Technical note: Simulation of square-root processes

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Noncentral chi-squared distribution

Definition. Let $(X_1, \dots, X_k)$ be k independent, normally distributed random variables such that $X_i \sim \mathcal{N}(\mu_i, 1)$. Then

$$X = \sum_{i=1}^{k} X_i^2 \sim \widetilde{\chi}^2(k, \lambda), \quad \lambda := \sum_{i=1}^{k} \mu_i^2.$$

In other words, X is distributed according to the noncentral chi-squared distribution with $k \in \mathbb{N}^*$ degrees of freedom. The parameter $\lambda \geqslant 0$ is sometimes called the noncentrality parameter. Obviously, $\widetilde{\chi}^2(k, 0) = \chi^2(k)$. The probability density function is given by

$$f_{\widetilde{\chi}^2(k,\lambda)}(x) = \sum_{i=0}^{\infty} \frac{e^{-\lambda/2}(\lambda/2)^i}{i!} f_{\chi^2(k+2i)}(x), \quad f_{\chi^2(q)}(x) := \frac{x^{q/2-1}e^{-x/2}}{2^{q/2}\Gamma(q/2)} \mathbb{1}_{x>0}.$$

As a consequence,

$$F_{\widetilde{\chi}^2(k,\lambda)}(x) = \sum_{i=0}^{\infty} \frac{e^{-\lambda/2}(\lambda/2)^i}{i! 2^{k/2+1}\Gamma(k/2+i)} \int_0^x u^{k/2+i-1} e^{-u/2} \, du.$$

Link with the square root process V. Recall that in our setting, $dV_t = (a + bV_t)\,dt + c\sqrt{V_t}\,dW_t$ with $b < 0$. For $s \leqslant t$,

$$\mathbb{P}\big(V_t \leqslant x | V_s\big) = F_{\widetilde{\chi}^2(d, V_s n(s,t))}\left(\frac{x \times n(s,t)}{e^{b(t-s)}}\right), \quad d := \frac{4a}{c^2}, \quad n(s,t) := \frac{4be^{b(t-s)}}{c^2(e^{b(t-s)} - 1)}$$

Therefore, using the fact that $\mathbb{E}\big[\widetilde{\chi}^2(k,\lambda)\big] = k + \lambda$ and $\mathrm{Var}(\widetilde{\chi}^2(k,\lambda)) = 2(k + 2\lambda)$ it is possible to compute explicits expressions for the first two conditional moments of V. One can check that we retrieve the same quantities with the computations below.

Using the fact that

$$V_t = e^{b(t-s)}V_s + a\frac{e^{b(t-s)} - 1}{b} + c\int_s^t e^{b(t-u)}\sqrt{V_u}\,dW_u,$$

it leads to

$$\begin{aligned} \mathbb{E}\big[V_t | V_s\big] &= e^{b(t-s)}V_s + a\frac{e^{b(t-s)} - 1}{b} \\ \mathrm{Var}\big(V_t | V_s\big) &= c^2 \int_s^t e^{2b(t-u)}\mathbb{E}[V_u | V_s]\,du = c^2\left(\frac{e^{b(t-s)}\left(e^{b(t-s)} - 1\right)}{b}V_s + \frac{a}{2b^2}\left(e^{b(t-s)} - 1\right)^2\right) \end{aligned}$$

Now, suppose that $V_0 > 0$. If $2a \geqslant c^2$ (i.e. $d \geqslant 2$) then the process V can never reach 0. In typical market regime the Feller condition above is no longer satisfied, so the likelihood of hitting zero is often quite significant.

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It is well-known that $\widetilde{\chi}^2(k,\lambda)$ approaches a Gaussian distribution as the noncentrality parameter λ approaches $+\infty$. We know that $V_{t_{i+1}}$ is proportional to a noncentral chi-square distribution with $k=d$ and $\lambda = V_{t_i} n(t_i, t_{i+1})$ with $n(t_i, t_{i+1})$ independent of V_{t_i}. For "sufficiently large" V_{t_i} a good proxy for $V_{t_{i+1}}$ would be a Gaussian variable with the first two moments fitted to match those given above.

On the other hand, for small V_{t_i}, the noncentrality paramater λ is near 0, and the distribution of $V_{t_{i+1}}$ becomes proportional to $\chi^2(d)$, and as said before the probability density function is defined as:

$$f_{\chi^2(k)}(x) := \frac{x^{k/2-1}e^{-x/2}}{2^{k/2}\Gamma(k/2)}\mathbb{1}_{x>0}.$$

When $4a/c^2 \ll 2$, the presence of the term $x^{d/2-1} = x^{2a/c^2-1}$ in the probability density function implied that, for small V_{t_i}, the density of $V_{t_{i+1}}$ will be very large around 0. It should be clear that approximation of $V_{t_{i+1}}$ with a Gaussian random variable is typically <u>not</u> accurate when V_{t_i} is close to zero.

TG (Truncatured Gaussian) scheme

In this scheme the idea is to sample from a moment-matched Gaussian density where all probability mass below zero is inserted into a delta-function at the origin. For large values of V_{t_i} (where the likelihood of reaching zero is low) this scheme will automatically reproduce the asymptotic behavior of $V_{t_{i+1}}$ described earlier. For small V_{t_i}, the resulting scheme will approximae the chi-square density by a mass in 0 combined with an upper density tail proportional to $e^{-x^2/2}$. To put in a nutshell, the scheme writes

$$\widehat{V}_{t_{i+1}} = (\mu + \sigma Z)^+ ,$$

where Z is a standard Gaussian random variable, μ and σ are constants that will depend on the time step $\Delta := t_{i+1} - t_i$ and $\widehat{V}_{t_i}$, as well as the parameters (a,b,c).

To set μ and σ, we will proceed by moment-matching as prescribed before. More precisely, the goal is the match both $\mathbb{E}[\widehat{V}_{t_{i+1}}]$ and $\mathbb{E}[\widehat{V}^2_{t_{i+1}}]$ to the exact values of $\mathbb{E}[V_{t_{i+1}}|V_{t_i}]$ and $\mathbb{E}[V^2_{t_{i+1}}|V_{t_i}]$.

Proposition. *Let φ (resp. ϕ) the standard Gaussian probability density function (resp. cumulative distribution function), and define a function $r:\mathbb{R}\to\mathbb{R}$ by the following relation*

$$r(x)\times(\varphi\circ r)(x) + (\phi\circ r)(x)\times(1+r(x)^2) = (1+x)\left((\varphi\circ r)(x) + r(x)\times(\phi\circ r)(x)\right)^2$$

Also define

$$\begin{cases} m & := \mathbb{E}[V_{t_{i+1}}|V_{t_i}], \\ s^2 & := \mathrm{Var}(V_{t_{i+1}}|V_{t_i}), \\ \psi & := s^2/m^2 > 0. \end{cases}$$

If $\widehat{V}_{t_{i+1}}$ is generated by the TG scheme, with parameters settings

$$\mu = \frac{m}{(\varphi\circ r)(\psi)\times r(\psi)^{-1} + (\phi\circ r)(\psi)}, \quad \sigma = \frac{m}{(\varphi\circ r)(\psi) + r(\psi)\times(\phi\circ r)(\psi)},$$

then $\mathbb{E}[\widehat{V}_{t_{i+1}}] = m$ and $\mathrm{Var}(\widehat{V}^2_{t_{i+1}}) = s^2$.

Proof. It is easy to show that

$$\mathbb{E}[\widehat{V}_{t_{i+1}}] = \int_{-\mu/\sigma}^{\infty}(\mu+\sigma x)\varphi(x)\,dx = \mu\phi(\mu/\sigma) + \sigma\varphi(\mu/\sigma)$$

$$\mathbb{E}[\widehat{V}^2_{t_{i+1}}] = \int_{-\mu/\sigma}^{\infty}(\mu+\sigma x)^2\varphi(x)\,dx = \mathbb{E}[\widehat{V}_{t_{i+1}}]\mu + \sigma^2\phi(\mu/\sigma)$$

Due to the non-linear form of the above relationships, the moment-matching cannot be done analytically, so we will have to rely on numerical methods. To do so, we define the ratio $r = \mu/\sigma$. Matching the mean to m results in

$$\mu\phi(r) + \sigma\varphi(r) = m \iff \phi(r) + r^{-1}\varphi(r) = m/\mu \iff \mu = \frac{m}{r^{-1}\varphi(r)+\phi(r)}, \quad \sigma = \mu/r = \frac{m}{\varphi(r)+r\phi(r)}.$$

Inserting this expression into the second order moment,

$$\mathbb{E}[\widehat{V}_{t_{i+1}}^2] = m^2 \left(\frac{1}{r^{-1}\varphi(r) + \phi(r)} + \frac{\phi(r)}{(\varphi(r) + r\phi(r))^2} \right)$$

Matching with $s^2 + m^2$ yields

$$\psi + 1 = \frac{1}{r^{-1}\varphi(r) + \phi(r)} + \frac{\phi(r)}{(\varphi(r) + r\phi(r))^2}$$

This expression translate that r is only of ψ, which concludes the proof. $\square$

The recovery of the function r could (should) be done offline the simulation. In practice, we would do this mapping on a discrete, equidistant grid for ψ, on a bounded domain. To determine the limits of this domain, we notice that

$$\begin{aligned} m &= e^{b\Delta}\widehat{V}_{t_i} + a\frac{e^{b\Delta} - 1}{b} \\ s^2 &= c^2 \left(\frac{e^{b\Delta}\left(e^{b\Delta} - 1\right)}{b}\widehat{V}_{t_i} + \frac{a}{2b^2}\left(e^{b\Delta} - 1\right)^2 \right) \end{aligned}$$

which leads to

$$\psi = \frac{s^2}{m^2} = \frac{c^2 \left(\frac{e^{b\Delta}\left(e^{b\Delta} - 1\right)}{b}\widehat{V}_{t_i} + \frac{a}{2b^2}\left(e^{b\Delta} - 1\right)^2 \right)}{e^{b\Delta}\widehat{V}_{t_i} + a\frac{e^{b\Delta} - 1}{b}}.$$

Differentiating this expression with respect to $\widehat{V}_{t_i}$ shows that $\partial\psi/\partial\widehat{V}_{t_i} < 0$ for all $\widehat{V}_{t_i} \geqslant 0$ such that the largest possible value for ψ is obtained for $\widehat{V}_{t_i} = 0$, and the smallest possible for $\widehat{V}_{t_i} = \infty$. Inserting these values yields $\psi \in (0, c^2/(2a)]$.

In practice, there is no need to map $r(\psi)$ all the way fown to $\psi = 0$. If the probability of $\widehat{V}_{t_{i+1}}$ reaching 0 is negligible, we can skip the moment-fitting step entirely and simply set $\mu = m$ et $\sigma = s$. If we introduce a confidence multiplier α, we can decide to skip the fitting step when $m/s = 1/\sqrt{\psi} > \alpha$. In practice, the relevant domain for ψ on which we, as a minimum, need to map the function $r(\psi)$, is thus : $\psi \in [1/\alpha^2, c^2/(2a)]$.

As a final computational trick, note that once we have established the function r, we can write

$$\begin{aligned} \mu &= f_\mu(\psi) \times m, \quad f_\mu(\psi) := \frac{r(\psi)}{(\varphi \circ r)\psi + r(\psi) \times (\phi \circ r)(\psi)}, \\ \sigma &= f_\sigma(\psi) \times s, \quad f_\sigma(\psi) := \frac{1/\sqrt{\psi}}{(\varphi \circ r)(\psi) + r(\psi) \times (\phi \circ r)(\psi)}. \end{aligned}$$

QE (Quadratic Exponential) scheme

The TG scheme models the upper tail of the density for $\widehat{V}_{t_{i+1}}$ as proportional to $e^{-x^2/2}$. For low values of $\widehat{V}_{t_i}$, however, this density decay is too fast. We now introduce a scheme that is designed to address this issue, as an added benefit, the resulting scheme will not require the same amount of pre-caching as was necessary for the TG scheme.

The first step is based on an observation that a noncentral chi-square with moderate or high noncentrality parameter λ can be well-represented by a power function applied to a Gaussian variable. For "sufficiently large" values of $\widehat{V}_{t_i}$, we write

$$\widehat{V}_{t_{i+1}} = \alpha(\beta + Z)^2.$$

Here and as before, $Z \sim \mathcal{N}(0, 1)$ and α, β some constants, to be determined by moment-matching, depending on Δ, (a, b, c) and $\widehat{V}_{t_i}$.

The above scheme doesn't work well for low values of $\widehat{V}_{t_i}$ (the moment-matching exercise fails to work) : so we supplement it with a scheme to be used for low values of $\widehat{V}_{t_i}$. For this, recall the expression of the probability density function of the standard chi-square distribution with k degrees of freedom :

$$f_{\chi^2(k)}(x) = \frac{x^{k/2-1}e^{-x/2}}{2^{k/2}\Gamma(k/2)}\mathbb{1}_{x>0}.$$

We will approximate the density of $\widehat{V}_{t_{i+1}}$ by

$$\mathbb{P}\left(\widehat{V}_{t_{i+1}} \in [x, x+dx]\right) \approx \left(p\delta_0 + q(1-p)e^{-qx}\right)\, dx, \quad x \geqslant 0,$$

where p and q are non-negative constants to be determined. As in the TG scheme, we have a probability mass at the origin, but now the strength of this mass (p) is explicitly specified, rather than implied from other parameters. The mass at the origin is supplemented with a exponential tail. It can be verified that if $p \in [0,1]$ and $q \geqslant 0$, this expression constitutes a valid density function (non-negative and the integral over $\mathbb{R}$ equals 1).

To sample according this distribution, we integrate in order to obtain a cumulative distribution function:

$$\Psi(x) = \mathbb{P}\left(\widehat{V}_{t_{i+1}} \leqslant x\right) = \left(p + (1-p)\left(1-e^{-qx}\right)\right)\mathbb{1}_{x\geqslant 0}$$

The inverse is computable in a closed way:

$$\Psi^{-1}(u) = \begin{cases} 0 & \text{if } 0 \leqslant u \leqslant p, \\ q^{-1}\ln\left(\frac{1-p}{1-u}\right) & \text{if } p < u \leqslant 1. \end{cases}$$

Consequently, it opens the door to an application of the so-called inverse transform sampling, i.e.

$$\widehat{V}_{t_{i+1}} = \Psi^{-1}(U), \quad U \sim \mathcal{U}([0,1]).$$

Regarding on the computation of α and β, the procedure is impulsed by the following result:

Proposition. *Recall that*

$$\begin{cases} m & := \mathbb{E}[V_{t_{i+1}}|V_{t_i}], \\ s^2 & := \mathrm{Var}(V_{t_{i+1}}|V_{t_i}), \\ \psi & := s^2/m^2 > 0. \end{cases}$$

Provided that $\psi \leqslant 2$, set

$$\beta^2 = 2\psi^{-1} - 1 + \sqrt{2\psi^{-1}}\sqrt{2\psi^{-1}-1} \geqslant 0, \quad \alpha = \frac{m}{1+\beta^2}.$$

With this parametrization, $\widehat{V}_{t_{i+1}}$ is such that $\mathbb{E}[\widehat{V}_{t_{i+1}}] = m$ and $\mathrm{Var}(\widehat{V}_{t_{i+1}}) = s^2$.

Proof. It is (almost) straightforward. In fact, $\widehat{V}_{t_{i+1}}$ is being distributed as a times a non-central chi-square distribution with a degree of freedom $k=1$ and a noncentrality paramater $\lambda = \beta^2$. Therefore by definition

$$\mathbb{E}\left[\widehat{V}_{t_{i+1}}\right] = \alpha(1+\beta^2), \quad \mathrm{Var}\left(\widehat{V}_{t_{i+1}}\right) = 2\alpha^2(1+2\beta^2).$$

Now, set $x = \beta^2$. The system to solve could be rewrite as

$$\begin{cases} \alpha(1+x) & = m \\ 2\alpha^2(1+2x) & = s^2 \end{cases} \iff x^2 + 2x(1-2\psi^{-1}) + 1 - 2\psi^{-1} = 0.$$

The conclusion naturally follows. $\square$

We emphasize that the values of α and β only apply for the case where $\psi \leqslant 2$. For higher values of ψ (corresponding to low values pf $\widehat{V}_{t_i}$), the scheme will fail.

Proposition. *Let m, s and ψ be as defined in the last Proposition. Assume that $\psi \geqslant 1$ and set*

$$p = \frac{\psi-1}{\psi+1} \in [0,1), \quad q = \frac{1-p}{m} = \frac{2}{m(\psi+1)} > 0.$$

With this parametrization, $\widehat{V}_{t_{i+1}}$ is such that $\mathbb{E}[\widehat{V}_{t_{i+1}}] = m$ and $\mathrm{Var}(\widehat{V}_{t_{i+1}}) = s^2$.

Proof. It is clear that

$$\begin{aligned}
\mathbb{E}\left[\widehat{V}_{t_{i+1}}\right] &= \int_0^\infty q(1-p)xe^{-qx}\,dx = (1-p)\left[-xe^{-qx}\right]_0^\infty + (1-p)\int_0^\infty e^{-qx}\,dx = \frac{1-p}{q}\\
\mathbb{E}\left[\widehat{V}_{t_{i+1}}^2\right] &= \int_0^\infty q(1-p)x^2e^{-qx}\,dx = 2(1-p)\int_0^\infty xe^{-qx}\,dx = 2\frac{1-p}{q^2}\\
\mathrm{Var}\left(\widehat{V}_{t_{i+1}}\right) &= \frac{1-p^2}{q^2}
\end{aligned}$$

which leads to the following system

$$\begin{cases} \frac{1-p}{q} &= m \\ \frac{1-p^2}{q^2} &= s^2 \end{cases} \iff (1+\psi)p^2 - 2\psi p + \psi - 1 = 0.$$

The conclusion naturally follows. We stress that for the solution to make sense, we need for p to be non-negative. That is, we must demand $\psi \geqslant 1$.

With the genuine $\psi = \mathrm{Var}\left(V_{t_{i+1}}|V_{t_i} = \widehat{V}_{t_i}\right) \times \mathbb{E}\left[V_{t_{i+1}}|V_{t_i} = \widehat{V}_{t_i}\right]^{-2}$, we have shown that the quadratic sampling scheme can only be moment matched for $\psi \leqslant 2$. On the other hand, the exponential scheme can only be moment matched for $\psi \geqslant 1$. Fortunately, these domains of applicability overlap, such that at lest one of the two schemes can only always be used. A natural procedure is to introduce some critial level $\psi_c \in [1,2]$, and use the quadratic sampling if $\psi \leqslant \psi_c$ and the exponential one otherwise. We use in practice $\psi_c = 1.5$. ☐

On the simulation of $X := \ln S$

I. How <u>not</u> to discretize the process X

Assume first that we have chose, to use the TG scheme as method to choice for the generation of random paths for the variance process V. That is, the advancement of V on the time interval $[t_i, t_i + \Delta]$ takes the form $V_{t_{i+1}} = (\mu + \sigma Z)^+$ where μ and σ are certain moment-matched constants, and $Z \sim \mathcal{N}(0,1)$. Suppose taht we combine this scheme with an Euler scheme in X, but with no need to trcuncate V at 0 :

$$\widehat{X}_{t_{i+1}} = \widehat{X}_{t_i} - \frac{1}{2}\widehat{V}_{t_i}\Delta + \sqrt{\widehat{V}_{t_i}\Delta}\left(\rho Z + \sqrt{1-\rho^2}Z^\perp\right),$$

with $Z^\perp$ another standard Gaussian random variable which is independent from Z.

Notice that the strongly non-linear relationship between $\widehat{V}_{t_{i+1}}$ and Z will imply that the effective correlation between $\widehat{X}_{t_{i+1}}$ and $\widehat{V}_{t_{i+1}}$ will be closer to zero than ρ for the cases where $\mathbb{P}(\mu + \sigma Z < 0)$ is significant, as it would be if $\widehat{V}_{t_i}$ is close to zero. In reality, however, it can be verified that the true correlation between $X_{t_{i+1}}$ and $V_{t_{i+1}}$ (conditioned on V_{t_i} and X_{t_i}) will always be close to ρ, even for large values of Δ and when V_{t_i} is close to the origin.

If one were to nevertheless ignore the problem of "leaking correlation" and insist on using this simulation scheme for the log-spot, at practical levels of Δ one would experience a strong tendency for the Monte Carlo simulation to generate too feeble effective correlation and, consequently, paths of X with poor distribution tails. In call option pricing terms, this would manifest itself in a overvall poor ability to price options away from the money.

II. How to discretize the process X

In light of the problems highlighted in the last part, we don't deal with the naive Euler discretization, and instead turn our focus to an the exact representation. To proceed, note that

$$\begin{aligned}
X_{t_{i+1}} - X_{t_i} &= -\frac{1}{2}\int_{t_i}^{t_{i+1}} V_u\,du + \int_{t_i}^{t_{i+1}} \sqrt{V_u}\,dB_u, \quad dB_u = \rho\,dW_u + \sqrt{1-\rho^2}\,dW_u^\perp\\
V_{t_{i+1}} - V_{t_i} &= a\Delta + b\int_{t_i}^{t_{i+1}} V_u\,du + c\int_{t_i}^{t_{i+1}} \sqrt{V_u}\,dW_u\\
&\iff \int_{t_i}^{t_{i+1}} \sqrt{V_u}\,dW_u = \frac{1}{c}\left(V_{t_{i+1}} - V_{t_i} - a\Delta - b\int_{t_i}^{t_{i+1}} V_u\,du\right)
\end{aligned}$$

Which obviously leads to

$$X_{t_{i+1}} - X_{t_i} = \frac{\rho}{c}\left(V_{t_{i+1}} - V_{t_i} - a\Delta\right) + \left(-\frac{b\rho}{c} - \frac{1}{2}\right)\int_{t_i}^{t_{i+1}} V_u\, du + \sqrt{1-\rho^2}\int_{t_i}^{t_{i+1}} \sqrt{V_u}\, dW_u^{\perp}$$

To use this scheme, we need to consider how to handle the time-integral of V. Rather than using Fourier methods, we here simply write:

$$\int_{t_i}^{t_{i+1}} V_u\, du \approx \Delta\left(\gamma_i V_{t_i} + \gamma_2 V_{t_{i+1}}\right).$$

There are several ways for setting γ_1 and γ_2, the simplest being the Euler-type setting with $\gamma_1 = 1$ and $\gamma_2 = 0$. A central discretization, on the other hand, would set $\gamma_1 = \gamma_2 = 1/2$.

As $V \perp\!\!\!\perp W^{\perp}$,

$$\int_{t_i}^{t_{i+1}} \sqrt{V_u}\, dW_u^{\perp} \bigg| \int_{t_i}^{t_{i+1}} V_u\, du \sim \mathcal{N}\left(0, \int_{t_i}^{t_{i+1}} V_u\, du\right).$$

This yields to the following scheme:

$$\begin{aligned}
\widehat{X}_{t_{i+1}} &= \widehat{X}_{t_i} + \frac{\rho}{c}\left(\widehat{V}_{t_{i+1}} - \widehat{V}_{t_i} - a\Delta\right) + \Delta\left(-\frac{b\rho}{c} - \frac{1}{2}\right)\left(\gamma_1\widehat{V}_{t_i} + \gamma_2\widehat{V}_{t_{i+1}}\right) + \sqrt{\Delta(1-\rho^2)}\sqrt{\gamma_1\widehat{V}_{t_i} + \gamma_2\widehat{V}_{t_{i+1}}}\,Z^{\perp} \\
&= \widehat{X}_{t_i} + K_0 + K_1\widehat{V}_{t_i} + K_2\widehat{V}_{t_{i+1}} + \sqrt{K_3\widehat{V}_{t_i} + K_4\widehat{V}_{t_{i+1}}}\,Z^{\perp}
\end{aligned}$$

with $K_0 = -\frac{a\Delta\rho}{c}$, $K_1 = \gamma_1\Delta\left(-\frac{b\rho}{c} - \frac{1}{2}\right) - \frac{\rho}{c}$, $K_2 = \gamma_2\Delta\left(-\frac{b\rho}{c} - \frac{1}{2}\right) + \frac{\rho}{c}$, $K_3 = \gamma_1\Delta(1-\rho^2)$ and $K_4 = \gamma_2\Delta(1-\rho^2)$.

III. Martingale correction

The above genuine scheme is equivalent to

$$\widehat{S}_{t_{i+1}} = \widehat{S}_{t_i}\exp\left(K_0 + K_1\widehat{V}_{t_i}\right)\exp\left(K_2\widehat{V}_{t_{i+1}} + \sqrt{K_3\widehat{V}_{t_i} + K_4\widehat{V}_{t_{i+1}}}\,Z^{\perp}\right)$$

But in a general setting (and in particular for this scheme)

$$\mathbb{E}\left[S_{t_{i+1}}|S_{t_i}\right] = S_{t_i} < \infty \quad \not\Longrightarrow \quad \mathbb{E}\left[\widehat{S}_{t_{i+1}}|\widehat{S}_{t_i}\right] = \widehat{S}_{t_i}.$$

The practical relevance of this is often minor, as the net drift away from the martingale is typically very small and controllable by reduction of the time step Δ.

Proposition. *Let $K_i, i = 1, \ldots, 4$ be defined as before. Define*

$$M = \mathbb{E}\left[e^{A\widehat{V}_{t_{i+1}}}\Big|\,\widehat{V}_{t_i}\right] > 0, \quad A = K_2 + \frac{1}{2}K_4.$$

If $M < \infty$, then $\mathbb{E}[\widehat{S}_{t_{i+1}}|\widehat{S}_{t_i}] < \infty$. Assuming that M is finite, set

$$K_0^* = -\ln M - \left(K_1 + \frac{1}{2}K_3\right)\widehat{V}_{t_i}$$

and

$$\widehat{X}_{t_{i+1}} = \widehat{X}_{t_i} + K_0^* + K_1\widehat{V}_{t_i} + K_2\widehat{V}_{t_{i+1}} + \sqrt{K_3\widehat{V}_{t_i} + K_4\widehat{V}_{t_{i+1}}}\,Z^{\perp}.$$

In this case, $\mathbb{E}[\widehat{S}_{t_{i+1}}|\widehat{S}_{t_i}] = \widehat{S}_{t_i}$.

Proof. By the tower property of the conditional expectation,

$$
\begin{aligned}
\mathbb{E}[\widehat{S}_{t_{i+1}}|\widehat{S}_{t_i}] &= \mathbb{E}\left[\mathbb{E}[\widehat{S}_{t_{i+1}}|\widehat{S}_{t_i}, \widehat{V}_{t_{i+1}}]\right] \\
&= \widehat{S}_{t_i} e^{K_0^* + K_1 \widehat{V}_{t_i}} \mathbb{E}\left[e^{K_2 \widehat{V}_{t_{i+1}}} \mathbb{E}\left[e^{\sqrt{K_3 \widehat{V}_{t_i} + K_4 \widehat{V}_{t_{i+1}}} Z^{\perp}} \middle| \widehat{S}_{t_i}, \widehat{V}_{t_{i+1}}\right]\right] \\
&= \widehat{S}_{t_i} e^{K_0^* + (K_1 + \frac{1}{2}K_3)\widehat{V}_{t_i}} \mathbb{E}\left[e^{A\widehat{V}_{t_{i+1}}}\right]
\end{aligned}
$$

To conclude, we note that

$$
1 = e^{K_0^* + (K_1 + \frac{1}{2}K_3)\widehat{V}_{t_i}} \mathbb{E}\left[e^{A\widehat{V}_{t_{i+1}}}\right] \quad \Longleftrightarrow \quad K_0^* = -\ln M - \left(K_1 + \frac{1}{2}K_3\right)\widehat{V}_{t_i}
$$

□

To summarize, the martingale corrected scheme involves substituting K_0^* for K_0 in the genuine scheme. As stated in the proposition, we require that M be finite. Assuming that $\gamma_2 \geqslant 0$ (which would always be the case in practice), and $\widehat{V}_{t_{i+1}} \geqslant 0$ (which is always the case with TG and QE schemes), it can be verified that $A \leqslant 0$ for $\rho \leqslant 0$, which in turn shows that : $\rho \leqslant 0 \Longrightarrow M < \infty$. In fact, it is an obviously consequence of the fact that $e^{A\widehat{V}_{t_{i+1}}}$ is bounded to the interval $[0, 1]$.

Proposition. [TG scheme] *Let $\widehat{V}_{t_{i+1}} = (\mu + \sigma Z)^+$. Then, for any values of A, we have*

$$
\mathbb{E}\left[e^{A\widehat{V}_{t_{i+1}}} \middle| \widehat{V}_{t_i}\right] = \exp\left(A\mu + \frac{1}{2}A^2\sigma^2\right)\phi(d_1) + \phi(-d_2),
$$

with $d_1 = \mu/\sigma + A\sigma$ and $d_2 = \mu/\sigma$.
It leads to

$$
K_0^* = -\ln\left(\exp\left(A\mu + \frac{1}{2}A^2\sigma^2\right)\phi(d_1) + \phi(-d_2)\right) - \left(K_1 + \frac{1}{2}K_3\right)\widehat{V}_{t_i}
$$

Proposition. [QE scheme] *Recall that the QE scheme is characterized by the constants (α, β), and (p, q). Also, let $\psi_c \in [1, 2]$ be given. If $\psi \leqslant \psi_c$, then*

$$
\mathbb{E}\left[e^{A\widehat{V}_{t_{i+1}}}|\widehat{V}_{t_i}\right] = \frac{\exp\left(\frac{A\beta^2\alpha}{1-2A\alpha}\right)}{\sqrt{1-2A\alpha}},
$$

where A must satisfy $A < 1/(2\alpha)$. If, on the other hand, $\psi > \psi_c$, then

$$
\mathbb{E}\left[e^{A\widehat{V}_{t_{i+1}}}|\widehat{V}_{t_i}\right] = p + \frac{q(1-p)}{q-A},
$$

provided $A < q$.

Proof. For $\psi \leqslant \psi_c$, we recall that the QE sets $\widehat{V}_{t_{i+1}} = \alpha(\beta + Z)^2$, the distribution of which is a times a noncentral chi-squared distribution with $k = 1$ and $\lambda = \beta^2$. Using the moment-generating function of the noncentral chi-squared distribution, we get the first result of the Proposition. Now, for $\psi > \psi_c$, we have

$$
\mathbb{E}\left[e^{A\widehat{V}_{t_{i+1}}}|\widehat{V}_{t_i}\right] = p + q(1-p)\int_0^{\infty} e^{(A-q)u}\, du = p + \frac{q(1-p)}{q-A}.
$$

□

We emphasize that for the QE scheme the expectation $\mathbb{E}\left[e^{A\widehat{V}_{t_{i+1}}}|\widehat{V}_{t_i}\right]$ doesn't exist for all values of A. It leads to

$$
K_0^* = \begin{cases} -\frac{A\beta^2\alpha}{1-2A\alpha} + \frac{1}{2}\ln(1-2A\alpha) - \left(K_1 + \frac{1}{2}K_3\right)\widehat{V}_{t_i} & \text{if } \psi \leqslant \psi_c \\ -\ln\left(p + \frac{q(1-p)}{q-A}\right) - \left(K_1 + \frac{1}{2}K_3\right)\widehat{V}_{t_i} & \text{if } \psi > \psi_c \end{cases}
$$

Weak second order scheme (Alfonsi)

When $c^2 \leqslant 4a$, the scheme of Ninomiya and Victoir is well dfined and gives a second order scheme. For $c^2 > 4a$, this scheme is no longer defined when the scheme comes near 0. The solution consists in keeping the nonnegativity of the discretization scheme, taking different schemes whether the discretization is in a neighborhood of 0 or not. When $c^2 \leqslant 4a$, the Ninomira-Victoir scheme writes as follows : $\widehat{V}_t = \varphi(V_0, t, \sqrt{t}N)$, $N \sim \mathcal{N}(0,1)$, and

$$\varphi(x,t,w) = e^{\frac{bt}{2}} \left(\sqrt{\left(a - \frac{c^2}{4}\right) \frac{e^{\frac{bt}{2}} - 1}{b} + e^{\frac{bt}{2}} x} + \frac{c}{2} w \right)^2 + \left(a - \frac{c^2}{4}\right) \frac{e^{\frac{bt}{2}} - 1}{b}.$$

When the Feller is violated i.e. $c^2 > 4a$, the scheme is only well-define and positive above the following threshold:

$$\boldsymbol{K}_2(t) := \mathbb{1}_{\{c^2 > 4a\}} e^{-\frac{bt}{2}} \left(\left(\frac{c^2}{4} - a\right) \frac{e^{\frac{bt}{2}} - 1}{b} + \left[\sqrt{e^{-\frac{bt}{2}} \left(\frac{c^2}{4} - a\right) \frac{e^{\frac{bt}{2}} - 1}{b}} + \frac{c}{2}\sqrt{3t} \right]^2 \right)$$

From now on, we turn to the simulation of the CIR near 0, namely on $[0, \boldsymbol{K}_2(t)]$. Near the origin, as soon as $c^2 > 4a$, it does not seem possible to find even a first-order scheme that writes $= \varphi(x, t, \sqrt{t}Y)$ with Y matching the two first moments of a standard Gaussian variable, and that ensures nonnegativity. We therefore have to consider a different kind of scheme when a discretization scheme approaches 0 to keep nonnegativity, as it is also done in the TG(-M)/QE(-M) scheme.

We decide here to take a discrete random variable that matches the two first moments. Namely, we are looking for $\widehat{V}_t$ that takes two possibles values $0 \leqslant x_-(t,x) \leqslant x_+(t,x)$ with respective probabilities $1 - \pi(t,x)$ and $\pi(t,x)$, such that:

$$\begin{cases} \pi(t,x)x_+(t,x) + (1-\pi(t,x))x_-(t,x) & = \tilde{u}_1(t,x) \\ \pi(t,x)x_+(t,x)^2 + (1-\pi(t,x))x_-(t,x)^2 & = \tilde{u}_2(t,x) \end{cases} \quad \text{with} \quad \tilde{u}_q(t,x) := \mathbb{E}\left[\widehat{V}_t \middle| V_0 = x\right], \quad q \in \mathbb{N}.$$

We have seen before that

$$\tilde{u}_1(t,x) = e^{bt}x + a\frac{e^{bt}-1}{b}, \quad \tilde{u}_2(t,x) = \tilde{u}_1(t,x)^2 + c^2\left(e^{bt}\frac{e^{bt}-1}{b}x + \frac{a}{2b^2}\left(e^{bt}-1\right)^2\right)$$

Now, define $\gamma_\pm(t,x) := \frac{x_\pm(t,x)}{\tilde{u}_1(t,x)}$. It leads to the following system

$$\begin{cases} \pi(t,x)\gamma_+(t,x) + (1-\pi(t,x))\gamma_-(t,x) & = 1 \\ \pi(t,x)\gamma_+(t,x)^2 + (1-\pi(t,x))\gamma_-(t,x)^2 & = \frac{\tilde{u}_2(t,x)}{\tilde{u}_1(t,x)^2} \end{cases}$$

We arbitrarily take $\gamma_+(t,x) = \frac{1}{2\pi(t,x)}$ and $\gamma_-(t,x) = \frac{1}{2(1-\pi(t,x))}$, which ensures that the first equation is satisfied. For the second one, it recast to the following

$$\pi^2(t,x) - \pi(t,x) + \frac{\tilde{u}_1(t,x)^2}{4\tilde{u}_2(t,x)} = 0,$$

which obviously yields

$$\pi(t,x) = \frac{1 - \sqrt{1 - \frac{\tilde{u}_1(t,x)^2}{\tilde{u}_2(t,x)}}}{2},$$

since we want $\gamma_+ > \gamma_-$. Note that the discriminant $\Delta(t,x) \in [0,1]$ in both cases. We have thus $0 \leqslant \pi(t,x) \leqslant \frac{1}{2}$. Besides, we have $\frac{\tilde{u}_2(t,x)}{\tilde{u}_1(t,x)^2} \leqslant 1 + \frac{c^2}{a}$. Therefore, $\Delta(t,x) \geqslant 1 - \frac{1}{1+\frac{c^2}{a}}$, and we get $0 < \pi_{\min} := \frac{1-\sqrt{1-\frac{1}{1+\frac{c^2}{a}}}}{2} \leqslant$

$\pi(t,x) \leqslant \frac{1}{2}$. Since $\boldsymbol{K}_2(t) \underset{t\to 0}{\sim} \left[\frac{1}{2}\left(\frac{c^2}{4}-a\right) + \left(\sqrt{\frac{1}{2}\left(\frac{c^2}{4}-a\right)} + \frac{c}{2}\sqrt{3}\right)^2\right] t$, there exists $C = C(a,b,c) > 0$ s.t. $\widetilde{u}_1(t,x) \leqslant Ct$ for $x \in [0, \boldsymbol{K}_2(t)]$ and $t \leqslant 1$. Therefore, one should consider the following scheme

$$\widehat{V}_t = \mathbb{1}_{\{U \leqslant \pi(t,x)\}} \frac{\widetilde{u}_1(t,x)}{2\pi(t,x)} + \mathbb{1}_{U > \pi(t,x)} \frac{\widetilde{u}_1(t,x)}{2(1-\pi(t,x))}, \quad U \sim \mathcal{U}([0,1]).$$

If $x \geqslant \boldsymbol{K}_2(t)$, we make the update $x \leftarrow \varphi(x, t, \sqrt{t}Y)$, with Y the discrete random variable such that $\mathbb{P}(Y = \sqrt{3}) = \mathbb{P}(Y = -\sqrt{3}) = \frac{1}{6}$ and $\mathbb{P}(Y = 0) = \frac{2}{3}$, which fits the five firsts moments of the standard Gaussian. This latter could be straightforwardly sampled using an uniform random variable u :

```
def sample_Y(u) :
    if u < 1.0/6.0 :
        return −√3
    else if u < 5.0/6.0 :
        return 0
    else :
        return √3
```