because we can change the order of the expectation operator and the gradient, leaving us with

$$\begin{aligned}\nabla_{\theta} \mathcal{L}_{\theta, \phi}(\mathbf{x}) &= \nabla_{\theta} \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} [\log p_{\theta}(\mathbf{x}, \mathbf{z}) - \log q_{\phi}(\mathbf{z}|\mathbf{x})] \\ &\simeq \nabla_{\theta} (\log p_{\theta}(\mathbf{x}, \mathbf{z}) - \log q_{\phi}(\mathbf{z}|\mathbf{x})) \\ &= \nabla_{\theta} (\log p_{\theta}(\mathbf{x}, \mathbf{z})),\end{aligned}\tag{B.1}$$

where  $\simeq$  denotes an unbiased estimator. This reversing of the order of operations is not possible when taking gradients w.r.t variational parameters  $\phi$  because the expectation  $\mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})}$  is performed w.r.t the approximate posterior  $q_{\phi}(\mathbf{z}|\mathbf{x})$ . The gradient could be estimated with a vanilla Monte Carlo estimator, but it has very high variance and is not practical [4].

The problem of stochastic gradient estimation of an expectation of a function is a well studied problem that transcends machine learning and has a variety of applications [1, 6]. Different estimators differ in from and their properties, variance being one of the most important. In their review [5] Mohamed et al. categorise MC gradient estimators into three categories

1. *Score-function estimator*: The score function is a logarithm of a probability distribution w.r.t to distributional parameters. It can be used as a gradient estimator

$$\begin{aligned}\nabla_{\theta} \mathbb{E}_{p_{\theta}(\mathbf{x})}[f(\mathbf{x})] &= \nabla_{\theta} \int p_{\theta}(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} \\ &= \mathbb{E}_{p_{\theta}(\mathbf{x})}[f(\mathbf{x}) \nabla_{\theta} \log p_{\theta}(\mathbf{x})].\end{aligned}\tag{B.2}$$

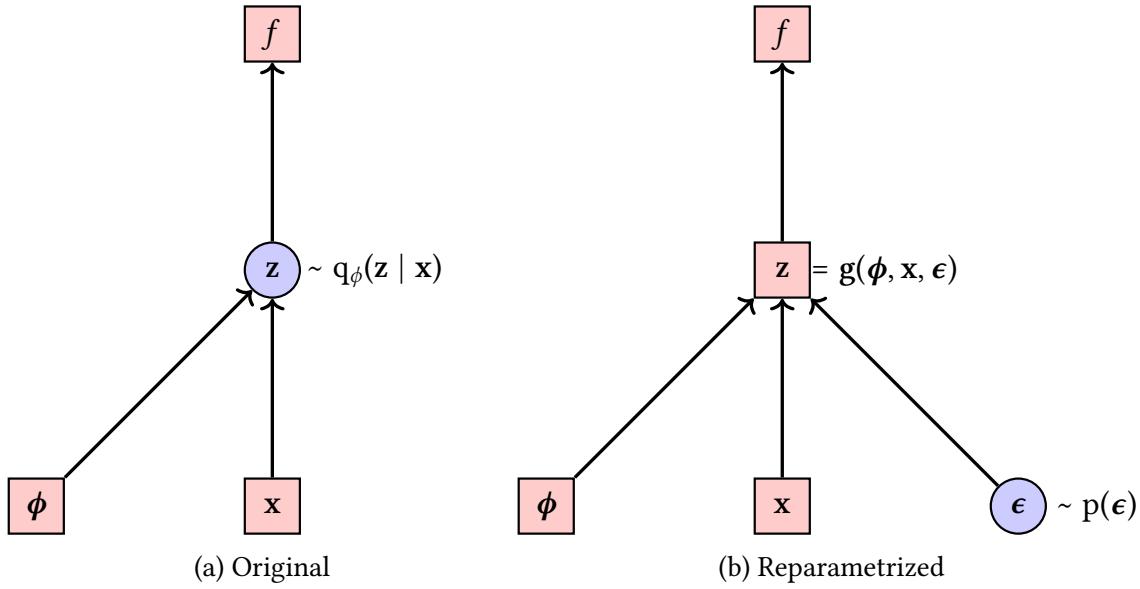


Fig. B.1 The reparametrization trick, adapted from [3]. The stochasticity of the  $z$  node is pushed out into a separate input to the same node, resulting in deterministic gradients w.r.t  $\phi$  through the node.

The score-function estimator is compatible with any cost function, it requires that the measure  $p_\theta(x)$  is differentiable and easy to sample. Very importantly it is applicable to both discrete and continuous distribution, but has a drawback of having high variance.

2. *Pathwise estimator:* Continuous distributions can be sampled either directly by generating samples from the distribution  $p_\theta(x)$  or indirectly, by sampling from a simpler base distribution  $p(\epsilon)$  and transforming the variate through a deterministic path  $g_\theta(\epsilon)$ . Using this, it is possible to move the source of randomness in such a way that the objective is differentiable. In essence this approach pushes the parameters of the measure into the cost function which is then differentiated. The estimator is

$$\begin{aligned}
 \nabla_\theta \mathbb{E}_{p_\theta(x)}[f(x)] &= \nabla_\theta \int p_\theta(x)f(x)dx \\
 &= \nabla_\theta \int p(\epsilon)f(g_\theta(\epsilon))d\epsilon \\
 &= \mathbb{E}_{p(\epsilon)}[\nabla_\theta f(g_\theta(\epsilon))].
 \end{aligned} \tag{B.3}$$

This was the gradient estimator originally used in the VAE implementation [4] there named as the *reparametrization trick*, see also Figure B.1. In many cases the transformation paths are so simple they can be implemented in one line of code,

referred to as *one-liners*. The pathwise-estimator can only be used on differentiable cost functions, but is easy to implement and crucially has lower variance than the score-function estimator.

3. *Measure-valued gradient estimator*, which exploits the properties of signed-measures, is beyond the scope of this report.

Unbiased gradient estimation makes training on the ELBO objective possible. During training the VAE learns a mapping between a complicated observed space of  $\mathbf{x}$  and the latent space of  $\mathbf{z}$ , which is usually defined to be relatively simple. The *decoder* network or the *generative* part of the VAE  $p_\theta(\mathbf{x}|\mathbf{z})$  learns to map from the latent space to the data space, while the *inference* or *encoder* network  $q_\phi(\mathbf{z}|\mathbf{x})$  approximates the true posterior  $p_\theta(\mathbf{z}|\mathbf{x})$  of this process, see Figure.



## **Appendix C**

### **Probability distributions**

