OPTIMAL STRATEGY FOR PREPAYMENT OF MORTGAGES

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OPTIMAL STRATEGY FOR PREPAYMENT OF MORTGAGES

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We study a borrower's optimal strategies to terminate a mortgage with a fixed interest rate by paying the outstanding balance all at once. The problem is modelled as a free boundary problem for a Black-Scholes type pricing equation under the assumption of the Vasicek model for the short rate of investment. Here the free boundary provides the optimal time at which the mortgage contract is to be terminated. A number of integral identities are derived and then used to design efficient numerical codes for computing the free boundary. For numerical simulation, parameters for the Vasicek model are estimated via the method of maximum likelihood estimate using 40 years of data from US government bonds. The asymptotic behavior of the free boundary for the infinite horizon is fully analyzed. Interpolating this infinite horizon behavior and a known near expiry behavior, two simple analytical approximation formulas for the optimal exercise boundary are proposed. Numerical evidence shows that the enhanced version of the approximation formula is amazingly accurate; in general, its relative error is less than 1%, for all time before expiry.

TABLE OF CONTENTS

LIST OF FIGURES

PREFACE

This dissertation is an achievement of the efforts and contributions of many people I am sincerely grateful for. I am deeply indebted to all those who have supported my research and have given me encouragement from various aspects and at various stages.

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1.0 INTRODUCTION

We consider a mortgage contract with a given maturity and a fixed mortgage interest rate, where the borrower has the right to terminate the contract prematurely by paying off the outstanding loan all at once. It is of interest to investigate this contract from the perspectives both of the borrower and of the bank.

Suppose the borrower always has a sufficient amount of money to settle the outstanding loan balance, then the optimal decision at any time, from the borrower's point of view, depends on the how much return can be earned if an equal amount of money be invested in the financial market, whose yield follows the assumed interest rate model. On the other hand, the bank may, for many good reasons, want to know the fair price of such a contract. Standard option pricing theory tells us that we must discount all future cash inflow to the bank by a discount factor determined by the future movement of risk-free rate. However, the future cash inflow to the bank is complicated by the fact that the time of prepayment from the borrower is not yet explicitly known. So the value of the contract must be solved simultaneously with the consideration of the early termination.

Suppose the mortgage contract under consideration has a duration T (years) and a fixed mortgage interest rate c (year^{-1}). At any time t during the term of the mortgage, the outstanding balance owed, $M(t)$, is reduced in the time period $[t, t+dt)$ by

$$dM(t) = cM(t)dt - mdt \quad \forall t \leqslant T$$

where $cM(t)dt$ is the interest accrued on the balance and mdt is the payment resulting from a constant continuous rate of payment of m (\$/year). In order that the mortgage be retired at $t = T$, the condition $M(T) = 0$ applies so that

$$M(t) = \frac{m}{c}\Big\{1 - e^{c(t-T)}\Big\}.$$

In this contract, the borrower is allowed to terminate the contract at any time t ($t < T$) of his choice by paying a lump sum $M(t)$ to the contract issuer.

This decision for the borrower to terminate the contract depends on the alternate investment strategy available to him. Assume for simplicity that the borrower has sufficient funds, say from an unexpected windfall, a valuable collateral, or an arrangement from a financial institution, to pay back the outstanding balance at any time. Then at any moment while the contact is in effect, the decision of the borrower on whether to terminate the contract depends on the rate of (short term) return that an investment can yield on the financial market. In this paper, we shall use the Vasicek model [13] for this short term market return rate, r_t, described by the stochastic differential equation

$$dr_t = k(\theta - r_t)dt + \sigma\, dW_t$$

where k, θ, and σ are assumed to be positive known constants and W_t is the standard Wiener process. Here the units for k, θ, σ, and W_t are year^{-1}, year^{-1}, year$^{-3/2}$ and year$^{1/2}$ respectively. To address the fact that the Vasicek model is not sufficient to describe the whole term structure, here we assume for simplicity that in this model the market price of risk has been incorporated into the drift $k(\theta - r_t)$; that is to say, the probability associated with the Brownian motion $\{W_t\}$ is the risk-neutral probability; see, for example, the mathematical finance books [1, 14].

Intuitively if an overall market return rate is expected to be low (relative to c) for a certain amount of time, one should choose to terminate the contract early. On the other hand, if the market return rate is strictly larger than c or if an overall market return rate is expected to be higher than c for a certain amount of time, one should choose to defer the closing date by an investment in the market of the capital $M(t)$ less the obligatory payment of m per unit time. Hence, at every moment that the contract is in effect the borrower must monitor the market return rate and decide whether to immediately close the contract. Statistically, there is an optimal strategy in making such a decision.

To find such a strategy, we introduce a function $V(r,t)$ being the (expected) value of the contract at time t and current market return rate $r_t = r$. This value can be regarded as an asset that the contract issuer (the mortgage company) possesses, or a fair price that a buyer would offer to the contract issuer in taking over the contract, say, in an issuer's restructuring or liquidation process. The value V is calculated according to the borrower's optimal decision; i.e. the issuer is a passive player. Since the borrower can terminate the contract by paying $M(t)$ at any time t, we have

$$0 \leqslant V(r,t) \leqslant M(t) \qquad \forall r \in \mathbb{R},\ t \leqslant T.$$

This automatically implies that $V(r,T) = 0$ for all r.

According to general mathematical finance theory, for every $r \in \mathbb{R}$ and $t < T$, we have

$$V(r,t) = \min\{M(t), \quad V(r,t) + [LV(r,t) + m]dt\} \tag{1.0.1}$$

where

$$LV(r,t) = \frac{\partial V(r,t)}{\partial t} + \frac{\sigma^2}{2}\frac{\partial^2 V(r,t)}{\partial r^2} + k(\theta - r)\frac{\partial V(r,t)}{\partial r} - rV(r,t) \tag{1.0.2}$$

Thus V is the solution to the variational inequality

$$0 = \min\{M(t) - V(r,t), \quad LV(r,t) + m\}, \quad 0 \leqslant V(r,t), \quad \forall r \in \mathbb{R}, \quad t \leqslant T \tag{1.0.3}$$

Using a classical method, such as that used in [3] for an American put option, it is easy to show that the above variational problem admits a unique solution and the solution has bounded derivatives V_{rr} and V_t . With this regularity, one can construct a delta hedging portfolio (using zero coupon bonds of various maturities) to replicate the mortgage contract and to conclude that at any time t ($t \leqslant T$) and spot rate $r_t = r$, the value of the mortgage contract is $V(r,t)$. In addition, one can show, by a comparison principle, we see that $V_r(r,t) \leqslant 0$ for all $r \in \mathbb{R}, t \leqslant T$. Therefore, there is a function $R(\cdot) : (-\infty, T) \to [-\infty, \infty)$ such that for each $t < T$,

$$V(r,t) < M(t) \quad \Longleftrightarrow \quad r > R(t). \tag{1.0.4}$$

We call $r = R(t)$ the **optimal boundary of mortgage contract termination**. That is,

> *the best strategy for the borrower is to terminate the mortgage contract at the first time that the spot market return rate r_t is below $R(t)$.*

One can further show that $R(T-) = c$, $R'(t) \geqslant 0$ for all $t < T$, and $R(-\infty) > -\infty$. Hence, (R, V) solves the following free boundary problem:

$$\begin{cases} \dfrac{\partial V}{\partial t} + \dfrac{\sigma^2}{2}\dfrac{\partial^2 V}{\partial r^2} + k(\theta - r)\dfrac{\partial V}{\partial r} - rV + m = 0 < M(t) - V(r,t) & \text{if } \ r > R(t), t < T, \\ 0 \leqslant V((R(t), t) = M(t), \quad V_r(R(t), t) = 0, & \forall\, t \leqslant T, \\ V(r,T) = 0, & \forall\ r \geqslant R(T) = c. \end{cases} \tag{1.0.5}$$

Once a solution of this free boundary problem is found, a solution of the variational inequality problem can be obtained by extending V to $\mathbb{R} \times (-\infty, T]$ by setting $V(r,t) = M(t)$ for every $r < R(t)$ and $t \leqslant T$.

In the following Figure 1, we provide a graphic illustration of the problem and the optimal strategy that the mortgage borrower should follow.

Similar problems have been studied from option-theoretical viewpoint by Buser & Hendershott [2], Epperson, Kau, Keenan, & Muller [4, 9, 10], Pozdena & Iben [12], Kau & Keenan [8], etc. The mathematical formulation for problem (1.0.5) has been carried out by Bian, Jiang, and Yi [7]; see also relevant mathematical work by Yuan, Jiang and Luo [15]. In [7], the authors proved that the problem is well-posed; namely problem (1.0.5) admits a unique solution which is smooth up to to the free boundary $r = R(t)$. Also, the free boundary $R(\cdot)$ is a smooth function strictly increasing on $(-\infty, T)$, and has the asymptotic behavior

$$R(t) \sim c - \sigma\bar{\kappa}\sqrt{T-t} \qquad \text{as } t \nearrow T, \qquad \bar{\kappa} = 0.47386... \tag{1.0.6}$$

In this work we shall mainly consider numerical aspects of this problem. But intensive mathematical analysis has also been used to derive the delicate natures of the prepayment boundary. In the course of the study, we shall provide an analytical solution to the infinite horizon problem and show that

$$R(t) \sim R^* + \rho^* e^{-c(T-t)} \text{ as } t \to -\infty \tag{1.0.7}$$

where R^* and ρ^* are constants that can be easily calculated by solving an algebraic equation involving Hermite functions. Based on the existing near expiry behavior (1.0.6) and our new long term behavior (1.0.7), we provide two global approximations. For all $t \leqslant T$,

$$\begin{aligned} R(t) \approx R_I(t) &:= c - (c - R^*)\sqrt{1 - e^{-b^*(T-t)}}, \qquad b^* := \left(\frac{0.474\sigma}{c - R^*}\right)^2, \\ R(t) \approx R_{II}(t) &:= c - \frac{0.474\sigma}{\sqrt{2c}}\sqrt{1 - e^{-2c(T-t)}} + \rho^*\left[e^{-c(T-t)} - 1\right] \\ &\quad + \left[R^* - c + \frac{0.474\sigma}{\sqrt{2c}} + \rho^*\right]\left[1 - e^{-2c(T-t)}\right]. \end{aligned}$$

We shall numerically demonstrate that these approximations are very accurate. In the special case when typical US economy parameters are used, we have

$$\max_{t \leqslant T} \frac{|R(t) - R_I(t)|}{R(T) - R(-\infty)} \leqslant 2\%, \qquad \frac{\max_{t \leq T} |R(t) - R_{II}(t)|}{R(T) - R(-\infty)} < 0.4\%.$$

Here $R(T) - R(-\infty) = c - R^*$ is the total oscillation of $R(\cdot)$ on $(-\infty, T]$.

In Chapter 2 we use the statistical procedure of Maximum Likelihood Estimation (MLE) to determine reasonable values for the parameters k, θ and σ appearing in the

Vasicek model to be used for the stochastic market rate of return. Without knowledge of the market price of risk, we can only speculate that these values should be in the vicinity of those values that incorporate the market price of risk. In Chapter 3, we make a series of transformations of variables to reduce problem (1.0.5) to a simpler version in terms of the heat equation. Chapter 4 develops integral identities that will be used in Chapter 5 to obtain fast and accurate numerical schemes based on Newton's method. Estimates for the asymptotic behavior of the termination boundary near and far from expiry of the mortgage are obtained in Chapter 6 and Chapter 7 respectively. These are combined in Chapter 8 to obtain the simple global estimates mentioned above. In Chapter 9 we provide numerical results as well as various important aspects pertaining to our theoretical and numerical claims. In the Appendix, we derived the Fundamental Solution to the problem. While change of variables is an effective way for the theoretical analysis, as it transforms a complicated system into a heat equation, the Fundamental Solution can be very useful and direct in numerical computation.

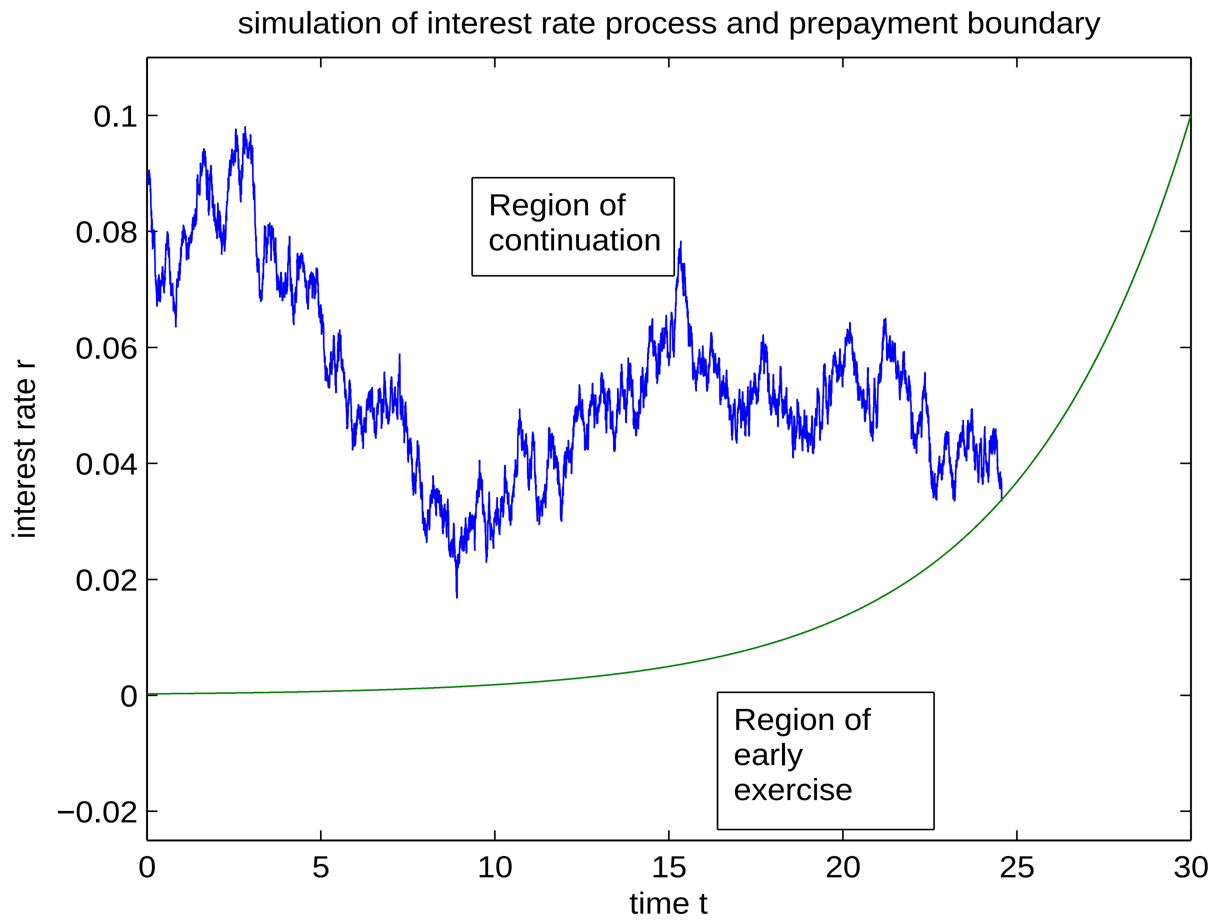

Figure 1: This is a graphic illustration of the problem. The smooth curve representsthe theoretically optimal prepayment boundary for the mortgage borrower. The jagged curveis one simulated path of the interest process. At each moment, theborrower needs to compare the real market interest rate and the theoretically computed optimal rate.When the market interest rate is relatively higher, it is not in his best interest to make prepayment.Rather, he should invest in the market in this case. On the other hand, when the market interest is belowthe optimal prepayment boundary, he should pay off the loan balance.

2.0 INTEREST RATE MODEL AND PARAMETER ESTIMATION

2.1 THE MODEL

In the Vasicek model [13] for the behavior of the rate of return of, say a US government bond, the yield r_t at time t is treated as a Markov process, governed by the stochastic differential equation

$$dr_t = k(\theta - r_t)dt + \sigma dW_t$$

where k, θ, and σ are positive parameters and $\{W_t\}$ is the standard Wiener (Brownian) process.

The Vasicek model is one of the most well-known and widely used models for interest rate and the pricing of its derivatives. It is composed of one deterministic term and one random term. The deterministic term (also "the drift term") is chosen to produce the so called "mean-reverting" property. And the random term is to model the volatility caused by (infinite) unpredictable factors. Specifically, θ is the long term mean of the spot interest rate, σ is the instantaneous standard deviation, and k is the speed measuring how fast the process will be reverted back to the mean once it evolves away from the mean.

Besides these nice physical features, the Vasicek model is also very tractable from mathematical point of view. Suppose we know the interest rate at time τ is r_τ , and the interest process is governed by the Vasicek model. Using integrating factor method, one can solve the stochastic differential equation

$$dr_t = k(\theta - r_t)dt + \sigma dW_t \tag{2.1.1}$$

and get the explicit (stochastic) solution for the interest rate at any time $t > \tau$.

$$r_t = \theta + e^{-k(t-\tau)}(r_\tau - \theta) + \sigma \int_\tau^t e^{-k(t-\tau-u)} dW_u \tag{2.1.2}$$

A standard theory in stochastic calculus tells us that r_t is a Gaussian process with mean

$$\text{Mean}[r_t|r_\tau] = \theta + e^{-k(t-\tau)}(r_\tau - \theta) \tag{2.1.3}$$

and variance

$$\text{Variance}[r_t|r_\tau] = \frac{\sigma^2}{2k}(1 - e^{-2k(t-\tau)}) \tag{2.1.4}$$

Since r_t is a normal distribution, the first two moments given in (2.1.3) and (2.1.4) are sufficient to determine the the probability density function of the process. Starting from an initial rate $r_\tau = x$, at a later time t ($t > \tau$), the probability density p for the rate r_t to be equal to y is given by

$$\begin{aligned} p(\tau, x; t, y) &:= \frac{\text{Probability } (r_\tau = x, r_t \in (y, y + dy)\ )}{dy} \\ &= \sqrt{\frac{k}{\pi\sigma^2(1 - e^{-2k(t-\tau)})}} \exp\Big(- \frac{k[(y-\theta) - (x-\theta)e^{-k(t-\tau)}]^2}{\sigma^2(1 - e^{-2k(t-\tau)})}\Big). \end{aligned}$$

Instead of using the first two moments and Guassian property of the process, one can also use the Kolmogorov forward equation to derive the probability density function. Let

$s = t - \tau$, From the Kolmogorov forward equation, we have that the probability density for r_t in the Vasicek model satisfies

$$\begin{cases} \dfrac{\partial p}{\partial s} = \dfrac{\sigma^2}{2}\dfrac{\partial^2 p}{\partial y^2} - \dfrac{\partial}{\partial y}[k(\theta - y)p], \\ \\ p(\tau, x; \tau+, y) = \delta(x - y). \end{cases}$$

This PDE can be solved using the Fourier transform method. The details of derivation of the solution are omitted here. However, In the Appendix, I have used the same method to solve for the Fundamental Solution of the mortgage contract value, which can be seen as a derivative of interest rate process. That PDE is similar to this one but more difficult since it has one extra term.

2.2 MAXIMUM LIKELIHOOD ESTIMATION

To determine the numerical values of the parameters k, θ, σ in the Vasicek model, we use the method of maximum likelihood. This is possible because, as introduced in previous section, the transitional probability density function of the process is explicitly solved.

Let $\{(\tau_i, x_i, t_i, y_i)\}_{i=1}^n$ be a collection of sample data where $x_i = r_{\tau_i}$, $y_i = r_{t_i}$, and $t_i > \tau_i$ for all i. Assume that the time increment $\Delta t := t_i - \tau_i$ is independent of i and that the intervals $\{[\tau_i, \tau_i + \Delta t)\}_{i=1}^n$ are non-overlapping. Using

$$d(e^{-kt}(r_t - \theta)) = \sigma e^{-kt} dW_t$$

we can show that $\{(y_i - \theta) - (x_i - \theta)e^{-k\Delta t}\}_{i=1}^n$ are i.i.d random variables. Hence, we can define the maximum likelihood function

$$\Phi(k, \theta, \sigma) := \prod_{i=1}^n p(0, x_i; \Delta t, y_i).$$

Consequently, the maximum likelihood estimators (MLE) for k, θ, σ are defined as the maximizer of the function Φ. This results in the algebraic system

$$\begin{cases} \dfrac{\partial \Phi(k,\theta,\sigma)}{\partial k} = 0, \\[2ex] \dfrac{\partial \Phi(k,\theta,\sigma)}{\partial \theta} = 0, \\[2ex] \dfrac{\partial \Phi(k,\theta,\sigma)}{\partial \sigma} = 0. \end{cases}$$

To simplify the system, we use the change of variables

$$\begin{gathered} b = e^{-k\Delta t}, \qquad a = \sigma^2(1-\beta^2)/k, \qquad \theta = \theta, \\ \Psi(a,b,\theta) = \ln(\sqrt{\pi}\Phi) = -\tfrac{n}{2}\ln a - \tfrac{1}{a}\textstyle\sum_{i=1}^{n}[(y_i-\theta)-(x_i-\theta)b]^2. \end{gathered}$$

Then the system $\nabla_{k,\theta,\sigma}\Phi = (0,0,0)$ is equivalent to $\nabla_{b,\theta,a}\Psi = (0,0,0)$. This provides the algebraic system

$$\begin{cases} \dfrac{1}{a}\displaystyle\sum_{i=1}^{n}[(y_i-\theta)-b(x_i-\theta)] = 0, \\[2ex] \dfrac{1}{a}\displaystyle\sum_{i=1}^{n}[(y_i-\theta)-b(x_i-\theta)](x_i-\theta) = 0, \\[2ex] -\dfrac{n}{2a} + \dfrac{1}{a^2}\displaystyle\sum_{i=1}^{n}[(y_i-\theta)-b(x_i-\theta)]^2 = 0. \end{cases}$$

Introduce the random variables $X = (x_1, \cdots, x_n)$, $Y = (y_1, \cdots, y_n)$ and their statistics

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} x_i, \tag{2.2.1}$$

$$\bar{Y} = \frac{1}{n}\sum_{i=1}^{n} y_i, \tag{2.2.2}$$

$$\mathrm{Cov}[X, Y] = \frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{Y})(x_i - \bar{X}), \tag{2.2.3}$$

$$\mathrm{Cov}[X, X] = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{X})^2, \tag{2.2.4}$$

$$\mathrm{Cov}[Y, Y] = \frac{1}{n-1}\sum_{i=1}^{n}(Y_i - \bar{Y})^2. \tag{2.2.5}$$

Then solving the equations for a, b, θ and transforming back to k, θ, σ we obtain the following statistics for the maximum likelihood estimators, also known as the MLEs,

$$b = \frac{\mathrm{Cov}[X, Y]}{\mathrm{Cov}[X, X]},$$

$$k = -\frac{1}{\Delta t}\log b,$$

$$\theta = \frac{\bar{Y} - b\bar{X}}{1 - b},$$

$$\sigma^2 = 2k\,\frac{n-1}{n}\,\frac{\mathrm{Cov}[Y, Y] - b^2\mathrm{Cov}[X, X]}{1 - b^2}.$$

2.3 AN EMPIRICAL EXPERIMENT ON US BONDS

Now suppose we have a list $\{(\tau_i, r_i)\}_{i=0}^n$ of rates of return r_i at time τ_i. Assume that all $\tau_{i+1} - \tau_i$ are positive and equal. Then we can take

$$\Delta t = \tau_{i+1} - \tau_i, \qquad X = (r_0, \cdots, r_{n-1}), \qquad Y = (r_1, \cdots, r_n)$$

and use these data to estimate the parameters k, θ, and σ in the Vasicek model using the formulas derived in the previous section.

The following Table (Figure 2) is a summary of the MLEs we did for the Vasicek model, one for a 13 week US Treasury Bill and the other for a 10 year US Treasury Note. We use three different time intervals $\Delta t = t_{i+1} - t_i$: daily, weekly, and monthly. (We assume, as usual, that the weekend is approximately equivalent to a single trading day.) We calculated these data using 10, 20, 30, 40 year periods. One can see that within the same period, say from 1996 to 2006, the MLEs obtained by using the daily data, or the weekly data or the monthly data are basically the same. This is part of the evidence that MLEs provide reasonable estimates for the parameters we are using for our problem.

We would like to remark that the MLEs are not necessarily unbiased. Assume that k and $b = e^{-k\Delta t}$ are known. Then $Z = \{z_i := r_{\tau_i+\Delta t} - br_{\tau_i}\}$ are i.i.d. random variables, normally distributed with mean $(1-b)\theta$ and variance $\sigma^2(1-b^2)/(2k)$, so

$$\bar{\theta} := \frac{\bar{Z}}{1-b} = \frac{\sum_{i=1}^n z_i}{n(1-b)} := \frac{\bar{Y} - b\bar{X}}{1-b}, \tag{2.3.1}$$

$$\bar{\sigma}^2 := \frac{2k}{1-b^2}\mathrm{Cov}[Z, Z] = \frac{2k}{1-b^2}\mathrm{Cov}[Y - bX, Y - bX] \tag{2.3.2}$$

are unbiased statistics for θ and σ. This is demonstrated by the fact that the parameters σ and θ in Figure 2 are quite stable, namely, not very sensitive to the method of sampling.

To estimate b, note that $\{z_i := y_i - bx_i\}$ being i.i.d random variables can be interpreted as saying that b is the best linear indicator between $Y = (y_1, \cdots, y_n)$ and $X = (x_1, \cdots, x_n)$ so we have a reasonable estimator

$$e^{-\bar{k}\Delta t} = \bar{b} = \frac{\text{Cov}[Y, X]}{\text{Cov}[X, X]} = 1 - \frac{\text{Cov}[Y - X, X]}{\text{Cov}[X, X]}.$$

Here since $\tau_{i+1} = \tau_i + \Delta t$, i.e., $y_i = x_{i+1}$, the distribution of $\bar{b}$ is quite complicated. For the moment, we do not know if $\bar{b}$ is unbiased. There is an extensive statistical literature dealing with the issues of biased estimations. Since this is not the main topic in this work, we will not elaborate further.

To give an idea of the interest rate evolution under the Vasicek model, we provide a simulation using the the typical parameters values θ=0.05, k=0.2, σ=0.015. Please see the following Figure 3.

13 week Treasury Bill

From to	sample	mean	StdDev	k	theta	sigma
1996--2006	daily	0.035	0.017	0.101	0.032	0.007
1996--2006	weekly	0.035	0.017	0.119	0.032	0.008
1996--2006	monthly	0.036	0.017	0.100	0.033	0.007
1986--2006	daily	0.045	0.019	0.108	0.039	0.008
1986--2006	weekly	0.045	0.019	0.120	0.040	0.009
1986--2006	monthly	0.045	0.019	0.103	0.039	0.008
1976--2006	daily	0.060	0.031	0.148	0.058	0.017
1976--2006	weekly	0.060	0.031	0.169	0.059	0.018
1976--2006	monthly	0.060	0.031	0.177	0.059	0.018
1966--2006	daily	0.059	0.028	0.178	0.059	0.017
1966--2006	weekly	0.059	0.028	0.208	0.059	0.018
1966--2006	monthly	0.059	0.028	0.229	0.059	0.019

10 year Treasury Note

From to	sample	mean	StdDev	k	theta	sigma
1996--2006	daily	0.051	0.009	0.731	0.049	0.009
1996--2006	weekly	0.051	0.009	0.769	0.049	0.009
1996--2006	monthly	0.051	0.009	0.707	0.049	0.009
1986--2006	daily	0.063	0.016	0.188	0.057	0.010
1986--2006	weekly	0.063	0.016	0.198	0.058	0.010
1986--2006	monthly	0.063	0.016	0.196	0.057	0.010
1976--2006	daily	0.077	0.027	0.091	0.067	0.013
1976--2006	weekly	0.077	0.027	0.098	0.068	0.013
1976--2006	monthly	0.077	0.027	0.108	0.069	0.014
1966--2006	daily	0.074	0.025	0.109	0.075	0.011
1966--2006	weekly	0.075	0.025	0.117	0.075	0.012
1966--2006	monthly	0.075	0.025	0.134	0.075	0.013

Figure 2: Summary of the yields for USA Government Bonds and the corresponding maximum likelihood estimators for the parameters in the Vasicek model. Where"mean" and "StdDev" represent the mean and standard deviation of the yield, measured in annual units.

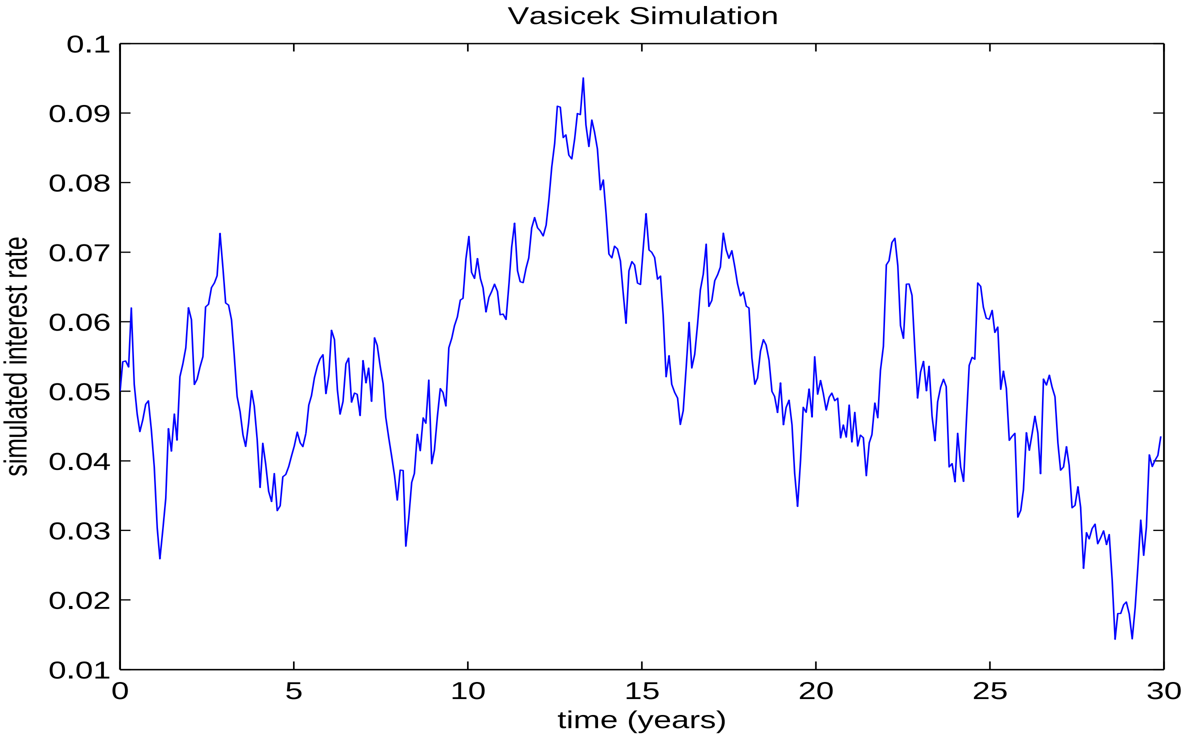

Figure 3: A sample path of interest rate simulation based on Vasicek model. For this particular simulation, we used θ=0.05, k=0.2, σ=0.015, r_0=0.05, $dt = 1/12$ years.

3.0 TRANSFORMATION

In this chapter, we shall make certain transformations to simplify the mathematical analysis of the equation for V; namely, we transfer the Black–Scholes type equation under investigation into a heat equation. For simplicity, we shall use subscripts to denote partial derivatives. These transformations are naturally suggested by the terms in the Fundamental Solution of the original PDE, which is derived in the Appendix.

3.1 REFORMULATION OF THE CONTRACT VALUE

We propose the following new variables

$$\tau := T - t, \tag{3.1.1}$$

$$\psi(r, \tau) := \frac{c}{m}\Big\{M(t) - V(r, t)\Big\}. \tag{3.1.2}$$

First note that τ is the time to expiry. This is convenient because we always know the value of the contract, early terminated or not, must have value zero at expiry. Secondly, note that ψ is a dimensionless quantity measuring the advantage of deferring termination. $M(t) - V(r, t)$ represents the amount of premium loss if the contract is closed at the current time t and market rate r and if, according to our theoretical result, it is actually not optimal to do so. Multiplying by the ratio c/m is nonessential in terms of financial interpretation, but is convenient for mathematical analysis.

In the new variables, (1.0.5) is equivalent to

$$\begin{cases} \psi_\tau - \frac{\sigma^2}{2}\psi_{rr} - k(\theta - r)\psi_r + r\psi = (r-c)(1-e^{-c\tau}) & \text{if } \psi(r,\tau) > 0, \tau > 0, \\ 0 \leqslant \psi(r,\tau) \leqslant 1 - e^{-c\tau} & \forall\, \tau \geqslant 0, r \in \mathbb{R}. \end{cases}$$

We remark that the constraint $\psi(r,\tau) \leqslant 1 - e^{-c\tau}$ on the upper bound, which corresponds to the original constraint $V \geqslant 0$, is not needed, since one can show that $1 - e^{-c\tau}$ is a super-solution so that by comparison

$$\psi(r,\tau) < 1 - e^{-c\tau} \qquad \forall\, r \in \mathbb{R}, \tau > 0.$$

Also, differentiating in r one sees that

$$\Big\{\frac{\partial}{\partial \tau} - \frac{\sigma^2}{2}\frac{\partial^2}{\partial r^2} - k(\theta - r)\frac{\partial}{\partial r} + (r+k)\Big\}\psi_r = 1 - e^{-c\tau} - \psi \geqslant 0 \qquad \text{if } \psi > 0.$$

The maximum principle then implies that $\psi_r(r,t) \geqslant 0$ for all $r \in \mathbb{R}, \tau \geqslant 0$. Therefore, there exists a function $R : (-\infty, T) \to [-\infty, \infty)$ such that for each $\tau > 0$,

$$\psi(r,\tau) > 0 \qquad \Longleftrightarrow \qquad r > R(T-\tau).$$

This is an equivalent way of stating (1.0.4).

3.2 DEPENDENT VARIABLE CHANGE

Let $h = h(r,\tau)$ be a function to be determined shortly. We make the change of variables for the unknown function ψ by

$$\phi(r,\tau) := e^{-h(r,\tau)}\psi(r,\tau).$$

Then the constraint for ψ becomes the constraint $\phi \geqslant 0$ for ϕ. When $\phi > 0$ we have $\psi > 0$ and the differential equation for ψ is transformed to the following differential equation for ϕ:

$$\phi_\tau - \tfrac{\sigma^2}{2}\phi_{rr} - [\sigma^2 h_r + k(\theta - r)]\phi_r + q\phi = (r-c)(1-e^{-c\tau})e^{-h}$$

where

$$q := h_\tau - \tfrac{\sigma^2}{2}h_{rr} - h_r\{\tfrac{\sigma^2}{2}h_r + k(\theta - r)\} + r.$$

We want to find a special h such that $q \equiv 0$. To this end we choose

$$h(r,\tau) \quad = \quad \frac{k}{\sigma^2}\Big(r + \frac{\sigma^2}{2k^2} - \theta\Big)^2 + \Big(k + \frac{\sigma^2}{2k^2} - \theta\Big)\tau.$$

The equation for ϕ becomes

$$\begin{cases} \phi_\tau - \tfrac{\sigma^2}{2}\phi_{rr} - \{kr + \tfrac{\sigma^2}{k} - k\theta\}\phi_r = (r-c)(1-e^{-c\tau})e^{-h} & \text{if } \ \phi > 0, \\ \\ \phi(r,\tau) \geqslant 0 = \phi(r,0) \quad \forall\, r \in \mathbb{R}, \tau > 0. \end{cases}$$

3.3 INDEPENDENT VARIABLE CHANGE

Finally, we make the change of variables

$$
\begin{aligned}
x &= \frac{k^{1/2}e^{k\tau}}{\sigma}\Big[r + \frac{\sigma^2}{k^2} - \theta\Big],\\
s &= e^{2k\tau},\\
u(x,s) &= \frac{2\sqrt{\pi}k^{3/2}}{\sigma}\phi(r,\tau).
\end{aligned}
$$

Then the system for ϕ becomes

$$
\begin{cases}
u_s - \frac{1}{4}\,u_{xx} = f(x,s) & \text{if } \ u(x,s) > 0, s > 1,\\
\\
u(x,s) \geqslant 0 = u(x,1) & \forall\, s > 1, x \in \mathbb{R}
\end{cases}
\tag{3.3.1}
$$

where

$$
\begin{aligned}
f(x,s) &= \frac{\sqrt{\pi}k^{1/2}}{\sigma}(r-c)(1-e^{-c\tau})e^{-2k\tau-h}\\
&= \sqrt{\pi}\Big(\frac{x}{\sqrt{s}} - \frac{k^2(c-\theta)+\sigma^2}{\sigma k^{3/2}}\Big)(1-s^{-c/(2k)})s^{\theta/(2k)-3/2-\sigma^2/(4k^2)}e^{-[x/\sqrt{s}-\sigma/(2k^{3/2})]^2}.
\end{aligned}
$$

For the system (3.3.1) to be well-posed, it is necessary to write the system for $u = u(x,s)$ as

$$
\begin{cases}
\min\Big\{u, \quad u_s - \frac{1}{4}u_{xx} - f\ \Big\} = 0 & \text{in } \ \mathbb{R}\times(1,\infty),\\
\\
u(x,1) = 0 \quad \forall x \in \mathbb{R}.
\end{cases}
\tag{3.3.2}
$$

Note that f can be written as

$$
f(x,s) = \sqrt{\pi}(s^\gamma - 1)s^{-\nu-1}(x-\beta\sqrt{s})e^{-(\frac{x}{\sqrt{s}}-\alpha)^2},
$$

where α, β, γ, and ν are dimensionless constants given by

$$
\alpha := \frac{\sigma}{2k^{3/2}}, \quad \gamma := \frac{c}{2k}, \quad \beta := \frac{\sqrt{k}}{\sigma}\Big(c - \theta + \frac{\sigma^2}{k^2}\Big), \quad \nu := 1 + \frac{\sigma^2}{4k^3} + \frac{c-\theta}{2k}.
$$

Once we find the free boundary $x = X(s)$ such that for each $s > 1$,

$$u(x, s) > 0 \quad \Longleftrightarrow \quad x > X(s),$$

the optimal boundary $r = R(t)$ for terminating the mortgage is given by

$$\begin{aligned} R(t) &= c + \frac{\sigma}{\sqrt{k}}\Big[\frac{X(s)}{\sqrt{s}} - \beta\Big] \\ &= c + \frac{\sigma}{\sqrt{k}}\Big[\frac{X(e^{2k(T-t)})}{e^{k(T-t)}} - \beta\Big]. \end{aligned} \tag{3.3.3}$$

4.0 INTEGRAL EQUATIONS

4.1 WELL-POSEDNESS

Using a standard theory of variational inequalities (e.g. [5]), one can show (c.f. [7]) that (3.3.2) admits a unique solution. In addition, there exists X such that

$$\begin{cases} u_s - \frac{1}{4}u_{xx} = f(x,s)\,\mathbf{1}_{[X(s),\infty)}(x) \quad \text{in } \mathbb{R}\times(1,\infty), \\ u(x,s) > 0 \quad \forall x > X(s), s > 1, \\ u(x,1) = 0 \quad \forall x \in \mathbb{R}, \qquad u(x,s) = 0 \quad \forall s > 1, x \leqslant X(s) \end{cases} \tag{4.1.1}$$

where

$$\mathbf{1}_{[z,\infty)}(x) = 1 \text{ if } x \geqslant z, \qquad \mathbf{1}_{[z,\infty)}(x) = 0 \quad \text{if } \ x < z.$$

Here the differential equation for u is in the L^p sense, i.e., both u_s and u_{xx} are in $L^p_{loc}(\mathbb{R}\times[0,\infty))$ for any $p \in (1,\infty)$.

Denote by

$$\Gamma(x,s) := \frac{e^{-x^2/s}}{\sqrt{\pi s}}$$

the fundamental solution associated with the heat operator $\partial_s - \frac{1}{4}\partial^2_{xx}$. Using Green's identity, the solution u to the differential equation in (4.1.1) can be expressed as

$$u(x,s) = \int_1^s d\varsigma \int_{X(\varsigma)}^{\infty} \Gamma(x-y, s-\varsigma) f(y,\varsigma)\, dy \quad \forall x \in \mathbb{R}, s \geq 1. \tag{4.1.2}$$

4.2 THE INTEGRAL IDENTITIES

In the following sections, we shall derive the following three integral identities for the unknown free boundary function $X(\cdot)$ defined on $(1, \infty)$:

$$0 = \int_1^s d\varsigma \int_{X(\varsigma)}^{\infty} \Gamma(X(s) - y, s - \varsigma) f(y, \varsigma)\, dy = 0 \quad \forall s > 1, \tag{4.2.1}$$

$$0 = \int_1^s d\varsigma \int_{X(\varsigma)}^{\infty} \Gamma_x(X(s) - y, s - \varsigma) f(y, \varsigma)\, dy = 0 \quad \forall\, s > 1, \tag{4.2.2}$$

$$\begin{aligned} 2f(X(s), s) &= -\int_1^s \Gamma_x(X(s) - X(\varsigma), s - \varsigma) f(X(\varsigma), \varsigma) d\varsigma \\ &\quad + \int_s^1 \int_{X(\varsigma)}^{\infty} \Gamma_x(X(s) - y, s - \varsigma) f_y(y, \varsigma)\, dy d\varsigma \quad \forall\, s > 1. \end{aligned} \tag{4.2.3}$$

These identities correspond, respectively, to the facts

$$u(X(s), s) = 0, \tag{4.2.4}$$

$$u_x(X(s), s) = 0, \tag{4.2.5}$$

$$u_{xx}(X(s)+, s) - u_{xx}(X(s)-, s) = -4f(X(s), s). \tag{4.2.6}$$

Once these integral identities are established, we can try to design a Newton scheme to solve for the free boundary iteratively. First of all, we can verify that $X(1) = \beta$. Financially this means that as time approaches to expiry date, the optimal prepayment boundary must approach to the mortgage rate c, otherwise an arbitrage opportunity will be possible. The initial value of the free boundary $X(1)$ is known, and at each moment $s > 1$, the value of the free boundary $X(s)$ must be chosen such that each of the above integral identities hold. This provides the theoretical foundation for our numerical schemes.

4.3 THE FIRST INTEGRAL IDENTITY

Setting $x = X(s)$ in (4.1.2) we immediately obtain the first integral equation (4.2.1) for the unknown $X(\cdot)$. Although $u(x,s) = 0$ for all $x \leqslant X(s)$, the equation (4.2.1) always produces the correct free boundary, as shown in the following Theorem.

Theorem 1. *Suppose $X : s \in [1,\infty) \to \mathbb{R}$ is a continuous function satisfying (4.2.1). Define u as in (4.1.2). Then (X,u) solves (4.1.1) and u is the unique solution to (3.3.2). In addition,*

$$X(s) < \beta\sqrt{s} \quad \forall s > 1. \tag{4.3.1}$$

Proof. Since X is continuous and f is smooth and bounded, the function u defined in (4.1.2) satisfies the differential equation in (4.1.1). In the domain $\{(x,s) \mid s > 1, x < X(s)\}$, u satisfies the heat equation $u_s = \frac{1}{4}u_{xx}$ and the zero boundary condition so $u \equiv 0$ in the domain. After transforming to the original variable (r,τ,ψ) one can show that the corresponding function ψ satisfies $\psi_r \geqslant 0$. From this we can derive that $u > 0$ when $x > X(s)$ and $s > 1$. Hence, (X,u) solves (4.1.1).

Next we prove (4.3.1). Let U be the solution to

$$\begin{cases} U_s - \frac{1}{4}U_{xx} = f(x,s), \quad (x,s) \in \Omega := \{(x,s) \mid s > 1, x > \beta\sqrt{s}\}, \\ U = 0 \text{ on } \ \partial_p\Omega := [\beta,\infty) \times \{0\} \cup \{(\beta\sqrt{s}, s) \mid s > 1\}. \end{cases}$$

Since $f > 0$ in Ω, we have $U > 0$ in Ω and $U_x(\beta\sqrt{s}, s) > 0$ for all $s > 1$. Comparing u and U on $\bar{\Omega}$ we see that $u \geqslant U$ on $\bar{\Omega}$. Since $u_x(X(s), s) = 0$, Hopf's Lemma implies that $u > U$ when $x = \beta\sqrt{s}, s > 1$. Thus, $X(s) < \beta\sqrt{s}$ for all $s > 1$.

Finally, notice that $f < 0$ whenever $x < \beta\sqrt{s}$, or whenever $x < X(s)$, so that u satisfies the variational inequality (3.3.2). It is a known fact that for any given smooth bounded f, (3.3.2) admit a unique solution; see for example, Friedman [5]. This completes the proof. □

We remark that (4.2.1) is derived from $u(X(s), s) = 0$. Since both $u_x(X(s), s) = 0$ and $u_s(X(s), s) = 0$, it would not be easy to find a stable and efficient scheme based solely on (4.2.1) and the standard Newton's method. We shall derive numerical schemes based on other integral equations for $X(\cdot)$.

4.4 THE SECOND INTEGRAL IDENTITY

Differentiation with respect to x for u in (4.1.2) gives, for every $x \in \mathbb{R}$ and $s \geqslant 1$,

$$u_x(x, s) \quad = \quad \int_1^s d\varsigma \int_{X(\varsigma)}^{\infty} \Gamma_x(x - y, s - \varsigma) f(y, \varsigma)\, dy.$$

Such differentiation is permitted since f is bounded and smooth, and

$$\int_1^s \int_{\mathbb{R}} \Big| \Gamma_x(x - y, s - \varsigma) \Big|\, dy\, d\varsigma = \frac{4\sqrt{s-1}}{\sqrt{\pi}} < \infty.$$

The condition $u_x(X(s), s) = 0$ immediately gives us the second integral equation (4.2.2).

For the same reason as above, although $u_x(x, t) = 0$ for all $x \leqslant X(s)$, a solution to (4.2.2) always provides us with the correct answer.

Theorem 2. *Suppose $X : s \in [1, \infty) \to \mathbb{R}$ is continuous and satisfies* (4.2.2)*. Then it is unique and the function u defined in* (4.1.2) *solves* (3.3.2) *and* (X, u) *solves* (4.1.1)*.*

The proof is analogous to that of Theorem 1 and hence is omitted.

Later we shall devise a numerical algorithm based on (4.2.2). For this, we need another integral identity.

4.5 THE THIRD INTEGRAL IDENTITY

In order to take another derivative, we use integration by parts to write

$$u_x(x,s) = \int_1^s \Big\{\Gamma(x - X(\varsigma), s-\varsigma) f(X(\varsigma),\varsigma) + \int_{X(\varsigma)}^\infty \Gamma(x-y, s-\varsigma) f_y(y,\varsigma)\, dy\Big\} d\varsigma.$$

Assume that $X(\cdot)$ is continuous. Then for $x \neq X(s)$, we can exchange the order of differentiation and integration to obtain

$$u_{xx}(x,s) = \int_1^s \Big\{\Gamma_x(x - X(\varsigma), s-\varsigma) f(X(\varsigma),\varsigma) + \int_{X(\varsigma)}^\infty \Gamma_x(x-y, s-\varsigma) f_y(y,\varsigma)\, dy\Big\} d\varsigma.$$

Suppose that $[X(s) - X(\varsigma)]/(s-\varsigma)^{3/2}$ is integrable over $\varsigma \in (1,s)$. Then

$$\int_1^s \Big|\Gamma_x(X(s) - X(\varsigma), s-\varsigma) f(X(\varsigma),\varsigma)\Big| d\varsigma = O(1) \int_1^s \frac{|X(s)-X(\varsigma)|}{(s-\varsigma)^{3/2}}\, d\varsigma < \infty.$$

As f is smooth, we derive that

$$\begin{aligned} \lim_{\varepsilon\to 0+} u_{xx}(X(s)\pm\varepsilon, s) \;&=\; \mp 2 f(X(s),s) + \int_1^s \Big\{\Gamma_x(X(s) - X(\varsigma), s-\varsigma) f(X(\varsigma),\varsigma) \\ &\quad + \int_{X(\varsigma)}^\infty \Gamma_x(X(s)-y, s-\varsigma) f_y(y,\varsigma)\, dy\Big\} d\varsigma. \end{aligned}$$

Consequently, since $u_{xx}(x,s) = 0$ for all $x < X(s)$, we have $u_{xx}(X(s)+,s) = -4f(X(s),s)$ and the integral identity (4.2.3).

The fact that $u_{xx}(X(s)+,s) > 0$ allows us to devise a stable and efficient Newton's iteration scheme to solve for X from the integral equation (4.2.2), originated from $u_x(\cdot,s) = 0$. As we shall see, the identity (4.2.3) will play an important role in simplifying our scheme.

5.0 A NEWTON ITERATION SCHEME

5.1 THE DERIVATION

We intend to numerically solve X from the integral equation (4.2.2). For this, we define an operator Q from $\rho \in C^1((1,\infty))$ to $Q[\rho]$ by

$$\begin{aligned} Q[\rho](s) &:= \int_s^1 \int_{\rho(\varsigma)}^\infty \Gamma_x(\rho(s)-y, s-\varsigma) f(y,\varsigma)\, dy d\varsigma \\ &= \int_s^1 \int_0^\infty \Gamma_x(\rho(s)-\rho(\varsigma)-z, s-\varsigma) f(\rho(\varsigma)+z,\varsigma)\, dz d\varsigma \quad \forall s>1. \end{aligned}$$

Thus, our problem is to find $X \in C([1,\infty)) \cap C^\infty((0,\infty))$ such that $Q[X] \equiv 0$. For this, we use Newton's method.

To implement Newton's method, we need to calculate the first variation of $Q[\rho]$. For every smooth function ζ, we compute

$$\begin{aligned} &Q'[\rho,\zeta](s) = \lim_{\varepsilon \searrow 0} \frac{Q[\rho+\varepsilon\zeta](s) - Q[\rho](s)}{\varepsilon} \\ =\ & \int_1^s \int_0^\infty \Big\{ (\zeta(s)-\zeta(\varsigma)) \Gamma_{xx}(\rho(s)-\rho(\varsigma)-z, s-\varsigma) f(\rho(\varsigma)+z,\varsigma) \\ &\quad + \zeta(\varsigma)\Gamma_x(\rho(s)-\rho(\varsigma)-z, s-\varsigma) f_y(\rho(\varsigma)+z,\varsigma) \Big\}\, dz\, d\varsigma \\ =\ & \zeta(s) \int_s^1 \Big\{ \Gamma_x(\rho(s)-\rho(\varsigma), s-\varsigma) f(\rho(\varsigma),\varsigma) + \int_{\rho(\varsigma)}^\infty \Gamma_x(\rho(s)-y, s-\varsigma) f_y(y,\varsigma)\, dy \Big\}\, d\varsigma \\ &\quad - \int_1^s \zeta(\varsigma)\Gamma_x(\rho(s)-\rho(\varsigma), s-\varsigma) f_y(\rho(\varsigma),\varsigma)\, d\varsigma. \end{aligned}$$

In particular, when $\rho = X$, we can use (4.2.3) to simplify the expression as

$$Q'[X,\zeta](s) = -2f(X(s),s)\zeta(s) - \int_s^1 \zeta(\varsigma)\Gamma_x(X(s)-X(\varsigma),s-\varsigma)f(X(\varsigma),\varsigma)\,d\varsigma.$$

Let Δs, representing a certain mesh size, be small. Suppose $\zeta \equiv 0$ on $[1, s-\Delta s]$. Then

$$\begin{aligned} Q'[X,\zeta](s) &= -2f(X(s),s)\zeta(s) - \int_{s-\Delta s}^{s} \zeta(\varsigma)\Gamma_x(X(s)-X(\varsigma),s-\varsigma)f(X(\varsigma),\varsigma)\,d\varsigma \\ &= -2f(X(s),s)\zeta(s) + o(1)\|\zeta\|_{L^\infty([s-\Delta s,s])}. \end{aligned} \tag{5.1.1}$$

Here we have used the assumption that the improper integral $\int_1^s |\Gamma_x(X(s)-X(\varsigma),s-\varsigma)|d\varsigma$ is convergent.

5.2 THE NEWTON ITERATION.

Now we use Newton's method to devise an iteration scheme for the unknown function X. Suppose we have already found X in $[1, s-\Delta s]$ and want to find X on $(s-\Delta s, s]$. Picking an initial guess $X^{old}(s)$, say $X^{old} \equiv X(s-\Delta s)$ on $[s-\Delta s, s]$. We can find an iterative update scheme from X^{old} to X^{new} according the following rationale. Let $\zeta = X(s) - X^{old}(s)$ be the amount of unknown correction needed. Then $X^{old} = X - \zeta$ and using $Q[X](s) = 0$ and (5.1.1) we have

$$Q[X^{old}](s) = Q[X-\zeta](s) - Q[X](s) \approx 2f(X(s),s)\zeta(s).$$

This gives us the approximation formula for the correction ζ in $X^{new} = X^{old} + \zeta$:

$$\zeta(s) \approx \frac{Q[X^{old}](s)}{2f(X(s),s)}.$$

Thus, we have the following Newton scheme, in a continuous setting,

$$X^{new}(\varsigma) = X^{old}(\varsigma) + \frac{Q[X^{old}](\varsigma)}{2f(X^{old}(\varsigma),\varsigma)} \quad \forall \varsigma \in (s-\Delta s, s].$$

We remark that in the interval $(1, 1+\Delta s]$, one could pick the very first initial guess $X^{old} \equiv \beta$.

For theoretical analysis, we propose the following scheme for the existence of a solution X to (4.2.2). Let $1 = s_0 < s_1 < s_2 < \cdots$ be mesh points in the sense that $\Delta s_n = s_n - s_{n-1}$ is not large (so that $o(1)$ in (5.1.1) is indeed small). Our objective is to show the existence of a solution X to

$$Q[X] \equiv 0$$

via the following scheme: Set $X(0) = \beta$. We find iteratively the function X on $(s_{n-1}, s_n]$, for $n = 1, 2, \cdots$, via the following

$$\begin{cases} X^0(\varsigma) = X(s_{n-1}), \quad \forall \varsigma \in (s_{n-1}, s_n], \quad \Big(X^0 \equiv X \ \text{ on } \ [1, s_{n-1}]\Big), \\ X^{q+1}(\varsigma) = X^q(\varsigma) + \frac{Q[X^q](\varsigma)}{2f(X^q(\varsigma),\varsigma)} \quad \forall\, \varsigma \in (s_{n-1}, s_n],\ q = 0, 1, \cdots, \\ X(\varsigma) = \lim_{q\to\infty} X^q(\varsigma) \quad \forall \varsigma \in (s_{n-1}, s_n]. \end{cases} \quad . \tag{5.2.1}$$

5.3 THE OPERATOR Q

Since $Q[X](s) = u_x(X(s), s)$ involves a double integral over $y \in (X(\varsigma), \infty)$ and $\varsigma \in (1, s)$, to reduce the amount of calculation needed we shall make a simplification so that it involves only a boundary layer integral.

We begin with

$$\begin{aligned} u_x(x,s) &= \int_s^1 \int_{X(\varsigma)}^\infty \Gamma_x(x-y, s-\varsigma) f(y,\varsigma)\, dy\, d\varsigma \\ &= \int_1^s \frac{(\varsigma^\sigma - 1)d\varsigma}{s\varsigma^\nu \sqrt{s-\varsigma}} \int_{X(\varsigma)}^\infty \frac{2s(y-x)(y-\beta\sqrt{\varsigma})}{(s-\varsigma)\varsigma} e^{-A(x,y,s,\varsigma)}\, dy \end{aligned}$$

where

$$\begin{aligned} A(x,y,s,\varsigma) &:= \frac{(x-y)^2}{s-\varsigma}+\frac{(y-\alpha\sqrt{\varsigma})^2}{\varsigma}=\frac{(x-\alpha\sqrt{\varsigma})^2}{s}+\frac{s(y-\xi)^2}{(s-\varsigma)\varsigma},\\ \xi=\xi(x,s,\varsigma) &:= \frac{\varsigma x+(s-\varsigma)\alpha\sqrt{\varsigma}}{s}=x-\frac{s-\varsigma}{s}(x-\alpha\sqrt{\varsigma}). \end{aligned}$$

We write

$$\begin{aligned} &(y-x)(y-\beta\sqrt{\varsigma})=(y-\xi)(y+\xi-x-\beta\sqrt{\varsigma})+(\xi-x)(\xi-\beta\sqrt{\varsigma})\\ =\;&(y-\xi)(y+\xi-x-\beta\sqrt{\varsigma})-\frac{(s-\varsigma)\varsigma}{s}\Big(\frac{x}{\sqrt{\varsigma}}-\alpha\Big)\Big(\frac{\xi}{\sqrt{\varsigma}}-\beta\Big) \end{aligned}$$

and use

$$\begin{aligned} &\frac{2s}{(s-\varsigma)\varsigma}\int_{X(\varsigma)}^{\infty}(y-\xi)(y+\xi-x-\beta\sqrt{\varsigma})\exp\Big(-\frac{s(y-\xi)^2}{(s-\varsigma)\varsigma}\Big)dy\\ =\;&\Big\{X(\varsigma)+\xi-x-\beta\sqrt{\varsigma}\Big\}\exp\Big\{-\frac{s(X(\varsigma)-\xi)^2}{(s-\varsigma)\varsigma}\Big\}+\int_{X(\varsigma)}^{\infty}\exp\Big(-\frac{s(y-\xi)^2}{(s-\varsigma)\varsigma}\Big)dy. \end{aligned}$$

Introducing the complementary error function

$$\operatorname{Erfc}(x)=\frac{2}{\sqrt{\pi}}\int_x^{\infty}e^{-z^2}dz,$$

we can express

$$\int_{X(\varsigma)}^{\infty}\exp\Big(-\frac{s(y-\xi)^2}{(s-\varsigma)\varsigma}\Big)dy=\frac{\sqrt{\pi}}{2}\sqrt{\frac{(s-\varsigma)\varsigma}{s}}\operatorname{Erfc}\Big(\sqrt{\frac{s}{(s-\varsigma)\varsigma}}(X(\varsigma)-\xi)\Big).$$

Thus,

$$\begin{aligned} u_x(x,s)=&\int_1^s\frac{(\varsigma^\gamma-1)e^{-A(x,X(\varsigma),s,\varsigma)}\{X(\varsigma)-\beta\sqrt{\varsigma}+\xi-x\}}{s\varsigma^\nu\sqrt{s-\varsigma}}d\varsigma\\ &+\int_1^s\frac{\sqrt{\pi}(\varsigma^\gamma-1)e^{-\frac{(x-\alpha\sqrt{\varsigma})^2}{s}}\{\frac12-(\frac{x}{\sqrt{\varsigma}}-\alpha)(\frac{\xi}{\sqrt{\varsigma}}-\beta)\}\operatorname{Erfc}(\frac{\sqrt{s}(X(\varsigma)-\xi)}{\sqrt{(s-\varsigma)\varsigma}})}{s^{3/2}\varsigma^{\nu-1/2}}d\varsigma \end{aligned}$$

Therefore,

$$\begin{aligned} u_x(x,s) &= \int_1^s\frac{G_1(x,X(\varsigma),s,\varsigma)}{\sqrt{s-\varsigma}}d\varsigma+\int_1^s G_2(x,X(\varsigma),s,\varsigma)\,d\varsigma \quad \forall\, x\in\mathbb{R}, s>1,\\ Q[X](s) &= \int_1^s G_2(X(s),X(\varsigma),s,\varsigma)\,d\varsigma-2\int_1^s G_1(X(s),X(\varsigma),s,\varsigma)\,d\sqrt{s-\varsigma} \quad \forall s>1 \end{aligned}$$

where

$$
\begin{aligned}
G_1(x,y,s,\varsigma) &:= \frac{\varsigma^\gamma-1}{s\varsigma^\nu}\Big\{y-\beta\sqrt{\varsigma}-\tfrac{s-\varsigma}{s}(x-\alpha\sqrt{\varsigma})\Big\}e^{-\frac{(x-y)^2}{s-\varsigma}-\frac{(y-\alpha\sqrt{\varsigma})^2}{\varsigma}},\\
G_2(x,y,s,\varsigma) &:= \frac{\sqrt{\pi}(\varsigma^\gamma-1)e^{-(x-\alpha\sqrt{\varsigma})^2/s}}{s^{3/2}\varsigma^{\nu-1/2}}\Big\{\frac{1}{2}-\Big(\tfrac{x}{\sqrt{\varsigma}}-\alpha\Big)\Big(\tfrac{x\sqrt{\varsigma}}{s}+\tfrac{s-\varsigma}{s}\alpha-\beta\Big)\Big\} *\\
&\qquad \mathrm{Erfc}\Big(\sqrt{\tfrac{s}{(s-\varsigma)\varsigma}}(y-x)+(\tfrac{x}{\sqrt{\varsigma}}-\alpha)\sqrt{\tfrac{s-\varsigma}{s}}\Big),\\
G_1(x,x,s,s) &= \frac{(s^\gamma-1)(x-\beta\sqrt{s})e^{-(x/\sqrt{s}-\alpha)^2}}{s^{\nu+1}}=\frac{1}{\sqrt{\pi}}f(x,s),\\
G_2(x,x,s,s) &= \frac{\sqrt{\pi}(s^\gamma-1)e^{-(x/\sqrt{s}-\alpha)^2}}{s^{\nu+1}}\Big\{\frac{1}{2}-\Big(\frac{x}{\sqrt{s}}-\alpha\Big)\Big(\frac{x}{\sqrt{s}}-\beta\Big)\Big\}.
\end{aligned}
$$

5.4 THE STANDARD NUMERICAL SCHEME

Suppose we use mesh points

$$1=s_0<s_1<s_2<\cdots.$$

We denote by X_i the approximation of $X(s_i)$, $i=0,1,2,\cdots$. One can check that

$$X_0=X(s_0)=X(1)=\beta.$$

We can use the trapezoid rule to discretize the integral for $Q[X](s_n)$:

$$
\begin{aligned}
Q[X](s_n) &\approx \sum_{i=1}^{n}\Big(\sqrt{s_n-s_{i-1}}-\sqrt{s_n-s_i}\Big)\Big(G_1(X_n,X_i,s_n,s_i)+G_1(X_n,X_{i-1},s_n,s_{i-1})\Big)\\
&\quad+\sum_{i=1}^{n}\Big(s_i-s_{i-1}\Big)\frac{G_2(X_n,X_i,s_n,s_i)+G_2(X_n,X_{i-1},s_n,s_{i-1})}{2}.
\end{aligned}
$$

Consider $z=X_n$ as an unknown. Numerically, we solve for it from the equation

$$Q_n(z)=0$$

where, since $G_1(\cdot,\cdot,\cdot,1)\equiv 0$ and $G_2(\cdot,\cdot,\cdot,1)\equiv 0$, $Q_n(\cdot)$ is defined by, for $n=1$,

$$Q_1(z) \;:=\; \sqrt{s_1-1}\,G_1(z,z,s_1,s_1)+\frac{s_1-1}{2}\,G_2(z,z,s_1,s_1)$$

and for $n\geq 2$,

$$\begin{aligned} Q_n(z) \;:=\;& \sqrt{s_n-s_{n-1}}G_1(z,z,s_n,s_n)+\frac{s_n-s_{n-1}}{2}G_2(z,z,s_n,s_n)\\ &+\sum_{i=1}^{n-1}\Big\{(\sqrt{s_n-s_{i-1}}-\sqrt{s_n-s_{i+1}})G_1(z,X_i,s_n,s_i)+\frac{(s_{i+1}-s_{i-1})}{2}G_2(z,X_i,s_n,s_i)\Big\}. \end{aligned}$$

Suppose $X_0,X_1,\cdots,X_{n-1}$ are known. We solve for $X_n=z$ from $Q_n(z)=0$ by the following iteration:

$$\begin{cases} z_0 &= X_{n-1}+\frac{X_{n-1}-X_{n-2}}{s_{n-1}-s_{n-2}}(s_n-s_{n-1})\\ z_{q+1} &= z_q+\dfrac{Q_n(z_q)}{2f(z_q,s_n)}, \quad q=0,1,2,\cdots, \\ X_n &= z_{q+1} \quad \text{if} \;\; |z_{q+1}-z_q|\leq\varepsilon, \text{a given tolerance.} \end{cases} \tag{5.4.1}$$

Here z_0 is an initial guess derived from a linear interpolation. We point out that Newton's method is quite efficient. For instance, in the example summarized in the left table in Figure 4, when 1024 evenly distributed division points are use for the interval $[1,e^{2kT}]\ni s$ with $T=1$ (year) and the tolerance is set to be $\varepsilon=5\times10^{-7}$, the sum of all the q's in the 1024 steps are 275; that is, the average number q of iteration is about 0.3, which means $q=0$ in most updating steps from X_{n-1} to X_n.

Numerical simulation shows that this numerical scheme has error of size

$$X(s_n)-X_n=O((\Delta s))$$

where Δs is the mesh size. That is to say, when the mesh size is halved, the error reduces by half.

Finally, we remark that when $n = 1$, the equation for X_1 is equivalent to

$$X_1 - \beta\sqrt{s_1} = -\frac{\sqrt{\pi}\sqrt{s_1 - 1}}{2}\Big\{\frac{1}{2} - \Big(\frac{X_1}{\sqrt{s_1}} - \alpha\Big)\Big(\frac{X_1}{\sqrt{s_1}} - \beta\Big)\Big\}.$$

This gives a rough approximation

$$X_1 \approx \beta - \tfrac{\sqrt{\pi}}{4}\sqrt{s_1 - 1} \approx \beta - 0.443\sqrt{s_1 - 1}.$$

As we shall see in the next section, this approximation is close, but not very accurate. The error comes from our Trapezoid rule for singular integrals.

5.5 UPGRADED NUMERICAL SCHEME

In general, one can improve the rate of convergence for numerical integration by using higher order quadrature rules. Since in the current situation singular integrals are involved, higher order quadrature rules are not very effective. Here we introduce a **modified Trapezoid rule** designed specifically for the singular integrals at hand.

Notice that for any constants $a < b \leqslant s$ and linear function $g(x)$ on $[a, b]$ we have

$$\begin{aligned} &\int_a^b \frac{g(x)}{\sqrt{s-x}}dx = \int_a^b \frac{(b-x)g(a) + (x-a)g(b)}{(b-a)\sqrt{s-x}}dx \\ = \ & \frac{2(b-a)}{3(\sqrt{s-a} + \sqrt{s-b})^2}\Big\{[\sqrt{s-a} + 2\sqrt{s-b}]g(a) + [2\sqrt{s-a} + \sqrt{s-b}]g(b)\Big\}. \end{aligned}$$

Thus, we can use the following discretization for the function $Q[X](s_n)$. When $n = 1$,

$$\bar{Q}_1(z) = \frac{4\sqrt{s_1 - 1}}{3}G_1(z, z, s, s) + \frac{s_1 - 1}{2}G_2(z, z, s, s).$$

When $n \geq 2$,

$$\begin{aligned}
\bar{Q}_n(z) \quad &= \quad \frac{4\sqrt{s_n - s_{n-1}}}{3} G_1(z, z, s_n, s_n) + \frac{s_n - s_{n-1}}{2} G_2(z, z, s_n, s_n) \\
&\quad + \sum_{i=1}^{n-1} \frac{s_{i+1} - s_{i-1}}{2} G_2(z, X_i, s_n, s_i) \\
&\quad + \sum_{i=1}^{n-1} \frac{2G_1(z, X_i, s_n, s_i)}{3} \Big\{ \frac{(s_i - s_{i-1})(\sqrt{s_n - s_i} + 2\sqrt{s_n - s_{i-1}})}{(\sqrt{s_n - s_i} + \sqrt{s_n - s_{i-1}})^2} \\
&\qquad\qquad + \frac{(s_{i+1} - s_i)(\sqrt{s_n - s_i} + 2\sqrt{s_n - s_{i+1}})}{(\sqrt{s_n - s_i} + \sqrt{s_n - s_{i+1}})^2} \Big\}.
\end{aligned}$$

Setting $X_0 = \beta$ and a "ghost" value $X_{-1} = \beta + 0.334\sqrt{s_1 - 1}$, we can calculate $\{X_n\}$ iteratively for $n = 1, 2, \cdots$ by the following scheme

$$\begin{cases}
z_0 &= X_{n-1} + \frac{X_{n-1} - X_{n-2}}{s_{n-1} - s_{n-2}}(s_n - s_{n-1}), \\
z_{q+1} &= z_q + \dfrac{\bar{Q}_n(z_q)}{2f(z_q, s_n)}, \quad q = 0, 1, 2, \cdots, \\
X_n &= z_{q+1} \quad \text{if } \ |z_{q+1} - z_q| \leq \varepsilon, \text{a given tolerance.}
\end{cases} \tag{5.5.1}$$

When ε is set to be 5×10^{-7}, the average number of iteration needed is about 0.2, i.e., in most of the calculation, q in (5.5.1) is equal to 0. The rate of convergence is observed by numerical experimentation to be about $O((\Delta s)^{3/2})$:

$$X(s_n) - X_n = O(\Delta s)^{3/2}).$$

That is, when the mesh size Δs is halved, the error reduces by a factor $2\sqrt{2} = 2.8$.

Finally, we remark that when $n = 1$, the equation for X_1 is equivalent to

$$\frac{4}{3}\Big(X_1 - \beta\sqrt{s_1}\Big) = -\frac{\sqrt{\pi}\sqrt{s_1 - 1}}{2}\Big\{\frac{1}{2} - \Big(\frac{X_1}{\sqrt{s_1}} - \alpha\Big)\Big(\frac{X_1}{\sqrt{s_1}} - \beta\Big)\Big\}.$$

This gives a very accurate approximation

$$X_1 \approx \beta - \tfrac{3\sqrt{\pi}}{16}\sqrt{s_1 - 1} \approx \beta - 0.332\sqrt{s_1 - 1}.$$

As we shall see in the next section, this approximation is almost the true asymptotic expansion, which reads $X(s) = \beta - [0.334\ldots + o(1)]\sqrt{s - 1}$ as $s \searrow 1$.

5.6 A NUMERICAL EXAMPLE

The following two tables in Figure 4 illustrate the rate of convergence for uniform mesh size. In this example, we take a typical US economy in 2006: in annual units,

$$c = 0.055, \quad \theta = 0.05, \quad \sigma = 0.015, \quad k = 0.15.$$

One notices that the Newton iteration converges very fast; for example, when 1024 evenly distributed grid points are used for the interval $[1, e^{2kT}]$ with $T = 1$ (year), the total number of iterations for the two schemes are 287 and 213 respectively, which means iteration is not needed in most updates. Also one sees that the upgraded scheme is significantly better than the standard scheme.

Standard Tolerance= $5.\times 10^{-7}$

Grid	Iteration	Solution	Improvement	Rate
8	61	0.2161798	$3.\times 10^{-2}$	3.1
16	90	0.2303882	1.4×10^{-2}	2.1
32	127	0.2373004	6.9×10^{-3}	2.1
64	183	0.2406784	3.4×10^{-3}	2.0
128	238	0.2423363	1.7×10^{-3}	2.0
256	353	0.2431532	8.2×10^{-4}	2.0
512	326	0.2435571	$4.\times 10^{-4}$	2.0
1024	275	0.2437574	$2.\times 10^{-4}$	2.0

Upgraded Scheme Tolerance= $5.\times 10^{-7}$

Grid	Iteration	Solution	Improvement	Rate
8	21	0.2436451	2.9×10^{-4}	-0.0
16	37	0.2438225	1.8×10^{-4}	1.7
32	59	0.2439030	8.1×10^{-5}	2.2
64	85	0.2439357	3.3×10^{-5}	2.5
128	142	0.2439484	1.3×10^{-5}	2.6
256	266	0.2439531	4.7×10^{-6}	2.7
512	253	0.2439548	1.7×10^{-6}	2.7
1024	213	0.2439555	6.3×10^{-7}	2.8

Figure 4: Rate of convergence for the standard numerical scheme (left) and the upgraded scheme (right). Here "Grid" stands for the number of grids, "Iteration" is the total Newton iterations, "Solution" is the value of X at $s = e^{2k\tau}$ with $\tau = T - t = 1$ (year), "Improvement" is the difference between the current solution with that in the previous row, and "Rate" is the ratio of the consecutive improvements.

Similar tables of convergence rate have also been obtained for other typical parameters

The following Figure 5 illustrates the difference of the two schemes. Since the upgraded scheme treats the singularity of the integral, the improvement of the solution at the first node is significant.

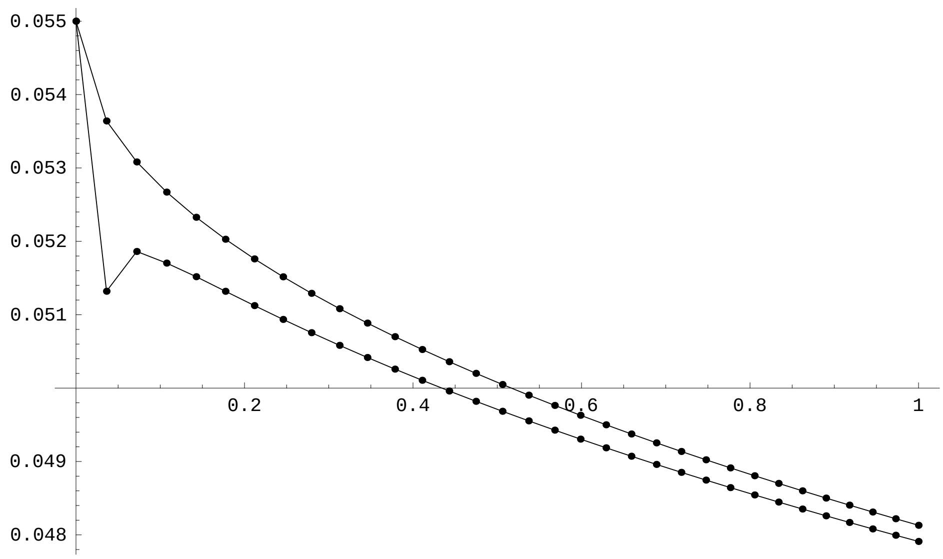

Figure 5: Numerical solutions of the curve $(t, R(t))$ in annual units with 32 grid points. Dots on the top curve are from the upgraded scheme; the dots on the bottom curve are for the standard scheme. The difference of the two solutions at the first node is large.

6.0 ASYMPTOTIC BEHAVIOR NEAR EXPIRY

Here we perform a formal derivation of the asymptotic behavior of X near $s = 1$. We will show that the free boundary in the formulated problem behaves like a constant multiple of the square root of the time to expiry. The desired value of the constant will be determined by a transcendental equation. Another derivation using a totally different method can be found in [7].

6.1 A FORMAL DERIVATION

One of the key observations here is that $f(x,s) > 0$ if $x > \beta\sqrt{s}$ and $f(x,s) < 0$ if $x < \beta\sqrt{s}$. Assume that $X(1) = \lim_{s\searrow 1} X(s)$ exists. We claim that $X(1) = \beta$. Indeed, we know that $X(s) < \beta\sqrt{s}$ for all $s > 1$. Should $X(1) < \beta$, then $X(s) < \beta - \varepsilon$ for all $s \in [1, 1+\varepsilon)$ for some $\varepsilon > 0$. It then follows that u is smooth near $(\beta - \varepsilon, 1)$, so that $u_{ss}(\beta-\varepsilon, 1) = f_s(\beta-\varepsilon, 1) < 0$ and hence $u(\beta-\varepsilon, s) < 0$ when $0 < s-1 \ll 1$, contradicting the fact that $u \geq 0$. Thus, we must have $X(1) = \beta$.

Now we postulate that

$$X(s) = \beta - \kappa\sqrt{s-1} + o(1)\sqrt{s-1} \quad \text{as} \quad s \searrow 1.$$

We then can derive the asymptotic expansion

$$\frac{Q[X](s)}{\sigma e^{-(\beta-\alpha)^2}} = \int_s^1 (\varsigma - 1)\Big\{ \int_{\frac{\kappa(\sqrt{s-1}-\sqrt{\varsigma-1})}{\sqrt{s-\varsigma}}}^{\infty} e^{-z^2} dz - \frac{\kappa\sqrt{\varsigma-1}}{\sqrt{s-\varsigma}} e^{-\frac{\kappa^2(\sqrt{s-1}-\sqrt{\varsigma-1})^2}{s-\varsigma}} \Big\} d\varsigma + o((s-1)^2).$$

Using the substitution $\varsigma = 1 + (s-1)t$ and sending $s \searrow 0$, we see that κ satisfies the equation

$$\begin{aligned} 0 &= \int_0^1 \Big\{ \int_{\frac{\kappa(1-\sqrt{t})}{\sqrt{1-t}}}^{\infty} e^{-z^2}\,dz - \frac{\kappa\sqrt{t}}{\sqrt{1-t}} e^{-\frac{\kappa^2(1-\sqrt{t})}{1+\sqrt{t}}} \Big\} t\,dt \\ &= \frac{\sqrt{\pi}}{4} - \kappa \int_0^1 e^{-\frac{\kappa^2(1-\sqrt{t})}{1+\sqrt{t}}} \frac{(5/4+\sqrt{t})t\sqrt{t}}{(1+\sqrt{t})\sqrt{1-t}}\,dt \end{aligned}$$

After the substitution $\sqrt{t} = \frac{\kappa^2 - z^2}{\kappa^2 + z^2}$, the equation for κ then becomes

$$\sqrt{\pi} = \int_0^{\kappa} \frac{e^{-z^2}(\kappa^2 - z^2)^4 (18\kappa^2 + 2z^2)}{(\kappa^2 + z^2)^5} dz. \tag{6.1.1}$$

It is easy to see that the right-hand is an increasing function of κ, equal to 0 when $\kappa = 0$ and equal to $9\sqrt{\pi}$ when $\kappa = \infty$. Thus, there exists a unique root κ to the equation. A numerical calculation shows that

$$\kappa = 0.3343641440309...$$

Hence,

$$X(s) = \beta - 0.334364\sqrt{s-1} + o(\sqrt{s-1}) \quad \text{as} \quad s \searrow 0.$$

We remark that in [7], the same asymptotic behavior is obtained by finding the root of

$$\int_{-\infty}^{\kappa} e^{-z^2} dz + e^{-\kappa^2} \frac{2\kappa^4 + 4\kappa^2 - 1}{4\kappa^5 + 10\kappa^3} = 0 \quad \Leftrightarrow \quad \int_{\kappa}^{\infty} \frac{15 e^{-z^2} dz}{2z^4 (5 + 2z^2)^2} = \sqrt{\pi}. \tag{6.1.2}$$

Although it is very difficult to show analytically that the two transcendental equations (6.1.1) and (6.1.2) have the same roots, an indication of why they provide the same answers is gotten in the next subsection.

Translating to the original variable, we have the asymptotic behavior:

Theorem 3. *[7] Near expiry the optimal mortgage termination boundary $r = R(t)$ has the asymptotic expansion*

$$R(t) \ \sim \ c - \sigma\bar{\kappa}\sqrt{T-t} \qquad \textit{as} \ \ t \nearrow T, \qquad \bar{\kappa} = \sqrt{2}\kappa = 0.47386... \tag{6.1.3}$$

6.2 AN EXACT SOLUTION FOR A SPECIAL CASE

In many applications, exact solutions play an important role. When f in (3.3.1) is given by $f(x,s) = \gamma\sqrt{\pi}e^{-(\beta-\alpha)^2}(x-\beta)(s-1)$, there is an exact solution of (4.1.1) given by

$$X(s) = \beta - \kappa\sqrt{s-1}, \qquad u(x,s) = \gamma\sqrt{\pi}e^{-(\beta-\alpha)^2}(s-1)^{5/2}g\Big(\frac{\beta-x}{\sqrt{s-1}}\Big)$$

where g, together with the unknown constant κ, solve the "free boundary" problem

$$g''(z) + 2zg'(z) - 10g(z) - 4z = 0 \quad \forall z < \kappa, \quad g(\kappa) = g'(\kappa) = 0,$$
$$g > 0 \text{ in } \ (-\infty, \kappa], \qquad g = 0 \text{ in } \ (\kappa, \infty), \quad g(z) = O(z) \text{ as } z \to -\infty.$$

We find that the solution to this free-boundary problem is given by

$$g(z) = \frac{1}{2}\Big\{\frac{\kappa\int_{-\infty}^{z}(z-t)^5e^{-t^2}dt}{\int_{-\infty}^{\kappa}(\kappa-t)^5e^{-t^2}dt} - z\Big\} \quad \forall\, z < \kappa,$$

where κ is the unique solution to the transcendental equation

$$5\kappa\int_{-\infty}^{\kappa}(\kappa-t)^4e^{-t^2}dt = \int_{-\infty}^{\kappa}(\kappa-t)^5e^{-t^2}dt \Leftrightarrow \quad \int_{\kappa}^{\infty}\frac{15e^{-t^2}dt}{2t^4(5+2t^2)^2} = \sqrt{\pi}.$$

A numerical calculation gives

$$\kappa = 0.3343641440309...$$

In [7], the asymptotic behavior (1.0.6) (with $\bar{\kappa} = \sqrt{2}\,\kappa$) is derived by a method equivalent to replacing f by its asymptotic expansion $\gamma\sqrt{\pi}e^{-(\beta-\alpha)^2}(x-\beta)(s-1)$.

6.3 A NUMERICAL EXAMPLE

In the following example (Figure 6), we provide a comparison between the numerical solution and the asymptotic expansion given by our formula (6.1.3). It shows that, for small time, the asymptotic expansion formula is very accurate. Here we used $c = 0.05$, $\theta = 0.05$, $k = 0.15$, $\sigma = 0.015$. For this set of parameters, $\max_{0<t<T} |R_{Asymptotic}(t) - R(t)| = 0.000018$, and

$$\frac{\max_{t<T} |R_{Asymptotic}(t) - R(t)|}{c - R(T)} \approx 0.4\%.$$

for $T = 0.36$.

Here $R_{Asymptotic}(t)$ is derived through the formula (6.1.3) in Theorem 3. $R(t)$ represents the true solution computed numerically. As to how we numerically computed the solution, we will elaborate in the following chapters. In the end, we will provide a comprehensive analysis on our numerical methods.

In Figure (7), we provide the detailed information about the errors between the asymptotic formula and the numerical solution recorded for each time between $[0, T]$ for T=0.36.

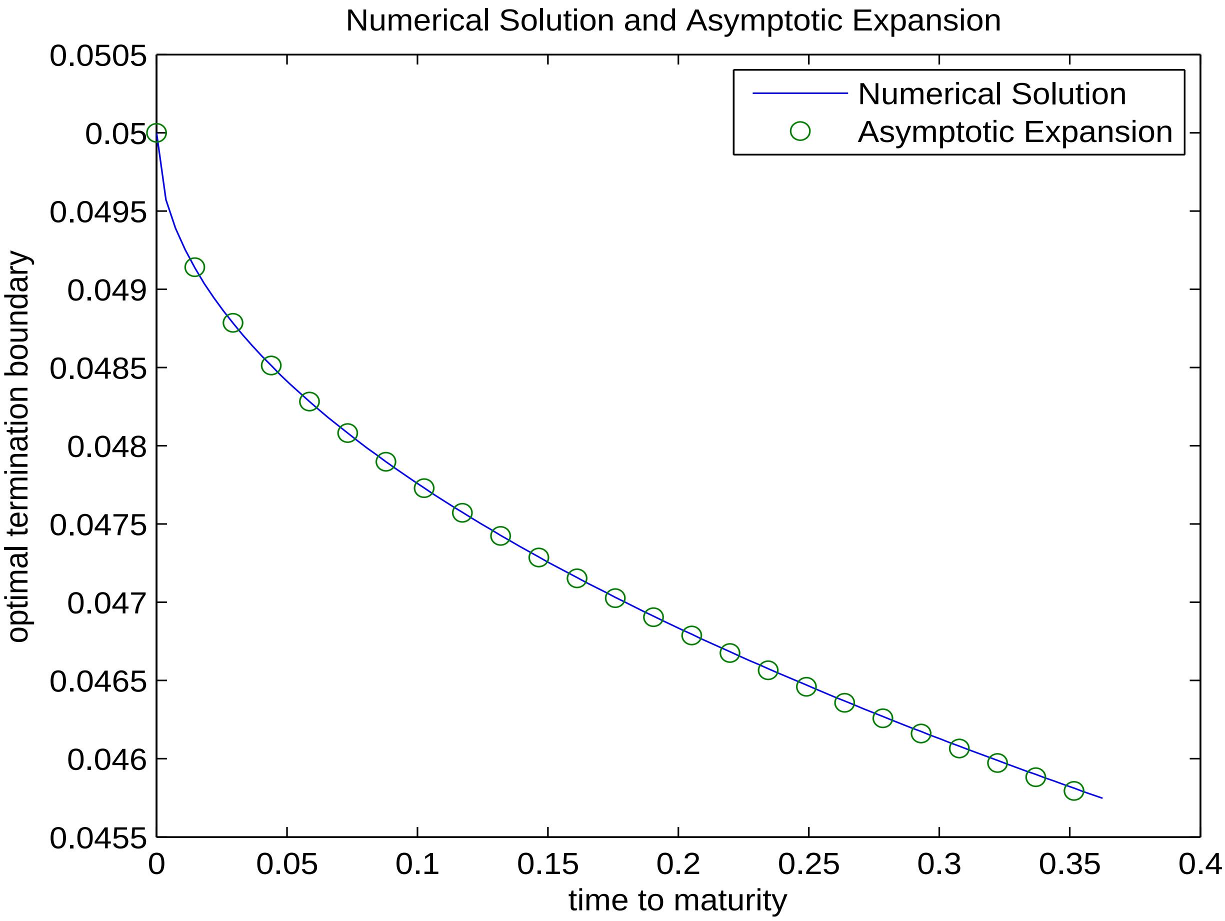

Figure 6: This is a comparison between the true numerical solution of the optimal terminationboundary (the smooth curve) and the asymptotic expansion (the circles) using the formula (6.1.3). It shows that, for small time, the asymptotic expansion formula is very accurate. For this particular example, the maximum error between the two is only 0.000018 for $0 < t < 0.36$. The parameters used in this example are: $c = 0.05, \quad \theta = 0.05, \quad k = 0.15, \quad \sigma = 0.015$.

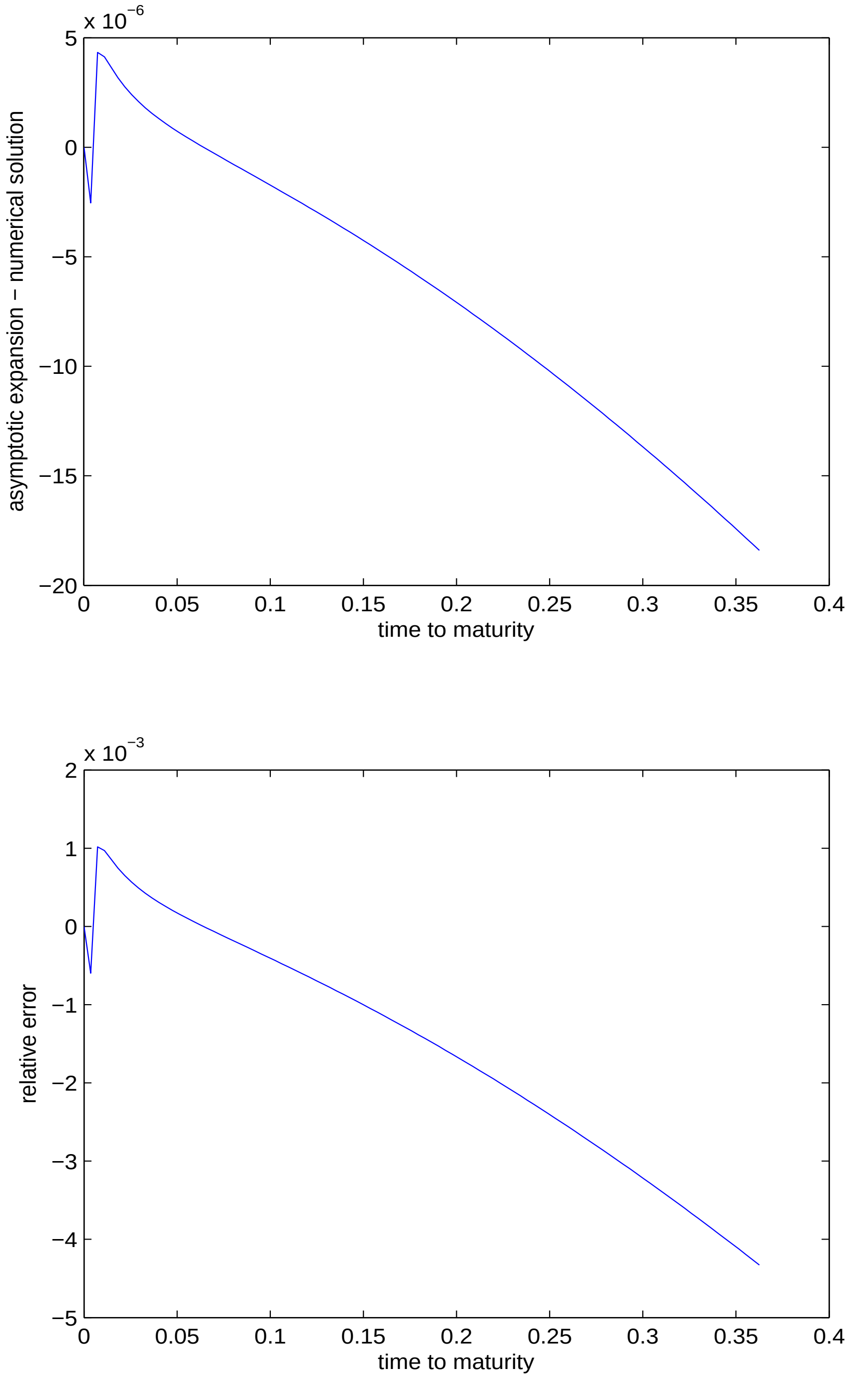

Figure 7: Errors between the asymptotic formula and the numerical solution recorded for each time. The top plot is for the error $R_{Asymptotic}(t) - R(t)$, and the bottom is for the relative error defined as $\frac{\max_{t<T} |R_{Asymptotic} - R(t)|}{c - R(T)}$ for T=0.36 . Here $c = 0.05, \theta = 0.05, k = 0.15, \sigma = 0.015$.

7.0 ASYMPTOTIC BEHAVIOR FOR LARGE TIME

In this section, we shall prove the following

Theorem 4. *There exist constants $R^* \in (-\infty, c)$ and $\rho^* > 0$ such that*

$$R(t) \sim R^* + \rho^* \, e^{c(t-T)} \quad \textit{as} \;\; t \to -\infty.$$

The idea here is to study first the limit $(R^*, V^*(\cdot)) := \lim_{t\to-\infty}(R(t), \frac{c}{m}V(\cdot,t))$, which solves a so-called **infinite horizon problem**, and then the limit $\zeta^*(r) := \lim_{t\to-\infty}\zeta(r,t)$ where

$$\zeta(r,t) := \frac{V_t(r,t)}{\dot{M}(t)} = -\frac{V_t(r,t)}{m\, e^{c(t-T)}}.$$

After deriving the relation

$$\dot{R}(t) \;\; = \;\; \frac{c\,\sigma^2}{2m}\frac{V_{tr}(R(t)+,t)}{(c-R(t))(1-e^{c(t-T)})} = \frac{ce^{c(t-T)}\,\sigma^2}{2}\frac{\zeta_r(R(t)+,t)}{(R(t)-c)(1-e^{c(t-T)})},$$

we see that

$$\rho^* := \frac{1}{c}\lim_{t\to-\infty}\dot{R}(t)e^{-c(t-T)} = \frac{\sigma^2}{2}\frac{\zeta^*_r(R^*)}{(R^*-c)}.$$

The theorem will be proven in the following subsections. In the process, we shall derive formulas for $R^*, V^*(\cdot), \zeta^*(\cdot)$ and ρ^*.

7.1 THE INFINITE HORIZON PROBLEM

In [7], it is shown that $\dot{R}(t) > 0$. Also, one can show that $V_t \leqslant 0$. Hence, there exists

$$\lim_{t\to-\infty}\Big(R(t)\ ,\ \frac{c}{m}V(\cdot,t)\Big) = \Big(R^*, V^*(\cdot)\Big)\ . \tag{7.1.1}$$

From (1.0.5), one derives that (R^*, V^*) is a solution to the following **infinite horizon problem**:

$$\begin{cases} \Big\{\frac{\sigma^2}{2}\frac{d^2}{dr^2} + k(\theta - r)\frac{d}{dr} - r\Big\}V^* = -c & \text{in } \ (R^*, \infty), \\ \\ 0 \leqslant V^* \leqslant 1 & \text{in } \ (R^*, \infty), \\ \\ V^*(R^*) = 1, \quad V_r^*(R^*) = 0. \end{cases} \tag{7.1.2}$$

Theorem 5. *Assume that σ, k, θ, c are positive constants. Then (7.1.2) admits a unique solution. In addition, the solution has the property that $R^* \in (-\infty, c)$ and $V_r^*(r) < 0$ for all $r \in (R^*, \infty)$.*

Before proving theorem 5, we first verify (7.1.2). Let (R^*, V^*) be as stated in the Theorem. We claim that $R(t) > R^*$ for all $t \leqslant T$. Suppose this is not true. Then since $R(T-) = c$, R is smooth and $\dot{R} < 0$ in $(-\infty, T)$, there exists a finite $t_* < T$ such that $R(t) > R^*$ for all $t \in (t_*, T]$ and $R(t_*) = R^*$. We calculate, for all $r > R(t)$ and $t \in [t_*, T]$,

$$\Big\{\frac{\partial}{\partial(T-t)} - \frac{\sigma^2}{2}\frac{\partial^2}{\partial r^2} - k(\theta - r)\frac{\partial}{\partial r} + r\Big\}\Big(V^*(r)M(t)\Big) = m + me^{c(t-T)}[V^*(r) - 1] < m$$

since $V^*(r) < 1$ for $r > R^*$. Also, $V(R(t), t) = M(t) \geq V^*(R(t))M(t)$ for all $t \in [t_*, T]$. It then follows from a strong comparison principle for $V(r,t)$ and $V^*(r)M(t)$ in the set $\{(r,t) \mid t_* \leq t \leq T, r \geq R(t)\}$ that $M(t)V^*(r) < V(r,t)$ for all $r > R(t), t \in [t_*, T)$. In addition, as R is smooth, by Hopf's Lemma, we should also have $V_r(R(t_*)+, t_*) > V_r^*(R(t_*))M(t_*) = 0$, which is impossible since we know that $M(t) = V(R(t_*), t_*) \geq$

$V(r,t_*)$ for all r. Hence, we must have $R(t) > R^*$ for all $t \leqslant T$. In addition, by the comparison just established,

$$R^* < R(t) < c, \quad V^*(r)M(t) < V(r,t) < M(t) \quad \forall\, t < T, r > R(t). \tag{7.1.3}$$

From these bounds and the fact that $\dot{R} > 0$ and $V_t \leqslant 0$ we then know that there exists $(R(-\infty), V(r,-\infty)) := \lim_{t\to-\infty}(R(t), V(r,t))$. As $R(t) \geq R^*$, a local regularity result for parabolic equations [11] shows that $\lim_{t\to-\infty} V_t(r,t) = 0$ for every $r > R(-\infty)$. Thus the $(R(-\infty), V(r,-\infty))$ is a solution to the infinite horizon problem (7.1.2). By the uniqueness result of Theorem 5, we see that (7.1.1) holds. We summarize the result as follows.

Lemma 7.1.1. *Let (R^*, V^*) be the unique solution to (7.1.2). Then both (7.1.1) and (7.1.3) hold.*

In the next two subsections, we prove Theorem 5, along with formulas for R^* and $V^*(\cdot)$.

7.2 THE HOMOGENEOUS EQUATION

We begin with the homogeneous equation

$$\left\{\frac{\sigma^2}{2}\frac{d^2}{dr^2} + k(\theta - r)\frac{d}{dr} - r\right\}G(r) = 0, \qquad r \in \mathbb{R}.$$

In self-adjoint form, this equation can be written as

$$\left\{e^{-k(r-\theta)^2/\sigma^2} G_r(r)\right\}_r = \tfrac{2}{\sigma^2}\, e^{-k(r-\theta)^2/\sigma^2} r\, G(r), \quad r \in \mathbb{R}. \tag{7.2.1}$$

If G_1 and G_2 are two linearly independent solutions, their Wronskian satisfies

$$G_{1r}(r)G_2(r) - G_{2r}(r)G_1(r) = Ce^{k(r-\theta)^2/\sigma^2}$$

where C is a non-zero constant. Thus, if there is a solution bounded at $r = \infty$, it is unique up to a constant multiple. We shall now find such a solution.

Lemma 7.2.1. *Assume that $\sigma > 0$ and $k > 0$. Then (7.2.1) admits a unique solution satisfying*

$$\lim_{r\to\infty} G(r)e^{r/k}r^{-\mu} = 1, \qquad \mu := \frac{\sigma^2 - 2\theta k^2}{2k^3}.$$

In addition, there exists $r_0 \in [-\infty, 0)$ such that

$$G_r < 0 < G \text{ in } (r_0, \infty), \qquad \int_{r_0}^{\infty} re^{-k(r-\theta)^2/\sigma^2}G(r)\,dr = 0. \tag{7.2.2}$$

In particular, (i) when $\sigma^2 \leq 2k^2\theta, r_0 = -\infty$; (ii) when $\sigma^2 > 2k^2\theta$, $r_0 > -\infty$ and $G_r(r_0) = 0$.

Proof. Make a change of variables

$$x = \frac{\sqrt{k}}{\sigma}\Big(r + \frac{\sigma^2}{k^2} - \theta\Big), \quad H(x) = e^{r/k}G(r).$$

Then $H = H(x)$ satisfies the Hermite equation

$$H_{xx} = 2xH_x - 2\mu H \quad \forall\, x \in \mathbb{R}.$$

A particular solution of this ode is the Hermite function defined as

$$H(\mu; x) = \frac{(-1)^m t^{-\mu-1}}{\Gamma(m-\mu)} \int_0^{\infty} t^m \frac{d^m e^{-t^2-2xt}}{dt^m} dt, \forall x, \mu \in \mathbb{C},\ m \in \mathbb{N} \cap (\mathrm{Re}(\mu), \infty). \tag{7.2.3}$$

Here $\Gamma(\cdot)$ is the Gamma function, $\mathbb{N} = \{0, 1, 2, \cdots\}$ is the set of non-negative integers, and most importantly, the integral on the right-hand side is independent of the integer m and hence $H(\mu; x)$ is an entire function of both variables $\mu \in \mathbb{C}$ and $x \in \mathbb{C}$. The integer

m here is introduced so that the integral is uniformly convergent. Without it, one can use contour integrals to express

$$H(\mu;x) = \frac{1}{\Gamma(-\mu)[1-e^{-2\pi\mu\mathbf{i}}]}\int_{\omega} t^{-\mu-1}e^{-t^2-2xt}dt \qquad \forall\, x\in\mathbb{C},\ \mu\in\mathbb{C}\setminus\mathbb{Z}$$

where ω is any contour starting from $\infty e^{2\pi\mathbf{i}}$, rotating around the origin clockwise without touching the origin and positive real axis, and finally ending at $\infty e^{0\mathbf{i}}$. One has the relations

$$\begin{aligned}
H_x(\mu;x) &= 2\mu H(\mu-1;x) && \forall\, x,\mu\in\mathbb{C},\\
H(\mu+1;x) &= 2xH(\mu;x) - 2\mu H(\mu-1;x) && \forall\, x,\mu\in\mathbb{C},\\
H(\mu;x) &\sim (2x)^{\mu} \quad \text{as}\ \ x\to\infty && \forall\,\mu\in\mathbb{C}\\
H(\mu;x) &\sim \tfrac{\sqrt{\pi}e^{x^2}}{\Gamma(-\mu)(-x)^{\mu+1}} \quad \text{as}\ \ x\to-\infty && \forall\,\mu\in\mathbb{C}\setminus\mathbb{N},\\
H(\mu;-x) &= (-1)^{\mu}H(\mu;x) && \forall\, x\in\mathbb{C},\ \mu\in\mathbb{N}.
\end{aligned}$$

Here the first two relations can be verified from the definition. For the asymptotic behavior, for every $\mu\in\mathbb{C}$, taking any $m\in\mathbb{N}\cap(\mathrm{Re}(\mu),\infty)$, we have,

$$\begin{aligned}
\lim_{x\to\infty}\frac{H(\mu;x)}{(2x)^{\mu}} &= \lim_{x\to\infty}\frac{(-1)^m}{\Gamma(m-\mu)}\int_0^{\infty} s^{m-\mu-1}\frac{d^m e^{-s^2/(4x^2)-s}}{ds^m}ds\\
&= \frac{(-1)^m}{\Gamma(m-\mu)}\int_0^{\infty} s^{m-\mu-1}\frac{d^m e^{-s}}{ds^m}ds = \frac{1}{\Gamma(m-\mu)}\int_0^{\infty} s^{m-\mu-1}e^{-s}ds = 1
\end{aligned}$$

by Lebesgue's Dominated Convergence theorem and the definition of the Gamma function.

When $\mu\in\mathbb{N}$, one can check that $H(\mu,x)$ is the Hermite polynomial of degree μ and that $H(\mu,-x) = (-1)^{\mu}H(\mu,x)$; in particular,

$$H(0;x)=1,\quad H(1;x)=2x,\quad H(2;x)=4x^2-2,\quad H(3;x)=2x(4x^2-6),$$
$$H(n+1;x) = 2xH(n;x) - 2nH(n-1;x),$$
$$e^{-t^2+2xt} = \sum_{n=0}^{\infty}\frac{H(n;x)}{n!}\,t^n \quad \forall\, x,t\in\mathbb{Z}.$$

When μ is not an integer, one can calculate

$$\begin{aligned}
\lim_{x\to-\infty}(-x)^{\mu+1}e^{-x^2}H(\mu;x) &= \lim_{x\to-\infty}\frac{1}{\Gamma(-\mu)[1-e^{-2\pi\mu\mathbf{i}}]}\int_\gamma\left(\frac{t}{-x}\right)^{-\mu-1}e^{-(t+x)^2}dt \\
&= \lim_{x\to-\infty}\frac{1}{\Gamma(-\mu)[1-e^{-2\pi\mu\mathbf{i}}]}\int_{x+\gamma}\left[1+\frac{s}{-x}\right]^{-\mu-1}e^{-s^2}ds \\
&= \frac{1}{\Gamma(-\mu)}\int_{-\infty}^{\infty}e^{-s^2}ds = \frac{\sqrt{\pi}}{\Gamma(-\mu)}.
\end{aligned}$$

When μ is a negative integer, one can use (7.2.3) with $k=0$ to derive the same limit.

Finally, from $[e^{-x^2}H_x]_x = -2\mu e^{-x^2}H$, one can derive that on the real axis, $H(\mu;\cdot) > 0 > H_x(\mu;\cdot)$ when $\mu\le 0$ and $H(\mu;\cdot)$ changes sign when $\mu>0$.

Now going back to the original variable, we find that

$$G(r)e^{-k(r-\theta)^2/\sigma^2} = e^{-x^2+x\sigma k^{-3/2}-\theta/k}H(\mu;x).$$

It follows that

$$\lim_{|r|\to\infty}\Big\{|G_r(r)|+|G(r)|\Big\}e^{-k(r-\theta)^2/\sigma^2}e^{|r|/(2k)} = 0. \tag{7.2.4}$$

Integrating (7.2.1) over $\mathbb{R}$ we obtain $\int_{\mathbb{R}} re^{-k(r-\theta)^2/\sigma^2}G(r)dr = 0$, where the improper integeral is uniformly convergent. Finally, we have the following:

(1) When $\sigma^2 > 2k^2\theta$, we have $\mu>0$. As $H(\mu;\cdot)$ changes sign, so does $G(\cdot)$. Thus, there exists a finite real r_0 such that $G_r(r_0)=0$ and $G_r<0$ in (r_0,∞). This implies that $G>0$ in $[r_0,\infty)$. After integrating (7.2.1) over $[r_0,\infty)$ we obtain the integral identity in (7.2.2).

(2) When $\sigma^2\le 2k^2\theta$, we have $\mu\le 0$, so that $H(\mu;x)>0$ for all $x\in\mathbb{R}$. Thus, $G>0$ in $\mathbb{R}$. As $[e^{-k(r-\theta)^2/\sigma^2}]_r$ is positive in $(0,\infty)$ and negative in $(-\infty,0)$, in view of (7.2.4), we derive $G_r<0$ on $\mathbb{R}$. Hence (7.2.2) holds with $r_0=-\infty$. This completes the proof.

7.3 EXISTENCE OF A UNIQUE SOLUTION

We divide the proof into several steps. Suppose (R^*, V^*) solves (7.1.2). We first establish certain properties of (R^*, V^*) and then derive a formula for it, thereby obtaining both existence and uniqueness.

1. First we show that $V^*_r < 0$ in (R^*, ∞).

Suppose otherwise. Then $V^*_r(r_1) \geqslant 0$ at some $r_1 > R^*$. Since $V^*(R^*) = 1$ is a global maximum, $r_2 := \sup\{r \in (R^*, r_1) \mid V^*_r(r) < 0\}$ is well-defined and by continuity $V^*_r(r_2) = 0$. The case $V^*_{rr}(r_2) < 0$ is impossible since it would imply $V^*_r > 0$ in $(r_2 - \varepsilon, r_2)$ for some small positive ε, contradicting the definition of r_2. The case $V^*_{rr}(r_2) = 0$ is also impossible since it would imply by the ode for V^* that $r_2 V^*(r_2) = c > 0$ and $\frac{\sigma^2}{2} V^*_{rrr}(r_2) = V^*(r_2) > 0$ so that $V^*_r > 0$ in $(r_2 - \varepsilon, r)$ for some small positive ε. Hence $V^*_{rr}(r_2) > 0$ and, by the ode, $r_2 V^*(r_2) > c$. Set $r_3 = \sup\{r > r_2 \mid V^*_r > 0 \text{ in } (r_2, r)\}$. Then for every $r \in (r_2, r_3)$, $rV^*(r) > r_2 V(r_2) > c$ and $[e^{-k(r-\theta)^2/\sigma^2} V_r(r)]_r = (rV - c)e^{-k(r-\theta)^2/\sigma^2} > 0$. That is, $e^{-k(r-\theta)^2/\sigma^2} V_r$ is a strictly increasing function on $[r_2, r_3)$. This implies $r_3 = \infty$ and $\lim_{r\to\infty} e^{-k(r-\theta)^2/\sigma^2} V_r > 0$, which further implies $\lim_{r\to\infty} V^*_r = \infty$, contradicting the boundedness of V^*. Thus we must have $V^*_r < 0$ in (R^*, ∞). Consequently, $0 < V^* < 1$ in (R^*, ∞).

2. Next we show that $R^* > r_0$. For this, consider the weighted Wronskian

$$W(r) = \Big\{V^*_r(r)G(r) - V^*(r)G_r(r)\Big\}e^{-k(r-\theta)^2/\sigma^2}.$$

It satisfies $\frac{\sigma^2}{2} W_r = -ce^{-k(r-\theta)^2/\sigma^2} G$. Integrating this equation over (r, ∞) gives

$$W(r) = \frac{2c}{\sigma^2} \int_r^\infty G e^{-k(r-\theta)^2/\sigma^2} dt \quad \forall\, r \geqslant R^*. \tag{7.3.1}$$

First consider the case $r_0 > -\infty$. Should $R \leqslant r_0$, we would have, since $G_r(r_0) = 0$ and $G > 0$ on $[r_0, \infty)$, that $0 < W(r_0) = V^*_r(r_0)G(r_0)e^{-k(r-\theta)^2/\sigma^2} \leqslant 0$, a contradiction.

Next, we consider the case $r_0 = -\infty$. Then $G > 0$ on $\mathbb{R}$. Should $R^* = -\infty$, the boundedness of V^* implies that along a sequence $R_j \to -\infty$, $V_r(R_j) \to 0$ so that, in view of (7.2.4), $W \to 0$ along the sequence $\{R_j\}$, contradicting (7.3.1). Thus, we must have $R^* > r_0$.

3. Now we show that R^* needs to satisfy the following **solvability condition** for R^*:

$$\int_{R^*}^{\infty} (r-c)G(r)e^{-k(r-\theta)^2/\sigma^2}dr = 0, \qquad R^* > r_0. \tag{7.3.2}$$

In fact, substituting $V^*(R^*) = 1$ and $V_r^*(R^*) = 0$ into (7.3.1) at $r = r^*$ gives

$$e^{-k(r-\theta)^2/\sigma^2}G_r(R^*) = -\frac{2c}{\sigma^2}\int_{R^*}^{\infty} Ge^{-k(r-\theta)^2/\sigma^2}dt.$$

The equation in (7.3.2) then follows by noting that

$$e^{-k(r-\theta)^2/\sigma^2}G_r(R^*) = \int_{\infty}^{R^*} [e^{-k(r-\theta)^2/\sigma^2}G_r(r)]_r dr = -\frac{2}{\omega^2}\int_{R^*}^{\infty} re^{-k(r-\theta)^2/\sigma^2}G(r)dr.$$

4. Here we show that (7.3.2) has a unique solution R^*. Since

$$\int_{r_0}^{\infty} rG(r)e^{-k(r-\theta)^2/\sigma^2}dr = 0 \tag{7.3.3}$$

and $G > 0$ on $[r_0, \infty)$, we see that $r_0 < 0$ and that the function

$$\Psi(c,r) := \int_r^{\infty} (t-c)G(t)e^{-k(t-\theta)^2/\sigma^2}dt, \quad c > 0, r \in \mathbb{R}$$

has the property

$$\Psi(c,\infty) = 0, \quad \Psi_r(c,\cdot) < 0 \text{ in } (c,\infty), \quad \Psi_r(c,\cdot) > 0 \text{ in } (r_0,c), \quad \Phi(r_0) < 0.$$

It then follows that the algebraic equation $\Psi(c,\cdot) = 0$ has a unique root in (r_0,∞). Thus, R^* is the unique root to (7.3.2) and

$$r_0 < R^* < c, \qquad \lim_{c\searrow 0} R^* = r_0 \in [-\infty, 0).$$

One notices that $\Psi(c,r) > 0$ for all $r > R^*$.

5. We are ready now to derive a formula for V^*. Integrating over $[R^*, r)$ the equation (7.3.1) multiplied by $e^{-k(r-\theta)^2/\sigma^2}G^{-2}$ and using $V^*(R^*) = 1$ we obtain

$$V^*(r) := G(r)\Big\{\frac{1}{G(R^*)} + \frac{2c}{\sigma^2}\int_{R^*}^{r}\frac{e^{k(t-\theta)^2/\sigma^2}}{G^2(t)}\int_t^\infty G(s)e^{-k(s-\theta)^2/\sigma^2}dsdt\Big\}. \tag{7.3.4}$$

Using

$$\frac{1}{G(R^*)} - \frac{1}{G(r)} = \int_{R^*}^{r}\frac{G_r(t)}{G^2(t)}dt = -\frac{2}{\sigma^2}\int_{R^*}^{r}\frac{e^{k(t-\theta)^2/\sigma^2}}{G^2(t)}\int_t^\infty s\,G(s)e^{-k(s-\theta)^2/\sigma^2}dsdt$$

we can write the above expression as

$$V^*(r) = 1 - \frac{2G(r)}{\sigma^2}\int_{R^*}^{r}\frac{e^{k(t-\theta)^2/\sigma^2}}{G^2(t)}\int_t^\infty (s-c)\,G(s)e^{-k(s-\theta)^2/\sigma^2}dsdt. \tag{7.3.5}$$

In conclusion, if (R^*, V^*) solves (7.1.2), then R^* is the unique root to (7.3.2) and V^* is given by (7.3.4), which is equivalent to (7.3.5).

6. Finally, from (7.3.4), we see that $V^* > 0$ on $[R^*, \infty)$. Also, as $\Psi(c,r) > 0$ for all $r > R^*$, we see from (7.3.5) that $V^* < 1$ in (R^*, ∞) and that $V^*(R^*) = 1, V_r(R^*) = 0$. It is then an easy exercise to show that V^* in (7.3.4) satisfies the ode in (7.1.2). Thus, (R^*, V^*) obtained in this manner is indeed a solution to (7.1.2). We hence have established the existence of a unique solution to (7.1.2), thereby completing the proof of Theorem 5.

7.4 A PARAMETRIC RELATION BETWEEN R^* AND C

As a function of c, R^* defined in (7.3.2) is monotonic and the inverse function can be written as

$$c = \frac{\displaystyle\int_{R^*}^{\infty} re^{-k(r-\theta)^2/\sigma^2} G(r)\, dr}{\displaystyle\int_{R^*}^{\infty} e^{-k(r-\theta)^2/\sigma^2} G(r)\, dr}, \qquad R^* \in (r_0, \infty). \tag{7.4.1}$$

In terms of the Hermite function, the relation between R^* and c can be written in a parametric form with parameter x^* by

$$\begin{cases} R^* = \theta - \dfrac{\sigma^2}{k^2} + \dfrac{\sigma}{\sqrt{k}} x^*, \\ \\ c = \theta - \dfrac{\sigma^2}{k^2} + \dfrac{\sigma}{\sqrt{k}} \dfrac{\int_{x^*}^{\infty} yH(\mu; y)e^{-y^2+ay} dy}{\int_{x^*}^{\infty} H(\mu; y)e^{-y^2+ay} dy}, \end{cases} \qquad x^* \in (x_0, \infty), \tag{7.4.2}$$

or

$$\begin{cases} R^* = c + \dfrac{\sigma}{\sqrt{k}}(x^* - \beta), \quad x^* \in (x_0, \infty), \\ \\ c = \dfrac{k}{2} \dfrac{e^{ax^* - x^{*2}}\{aH(\mu, x^*) - H_x(\mu; x^*)\}}{\int_{x^*}^{\infty} e^{ay-y^2} H(\mu; y) dy}, \end{cases} \qquad x^* \in (x_0, \infty), \tag{7.4.3}$$

where

$$a := \frac{\sigma}{k\sqrt{k}}, \quad \mu := \frac{\sigma^2 - 2k^2\theta}{2k^3}, \quad \beta = \frac{\sqrt{k}}{\sigma}\Big(c + \frac{\sigma^2}{k^2} - \theta\Big)$$

$$x_0 := \inf\{x \mid H_y(\mu; y) < aH(\mu; y) \quad \forall\, y \in (x, \infty)\}.$$

Here the expression for c in (7.4.3) is obtained from (7.4.2) by integrating the identity

$$\frac{\sigma}{\sqrt{k}}\, yH(\mu; y)e^{ay-y^2} = \frac{k}{2}\frac{d}{dy}\Big\{e^{ay-y^2}[H_y - aH]\Big\} + \Big\{\frac{\sigma^2}{k^2} - \theta\Big\}He^{ay-y^2}.$$

7.5 ASYMPTOTIC BEHAVIOR OF $R(T)$ AS $T \to -\infty$

Recall that [7]

$$V_r(R(t),t) = 0, \qquad V_t(R(t),t) = \dot{M}(t) = -me^{c(t-T)}.$$

This implies, by the pde for V in (1.0.5) and by differentiating $V_r(R(t),t) = 0$ that

$$\begin{aligned} V_{rr}(R(t)+,t) &= \frac{2}{\sigma^2}\Big\{rM(t) - m - \dot{M}\Big\} = \frac{2m}{c\sigma^2}(r-c)(1-e^{c(T-t)}), \\ \dot{R}(t) &= -\frac{V_{rt}(R(t)+,t)}{V_{rr}(R(t)+,t)} = \frac{c\,\sigma^2}{2m}\frac{V_{tr}(R(t)+,t)}{(c-R(t))(1-e^{c(T-t)})}. \end{aligned}$$

Hence, to find the asymptotic behavior of $\dot{R}(t)$ as $t \to -\infty$, it suffices to find the asymptotic behavior of $V_{tr}(R(t)+,t)$ as $t \to -\infty$. For this, we consider the function V_t, whose boundary value at $r = R(t)$ is known to be $V_t = \dot{M}(t) = -me^{c(t-T)}$. Also V_t satisfies

$$\Big\{\frac{\partial}{\partial t} + \frac{\sigma^2}{2}\frac{\partial^2}{\partial r^2} + k(\theta - r)\frac{\partial}{\partial r} - r\Big\}V_t = 0, \quad r > R(t), t < T.$$

For the leading order expansion of V_t as $t \to -\infty$, it is natural to consider

$$\zeta(r,t) := \frac{V_t(r,t)}{\dot{M}(t)} = -\frac{V_t}{m\,e^{c(t-T)}}.$$

Then ζ satisfies the following problem:

$$\begin{cases} \Big\{\frac{\partial}{\partial t} + \frac{\sigma^2}{2}\frac{\partial^2}{\partial r^2} + k(\theta - r)\frac{\partial}{\partial r} + (c-r)\Big\}\zeta(r,t) = 0, \quad r > R(t), t < T, \\ \\ \zeta(r,t) = 1 \quad \forall r \leqslant R(t),\ t < T, \qquad \zeta(r,T) = 1 \quad \forall r \in \mathbb{R}. \end{cases} \tag{7.5.1}$$

Here the initial and boundary data for ζ follows from the fact that $V(r,t) = M(t)$ for all $r \leqslant R(t)$ and that $V(\cdot,T) = 0$. We shall prove in a subsequent subsection that there is a limit

$$\lim_{t\to-\infty} \zeta(r,t) = \zeta^*(r) \qquad \forall\, r > R^* \tag{7.5.2}$$

which satisfies the ode problem

$$\begin{cases} \{\frac{\sigma^2}{2}\frac{d^2}{dr^2} + k(\theta - r)\frac{d}{dr} + (c - r)\}\zeta^*(r) = 0 \quad \forall\, r > R^*, \\ \\ \zeta^*(R^*) = 1, \quad \sup_{r \geqslant R^*} \zeta^*(r) < \infty. \end{cases} \tag{7.5.3}$$

For this, we have the following:

Lemma 7.5.1. *Problem* (7.5.3) *has a unique solution, and the solution satisfies*

$$\zeta_r^*(r) < 0, \quad 0 < \zeta^*(r) \leqslant 1 \quad \forall\, r \geqslant R^*.$$

In addition, in terms of the Hermite function, it is given by

$$\zeta^*(r) = \frac{e^{(R^*-r)/k} H(\mu + c/k; x)}{H(\mu + c/k; x^*)},$$

$$x := \frac{\sqrt{k}}{\sigma}\Big(r + \frac{\sigma^2}{k^2} - \theta\Big), \quad x^* := \frac{\sqrt{k}}{\sigma}\Big(R^* + \frac{\sigma^2}{k^2} - \theta\Big), \quad \mu := \frac{\sigma^2 - 2k^2\theta}{2k^3}.$$

Now we can calculate

$$\begin{aligned} \lim_{t\to-\infty} \dot{R}(t)e^{-c(t-T)} &= \frac{c\,\sigma^2}{2} \lim_{t\to-\infty} \frac{\zeta_r(R(t)+, t)}{(R(t) - c)(1 - e^{c(t-T)})} \\ &= \frac{c\sigma^2\zeta_r^*(R^*)}{2(R^* - c)} = \frac{c\,\sigma\sqrt{k}}{2(c - R^*)}\Big\{\frac{\sigma}{k\sqrt{k}} - \frac{H_x(\mu + c/k; x^*)}{H(\mu + c/k; x^*)}\Big\}. \end{aligned}$$

Consequently, using

$$R(t) \;=\; R^* + \int_{-\infty}^{t} \Big\{\dot{R}(\hat{t})e^{-c(\hat{t}-T)}\Big\} e^{c(\hat{t}-T)} d\hat{t}$$

we obtain the asymptotic expansion $R(t) \sim R^* + \rho^* e^{c(t-T)}$ for large negative t, as stated in Theorem 4, where

$$\rho^* := \frac{\sigma^2\zeta_r^*(R^*)}{2(R^* - c)} = \frac{\sigma\sqrt{k}}{2\,(c - R^*)}\Big\{\frac{\sigma}{k\sqrt{k}} - \frac{H_x(\mu + c/k; x^*)}{H(\mu + c/k; x^*)}\Big\}. \tag{7.5.4}$$

Now to complete the proof of Theorem 4, it remains to prove Lemma 7.5.1 and (7.5.2), which will be the subject of the next two subsections.

7.6 ANOTHER HOMOGENEOUS EQUATION

The ode in (7.5.3) is homogeneous and has two linearly independent solutions, at least one of which is unbounded near $r = \infty$ (by using the Wronskian). Hence, if (7.5.3) has a solution, it is unique. Consider

$$\hat{G}(r) = e^{-r/\theta} H(\mu + c/\theta; x).$$

It satisfies

$$\Big\{\tfrac{\sigma^2}{2}\frac{d^2}{dr^2} + k(\theta - r)\frac{d}{dr} + (c - r)\Big\}\hat{G} = 0 \quad \forall\, r \in \mathbb{R}, \quad \hat{G}(\infty) = 0.$$

We shall show that $\hat{G}_r < 0$ on $[R^*, \infty)$. For this notice that V^* satisfies

$$\Big\{\tfrac{\sigma^2}{2}\frac{d^2}{dr^2} + k(\theta - r)\frac{d}{dr} + (c - r)\Big\}V^* = c(V^* - 1) < 0 \quad \forall r > R^*.$$

Thus, the Wronskian of $\hat{G}$ and V^* satisfies

$$\frac{d}{dr}\Big\{e^{-k(r-\theta)^2/\sigma^2}\Big[V_r^*\hat{G} - \hat{G}_r V^*\Big]\Big\} = c(V^* - 1)\hat{G}e^{-k(r-\theta)^2/\sigma^2}.$$

Suppose that $\hat{G}_r < 0$ on $[R^*, \infty)$ is not true. Then there exists $r_1 \geq R^*$ such that $\hat{G}_r(r_1) = 0$ and $\hat{G}_r < 0$ on (r_1, ∞). However, this would imply $\hat{G} > 0$ on $[r_1, \infty)$ and that, since $V_r^*(r_1) \leq 0$,

$$\begin{aligned} 0 &\geqslant V_r^*\hat{G} - \hat{G}_r V^*\Big|_{r=r_1} \\ &= e^{k(r_1-\theta)^2/\sigma^2}\int_{r_1}^{\infty} c(1 - V^*)\hat{G}e^{-k(r-\theta)^2/\sigma^2}dr > 0, \end{aligned}$$

a contradiction. Thus, $\hat{G}_r < 0$ on $[R^*, \infty)$. Consequently, $0 < \hat{G}(r) < \hat{G}(R^*)$ for all $r > R^*$ and

$$\zeta^*(r) = \frac{\hat{G}(r)}{\hat{G}(R^*)} = \frac{e^{(R^*-r)/k}H(\mu + c/k; x)}{H(\mu + c/k; x^*)},$$

is the unique solution to (7.5.3). This completes the proof of Lemma 7.5.1.

7.7 THE LIMIT OF ζ AS $T \to -\infty$.

Here we verify (7.5.2).

1. Since $V(r,t) = M(t)$ for all $r \leqslant R(t)$, we have $V_t(r,t) = M_t(t)$ for all $r \leqslant R(t)$. Also since $V(\cdot, T) = 0$, we know from the pde in (1.0.5) that $V_t(r,T) = -m$ for all $r > c = R(0)$. Thus,

$$\zeta(r,t) = 1 \quad \forall\, r \leqslant R(t), t \leqslant T, \qquad \zeta(r,T) = 1 \quad \forall r \in \mathbb{R}.$$

In addition, 0 is a subsolution and $e^{(c-R^*)(T-t)}$ is a supersolution to ζ so that

$$0 < \zeta(r,t) < e^{(c-R^*)(T-t)} \qquad \forall\, r \geqslant R^*, t < T.$$

This implies that for each $t \leqslant T$, $\zeta(\cdot, t)$ is a bounded function.

2. Let ζ^* be the unique solution to (7.5.3), stated in Lemma 7.5.1. Now using $\zeta(R(t),t) = 1 > \zeta^*(R(t))$ for all $t \leqslant T$ and comparing the function ζ and ζ^* on $\{(r,t) \mid r \geq R(t), t \leq T\}$ we see that $\zeta(r,t) > \zeta^*(r)$ for all $r \geqslant R(t)$. As $\zeta(r,t) = 1 > \zeta^*(r)$ for $r \in (R^*, R(t)]$, we see that

$$\zeta(r,t) > \zeta^*(r) \quad \forall r > R^*, t \leqslant T.$$

3. To estimate the upper bound, let

$$G_1(r) = \zeta^*(r)\Big\{1 + \int_{R^*}^{r} \frac{e^{k(t-\theta)^2/\sigma^2}}{\zeta^{*2}(t)} dt\Big\} \quad \forall r \in \mathbb{R}.$$

This is another solution to the ode in (7.5.3) and satisfies $\lim_{r\to\infty} G_1(r) = \infty$. Define

$$\delta(t) := \inf\{\delta > 0 \mid \zeta(r,t) \leq \zeta^*(r) + \delta G_1(r) \quad \forall r \geq R^*\}, \quad \forall t \leqslant T.$$

Since $\zeta(\cdot, t)$ is bounded and $G_1(\infty) = \infty$, $\delta(t)$ is positive and finite. In addition,

$$\zeta(r,t) \leqslant \zeta^*(r) + \delta(t) G_1(r) \quad \forall\, r \geqslant R^*, t \leqslant T.$$

Furthermore, since $\dot{R} > 0$, we have $\zeta(r) + \delta(\hat{t})G_1(r)|_{r=R(t)} \geq \zeta(R(t), \hat{t}) = 1$ for all $t < \hat{t}$. Hence, comparing $\zeta(r,t)$ and $\zeta^*(r) + \delta(\hat{t})G_1(r)$ on $\{(r,t) \mid r \geqslant R(t),\ t \leqslant \hat{t}\}$ we have

$$\zeta(r,t) < \zeta^*(r) + \delta(\hat{t})G_1(r) \quad \forall\, r > R(t), t < \hat{t} \leqslant T.$$

Hence, $0 < \delta(t) < \delta(\hat{t})$ for all $t < \hat{t}_1 \leqslant T$. Consequently, there exists

$$\delta_* := \lim_{t \to -\infty} \delta(t) \in [0, \infty).$$

4. Here we show that $\delta_* = 0$. Suppose on the contrary that $\delta_* > 0$.

(a) On the spatially bounded domain $\{(r,t) \mid r \in [R^*, c+2], t < T\}$, let $\hat{\zeta}$ be the solution to the boundary value problem

$$\begin{cases} \left\{\frac{\partial}{\partial t} + \frac{\sigma^2}{2}\frac{\partial^2}{\partial r^2} + k(\theta - r)\frac{\partial}{\partial r} + (c - r)\right\}\hat{\zeta}(r,t) = 0, \quad r \in (R(t), c+2), t < T, \\ \\ \hat{\zeta}(c+2, t) = \zeta^*(c+2) + \delta(t)G_1(c+2) \quad \forall t < T, \\ \\ \hat{\zeta}(r, T) = 1 \quad \forall r \in [R^*, c+2], \quad \hat{\zeta}(r,t) = 1 \quad \forall r \in [R^*, R(t)], t \leqslant T. \end{cases}$$

By comparison,

$$\zeta(r,t) \leqslant \hat{\zeta}(r,t) \quad \forall\, r \in [R^*, c+2], \quad t \leqslant T.$$

Also, using an elementary pde analysis, say the Fourier series, one can show that uniformly in $r \in [R^*, c+2]$, $\lim_{t \to -\infty} \hat{\zeta}(r,t) = \hat{\zeta}(r, -\infty)$ where $\hat{\zeta}(r, -\infty)$ is the solution to the ode in (7.5.3) on $[R^*, c+2]$ with the boundary value

$$\hat{\zeta}(R^*, -\infty) = 1, \quad \hat{\zeta}(c+2, -\infty) = \zeta^*(c+2) + \delta_* G_1(c+2).$$

By comparison, it is easy to see that $\hat{\zeta}(r, -\infty) < \zeta^*(r) + \delta_* G_1(r)$ for all $r \in [R^*, c+2)$. Thus, there exists $\delta_1 \in (0, \delta_*)$ such that

$$\hat{\zeta}(r, -\infty) < \zeta^*(r) + \delta_1 G_1(r) \quad \forall r \in [R^*, c+1].$$

This also implies that there exists $t_1 \ll -1$ such that

$$\zeta(r,t) < \zeta^*(r) + \delta_1 G_1(r) \quad \forall r \in [R^*, c+1],\ t \leqslant t_1.$$

(b) Now we compare the function $\zeta(r,t)$ and $\zeta^*(r)+\delta_1 G_1(r)$ on $[c+1,\infty)\times(-\infty,t_1]$. Since $\delta_1 < \delta_*$, for each fixed $t < t_1$, we see from the definition of δ_* that the maximum of

$$\varphi(r,t) := \zeta(r,t) - [\zeta^*(r) + \delta_1 G_1(r)], \quad r \in [R^*, \infty)$$

is positive. As $\varphi(r,t) < 0$ for all $r \in [R^*, c+1]$ and $\varphi(\infty,t) = -\infty$, there exists $\hat{r}(t) \in (c+1,\infty)$ such that $0 < \varphi(\hat{r},t) = \max_{r\geq R^*}\varphi(r,t)$. Using $\varphi_r(\hat{r},t) = 0 \geq \varphi_{rr}(\hat{r},t)$ and the pde for φ we have

$$\begin{aligned} 0 &= \varphi_t + \frac{\sigma^2}{2}\varphi_{rr} + (\eta-\theta r)\varphi_r + (c-r)\varphi\Big|_{r=\hat{r}} \\ &\leq \varphi_t(\hat{r},t) + (c-\hat{r})\varphi(\hat{r},t). \end{aligned}$$

Hence, denoting $K(t) := \varphi(\hat{r},t) = \max_{r>R(t)}\varphi(r,t)$, we have

$$\begin{aligned} \frac{d}{dt}K(t) &:= \liminf_{h\to 0}\frac{K(t+h)-K(t)}{h} \geq \lim_{h\to 0}\frac{\varphi(\hat{r},t+h)-\varphi(\hat{r},t)}{h} = \varphi_t(\hat{r},t) \\ &\geq (\hat{r}-c)\varphi(\hat{r},t) \geq \varphi(\hat{r},t) = K(t). \end{aligned}$$

Thus $\frac{d}{dt}[K(t)e^{-t}] \geqslant 0$ for all $t < t_1$. After integration, this gives

$$0 < K(t) \leq K(t_1)e^{t-t_1} \quad \forall\, t < t_1, \qquad \lim_{t\to-\infty} K(t) = 0.$$

This implies that for all sufficiently large negative t, $\max_{r\geqslant R^*}\varphi(r,t) = K(t) \leq \frac{1}{2}(\delta_* - \delta_1)\min_{r\geq R^*}G_1(r)$, so that $\zeta(r,t) \leq \zeta^*(r) + \frac{1}{2}(\delta_1+\delta_*)G_1(r)$ for all $r \geq R^*$ and sufficiently large negative t, contradicting the definition of δ_*.

In conclusion, we must have $0 = \delta_* = \lim_{t\to-\infty}\delta(t)$.

5. Denote $K_1(t) = \max_{r\in[R^*,c+2]}|\zeta(r,t)-\zeta^*(r)|$. Then

$$0 \leqslant \lim_{t\to-\infty} K_1(t) \leq \sup_{r\in[R^*,c+2]} G_1(r) \lim_{t\to-\infty}\delta(t) = 0.$$

Set

$$K_2(t) := \sup_{r \geqslant c+1} |\zeta(r,t) - \zeta^*| = \lim_{\varepsilon \searrow 0} \max_{r \geqslant c+1} [\zeta(r,t) - \zeta^*(r) - \varepsilon G_1(r)].$$

Using a similar idea as in **4(b)** one can show that

$$K_2(t) \leqslant K_1(t) + K_2(T) e^{(t-T)} \quad \forall\, t \leqslant T.$$

This implies that $\lim_{t \to -\infty} K_2(t) = 0$. Thus,

$$\lim_{t \to -\infty} \sup_{r \geqslant R^*} |\zeta(r,t) - \zeta^*(r)| = 0.$$

Finally since $\dot{R}$ is bounded in $(-\infty, T-1]$ (c.f.[7]), one can use a local regularity theory for parabolic equations to show that $\lim_{t \to -\infty} \zeta_r(R(t)+, t) = \zeta_r(R^*+)$. This completes the proof of (7.5.2) and also the proof of Theorem 4.

8.0 GLOBAL APPROXIMATION

Let $\tau = T - t$. So far we have discussed the behavior of $R(T-\tau)$ for small and large τ :

$$R(T-\tau) \sim \begin{cases} c - \bar{\kappa}\sigma\sqrt{\tau} & \text{when} \;\; 0 \leqslant \tau \ll 1, \\ \\ R^* + \rho^* e^{-c\tau} & \text{when} \;\; \tau \gg 1. \end{cases}$$

We can combine both to obtain a unified approximation that is valid for both small and large τ, and hopefully, for all τ. Here we propose two approximations.

8.1 THE SIMPLE GLOBAL APPROXIMATION

We seek a simple approximation formula for $R(T-\tau)$ such that (i) it has asymptotic expansion $c + \bar{\kappa}\sigma\sqrt{\tau}$ for small positive τ and (ii) it exponentially approaches R^* for large τ. For this, we seek an approximation of the form

$$R_I(T-\tau) := c - \bar{\kappa}\sigma\sqrt{\frac{1 - e^{-b^*\tau}}{b^*}}.$$

For any $b^* > 0$, this approximation has the right asymptotic behavior for small τ. To make it match with the large τ behavior, we need

$$R^* = c - \sigma\bar{\kappa}\sqrt{\frac{1}{b^*}} \quad \Longleftrightarrow \quad b = \Big(\frac{\bar{\kappa}\sigma}{c - R^*}\Big)^2$$

Hence, using the information that $R \sim R^*$ as $t \to -\infty$, we have the **first approximation for** R:

$$R_I(T-\tau) := c - (c - R^*)\sqrt{1 - e^{-b^*\tau}}, \tag{8.1.1}$$

where b^* is defined by

$$b^* := \Big(\frac{0.474\sigma}{c - R^*}\Big)^2. \tag{8.1.2}$$

Numerical evidence shows that when θ is close to c, the approximation is very accurate. In Figure 8, the relative error is as small as 2 percent:

$$\frac{\max_{t<T} |R(t) - R_I(t)|}{c - R^*} \approx 0.02.$$

8.2 AN ENHANCED APPROXIMATION

In the first approximation proposed above, we only used the information $R \sim R^*$ as $t \to -\infty$. Since we have more detailed information on the asymptotic behavior for very large time, $R \sim R^* + \rho^* e^{-c\tau} = O(e^{-2c\tau})$, as $t \to -\infty$, we can interpolate these information into our approximation and achieve an even better approximation $R(t) \approx R_{II}(t)$ where

$$R_{II}(T-\tau) := c - \frac{0.474\sigma\sqrt{1-e^{-2c\tau}}}{\sqrt{2c}} + \rho^*(e^{-c\tau} - e^{-2c\tau}) + \Big[R^* - c + \frac{0.474\sigma}{\sqrt{2c}}\Big](1 - e^{-2c\tau}).$$

To derive the above formula, we first propose that the terms $e^{-c\tau}$ and $e^{-2c\tau}$ should be incorporated, as suggested by $R \sim R^* + \rho^* e^{-c\tau} = O(e^{-2c\tau})$. The idea for incorporating term $c-\dfrac{0.474\sigma\sqrt{1-e^{-2c\tau}}}{\sqrt{2c}}$ into our formula is same as that for the first approximation, as it has asymptotic expansion $c-0.474\sigma\sqrt{\tau}$ for small τ. But the limit of this term as $\tau \to \infty$ is $c-\dfrac{0.474\sigma}{\sqrt{2c}}$ instead of R^*. To balance this we incorporate $\left[R^* - c + \frac{0.474\sigma}{\sqrt{2c}}\right](1-e^{-2c\tau})$ into our formula. Lastly, we notice $\rho^*(e^{-c\tau}-e^{-2c\tau}) \to 0$ as $\tau \to 0$.

It is a pleasant surprise to find in Figure 8 that for a typical parameter set, the relative error of the second approximation is reduced to 4 per thousand:

$$\frac{\max_{t<T}|R(t)-R_{II}(t)|}{c-R^*} \approx 0.004.$$

We have tested the accuracy of both approximations with various data input and the results are very consistent for all reasonable parameters derived from the MLE method.

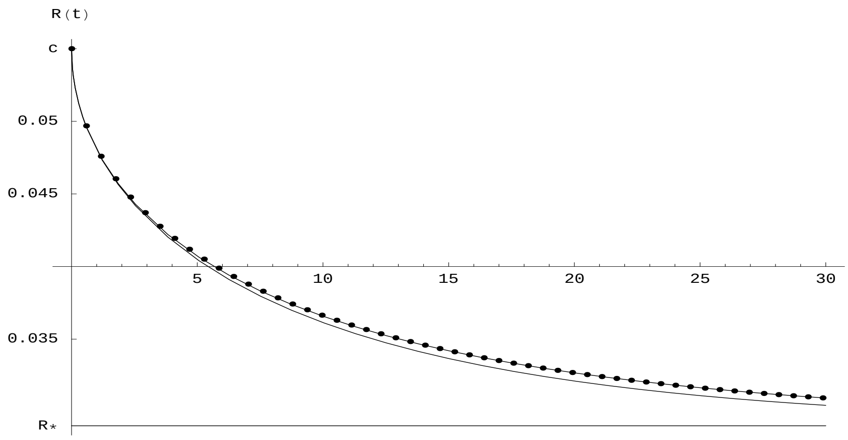

Figure 8: Dots represent the "true" solution, calculated by using 2048 division points in the upgraded scheme outlined in Chapter 5. The curve "on the dots" is the second approximation with maximum relative error 0.004 which is not discernable from the plot. The curve below the dots is the first approximation, with relative error 0.02. In this example, the following typical data from the US economy is used: $c = 0.055, \theta = 0.050, \sigma = 0.015, k = 0.150$. For this example, $R^* = 0.029, \rho^* = 0.0086$.

9.0 NUMERICAL EXPERIMENTS

In this Chapter we would like to provide more comprehensive examples of our numerical results and some details about various aspects of our numerical codes to get a glimpse of how these results were achieved, especially the claims made on the accuracy of our analytical approximation formulas.

First of all, we have tested the whole range of all the parameters appearing in the Vasicek model, which we have obtained via MLE method. Of course we cannot cover the continuous values of the parameters, but we tried with reasonable discrete values. We did numerical experiments by changing only one parameter, say c, for instance, at one time, and kept the three others fixed. Since historically c varies from 0.01 to 0.08, we simulated all cases for c=0.01, 0.02, ..., 0.08. Then we did the same for θ, and so on. Based on a large amount of numerical experimentation we made claims about our analytical formulas.

As shown in previous chapters, the free boundary of the problem is obtained by Newton iteration based on the integral identities. The accuracy requirement is 10^{-8} for each step of the iteration, i.e. the iteration loop will not stop until the difference of the results from two consecutive iterations falls within the tolerance of 10^{-8}. The convergence rate and the average number of iterations required is based on this tolerance.

When we calibrate our approximation formulas, we first need to decide a time interval on which we carry out the numerical computation. Since $T = 30$ years is the longest maturity for fixed rate mortgages, we decided on this value for all our numerical computations and for testing the accuracy of our approximation formulas.

We also need to make sure that the "true" boundary (numerically calculated) is precise enough before we compare its difference with our approximation formulas. In our computations, we set double tolerances requirements to address this. First, we set the accuracy requirement to be Tolerance1=10^{-6} at T=30. Note this is needed in addition to the tolerance for each Newton iteration because although each iteration is very accurate, the errors can accumulate after many steps. Secondly, we also require that the L^∞ error between two consecutive numerical boundaries (from time 0 to time 30) be within Tolerance2=10^{-5} as we change the mesh size in the time discretization. It is because of this double tolerance requirement that we believe the numerically computed boundary can be regarded as the "true" theoretical boundary.

9.1 A COMPREHENSIVE EXAMPLE

Here we first provide a complete example of our numerical output for one typical set of parameters. Figure 9 shows the numerical boundary, $R(t)$, the approximation boundary, R_I and R_{II}. The following are the various numerical parameters associated with the outputs.

1. T=30, $c = 0.06$, $\theta = 0.045$, $k = 0.15$, $\sigma = 0.015$,
2. the number of mesh points N=4096,
3. Tolerance for each Newton iteration = 10^{-8},
4. Tolerance for consecutive numerical boundaries at $T = 30$ as N increses = 10^{-6},
5. Tolerance of L^∞ error for consecutive numerical boundaries = 10^{-5},
6. $R^* = 0.0394434$, $\rho^* = 0.0044028$,
7. the constant appearing in the first approximation $b^* = 0.1191$,
8. time at which the error of $|R_I(t) - R(t)|$ reaches maximum=11.24,
9. time at which the error of $|R_{II}(t) - R(t)|$ reaches maximum=13.36,

10. $\max_{t<T} |R_I(t) - R(t)| = 0.001085$,

11. $\max_{t<T} |R_{II}(t) - R(t)| = 0.0000715$,

12.

$$\frac{\max_{t<T} |R_I(t) - R(t)|}{c - R^*} = 0.04906 < 5\%, \tag{9.1.1}$$

13.

$$\frac{\max_{t<T} |R_{II}(t) - R(t)|}{c - R^*} = 0.00348 < 0.4\%, \tag{9.1.2}$$

14. $|R_I(T) - R(T)| = 0.000575$,

15. $|R_{II}(T) - R(T)| = 0.0000249$,

16. $|R(T) - R^*| = 0.00086492$.

Since we are interested in where the maximum error will occur for each approximations, we provide the plots of the approximation error against time in Figure 10. While in Figure 11 the relative errors of the two approximations were recorded, where relative errors are defined as $\max_{t<T} \frac{|R(t)-R_I(t)|}{R(T)-R(-\infty)}$, $\quad \max_{t<T} \frac{|R_(t)-R_{II}(t)|}{R(T)-R(-\infty)}$.

Since we set very strict accuracy requirement for the numerical computation, so we cannot prescribe a uniform mesh size T/N for every computation. Rather, we let the program run until the prescribed accuracies are achieved. Fortunately the Newton algorithm has proven to be very fast in our scheme. For most of the several hundreds of cases we computed, the values of N are about 4096. For very extreme cases, N needed to be as large as 8192, but never more than 16384.

9.2 VARIATION OF THE OPTIMAL TERMINATION BOUNDARY

It is of interest to numerically investigate how the boundary behaves in time, and how it will change when the parameters change. Here we first display a few numerical results, where one can observe the pattern of the variations of the optimal termination boundary.

In Figure 12 and Figure 13 we display the optimal termination boundary as one of the parameter changes, keeping the others fixed. From the figure, one can reasonably conclude that the optimal mortgage termination boundary $r_t = R(c, \theta, k, \sigma; t)$ is

1. increasing in c,
2. decreasing in θ,
3. increasing in k,
4. decreasing in σ.

As the optimal termination boundary changes, so does the R^*. We to want to know for what kind of parameters R^*=0. As observed in a real economy, the probability of the interest rate being zero or negative is very low (if not impossible). So it is reasonable to say that, in reality, a zero or negative R^* will not likely be encountered. By investigating in which situation R^* is zero we will get another view of why c is usually greater than θ.

As we showed in our analysis as well as by the numerical demonstration, our approximation formulas are especially accurate for the cases where (1) c is closer to θ and (2) c is greater than θ. In Figure 14 we provide a plot of c against θ, where R^*=0. This plot roughly divides the c, θ plane into two regions, one is where $c > \theta$ and one where $c < \theta$. Since we also numerically demonstrated that R^* is increasing in c and decreasing in θ, we can safely conclude that for R^* to be positive, it is necessary for c to be greater than θ.

9.3 ACCURACY OF THE APPROXIMATION FORMULAS

Here we want to provide numerical demonstrations to show the accuracy of the two approximation formulas.

In Figures 15, 16, 17, 18, and 19 we display the relative errors of our two analytical approximation formulas for the optimal boundary, as one of the parameter changes and the others are kept fixed. One can see that when $0 < \theta \leqslant c$, both approximations are extremely accurate. As we can observe from the historical data, it is very rare (if not impossible) for the mortgage rate c to be lower than the treasury bill rate θ.

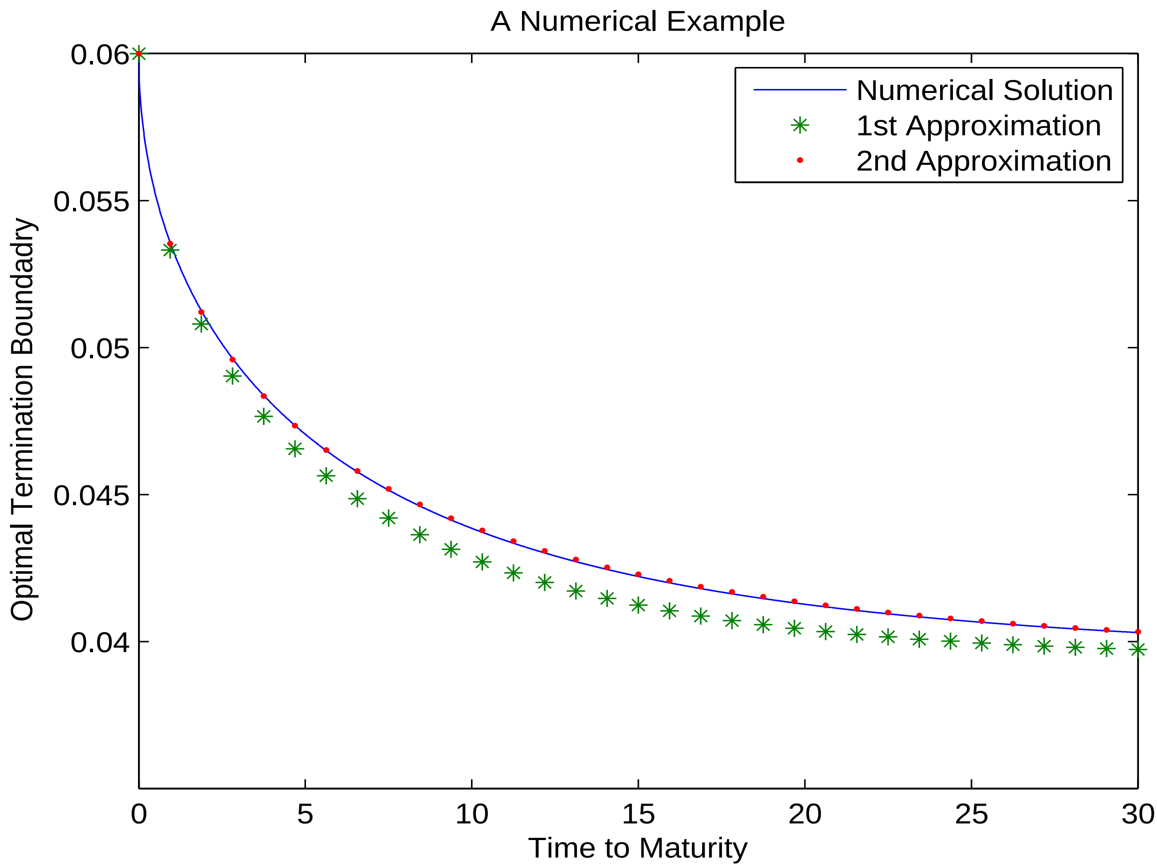

Figure 9: Optimal termination boundary $r_t = R(t)$ as function of time $T - t$ to maturity. The parameters used for this example are: $c = 0.06, \theta = 0.045, k = 0.15, \sigma = 0.015$.

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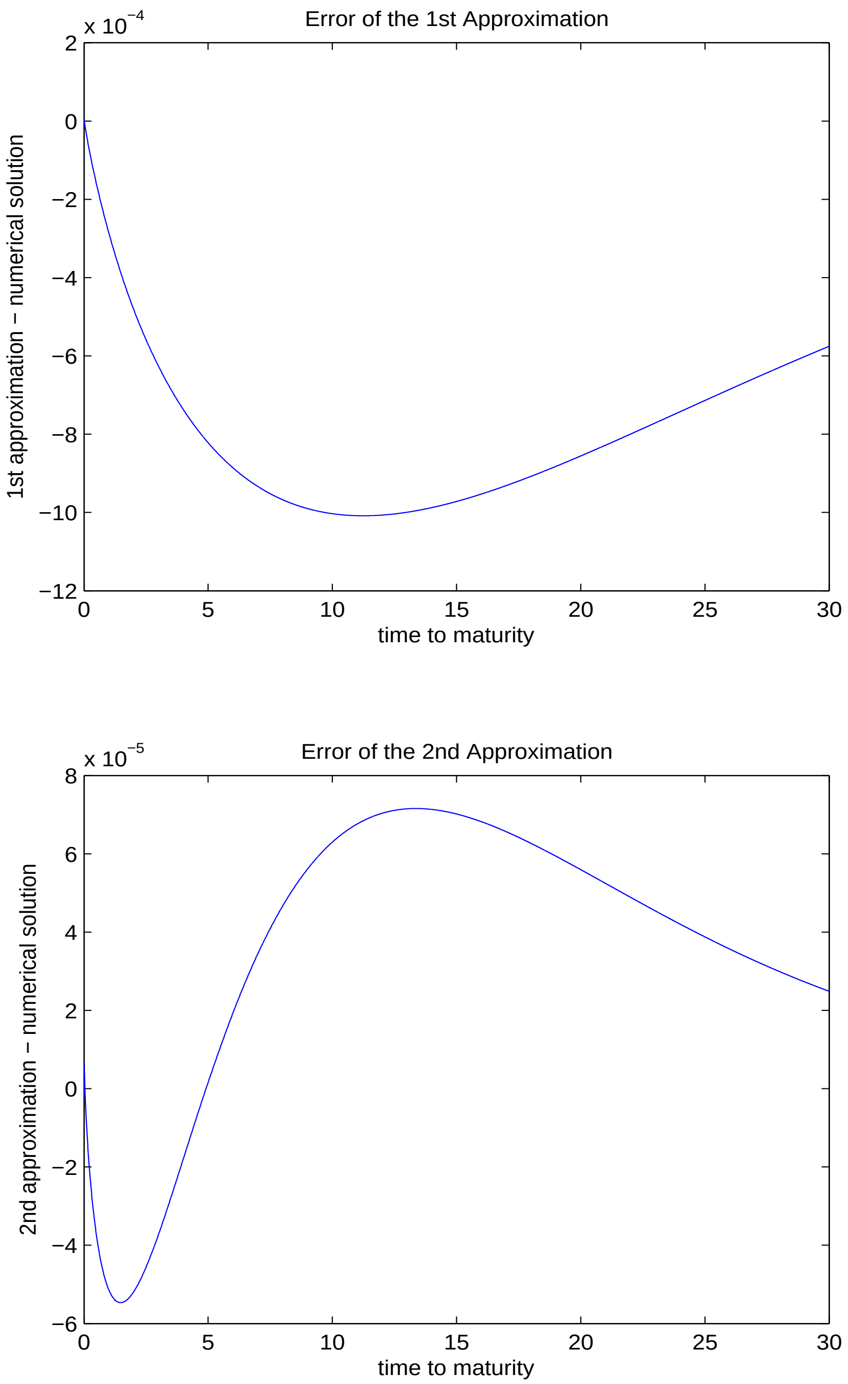


Figure 10: Approximation errors recorded for each time. The top plot is for the 1st approximation and the bottom one is for the 2nd approximation. Here $c = 0.06, \theta = 0.045, k = 0.15, \sigma = 0.015$.

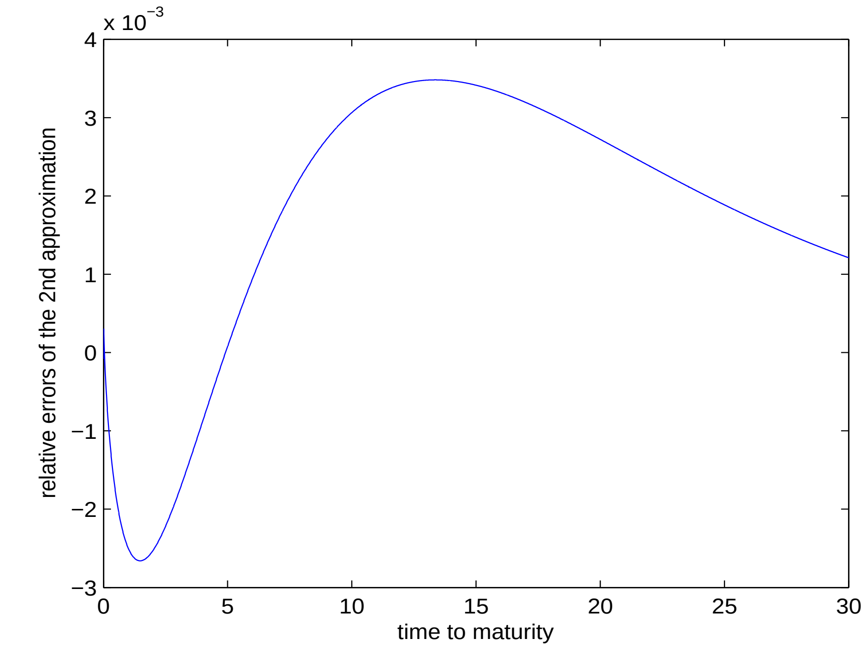
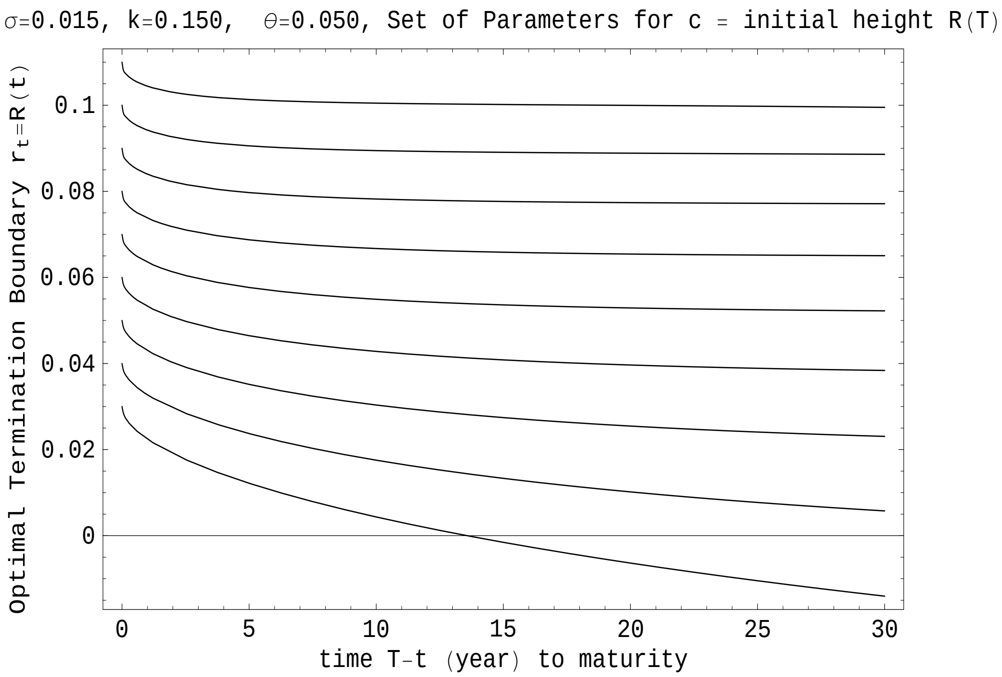


Figure 11: Relative approximation errors recorded for each time. The top plot is for the 1st approximation and the bottom one is for the 2nd approximation. Here $c = 0.06, \theta = 0.045, k = 0.15, \sigma = 0.015$.



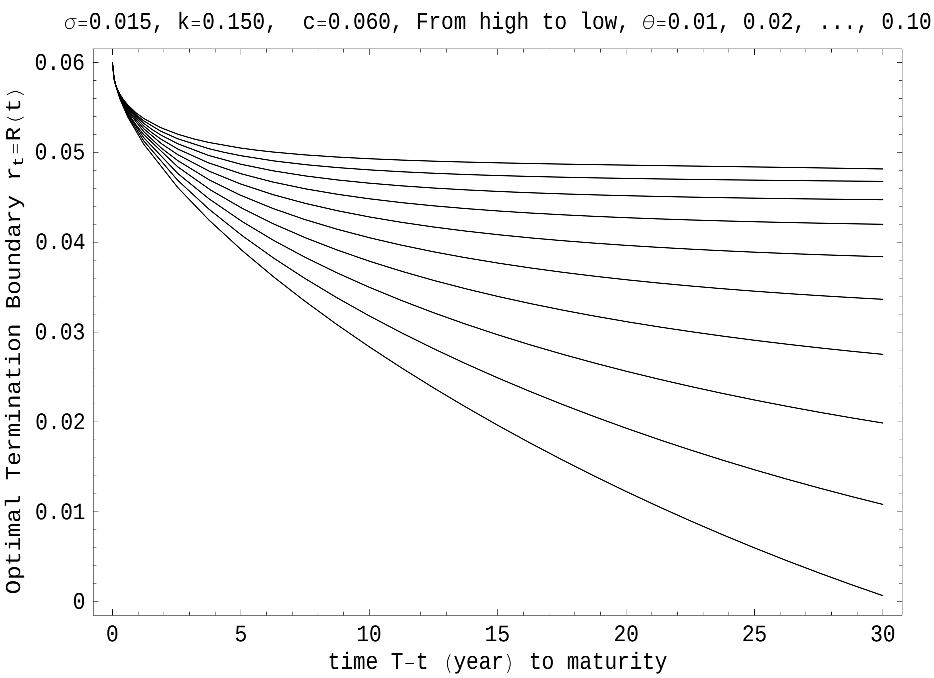
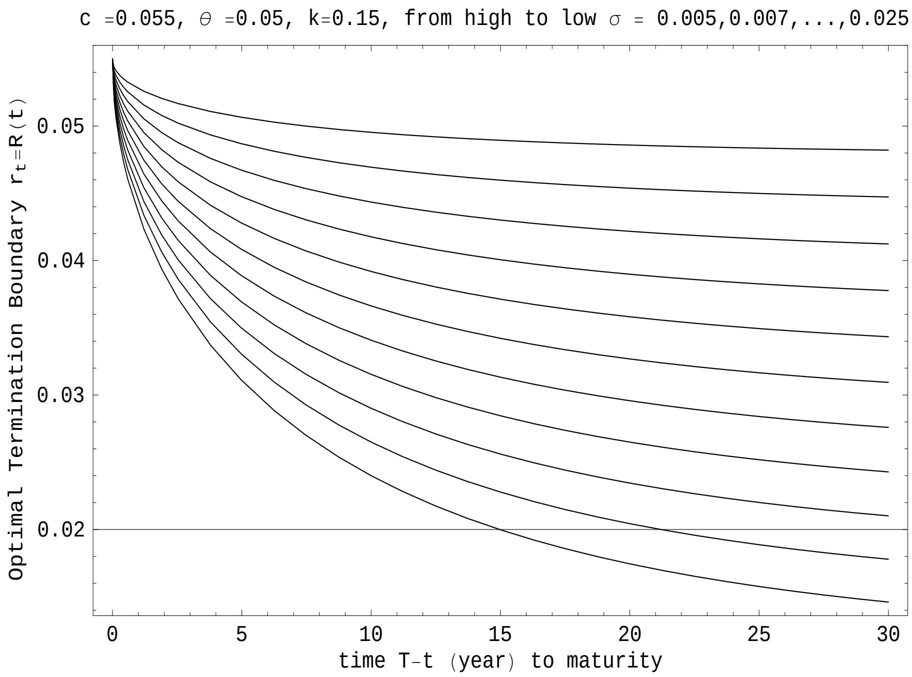


Figure 12: Optimal termination boundary $r_t = R(t)$ as function of time $T - t$ to maturity. Each set of curves corresponds to changing one of the parameters.



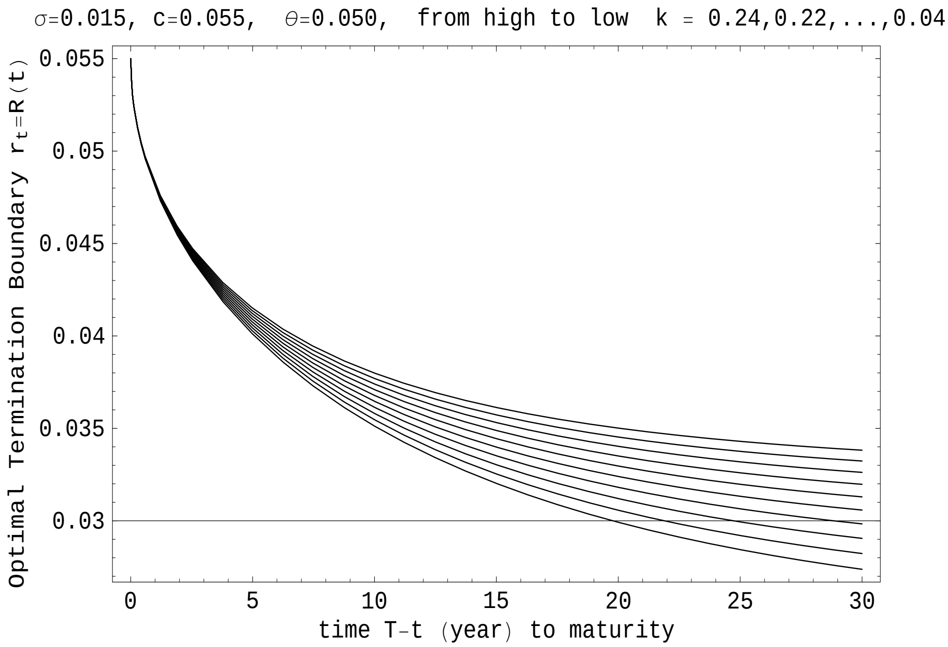


Figure 13: Optimal termination boundary $r_t = R(t)$ as function of time $T - t$ to maturity. Each set of curves corresponds to changing one of the parameters.

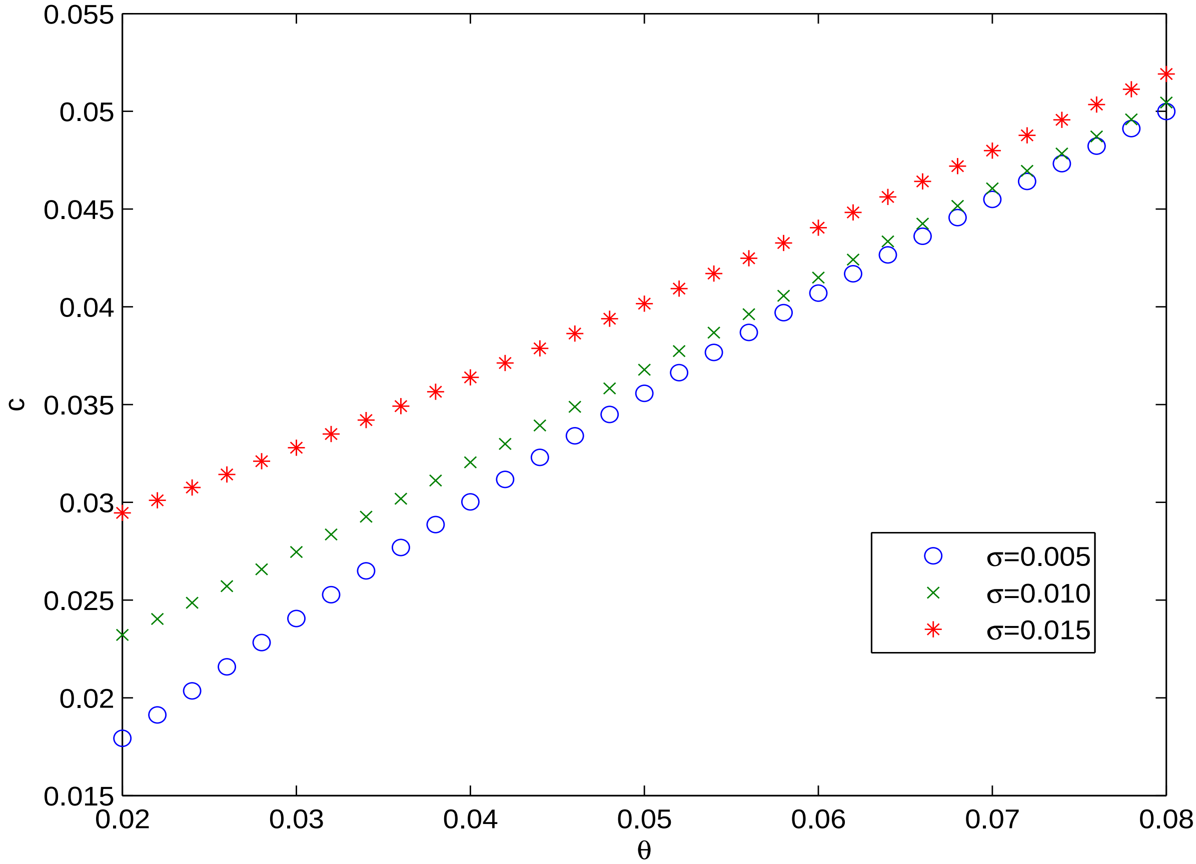


Figure 14: This figure shows the relation between c and θ when R^*=0. For this illustration, we have kept k=0.15, the average value obtained through MLE. Since in general $c > \theta$, so R^* is most often greater than 0.

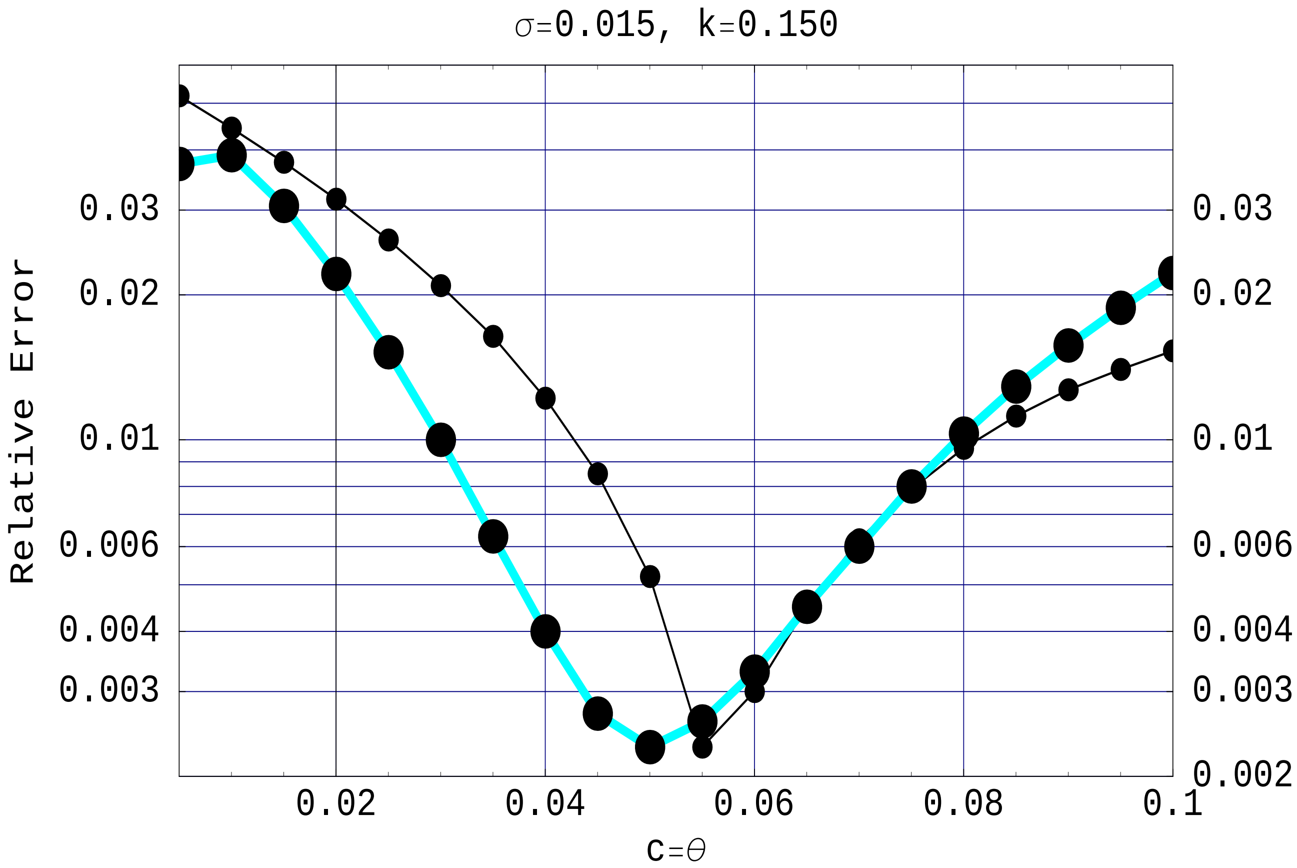


Figure 15: Relative errors of the first approximation R_I (thin curve) and the second approximation R_{II} (thick curve) as functions of parameters.

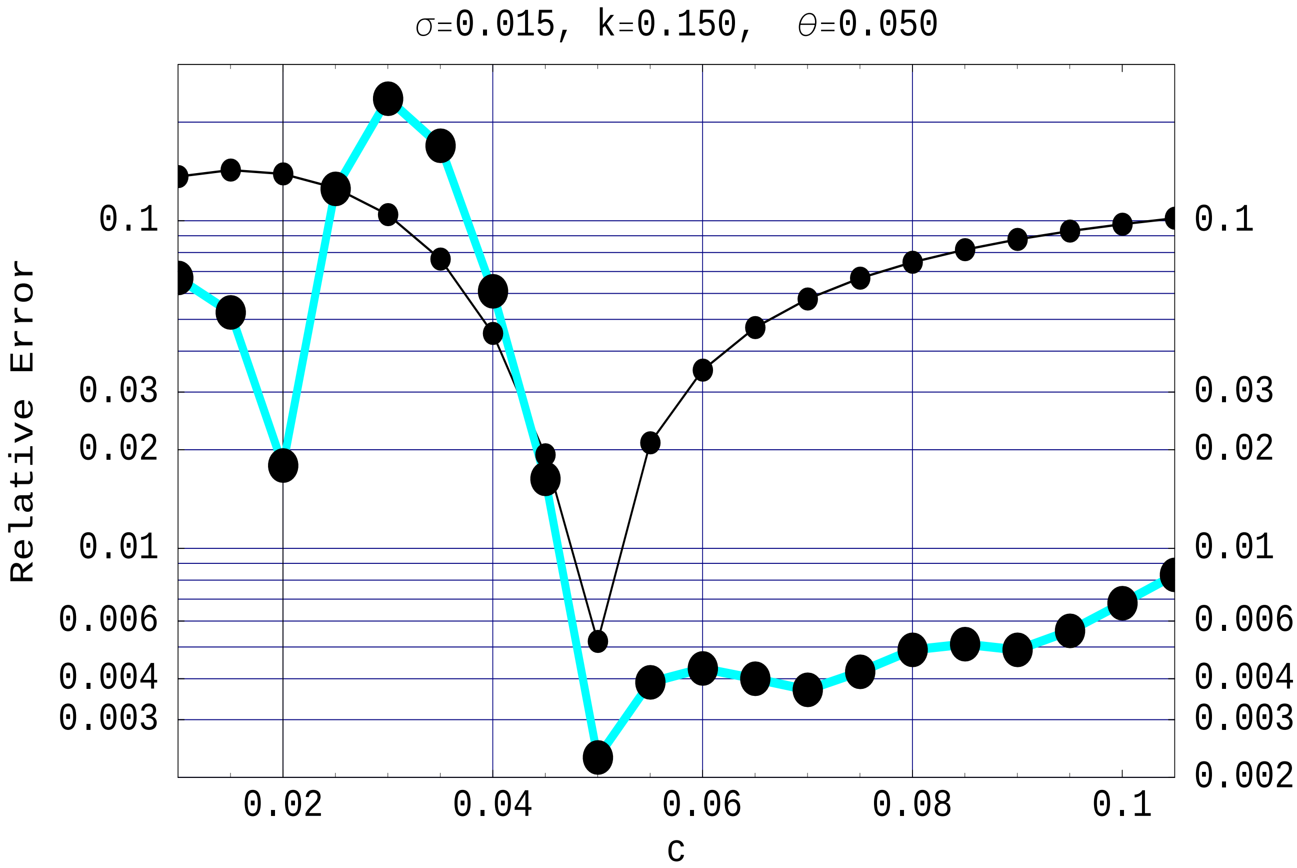


Figure 16: Relative errors of the first approximation R_I (thin curve) and the second approximation R_{II} (thick curve) as functions of parameters.

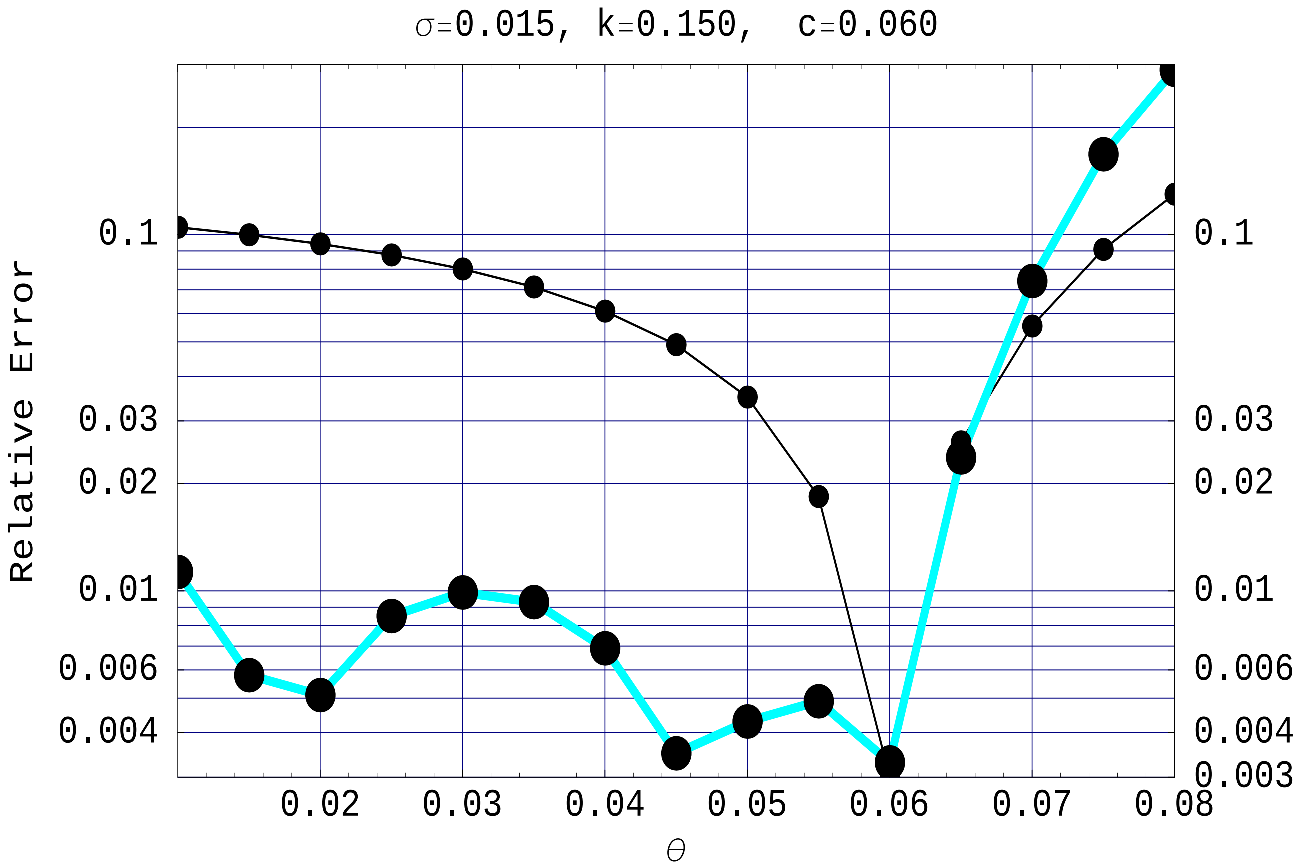


Figure 17: Relative errors of the first approximation R_I (thin curve) and the second approximation R_{II} (thick curve) as functions of parameters.

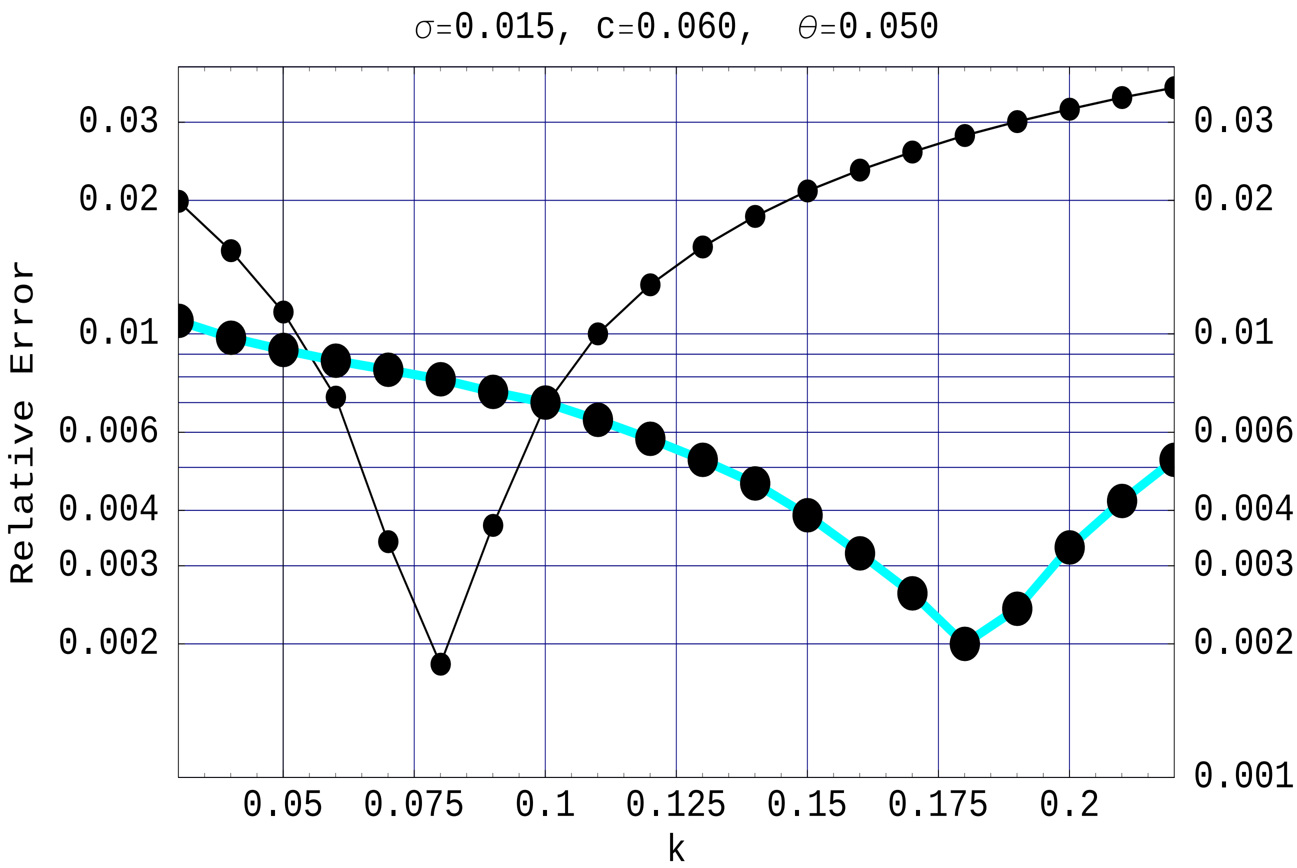


Figure 18: Relative errors of the first approximation R_I (thin curve) and the second approximation R_{II} (thick curve) as functions of parameters.

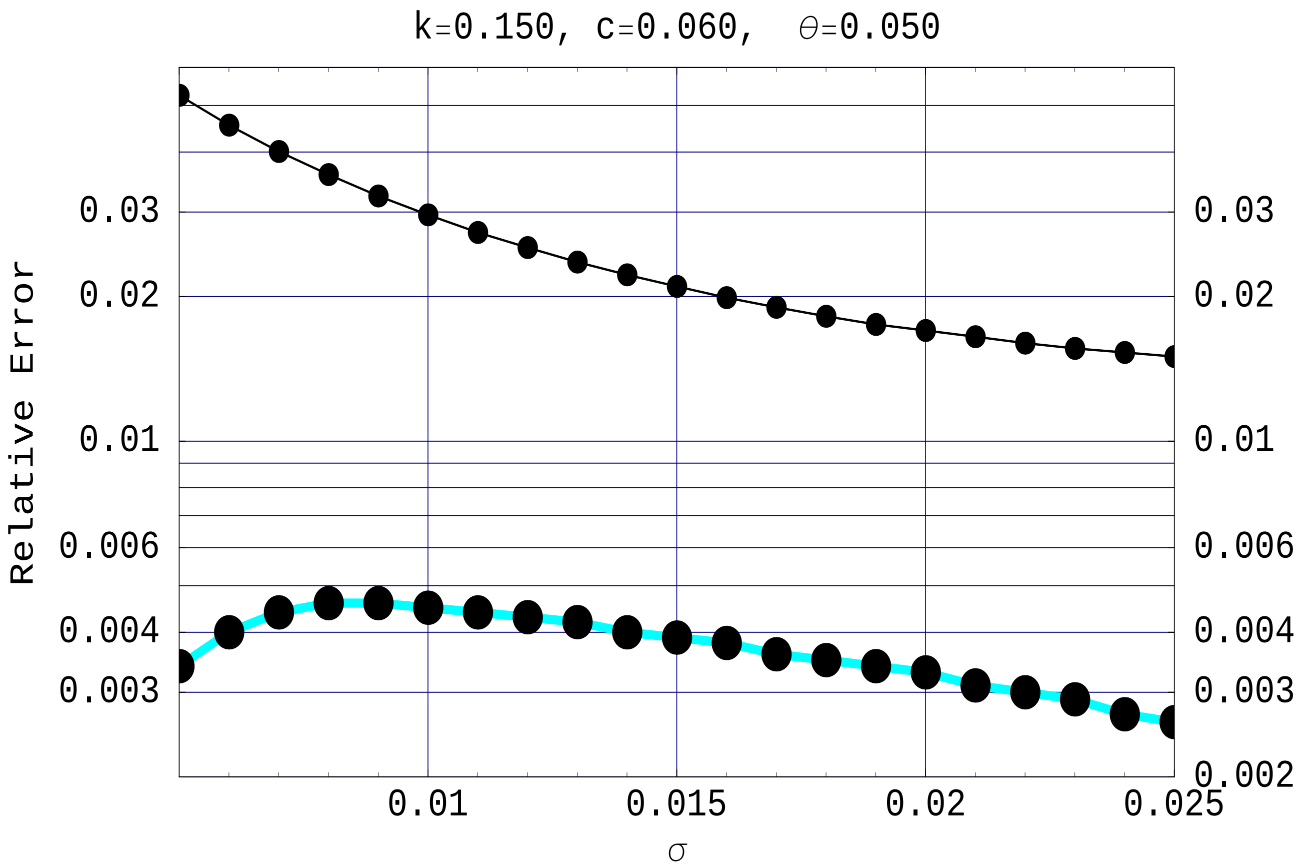


Figure 19: Relative errors of the first approximation R_I (thin curve) and the second approximation R_{II} (thick curve) as functions of parameters.

APPENDIX

FUNDAMENTAL SOLUTION

The main purpose of the Appendix is to show an equivalent approach to derive the key integral identities, appearing in Chapter 4, which were used for designing the Newton scheme to solve the free boundary. We first explain some mathematical motivation for this approach, then use the Fourier transformation method to derive the explicit Fundamental Solution associated with the problem. Lastly we end up with the desired integral equations.

A.1 MATHEMATICAL MOTIVATION

When handling a free boundary PDE system, it is often tempting to investigate if we can find a Fundamental Solution for the homogeneous PDE without boundaries. If this is can be done, then the solution to the system is easy to formulate. From now on, we let t be the time to expiry (note in Chapter 3, we used τ to denote time to expiry), then from (1.0.5) the value of the contract V, at any time $t > 0$ and the corresponding interest rate r, must satisfy

$$\begin{cases} \dfrac{\partial V}{\partial t} - \dfrac{\sigma^2}{2}\dfrac{\partial^2 V}{\partial r^2} - k(\theta - r)\dfrac{\partial V}{\partial r} + rV = m & \text{if } V(r,t) < M(t), t > 0, \\ 0 \leqslant V(r,t) \leqslant M(t) := \dfrac{m}{c}(1 - e^{-ct)}) & \forall\, t > 0, r \in \mathbb{R}. \end{cases} \tag{A.1.1}$$

Define

$$L(V) := \frac{\sigma^2}{2}\frac{\partial^2 V}{\partial r^2} + k(\theta - r)\frac{\partial V}{\partial r} - rV \ , \tag{A.1.2}$$

Without loss of generality, we can assume $m = 1$. We see that, according to the analysis done in the Chapter 1, (A.1.1) is equivalent to

$$\begin{cases} \dfrac{\partial V}{\partial t} - L(V) = F(r,t), & \text{for } \quad r \in \ \mathbb{R}, t > 0 \\ V = \frac{1}{c}(1 - e^{-ct}), & \text{for } \quad r \leq R(t), t > 0 \\ V(r,0) = 0 & \\ V_r \equiv 0 \text{ on } R(t) & \end{cases} \tag{A.1.3}$$

where

$$F(r,t) = \begin{cases} 1, & \text{for } \quad r > R(t), t > 0 \\ \dfrac{r}{c} + (1 - \dfrac{r}{c})e^{-ct}, & \text{for } \quad r \leq R(t), t > 0 \end{cases} \tag{A.1.4}$$

If we can find the Fundamental Solution, say $G(r, y, t, \tau)$ to the PDE for V, we would be able to write the solution to the above system as

$$V(x,t) = \int_0^t \int_{-\infty}^{\infty} F(y,\tau) G(x, y, t, \tau) dy d\tau.$$

And then the following manipulations can be made to find the integral identities on which a Newton iteration scheme can be designed.

$$V = \int_0^t \int_{-\infty}^{R(\tau)} (\frac{y}{c} + (1 - \frac{y}{c}))e^{-c\tau} G(r, y, t, \tau) dy d\tau + \int_0^t \int_{R(\tau)}^{\infty} G(r, y, t, \tau) dy d\tau$$

$$= \int_0^t \int_{-\infty}^{\infty} (\frac{y}{c} + (1 - \frac{y}{c}))e^{-c\tau} G(r, y, t, \tau) dy d\tau - \int_0^t \int_{R(\tau)}^{\infty} G(r, y, t, \tau)(1 - \frac{y}{c})(e^{-c\tau} - 1) dy d\tau$$

Denote

$$I = \int_{-\infty}^{\infty} (\frac{y}{c} + (1 - \frac{y}{c}))e^{-c\tau} G(x, y, t, \tau) dy$$

We are going to show that $I = M(t)$. To this end we do not evaluate I directly. Instead, we integrate the differential form of G with respect to y over the whole space. Let $s = t - \tau$. Because G, by the nature of being the Fundamental Solution to the PDE in (A.1.1), satisfies

$$G_s - \frac{\sigma^2}{2} G_{yy} + [k(\theta - y)G]_y + yG = 0$$

and G decays exponentially in y, as will become apparent after we derive its explicit formula, we can integrate the above equation with respect to y in the whole space, thus yield

$$\frac{d}{ds} \int_R G dy = - \int_R y G dy$$

Now

$$\begin{aligned} I &= e^{-c\tau} \int_R G dy + \frac{1 - e^{-c\tau}}{c} \int y G dy \\ &= e^{-c\tau} \int_R G dy - \frac{1 - e^{-c\tau}}{c} \frac{d}{ds} \int G dy \\ &= -\frac{1}{c} \frac{d}{ds} \{(1 - e^{-c\tau}) \int_R G dy\} \end{aligned}$$

Thus, using the fact that $\int_R G dy = 1$ at $\tau = t$, we get

$$\int_0^t I d\tau = \int_0 -\frac{1}{c}\frac{d}{ds}\{(1-e^{-c\tau})\int_R Gdy\} = \frac{1}{c}(1-e^{-ct}) \equiv M(t).$$

Let

$$U(x,t) = \int_0^t \int_{R(\tau)}^{\infty} G(r,y,t,\tau)(1-\frac{y}{c})(e^{-c\tau}-1)dyd\tau$$

Then

$$V(r,t) = M(t) - U(r,t)$$

And now it is straightforward to translate the the boundary condition of $V(r,t)$ into boundary conditions of $U(r,t)$, i.e., when $r = R(t)$,

$$U(r,t) = 0, \tag{A.1.5}$$

$$U_r(r,t) = 0, \tag{A.1.6}$$

It is also straightforward to verify that above integral identities are completely equivalent to those derived in the Chapter 4 using the method of change of variables. So far the above analysis is carried out as if we already know the Fundamental Solution. The following section is dedicated to the procedure of finding such a Fundamental Solution using the Fourier Transform method.

A.2 DERIVATION OF THE FUNDAMENTAL SOLUTION

The fundamental solution associated with the problem (A.1.3) is defined by the following.

For every (x, t) be fixed,

$$\begin{cases} \dfrac{\partial G}{\partial \tau} + \dfrac{\sigma^2}{2}\dfrac{\partial^2 G}{\partial y^2} - k(\theta - y)\dfrac{\partial G}{\partial y} + (k - y)G = 0, \quad \text{for } \tau < t, \ \ y \in R \\ G(x, y, t, \tau) = \delta(x - y), \ \text{if } \tau = t+ \end{cases} \tag{A.2.1}$$

Define the Fourier transform in the x variable by

$$F[G(r, y, t, \tau)] = \int_{-\infty}^{\infty} G(r, y, t, \tau)e^{-i\lambda r}dr = \hat{G}(\lambda, y, t, \tau)$$

Then we have

$$\begin{cases} \dfrac{\partial \hat{G}}{\partial \tau} + \dfrac{\sigma^2}{2}\dfrac{\partial^2 \hat{G}}{\partial y^2} - k(\theta - y)\dfrac{\partial \hat{G}}{\partial y} + (k - y)\hat{G} = 0, \quad \text{for } \tau < t, \ \ y \in R \\ \hat{G}(\lambda, y, t, t-) = e^{-i\lambda y} \end{cases} \tag{A.2.2}$$

We postulate that the above equation admits a solution of the form

$$\hat{G}(r, y, t, t-) = e^{A(t,\tau,\lambda)+yB(t,\tau,\lambda)}. \tag{A.2.3}$$

Substituting this solution back into the above PDE (A.2.2) for $\hat{G}$, we get

$$A' + yB' + \frac{\sigma^2}{2}B^2 - k(\theta - y)B + (k - y) = 0, \tag{A.2.4}$$

which must be true for all y. This (together with the limit condition for $t \to \tau$) implies that

$$\begin{cases} A' + \dfrac{\sigma^2}{2}B^2 - k\theta B + k = 0 \\ B' + kB - 1 = 0 \\ A(t, t, \lambda) = 0 \\ B(t, t, \lambda) = -i\lambda \end{cases} \tag{A.2.5}$$

After tedious but straightforward solving of the ODE, we arrive at

$$A + yB = -\alpha_2\lambda^2 + \alpha_1 i\lambda + \alpha_0\lambda, \tag{A.2.6}$$

where

$$\begin{cases} \alpha_2 = \dfrac{\sigma^2}{4k}(e^{2k(t-\tau)} - 1), \\ \alpha_1 = \frac{\sigma^2}{2k^2}e^{2k(t-\tau)} + \left(\theta - \frac{\sigma^2}{k^2} - y\right)e^{k(t-\tau)} + (-\theta + \frac{\sigma^2}{2k^2}), \\ \alpha_0 = \frac{1}{k}(-\theta + \frac{3\sigma^2}{4k^2} + y) + (-\theta + \frac{\sigma^2}{2k^2} + k)(t-\tau) + \frac{1}{k}(\theta - \frac{\sigma^2}{k^2} - y)e^{k(t-\tau)} + \frac{\sigma^2}{4k^3}e^{2k(t-\tau)}. \end{cases} \tag{A.2.7}$$

With the above constants in mind, we can now apply the inverse of Fourier transform to derive the desired expression of the Fundamental Solution

$$\begin{aligned} G(r,y,t,\tau) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{G}(r,y,t,\tau)e^{i\lambda r}d\lambda \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\alpha_2\lambda^2+\alpha_1 i\lambda+\alpha_0\lambda}e^{i\lambda r}d\lambda \\ &= \frac{1}{\sqrt{4\pi\alpha_2}}e^{\alpha_0 - \frac{(\alpha_1+r)^2}{4\alpha_2}} \end{aligned}$$

Thus we arrive at the Fundamental Solution of the original problem (A.1.1). It is easy to see that this G is exponentially decaying in y and the spatial integral w.r.t. y is always equal to 1 for fixed $\tau = t$, i.e. $\int_R G dy = 1$ at $\tau = t$. These properties were used early on to derive the integral identities.

A.3 KEY INTEGRAL IDENTITIES

Since the expression for $U_r(r,t)$ involves a double integral over an infinite domain, it is not easy to find an effective and fast Newton algorithm if we do not reduce the double integral to a single one. To evaluate the inside integral w.r.t. y explicitly, we need appeal to a change of variables. Again the computation is straightforward, although tedious. The desired changes of variables are

$$\begin{cases} s = e^{k(t-\tau)} \\ \alpha = \frac{\sigma^2}{\theta}(s^2-1) \\ \beta_0 = \frac{3\sigma^2}{4k^3}s^2 + \frac{1}{k}(\theta - \frac{\sigma^2}{k^2})s + (-\theta + \frac{\sigma^2}{2k^2} + k)(t-\tau) + \frac{1}{k}(-\theta + \frac{\sigma^2}{4k^2}) \\ \beta_1 = \frac{\sigma^2}{2k^2}s^2 + (\theta - \frac{\sigma^2}{k^2})s + (-\theta + \frac{\sigma^2}{2k^2}) \\ k_2 = s^2 \\ k_1 = \frac{\alpha(1-s)}{\theta} + 2(\beta_1 + r)s \\ k_0 = -(\beta_1 + r)^2 \\ \tilde{y} = \frac{y}{\sqrt{\alpha}} - \frac{k_1}{2\sqrt{\alpha}k_2} \end{cases} \tag{A.3.1}$$

Such a set of change of variables and substitutions allow us to evaluate the inside integral with respect to y explicitly.

$$\begin{aligned} U_r(r,t) &= \int_0^t \int_{h(\tau)}^{\infty} G_r(r,y,t,\tau)(1-\frac{y}{c})(e^{-c\tau}-1)dyd\tau \\ &= \int_0^t \frac{-2e^{\beta_0}(e^{-c\tau}-1)}{\sqrt{\pi}} e^{\frac{k_1^2}{4\alpha k_2}+\frac{k_0}{\alpha}} \{ \frac{1}{\sqrt{\alpha}} \frac{s(h(\tau)+\frac{k_1}{2k_2}) - (\beta_1+r) - cs}{2ck_2} e^{-k_2(\tilde{h}(\tau))^2} \\ &+ \{ \frac{s}{2ck_2} + \frac{\frac{s(1-s)^2\alpha}{\theta^2} + \frac{2s^2(1-s)(\beta_1+r-cs)}{\theta}}{4ck_2^2} \} \frac{\sqrt{\pi}}{2\sqrt{k_2}} \mathrm{Erfc}(\sqrt{k_2}\tilde{h}(\tau)) \} d\tau \end{aligned} \tag{A.3.2}$$

A further substitution of

$$\begin{cases} \beta_3 = \frac{1}{k}(-\theta + \frac{\sigma^2}{k^2} + r)s^{-1} - \frac{\sigma^2}{4k^3}s^{-2} + (-\theta + \frac{\sigma^2}{2k^2} + k)(t-\tau) + \frac{1}{k}(\theta - \frac{3\sigma^2}{4k^2} - r) \\ L_1 = (h(\tau) - c + \tfrac{\sigma^2}{2k^2})s^{-1} + \tfrac{\sigma^2}{2k^2}s^{-2} - \tfrac{\sigma^2}{2k^2}s^{-3} - \tfrac{\sigma^2}{2k^2} \\ L_2 = \tfrac{1}{k}(-\theta + \tfrac{3\sigma^2}{2k^2} + c)s^{-1} + \tfrac{1}{k}(k + 2\theta - c - r - \tfrac{3\sigma^2}{2k^2})s^{-2} \\ \quad\quad + \tfrac{1}{k}(-\theta + \tfrac{3\sigma^2}{2k^2} + r)s^{-3} - \tfrac{\sigma^2}{2k^3}s^{-4} \\ \hat{h} = \tfrac{s}{\sqrt{\alpha}}\{(h(\tau) - \theta + \tfrac{\sigma^2}{2k^2}) - (-\tfrac{\theta}{k} + \tfrac{\sigma^2}{k^2} + r)s^2 + \tfrac{\sigma^2}{2k^2}s^{-2}\}, \text{ if } \tau \neq t \\ \hat{h} = 0, \text{ if } \tau = t \end{cases} \tag{A.3.3}$$

will enable us to further simplify the above expression into

$$U_r(r,t) = \int_0^t \frac{e^{\beta_0}(1 - e^{-c\tau})}{\sqrt{\pi}c} e^{\beta_3}\{\frac{1}{\sqrt{\alpha}}L_1 e^{-(\hat{h}(\tau))^2} + L_2\frac{\sqrt{\pi}}{2}\text{Erfc}(\hat{h}(\tau)\}d\tau \tag{A.3.4}$$

It can be verified that this integral identity is exactly equivalent to the one derived in Chapter 4.

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