

# End-of-Studies Internship Report

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## Modeling Forward Initial Margin and Counterparty Risk in Uncleared Derivatives

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# Abstract

This report focuses on the modeling of forward initial margin (IM) in the context of counter-party credit risk. A Github repository is available at [Nathan-Sanglier/EY-Initial-Margin](#).

**In Section 1**, we highlight the need to model such quantity as part of the prudential framework, ie. the bank capital requirements. We follow a top-down approach starting from the computation of RWA, up to the modeling of collateralized exposure. **In Section 2**, we investigate where spot and forward IM appear beyond the prudential framework and we provide the main methods for calculating the spot initial margin. We also give the mathematical definition of forward IM and the general procedure for its estimation in the context of Monte-Carlo simulations, which are necessary for computing the expected exposure. **In Section 3**, we focus on the forward IM models studied in this report: nested Monte-Carlo, Monte-Carlo with Gaussian distribution, Monte-Carlo with Johnson distribution, and neural networks quantile regression. We also provide a exhaustive state-of-the-art of the other techniques. **In Section 4**, we present a detailed analysis of the performance of the forward IM models for two case studies: a European put option where the stock price follows a Black-Scholes dynamics, and a swaption where the riskfree rate follows a one factor Hull-White dynamics. **Finally, Section 5** summarizes the findings of this report and discuss potential further developments in the field of forward initial margin modeling. Several technical appendices are also available for the reader unfamiliar with the mathematical topics discussed.

Throughout this report, we consider a frictionless and arbitrage-free continuous-time financial market with a finite time horizon  $T$ . In addition and unless stated otherwise, let  $(\Omega, \mathcal{F}, \mathbb{Q})$  be the probabilistic space with the market filtration  $\mathcal{F} = (\mathcal{F}_t)_{0 \leq t \leq T}$  and the risk-neutral probability measure  $\mathbb{Q}$ , with  $\mathbb{E}[\cdot]$  being the expectation under  $\mathbb{Q}$ . We also denote the physical probability measure  $\mathbb{P}$ .

# Contents

<b>1 Initial Margin in the Regulatory Framework</b>	<b>5</b>
1.1 The Basel frameworks . . . . .	5
1.2 CCR for uncleared OTC derivatives . . . . .	7
1.3 Modeling collateralized exposure . . . . .	9
<b>2 Computing Initial Margin</b>	<b>12</b>
2.1 Initial margin in the XVA framework . . . . .	12
2.2 Spot initial margin . . . . .	13
2.2.1 Standardized margin schedule . . . . .	13
2.2.2 ISDA standard initial margin model (SIMM) . . . . .	13
2.2.3 Internal model . . . . .	14
2.3 Forward initial margin . . . . .	15
<b>3 Forward Initial Margin Models</b>	<b>18</b>
3.1 A first approach: nested Monte-Carlo . . . . .	18
3.2 State-of-the-art . . . . .	19
3.3 Monte-Carlo with Gaussian distribution . . . . .	21
3.4 Monte-Carlo with Johnson distribution . . . . .	23
3.4.1 Johnson least-squares Monte-Carlo . . . . .	24
3.4.2 Johnson percentile matching Monte-Carlo . . . . .	26
3.5 Neural networks quantile regression . . . . .	27
3.5.1 A larger scope of study . . . . .	27
3.5.2 Learning conditional value-at-risk and expected shortfall . . . . .	28
3.5.3 A priori error, a posteriori error, and multi-quantile setup . . . . .	30

<b>4 Case Study and Numerical Results</b>	<b>32</b>
4.1 European put option in Black-Scholes model . . . . .	32
4.1.1 Model setup and analytical expressions . . . . .	32
4.1.2 Numerical results . . . . .	33
4.2 Swaption in Hull-White model . . . . .	40
4.2.1 Model setup and analytical expressions . . . . .	40
4.2.2 Numerical results . . . . .	42
4.3 Conclusion . . . . .	47
<b>5 Further Developments and Conclusion</b>	<b>49</b>
<b>A On Conditional Expectation, Quantile, and Superquantile</b>	<b>55</b>
A.1 Conditional expectation . . . . .	55
A.2 Conditional quantile . . . . .	56
A.3 Conditional superquantile . . . . .	59
<b>B On Neural Networks and Stochastic Gradient Descent</b>	<b>60</b>
<b>C On Johnson Distributions</b>	<b>64</b>
C.1 The types of Johnson distributions . . . . .	64
C.2 Johnson parameters estimation . . . . .	66
C.2.1 Moment matching . . . . .	66
C.2.2 Percentile matching . . . . .	67
<b>D On One Factor Hull-White Model and Swaption Pricing</b>	<b>68</b>
D.1 The one factor Hull-White model . . . . .	68
D.2 Swaption pricing in HW1F . . . . .	69

# 1 Initial Margin in the Regulatory Framework

In this section, we introduce the necessity to model forward IM in the context of the prudential Basel frameworks. Thus, it is important to understand and define the metrics used for capital requirement of banks.

## 1.1 The Basel frameworks

The Basel Committee of Banking Supervision (BCBS) is a committee of the Bank for International Settlements (BIS) responsible for defining global standards for banking regulation worldwide. Notice that the Basel frameworks focus only on the banking sector and have no legal power. Indeed, each jurisdictional regulatory body is responsible for adopting and adapting the BCBS guidance into local regulation. For instance, in the European Union (EU), the European Commission proposes legislative texts with the help of the European Parliament, the European Banking Authority (EBA), and the European Central Bank (ECB). Some of them are directly applicable in all EU member States (regulations) while others (directives) must be transposed into the national law by national competent authorities, like Autorité de Contrôle Prudentiel et de Résolution (ACPR) in France.

The first Basel Accord was published in the 1980's and has evolved through subsequent Accords into the cumulative Basel framework, which is based on three pillars (in addition to separate regulatory tools for leverage and liquidity aspects which are not studied here):

1. **Capital requirements.** The bank has to meet a minimum level of solvency at all times by having enough capital to cover the risk of expected and unexpected losses, based on capital ratio (CR):

$$CR := \frac{\text{Capital}}{\text{RWA}}, \quad (1)$$

where RWA are the risk-weighted assets, which will be detailed later. Capital is highly important, because if the value of assets falls, the losses are subtracted from capital and not from customer deposits or debt holders. We can distinguish 3 types of capital. The first one is Common Equity Tier 1 (CET1) which includes common shares, retained earnings and is considered the most stable. The second one is Additional Tier 1 whose purpose is to absorb losses prior to or at the point of insolvency<sup>1</sup> and forms the Tier 1 capital with

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<sup>1</sup>Notice that insolvency is different from default and bankruptcy. Default occurs when a bank fails to miss a specific debt obligation (eg. missed coupon payment) and may lead to bankruptcy if the default can't be cured. Bankruptcy refers to the legal process through which the bank seeks relief from some of its debts by liquidating assets. On the other hand, insolvency means that the bank has not enough assets or cash flows to cover its liabilities. Insolvency does not always imply default as the bank could still meet its debt obligations by borrowing money or acknowledging incapacity to meet future payments. However, it may lead to debt restructuring (modify terms with creditors to survive) or bankruptcy directly if no other solution is conceivable.

CET1. The last one is Tier 2 capital, used to absorb losses in the event of liquidation and forms the total capital with the tier 1 capital. Since the Basel III framework published by the BCBS in 2010, and implemented legally in the EU as Capital Requirement Regulation (CRR) III and Capital Requirement Directive (CRD) VI as of 1st January 2014, the minimum capital requirements (MCR) are:

$$MCR := \begin{cases} 4.5\% & \text{if Capital} = \text{CET1}, \\ 6.0\% & \text{if Capital} = \text{Tier 1}, \\ 8.0\% & \text{if Capital} = \text{Total Capital}. \end{cases} \quad (2)$$

There also exist capital buffers (conservation, countercyclical and systemic) to protect banks against the variability of their capital requirements. For more information, consult RBC20 [[oBS20a](#)].

2. **Supervisory review process.** This pillar focuses on forward-looking capital adequacy of the bank, assessed internally for each material risk and is required annually through the Internal Capital Adequacy Assessment Process (ICAAP) as part of the Supervisory Review and Evaluation Process (SREP). Moreover, it provides sound guidelines about risk management and reporting, as well as stress tests (banks performance during simulated macroeconomic and market adverse scenarios), which are also controlled by supervisors during the SREP, who could require higher capital ratios or impose qualitative measures for risk management.
3. **Market disclosure.** In order to ensure transparency and accountability, this last pillar requires banks to publicly disclose key information on their risk exposure, capital adequacy, and governance and risk management practices.

Since its publication, the Basel III framework has been reformed and the latest modifications have been proposed in December 2017. They have been legally implemented in the EU since 1st January 2025 with CRR III and CRD VI.

In this report, we consider the regulations related to Counterparty Credit Risk (CCR), defined as the risk that a counterparty to a transaction could default before the final settlement of the transaction's cash flows in cases where there is a bilateral risk of loss (see CRE50 [[oBS24a](#)]). CCR mainly relates to the trading book, where financial instruments are recorded in the balance sheet as mark-to-market if they are exchange-traded (eg. futures), or mark-to-model if they are traded over-the-counter (OTC). Notice that some OTC derivatives can be traded through clearing houses (cleared OTC derivatives). Moreover, even if a credit valuation adjustment (CVA) has been charged to the client in addition to the derivative price, the bank still needs to put aside capital reserves as the credit situation of the counterparty can change during the instrument life. CCR is opposed to credit risk associated with the banking book, where financial instruments are recorded by their amortized cost (eg. loans, mortgages). For more information,

see CRE51 [oBS20b].

## 1.2 CCR for uncleared OTC derivatives

When computing its RWA, the bank has the choice to either use internal methods or standard approaches. While internal methods are tailored to the portfolio of the bank, they must also be authorized by the competent authorities and require more investment. According to CRE51 [oBS20b], the CCR RWA for uncleared OTC derivatives are calculated either by the standardized or the IRB<sup>2</sup> approach to credit risk. In all cases (see CRE20 [oBS24b] and CRE31 [oBS20f]):

$$\text{RWA} := \frac{1}{0.08} \cdot \sum_j w_j \text{EAD}_j, \quad (3)$$

where  $\text{EAD}_j$  is the Exposure at Default of counterparty  $j$ , and  $w_j$  is the weight attributed to this counterparty. Notice that  $1/0.08 = 12.5$  enables to express total required capital directly as RWA. The difference between the standardized and the IRB approaches lies in the calculation of  $w_j$ . While it follows simple predetermined grids for standardized approach (see CRE20 [oBS24b]), it is more complex for the IRB approach. According to see CRE31 [oBS20f] it features the one year probability of default (PD) calculated based on the rating of the counterparty, and the loss given default (LGD) calculated based on the EAD of the counterparty:

$$w_j := \left( \Phi \left( \sqrt{\frac{1}{1-R_j}} \Phi^{-1}(\text{PD}_j) + \sqrt{\frac{R_j}{1-R_j}} \Phi^{-1}(0.999) \right) - \text{PD}_j \right) \times \text{LGD}_j \cdot \frac{1 + (M_j - 2.5)b_j}{1 - 1.5b_j}, \quad (4)$$

where  $b_j = (0.11852 - 0.05478 \ln(\text{PD}_j))^2$ ,  $R_j$  is the correlation parameter (see CRE31 [oBS20f]) and  $M_j$  the maturity factor (see CRE53 [oBS20c]), such that in the general case:

$$\begin{cases} R_j &:= 0.12 \frac{1-e^{-50\text{PD}_j}}{1-e^{-50}} + 0.24 \left( 1 - \frac{1-e^{-50\text{PD}_j}}{1-e^{-50}} \right), \\ M_j &:= \min \left( 1 + \frac{\int_1^T \text{EE}(t) B_0(t) dt}{\int_0^1 \text{EEE}(t) B_0(t) dt}, 5 \right), \end{cases} \quad (5)$$

where  $B_0(t)$  is the discount factor (ie. the price of the zero-coupon of maturity  $t$ ),  $T$  is the last maturity of contracts related to counterparty  $j$  (considering a run-off portfolio), and  $\text{EE}(t)$  is the expected exposure at time  $t$ , which will be detailed later. For the IRB approach presented here, notice that the PD is always estimated internally (see CRE36 [oBS20d]), and the LGD can be estimated using either the F-IRB approach or a fully internal one (A-IRB), see CRE32 [oBS20e]. Herafter, we will only focus on the estimation of EAD.

While the calculation of EAD obeys to simple accounting rules in the context of credit risk related to on-balance sheet items (see article 166 of CRR III), it is a much tougher task in

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<sup>2</sup>IRB: Internal Rating Based.

the context of CCR for uncleared OTC derivatives as they are marked-to-model and require posting/receiving collateral in order to mitigate excessive credit exposure. Indeed, the derivatives contracts related to a counterparty are grouped into a unique legal framework called the ISDA Master Agreement (IMA), which defines the general terms of the transactions. In this structure, derivatives can be grouped (not a requirement) into several Master Netting Agreements (MNA), which are in turn made of different Credit Support Annexes (CSA).

When computing EAD for uncleared OTC derivatives, the bank has the choice to use either the standardized approach (SA-CCR) based on CRE52 [oBS20h], or the internal model method IMM). We will only focus on the IMM. For a counterparty  $j$ , denoting  $EAD := EAD_j$  for simplicity, we have based on CRE53 [oBS20c]:

$$EAD := \alpha \cdot \max (EEPE, EEPE_{stressed}), \quad (6)$$

where  $\alpha \geq 1.4$  is the regulatory multiplier, and  $EEPE$  and  $EEPE_{stressed}$  are the Effective Expected Positive Exposures calculated respectively under unstressed and stressed market conditions (calibration of model parameters will change), and such that:

$$EEPE := \int_0^{T \wedge 1} EEE(t) dt, \quad (7)$$

where

$$EEE(t) := \sup_{0 \leq s \leq t} EE(s) \quad (8)$$

is the Effective Expected Exposure at time  $t$ . This formula enables to have a conservative estimation on the calculation of EEE to reflect the fact we consider in theory a run-off portfolio (the portfolio values amortizes through time), whereas it is not true in practice. Moreover,

$$EE(t) := \mathbb{E}[E_t | \mathcal{F}_0] \quad (9)$$

is the Expected Exposure at time  $t$  (assuming the counterparty defaults at time  $t$ ), where  $(E_t)$  is the collateralized exposure which needs to be modeled taking into account the IMA legal framework (see Section 1.3). Notice that the expectation is computed under the risk-neutral one  $\mathbb{Q}$  (ie. calibrating with market implied data), but it can also be computed under the historical probability measure  $\mathbb{P}$  (ie. calibrating the modeling of  $(E_t)$  with at least three years historical market data). For more information, see article 292 of CRR III.

In the definition (9) of expected exposure, we have assumed that there is no specific wrong-wray risk. According to [oBS24a], such risk arises when the exposure to the counterparty is positively correlated with its probability of default, due to the nature of the transaction. In

other words, we have assumed that:

$$\mathbb{E}[E_t | \tau^* = t, \mathcal{F}_0] = \mathbb{E}[E_t | \mathcal{F}_0], \quad (10)$$

where  $\tau^*$  is the materialized default time of the counterparty<sup>3</sup>. From articles 284 and 291 of CRR III, expected exposures for instruments subject to specific wrong-way risk should be calculated separately. For instance, [Pyk24] and [AK24] investigate the modeling of expected exposure subject to a modified "leveraged" wrong-way risk by applying a Gaussian copula to link the counterparty default event with the increment of the portfolio value over the MPOR defined in Section 1.3.

### 1.3 Modeling collateralized exposure

The Expected Exposure defined in (9) relies on the stochastic process  $(E_t)_{0 \leq t \leq T}$ , which is the collateralized exposure. It represents the estimated "net" exposure of the bank if the counterparty defaults and the amount of losses becomes known at a future time  $t$ . Let us denote  $M$  a MNA inside the ISDA agreement<sup>4</sup>  $I$ , and  $C$  a CSA inside a specific MNA. We then have:

$$E_t = \sum_{M \in I} E_t^{(M)} = \sum_{M \in I} \left( \sum_{C \in M} \left( V_t^{(C)} + \text{UTF}_t^{(C)} - K_t^{(C)} \right) \right)_+, \quad (11)$$

where  $V_t^{(C)}$  is the mark-to-market process (to the bank) associated to CSA  $C$ , so MtMs are aggregated (netted) at the CSA level. Notice that we use the term "mark-to-market", but it is in fact a mark-to-model process as we focus on the pricing of OTC products at future dates. Moreover,  $\text{UTF}_t^{(C)}$  represents the unpaid trade flows to the bank (flows related to contractual cash flows) at the CSA level during the margin period of risk (MPOR).  $K_t^{(C)}$  is the effective collateral available to the bank. For simplicity, assume we have only one CSA (equivalently a "portfolio") in our ISDA agreement, ie.

$$E_t := (V_t + \text{UTF}_t - K_t)_+, \quad (12)$$

where  $(V_t)$  is the portfolio value. In order to model the quantities in (12), we need to make some hypotheses about collateral exchanges (margin flows) and trade flows. We will use the model of [Pyk09], described in [ASP16] as the "Classical+" model, but enhanced with an Initial Margin (IM) component.

**Assumptions on margin flows.** First, we define the MPOR represented in Figure 1 as the period of time between the last successful margin call and the time when the amount of loss

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<sup>3</sup>This means the time at which the counterparty defaults is known. In practice the true default time can happen any time during the MPOR defined in Section 1.3.

<sup>4</sup>One may find the term "netting set" in the Basel documentation. Under the IMM, this represents in general a CSA, see Article 272 of CRR III.

becomes known and transaction is closed out (ETD<sup>5</sup>), assuming the counterparty has defaulted between these two dates.

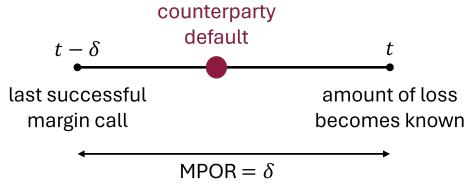


Figure 1: Stylized representation of the MPOR.

Indeed, a firm under stress may stop fully honoring margin calls by attempting a dispute over the collateral requirement calculation, before an Event of Default would be officially issued, and a portfolio termination date decided. Here, we set a fixed MPOR  $\delta = 10$  business days, which is coherent with the standard case in the regulation (see article 304 of CRR III). In practice, the timeline of events prior ETD is more complex, so that the model may be enhanced as in [ASP16]. We also consider that both the bank and its counterparty stop paying margins at  $t - \delta$  ( $t$  being the ETD) and that there is no minimal amount threshold for receiving or posting collateral (ie. no margin threshold). Thus, for all  $t \in [\delta, T]$ :

$$\begin{cases} K_t &= \text{VM}_{t-\delta} + \text{IM}_{t-\delta} \\ \text{VM}_t &= V_t, \end{cases} \quad (13)$$

where VM and IM are respectively the Variation Margin and *received* Initial Margin (ie. IM posted by the counterparty to the bank), calculated at the CSA level<sup>6</sup>. VM captures the day-to-day movement of the portfolio, and we have assumed perfect continuous variation margining as it is not the focus of our study. IM covers portfolio gap risk (also called close-out risk) which is the risk of adverse market movement during the MPOR, at some high percentage. Although the term “initial” may be misleading, notice that both these quantities are dynamically refreshed. However, the IM amount must be held in a default-remote way (eg. by a custodian), so that IM posted by a counterparty should be immediately available to it should the other counterparty default. Since 2015, posting/receiving VM and IM is mandatory on a regular basis (eg. daily) and follows specific uncleared margin rules (UMR) under the BCBS-IOSCO guidelines [oBS20g]. The MPOR implies that the counterparty cannot default before  $\delta$  (otherwise the bank would not enter the trade), hence the integral in EEPE starts at  $t = \delta$ .

**Assumptions on trade flows.** We consider that both the bank and the counterparty continue paying all trade flows during the MPOR:

$$\text{UTF}_t = 0. \quad (14)$$

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<sup>5</sup>Early Termination Date.

<sup>6</sup>Notice one could accrue collateral from  $t - \delta$  to  $t$  at the riskfree rate, such that  $K_t = e^{\int_{t-\delta}^t r_s ds} (\text{VM}_{t-\delta} + \text{IM}_{t-\delta})$ .

Notice that this is not a too restrictive hypothesis (and greatly simplifies implementations) as most of the time, there is no trade flow between  $t - \delta$  and  $t$  ( $\delta = 10$  days). Moreover, the final quantity EAD is based on an integral of the collateralized exposure during the portfolio life, making the consideration of trade flows less significant. Nonetheless, any possibility of the bank making a trade payment to the counterparty in the future results in upward spikes in the expected exposure profile. These spikes appear because the portfolio value will jump following the payment by the bank, but the counterparty does not update the VM in consequence, ie. there is not offsetting. In some situations, it could yield to an undesirable instability in expected exposure (or CVA, defined later)<sup>7</sup>. As mentioned before, this exposure model can be refined, to better account for the timeline complexity of IMA/CSA events, eg. see [ASP16].

In summary, one needs to estimate  $\forall \delta \leq t \leq T \wedge 1$ :

$$\text{EE}(t) = \mathbb{E} [(V_t + \text{UTF}_t - \text{VM}_{t-\delta} - \text{IM}_{t-\delta})_+ \mid \mathcal{F}_0]. \quad (15)$$

In particular, we need to define the quantity  $\text{IM}_t$ . Typically, the expectation under  $\mathbb{Q}$  will be approximated by its empirical version, and the expected exposure will be computed on a time grid<sup>8</sup>  $G := [\delta =: t_0, \dots, t_K := T \wedge 1]$ , such that for all  $k \in 0 : K$ ,

$$\text{EE}(t_k) \approx \frac{1}{M} \sum_{m=1}^M \left( V_{t_k}^{(m)} + \text{UTF}_{t_k}^{(m)} - \text{VM}_{t_k-\delta}^{(m)} - \text{IM}_{t_k-\delta}^{(m)} \right)_+. \quad (16)$$

It implies the necessity to:

1. Model and compute the mark-to-market process on each path  $(m)$  and *at least*<sup>9</sup> at each timestep  $t_k$ .
2. Model and compute the initial margin on each path  $(m)$  and at each date  $t_k - \delta$ . It amounts to calculating the spot IM value for  $t_k = \delta$  (ie.  $t_k - \delta = 0$ ), but also a **forward** IM value for  $t_k > \delta$ .

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<sup>7</sup>For a comprehensive study, see [ASP17].

<sup>8</sup>A finer mesh is usually used for short-term dates in the time grid  $G$ , with increasing timestep towards maturity.

<sup>9</sup>We will see that computing IM also requires computing portfolio value at given dates that may not be in our time grid  $G$ .

## 2 Computing Initial Margin

### 2.1 Initial margin in the XVA framework

As explained in Section 1, computing spot IM is needed for “real-world” transactions of OTC derivatives under the BCBS-IOSCO guidelines [oBS20g], and both spot and forward IM are mandatory from a prudential point of view. Moreover, they are also required in the context of fair value pricing of a derivative product. In incomplete markets, a model price assuming a completeness hypothesis has to be adjusted by the valuation of market imperfections. Derivative dealers charge to their clients so-called XVAs, standing for the different value adjustments, meant to account for counterparty risk and its capital and funding implications. In particular, posting initial margin dynamically during the life of the contract induces a funding cost which is known as margin value adjustment (MVA) [VL24]:

$$\text{MVA}_0 = \int_0^T f(t) \mathbb{E} \left[ e^{-\int_0^t r_s ds} \text{PIM}_t \mid \mathcal{F}_0 \right] dt, \quad (17)$$

where  $f$  is the risky funding spread of the bank,  $(r_t)$  is the risk-free rate, and  $\text{PIM}_t$  is the *posted* IM by the bank. In addition, the credit value adjustment (CVA) represents the difference between the price of the product with and without default risk the counterparty. Let us assume default time of the bank is beyond  $T$  and denote  $\tau = \tau^* - \delta$  where  $\tau^*$  is the materialized default time (as explained in Section 1.2). we have according to [BCG<sup>+</sup>24] and [CBB14]:

$$\text{CVA}_t = \mathbb{E} \left[ e^{-\int_t^{\tau+\delta} r_s ds} \mathbf{1}_{t < \tau + \delta < T} (1 - R) E_{\tau + \delta} \mid \mathcal{F}_t \right] \quad (18)$$

$$= (1 - R) \mathbf{1}_{t < \tau + \delta} \mathbb{E} \left[ e^{-\int_t^{\tau+\delta} r_s ds} \mathbf{1}_{\tau + \delta < T} E_{\tau + \delta} \mid \mathcal{F}_t \right], \quad (19)$$

here  $R$  is the recovery rate of the counterparty upon default, and  $E_\tau$  is the collateralized exposure defined in (12) which features the IM received by the bank. We then have:

$$\begin{aligned} \text{CVA}_t = & (1 - R) \mathbf{1}_{t < \tau} \mathbb{E} \left[ \mathbb{E} \left[ e^{-\int_t^{\tau+\delta} r_s ds} \mathbf{1}_{\tau + \delta < T} E_{\tau + \delta} \mid \mathcal{F}_\tau \right] \mid \mathcal{F}_t \right] \\ & + (1 - R) \mathbf{1}_{\tau < t < \tau + \delta} \mathbb{E} \left[ e^{-\int_t^{\tau+\delta} r_s ds} \mathbf{1}_{\tau + \delta < T} E_{\tau + \delta} \mid \mathcal{F}_t \right]. \end{aligned} \quad (20)$$

Assuming a reduced-form credit default model for the counterparty and denoting  $\gamma(t)$  its default intensity (ie. the hazard rate), we have:

$$\begin{aligned} \text{CVA}_t = & (1 - R) \mathbf{1}_{t < \tau} \mathbb{E} \left[ \int_t^{T-\delta} \mathbb{E} \left[ e^{-\int_t^{s+\delta} r_u du} E_{s+\delta} \mid \mathcal{F}_s \right] \gamma(s) e^{-\int_t^s \gamma(u) du} ds \mid \mathcal{F}_t \right] \\ & + (1 - R) \mathbf{1}_{\tau < t < \tau + \delta} \mathbb{E} \left[ e^{-\int_t^{\tau+\delta} r_s ds} \mathbf{1}_{\tau + \delta < T} E_{\tau + \delta} \mid \mathcal{F}_t \right]. \end{aligned} \quad (21)$$

For more information on CVA, MVA, other XVA and the implications of collateralization, please refer to [CBB14], [Gre15]. In conclusion, as for the regulatory point of view, we face the challenge

of computing a forward (and spot) Initial Margin, re-affirming the importance of such problem.

## 2.2 Spot initial margin

As explained above, calculating spot IM (ie. IM at the date  $t = 0$ ) is done on a daily basis by the banks, in order to announce margin calls to their counterparties. It falls under clear regulations and requirements described in [oBS20g], where financial institutions can either use a standardized margin schedule or an initial margin model.

### 2.2.1 Standardized margin schedule

This standardized method is provided by the BCBS and the International Organization of Securities Commissions (IOSCO), such that:

$$\text{IM}_0 = (0.4 + 0.6 \cdot \text{NGR}) \cdot \sum_j \text{GIM}_j, \quad (22)$$

where  $\text{GIM}_j = w_j \cdot \text{Notional}_j$ , is the gross initial margin amount expressed based on the notional size of the derivative contract  $j$  inside the portfolio (ie. inside a CSA), and a margin rate  $w_j$  pre-determined for specific asset classes given in Appendix A of [oBS20g]. Notice that a limited degree of netting may be performed to compute the notional amount that is applied to the margin rate. Moreover, according to [Aut19], the NGR ratio<sup>10</sup> is:

$$\text{NGR} := \frac{\left( V_0^{(C)} \right)_+}{\sum_{j \in C} \left( V_0^{(j)} \right)_+}, \quad (23)$$

where  $V_0^{(C)} := \sum_{j \in C} V_0^{(j)}$  is the (netted) mark-to-market value of the portfolio at CSA level, and  $V^{(j)}$  the mark-to-market value of instrument  $j$  inside the CSA considered.

### 2.2.2 ISDA standard initial margin model (SIMM)

If the bank does not use the standardized approach, then it uses its own initial margin model, which regroups either the ISDA<sup>11</sup> SIMM or an internal model. In accordance with regulatory standards [oBS20g], the ISDA suggested a method in [Ass23] (first version in 2016) to prevent disputes between counterparties, that is straightforward to implement while being more complex than the standardized approach. This method is now widely used by the industry.

In a portfolio made of several instruments, the methodology considers four product classes:

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<sup>10</sup>NGR: ratio of the net current replacement cost to gross current replacement cost.

<sup>11</sup>ISDA: Interest Swap Derivatives Association.

Interest Rates and Foreign Exchange (RatesFX), Credit, Equity, and Commodity. Moreover, there are six risk classes: Interest, Credit (Qualifying), Credit (Non-Qualifying), Equity, Commodity, FX. The margin that will be calculated for each risk class is defined as the sum of (potentially) four margin classes: Delta, Vega, Curvature<sup>12</sup>, and Base Correlation margins<sup>13</sup>. These margins are defined based on sensitivities with respect to risk factors. Notice that the method to compute these sensitivities is left up to the bank. Moreover, they are assigned to risk buckets according to the characteristics of the risk factor associated. The first step is to classify our instruments and related sensitivities with Algorithm 1. We can then calculate the margins with Algorithm 2 (see [Ass23] for more details).

---

**Algorithm 1:** ISDA SIMM - Sensitivities Classification

---

```

for each instrument  $I_j$  do
    assign it to a product class  $PC_p$  and risk class  $RC_r$ 
    for each risk factor  $RF_k$  related to  $I_j$  do
        assign it to a risk bucket  $RB_b$ 
        for each margin class  $MC_m$  do
            compute the sensitivity  $s_{j,k,m}$  of  $I_j$  wrt.  $RF_k$ , for  $MC_m$ 
            compute the weighted sensitivity  $ws_{j,k,m}$  based on  $RB_b$ 

```

---

**Algorithm 2:** ISDA SIMM - Initial Margin Computation

---

```

Input:  $\forall r \neq s$ , risk classes correlation  $\psi_{r,s}$ 
for each product class  $PC_p$  do
    for each risk class  $RC_r$  do
        for each margin class  $MC_m$  do
            for each risk bucket  $RB_b$  do
                 $K_b \leftarrow$  aggregation of  $\{ws_{j,k,m} \text{ st. } I_j \in PC_p \text{ and } RC_r, RF_k \in RB_b, \forall(j, k)\}$ 
                 $margin_m \leftarrow$  aggregation of  $\{K_{m,b}, \forall b\}$ 
                gross initial margin  $IM_{p,r} \leftarrow \sum_m margin_m$ 
            initial margin  $SIMM_p \leftarrow \sqrt{\sum_r IM_{p,r}^2 + \sum_{s \neq r} \psi_{r,s} IM_{p,r} IM_{p,s}}$ 
        total initial margin  $IM_0 \leftarrow \sum_p SIMM_p$ 

```

---

### 2.2.3 Internal model

If the financial institution does not use the ISDA SIMM for its own initial margin model, then it can use an internal one, which should be approved by the EBA (European Banking Authority) [Par24], and should respect the BCBS-IOSCO guidelines (see [oBS20g]). In this section, we do

<sup>12</sup>It represents the Gamma sensitivity.

<sup>13</sup>Only for credit qualifying, sensitivity to correlation between defaults of different credits within a basket.

not provide examples of such model as more general models for calculating the forward initial margin (and so the spot initial margin) will be investigated later.

The initial margin must reflect an extreme but plausible estimate of an increase in the value of the instrument that is consistent with a one-tailed 99 per cent confidence interval over a 10-day horizon (in case variation margin is exchanged daily). The model calibration should be done based on an historical data period that do not exceed 5 years and that incorporates a period of significant financial stress. This period of financial stress should be identified and applied separately for each broad asset class in the portfolio. Notice that this calibration step is different from the one implied by the Basel capital requirements detailed in Section 1.2.

Moreover, a bank should not be allowed to switch between model and schedule-based margin calculations in an effort to cherry-pick the most favorable initial margin terms. However, it can use a model-based initial margin for one class of derivatives commonly dealt, and a schedule-based one for derivatives that are less routinely employed in its trading activity.

### 2.3 Forward initial margin

Contrary to the computation of spot IM analyzed in Section 2.2, there are no regulatory requirements nor standardized approaches for calculating the forward IM. Nonetheless, in compliance with guidelines for the spot IM provided in Section 2.2.3 and in [Aut19], we define the forward IM for our portfolio as<sup>14</sup>  $\forall t \in [0, T]$ :

$$\text{IM}_t := (\text{VaR}^\alpha(\Delta V_{t+\delta} | \mathcal{F}_t))_+, \quad (24)$$

where  $\Delta V_{t+\delta} := V_{(t+\delta)\wedge T} - V_t$ , and  $\text{VaR}^\alpha(Y) = \inf \{y \in \mathbb{R} \text{ st. } F_Y(y) \geq \alpha\}$  is the quantile of the random variable  $Y$  at level  $\alpha$ , with  $F_Y(\cdot)$  being the cumulative density function (cdf.) of  $Y$  under probability  $\mathbb{Q}$ . Thus, estimating the forward initial margin amounts to estimating a conditional quantile under  $\mathbb{Q}$ . In practice, we will choose  $\alpha = 99\%$ , as described in [oBS20g]. Notice that if the cdf. of  $Y$  is continuous, then  $\mathbb{Q}(Y \leq \text{VaR}^\alpha(Y)) = \alpha$ . For rigorous mathematical definitions of conditional expectation and conditional value-at-risk (or conditional quantile), we refer the reader to Appendix A.1. of [MKN<sup>+</sup>18], Section 2. of [BCG<sup>+</sup>24], as well as [Kal02]. We assume here that all the assumptions are satisfied so that both these operators are defined and applied accordingly.

The construction of a forward IM model is typically done in five main steps. As described in Section 1.3 and given the expressions in Section 2.1, we need to model and compute the initial

---

<sup>14</sup>Notice that one could add the term  $\text{UTF}_{t+\delta}$  inside the value-at-risk. One could also discount the portfolio value at  $t + \delta$  by  $e^{-\int_t^{t+\delta} r_s ds}$ . In order to be consistent with our collateralized exposure model of Section 1.3, we did not take them into account.

margin  $\text{IM}_{t_i}^{(m)}$  on each path  $(m) \in [|1, M|]$  at each evenly spaced date  $t_i$  in the grid:

$$\pi := \{0 =: t_0, \dots, t_N := T \wedge 1\}, \quad (25)$$

with timestep  $h$ . For simplicity, we assume  $\delta \in \pi$  so that  $(t_i + \delta) \wedge T \in \pi$ , since we need to simulate our portfolio value both at  $t_i + \delta$  and  $t_i$  given the formula (24). As in Section 1.3, we choose  $\delta = 10$  days and we will take  $h = 1$  day. Notice that the time grid  $G$  from Section 1.3 is not necessarily the same as the time grid  $\pi$ , even if in general we have  $G \subseteq \pi$ .

1. **Diffusing the risk factors.** In order to calculate our portfolio value at each  $t \in \pi$  in a model-based approach, we first need to identify the risk factors  $(X_t)_t$  associated to the portfolio (taking values in  $\mathbb{R}^d$ ,  $d \in \mathbb{N}^*$ ), and model their dynamics by stochastic differential equations (SDEs), eg. Black-Scholes model. Then, one should calibrate the model parameters with market-implied or historical data. Finally, simulate the  $(m)$ -th path  $\{X_{t_0}^{(m)}, \dots, X_{t_N}^{(m)}\}$  of these risk factors with a given discretization scheme. Notice that for complex models, the scheme used could produce numerical errors, that should be quantified.
2. **Pricing the portfolio.** Based on the  $(m)$ -th path of risk factors previously computed, calculate the  $M$ -th path of portfolio value  $\{V_{t_0}^{(m)}, \dots, V_{t_N}^{(m)}\}$  through the usual techniques such as closed-form formulas, Monte-Carlo methods, partial differential equations (PDEs) resolution, etc.
3. **Estimating the value-at-risk.** Assuming the risk factors to be a Markov process, we now need to calculate for each  $i \in [|0, N|]$  and for each  $m \in [|1, M|]$ :

$$f_i(X_{t_i}^{(m)}) := \text{VaR}^\alpha(\Delta V_{t_i+\delta} | X_{t_i}^{(m)}), \quad (26)$$

where  $(\Delta V_{t+\delta} | x) := (V_{t+\delta} - V_t | X_t = x)$ , for  $x \in \mathbb{R}^d$ . For each  $i \in [|0, N|]$ , the function  $f_i(\cdot)$  (or directly the values  $f_i(V_{t_i}^{(m)})$  in the case of nested Monte-Carlo) will be estimated from our ‘‘training’’ dataset:

$$\mathcal{D} := \left\{ \left( X_{t_i}^{(1)}, \Delta V_{t_i+\delta}^{(1)} \right), \dots, \left( X_{t_i}^{(M)}, \Delta V_{t_i+\delta}^{(M)} \right) \right\}, \quad (27)$$

and/or from new simulations of risk factors<sup>15</sup>. We will see that it is often simpler to calculate for each  $i \in [|0, N|]$  and for each  $m \in [|1, M|]$ :

$$g_i(V_{t_i}^{(m)}) := \text{VaR}^\alpha(\Delta V_{t_i+\delta} | V_{t_i}^{(m)}) \approx f_i(X_{t_i}^{(m)}), \quad (28)$$

where  $(\Delta V_{t+\delta} | v) := (V_{t+\delta} - V_t | V_t = v)$ . Again, for each  $i \in [|0, N|]$ , one can estimate

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<sup>15</sup>It will be the case for techniques involving nested Monte-Carlo simulations.

the function  $g_i(\cdot)$  from the following training dataset:

$$\mathcal{D}' := \left\{ \left( V_{t_i}^{(1)}, \Delta V_{t_i+\delta}^{(1)} \right), \dots, \left( V_{t_i}^{(M)}, \Delta V_{t_i+\delta}^{(M)} \right) \right\}. \quad (29)$$

4. **Adjusting to external methodology.** At this point, there is little chance that our IM estimation at  $t_0$  is consistent with the realized IM value for this portfolio (eg. given by SIMM), as the associated external IM methodology usually differs from our model, and our risk factors model may not be accurate enough. In order to adjust the two quantities at  $t = t_0$  and trying to reduce the gap at  $t > t_0$  to limit the number of exceptions in the back-testing (and to have a conservative value), it is possible to scale the IM estimations by a deterministic coefficient  $\alpha(t)$ , as in [AAGL17]. However, this raises a number of questions about stability and back-testing of this scaling function, investigated in [CA24]. If the external methodology is based on datasets of historical information, [THM16] proposes to scale the IM estimation at  $t_0$  and to re-weight  $\{V_t^{(1)}, \dots, V_t^{(M)}\}$  for  $t > t_0$ . This re-weighting step can be seen as a kind of measure change to the subjective measure  $\mathbb{P}^*$  (perception of the probability  $\mathbb{P}$ ) that is implied by the historical data available.
5. **Backtesting the method.** According to article 294 of CRR III, the last *mandatory* step is to backtest our estimation of value-at-risk. The standard approach in the industry (see [CA24] for an exhaustive review) is to define a back-testing that examines jointly the model's risk factors generation and accuracy of IM forecast. More precisely, [AAGL17] defines a procedure which involves diffusing  $B$  risk factors paths from their observed value at a given past time  $t$  during a backtesting horizon  $H$  (ie. up to time  $t + H$ ). Then, one should calculate calibrate<sup>16</sup> and estimate IM for these  $B$  risk factor values and compare them to the realized IM value. Finally, one should aggregate the results for different past times and horizons. It is also possible to backtest the top-level expected exposure metric as in [AKN13].

Notice that in this report, we do not focus on the calibration of risk factors model parameters, although it is a crucial task. The emphasis is put on the method used to estimate the value-at-risk functions  $f_i(\cdot)$  (or at least the function  $g_i$ ).

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<sup>16</sup>It implies to diffuse the risk factors up to  $t + h + \delta$ .

### 3 Forward Initial Margin Models

#### 3.1 A first approach: nested Monte-Carlo

A first naive approach to directly estimate the values  $f_i(X_{t_i}^{(m)})$  is to calculate the quantile in equation (26) empirically, giving rise to a nested Monte-Carlo. Indeed, for a given  $m \in [|1, M|]$  we first need to simulate  $K$  iid. realizations of  $X_{t_i+\delta}$  conditional on  $X_{t_i} = X_{t_i}^{(m)}$ , denoted  $X_{t_i+\delta}^{(m,k)}$  for each  $k \in [|1, K|]$ . Then, we can compute the portfolio values  $V_{t_i+\delta}^{(m,k)}$  associated, and the sample quantile at level  $\alpha$  based on the  $K$  iid. samples  $\Delta V_{t_i+\delta}^{(m,k)} := V_{t_i+\delta}^{(m,k)} - V_{t_i}^{(m)}$  of  $(\Delta V_{t_i+\delta} | X_{t_i}^{(m)})$ .

In Figure 2, we show a stylized methodology of such approach, for a specific time  $t_i \in \pi$  and a specific path  $m \in [|1, M|]$ . On the left graph, we generate the nested paths of the risk factor ( $d = 1$ ). They are used on the right graph to compute the nested paths of portfolio value (in red), from which we display (in green) the empirical distribution of  $(\Delta V_{t_i+\delta} | X_{t_i}^{(m)})$  and the associated empirical quantile  $\hat{q}_i^{(m)}$ . This value is the estimation of  $f_i(X_{t_i}^{(m)})$  defined in equation (26).

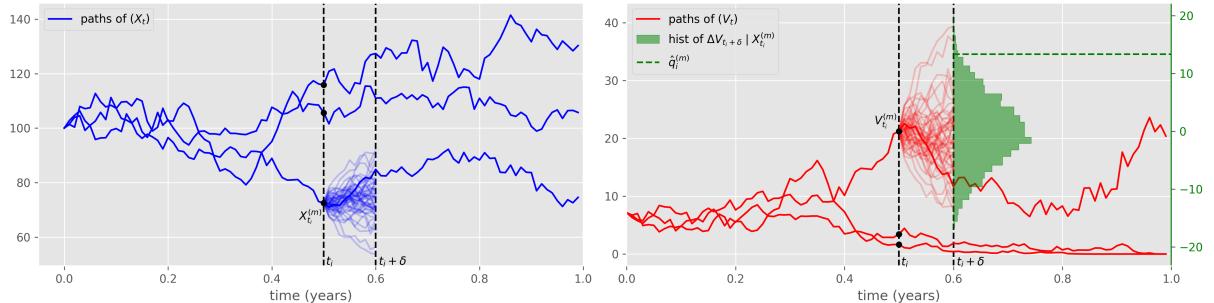


Figure 2: Nested Monte-Carlo, stylized methodology at a specific  $(t_i, m)$ .

At this point, we need to specify what we mean by a sample/empirical quantile  $\hat{q}_i^{(m)}$ . Indeed, according to [HY96], there exist a large number of different definitions used for sample quantiles in statistical packages. Here, we consider the oldest and most studied version.

**Definition 1** (Sample quantile). *Let  $\{Y_1, \dots, Y_K\}$  be a set of iid. observations of a random variable  $Y$  with probability density function  $h$ , and denote  $\{Y_{(1)}, \dots, Y_{(K)}\}$  the associated order statistics. Then, the sample quantile at level  $\alpha$  is:*

$$\hat{q} := \begin{cases} Y_{(\lfloor \alpha K \rfloor + 1)} & \text{if } \lfloor \alpha K \rfloor < \alpha K \leq \lfloor \alpha K \rfloor + 1 \\ Y_{(\lfloor \alpha K \rfloor)} & \text{if } \alpha K = \lfloor \alpha K \rfloor, \end{cases}$$

where  $\lfloor \cdot \rfloor$  denotes the integer part. A visualization is given in Figure 3.

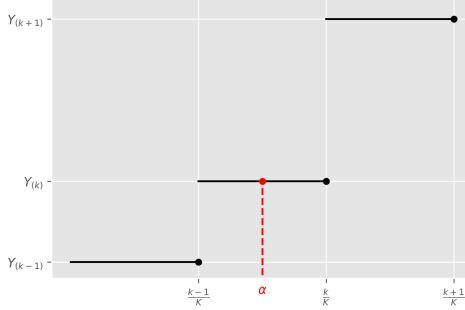


Figure 3: Sample quantile of Definition 1.

[OR01] shows that this estimator is biased<sup>17</sup> (ie.  $\mathbb{E}[\hat{q}] \neq q$ , where  $q$  is the true quantile), and all the more for extreme quantiles compared to central ones. However, [OR01] provides a “quantile Central Limit Theorem”.

**Theorem 1** (Quantile CLT). *Let  $\hat{q}$  be the sample quantile of Definition 1 and  $q$  the true quantile, both at level  $\alpha$ . Then we have:*

$$\sqrt{K}(\hat{q} - q) \xrightarrow[K \rightarrow +\infty]{\mathcal{D}} \mathcal{N}\left(0, \frac{\alpha(1-\alpha)}{h(q)^2}\right). \quad (30)$$

Further detail on sample and asymptotic bounds are investigated in [OR01] and [Leh98]. Thus, we see that the sample quantile is an asymptotically unbiased estimator, which implies that we need to simulate a high number  $K$  of nested paths, but simulating risk factors and pricing portfolio  $K \times M \times N$  times is too costly. [GJ10] investigates in details the computational budget to be allocated based on a mean-square error criterion. Notice that [ATCD18] provides advanced nested Monte-Carlo based on GPU optimization to mitigate this issue in the more general context of XVA computations.

### 3.2 State-of-the-art

In order to alleviate the computational burden implied by nested Monte Carlo methods, it is common practice in the industry to rely on more advanced techniques that we group into different broad categories.

1. **Distribution-based methods.** The first step is to make an assumption on the distribution of  $(\Delta V_{t+\delta} | v)$ . Indeed, we will estimate the function  $g_i(\cdot)$  instead of  $f_i(\cdot)$  (see equations (26)-(28)) to avoid specifying a distribution in high dimension and estimating mixed moments that would not be feasible in practice. In particular, we will study the method GLSMC [AAGL17] where we make the hypothesis that  $(\Delta V_{t+\delta} | v)$  follows a Gaussian distribution (see Section 3.3), as well as the method JLSMC [MKN<sup>+</sup>18] which makes

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<sup>17</sup>This is not specific to the estimator studied here.

the assumption that  $(\Delta V_{t+\delta} | v)$  follows a Johnson distribution (see Section 3.4.1). Once we have determined the adequate distribution, the next step is to estimate some metrics of the distribution (eg. moments, quantiles, etc.) and fit the distribution parameters based on these estimations. Usually, one estimates the first conditional raw moments of  $(\Delta V_{t+\delta} | v)$  up to a given order and performs a moment-matching procedure. In this case, the conditional raw moments functions are estimated by regression using the dataset  $D'$  defined in (29). At this point, we can either use non-parametric methods like kernel regression,  $k$ -NN, Random Forest, etc. or parametric methods. If one chooses the last option, the regression is performed by specifying the conditional raw moment function as a linear combination of functions from a given truncated basis. It amounts to a least-squares Monte-Carlo approach as in the standard American option pricing (see eg. the Longstaff-Schwartz method [LS01]). Although ordinary least squares (OLS) approach is the most natural for parametric regression, other approaches can be explored such as Huber regression [HR09], generalized linear models [NW72], ridge regression etc. Finally, value-at-risk can be estimated as the quantile at level  $\alpha$  of the fitted distribution.

2. **Parametric distribution-free methods.** While assuming a given distribution for  $(\Delta V_{t+\delta} | v)$  yields a more tractable problem, it is also prone to high bias (eg. invalid distribution) and high variance (eg. estimation of high-order moments for moment matching). Fortunately, some techniques do not require such hypothesis and can be coined as parametric quantile regression methods. It can be seen that the function representing the conditional value-at-risk minimizes the expectation of the “pinball loss” (see equation (105) of Appendix A). Minimizing this loss over the set of neural networks yield a non-convex optimization problem, which involves the use of stochastic gradient descent (SGD)-like algorithms. The task of estimating the value-at-risk function by minimizing this loss is called *quantile regression*. We will explore the approach of [BCG<sup>+</sup>24] (see Section 3.5) who propose a two-steps methodology for estimating value-at-risk and expected shortfall in a potentially multi-quantile setup (ie. estimating value-at-risk at different levels  $\alpha$ ). Regulators are not especially eager to the adoption of such approach as they consider Deep Learning techniques to be black boxes with little control. However, as we will recall, there are many theoretical results on neural networks that enable to provide so-called *a priori* and *a posteriori* bounds on the error between neural network estimation of value-at-risk (or expected shortfall) and the corresponding groundtruth.
3. **Non-parametric methods.** If one does not want to specify a parametric form for the function  $f_i(\cdot)$  of equation (26), it is possible to use kernel quantile regression [LLZ07], which includes the entire family of smoothing splines and additive and interaction spline models. Moreover, one can use quantile regression tree [CL02] or quantile regression forest [Mei06] that are build upon regression trees and random forests. While these methods are non-supervised, one may instead try supervised learning methods such as Gaussian process regression (see [MZ21] and [BBC12]), which assumes a Gaussian process prior

over the function to estimate. However, it requires labels (ie. true value-at-risk function valued at given points) that we don't have at first hand. Hence, we need to produce noisy labels using nested Monte-Carlo simulations, which adds computational burden over the Gaussian process regression.

4. **Sensitivity-based methods.** Another approach is to use sensitivity-based methods, which focus on the sensitivity of the portfolio value to changes in risk factors. The Delta-Gamma method (see [GH21], [BJS99]) is based on a second-order Taylor expansion of the portfolio pricing function  $u(t, x)$  around  $(t + \delta, X_{t+\delta})$ , and further assumes that the risk factors return during the MPOR follows a normal distribution (ie. it is coherent when we have a multivariate Black-Scholes diffusion). Then, value-at-risk can be obtained as a function of Delta and Gamma (and potentially Theta) sensitivities either through Cornish-Fisher expansion or a Gaussian distribution hypothesis for  $(\Delta V_{t+\delta} | v)$ , matching the moments with the ones implied by the Taylor expansion. However, this Delta-Gamma approach is not very useful in our Monte-Carlo framework since we can directly estimate any moment of  $(\Delta V_{t+\delta} | v)$  by regression, as we do for GLSMC/JLSMC. One can also adapt the SIMM method of Section 2.2.2 by setting the sensitivities to the corresponding derivatives of the portfolio pricing function  $u(t, x)$ , see eg. [FKLV18]. However, if there are no analytical expressions (or already computed estimates) of sensitivities available, then these sensitivity-based techniques imply a high computational burden. For instance, they may be computed automatic adjoint differentiation (AAD) in the context of differential Machine Learning as in [HS20].

### 3.3 Monte-Carlo with Gaussian distribution

The Gaussian Least-Squares Monte Carlo (GLSMC) method of [AAGL17] falls into the category of distribution-based method described in Section 3.2 assumes that<sup>18</sup>:

$$(\Delta V_{t_i+\delta} | v) \sim \mathcal{N}(0, \sigma_i^2(v)). \quad (31)$$

As explained in Appendix A, we can approximate  $\sigma_i^2(\cdot)$  as a linear combination of some basis functions:

$$\sigma_i^2(v) \approx \hat{\sigma}_i^2(v) := \sum_{k=0}^K \hat{a}_k L_k(v), \quad (32)$$

where  $\hat{a} := (\hat{a}_0, \dots, \hat{a}_K)^T$  is estimated using the dataset  $\mathcal{D}'$  defined in (29). In practice, [AAGL17] takes  $L_k(x) = x^k$  as basis functions. Although they are simple, they are not valid theoretically. Indeed, because of multicollinearity, the Gram matrix  $\mathbf{L}^T \mathbf{L}$  in equation (102) tends to be ill-conditioned, which can make our coefficient estimates highly sensitive to noise. As

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<sup>18</sup>For the reasons mentioned in Section 3.2, we do not model directly the law of  $(\Delta V_{t+\delta} | x)$ .

explained in Appendix A, a solution would be to choose an orthogonal basis in a well-chosen weighted  $L^2$  space, such as the Laguerre polynomials used in [MKN<sup>+</sup>18]. However, we have found that empirically, the choice of the basis functions (among the usual ones) has little importance on the quality of the estimation. The function  $g_i(\cdot)$  of equation (28) is then estimated by  $\hat{g}_i(\cdot)$  such that:

$$\hat{g}_i(v) = \hat{\sigma}_i(v) \Phi^{-1}(\alpha), \quad (33)$$

where  $\Phi(\cdot)$  is the cdf of the standard normal distribution.

Nonetheless, there is an important issue with this method. Depending on the value taken by  $v = V_{t_i}^{(m)}$ , it is possible that our estimated function  $\hat{\sigma}_i^2$  may take negative values, which happened in our numerical experiments. Unfortunately, the authors in [AAGL17] do not investigate this problem and we have tried several methods. First, one can enforce positivity of  $\sigma_i^2(v)$  by using a so-called generalized linear model (GLM) with the logarithm as the link function (log-linear model). Thus, it assumes we can write:

$$\ln \left( \mathbb{E} \left[ (\Delta V_{t_i+\delta})^2 \mid v \right] \right) = \sum_{k=0}^K \hat{a}_k L_k(v) \quad (34)$$

$$\Leftrightarrow \mathbb{E} \left[ (\Delta V_{t_i+\delta})^2 \mid v \right] = \exp \left( \sum_{k=0}^K \hat{a}_k L_k(v) \right) =: \hat{\sigma}_i^2(v). \quad (35)$$

Although it does not yield an OLS type minimization problem (because we don't have a linear combination of basis functions), it is possible to find the optimal  $\hat{a}_k$  by Maximum Likelihood Estimation (MLE), through an iteratively reweighted Least-Squares procedure (IRLS), see [NW72]<sup>19</sup>. An other method is simply to discard the points for which it produces a negative variance. Indeed, as the final goal is to take an empirical mean, we can afford to discard some points as long as they are not too numerous. More precisely, assuming that the timegrid  $\pi$  defined in Section 2.3 is the same as the timegrid  $G$  and recalling equation (16), the estimated expected exposure at a time  $t_i$  will be calculated as:

$$\widehat{\text{EE}}(t_i) \approx \frac{1}{\text{Card}(A)} \sum_{m \in A} \left( V_{t_i}^{(m)} + \text{UTF}_{t_i}^{(m)} - \text{VM}_{t_i-\delta}^{(m)} - \hat{g}_i \left( V_{t_i-\delta}^{(m)} \right)_+ \right)_+, \quad (36)$$

where  $A$  is the set of points  $m \in [|1, M|]$  for which  $\hat{\sigma}_i^2 \left( V_{t_i}^{(m)} \right) > 0$ . Notice that this reasoning is also applicable for any other metric estimated by an empirical expectation, eg. the dynamic initial margin:

$$\widehat{\text{DIM}}(t_i) \approx e^{-rt_i} \frac{1}{\text{Card}(A)} \sum_{m \in A} \hat{g}_i \left( V_{t_i}^{(m)} \right)_+. \quad (37)$$

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<sup>19</sup>As a warning, notice that our application of the GLM framework is not fully satisfying from a theoretical point of view.

Notice that we have tested to set the mean of  $(\Delta V_{t+\delta} | v)$  different from zero by assuming that:

$$(\Delta V_{t_i+\delta} | v) \sim \mathcal{N}(\eta_{i,1}(v), \sigma_i^2(v)), \quad (38)$$

where  $\eta_{i,j}(v)$  is the  $j$ -th conditional raw (ie. not centred) moment of  $(\Delta V_{t_i+\delta} | v)$ . In order to estimate  $\eta_{i,1}(\cdot)$  and  $\sigma_i^2(\cdot)$ , we need to estimate both the conditional raw moments of order one and two by regression:

$$\hat{\sigma}_i^2(v) = \hat{\eta}_{2,i}(v) - \hat{\eta}_{1,i}(v)^2. \quad (39)$$

However, even when enforcing positivity of  $\hat{\eta}_{2,i}(\cdot)$  by regressing using GLM with log-link, it does not mean that  $\hat{\sigma}_i^2(\cdot) > 0$ . This case is extended in details in Section 3.4, and investigated empirically in Section 4.

### 3.4 Monte-Carlo with Johnson distribution

While the Gaussian hypothesis may be valid for a portfolio with a large number of instruments with different payoffs, it is clearly not valid when the portfolio is made off a few instruments with sharp payoffs as encountered in most cases. For instance, consider the put example of Section 4.1 at a given time  $t_i = 1/12$  and for a given portfolio value  $V_{t_i} = 6.875$  (corresponding to  $X_{t_i} = 100$ ). On the left graph of Figure 4, we plot the histogram of  $(\Delta V_{t+\delta} | X_{t_i} = 100)$  and the estimated Gaussian density<sup>20</sup>, based on Monte-Carlo simulations. We also plot the empirical quantile and the estimated quantile under the Gaussian hypothesis at level  $\alpha = 99\%$ . On the right graph, we display the QQ-plot.

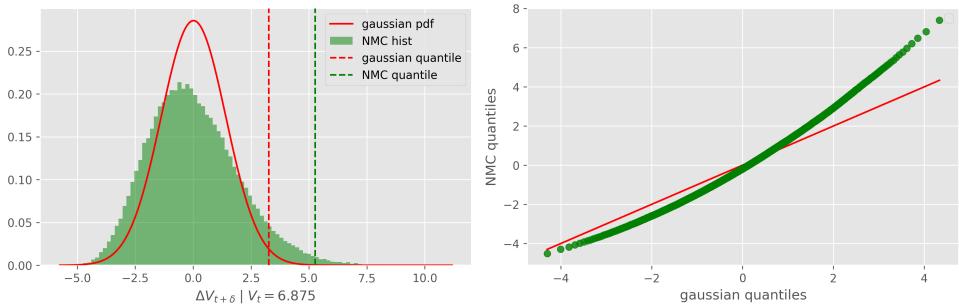


Figure 4: Distribution of  $(\Delta V_{t_i+\delta} | X_{t_i} = 100)$  for  $t_i = 1/12$ .

We clearly see that even in the simple case of a put in a Black-Scholes model, the Gaussian assumption is not valid. This has been confirmed statistically with Andersen-Darling and Kolmogorov-Smirnov tests reporting  $p$ -values well below the 5% threshold. It implies the need

<sup>20</sup>It is computed here based on Monte-Carlo simulations, and not based on the GLSMC method that assumes a centred Gaussian distribution with variance estimated as described in Section 3.3. Indeed, we don't want to take into account the bias in our estimation of the distribution parameters to justify that a Gaussian distribution is not adapted.

to model the distribution of  $(\Delta V_{t_i+\delta} | v)$  in a more flexible way. We will assume that:

$$(\Delta V_{t_i+\delta} | v) \sim \text{Johnson}(J_{i,v}(\cdot), \gamma_{i,v}, \delta_{i,v}, \xi_{i,v}, \lambda_{i,v}). \quad (40)$$

We recall the main properties of this family of distributions as well as parameters estimation methods in Appendix C.

### 3.4.1 Johnson least-squares Monte-Carlo

In the Johnson Least-Squares Monte-Carlo (JLSMC) method of [MKN<sup>+</sup>18], the estimation of the Johnson distribution parameters is done using a moment matching method, described in Appendix C.2.1. It requires computing the mean, variance, skewness and kurtosis of  $(\Delta V_{t_i+\delta} | v)$ . Although conditional variance, skewness and kurtosis functions can't be estimated directly by regression, they are based on conditional raw moments of order one to four, which can be estimated by regression. Indeed, from equation (153), the estimated skewness and kurtosis of  $(\Delta V_{t_i+\delta} | v)$  are respectively given by:

$$\begin{cases} \hat{\gamma}_i(v) := \frac{\hat{\mu}_{i,3}(v)}{\hat{\mu}_{i,2}(v)^{3/2}}, \\ \hat{\kappa}_i(v) := \frac{\hat{\mu}_{i,4}(v)}{\hat{\mu}_{i,2}(v)^2}, \end{cases} \quad (41)$$

where  $\hat{\mu}_{i,j}(v)$  is the estimation of  $\mu_{i,j}(v)$ , the  $j$ -th conditional centred moment<sup>21</sup> of  $(\Delta V_{t_i+\delta} | v)$ , such that:

$$\hat{\mu}_{i,j}(v) := \sum_{k=0}^j \binom{j}{k} (-1)^{j-k} \hat{\eta}_{i,k}(v) \hat{\eta}_{i,1}(v)^{j-k}, \quad (42)$$

where  $\hat{\eta}_{i,j}(v)$  is the estimated  $\eta_{i,j}(v)$  by regression, defined as in Section 3.3.

Although [MKN<sup>+</sup>18] do not mention this problem, a first remark we can make is that  $\hat{\eta}_{i,2}(\cdot)$  and  $\hat{\eta}_{i,4}(\cdot)$  may be negative, whereas it is not possible theoretically. It implies that  $\hat{\mu}_{i,j}(v)$  for  $j \in [|2, 4|]$  may be ill-defined for some values of  $v$ . It impacts in turn the regions where estimated conditional skewness  $\hat{\gamma}_i(\cdot)$  and kurtosis  $\hat{\kappa}_i(\cdot)$  functions are well-defined. There are not many approaches to deal with this issue, and one can only partially solve the problem. As explained in Section 3.3, we can either discard the values  $v = V_{t_i}^{(m)}$  for which the estimated conditional raw moments of order two and four are negative, and discard in addition the values for which the estimated conditional centred moments of order two and four are negative. Notice that depending on the quality of our regression, it could yield to discard a too large number of points, which is not desirable. As explained in Section 3.3, an alternative is to use a GLM with log-link function for the regression of  $\eta_{i,2}(\cdot)$  and  $\eta_{i,4}(\cdot)$  to ensure their estimate is positive.

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<sup>21</sup>Notice that the variance of  $(\Delta V_{t_i+\delta} | v)$  is then denoted  $\mu_{i,2}(v)$ .

However, it does not mean that the estimates of  $\mu_{i,2}(\cdot)$  and of  $\mu_{i,4}(\cdot)$  are positive. It only reduces the number of points to discard but at the cost of a potentially high bias in the regression.

A second observation is that the biases in estimations of the conditional raw moments accumulate when computing variance, skewness and kurtosis. It may lead to Johnson distribution parameters totally misspecified while  $(\Delta V_{t_i+\delta} | v)$  may indeed follow a Johnson distribution but with very different parameters values. The only way to limit this issue is to try several regression methods beyond the natural OLS formulation from Appendix A, as mentionned in Section 3.2.

Moreover, as explained in Appendix C.2.1, the moment matching procedure is highly costly in time and represents too much computational burden if we want to fit a Johnson distribution (ie. finding its parameters) to  $(\Delta V_{t_i+\delta} | v)$  for each value  $v = V_{t_i}^{(m)}$  with  $m \in [|1, M|]$ . Thus, we will fit a Johnson distribution at time  $t_i$  only for some given *support values* denoted:

$$\mathcal{V}_i = \left\{ V_{t_i}^{(m_{i,1})}, \dots, V_{t_i}^{(m_{i,R})} \right\}, \quad (43)$$

where  $R$  is the number of support values chosen. Then, the function  $g_i(\cdot)$  of equation (28) is estimated by minimizing a given empirical loss function on a given set of functions or by non-parametric techniques<sup>22</sup>, based on the theoretical quantiles  $\{q_{i,1}, \dots, q_{i,R}\}$  at level  $\alpha$  of the Johnson distributions fitted to  $(\Delta V_{t_i+\delta} | v)$  for each  $v \in \mathcal{V}_i$ . Indeed, it is possible to compute the quantile of a Johnson distribution in closed-form, as explained in Appendix C. In [MKN<sup>+</sup>18], the authors simply minimize a mean square error criterion over the set  $\mathcal{G}$  of linear combination of Laguerre polynomials truncated at fourth order:

$$\hat{g}_i(v) = \arg \min_{g \in \mathcal{G}} \frac{1}{R} \sum_{r=1}^R \left( g \left( V_{t_i}^{(m_{i,r})} \right) - q_{i,r} \right)^2, \quad (44)$$

where  $g(v) := \sum_{k=0}^4 a_k L_k(v)$ .

A fundamental question lies in how to choose the support values  $\mathcal{V}_i$  at a given time  $t_i$ . In [MKN<sup>+</sup>18], they are chosen as some empirical quantiles<sup>23</sup> of  $V_{t_i}$ , based on the dataset of iid. observations  $\{V_{t_i}^{(1)}, \dots, V_{t_i}^{(M)}\}$ . More precisely, we use  $M_q = 100$  empirical quantiles at evenly-spaced levels, and we add more evenly-spaced levels in the tails below 1% and above 99%, such that the added number of empirical quantiles in each tail is  $\left\lfloor \frac{0.1 \cdot M_q}{2} \right\rfloor$  (if no duplicate with the previous levels related to  $M_q$ ). These added quantiles enable us to capture effectively the behaviour in the distribution tail, which is crucial for risk management applications. However, there is no clear justification on the extreme quantile levels taken (1% and above 99%), which should ideally depend on the empirical distribution  $V_{t_i}$ , ie. the number of support values should

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<sup>22</sup>Any classical technique may be worth it to consider, as long as the computational cost remains low. Thus, OLS formulations are usually preferred.

<sup>23</sup>We have estimated conditional mean, variance, skewness and kurtosis of  $(\Delta V_{t_i+\delta} | v)$  as *functions* of  $v$ , thus we can choose any definition of empirical quantile. For simplicity, we take the Definition 1 already seen, so that the support values are existing portfolio values among  $\{V_{t_i}^{(1)}, \dots, V_{t_i}^{(M)}\}$ .

depend on  $i \in [|0, N|]$ . Thus, an alternative idea to build the set of support values could be to use a weak discrepancy sequence over the interval  $\left[ \min_m V_{t_i}^{(m)}, \max_m V_{t_i}^{(m)} \right]$ . For instance, in the spirit of [MZ21], we may generate the support values from  $R$  points of a Sobol sequence [Sob67] on  $[0, 1]$ , such that  $\mathcal{V}_i = \left\{ V_i^{(1)}, \dots, V_i^{(R)} \right\}$  where:

$$V_i^{(r)} = \min_m V_{t_i}^{(m)} + \text{sob}_r \cdot \left( \max_m V_{t_i}^{(m)} - \min_m V_{t_i}^{(m)} \right) \quad (45)$$

with  $\text{sob}_r$  being the  $r$ -th element of a Sobol sequence over  $[0, 1]$ . Notice that we have not tested this idea in practice, but it may be good to analyze it in the future.

Notice that we have tested other methods for estimating  $g_i(\cdot)$  based on the theoretical quantiles  $\{q_{i,1}, \dots, q_{i,R}\}$ , which are investigated in details in Section 4. Moreover, one may argue that we could use nested Monte-Carlo simulations in order to compute the raw moments of  $(\Delta V_{t_i+\delta} | v)$  for  $v \in \mathcal{V}_i$  instead of doing a regression. Nonetheless, it would be too costly in practice, even for a reasonable number of support values as the algorithm AS99 already requires a high computation time.

### 3.4.2 Johnson percentile matching Monte-Carlo

In order to alleviate the drawbacks of the JLSMC method, we propose a new method called Johnson Percentile Matching Monte-Carlo (JPMMC), which has also been investigated in [GH21]. The main idea is to use an other technique to perform the fitting of Johnson distributions to  $(\Delta V_{t_i+\delta} | v)$  for each support value  $v \in \mathcal{V}_i$ , which does not have the flaws of the moment matching procedure explained in Section 3.4.1. We have chosen to use the percentile matching method detailed in Appendix C.2.2 since it does not require the estimation of high-order metrics like skewness and kurtosis and one has more control over the computational cost. As mentionned in Appendix C.2.2, the cost only comes from estimating some quantiles of  $(\Delta V_{t_i+\delta} | v)$  for each support value  $v \in \mathcal{V}_i$  defined in Section 3.4.1, through nested Monte-Carlo. It is controlled by the number of inner paths  $M_{\text{IN}}$ , where we have found  $M_{\text{IN}} = 1000$  to be a good compromise between accuracy and computational cost. Notice we don't estimate quantiles, ie. perform a nested Monte-Carlo, for all the values  $v = V_{t_i}^{(m)}$  with  $m \in [|1, M|]$  but only for the support values  $v \in \mathcal{V}_i$ . Indeed, it would be too costly to simulate  $N \times M \times K$  paths of the risk factors and to price our portfolio on these paths. In this case, we would be better of doing a quantile regression, explained in Appendix A and investigated in Section 3.5.

Finally, the same procedure as in Section 3.4.1 can be employed to estimate the function  $g_i(\cdot)$ , but notice that the support values cannot be chosen as freely as for the JLSMC method. Indeed, for each support value  $v \in \mathcal{V}_i$ , the nested Monte-Carlo simulations imply to generate  $K$  iid. samples of  $(\Delta V_{t_i+\delta} | v)$ . Recalling the procedure of Section 3.1, we first need to generate risk factors paths starting from the risk factors value  $X_{t_i}^*$  that would produce the protfolio value

$v$ . However, it is not clear how to obtain this value  $X_{t_i}^*$  if there is not a bijection between the risk factors and portfolio values, or if the function that relates them is not easily invertible. Thus, our only choice is to take the support values as some of the portfolio values  $V_{t_i}^{(m)}$  for  $m \in [|1, M|]$  already generated, because we know the risk factors value  $X_{t_i}^{(m)}$  associated to each portfolio value  $V_{t_i}^{(m)}$ . For simplicity, we choose the support values as in Section 3.4.1 where the empirical quantile is given in Definition 1.

The only drawback of this method is that the nested Monte-Carlo simulations may be too costly in two cases. First, the risk factors simulation could require numerical methods other than the classic schemes like Euler-Maruyama. Second, there may not be analytical (or fast enough semi-analytical) expressions for the portfolio price and one may be forced to use Monte-Carlo simulations or other costly techniques to estimate the portfolio value at each time  $t_i$  and for each path  $m$ . In this case, it is not a good option to rely on the JMMC method and one may use a simpler technique like GLSMC explained in Section 3.3. Nonetheless, there may be ways to reduce the variance in the estimation of the four quantiles, hence enabling to reduce the number of inner paths for the same degree of accuracy. For instance, one may use techniques like antithetic variables, control variates [HN98] or importance sampling [EL10] [Gly96], but their implementation depends on the risk factors diffusion and portfolio specified. One may also try to estimate the four quantiles by doing quantile regression in a multi-level setup with a very small neural network, but it is not clear how much accuracy we can achieve with such a small model and we may be better off using a larger model and follow the distribution-free approach of [BCG<sup>+</sup>24] described in Section 3.5.

## 3.5 Neural networks quantile regression

In this section, we investigate the work of [BCG<sup>+</sup>24] who propose a two-steps methodology for estimating value-at-risk and expected shortfall in a potentially multi-quantile setup, leveraging neural networks and transfer learning. We recommend the reader unfamiliar with this topic to go through Appendix A.2, Appendix A.3, and Appendix B before all.

### 3.5.1 A larger scope of study

The estimation of both value-at-risk (or quantile) and expected shortfall (or superquantile) don't arise directly in forward initial margin, and we exceptionnally take a larger perspective in this section. Indeed, expected shortfall appears from a risk management point of view or when calculating the CVA (see [BCG<sup>+</sup>24], [AAC20]). Let us provide a short explanation and assume the riskfree rate is deterministic for the sake of simplicity. Then, from equation (21) we need to

calculate for all  $t \in [0, T - \delta]$  and for all  $s \in [t, T - \delta]$ :

$$\mathbb{E}[E_{s+\delta} | \mathcal{F}_s] = \mathbb{E}[(\Delta V_{s+\delta} - \text{IM}_s)_+ | \mathcal{F}_s] \quad (46)$$

$$= \mathbb{E}\left[\left(\Delta V_{s+\delta} - \text{VaR}^\alpha(\Delta V_{s+\delta} | \mathcal{F}_s)_+\right)_+ | \mathcal{F}_s\right]. \quad (47)$$

Assuming that taking  $\text{VaR}^\alpha(\Delta V_{s+\delta} | \mathcal{F}_s)_+ \approx \text{VaR}^\alpha(\Delta V_{s+\delta} | \mathcal{F}_s)$  has little impact on the CVA value, it yields:

$$\begin{aligned} \mathbb{E}[E_{s+\delta} | \mathcal{F}_s] &= \mathbb{E}\left[(\Delta V_{s+\delta}) \mathbf{1}_{\Delta V_{s+\delta} > \text{VaR}^\alpha(\Delta V_{s+\delta} | \mathcal{F}_s)}\right] \\ &\quad - \text{VaR}^\alpha(\Delta V_{s+\delta} | \mathcal{F}_s) \mathbb{Q}(\Delta V_{s+\delta} > \text{VaR}^\alpha(\Delta V_{s+\delta} | \mathcal{F}_s)). \end{aligned} \quad (48)$$

Using the identity in Proposition 2, we have:

$$\mathbb{E}[E_{s+\delta} | \mathcal{F}_s] = (1 - \alpha)(\text{ES}^\alpha(\Delta V_{s+\delta} | \mathcal{F}_s) - \text{VaR}^\alpha(\Delta V_{s+\delta} | \mathcal{F}_s)), \quad (49)$$

where  $\text{ES}^\alpha(Y) = \mathbb{E}[Y | Y > \text{VaR}^\alpha(Y)]$ . For rigorous mathematical definition of conditional expected shortfall (or conditional superquantile), we refer the reader to Section 2. of [BCG<sup>+</sup>24].

### 3.5.2 Learning conditional value-at-risk and expected shortfall

It implies that for each  $i \in [|0, N|]$  and for each  $m \in [|1, M|]$ , we need to estimate the function  $f_i(\cdot)$  defined in equation (26), as well as the function  $\text{es}_i(\cdot)$  such that:

$$\text{es}_i(X_{t_i}^{(m)}) := \text{ES}^\alpha(\Delta V_{t_i+\delta} | X_{t_i}^{(m)}). \quad (50)$$

As mentionned in the procedure for estimating expected shortfall in Appendix A.3, the first step is to estimate the value-at-risk function  $f_i(\cdot)$ . In [BCG<sup>+</sup>24], the authors propose to learn this function using neural networks, in order to lower the bias compared to a basis functions approach investigated in Appendix A.2. Moreover, notice that this basis function approach would require to estimate the function  $g_i(\cdot)$  defined in equation (28) instead of the function  $f_i(\cdot)$ , as we have done for the Johnson and Gaussian Monte-Carlo methods. Indeed, we need to make this approximation because we define the basis functions as taking their inputs in  $\mathbb{R}$  and not  $\mathbb{R}^d$ . Building on the results of Appendix A.2 and using the approach from Appendix B, we solve the following stochastic optimization problem for each  $i \in [|0, N|]$ :

$$h_{\theta^*} := \arg \min_{h_\theta \in \mathcal{H}_\theta} \mathbb{E}[p(\Delta V_{t_i+\delta}, h_\theta(X_{t_i}))], \quad (51)$$

where  $p(\cdot, \cdot)$  is the pinball loss of equation (106), and  $\mathcal{H}_\theta$  defined in equation (142) is the set of (feed-forward) neural network functions parametrized by  $\theta$ . Here, we use mini-batch SGD given by Algorithm 4 in Appendix B, and Ridge regularisation with parameter  $\kappa > 0$ , so that the loss

used in the SGD procedure is:

$$\mathcal{L}(x, y; \theta) = p(y, h_\theta(x)) + \kappa \|\theta\|_2^2, \quad (52)$$

with the dataset  $\mathcal{D}$  defined in equation (27) where  $\|\theta\|_2$  is the euclidian norm of the flattened vector  $\theta$ . We then have:

$$\hat{f}_i(\cdot) = h_{\hat{\theta}}(\cdot), \quad (53)$$

where  $\hat{\theta}$  is the output of the mini-batch SGD algorithm. Then, one can estimate the expected shortfall function as we have  $\text{es}_i(\cdot) = f_i(\cdot) + r_i(\cdot)$ , and in view of equation (133) from Appendix A.3:

$$r_i = \arg \min_{h \in \mathcal{B}} \mathbb{E} \left[ (p(\Delta V_{t_i+\delta}, f_i(X_{t_i})) - f_i(X_{t_i}) - h(X_{t_i}))^2 \right]. \quad (54)$$

Replacing  $f_i(\cdot)$  by  $\hat{f}_i(\cdot)$  and using a new neural network to estimate  $r_i(\cdot)$  in order to have minimal bias, we obtain the following stochastic optimization problem for each  $i \in [|0, N|]$ :

$$\zeta_{\theta^*} := \arg \min_{h_\theta \in \mathcal{H}_\theta} \mathbb{E} \left[ \left( p(\Delta V_{t_i+\delta}, \hat{f}_i(X_{t_i})) - \hat{f}_i(X_{t_i}) - h_\theta(X_{t_i}) \right)^2 \right]. \quad (55)$$

Performing the mini-batch SGD algorithm on this problem, we would obtain  $\hat{r}_i(\cdot) = \zeta_{\hat{\theta}}(\cdot)$  as an estimation of  $r_i(\cdot)$ , where  $\hat{\theta}$  is the output of the mini-batch SGD algorithm. However, [BCG<sup>+</sup>24] propose a transfer learning approach to free from the computational burden of training a new neural network from scratch. Indeed, we can use the trained hidden layers of the value-at-risk neural network function  $\hat{f}_i(\cdot)$  to estimate the residual function  $r_i(\cdot)$ . More precisely, they use the following procedure:

1. Define a neural network  $\zeta_{\tilde{\theta}}$  for learning the residual function  $r_i(\cdot)$ , with the same architecture as the value-at-risk neural network  $\hat{f}_i(\cdot) = h_{\hat{\theta}}(\cdot)$ .
2. Freeze the weight matrices of the hidden layers of the expected shortfall neural network  $\zeta_{\tilde{\theta}}$  to be equal to the weight matrices of the hidden layers of the value-at-risk neural network  $h_{\hat{\theta}}$ . Similarly to equation (143) of Appendix B, let us denote  $\hat{\theta} = \{\hat{W}_1, \dots, \hat{W}_{l+1}\}$  and  $\tilde{\theta} = \{\tilde{W}_1, \dots, \tilde{W}_{l+1}\}$ . It means we set:

$$\tilde{W}_k := \hat{W}_k, \quad \forall k \in [|1, l|]. \quad (56)$$

3. Thus, the only parameter to optimize is the output weight matrix, such that:

$$\tilde{W}_{l+1} = \arg \min_{W \in \mathbb{R}^{1 \times n_l}} \mathbb{E} \left[ \left( p(\Delta V_{t_i+\delta}, \hat{f}_i(X_{t_i})) - \hat{f}_i(X_{t_i}) - W \zeta_l(X_{t_i}) \right)^2 \right], \quad (57)$$

where  $\zeta_l(\cdot)$  is the output (taking values in  $\mathbb{R}^{n_l}$ ) of the last hidden layer of the expected

shortfall neural network  $\zeta_{\tilde{\theta}}(\cdot) = \tilde{W}_{l+1}\zeta_l(\cdot)$ . Taking the empirical version of this loss function over the whole dataset, we then have a classic linear regression problem (ie. OLS formulation), which can be solved in closed-form:

$$\tilde{W}_{l+1} \approx \arg \min_{W \in \mathbb{R}^{1 \times n_l}} \frac{1}{M} \sum_{m=1}^M \left( p \left( \Delta V_{t_i+\delta}^{(m)}, \hat{f}_i \left( X_{t_i}^{(m)} \right) \right) - \hat{f}_i \left( X_{t_i}^{(m)} \right) - W \zeta_l \left( X_{t_i}^{(m)} \right) \right)^2. \quad (58)$$

4. Finally, we set  $\hat{e}s_i(\cdot) = \hat{f}_i(\cdot) + \hat{r}_i(\cdot)$  where  $\hat{r}_i(\cdot) = \tilde{W}_{l+1}\zeta_l(\cdot) = \zeta_{\tilde{\theta}}(\cdot)$ .

Notice that this transfer learning approach is only possible if we estimate the value-at-risk function  $f_i(\cdot)$  by a neural network. Moreover, we have one neural network training (to estimate the value-at-risk function) per timestep  $i \in [|0, N|]$ . If  $N$  is large, one may wonder if we can leverage the knowledge gained from  $\hat{f}_i(\cdot)$  learned at previous timesteps to improve the training process for later timesteps. In [BCG<sup>+</sup>24], the authors build upon the work of [ATCS22] by doing first the training of  $\hat{f}_N(\cdot)$  and then using the learned parameters to initialize the training of  $\hat{f}_{N-1}(\cdot)$ , and so on, until  $\hat{f}_0(\cdot)$ . Hence, if we denote the learned parameters  $\hat{\theta}_i$  at step  $i$ , then we initialize  $\hat{\theta}_{i-1} = \hat{\theta}_i$  for the training of  $\hat{f}_{i-1}(\cdot)$ . For the last timestep, the parameters are initialized using the default pytorch procedure ie. each value is drawn from  $\mathcal{U} \left( -\frac{1}{\sqrt{n_l}}, \frac{1}{\sqrt{n_l}} \right)$ .

### 3.5.3 A priori error, a posteriori error, and multi-quantile setup

Although using neural networks may be seen as a black-box approach, there are actually many theoretical results on the SGD and value-at-risk error bound. Assuming that the optimization procedure converges to the global minimum of the empirical version of the loss function from equation (51) (which is a very strong assumption though), then the upper bound of the statistical error between  $\hat{f}_i(\cdot)$  (which the theoretical estimate here and not the actual one) and  $f_i(\cdot)$  exhibits a rate of order<sup>24</sup>  $\mathcal{O}(M^{-1/4})$ . We call this error the *a priori error* as it does not consider the error arising in practice from the optimization procedure. Analyzing *a priori* the error resulting from the optimization procedure is a highly difficult task that has not been completely solved yet.

Thus, [BCG<sup>+</sup>24] also provide a way to estimate the distance of  $\hat{f}_i(\cdot)$  and  $\hat{e}s_i(\cdot)$  (which are the actual estimates we get with our data and the SGD procedure) to the groundtruth  $f_i(\cdot)$  and  $e{s}_i(\cdot)$  respectively. These *a posteriori errors* involve a companion out-of-sample “twin” Monte-Carlo procedure, and are not restricted to neural network estimators. Notice that the twin Monte-Carlo is only appropriate to ensure that the a posteriori error is small enough for a given type of estimator, but not for comparing the performance across different types of estimators. For instance, if we find an a posteriori error too large for our neural network estimator, we can try to modify its architecture or the optimization procedure and recompute the a posteriori error.

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<sup>24</sup>Notice that [BCG<sup>+</sup>24] provide explicitly the upper bound of this error.

Comparing different types of estimators is simply done computing a MSE based on either the groudtruth or nested Monte-Carlo.

Finally, [BCG<sup>+</sup>24] provide an extension of this approach to the problem of learning value-at-risk and expected shortfall at different levels  $\alpha$ . In particular, their extension tackles the crossing quantile issue, which refers to the violation of value-at-risk monotonicity with respect to  $\alpha$ .

## 4 Case Study and Numerical Results

### 4.1 European put option in Black-Scholes model

#### 4.1.1 Model setup and analytical expressions

In this section, we consider that our portfolio is a European put option on an underlying stock price  $X$ , with strike  $K$  and maturity  $T$ . The payoff at maturity is given by:

$$V_T = (K - X_T)_+. \quad (59)$$

We assume the stock price follows a Black-Scholes model [BS73] under  $\mathbb{Q}$  such that:

$$dX_t = rX_t dt + \sigma X_t dW_t, \quad (60)$$

where  $r$  is the constant riskfree rate,  $\sigma$  is the constant volatility, and  $W$  is a  $\mathbb{Q}$ -Brownian motion. From Itô lemma applied to the function  $f(x) = \ln(x)$ , we know that on the timegrid  $\pi$  defined in Section 2.3, we have:

$$\begin{cases} X_{t_i} = X_{t_{i-1}} e^{(r - \frac{\sigma^2}{2})h + \sigma(W_{t_i} - W_{t_{i-1}})}, \\ X_{t_0} = X_0, \end{cases} \quad (61)$$

We construct an exact approximation<sup>25</sup> of  $X$  using independent Gaussian random variables  $Z_i \sim \mathcal{N}(0, 1)$  such that:

$$\begin{cases} X_{t_i} = X_{t_{i-1}} e^{(r - \frac{\sigma^2}{2})h + \sigma\sqrt{h}Z_i}, \\ X_{t_0} = X_0. \end{cases} \quad (62)$$

Thus, we simulate our risk factor ( $d = 1$ ) paths such that:

$$\begin{cases} X_{t_i}^{(m)} = X_{t_{i-1}}^{(m)} e^{(r - \frac{\sigma^2}{2})h + \sigma\sqrt{h}Z_{i,m}}, \\ X_{t_0}^{(m)} = X_0, \end{cases} \quad (63)$$

where  $Z_{i,m} \stackrel{\text{iid.}}{\sim} \mathcal{N}(0, 1)$ . Moreover, we know that we have an analytical expression for the price of our portfolio for all  $t < T$ , given by:

$$V_t = u(t, X_t) := K e^{-r(T-t)} \Phi(-d_2(t, X_t)) - X_t \Phi(-d_1(t, X_t)), \quad (64)$$

---

<sup>25</sup>ie. the joint distribution of our approximation given by equation (62) on  $\pi$  coincides with the joint distribution of the true process given by equation (61) on  $\pi$ .

where  $\Phi$  is the cdf of  $\mathcal{N}(0, 1)$  and:

$$\begin{cases} d_1(t, x) := \frac{\ln(\frac{x}{K}) + (r + \frac{\sigma^2}{2})(T - t)}{\sigma\sqrt{T - t}}, \\ d_2(t, x) := d_1(t, x) - \sigma\sqrt{T - t}. \end{cases} \quad (65)$$

Thus, we simulate with no additional cost our portfolio price paths such that  $V_{t_i}^{(m)} = u(t_i, X_{t_i}^{(m)})$ .

Although it is well known that the Black-Scholes model fails to capture important empirical features such as the volatility smile, it is still a good example to illustrate and benchmark our methods. In particular, we have an analytical expression for the true conditional value-at-risk function  $f_i(\cdot)$  (and so for initial margin) defined in equation (26) of Section 2.3, based on the monotonicity property of value-at-risk from Proposition 1 of Appendix A. We have:

$$f_i(x) = \text{VaR}^\alpha(\Delta V_{t_i+\delta} | x) \quad (66)$$

$$= \text{VaR}^\alpha \left( u \left( t_i + \delta', xe^{\left(r - \frac{\sigma^2}{2}\right)\delta' + \sigma(W_{t_i+\delta'} - W_{t_i})} \right) - u(t_i, x) \right) \quad (67)$$

$$= \text{VaR}^\alpha \left( u \left( t_i + \delta', xe^{\left(r - \frac{\sigma^2}{2}\right)\delta' + \sigma\sqrt{\delta'}Z_i} \right) - u(t_i, x) \right) \quad (68)$$

$$= \text{VaR}^\alpha(w_i(Z_i)), \quad (69)$$

where  $w_i(z) := u \left( t_i + \delta', xe^{\left(r - \frac{\sigma^2}{2}\right)\delta' + \sigma\sqrt{\delta'}z} \right) - u(t_i, x)$  and  $\delta' := \delta \wedge (T - t_i)$ . The derivative of  $w_i$  is given by:

$$w'_i(z) = x\sigma\sqrt{\delta'}e^{\left(r - \frac{\sigma^2}{2}\right)\delta' + \sigma\sqrt{\delta'}z} \cdot \partial_x u \left( t_i + \delta', xe^{\left(r - \frac{\sigma^2}{2}\right)\delta' + \sigma\sqrt{\delta'}z} \right), \quad (70)$$

where  $\Delta = \partial_x u(t, x)$  is the partial derivative of  $u$  with respect to its second variable  $x$ . It is well-known that the Greek  $\Delta$  of a European put option is strictly negative, so that  $w'_i < 0$ , ie.  $w_i$  is strictly decreasing. From Proposition 1, we have:

$$f_i(x) = w_i(\text{VaR}^{1-\alpha}(Z_i)) \quad (71)$$

$$= u \left( t_i + \delta', xe^{\left(r - \frac{\sigma^2}{2}\right)\delta' + \sigma\sqrt{\delta'}\Phi^{-1}(1-\alpha)} \right) - u(t_i, x). \quad (72)$$

#### 4.1.2 Numerical results

In this section, we present detailed numerical results of our initial margin estimation methods for the European put option in the Black-Scholes model. For consistency with [MKN<sup>+</sup>18], we will take the following parameters values in Table 1 assuming one year is 240 days.

riskfree rate	$r$	5%	MPOR	$\delta$	1/24
spot price	$X_0$	100	timestep	$h$	1/240
volatility	$\sigma$	30%	nb paths train set	$M_{\text{train}}$	$10^4$
maturity	$T$	1 year	nb paths test set	$M_{\text{test}}$	$10^3$
strike	$K$	95			
value-at-risk level	$\alpha$	99%			

Table 1: Parameters values European put Black-Scholes.

If one uses the JLSMC method of Section 3.4.1, the first step is to estimate by regression the first four raw moments of  $(\Delta V_{t_i+\delta} | v)$ . Although the natural way is to do a linear regression (ie. OLS-type), we have tested other techniques including Hubert regression and GLM, with/without Ridge penalization. We have also tested kernel regression with a Silvermann bandwidth and Gaussian kernel. Moreover, we tried Laguerre and polynomial basis functions with truncature degree of 2, 3, and 7. Finally, we considered assuming the mean of  $(\Delta V_{t_i+\delta} | v)$  equal or different from zero. As an example, we plot in Figure 5 the regressed mean, variance, skewness, and kurtosis of  $(\Delta V_{t_i+\delta} | v)$  for  $t_i = 1/12$ , using linear regression with Laguerre polynomials truncated at a degree of 2 and without Ridge penalty (JLSMC). The raw moments obtained by nested Monte-Carlo and the GLSMC setting of [AAGL17] are displayed for comparison purposes. We notice there are 7 invalid support values, ie. the values  $v \in \mathcal{V}_i$  for which the estimated metrics values do not belong to the corresponding definition domains. Moreover, we see that the estimations of skewness and kurtosis are not accurate for small values  $v$ , due to the accumulation of errors and invalid support values in regression of the conditional raw moments.

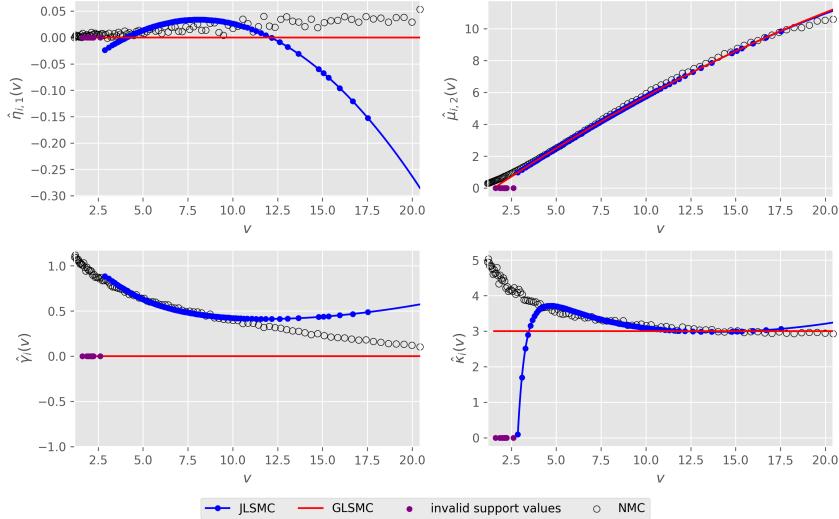


Figure 5: Regressed mean, variance, skewness, and kurtosis for  $t_i = 1/12$ .

The second step of the JLSMC method is to estimate the Johnson distribution parameters

(based on the estimated metrics described above) and calculate the associated quantile at level  $\alpha$ , for each support value  $v \in \mathcal{V}_i$ . In Figure 6, we display the quantiles of fitted Johnson distributions for each support value using the same setup as in Figure 5. We also display the estimated  $f_i(\cdot)$  obtained from the GLSMC method of Section 3.3 and the analytical expression given in equation (72) of Section 4.1.1.

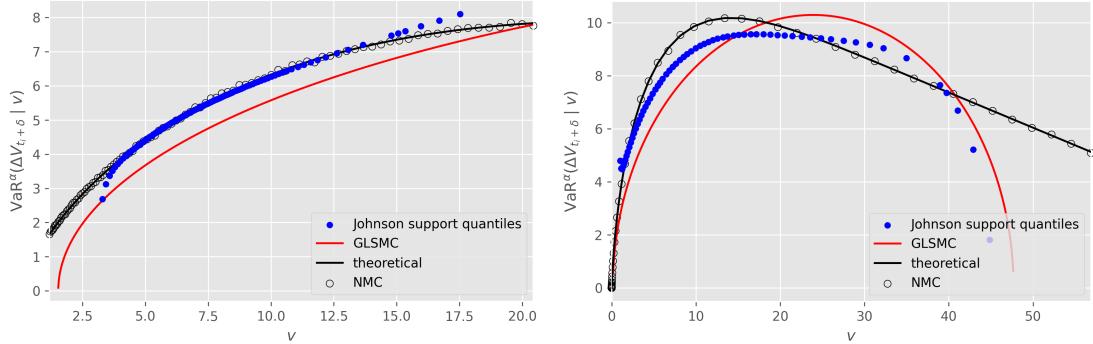


Figure 6: Estimated Johnson quantiles with moment matching. Left:  $t = 1/12$ . Right:  $t = 0.8$ .

Notice that we have respectively 9 and 44 invalid support values for  $t_i = 1/12$  and  $t_i = 0.8$ . Moreover, we see that the fitting of Johnson distribution to  $(\Delta V_{t_i+\delta} | v)$  for  $v \in \mathcal{V}_i$  is bad for  $t_i = 0.8$ . It is mainly due to the errors that accumulate in the estimation of skewness and kurtosis, leading to inaccurate Johnson parameters values. As an example, we display in Figure 7 the empirical distribution for the largest support value  $v \approx 44.864$  of Figure 6 for  $t_i = 0.8$ , computed using nested Monte-Carlo. Comparing with the pdf of the fitted Johnson distribution, we see that although a Johnson distribution is adapted to the distribution of  $(\Delta V_{t_i+\delta} | v)$ , the fitted parameters are not accurate enough to capture the distribution shape.

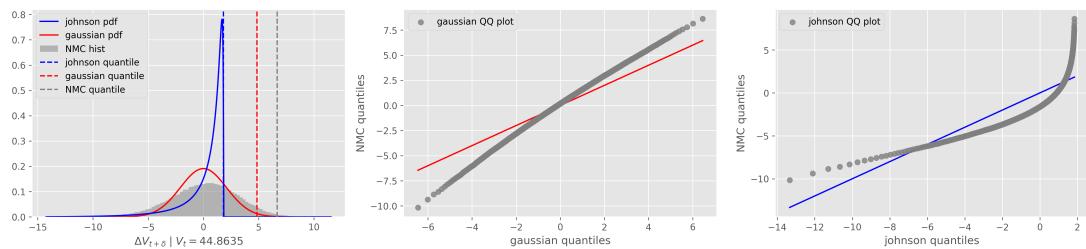


Figure 7: Fitted distributions for largest support value when  $t_i = 1/12$ .

One may wonder if we have the same problem with the JPMMC method of Section 3.4.2, ie. when we estimate the Johnson distribution parameters using the percentile matching method. In Figure 8, we display the same setting as in Figure 6 but using the percentile matching method instead of the moment-matching method, with  $M_{\text{IN}} = 1000$  (see Section 3.4.2) and  $z = 1$  (see Appendix C.2.2). We see that we have not the estimation issues of the moment-matching method, as we already mentionned before. In particular, we do not have any invalid support

values.

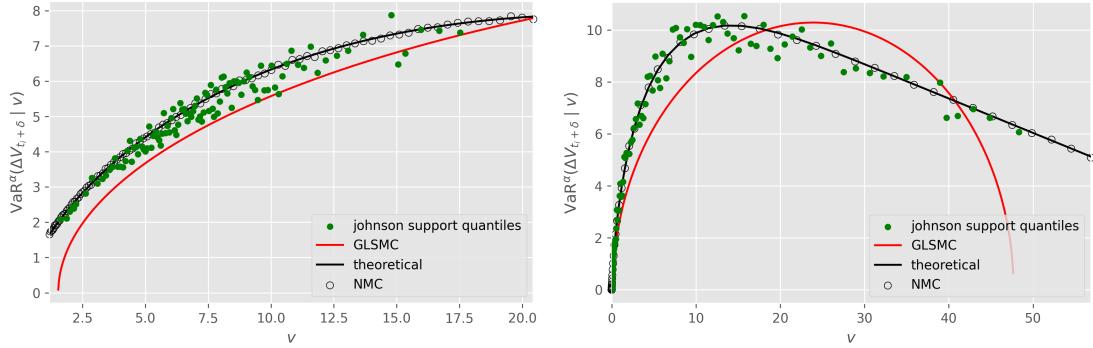


Figure 8: Estimated Johnson quantiles with percentile matching. Left:  $t_i = 1/12$ . Right:  $t_i = 0.8$ .

One may wonder if the hypothesis of Johnson distribution is well adapted to the distributions of  $(\Delta V_{t_i+\delta} \mid v)$  for  $v \in \mathcal{V}_i$  we face in this case study. In Figure 9, we show the empirical distribution for the 60-th smallest support value  $v \approx 0.496$  (corresponding to  $X_{t_i} \approx 97.051$ ) for  $t_i = 0.9875$  and the estimated Johnson density<sup>26</sup>, based on nested Monte-Carlo simulations.

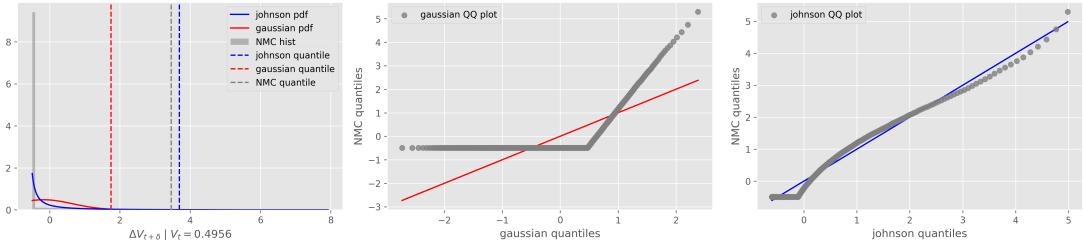


Figure 9: Distribution of  $(\Delta V_{t_i+\delta} \mid v)$  for  $t_i = 0.9875$ .

We see that the distribution of  $(\Delta V_{t_i+\delta} \mid v)$  has a spike on the left extremity of the support, which is not well captured by the Johnson distribution. Such case happens when  $t_i$  is near maturity and the put is at-the-money, ie.  $X_{t_i}^{(m)} \approx K$ . If we denote the considered support value by  $v = V_{t_i}^{(m)}$ , then some values  $X_{t_i+\delta}^{(m,k)}$  from the nested Monte-Carlo simulation (recall notations of Section 3.1) will be above the strike  $K$ , yielding some values  $V_{t_i+\delta}^{(k)} \approx 0$  and so a negative spike. The empirical and Johnson quantiles are roughly the same, but we have observed in practice that it is especially difficult to estimate the Johnson distribution parameters in the context of JLSMC/JPMMC methods in this case.

The last step is to estimate the function  $g_i(\cdot)$  of equation (28) using an error based on the fitted quantiles  $\{q_{i,1}, \dots, q_{i,R}\}$ . As mentioned in Section 3.4, we have tested parametric techniques like linear regression with Laguerre basis functions and truncature degree of 2, 3,

<sup>26</sup>It is computed here based on the nested Monte-Carlo simulations, and not based on the JLSMC/JPMMC method. Indeed, we don't want to take into account the bias in our estimation of the distribution parameters to justify that a Johnson distribution is not adapted in some cases.

and 4. Moreover, we investigated non-parametric techniques like kernel regression with cross-validated bandwidth, or  $k$ -nearest neighbors ( $k$ -NN) with  $k = 1, 3, 5$ . In Figure 10 and Figure 11, we display the function  $\hat{g}_i(\cdot)$  computed using respectively linear regression with order 2 and  $k$ -NN with  $k = 3$ , for  $t_i = 1/12$  and  $t_i = 0.8$ . In order to isolate the Johnson fittings quality from this final step, we take the Johnson quantiles given by the fitted Johnson distributions through percentile-matching procedure with  $z = 1$  and  $M_{\text{IN}} = 10^4$ .

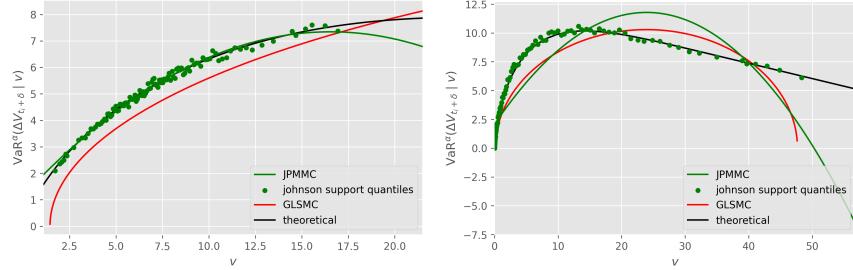


Figure 10:  $\hat{g}_i(\cdot)$  using linear regression. Left:  $t_i = 1/12$ . Right:  $t_i = 0.80$ .

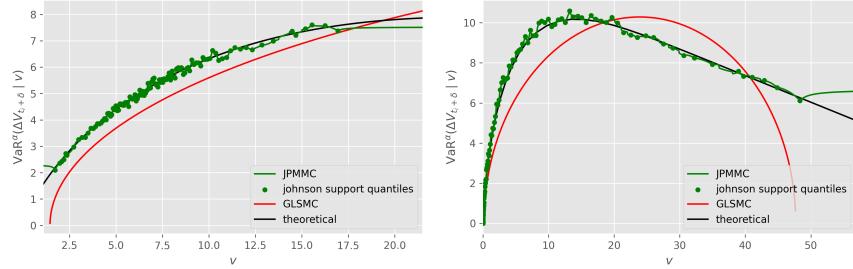


Figure 11:  $\hat{g}_i(\cdot)$  using  $k$ -NN. Left:  $t_i = 1/12$ . Right:  $t_i = 0.80$ .

We observe that extrapolation (ie. estimating  $g_i(\cdot)$  outside the two extreme support values) is especially challenging, as the function has many degrees of freedom. Nonetheless, bad extrapolation is not critical (unless it is very bad, like rapidly decreasing function). Indeed, the support values cover around 99.66% of values taken by  $V_{t_i}$  in our Monte-Carlo experiment, so that extrapolation is relevant only for a very small number of paths at  $t_i$  (around 30 points for  $M = 10^4$ ). Notice we have tried to add  $\max_m V_{t_i}^{(m)}$  and  $\min_m V_{t_i}^{(m)}$  to  $\mathcal{V}_i$ , or to have an even more finer resolution in the tails to improve extrapolation, but it did not change the final results of Table 2. There are many twists one can provide to the JLSMC/JMMC methods, but it is more of adding ingredients in a recipe than a solid theoretical framework.

**TODO machine learning**

préciser comment initialiser  $\theta$  pour le dernier timestep, comment choisir learning rate, batch size, nombre d'epochs, force de régularisation  $\kappa$ , nombre de hidden layers, nombre de neurones par layer, fonction d'activation

Finally, one can compare the methods investigated with the different settings using a mean-

square error between the estimated IM  $\hat{g}_i(\cdot)_+$  and the true IM  $f_i(\cdot)_+$  given by<sup>27</sup> equation (72) aggregated over all paths and timesteps:

$$\text{MSE} = \frac{1}{M \cdot (N+1)} \sum_{i=0}^N \sum_{m=1}^M \left[ \hat{g}_i \left( V_{t_i}^{(m)} \right)_+ - f_i \left( X_{t_i}^{(m)} \right)_+ \right]^2, \quad (73)$$

computed on both training set and test set to check for potential underfitting/overfitting issues. In Table 2, we show the MSE and the running time of the JLSMC and GLSMC methods for their initial regression setting in [MKN<sup>+</sup>18] and [AAGL17], as well as for variants in moments regressions and in the estimation of  $g_i(\cdot)$ . Here, “MM” and “PM” stand for moment-matching and percentile-matching procedures to fit the Johnson distribution. Then, “xk” represents the number of nested paths  $M_{\text{IN}} = x \times 1000$  used in percentile-matching. “LRx” is the linear regression method (ie. OLS-type expression) truncature degree  $x$  of Laguerre polynomials, for the regression of the conditional raw moments in the moment-matching method. In the same way, “GLMx” is the GLM method but only for regressing conditional raw moments of order two and four, the others being regressed with linear regression. Finally, “NNx” and “LRx” are respectively x-NN and linear regression with Laguerre polynomials of degree x, for the estimation of the function  $g_i(\cdot)$ . Notice that in this Table, we do not display all the variants we have tested for the sake of brevity.

Id	Fit. type	Fit. params	Reg. type	MSE train	MSE test	Runtime
GLSMC*	MM	LR4	-	0.78	<b>0.76</b>	1s
JPPMC*	PM	10k	LR4	0.76	<b>0.77</b>	3mn9s
JPPMC	PM	1k	LR4	0.90	<b>0.92</b>	29s
-	PM	1k	NN3	0.98	0.98	28s
JLSMC*	MM	GLM4	NN3	1.19	<b>1.23</b>	5mn33s
GLSMC	MM	LR2	-	1.30	<b>1.30</b>	0s
-	MM	GLM4	LR4	1.40	1.49	6mn28s
-	MM	LR4	LR4	2.00	2.10	3mn36s
-	MM	LR4	NN3	2.16	2.23	3mn53s
JLSMC	MM	LR2	LR4	<b>2.23</b>	<b>2.34</b>	1mn53s
-	PM	10k	LR2	2.48	2.50	3mn51s
-	PM	1k	LR2	2.55	2.57	29s
-	MM	LR2	LR2	3.63	3.78	1mn55s
-	MM	GLM2	LR2	3.58	3.79	1mn03s
-	MM	GLM2	LR4	4.19	4.66	59s

Table 2: MSE of IM estimations for the European put in Black-Scholes model.

We observe that the methods using percentile matching for the fitting of the distributions perform better compared to the ones using moment-matching. It means that the estimation

<sup>27</sup>Notice that if no analytical formula was available, we could simply have used the nested Monte-Carlo estimations as ground truth, although it takes a long time to run.

of conditional skewness and kurtosis in the moment-matching method is too unstable. Thus, our JPMMC method is preferable compared to the JLSMC method of [MKN<sup>+</sup>18], although the computational cost is higher because of the need to generate some nested paths. In particular, the JPMMC\* method is not adapted in practice because of its high runtime, although it provides the best MSE. Moreover, we managed to improve the MSE of the JLSMC method by a factor of 2.5, compared to [MKN<sup>+</sup>18] by using other regression techniques (JLSMC\* vs. JLSMC). Finally, the JLSMC method performs poorer than the GLSMC one, which is better than half of the settings considered. It means the Gaussian assumption is robust enough although not realistic. The only difference between GLSMC and GLSMC\* is that we set the mean different from zero and regress the moments by linear regression with order four (instead of two) Lagrange polynomials. In Figure 12, we display the estimated IM profiles of some methods up to<sup>28</sup>  $T - \delta$  by representing the empirical mean and quantiles at 2.5% and 97.5% based on the training and test sets.

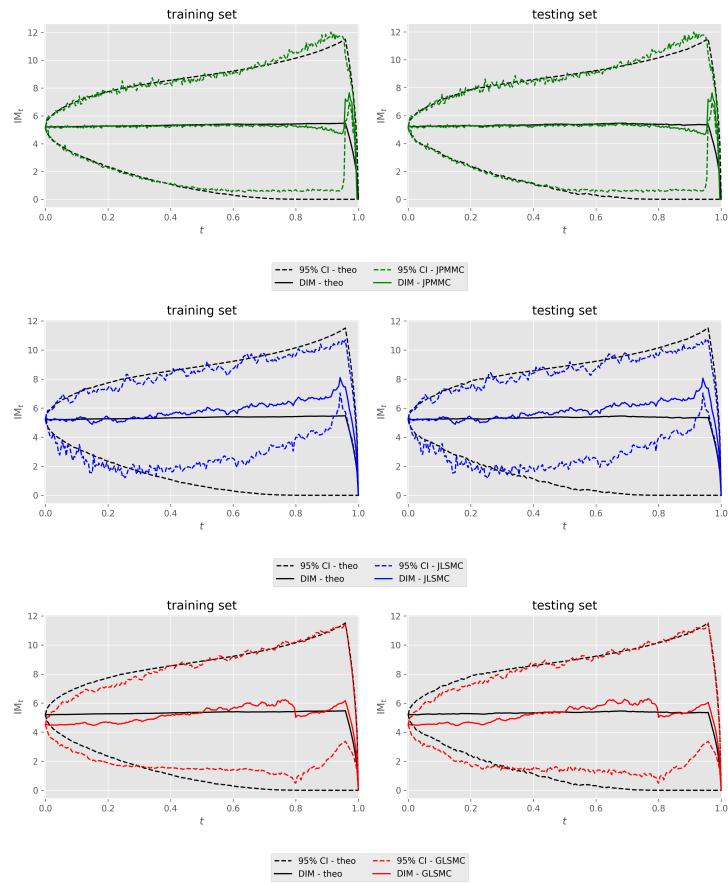


Figure 12: IM profiles up to  $T - \delta$ . Top: JPMMC. Middle: JLSMC. Bottom: GLSMC.

<sup>28</sup>Notice that we could have shown the IM profiles up to  $T$ , but the IM quickly decreases towards zero from  $T - \delta$  to  $T$  because of  $(\cdot \wedge T)$  in equation (24). The conclusions remain the same and it would only make the graphs less informative.

## 4.2 Swaption in Hull-White model

### 4.2.1 Model setup and analytical expressions

In this section, we consider that our portfolio is a European swaption with payoff at time  $T = T_0$  given by:

$$V_T = \left( V_{T_0}^{\text{swap}} \right)_+, \quad (74)$$

where  $V_{T_0}^{\text{swap}}$  is the price at time  $T_0$  of the payer swap exchanging a fixed rate  $R$  against the floating rate  $L(T_{i-1}, T_i)$  for the period  $[T_{i-1}, T_i]$  and for a notional FV, where  $\pi^* := \{T_1, \dots, T_n\}$  is the timegrid of the fixing dates (ie. swap payment dates) assumed to be equally spaced such that  $\Delta T := T_i - T_{i-1}$ . Moreover, we assume the riskfree rate under  $\mathbb{Q}$  follows a HW1F model, described in Appendix D.1 such that:

$$dr_t = (\theta(t) - kr_t)dt + \sigma dW_t, \quad (75)$$

From Appendix D.1, we know that on the timegrid  $\pi$  defined in Section 2.3, we have:

$$\begin{cases} r_{t_i} \mid \mathcal{F}_{t_{i-1}} & \sim \mathcal{N} \left( (r_{t_{i-1}} - \beta(t_{i-1}))e^{-kh} + \beta(t_i), \frac{\sigma^2}{2k} (1 - e^{-2kh}) \right), \\ r_{t_0} & = \hat{r}_0, \end{cases} \quad (76)$$

where  $\hat{r}_0$  is the observed spot short rate. Notice that here, we specify as in [MKN<sup>+</sup>18], that the observed continuously compounded zero-coupon yield curve  $T \mapsto \hat{y}(T)$  is given by:

$$\hat{y}(T) := C_1 + C_2 e^{C_3 T}, \quad (77)$$

with  $\hat{B}_0(T) = e^{-\hat{y}(T) \cdot T}$  being the observed price of the ZC with maturity  $T$ . It yields that  $\hat{r}_0 := \lim_{T \rightarrow 0} \hat{y}(T) = C_1 + C_2$  and the observed instantaneous forward rate is given by:

$$\hat{f}(0, T) = -\partial_T \ln \hat{B}_0(T) \quad (78)$$

$$= \hat{y}'(T) \cdot T + \hat{y}(T), \quad (79)$$

with  $\hat{y}'(T) = C_2 C_3 e^{C_3 T}$  and  $B_t(T)$  is the price of the zero-coupon with maturity  $T$ . Notice that we could have used a real zero-coupon prices curve taken from Refinitiv, but for replication purposes we have chosen to use the same (possibly unrealistic) setup as in [MKN<sup>+</sup>18] since it does not change the analysis. We construct an exact approximation of  $r$  using independent Gaussian random variables  $Z_i \sim \mathcal{N}(0, 1)$  such that:

$$\begin{cases} r_{t_i} & = (r_{t_{i-1}} - \beta(t_{i-1}))e^{-kh} + \beta(t_i) + \sqrt{\frac{\sigma^2}{2k} (1 - e^{-2kh})} Z_i, \\ r_{t_0} & = \hat{r}_0. \end{cases} \quad (80)$$

Thus, we simulate our risk factor  $X_t = r_t$  ( $d = 1$ ) paths such that:

$$\begin{cases} X_{t_i}^{(m)} = (X_{t_{i-1}}^{(m)} - \beta(t_{i-1}))e^{-kh} + \beta(t_i) + \sqrt{\frac{\sigma^2}{2k}(1 - e^{-2kh})}Z_{i,m}, \\ X_{t_0}^{(m)} = \hat{r}_0, \end{cases} \quad (81)$$

where  $Z_{i,m} \stackrel{\text{iid.}}{\sim} \mathcal{N}(0, 1)$ . Notice that equation (80) can be seen as a shifted AR(1) filter, so that we can leverage the function `scipy.signal.lfilter` in `python` for simulating our risk factor. Moreover, we know from the results in Appendix D.2 that we have an analytical expression for the price of our portfolio (made of one swaption) for all  $t < T$ , given by:

$$V_t = u(t, X_t) = \text{FV} \cdot \sum_{k=1}^n c_k u_k^{\text{put}}(t, X_t), \quad (82)$$

where the price function of a put with maturity  $T = T_0$  and strike  $K_k$  on the zero-coupon with maturity  $T_k$  is given by:

$$u_k^{\text{put}}(t, x) := K_k u_0^{\text{zc}}(t, x) \Phi(-d_{2,k}(t, x)) - u_k^{\text{zc}}(t, x) \Phi(-d_{1,k}(t, x)), \quad (83)$$

with:

$$\begin{cases} d_{1,k}(t, x) := \frac{\ln\left(\frac{u_k^{\text{zc}}(t, x)}{K_k u_0^{\text{zc}}(t, x)}\right) + \frac{1}{2}\bar{v}(t, T, T_k)}{\sqrt{\bar{v}(t, T, T_k)}}, \\ d_{2,k}(t, x) := d_{1,k}(t, x) - \sqrt{\bar{v}(t, T, T_k)}. \end{cases} \quad (84)$$

Moreover, we recall the price function of the zero-coupon with maturity  $T_k$  is:

$$u_k^{\text{zc}}(t, x) := e^{m(t, T_k) - n(t, T_k)x}. \quad (85)$$

Thus, we simulate with almost no additional cost our portfolio price paths such that  $V_{t_i}^{(m)} = u(t_i, X_{t_i}^{(m)})$ . Notice that calculating the cdf of the standard normal distribution  $2n$  times for computing one portfolio value  $v = V_{t_i}^{(m)}$  is not negligible when the number of fixing dates is large. Now, one may wonder if we have an analytical expression for conditional value-at-risk function  $f_i(\cdot)$  defined in equation (26) of Section 2.3, as in Section 4.1.1. We have:

$$f_i(x) = \text{VaR}^\alpha(\Delta V_{t_i+\delta} | x) \quad (86)$$

$$= \text{VaR}^\alpha \left( u \left( t_i + \delta', (x - \beta(t_i - \delta'))e^{-k\delta'} + \beta(t_i) + \sqrt{\frac{\sigma^2}{2k}(1 - e^{-2k\delta'})}Z_i \right) - u(t_i, x) \right) \quad (87)$$

$$= \text{VaR}^\alpha(w_i(Z_i)), \quad (88)$$

where  $w_i(z) := u \left( t_i + \delta', (x - \beta(t_i - \delta'))e^{-k\delta'} + \beta(t_i) + \sqrt{\frac{\sigma^2}{2k}(1 - e^{-2k\delta'})}z \right) - u(t_i, x)$ . We need to check if the derivative of this function  $w_i$  is strictly positive/negative. The derivative of  $w_i$  is

given by:

$$w'_i(z) = \sqrt{\frac{\sigma^2}{2k} (1 - e^{-2k\delta'})} \cdot \partial_x u \left( t_i + \delta', (x - \beta(t_i - \delta'))e^{-k\delta'} + \beta(t_i) + \sqrt{\frac{\sigma^2}{2k} (1 - e^{-2k\delta'})} z \right), \quad (89)$$

where  $\Delta = \partial_x u(t, x)$  is the partial derivative of  $u$  with respect to its second variable  $x$ . Checking the sign of  $w'_i$  is not straightforward as  $\partial_x u(t, \cdot)$  is made of a sum of complex functions that are not all positive or all negative. Relying on numerical simulations, we observed that for some  $i \in [|1, N|]$ ,  $u(t, \cdot)$  is not strictly monotonic contrary to what is mentionned in [MKN<sup>+</sup>18], who gives this result without any proof. We have found that, with our parameters values,  $w_i$  is strictly increasing on an interval containing most of the values of  $z$  (which would be drawn from  $\mathcal{N}(0, 1)$ ) for most of  $i \in [|1, N|]$  and for most values of  $x$  (which would be drawn from a Gaussian distribution with a given mean and variance). Nonetheless, for more extreme parameters values, we have found that  $w_i$  is strictly decreasing on this interval up to  $i = i^*$  and is strictly increasing for  $i > i^*$ , where  $i^*$  strongly depends on the paramaters values and is not easily determined analytically. Since this shift of regime appears only for extreme paramaters values, we will assume that  $w_i(\cdot)$  is strictly increasing. Hence, we have the following approximated analytical formula using the Proposition 1 of Appendix A:

$$f_i(x) \approx w_i(\text{VaR}^\alpha(Z_i)) \quad (90)$$

$$= u \left( t_i + \delta', (x - \beta(t_{i-1}))e^{-k\delta'} + \beta(t_i) + \sqrt{\frac{\sigma^2}{2k} (1 - e^{-2k\delta'})} \Phi^{-1}(\alpha) \right) - u(t_i, x). \quad (91)$$

Notice it is difficult to quantify the error we make by assuming that  $w_i$  is strictly increasing, and to quantify the interval of parameters values for which this assumption is violated. For our numerical experiments, we observed that the nested Monte-Carlo provides the same results as equation (91).

#### 4.2.2 Numerical results

In this section, we present detailed numerical results of our initial margin estimation methods for the swaption in the HW1F model. For consistency with [MKN<sup>+</sup>18], we will take the following parameters values in Table 3 assuming one year is 240 days. We recall that the initial value of risk factors  $X_0 = \hat{r}_0$  is entirely determined by the zero-coupon yield curve.

long-term mean	$k$	1.5%	MPOR	$\delta$	1/24
param ZC yield curve	$C_1$	0.05	timestep	$h$	1/240
-	$C_2$	-0.03	nb paths train set	$M_{\text{train}}$	$10^4$
-	$C_3$	-0.18	nb paths test set	$M_{\text{test}}$	$10^3$
volatility	$\sigma$	1%			
swaption maturity	$T$	1 year			
swap length	$T^*$	5 years			
swap strike	$R$	4%			
swap notional	FV	10000€			
swap accrual period	$\Delta T$	0.25 years			
value-at-risk level	$\alpha$	99%			

Table 3: Parameters values swaption HW1F.

As we follow the same methodology as for the put in the Black-Scholes model of Section 4.1.2, we do not repeat the details mentionned, but provide a brief analysis of the results. In Figure 13, we plot the regressed mean, variance, skewness, and kurtosis of  $(\Delta V_{t_i+\delta} | v)$  for  $t_i = 1/12$  using the same setting as in Figure 5. We notice there are 0 invalid support values.

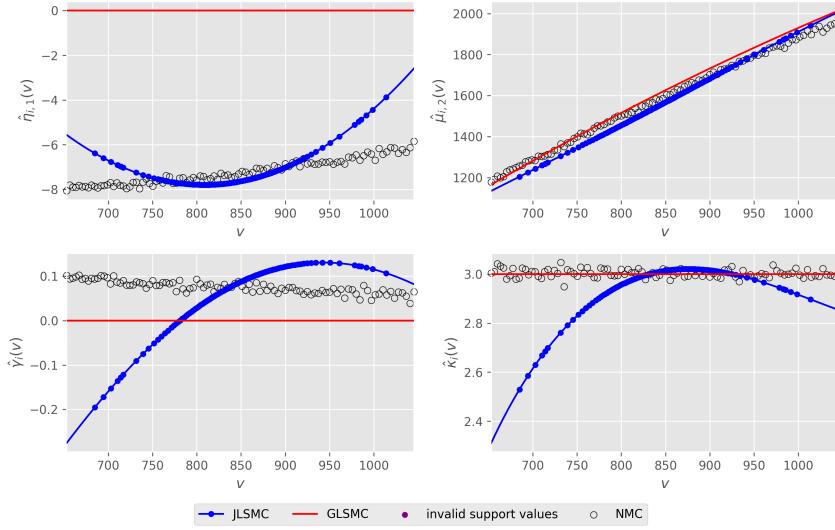


Figure 13: Regressed mean, variance, skewness, and kurtosis for  $t_i = 1/12$ .

In Figure 14 and Figure 15, we display the quantiles of fitted Johnson distributions for each support value respecitvely in the same way as in Figure 6 and Figure 8. In these graphs, we add the nested Monte-Carlo estimations of value-at-risk since the analytical formula for  $f_i(\cdot)$  in equation (91) is only valid as an approximation, recall the discussion of Section 4.2.1.

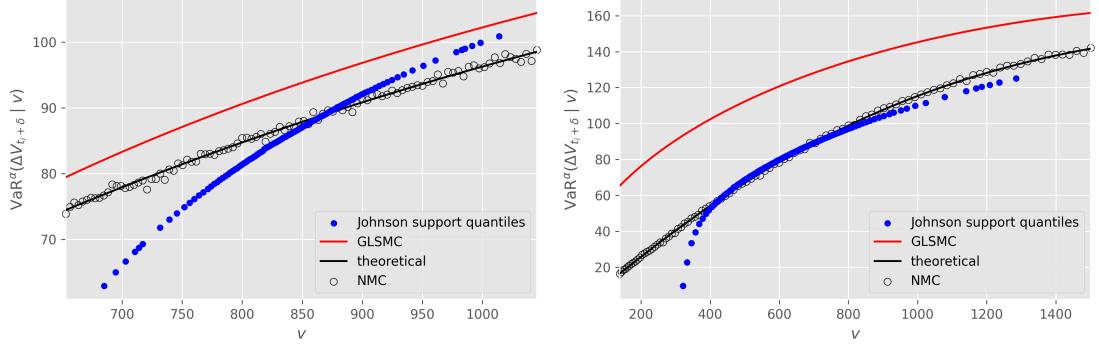


Figure 14: Estimated Johnson quantiles with moment matching. Left:  $t = 1/12$ . Right:  $t = 0.8$ .

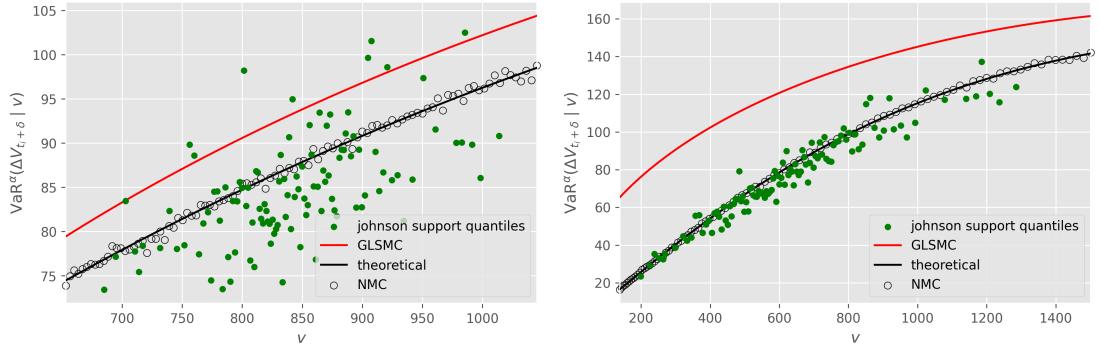


Figure 15: Estimated Johnson quantiles with percentile matching. Left:  $t = 1/12$ . Right:  $t = 0.8$ .

We observe that in both cases, we do not have any invalid support values, and the fittings of the Johnson distributions using moment-matching is good (at least at these two timesteps). However, we have much more variance in the quantiles of the fitted Johnson distributions using the percentile matching procedure, although taking the same number of nested paths  $M_{IN} = 1000$  as in the Black-Scholes case. We have checked that by increasing the number of nested paths to  $M_{IN} = 10^4$ , we obtain a much better fitting. In Figure 16, we display the function  $\hat{g}_i(\cdot)$  computed using respectively linear regression with order 2 and  $k$ -NN with  $k = 3$ , only for  $t_i = 1/12$  which is the interesting case here. In order to investigate the estimation of  $g_i(\cdot)$  in a more delicate situation, we take the Johnson quantiles given by the fitted Johnson distributions through the percentile matching procedure with  $z = 1$  and  $M_{IN} = 10^3$  in the same way as in Figure 10 and Figure 11, but only for  $t_i = 1/12$  here which is the interesting case.

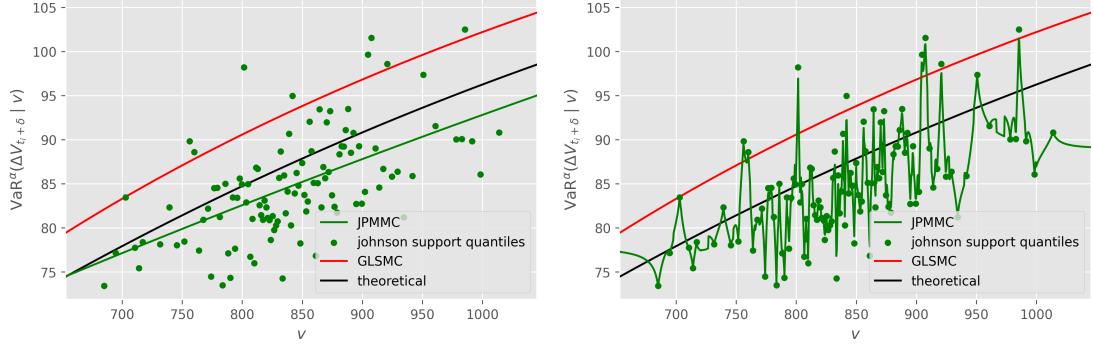


Figure 16:  $\hat{g}_i(\cdot)$  when  $t_i = 1/12$ . Left: using linear regression. Right: using  $k$ -NN.

We remark that using  $k$ -NN is not adapted here, because of the large variance in the quantiles of fitted Johnson distributions. On the other hand, linear regression techniques provide smoother estimates that are more appreciated by regulators.

### TODO machine learning

comment choisir learning rate, batch size, nombre d'epochs, force de reégularisation  $\kappa$ , nombre de hidden layers, nombre de neurones par layer, fonction d'activation

Finally, one can compare the methods investigated using a mean-square error as in Section 4.1.2, by displaying the Table 4 similarly to Table 2. However, notice that it was not possible to use the GLM technique for the moments regression in the moment matching procedure because of numerical failure in the optimization algorithm. Indeed, we mentionned in a footnote of Section 3.3 that our application of the GLM framework is not fully satisfying from a theoretical point of view.

Id	Fit. type	Fit. params	Reg. type	MSE train	MSE test	Runtime
JPMMC*	PM	10k	LR4	3.10	<b>2.66</b>	12mn44s
JPMMC	PM	1k	LR4	5.59	<b>5.00</b>	4mn20s
JLSMC*	MM	LR4	NN3	18.53	<b>17.12</b>	1mn55s
-	MM	LR2	NN3	19.68	18.75	2mn46s
-	PM	1k	NN3	22.66	22.63	5mn19s
GLSMC*	MM	LR2	-	<b>25.63</b>	<b>25.89</b>	1s
-	MM	LR4	LR2	32.21	31.28	1mn45s
-	MM	LR4	LR4	50.30	40.63	1mn52s
-	PM	1k	NN3	46.43	45.85	4mn27s
JLSMC	MM	LR2	LR4	<b>60.56</b>	<b>51.31</b>	2mn40s
-	MM	LR2	LR2	143.03	133.25	2mn42s
JLSMC†	MM	GLM4	NN3	1942.54	<b>1944.58</b>	22mn33s
GLSMC	MM	LR2	-	<b>11777.55</b>	<b>11810.43</b>	1s
-	MM	GLM2	LR4	27008.60	25066.21	16mn31s

Table 4: MSE of IM estimations for the swaption in HW1F model.

dire que regress mean no impact sur put mais que gros impact upward sur swaption

As for the put in the Black-Scholes model, we observe that the JPMMC performs better than the JLSMC method. Nonetheless, the best JPMMC setting for the put in the Black-Scholes model (denoted JPMMC in Table 2) is one of the worst for the swaption in the HW1F model (denoted JPMMC† in Table 4). It means that the choice of the technique to estimate  $g_i(\cdot)$  based on the quantiles of fitted Johnson distributions is crucial, and  $k$ -NN is not adapted. Finally, the GLSMC setting if [AAGL17] is very bad, but the performance improve drastically if we consider the mean different from zero and regress the first conditional raw moment using eg. linear regression with truncature degree 2 (GLSMC\*). Notice the MSE is calculated based on the approximated analytical formula of  $f_i(\cdot)$  given by equation (91), as we have checked that the initial margin profile obtained by nested Monte-Carlo matches the IM profile obtained with the analytical expression. In Figure 17 and Figure 18, we display the estimated IM profiles of some methods up in the same way as for Figure 12.

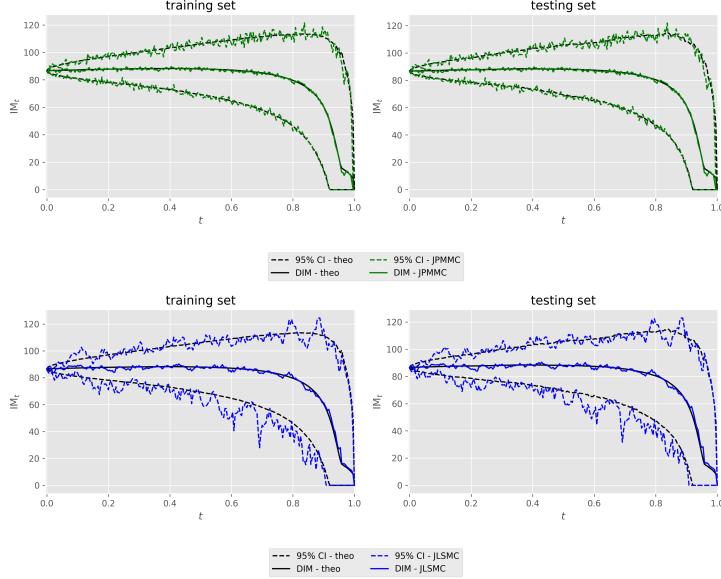


Figure 17: IM profiles up to  $T - \delta$ . Top: JPMMC. Bottom: JLSMC.

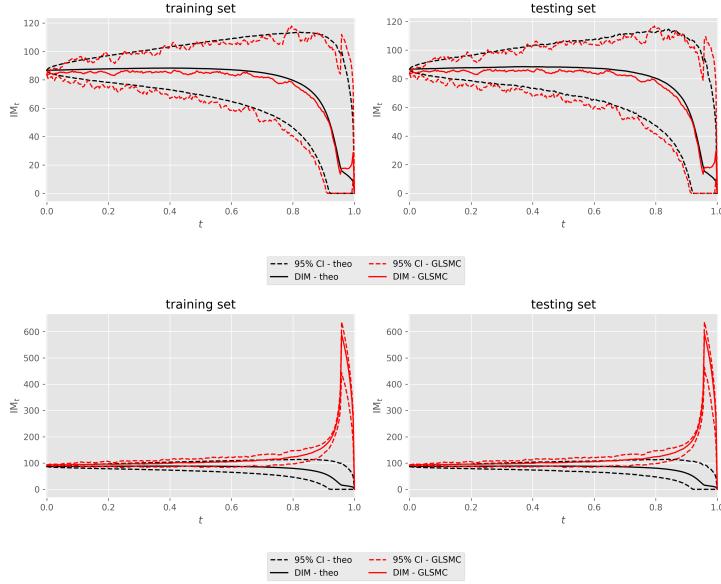


Figure 18: IM profiles up to  $T - \delta$ . Top: GLSMC\*. Bottom: GLSMC.

The results are of course more noisy than in Figure 12 because we use a lower number of paths in the training set. Moreover, the IM profile obtained by nested Monte-Carlo does not match the IM profile obtained with the analytical expression, only because of the reduced number of nested paths we have used, to avoid a too long runtime.

### 4.3 Conclusion

Throughout these numerical applications, we have seen that Monte-Carlo with Johnson distribution hypothesis is not recommended if one uses the JLSMC method of [MKN<sup>+</sup>18]. Indeed,

the moment-matching procedure to fit the Johnson distributions requires conditional skewness and kurtosis, whose estimation is highly unstable and cannot guarantee robust results. Still, Monte-Carlo with Johnson distribution is a good alternative to the Gaussian assumption if (and only if) one uses the JPMMC method we provide (and briefly mentionned in [GH21]), with the percentile-matching procedure to fit the Johnson distributions and minimizing a MSE to estimate  $g_i(\cdot)$ .

However, if simulating risk factors and pricing portfolio is too costly, then the JPMMC method is not adapted as it involves some nested Monte-Carlo simulations. In this case, we recommend to use the GLSMC method of [AAGL17]. Although the Gaussian hypothesis is not realistic, it provides stable performance since it does not require to estimate high-order conditional metrics. In particular, we recommend to assume the mean of the Gaussian distribution to be different from zero, so that one should estimate the first two conditional raw moments.

A last point of attention is that we have dealt with cases involving bijection between risk factors and portfolio value, which is often not the case in practice. Under this bijection property, it is equivalent to estimate the function  $f_i(\cdot)$  or the function  $g_i(\cdot)$ . Otherwise (eg. simply consider a European put option in a Heston model), there is no equivalence and we would observe further discrepancies between the true IM profile based on  $f_i(\cdot)$  and the estimated one based on  $\hat{g}_i(\cdot)$ . **obv we have not this problem with the Machine Learning approach.**

**TODO**

## **5 Further Developments and Conclusion**

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## A On Conditional Expectation, Quantile, and Superquantile

We highlight here the property of conditional expectation as the minimizer of a least-squares criterian which is not the case for conditional quantile. Let  $(\Omega, \mathcal{F}, \mathbb{P})$  a probability space with  $\mathbb{E}[\cdot]$  being the expectation under  $\mathbb{P}$ . Let  $X$  and  $Z$  be two random variables with values in  $\mathbb{R}$ , and let  $\mathcal{G}$  be a sub  $\sigma$ -field of  $\mathcal{F}$ . Assume that  $X$  is  $\mathcal{G}$ -measurable and that  $Z$  is independent of  $\mathcal{G}$ .

### A.1 Conditional expectation

We know that for any nonnegative (or bounded) Borel function  $\Phi$ , the function  $\phi$  defined for all  $x \in \mathbb{R}$  by  $\phi(x) := \mathbb{E}[\Phi(x, Z)]$  is a measurable function and we have with probability one:

$$\phi(X) = \mathbb{E}[\Phi(X, Z) | \mathcal{G}]. \quad (92)$$

Moreover, assume  $Y := \Phi(X, Z) \in L^2(\Omega, \mathbb{P})$ :

$$\mathbb{E}[Y^2] = \int_{\Omega} Y(\omega)^2 \mathbb{P}(d\omega) \quad (93)$$

$$= \int_{\mathbb{R}} y^2 \mu_Y(dy) < +\infty, \quad (94)$$

where  $\mu_Y(\cdot)$  is the law of  $Y$  under  $\mathbb{P}$  and  $Y(\Omega) \subset \mathbb{R}$ . Then  $\phi(X)$  is the (unique) orthogonal projection of  $Y$  in Hilbert space  $L^2(\Omega, \mathbb{P})$  onto the set of functions  $\{g(X) : g \in L^2(\mathbb{R}, \mu_X)\} \subset L^2(\Omega, \mathbb{P})$ . Moreover, it is easy to show that:

$$\phi = \arg \min_{h \in \mathcal{B}} \mathbb{E}[(Y - h(X))^2], \quad (95)$$

where  $\mathcal{B}$  is the set of all functions in  $L^2(\mathbb{R}, \mu_X)$ . Now, from the properties of this Hilbert space, we know there exists an orthonormal basis of functions  $\{L_k(\cdot)\}_k$  (possibly uncountable) such that:

$$\phi = \sum_{k=0}^{+\infty} \tilde{a}_k L_k, \quad (96)$$

where  $\tilde{a}_k := \langle \phi, L_k \rangle$ , with  $\langle \cdot, \cdot \rangle$  being the natural inner product in  $L^2(\mathbb{R}, \mu_X)$ . If  $X$  is a continuous random variable with probability density function (pdf)  $f_X(\cdot)$ , then:

$$\langle \phi, L_k \rangle = \int_{\mathbb{R}} \phi(x) L_k(x) f_X(x) dx, \quad (97)$$

and  $L^2(\mathbb{R}, \mu_X)$  can be seen as the  $L^2(\mathbb{R})$ <sup>29</sup> space weighted by  $f_X$ . Since equation (95) yields an infinite-dimensional optimization, we truncate the series in equation (96):

$$\phi(X) \approx \sum_{k=0}^K \tilde{a}_k L_k(X), \quad (98)$$

with  $\tilde{a} := (\tilde{a}_0, \dots, \tilde{a}_K)^T$  being such that:

$$\tilde{a} = \arg \min_{a \in \mathbb{R}^{K+1}} \mathbb{E} \left[ (Y - L(X)a)^2 \right], \quad (99)$$

where  $L(X) = (L_0(X), \dots, L_K(X))$ . Assuming we are not able to express easily the probability density functions involved, it may be difficult to find an orthonormal basis  $\{L_k\}_k$  of  $L^2(\mathbb{R}, \mu_X)$ . Thus, we usually rely on a simpler weighted  $L^2(\mathbb{R})$  space. For instance, the weight  $x \mapsto e^{-x}$  would be the pdf of  $X \sim \mathcal{E}(1)$ , and we would look for a basis  $\{L_k(\cdot)\}_k$  such that:

$$\langle L_i, L_j \rangle = \int_{\mathbb{R}_+} L_i(x) L_j(x) e^{-x} dx = \delta_{ij}. \quad (100)$$

Such basis can be given by the Laguerre polynomials, which are obtained thanks to the Gram-Schmidt algorithm that orthogonalizes the monomials  $\{x \mapsto x^k\}_k$  in this weighted  $L^2(\mathbb{R})$  space. Notice that the Laguerre polynomials can be normalized so that they form an orthonormal basis.

Most of the time, we are not able to calculate explicitly the expectation in equation (99). However, if we have access to iid. samples  $\{(X_1, Y_1), \dots, (X_M, Y_M)\}$ , we can approximate it by its empirical counterpart, building on the Ordinary Least Squares (OLS) method:

$$\hat{a} = \arg \min_{a \in \mathbb{R}^{K+1}} \frac{1}{M} \sum_{m=1}^M (Y_m - \mathbf{L}(X_m)a)^2 \quad (101)$$

$$= (\mathbf{L}^T \mathbf{L})^{-1} \mathbf{L}^T \mathbf{Y}, \quad (102)$$

where  $\mathbf{L} := [L(X_1), \dots, L(X_M)]^T \in \mathbb{R}^{M \times K+1}$  and  $\mathbf{Y} := (Y_1, \dots, Y_M) \in \mathbb{R}^M$ . Then, we have:

$$\phi(X) \approx \hat{\phi}(X) = \sum_{k=0}^K \hat{a}_k L_k(X). \quad (103)$$

## A.2 Conditional quantile

Assume now we want to estimate a conditional quantile (ie. a conditional value-at-risk) instead of a conditional expectation. We know there exist a function  $\psi$  such that:

$$\psi(X) = \text{VaR}^\alpha(\Phi(X, Z) \mid \mathcal{G}). \quad (104)$$

---

<sup>29</sup>The measure being the Lebesgue measure.

It is easy to show that such function is given by:

$$\psi = \arg \min_{h \in \mathcal{B}} \mathbb{E} [p(Y, h(X))], \quad (105)$$

where  $Y := \Phi(X, Z)$  and  $p(\cdot, \cdot)$  is the pinball loss also displayed in Figure 19, such that:

$$p(y, \hat{y}) := \frac{1}{1 - \alpha} (y - \hat{y})^+ + \hat{y}. \quad (106)$$

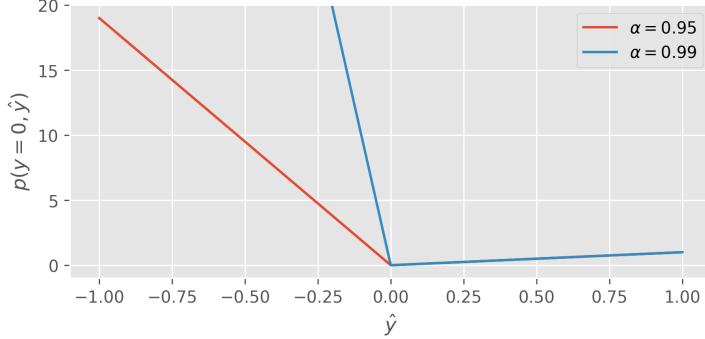


Figure 19: Pinball loss for  $y = 0$  and  $\alpha = 0.95, 0.99$ .

If we have access to iid. samples  $\{(X_1, Y_1), \dots, (X_M, Y_M)\}$ , we can approximate the expectation in equation (105) by its empirical counterpart:

$$\psi \approx \arg \min_{h \in \mathcal{B}} \frac{1}{M} \sum_{m=1}^M p(Y_m, h(X_m)). \quad (107)$$

As in Appendix A.1, one could be tempted to use Hilbert space properties by performing the minimization over functions  $h(\cdot)$  defined as in equation (98):

$$\hat{a} = \arg \min_{a \in \mathbb{R}^{K+1}} \frac{1}{M} \sum_{m=1}^M p(Y_m, L(X_m)a). \quad (108)$$

Notice that this empirical loss is convex wrt.  $a$ , but does not feature a quadratic expression as for the conditional expectation. Although we don't have an analytical expression for  $\hat{a}$ , the minimization problem can be solved by the simplex method (eg. `scipy.optimize.linprog` in Python) applied to the following linear program:

$$\begin{aligned} & \min_{a \in \mathbb{R}^{K+1}, b \in \mathbb{R}^M} \frac{1}{M} \sum_{m=1}^M \frac{1}{1 - \alpha} b_m + L(X_m)a, \\ & \text{st. } \begin{cases} b_m \geq Y_m - L(X_m)a, & \forall m \in [|1, M|], \\ b_m \geq 0, & \forall m \in [|1, M|]. \end{cases} \end{aligned} \quad (109)$$

Then, we would have:

$$\hat{\psi}(X) = \sum_{k=0}^K \hat{a}_k L_k(X), \quad (110)$$

where  $\hat{a}$  is the solution of the linear program (109) corresponding to  $a$ . Moreover, if one wants to derive an analytical expression for the value-at-risk of a given random variable, the following property is of high interest.

**Proposition 1.** *Assume in addition that  $\Phi(X, \cdot)$  is strictly increasing. Then, we have:*

$$\begin{aligned} \psi(X) &= \text{VaR}^\alpha(\Phi(X, Z) | \mathcal{G}) \\ &= \Phi(X, \text{VaR}^\alpha(Z)). \end{aligned} \quad (111)$$

If  $\Phi(X, \cdot)$  is strictly decreasing, then  $\psi(X) = \Phi(X, \text{VaR}^{1-\alpha}(Z))$ .

*Proof.* First, let us denote  $U := \Phi(x, Z)$  and  $g(z) := \Phi(x, z)$  for a given  $x \in \mathbb{R}$ . Notice that if  $g$  is strictly increasing, then  $g^{-1}$  is also strictly increasing. Indeed,

$$g \circ g^{-1}(z) = z \Rightarrow (g^{-1})'(z) \cdot g' \circ g^{-1}(z) = 1 \quad (112)$$

$$\Leftrightarrow (g^{-1})'(z) = \frac{1}{g' \circ g^{-1}(z)}. \quad (113)$$

Since  $g' > 0$ , we have  $(g^{-1})' > 0$  and so  $g^{-1}$  is strictly increasing. Thus, we have:

$$F_U(u) := \mathbb{P}(U \leq u) = \mathbb{P}(g(Z) \leq u) \quad (114)$$

$$= \mathbb{P}(Z \leq g^{-1}(u)) \quad (115)$$

$$= F_Z(g^{-1}(u)), \quad (116)$$

where  $F_U$  and  $F_Z$  are the cdf of  $U$  and  $Z$ , respectively. Then, we get:

$$u \geq \text{VaR}^\alpha(\Phi(x, Z)) \Leftrightarrow F_U(u) \geq \alpha \quad (117)$$

$$\Leftrightarrow F_Z(g^{-1}(u)) \geq \alpha \quad (118)$$

$$\Leftrightarrow g^{-1}(u) \geq \text{VaR}^\alpha(Z) \quad (119)$$

$$\Leftrightarrow u \geq g(\text{VaR}^\alpha(Z)) \quad (120)$$

$$\Leftrightarrow u \geq \Phi(x, \text{VaR}^\alpha(Z)). \quad (121)$$

Thus,  $\text{VaR}^\alpha(\Phi(x, Z)) = \Phi(x, \text{VaR}^\alpha(Z))$  for all  $x \in \mathbb{R}$ . Now if  $g$  is strictly decreasing, it is easy

to show that  $g^{-1}$  is also strictly decreasing and that  $F_U(u) = 1 - F_Z(g^{-1}(u))$ . Thus, we have:

$$u \geq \text{VaR}^\alpha(\Phi(x, Z)) \Leftrightarrow F_U(u) \geq \alpha \quad (122)$$

$$\Leftrightarrow 1 - F_Z(g^{-1}(u)) \geq \alpha \quad (123)$$

$$\Leftrightarrow F_Z(g^{-1}(u)) \leq 1 - \alpha \quad (124)$$

$$\Leftrightarrow g^{-1}(u) \leq \text{VaR}^{1-\alpha}(Z) \quad (125)$$

$$\Leftrightarrow u \geq g(\text{VaR}^{1-\alpha}(Z)) \quad (126)$$

$$\Leftrightarrow u \geq \Phi(x, \text{VaR}^{1-\alpha}(Z)), \quad (127)$$

and we find that  $\text{VaR}^\alpha(\Phi(x, Z)) = \Phi(x, \text{VaR}^{1-\alpha}(Z))$  for all  $x \in \mathbb{R}$ .  $\square$

### A.3 Conditional superquantile

Assume we now want to estimate a conditional superquantile (ie. a conditional expected shortfall) in addition to a conditional quantile. We know there exist a function  $s$  such that:

$$s(X) = \text{ES}^\alpha(\Phi(X, Z) | \mathcal{G}) \quad (128)$$

$$= \mathbb{E}[p(Y, \psi(X)) | X], \quad (129)$$

where  $Y := \Phi(X, Z)$ ,  $\psi(\cdot)$  is the conditional quantile function defined in equation (105), and  $p(\cdot, \cdot)$  is the pinball loss of equation (106). Thus, it is easy to see that:

$$s(X) = \mathbb{E}[p(Y, \psi(X)) | X] \quad (130)$$

$$\Leftrightarrow (s - \psi)(X) = \mathbb{E}[p(Y, \psi(X)) - \psi(X) | X] \quad (131)$$

$$\Leftrightarrow r(X) = \mathbb{E}[p(Y, \psi(X)) - \psi(X) | X], \quad (132)$$

where  $r = s - \psi$ . Learning  $r$  is then equivalent to learning a conditional expectation as in Appendix A.1:

$$r = \arg \min_{h \in \mathcal{B}} \mathbb{E} \left[ (p(Y, \psi(X)) - \psi(X) - h(X))^2 \right], \quad (133)$$

so that<sup>30</sup>  $s = \psi + r$ . If we have access to iid. samples  $\{(X_1, Y_1), \dots, (X_M, Y_M)\}$ , we first estimate the function  $\psi$  by  $\hat{\psi}$ , and we then approximate the expectation in equation (133) by its empirical counterpart:

$$r \approx \arg \min_{h \in \mathcal{B}} \frac{1}{M} \sum_{m=1}^M \left( p(Y_m, \hat{\psi}(X_m)) - \hat{\psi}(X_m) - h(X_m) \right)^2. \quad (134)$$

---

<sup>30</sup>There may be several functions that satisfy equations (105)-(133), but one can take any of them to determine the expected shortfall function.

As in Appendix A.1, we can perform minimization over functions  $h(\cdot)$  defined as in equation (98):

$$\hat{a} = \arg \min_{a \in \mathbb{R}^{K+1}} \frac{1}{M} \sum_{m=1}^M \left( p(Y_m, \hat{\psi}(X_m)) - \hat{\psi}(X_m) - L(X_m)a \right)^2 \quad (135)$$

$$= (\mathbf{L}^T \mathbf{L})^{-1} \mathbf{L}^T \chi, \quad (136)$$

where  $\chi := (\chi_1, \dots, \chi_M) \in \mathbb{R}^M$  with  $\chi_m := p(Y_m, \hat{\psi}(X_m)) - \hat{\psi}(X_m)$ . Then, we would have:

$$r(X) \approx \hat{r}(X) = \sum_{k=0}^K \hat{a}_k L_k(X), \quad (137)$$

so that  $\hat{s} = \hat{\psi} + \hat{r}$ . Notice that we usually learn the residual  $r = s - \psi$  instead of the expected shortfall  $s$  directly, because it may speed up convergence if one uses neural network techniques.

It is also useful to recall the following property between superquantile and quantile, derived from Bayes theorem.

**Proposition 2.** *The following property holds.*

$$\mathbb{E} [Y \mathbf{1}_{Y > VaR^\alpha(Y|\mathcal{G})} \mid \mathcal{G}] = (1 - \alpha) ES^\alpha(Y \mid \mathcal{G}). \quad (138)$$

## B On Neural Networks and Stochastic Gradient Descent

In this Appendix, we recall the main theoretical results on feed-forward neural networks and stochastic gradient descent (SGD). Assume we want to solve the following stochastic optimization problem over the set of Borel functions  $\mathcal{B}$  from  $\mathbb{R}^d$  to  $\mathbb{R}$ :

$$\min_{h \in \mathcal{B}} \mathbb{E} [L(Y, h(X))], \quad (139)$$

where  $L(\cdot, \cdot) : \mathbb{R} \times \mathbb{R} \mapsto \mathbb{R}$  is a given function, and  $(X, Y)$  is a couple of random variables with values in  $\mathbb{R}^d \times \mathbb{R}$ , defined on a given probability space. As this problem has infinite dimension, assume we minimize the loss over the set of neural networks functions  $\mathcal{H}_\theta$  parameterized by  $\theta$ , such that:

$$\theta^* := \arg \min_{\theta} \mathbb{L}(\theta), \quad (140)$$

where  $\mathbb{L}(\theta) := \mathbb{E} [\mathcal{L}(X, Y; \theta)]$  and  $\mathcal{L}(x, y; \theta) := L(y, h_\theta(x))$ , which leads to:

$$h_{\theta^*} = \arg \min_{h_\theta \in \mathcal{H}_\theta} \mathbb{E} [L(Y, h_\theta(X))]. \quad (141)$$

At this point, we should specify what we exactly mean by a neural network function  $h_\theta$ . Here, we consider a simple feedforward neural network structure mapping an input in  $\mathbb{R}^d$  to an output

in  $\mathbb{R}$ :

$$\mathcal{H}_\theta = \left\{ \mathbb{R}^d \ni x \mapsto W_{l+1}\sigma(W_l\sigma(\dots\sigma(W_1\tilde{x}))) \in \mathbb{R} \right\}, \quad (142)$$

where  $\tilde{x} = [x, 1]^T \in \mathbb{R}^{d+1}$  is the augmented input vector to account for bias terms, and  $W_i \in \mathbb{R}^{n_i \times n_{i-1}}$  is the weight matrix of the  $i$ -th layer, with  $n_0 = d+1$  and  $n_{l+1} = 1$ . Moreover,  $\sigma(\cdot)$  is a (potentially) non-linear activation function (eg. ReLU, sigmoid, tanh) that is applied element-wise to a given vector. A stylized representation of such neural network function is displayed in Figure 20.

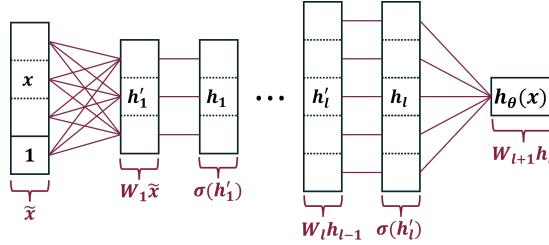


Figure 20: Stylized representation of a feedforward neural network.

The parameter  $\theta$  is then defined as:

$$\theta = \{W_1, W_2, \dots, W_{l+1}\}. \quad (143)$$

Coming back to our stochastic optimization problem, one usually doesn't know the joint law of  $(X, Y)$ , so that it is not possible to explicitly compute  $\mathbb{L}(\theta)$  or  $\nabla \mathbb{L}(\theta)$ . Notice that we consider  $\theta$  to be the flattened array of all weight matrices coordinates when writing gradient with respect to  $\theta$ . If we have access to iid. samples  $\{(X_1, Y_1), \dots, (X_M, Y_M)\}$ , we can use the trick of stochastic gradient descent given in its simplest version by Algorithm 3.

---

**Algorithm 3:** SGD for a feedforward neural network

---

**Input:** a sequence of learning rates  $(\alpha_k)_{k \geq 1}$  and a number of epochs  $K$ .

Initialize  $\hat{\theta}$

**for** epoch  $k = 1$  **to**  $K$  **do**

Shuffle the dataset  $\{(X_1, Y_1), \dots, (X_M, Y_M)\}$

**for**  $m = 1$  **to**  $M$  **do**

$\hat{\theta} \leftarrow \hat{\theta} - \alpha_k \nabla_\theta \mathcal{L}(X_m, Y_m; \hat{\theta})$

---

The trick is that  $\nabla_\theta \mathcal{L}(X_m, Y_m; \hat{\theta})$  is an unbiased estimator of  $\nabla \mathbb{L}(\hat{\theta})$  at each step, so that we may converge to a local minimum of the loss function  $\mathbb{L}(\cdot)$  with an appropriate learning rate sequence. As neural network functions are non-convex in  $\theta$ , there is no guarantee to converge to a global minimum but the noisy property of SGD (through dataset shuffling) helps escaping saddle points of the loss function landscape. Notice that this algorithm belongs to the broader

class of stochastic approximation algorithms. This approach is effective in practice and has been extended to have a better control over the variance, numerical stability, or global convergence. For instance, we can penalize the loss (Lasso, Ridge), use mini-batches in SGD, or choose more advanced techniques such as Adam (see [KB17]) and others. The mini-batch SGD is presented in Algorithm 4.

---

**Algorithm 4:** Mini-batch SGD for a feedforward neural network

---

**Input:** a sequence of learning rates  $(\alpha_k)_{k \geq 1}$ , a number of epochs  $K$ , and a partition  $\mathcal{J}$  of  $\{1, \dots, M\}$ .

Initialize  $\hat{\theta}$

**for** epoch  $k = 1$  **to**  $K$  **do**

- Shuffle the dataset  $\{(X_1, Y_1), \dots, (X_M, Y_M)\}$
- for** batch  $J \in \mathcal{J}$  **do**
- $\hat{\theta} \leftarrow \hat{\theta} - \alpha_k \frac{1}{\text{Card}(J)} \sum_{m \in J} \nabla_{\theta} \mathcal{L}(X_m, Y_m; \hat{\theta})$

---

It enables to reduce the variance of the gradient unbiased estimator:

$$\mathbb{V} \left[ \frac{1}{|J|} \sum_{m \in J} \nabla_{\theta} \mathcal{L}(X_m, Y_m; \hat{\theta}) \right] = \frac{1}{\text{Card}(J)} \mathbb{V} \left[ \nabla_{\theta} \mathcal{L}(X, Y; \hat{\theta}) \right]. \quad (144)$$

Although these smoother iterates may increase the quality of convergence, taking a too large batch size  $\text{Card}(J)$  may prevent the algorithm to escape local minima and may decrease convergence speed since updating the parameters is more costly. Notice that the classic SGD corresponds to the case where  $\mathcal{J} = \{\{1\}, \dots, \{M\}\}$ , ie. each batch contains only one observation.

The SGD algorithm (or any of its variants) then produces an estimator  $\hat{\theta}$  of the optimal parameter  $\theta^*$ , so that we can define the learned neural network function by  $\hat{h} := h_{\hat{\theta}}$ . Notice that  $\theta \mapsto \mathcal{L}(x, y, \theta)$  may not be differentiable everywhere<sup>31</sup> for all coordinates of  $\theta$ , eg. if we have ReLu activation functions or if  $\hat{y} \mapsto L(y, \hat{y})$  is not differentiable everywhere, like the pinball loss in equation (106) of Appendix A.2. In this case, one simply replaces the gradient by a given subgradient in the SGD algorithm. Fortunately, most deep learning libraries such as `pytorch` or `tensorflow` implement this twist in their SGD and backpropagation (see later) algorithms, so that we do not have to worry about it.

One may argue that we could have taken the empirical version of  $\mathbb{L}(\cdot)$  based on our dataset of iid. observations, as we have done in Appendix A.1 or Appendix A.2:

$$\theta^* \approx \arg \min_{\theta} \bar{L}(\theta), \quad (145)$$

where  $\bar{L}(\theta) := \frac{1}{M} \sum_{m=1}^M \mathcal{L}(X_m, Y_m; \theta)$ . Then, we would perform the minimization over  $\theta$  using

---

<sup>31</sup>The function should be at least continuous in all the coordinates of  $\theta$ .

a simple gradient descent algorithm as presented in Algorithm 5.

---

**Algorithm 5:** Gradient Descent for a feedforward neural network

---

**Input:** a sequence of learning rates  $(\alpha_k)_{k \geq 1}$  and a number of epochs  $K$ .

Initialize  $\hat{\theta}$

**for** epoch  $k = 1$  **to**  $K$  **do**

$\hat{\theta} \leftarrow \hat{\theta} - \alpha_k \nabla \bar{L}(\hat{\theta})$

---

However, as guessed before for the limits of mini-batch SGD, this approach is not suitable for neural networks and large datasets for several reasons. First, as there is no random effect in the classic gradient descent, we have less chance to reach the global minima (or a good local minima) since  $\bar{L}(\cdot)$  is not convex. Second, the gradient of  $\bar{L}(\cdot)$  is given by:

$$\nabla \bar{L}(\theta) = \frac{1}{M} \sum_{m=1}^M \nabla_{\theta} \mathcal{L}(X_m, Y_m, \theta) \quad (146)$$

which requires to evaluate the gradient for each observation of the dataset *before* making a weight update, so that the cost of a weight update is  $\mathcal{O}(M)$  versus  $\mathcal{O}(1)$  for SGD. Hence, SGD provides rapid and noisy updates, speeding up convergence and potentially escaping shallow minima, contrary to the classic gradient descent.

Finally, one should mention how to compute gradient of the loss function  $\mathcal{L}(x, y, \theta)$  with respect to the parameters  $\theta$ . First, one has to compute  $h_{\theta}(x)$  by a “forward pass” through the neural network, starting from the input layer and going through each layer until the output layer. Then, one calculates the value of  $\nabla_{\theta} \mathcal{L}(x, y, \theta)$  using the so-called “backpropagation” technique, which is the Automatic Adjoint Differentiation (AAD) method applied to neural networks. The idea is that every evaluation of the neural network (and hence of the loss function) can be seen as a directed acyclic graph of elementary operations, and the backpropagation algorithm allows to compute the gradient of the loss function with respect to the parameters  $\theta$  by traversing this graph backwards. This technique also enables to accomodate immediatly for different neural network architectures contrary to a symbolic (ie. analytical) differentiation approach. The cost of backpropagation is only a small constant multiple of the cost of a forward pass, making large-scale neural networks training tractable. Moreover, this algorithm is implemented in most deep learning libraries, so that one does not have to focus on the details of the backpropagation algorithm. For more information on AAD, we refer the interested reader to [Sav18].

## C On Johnson Distributions

### C.1 The types of Johnson distributions

The Johnson distribution family is a flexible family of probability distributions that can model a wide range of shapes, including those with skewness and kurtosis. More precisely, it is possible to match any value of skewness and kurtosis. It is particularly useful for modeling financial data, which often exhibit non-normal characteristics. The Johnson distribution family consists of four types:  $S_L$  for *log-normal*,  $S_U$  for *unbounded*,  $S_B$  for *bounded*,  $S_T$  for *two-ordinate* (which is a special case of  $S_B$ ), and  $S_N$  for *normal*. If  $X$  follows a Johnson distribution, then we denote  $X \sim \text{Johnson}(J(\cdot), \gamma, \delta, \xi, \lambda)$  such that:

$$\gamma + \delta \cdot J\left(\frac{X - \xi}{\lambda}\right) \sim \mathcal{N}(0, 1), \quad (147)$$

where the parameters  $(\gamma, \delta, \xi, \lambda)$  control the location, scale, and shape of the distribution, while  $J(\cdot)$  is a transformation function that depends on the type of Johnson distribution:

$$J(u) := \begin{cases} \ln(u) & (S_L), \\ \ln(u + \sqrt{u^2 + 1}) = \sinh^{-1}(u) & (S_U), \\ \ln(u/(1-u)) & (S_B) \text{ or } (S_T), \\ u & (S_N). \end{cases}$$

Noticing that the cdf of  $X$  is given by:

$$F_X(x) = \Phi\left(\gamma + \delta \cdot J\left(\frac{x - \xi}{\lambda}\right)\right), \quad (148)$$

where  $\Phi(\cdot)$  is the cdf of  $\mathcal{N}(0, 1)$ , it is easy to show that the pdf of  $X$  is given by:

$$f_X(x) = \frac{\delta}{\lambda} J'\left(\frac{x - \xi}{\lambda}\right) \cdot \phi\left(\gamma + \delta \cdot J\left(\frac{x - \xi}{\lambda}\right)\right), \quad (149)$$

where  $\phi(\cdot)$  is the pdf of  $\mathcal{N}(0, 1)$ . The derivative of  $J$  is given by:

$$J'(u) = \begin{cases} 1/u & (S_L), \\ \frac{1}{\sqrt{1+u^2}} & (S_U), \\ \frac{1}{u(1-u)} & (S_B) \text{ or } (S_T), \\ 1 & (S_N). \end{cases} \quad (150)$$

Moreover, from equation (148), the quantile at level  $\alpha$  of  $X$  is given by:

$$q = \xi + \lambda J^{-1}\left(\frac{\Phi^{-1}(\alpha) - \gamma}{\delta}\right), \quad (151)$$

where the inverse of  $J(\cdot)$  is given by:

$$J^{-1}(u) = \begin{cases} e^u & (S_L), \\ \sinh(u) & (S_U), \\ \frac{1}{1+e^{-y}} & (S_B) \text{ or } (S_T), \\ u & (S_N). \end{cases} \quad (152)$$

Notice that in practice, one can set  $\xi = 0$  when the family is  $S_N$  without loss of generality, implying an appropriate rescaling of  $\gamma$ . Indeed in this case,  $X \sim \mathcal{N}\left(\frac{\xi-\gamma\lambda}{\delta}, \frac{\lambda^2}{\delta^2}\right)$  so that  $\xi$  and  $\gamma$  only act on one parameter of the distribution. Moreover, one should be very careful when using the `scipy.stats` functions available in `python` as they do not follow the same convention as the one used in this report. One should use them in the following way:

$$\begin{cases} \text{lognorm.xxx}\left(yyy, s=\frac{1}{|\delta|}, loc=\xi, scale=\lambda e^{\frac{-\gamma}{\delta}}\right) & (S_L), \\ \text{johnsonsu.xxx}\left(yyy, a=\gamma, b=\delta, loc=\xi, scale=\lambda\right) & (S_U), \\ \text{johnsonsb.xxx}\left(yyy, a=\gamma, b=\delta, loc=\xi, scale=\lambda\right) & (S_B) \text{ or } (S_T), \\ \text{norm.xxx}\left(yyy, loc=\frac{\xi-\gamma\lambda}{\delta}, scale=\frac{|\lambda|}{|\delta|}\right) & (S_N). \end{cases}$$

The function  $J(\cdot)$  is uniquely determined by the square of the skewness  $\gamma$  and the kurtosis  $\kappa$  defined as:

$$\begin{cases} \gamma := \frac{\mathbb{E}[(X - \mathbb{E}[X])^3]}{(\mathbb{E}[(X - \mathbb{E}[X])^2])^{3/2}}, \\ \kappa := \frac{\mathbb{E}[(X - \mathbb{E}[X])^4]}{(\mathbb{E}[(X - \mathbb{E}[X])^2])^2}. \end{cases} \quad (153)$$

Figure 21 shows the regions of Johnson functions (and so Johnson types) in the  $(\gamma^2, \kappa)$  plane. We see that the  $(S_T)$  type is indeed a special case of the  $(S_B)$  type when  $\gamma^2 = \kappa + 1$ . Moreover, we recover  $(\gamma, \kappa) = (0, 3)$  for the normal distribution corresponding to the  $(S_N)$  type. Notice that the impossible region corresponds to the case where  $\gamma^2 < \kappa + 1$ . Although such region is theoretically impossible for any distribution, it can be observed in practice due estimation issues.

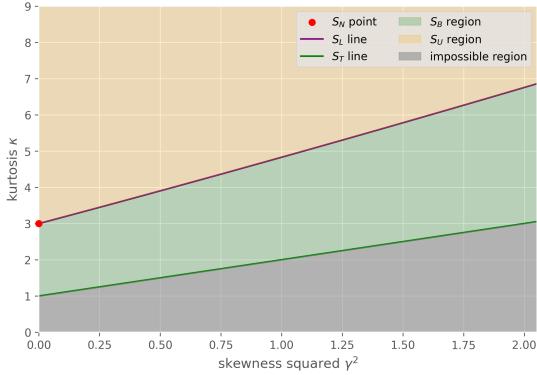


Figure 21: Johnson distribution types in the  $(\gamma^2, \kappa)$  plane.

## C.2 Johnson parameters estimation

From the theoretical developments explained above, it is necessary to have a procedure to estimate the parameters of a Johnson distribution. We do not focus here on maximum likelihood estimation (MLE) for two reasons. First, it is not possible to compute analytically the maximum likelihood estimates, and maximizing the likelihood function is difficult because of its non-regularity [GR11]. Second, MLE methods involve computing various statistics based on iid. samples of  $X$ . However, in our case of initial margin and counterparty credit risk, we do not have access to iid. samples of  $X = (\Delta V_{t+\delta} | v)$  for a given  $t$  and a given  $v$ . More precisely, we can generate iid. samples of  $X$  at a high cost, so that the MLE numerical method should be fast enough, which is not the case. We refer the reader to [GR11] for a detailed discussion on MLE methods for Johnson distributions.

### C.2.1 Moment matching

Putting maximum likelihood methods aside, the most natural way to estimate the parameters of a Johnson distribution is to use the method of moments (also called moment fitting or moment matching). It consists in finding the parameters  $(\gamma, \delta, \xi, \lambda)$  such that the first four theoretical Johnson moments match the moments we have specified. The function  $J(\cdot)$  is entirely determined by the squared skewness and kurtosis computed based on our first four raw moments. In our case of initial margin and counterparty credit risk, the first four moments of  $X = (\Delta V_{t+\delta} | v)$  are estimated by regression. However, the procedure of matching moments is non trivial and costly with little control on the running time. It is given by the algorithm AS99 of [HHH76] which requires the mean, variance, skewness, and kurtosis of  $X$  as an input. It was initially written in Fortran in 1976, then translated into an unofficial Matlab package in the 2010's, and finally implemented in Python through a Github project<sup>32</sup> in the last years. However, it is important to note that the Matlab code contains some errors that are also repeated in

<sup>32</sup>available [here](#).

the Python implementation. I have corrected those I have seen in my Python code, which is available upon request. Notice that in practice it may be possible that some parameters are not well defined because of the estimation of raw moments and higher order metrics such as variance, skewness, and kurtosis. Moreover, the moment fitting procedure could simply fail. In these case, we say that we have an impossible region and cancel the estimation.

### C.2.2 Percentile matching

Because of the drawbacks of the moment matching method described above, it is interesting to explore other approaches. We consider here the percentile matching method from [SS80]. The first step is to compute four quantiles of  $X$  denoted  $x_{3z}$ ,  $x_z$ ,  $x_{-z}$  respectively at the levels  $\Phi(3z)$ ,  $\Phi(z)$ ,  $\Phi(-z)$ , and  $\Phi(-3z)$  for a given  $z > 0$ , where  $\Phi(\cdot)$  is the cdf of  $\mathcal{N}(0, 1)$ . In our case of initial margin and counterparty credit risk, it involves simulating iid. samples of  $X = (\Delta V_{t+\delta} \mid v)$  at a high cost, so that the quantiles can be estimated by the corresponding empirical quantiles, potentially considering smoother definitions than the one of Definition 1. Based on these quantiles, we define the following metrics:

$$\begin{cases} m &:= x_{3z} - x_z, \\ n &:= x_{-z} - x_{-3z}, \\ p &:= x_z - x_{-z}, \end{cases} \quad (154)$$

The Johnson distribution type is then  $(S_B)$  if  $d < 0.999$ ,  $(S_U)$  if  $d > 1.001$ , and  $(S_L)$  otherwise, where  $d := \frac{m \cdot n}{p^2}$ . Notice that theoretically, the  $(S_L)$  type is set iff.  $d = 1$ . As this event has probability zero, we use in practice a tolerance threshold of  $\pm 0.001$ . Moreover, the case of  $(S_T)$  is embedded in  $(S_B)$  while the case of  $(S_N)$  is not possible here as we assume that  $X$  is not normally distributed (otherwise we would have used a Gaussian distribution directly). Then, we can compute the parameters  $(\gamma, \delta, \xi, \lambda)$  from Table 5, by denoting  $q := m/p$ ,  $\bar{q} := 1/q$ ,  $r := n/p$ , and  $\bar{r} := 1/r$ .

Type	$S_L$	$S_U$	$S_B$
$\gamma$	$\delta \ln \left( \frac{q-1}{p\sqrt{\bar{q}}} \right)$	$\delta \sinh^{-1} \left( \frac{r-q}{2\sqrt{qr-1}} \right)$	$\delta \sinh^{-1} \left( \frac{(\bar{r}-\bar{q})\sqrt{(1+\bar{q})(1+\bar{r})-4}}{2(\bar{q}\bar{r}-1)} \right)$
$\delta$	$\frac{2z}{\ln q}$	$\frac{2z}{\cosh^{-1} \left( \frac{q+r}{2} \right)}$	$\frac{z}{\cosh^{-1} \left( \frac{1}{2}\sqrt{(1+\bar{q})(1+\bar{r})} \right)}$
$\xi$	$\frac{x_z+x_{-z}}{2} - \frac{p}{2} \cdot \frac{q+1}{q-1}$	$\frac{x_z+x_{-z}}{2} + \frac{p(r-q)}{2(q+r-2)}$	$\frac{x_z+x_{-z}}{2} - \frac{\lambda}{2} + \frac{p(\bar{r}-\bar{q})}{2(\bar{q}\bar{r}-1)}$
$\lambda$	1	$\frac{2p\sqrt{qr-1}}{(qr-2)\sqrt{q+r-2}}$	$\frac{p\sqrt{((1+\bar{q})(1+\bar{r})-2)^2-4}}{\bar{q}\bar{r}-1}$

Table 5: Johnson parameters estimation in the percentile matching method.

As for the moment-matching method of Appendix C.2.1, it may be possible that some parameters are not well defined, because of the estimation of the quantiles  $x_{3z}$ ,  $x_z$ ,  $x_{-z}$ , and  $x_{-3z}$ . In this case, we can use the following heuristics:

- If  $d \in [0.999, 1)$  and  $q \leq 1$ , we set the type to  $(S_B)$  instead of  $(S_L)$ .
- If  $d \in (1, 1.001]$  and  $q \leq 1$ , we set the type to  $(S_U)$  instead of  $(S_L)$ .
- If  $d = 1$  and  $q \leq 1$ , or if some parameters are not well defined for a given type, we say that it is an impossible region and we cancel the estimation.

An important question is how to choose the value of  $z$ . We have found that for our application,  $z = 0.524$  or  $z = 1$  usually yield robust results. Finally, notice that the percentile matching method has been shown empirically to be more robust than the moment matching method, see [SS80].

## D On One Factor Hull-White Model and Swaption Pricing

### D.1 The one factor Hull-White model

The one factor Hull-White model (HW1F) of [WH90], also called extended Vasicek Hull-White model, is a popular model used to describe the evolution of the short rate ( $r_t$ ) over time. In this section, we recall its main properties that we will use for the pricing of swaption in Appendix D.2 and we recall the expectation under  $\mathbb{Q}$  is denoted  $\mathbb{E}[\cdot]$ . The interested reader can find more details in [BM13] although the notations are not exactly the same. More precisely, it assumes the following dynamics under the risk-neutral probability measure  $\mathbb{Q}$ :

$$dr_t = (\theta(t) - kr_t)dt + \sigma dW_t, \quad (155)$$

where  $\theta(t)$  is a deterministic long-term mean function chosen to match the initial curve of zero-coupon prices,  $k$  is the mean reversion speed,  $\sigma$  is the volatility of the short rate, and  $W$  is a  $\mathbb{Q}$ -Brownian motion. Let us denote  $T \mapsto \hat{B}_0(T)$  the observed zero-coupon (ZC) price curve, and  $B_t(T)$  the price of the ZC with maturity  $T$  at time  $t$  in our HW1F model. Notice that we don't specify here how to construct this observed ZC price curve from available market instruments with the so-called bootstrapping technique, see eg. [HW08]. Instead, we assume the ZC price curve is given, for instance from Refinitiv. It can be shown that we calibrate perfectly to the observed ZC price curve<sup>33</sup> by setting:

$$\theta(t) = \partial_t \hat{f}(0, t) + k \cdot \hat{f}(0, t) + \frac{\sigma^2}{2k} \left( 1 - e^{-2k(T-t)} \right), \quad (156)$$

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<sup>33</sup>ie.  $B_0(T) = \hat{B}_0(T)$ .

where  $T \mapsto \hat{f}(0, T) = -\partial_T \ln \hat{B}_0(T)$  is the observed instantaneous forward rate curve<sup>34</sup>. Moreover, the random variable  $r_t$  is Gaussian conditional on  $\mathcal{F}_s$  under  $\mathbb{Q}$ :

$$r_t \mid \mathcal{F}_s \sim \mathcal{N} \left( (r_s - \beta(s))e^{-k(t-s)} + \beta(t), \frac{\sigma^2}{2k} (1 - e^{-2k(t-s)}) \right), \quad (157)$$

where  $\beta(t) = \hat{f}(0, t) + \frac{\sigma^2}{2k} (1 - e^{-k(T-t)})^2$ . Moreover, notice that the HW1F model is an affine structure model:

$$B_t(T) = \mathbb{E} \left[ e^{-\int_t^T r_s ds} \mid \mathcal{F}_t \right] = e^{m(t, T) - n(t, T)r_t}, \quad (158)$$

where:

$$\begin{cases} n(t, T) &= (1 - e^{-k(T-t)}) / k, \\ m(t, T) &= \ln \left( \frac{\hat{B}_0(T)}{\hat{B}_0(t)} \right) + n(t, T)\hat{f}(0, t) - \frac{\sigma^2}{4k}n(t, T)^2 (1 - e^{-2kt}). \end{cases} \quad (159)$$

Finally, the HW1F model can be seen as a special case of a (Gaussian) HJM model under  $\mathbb{Q}$ :

$$df(t, T) = \alpha(t, T)dt + \sigma(t, T)dW_t, \quad (160)$$

where  $f(0, T) = \hat{f}(0, T)$ ,  $\sigma(t, T) := \sigma e^{-k(T-t)}$ , and the drift  $\alpha(t, T)$  is entirely determined by the HJM drift condition under absence of arbitrage opportunities:

$$\alpha(t, T) = \Sigma(t, T)\sigma(t, T), \quad (161)$$

where  $\Sigma(t, T) := \frac{\sigma}{k}(1 - e^{-k(T-t)})$ .

## D.2 Swaption pricing in HW1F

Assume we want to price a swaption in the HW1F model described in Appendix D.1. We denote  $T_0$  the swaption maturity,  $T_1$  the start of the underlying payer swap with evenly spaced fixing dates  $\{T_1, \dots, T_n\}$  such that  $\Delta T := T_i - T_{i-1}$ . In this swap with a notional amount FV, we pay a fixed rate  $K$  and receive the interest rate  $L(T_{i-1}, T_i)$  simply compounded on the period  $[T_{i-1}, T_i]$  at time  $T_i$ , such that:

$$L(t, T) = \frac{1}{T-t} \left( \frac{1}{B_t(T)} - 1 \right). \quad (162)$$

We display the stylized payer swap cash flows in Figure 22.

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<sup>34</sup>Recall that the instantaneous forward rate  $f(t, \cdot)$  is such that  $B_t(T) = e^{-\int_t^T f(t,s)ds}$ .

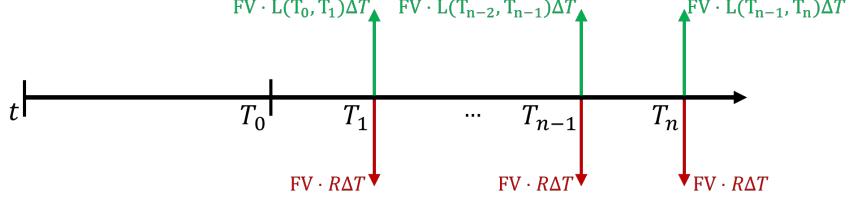


Figure 22: Stylized payer swap cash flows.

Thus, the payoff of the swaption at maturity  $T_0$  is given by:

$$V_{T_0} = \left( V_{T_0}^{\text{swap}} \right)_+, \quad (163)$$

where  $V_{T_0}^{\text{swap}}$  is the price at time  $T_0$  of the swap described above. It is easy to show that:

$$V_{T_0}^{\text{swap}} = \text{FV} \cdot \left( 1 - \sum_{k=1}^n c_k B_{T_0}(T_k) \right), \quad (164)$$

where  $c_k = \mathbf{1}_{k=n} + \Delta T \cdot R$  for all  $k \in [|1, n|]$ . Let us denote the  $T_0$ -forward measure  $\mathbb{Q}^{T_0}$  such that for all  $t \leq T_0$ :

$$\frac{d\mathbb{Q}^{T_0}}{d\mathbb{Q}} \Big|_{\mathcal{F}_t} := \frac{B_t(T_0)}{B_0(T_0)B_t}. \quad (165)$$

The swaption price is a put price on a coupon-bearing bond, given under this probability measure by:

$$V_t = \text{FV} \cdot B_t(T_0) \cdot \mathbb{E}^{\mathbb{Q}^{T_0}} \left[ \left( 1 - \sum_{k=1}^n c_k B_{T_0}(T_k) \right)_+ \mid \mathcal{F}_t \right]. \quad (166)$$

We recall that the HW1F model is a Gaussian Heath-Jarrow-Morton (HJM) model (see [HJM92]) since  $r_t$  is Gaussian under  $\mathbb{Q}$  from equation (157). Moreover, it has separable volatility so that  $\sigma(t, T) = \zeta(t)\rho(T)$  with  $\zeta(t) = e^{kt}$  and  $\rho(T) = \sigma e^{-kT}$ . Using equation (158), it can be shown that:

$$B_{T_0}(T_k) = e^{\mu(T_0, T_k) - \psi(T_0, T_k)Y_{T_0}}, \quad (167)$$

where  $Y_{T_0} \sim \mathcal{N}(0, 1)$  under  $\mathbb{Q}^{T_0}$ , and  $\psi(T_0, T_k) = \frac{\sigma}{k}(e^{-kt} - e^{-kT})$ . Moreover, we have:

$$\mu(t, T) = \ln \left( \frac{B_0(T)}{B_0(t)} \right) - I_1(t, T) + I_2(t, T), \quad (168)$$

where:

$$I_1(t, T) := \frac{1}{2} \int_0^t (\Sigma(u, T)^2 - \Sigma(u, t)^2) du \quad (169)$$

$$= \frac{\sigma^2}{k^3} \left( 1 + e^{-kT} - e^{-kt} - e^{-k(T-t)} + \frac{1}{4} (e^{-2k(T-t)} - 1) \right), \quad (170)$$

and  $I_2(t, T) := \int_0^t \Sigma(u, T_0) (\Sigma(u, T) - \Sigma(u, t)) du$ , so that:

$$\begin{aligned} I_2(t, T) &= \frac{\sigma^2}{k^3} \left( e^{-k(T-t)} - e^{-kT} - 1 + e^{-kt} - e^{-k(T+T_0-2t)} \right. \\ &\quad \left. + e^{-k(T+T_0)} + e^{-k(T_0-t)} - e^{-k(t+T_0)} \right). \end{aligned} \quad (171)$$

Now, we would like to take the sum out of the positive part in equation (166), to get a sum of put prices. We will use the Jamshidian trick described in [Jam89] to do so. Let us define:

$$f(y) := \sum_{k=1}^n f_k(y), \quad (172)$$

where  $f_k(y) := c_k e^{\mu(T_0, T_k) - \psi(T_0, T_k)y}$ . Let us solve numerically  $\bar{y}$  such that  $f(\bar{y}) = 1$ . Notice that there is a unique solution as  $f$  is continuous and strictly decreasing as a sum of strictly decreasing functions  $(f_k)_k$  with limits 0 and  $+\infty$  at  $\pm\infty$ . From the monotonicity and positivity of  $f_k$  and  $f$ , we have:

$$\left( 1 - \sum_{k=1}^n c_k B_{T_0}(T_k) \right)_+ = (f(\bar{y}) - f(Y_{T_0})) \mathbf{1}_{f(\bar{y}) > f(Y_{T_0})} \quad (173)$$

$$= (f(\bar{y}) - f(Y_{T_0})) \mathbf{1}_{\bar{y} < Y_{T_0}} \quad (174)$$

$$= \sum_{k=1}^n (f_k(\bar{y}) - f_k(Y_{T_0})) \mathbf{1}_{\bar{y} < Y_{T_0}} \quad (175)$$

$$= \sum_{k=1}^n (f_k(\bar{y}) - f_k(Y_{T_0})) \mathbf{1}_{f_k(\bar{y}) > f_k(Y_{T_0})} \quad (176)$$

$$= \sum_{k=1}^n c_k (K_k - B_{T_0}(T_k))_+, \quad (177)$$

where  $K_k := f_k(\bar{y})/c_k$ . Thus, the swaption price is given by a weighted sum of the prices  $\Pi^{\text{put}}(t, T_0, T_k, K_k)$  at time  $t$  of put options with maturity  $T_0$  and strike  $K_k/c_k$  on the ZC with maturity  $T_k$ :

$$V_t = \text{FV} \cdot \sum_{k=1}^n c_k \cdot B_t(T_0) \mathbb{E}^{\mathbb{Q}^{T_0}} [(K_k - B_{T_0}(T_k))_+ \mid \mathcal{F}_t] \quad (178)$$

$$= \text{FV} \cdot \sum_{k=1}^n c_k \cdot \Pi^{\text{put}}(t, T_0, T_k, K_k). \quad (179)$$

Finally, as the HW1F model is a Gaussian HJM model, it can be shown that:

$$\Pi^{\text{put}}(t, T, S, K) = KB_t(T)\Phi(-d_2) - B_t(S)\Phi(-d_1), \quad (180)$$

where  $\Phi$  is the cdf of  $\mathcal{N}(0, 1)$  and  $d_{1,2} := \frac{\ln\left(\frac{B_t(S)}{KB_t(T)}\right) \pm \frac{1}{2}\bar{v}(t, T, S)}{\sqrt{\bar{v}(t, S, T)}}$  with:

$$\bar{v}(t, T, S) := \frac{\sigma}{k} \left(1 - e^{-k(T-S)}\right) \sqrt{\frac{1 - e^{-2k(T-t)}}{2k}}. \quad (181)$$

Notice that since the zero-coupon price is a an analytical function of  $(t, r_t)$  from equation (158), the swaption price is also an analytical function  $V_t =: u(t, r_t)$ .